DICTIONARY OF

MARINE NATURAL PRODUCTS

with CD-ROM

Edited by
JOHN W. BLUNT
MURRAY H. G. MUNRO

Chapman & Hall/CRC
Taylor & Francis Group

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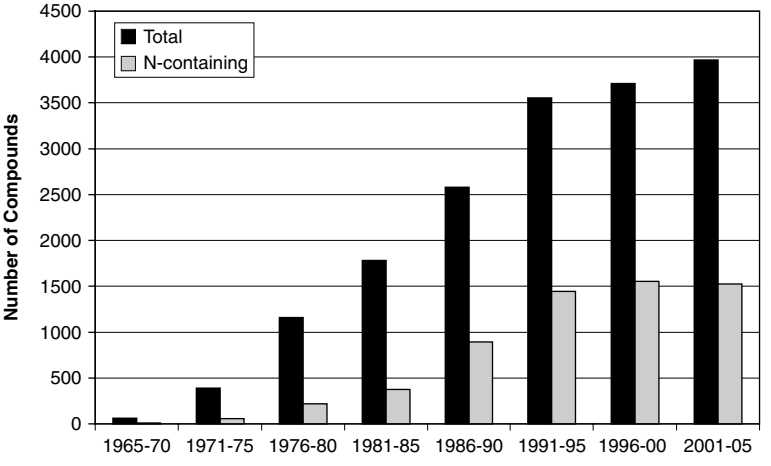
Preface

This production of the *Dictionary of Marine Natural Product*s has been made in response to the growing importance of marine natural products (MNPs) as a subset of all natural product studies. Whilst the study of natural products has been a major focus of the discipline of chemistry for well over a century, most of the effort has been on those derived from terrestrial sources. This emphasis began to change after the 1950s when the impact and significance of Werner Bergmann's pioneering work on natural products from the marine environment was recognised. Bergmann started his work on MNPs in 1933 and published the 50th article in his "Marine Product" series in 1961. The work for which he is widely recognised was the isolation and characterisation in the early 1950s of the non-ribose nucleosides, spongothymidine and spongouridine, from the Caribbean sponge *Cryptotethia crypta.* Within a decade of these discoveries the biomedical importance of non-ribose nucleosides was being realised and the development of drugs such as Ara-C, Ara-A and AZT can be traced directly back to Bergmann's work. The delayed onset of more extensive research into MNPs was partly a consequence of the relatively limited access that biologists and chemists had to that part of the marine environment beyond the sub-tidal zones. This was remedied by the popularisation of SCUBA which dramatically enhanced the ability to collect in the aquatic environment as well as opening up possibilities for marine environmental chemistry. SCUBA was followed in turn by the use of ROVs and various submersibles that have allowed access to very much deeper water. Along with the enhanced collecting opportunities came the recognition that most of the biodiversity on earth was actually present in the oceans.

From the recognition of the importance of marine natural products in the 1950s the field progressed steadily with the next champion, Paul Scheuer, who played a dominant role from the mid-1960s until recently. Joining Scheuer as leaders in the field from the 1970s onwards were Ken Rinehart and John Faulkner (sadly, all three recently deceased). Further MNP studies from the 1970s onwards were assisted by advances in spectroscopic methods and separation science that allowed for the rapid isolation and characterisation of many new structural types. Since then the number of groups undertaking research in the area has grown rapidly, as reflected by the rapid increase in MNP publications and the establishment of MNPs as a separate focal point for conferences. Currently, studies on MNPs are carried out by a wide range of research groups (in excess of 150) scattered across at least 40 countries, but with many of the current leaders of the field able to trace an academic ancestry back to having worked for, or with, Scheuer, Rinehart or Faulkner. Over the years the number of new compounds reported has been rising steadily and is shown graphically below from 1965 until 2005. In 2006 814 new compounds were reported in 302 refereed publications. The total number of MNPs is now approximately 18,000.



Early investigations focussed on the diversity of chemical structures elaborated by marine organisms readily accessible to collectors, notably algae, sponges, tunicates and other invertebrates. The best illustration of this approach was the degree of attention that was focused on halogenated metabolites available from red algae (Rhodophycota). Genera such as *Plocamium* and *Laurencia* were readily available by shore wading, could be collected in relatively large amounts and the metabolites present were relatively non-polar and could be readily

extracted and separated by the conventional separation techniques available at that time (1970s). However, by the 1980s the focus of attention was switching to the role of these diverse structures in ecological interactions and especially to the potential of compounds of marine origin as pharmaceutical agents. Considering the dramatic start that Bergmann's discovery of the non-ribose nucleosides had on the biomedical role of MNPs some 20 years earlier, this preoccupation with non-polar non-nitrogenous compounds was a distraction. In John Faulkner's first review on marine metabolites (1977) covering the period 1974-6 only 10% of the metabolites covered were nitrogenous. However, for the period 1977-85 this figure had almost doubled to 19.5% with 332 out of 1706 metabolites containing at least one N. Long before Lipinski's "rule of five" had been enunciated it was well recognised that nitrogen was an important structural feature in bioactive compounds. Fortuitously, rapid advances in chromatographic techniques and phases were occurring at this time that dramatically eased the problems of working on the (usually) more polar bioactive compounds. This move towards searching for bioactive compounds was a major driving force for the expansion of interest in MNPs and continues to provide a strong rationale for new discovery programmes. Structural elucidation aspects of MNPs continue as a core activity. With the advent of more sensitive NMR techniques, the mass requirements for obtaining good 1D- and 2D-NMR data have been reduced by two orders of magnitude. The effects of this have been two-fold. Firstly, it is easier to examine and characterise the very minor metabolites. Secondly, these advances have had a distinct influence on the mass requirements for field collections - smaller samples are possible as well as the opening up of a whole new range of marine organisms that are only ever available in small amounts.

Also dating back to the 1980s was the move towards the study of marine microorganisms. A continuing leader in this field is William Fenical. Initially, Fenical and his group focused on bacteria, especially those colonising the surfaces of marine algae and invertebrates, but in time changed their emphasis more towards marine fungi. This focus is now a major preoccupation of many of the marine research groups. For the literature on marine microorganisms, 45% of the total citations over the 1965 to 2005 period have been published since 2001. A significant find has been the discovery of new obligate marine actinomycete genera that produce unique metabolites. Accompanying the study of marine microorganisms has been the recognition that many of the MNPs described in the literature may well be of microbial origin and produced by microorganisms that are symbiotic, commensal or dietary components of the host invertebrate species. Modern developments in the tools of molecular biology are making the studies of these relationships more accessible. There has been a hiatus in the use or development of compounds of marine origin as pharmaceuticals. The recent licensing of Prialt, from the toxin of a *Conus* species, for the treatment of intractable pain comes some 50 years since the introduction of Ara-A and Ara-C and is the first direct drug from a marine invertebrate. It is likely that others, such as Yondelis for the treatment of cancer, will now soon follow.

No matter what the role or the source of MNPs might be, or what the focus of the research, the type of assays or analytical techniques that are directing the purification, chemists needs to quickly establish the novelty of compounds that they are working on (dereplication), and to explore the relatedness of new compounds to others in the same class of structural types. The dereplication process in a modern context relies heavily on UV libraries (from HPLC data), mass spectrometry (from LC-MS data) and NMR pattern recognition (from cryoprobe or capillary probe NMR spectroscopy). The scale of such operations is now at the μg level and effectively telescopes the traditional process of several steps (crude extract evaluation, isolation, dereplication and characterisation) into just one process. The dereplication of MNPs relies heavily on access to appropriate collections of data, especially those with substructure searching capability, MW and UV data, that enable researchers to rapidly distinguish unique molecules from known compounds.

Such collections of data include the *Dictionary of Natural Products* (DNP) which is an all-encompassing compilation of natural product compound information from all sources including compound data, taxonomy and key references to structural, synthetic, ecological and biological activity studies. DNP was first published in 1992, and since that time has been continually updated by a team of specialist contributors and republished every six months in electronic form (CD-ROM, and more recently also as a web product). The *Dictionary of Marine Natural Products* is a specialist subset of the DNP. During 2004 to 2006, all entries in the DNP database referring to marine natural products were extracted, reviewed and where necessary expanded with reference to specialist literature sources such as MarinLit, and with the input of further levels of expertise from the marine natural specialists (John Blunt and Murray Munro).

The resulting *Dictionary of Marine Natural Products* in printed/CD-ROM format consists of approximately one-sixth of the DNP database, specially enhanced with new types of information particularly relevant to the marine environment. In particular, during the compilation, Type of Organism codes were added to the (whole) database for the first time, allowing the data to be searched by broad taxonomic criteria in parallel with other

parameters. This information, along with the MS, MF and UV data, can be directly searched in the CD-ROM version of *Dictionary of Marine Natural Products* and can give a rapid, unambiguous answer on the novelty of any metabolite isolated or partially characterised.

It is intended that the *Dictionary of Marine Natural Products* will be republished periodically, probably in CD-ROM format only. Users can obtain access to more frequent updates of the whole DNP database (including new marine information) by subscription. This first compilation of the *Dictionary of Marine Natural Products* will be of significant value to the growing number of investigators in the field of marine natural products. The efforts of John Buckingham and Steve Walford, coordinating a team of contributors (principally Keith Baggaley, Bob Hill and Andy Roberts) will be greatly appreciated.

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Murray H.G. Munro
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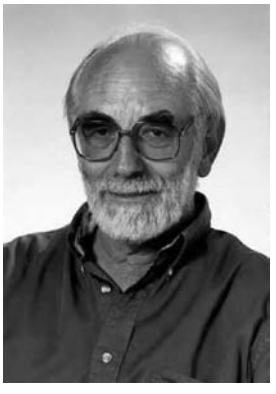
New Zealand
June 2007

Editorial Board

Biography

John Blunt obtained his BSc (Hons) and PhD degrees from the University of Canterbury, followed by postdoctoral appointments in Biochemistry at the University of Wisconsin-Madison, and with Sir Ewart Jones at Oxford University. He took up a lectureship at the University of Canterbury in 1970, where he is now a Professor. His research interests are with natural products, and the application of NMR techniques to structural problems.



Murray Munro, University of Canterbury, Christchurch New Zealand, has worked on natural products, mainly of New Zealand origin, right through his career. Following a sabbatical with Ken Rinehart at the University of Illinois in 1973 interest in marine natural products developed with a particular focus on bioactive compounds. In recent years his research interests have widened to include terrestrial and marine fungi and actinomycetes as well as marine invertebrates.

Introduction

1. COVERAGE

The *Dictionary of Marine Natural Products* is a comprehensive database containing over 30,000 compounds. It is a subset of the *Dictionary of Natural Products* (DNP) database. DNP is an ongoing project based on a 25-year review of the natural product literature. For the present project, the subset of DNP entries referring to marine natural products were carefully checked and reviewed and enhanced with a considerable amount of additional information relating to their natural occurrence. Several careful reviews were also carried out to ensure that the coverage of marine natural products in the finished publication was as complete as possible.

The compounds present in the Dictionary have been classified under the following major headings, which are described in more in the **Structural Types** section below. (There are obvious overlaps between the categories.)

Aliphatic natural products
Carbohydrates
Oxygen heterocycles
Simple aromatic natural products
Terpenoids
Steroids
Aminoacids and peptides
Alkaloids
Polypyrroles

Biosynthetic information on these compound classes can also be found in the Structural Types section. Taxonomic information on the organisms and their metabolites is covered in the **Classification of Organisms** section.

In compiling the printed version and the CD-ROM, the primary literature has been reviewed up to mid-2006.

The definition of a marine natural product is imprecise. The coverage of this Dictionary in terms of 'mainstream' natural products is intended to be comprehensive and as far as can be determined by various cross-checks carried out in the later stages of compilation, it comes extremely close to achieving that aim. Natural products which may be considered marginal are present to a great extent, but to include every compound that might be found somewhere in the sea would be an unrealistic target. In particular, compounds of the following type may not necessarily be present:

(1) Biochemicals endogenous to the higher marine animals, e.g. bile acids of marine mammals, endocrine hormones of crustaceans.
(2) Microbial products isolated from organisms that are widespread on both sea and land and have in fact been isolated from a marine-related source, e.g. an antibiotic from *Streptomyces* harvested from driftwood.
(3) Natural products of a 'terrestrial' type isolated from plants and animals in marginal environments, e.g. mangrove saltmarshes, may not be fully covered.
(4) Widespread polysaccharides, e.g. Amylose, Amylopectin.

All of these are included in the parent database *Dictionary of Natural Products*, available on DVD or online from CRC Press.

The coverage of lipids is extensive but not completely comprehensive. Numerous homologous series of fatty acids with different unsaturation patterns occur in both terrestrial and marine organisms, and there may not be an individual entry for every minor congener.

1.1 Natural products in the marine environment; general observations

The marine environment is an extremely complex one, showing immense biodiversity. Marine organisms produce all of the main type of natural product found among their terrestrial counterparts, but with a very different range of chemodiversity, so that, for example, the range of terpenoid skeletons includes some not found on land. Conversely, there are large groups of natural product found in some higher plants (e.g. many terpenoid skeletons; large categories of alkaloids) for which the enzymatic pathways have not evolved among marine organisms; higher plants are essentially absent from the sea.

1.1.1 Elemental composition

Many marine natural products contain the elements nitrogen, sulfur and halogens available in seawater, but with very uneven distribution across the phyla. A few compounds containing other elements such as arsenic and boron are also known, and also metal complexes (Ni, V, Zn). Vanadium bromoperoxidases are involved in the production of brominated marine natural products (but chlorinated metabolites arise by a different route). The proportion of nitrogenous compounds is much higher in cyanobacteria, bryozoans and ascidians, and the proportion of halogenated compounds is very high in the red algae (in marked contradistinction to the brown algae). More details are given in the sections below describing these organisms.

Kornprobst, J.M. *et al, Comp. Biochem. Physiol. B,* 1998, **119**, 1–51 (*rev, sulfates*)
Jiménez, C., *Stud. Org. Chem*., 2001, **25**, 811-917 (*rev, sulfur-containing marine natural products*)
Butler, A. *et al, Nat. Prod. Rep*., 2004, **21**, 180-188 (*vanadium bromoperoxidases*)

1.1.2 Interspecific interactions

It is now clear that, whilst many marine natural products are located in the tissues of the larger marine animals and plants, and are thus genuine natural products of those organisms, many others are produced by associated endo- and epibiotic microorganisms. Most marine microorganisms have not yet been successfully cultured, and definitive proof of origin is in most cases currently lacking. These products produced by symbiotic or epiphytic microorganisms appear in many cases to play a role in chemical defence mechanisms.

In the past five years, however, much progress has been made in assigning a definite microbial origin to many natural products. For example, in the case of **Swinholide A**, originally isolated from the sponge *Theonella swinhoei*, centrifugation of macerated cell samples from the sponge showed that the alkaloid was located within heterotrophic unicellular bacterial cells, was absent from the sponge cells themselves, but was also in the cells of the co-occurring cyanobacterium *Aphanocapsa feldmanni* also present. More recently, however, Swinholide A has been found in some cyanobacteria, and it has been speculated that it may be produced by one component of this symbiont system, and stored by another. In the case of the isocyano- and related metabolites found in marine invertebrate extracts, the isocyano group, possibly derived from cyanide ion, may be produced by an associated microorganism, while the terpenoid component derives from the animal. Genomic techniques are now being used; for example to show that **Patellamides A** and **C** are biosynthesised by a cyanobacterial symbiont of the originally cited source. Other natural products isolated from the higher marine organisms, however, have a known dietary origin, while a definite *de novo* biosynthesis of some mollusc products has been demonstrated.

It may be true in some cases that although a particular type of metabolite isolated from a higher animal has not yet been found among the lower forms such as cyanophytes forming part of the same ecosystem, this is merely an accident of the search process.

Haygood, M.G. *et al, J. Mol. Microbiol. Biotechnol*., 1999, **1**, 33–43 (*rev, microbial symbionts*)
Paul, V.J. *et al, Nat. Prod. Rep.,* 2004, **21**, 189–209 *(rev, chemical mediation of interorganism interactions*)
Salomon, C.E. *et al, Nat. Prod. Rep*., 2004, **21**, 105–121 (*rev, microbial genetics and chemical diversity*)
Hildebrand, M. *et al, Nat. Prod. Rep*., 2004, **21**, 122–142 (*rev, symbiont genetics*)
Proksch, P. *et al, BIOforum Eur*., 2004, **8**, 44
Moore, B.S., *Nat. Prod. Rep*., 2005, **22**, 580–593; 2006, **23**, 615–629 (*rev, biosynth*)

2. ORGANISATION OF ENTRIES

The Dictionary is arranged alphabetically by entry name. Every entry is numbered to assist ready location. Many compounds are included as derivatives of main entry compounds but important derivatives have their own individual cross-referenced entries. Use of the CD-ROM indexes enables the rapid location of all compounds in the Dictionary by name or compound type, regardless of their location. Entries may sometimes contain data on natural products which are not of marine origin, but this is obvious from the context and may provide valuable links to relationships between marine and terrestrial sources. This is especially true of entries dealing with fungal metabolites (see the section dealing with fungi, below).

A representative dictionary entry is shown in **Figure 1.**

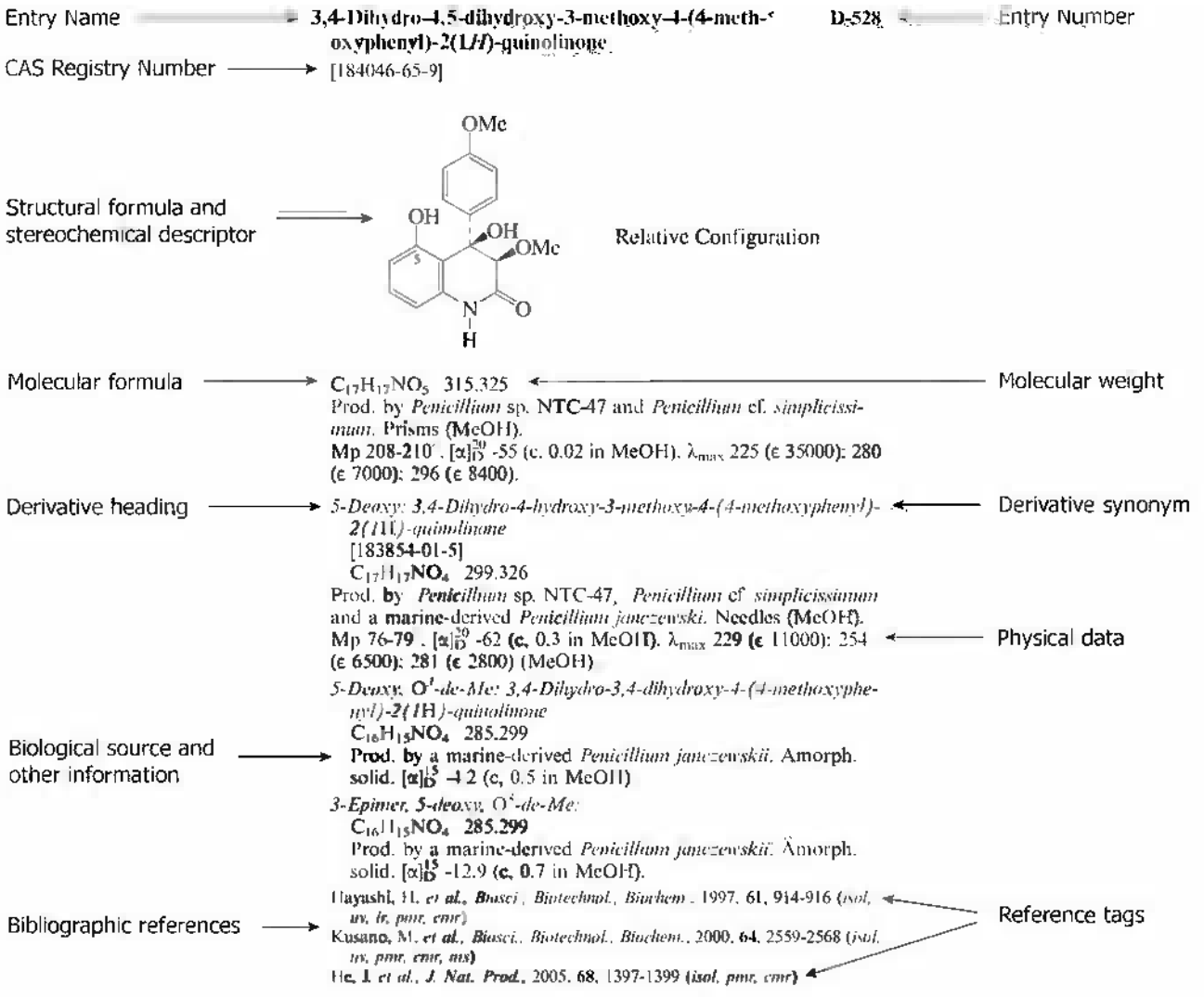


FIGURE 1

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2.1 Chemical names and synonyms

The Dictionary contains a wide range of synonyms which may be (a) those found in the primary literature, (b) *Chemical Abstracts* names, or (c) names added editorially to achieve as much consistency as possible with other closely related substances. Names corresponding to those used by CAS during the 9th and subsequent Collective Index periods (1973) are labelled 9CI Names. All important derivatives embedded within entries are named (but see comment on CAS nomenclature below). If a compound cannot be located immediately in the main body of the entries, it is important to use the indexes. The CD-ROM version of the Dictionary is much more highly indexed than the printed version.

The most authoritative current statement of good practice on natural product nomenclature is the document *IUPAC Recommendations 1999* (*Pure Appl. Chem.,* 1999, **71**, 587–643) the full text of which can be read on the *Dictionary of Marine Natural Products on CD-ROM* (access from the Windows® Start menu item or via the Help menu in the main program).

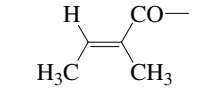
Some marine natural products have been given trivial names which duplicate those already in the literature, or which are simultaneously published for two or more non-identical substances. Where such a duplication is noticed this is indicated by the dagger symbol (‡) immediately following the name. Borderline cases, especially as between presence or absence of terminal e or suffix A or 1, are considered to constitute duplicates for this purpose.

2.1.1 Nomenclature

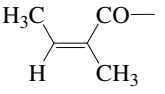
It is expected that this Dictionary will be used by a wide variety of scientists, not all of whom will be specialist organic chemists. Therefore compounds have been named so as to facilitate access to their factual data by keeping the nomenclature as simple as possible, whilst still adhering to good practice as determined by IUPAC (the International Union of Pure and Applied Chemistry). A great deal of care has been taken to achieve this aim as nearly as possible.

A much fuller description of the detailed nomenclature of individual classes of marine natural product is given in the **Structural Types** section. The following notes are of general applicability throughout the Dictionary.

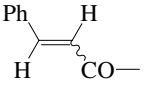
1. There are many examples in the primary literature of compounds being named in ways which are violations of good IUPAC practice, e.g. where the substituents are ordered non-alphabetically. These are not reported in their incorrect form but have been corrected.
2. The number of trivial names used for acylating substituents has been kept to a minimum but the following are used throughout the Dictionary.



Tigloyl = *E*-2-methyl-2-butenoyl



Angeloyl = *Z*-2-methyl-2-butenoyl



Cinnamoyl = 3-phenyl-2-propenoyl

3. Many other trivial appellations have from time to time appeared in the literature for other acyl groups (e.g. Senecioyl = 3-methyl-2-butenoyl, Feruloyl = 3-(4-hydroxy-3-methoxypheny1)-2-propenoyl or 4-hydroxy-3-methoxycinnamoyl).

The term **prenyl** for the common 3-methyl-2-butenyl substituent, $(H_3C)_2C{=}CHCH_2$-, is used throughout the Dictionary. Several other names for this substituent have from time to time been used and appear in the primary literature including the following:

3-Methyl-2-butenyl (systematic)
γ,γ-Dimethylallyl
3,3-Dimethylallyl
3,3-Dimethylpropenyl
Dimethallyl
Isoprenyl
Isopentenyl
β,β-Dimethylacrylyl

2.2 CAS REGISTRY NUMBERS

CAS numbers are identifying numbers allocated to each distinctly definable chemical substance indexed by CAS since 1965 (plus some retrospective allocation of numbers by CAS to compounds from earlier index periods). The numbers have no chemical significance but they provide a label for each substance independent of any system of nomenclature. They are extensively used for exchanging information between individuals and databases. The numbers take the form NNNNNN-NN-R, where the total number of digits is five or more and R is a check digit.

For practical purposes, CAS numbers have certain shortcomings arising from their free allocation, resulting in one substance having more than one potential number. Duplication may arise for one of several reasons to do with the detailed chemistry of the substance, for example tautomerism, solvent formation, partially unspecified stereochemistry. There are also replaced numbers. For this reason, Dictionary entries will often contain one or more *Additional CAS numbers* which may help the user to obtain further information about the substance, especially by online searching.

Clearly, the additional CAS numbers given in this Dictionary have to be used with care. Their inclusion in the entry is the result of an editorial decision by the Dictionary contributor that they refer to what is essentially the same substance, but this decision may be a subjective one. Care has been taken to ensure that the main CAS number given in this Dictionary for each substance is the correct one.

Further information on CAS number allocation policy can be obtained from CAS indexes or *The Organic Chemist's Desk Reference* (Chapman & Hall, 1995).

2.3 Structural formulae

Every attempt has been made to present the structures of chemical substances as accurately as possible according to best current practice and recommendations of IUPAC. As much consistency as possible has aimed at between closely-related structures. For example, all sugars are shown as Haworth formulae, and whenever possible in complex structures the rings are oriented in the standard Haworth convention so that structural comparisons can be quickly made.

2.4 Molecular formula and molecular weight

The elements in the molecular formula are given according to the Hill convention (C, H, then other elements in alphabetical order). The molecular weights given are formula weights (or more strictly, molar masses in daltons) and are rounded to three places in decimals. In the case of some high molecular mass substances, such as proteins, the value quoted may be that taken from an original literature source and may be an aggregate molar mass.

2.5 Physical data

The Dictionary gives the following physical characteristics of substances, when available: appearance, melting point, boiling point, optical rotation, density, refractive index, solubility, p*K*a. All of these fields are searchable by numerical value (including range searching) in the CD-ROM version of the Dictionary.

2.5.1 Appearance

Organic compounds are considered to be colourless unless otherwise stated. Where the compound contains a chromophore which would be expected to lead to visible colour, but no colour is mentioned in the literature, the Dictionary entry will mention this fact if it has been noticed by the contributor. An indication of crystal form and recrystallisation solvent is often given but these are imprecise items of data; most compounds can be crystallised from several solvent systems and the crystal form often varies. In the case of the small number of compounds where crystal behaviour has been intensively studied (e.g. pharmaceuticals), it is found that polymorphism is a very common phenomenon and there is no reason to believe that it is not widespread among organic compounds generally.

2.5.2 Melting Points and Boiling Points

The policy followed in the case of conflicting data is as follows:

a. Where the literature melting points are closely similar, only one figure (the highest or most probable) is quoted
b. Where two or more melting points are recorded and differ by several degrees (the most likely explanation being that one sample was impure) the lower figure is given in parentheses, thus Mp 139° (134–135°)
c. Where quoted figures differ widely and some other explanation such as polymorphism or incorrect identity seems the most likely explanation, both figures are quoted without parentheses, thus Mp 142°, Mp 205–206°
d. Known cases of polymorphism or double melting points are noted

Boiling point determination is less precise than that of melting points and conflicting boiling point data are not usually reported except when there appears to be a serious discrepancy between the different authors.

2.5.3 Optical rotations

These are given wherever possible, and normally refer to what the Dictionary contributor believes to be the best characterised sample of highest chemical and optical purity. Where available an indication of the optical purity

(op) or enantiomeric excess (ee) of the sample measured follows the specific rotation value. For a recent discussion of the validity and applicability of these terms, see Gawley, R.E., *J. Org. Chem*., 2006, **71**, 2411–2416.

Specific rotations are dimensionless numbers and the degree sign which was formerly universal in the literature has been discontinued.

2.6 Spectroscopic data

Many Dictionary entries include ultraviolet spectra which are presented in the format:

[neutral] λ_{max} 198(log ε 1.55); 224 (sh) (log ε 0.61); 241 (sh) (log ε 0.55)(H_2O)(Berdy)

where ε is the absorption coefficient for a given UV maxima value (λ_{max}). A description of the solvent conditions used, if reported in the literature, is listed at the beginning and end of the UV data in parentheses. All peak absorptions cited are maxima unless otherwise described, e.g. shoulder/inflection (sh) and end absorption (end). In addition, UV data may be followed by the term 'Berdy' or 'DEREP' indicating from which database the data originated. The absence of these terms implies that the data were abstracted from the primary literature.

On the CD-ROM, all the λ_{max} values are indexed in the UV Maxima field and can be searched for numerically including range searching. Similarly, the solvent data associated with the UV data are indexed in the UV Solvent field.

2.7 Hazard and toxicity information

2.7.1 General

Toxicity and hazard information is highlighted by the symbol and has been selected to assist in risk assessments for experimental, manufacturing and manipulative procedures with chemicals.

The Publishers cannot be held responsible for any inaccuracies in the reported information, neither does the omission of hazard data in the Dictionary imply an absence of this data from the literature. Widely recognised hazards are included, however, and where possible key toxicity reviews are identified in the references. Further advice on the storage, handling and disposal of chemicals is given in *The Organic Chemist's Desk Reference*.

2.7.2 RTECS® Accession Numbers*

Many entries in this Dictionary contain one or more RTECS® Accession Numbers. Possession of these numbers allows users to locate toxicity information on relevant substances from the NIOSH *Registry of Toxic Effects of Chemical Substances*, which is a compendium of toxicity data extracted from the scientific literature.

2.8 Bibliographic references

The selection of references is made with the aim of facilitating entry into the literature for the user who wishes to locate more detailed information about a particular compound. The contents of most references are indicated by reference tags (suffixes) indicating their content and in particular the stereoisomers and derivatives of the parent compound which they document. The number of references cited does not indicate the relative importance of a compound; one key recent citation may supersede a number of older ones.

Journal abbreviations generally follow the practice of the Chemical Abstracts Service Source Index (CASSI), except for a short list of very well known journals where the Dictionary gives shorter abbreviations to save space (e.g. *J.A.C.S.* instead of *J. Am. Chem. Soc.*)

2.8.1 Further References

Further useful information on a variety of topics concerned with the structure, description, stereochemistry and nomenclature of organic compounds can be found in the *Organic Chemist's Desk Reference*.

*RTECS® Accession Numbers are compiled and distributed by the National Institute for Occupational Safety and Health Service of the U.S. Department of Health and Human Services of The United States of America.

3. INDEXES

There are three printed indexes:

1. **Name Index** which lists every compound name and synonym in the Dictionary
2. **Type of Compound index** listing all compounds given in the Dictionary organised by structural type
3. **Type of Organism index** listing all compounds according to the species from which they have been isolated.

The indexes refer to the entry number. Searches on all text and numerical indexes, as well as structure and substructure searching can be carried out on the CD-ROM version of the Dictionary. For information on the Type of Compound codes used in the Type of Compound Index, please see the **Structural Types** section.

4. ABBREVIATIONS

The following is a selection of the most common Database abbreviations used:

Abbreviation	**Name**
[α]	specific rotation
abs config	absolute configuration
Ac	acetyl
acc	according
AcOH	acetic acid
Ac_2O	acetic anhydride
alk	alkaline
amorph	amorphous
amt	amount
anal	analytical applications, analysis of detection
anhyd	anhydrous
aq	aqueous
BAN	British Approved Name
bibl	bibliography
biosynth	biosynthesis
Bp	boiling point
c	concentration
ca	(*circa*) about
cd	circular dichroism
CAS	Chemical Abstracts Service
chromatog	chromatography
cmr	carbon (^{13}C) nuclear magnetic resonance
CNS	central nervous system
col	colour, coloration
coml	commercial(ly)
compd	compound
conc	concentrated
config	configuration
conformn	conformation
constit	constituent
cryst struct	X-ray crystal structure determination
d	density
dec	decomposes, decomposition
degradn	degradation
deg	degree
deriv(s)	derivative(s)
detn	detection, determination
dil	dilute, dilution
dimorph	dimorphic

diss	dissolves, dissolved
dist(n)	distil, distillation
DMF	dimethylformamide
DMSO	dimethyl sulfoxide
ee	enantiomeric excess
epr	electron paramagnetic (spin) resonance
equilib	equilibrium
esp	especially
Et	ethyl
EtOAc	ethyl acetate
EtOH	ethanol
EtOH aq	aqueous ethanol
exp	experimental
FEMA	Flavor and Extract Manufacturers' Association
fl p	flash point
fluor	fluoresces, fluorescence
formn	formation
Fp	freezing point
g	gram
glc	gas liquid chromatography
Glc	β-D-glucopyranosyl
GRAS	Generally Recognised As Safe
ham	hamster
haz	hazard
hplc	high performance liquid chromatography
hydrol	hydrolyses, hydrolysed, hydrolysis
ihl	inhalation
ims	intramuscular
INN	International Nonproprietary Name
intermed	intermediate
ipr	intraperitoneal
ir	infra-red spectrum
isol(n)	isolation, isolated
isom	isomerism, isomers, isomerises
ivn	intravenous
JAN	Japanese Accepted Name
JMAF	Japanese Ministry for Agriculture, Forestry and Fisheries
LC	lethal concentration
LD	lethal dose: LD_{50}, a dose which is lethal to 50% of the animals tested
M	molecular weight (formula weight)
manuf	manufacturer, manufactured
max	maximum
Me	methyl
MeOH	methanol
Me_2CO	acetone
MEL	maximum exposure limit
metab	metabolite, metabolism
misc	miscible
mixt	mixture
mod	moderately
Mp	melting point
ms	mass spectrum
mus	mouse
n	index of refraction, e.g. n_D^{20} for 20° and sodium light
nmr	nuclear magnetic resonance spectrum (general)
obt	obtained

oc	open cup
occup	occupational
OES	Occupational Exposure Standard
op	optical purity
ord	optical rotatory dispersion
orl	oral
Ph	phenyl (C_6H_5)
pharmacol	pharmacology
pmr	proton (^1H) nuclear magnetic resonance
polarog	polarography
polym	polymerises, polymer
ppd	precipitated
ppm	parts per million
props	properties
purifn	purification
Py	pyridine
rbt	rabbit
ref	reference
resoln	resolution
rev	review
rt	room temperature
scu	subcutaneous
sepn	separation
skn	skin
sl	slightly
sol	soluble
soln	solution
solv	solvent
sp	species (singular)
spar	sparingly
spp	species (plural)
ssp	subspecies
subl	sublimation, sublimes
synth	synthesis
tautom	tautomerism
THF	tetrahydrofuran
tlc	thin layer chromatography
TLV	Threshold Limit Value
tox	toxicity
unsatd	unsaturated
USAN	United States Adopted Name
uv	ultraviolet spectrum
v	very
var	variety
vis	visible
vol	volume

4.1 Reference tags

The following is a selection of the most common Reference Tag abbreviations used:

Abbreviation	**Name**
abs config	absolute configuration
anal	analysis
bibl	bibliography
biosynth	biosynthesis

cd	circular dichroism
chromatog	chromatography
cmr	^{13}C nuclear magnetic resonance spectrum
config	configuration
conformn	conformation
cryst struct	X-ray crystal structure determination
deriv(s)	derivative(s)
detn	determination, detection
dta	differential thermal analysis
glc	gas-liquid chromatography
hplc	high performance liquid chromatography
ir	infrared spectrum
isol	isolation
isom	isomerism
manuf	manufacture
metab	metabolism
ms	mass spectrum
nmr	nuclear magnetic resonance spectrum
occur	occurrence
ord	optical rotatory dispersion
pharmacol	pharmacology
pmr	proton (^1H) nuclear magnetic resonance spectrum
props	properties (chemical or physical)
Raman	Raman spectrum
resoln	resolution
rev	review
sepn	separation
struct	structure
synth	synthesis
tautom	tautomerism
tlc	thin layer chromatography
tox	toxicity
trans	transition(s)
uv	ultraviolet spectrum
uv-vis	ultraviolet visible spectrum

5. THE DICTIONARY OF MARINE NATURAL PRODUCTS ON CD-ROM

The *Dictionary of Marine Natural Products* is published together with a fully searchable CD-ROM. Space considerations have precluded the inclusion of indexes other than the Name, the Type of Compound and the Type of Organism indexes in the hard-copy version. By contrast, the CD-ROM contains searchable indexes on the following 35 fields:

Accurate Mass	Chemical Name	Molecular Weight	Supplier
All Entries	Density	Optical Rotation	Type of Compound
All Text	Development Status	Partition Coefficient (Calc.)	Type of Compound Words
Biological Source	Dissociation Constant	Percent Composition	Type of Organism
Biological Use/Importance	Hazard & Toxicity	References	Type of Organism Words
Boiling Point	Hazard Flag	Refractive Index	Use/Importance
Boiling Point Pressure	Ion Charge	Rotation Conditions	UV Maxima
CAS Registry Number	Melting Point	RTECS Accession No.	UV Solvent
Chapman & Hall Number	Molecular Formula	Source/Synthesis	

In addition to searching the above text fields, it is possible to search on structure and substructure.

Once installed, a Help file providing additional information on data content and guide to searching is available from the Chapman & Hall_CRC folder in the Start Menu and from the Help menu on the CD-ROM.

When accessing the *Dictionary of Marine Natural Products on CD-ROM* the first screen that is obtained is the Search Form window (**Figure 2**).

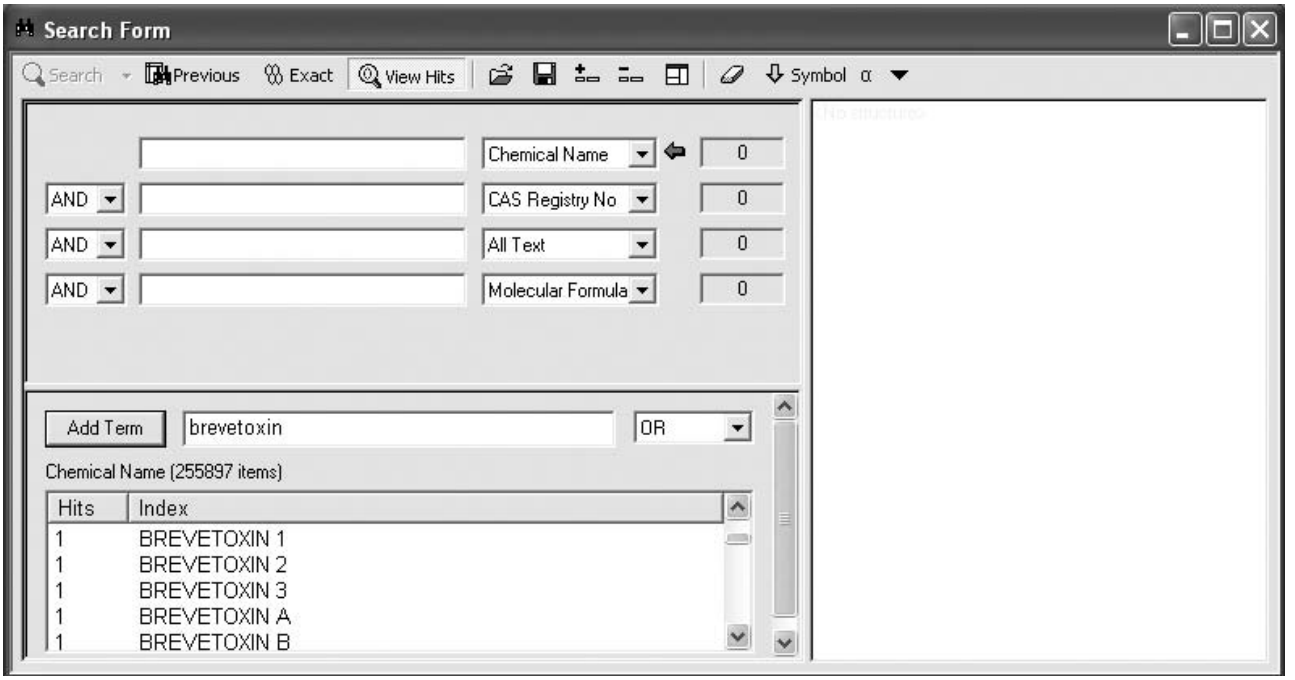


FIGURE 2

The Search Form window is split in to three panes:

1. Structure Search pane – allowing structure and substructure searching
2. Search Terms pane – search from one or more of the 35 available data/text fields
3. Index pane – displays the indexed terms within a selected field

From the Search Form window design your search profile using text, structure or text/structure searching. Once your search has been performed the resultant hits are listed alphabetically by chemical name in the Hit List screen. Clicking on any one of the hits in the hit list screen will result in that entry being displayed in the Entry Display screen (**Figure 3**).

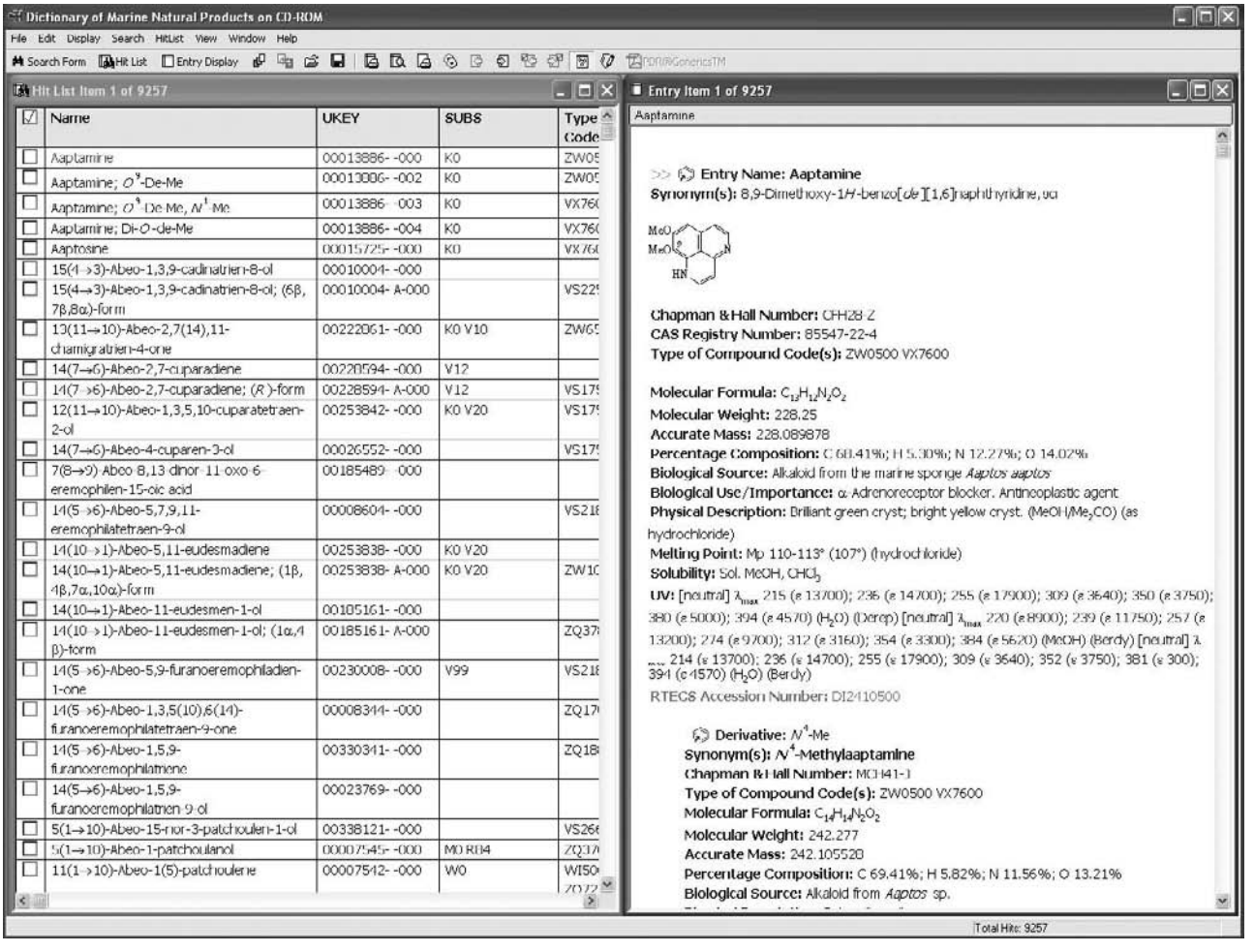


FIGURE 3

Any comments and suggestions for inclusion may be sent to:

The Editors, Dictionary of Marine Natural Products
Chapman & Hall/CRC
Albert House
1-4 Singer Street
London
EC2A 4BQ

Fax: +44 (0)20 7017 6747
Email: steve.walford@informa.com

Structural Types

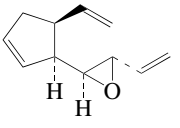
1. ALIPHATIC NATURAL PRODUCTS (VA)

A wide variety of small aliphatic and alicyclic compounds occur in nature. Because they are diverse, no attempt will be made here to give a general account; for information on specific aliphatics, their individual entries should be consulted. In the Type of Compound Index, the aliphatic compounds included in the Dictionary are simply classified by functional group and ring/chain structure.

1.1 Semiochemicals

Semiochemicals are defined as chemicals that mediate communication between individual organisms. When semiochemicals act between members of the same species they are known as pheromones. Pheromonal systems are usually the most highly developed semiochemical systems because the species directly benefits from any improvement. The phrase 'highly developed', in this context means that release of the pheromone is efficient and timely and that the receiver has a sensitive and selective detection system. Because most pheromones are involved in reproductive functions (mate attraction, courtship and copulation), increased efficacy is immediately apparent in higher fecundity. The most widely known semiochemicals in the marine environment are the pheromones of the brown algae which are described in more detail below (section ZH1000). Examples are **Dictyopterene B** and **Caudoxirene**.

Dictyopterene B
(Hormosirene)



Caudoxirene

Pohnert, G. *et al, Nat. Prod. Rep*., 2002, **19**, 108–122 (*algal pheromones*)

1.2 Lipids

Lipids have been defined in different ways at different times and there is still no agreed definition of the term. A simple definition is fatty acids and their derivatives, and substances related biosynthetically or functionally to them.

1.2.1 **Fatty acids** (VA0300, VA0600, VA1100, VA1500, VA1750)

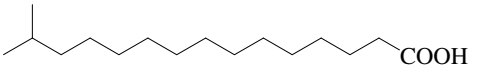
A wide variety of fatty acids are found in marine organisms. These include the common ones found in virtually all organisms, to rare types, typically polyunsaturated, which may be unique to certain phyla or classes of marine animal. No attempt will be made here to give an account of their distribution. Useful searches can be done on the CD-ROM version of this Dictionary by combining one or more codes for fatty acid type as given above (e.g. VA1100, with a code for organism type, e.g. ZE0001, green algae. A more detailed treatment is given in Kornprobst (2005) (various locations), Berge (2005), Rezanka (1989), Dalsgaard (2003) and Ackman (2006). The best general reference for lipids is Gunstone *et al*.

Fatty acids are given in this Dictionary under their systematic chemical names, and their trivial names (e.g. **Palmitic**, **Linoleic**) are given as synonyms and can readily be found in the CD-ROM version. The carbon chain is numbered from the carboxy group (COOH=1). The position of a double bond is sometimes denoted by Δ. Hence a Δ^9 indicates a double bond between the carbons 9 and carbon 10 and a Δ^9-desaturase inserts this unsaturation. An internationally accepted nomenclature uses abbreviations of the form A: B(C). A indicates the number of

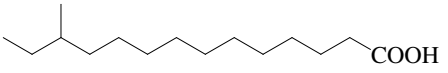
carbon atoms in the molecule, B represents the number of unsaturated centres which are usually *cis*-(*Z*-)-alkenic, and C indicates the position and configuration of the unsaturation counted from the *terminal* methyl of the carbon chain. Symbols such as ω3 or *n*-3 indicate the position of the unsaturated centre closest to the terminal CH_3 group. In this case it is assumed that all unsaturation is methylene-interrupted and has *cis*-(*Z*-) configuration.

Trivial	**Systematic**	**Abbreviation**
Palmitic acid	Hexadecanoic acid	16:0
Oleic acid	*cis*-9-Octadecenoic acid	18:1 (9*Z*)
Arachidonic acid	all-*cis*-5,8,11,14-Eicosatetraenoic acid	20:4 (*n*-6)

Acids with a single methyl substituent, most commonly have this at the penultimate position of the chain, and are named **isoacids**. If the methyl substituent is located on the antepenultimate carbon from the end of the chain the acids are named **anteiso** acids.



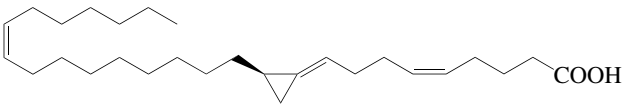
Isopalmitic acid
(14-Methylpentadecanoic acid)



Anteisopentadecanoic acid
(12-Methyltetradecanoic acid, Sarcinic acid)

The number of natural fatty acids known exceeds 1000 though only 20–50 are ubiquitous. From a survey of all these structures it is possible to make a number of generalisations, although there are significant exceptions to each statement. These statements were first based on chemical structure but it is clear that they also reflect underlying biosynthetic pathways.

(i) Natural fatty acids – both saturated and unsaturated – are mostly straight-chain compounds with an even number of carbon atoms. Chain lengths range from two to more than eighty carbon atoms but are most commonly between C_{12} and C_{22}. Odd-carbon acids (e.g. Hentriacontanoic acid) occur and are widespread in marine sources. Acids with branched structures (e.g. **Isopalmitic**, **Anteisononadecanoic**) or with carbocyclic units (e.g. **Amphimic acids**) also occur.



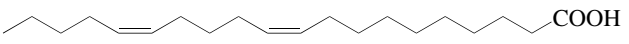
Amphimic acid B

(ii) Acids with one unsaturated centre are usually alkenic compounds with *cis*-(*Z*-) configuration and with the double bond in one of a limited number of preferred positions. This is most commonly Δ^9 (e.g. **Oleic acid**) or *n*-9 (e.g. **Erucic acid**) but the double bond can occur in other positions (e.g. **Petroselinic acid**) and monoacetylenic acids are also known (e.g. **7-Hexadecynoic acid**).

$$H_3C(CH_2)_7C{\equiv}C(CH_2)_5COOH$$

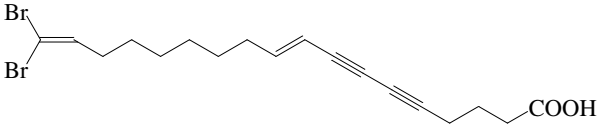
7-Hexadecynoic acid

(iii) Polyunsaturated acids are mainly polyalkenic (*cis*-/*Z*-configuration) with a methylene-interrupted arrangement of double bonds, i.e. double bonds are separated from each other by one CH_2 group. The pattern of 1,4-unsaturation is characteristic of fatty acids and differs from that in isoprenoids which are usually 1,3- or 1,5- conjugated. Polyunsaturated fatty acids occur in biochemically related families and the two most important are the *n*-6 family based on **Linoleic acid** and the *n*-3 family based on **α-Linolenic acid**. Some acids have conjugated unsaturation which is both *cis* and *trans* (e.g. **5,7,9,14,17-Eicosapentaenoic acid**), some have mixed ene/yne unsaturation both conjugated (e.g. **7,9,12-Octadecatrien-5-ynoic acid**) and non-conjugated (e.g. **16,16-Dibromo-15-hexadecen-5-ynoic acid**), and there is a group of acids in which unsaturation is not methylene-interrupted (e.g. **10,15-Eicosadienoic acid**).



10*Z*,15*Z*-Eicosadienoic acid

(iv) Fatty acids having additional functionality apart from the carboxyl group and unsaturation and are widespread. Acids are known with chloro, bromo, hydroxy, methoxy, oxo, and epoxy groups. Examples are **10-Chloro-9-hydroxy-hexadecanoic acid, 2-Methoxy-6-tetradecenoic acid, 18,18-Dibromo-9,17-octodecadiene-5,7-diynoic acid**.



(9*E*)-18,18-Dibromo-9,17-octadecadiene-5,7-diynoic acid

The major biosynthetic pathways leading to fatty acids are summarised in Figure 1. In the *de novo* pathway leading to saturated fatty acids, acetate (the primer) condenses with malonate (the extender) to produce a C_4 oxo acid which is reduced in three steps to butanoate. This cycle of condensation and reduction continues until, most commonly, palmitate has been obtained. The malonate is itself derived from acetate by carboxylation in the presence of a biotin enzyme and the carbon dioxide lost during condensation is that derived during carboxylation so that the carbon atoms in butanoate and in the longer chain acids are entirely acetate-derived. If the acetate is replaced by a different primer then other fatty acids are produced. This can be propanoate (major product: heptadecanoate), 2-methylpropionate (*iso* acids), or 2-methylbutanoate (*anteiso* acids).

The chain-elongation process is similar in outline to the *de novo* process but differs in some significant details. It operates with both saturated and unsaturated acids and occurs with either acetate or malonate. **Erucic acid** is made from Oleic acid by two chain-elongation steps:

$$18:1(9Z)\rightarrow 20:1(11Z)\rightarrow 22:1(13Z)$$

The most common route to monoene acids involves Δ^9 desaturation. This oxygen-requiring process occurs in plants, animals and microorganisms and furnishes acids with a *cis*-double bond between carbon atoms 9 and 10, e.g. **9-hexadecenoic**, **9-octadecenoic acids** (**Oleic acid**).

Further desaturation of **Oleic acid** to the 9,12-diene (**Linoleic acid**) and 9,12,15-triene (**α-Linolenic acid**) occurs only in plants. The additional double bonds assume a methylene interrupted pattern and lie between the existing double bond and the methyl group. Generally only plants are capable of biosynthesising *de novo* *n*-3 and *n*-6 polyunsaturated acids. Animals requiring these acids for the production of *n*-6 and *n*-3 polyene acids must obtain them through their dietary intake. Figure 1 shows the major pathways in marine algae and herbivorous calanoid copepods.

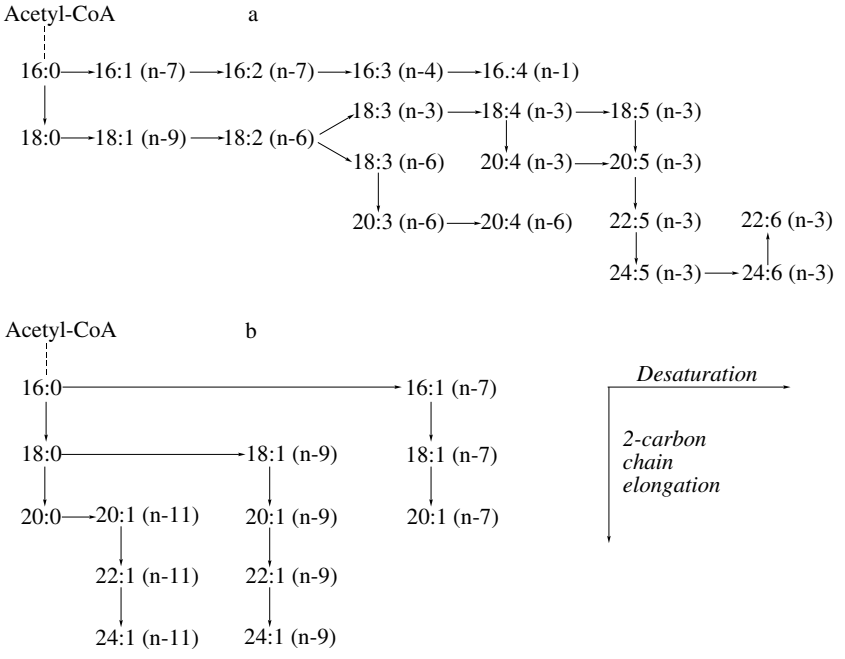


FIGURE 1. Major pathways of fatty acid biosynthesis in (a) marine algae and (b) herbivorous calanoid copepods (Dalsgaard et al)

Desaturation between an existing double bond and the carboxyl group occurs only rarely in plants (e.g. γ-Linolenic acid) but readily in animals. The additional double bonds have *cis*- configuration and are introduced in a methylene-interrupted pattern.

A wide variety of unusual fatty acids and phospholipids are found in sponges, and these arise by totally different biosynthetic pathways (Djerassi (1991). The fatty acids are derived by homologation of short chain fatty acid precursors largely derived from exogenous sources, most likely bacteria and plankton. Fatty acid desaturation in sponges has characteristics of both animal and plant processes. There is no conclusive evidence that sponges are incapable of *de novo* fatty acid biosynthesis, but so far the formation of short-chain acids from radiolabelled acetate had not been observed to any significant extent. Examples are 5*Z*,9*Z*,19*Z*-hexacosatrienoic acid and 6-bromo-5E,9Z-hexacosatrienoic acid.

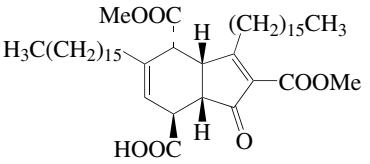
Rezanka, T., *Prog. Lipids Res*., 1989, **28**, 147–1879 (*very long fatty acids*)
Djerassi, C. *et al, Acc. Chem. Res*., 1991, **24**, 69–75 (*sponge fatty acids*)
Jie, M.S.F.L.K. *et al*, *Nat. Prod. Rep*., 1997, **14**, 163–189 (*rev*)
Debitsky, V.M. *et al, Prog. Lipid Research*, 2002, **41**, 315–367 (*halogenated fatty acids*)
Dalsgaard, J. *et al, Adv. Marine Biology*, 2003, **46**, 225–340 (*marine fatty acids, rev*)
Christie, W.W., *Lipid Analysis*, Oily Press, Bridgwater, U.K., 2003 (*analysis*)
Berge, J.-P. *et al*, *Adv. Biochem. Engin. Biotech*., 2005, **96**, 49–125 (*marine fatty acids, rev*)
Kornprobst, J.-M., *Substances Naturelles d'Origine Marine*, Lavoisier, Paris, 2005
Ackman, R.G., *Handbook of Functional Lipids*, (ed. Akoh, C.C.), CRC/Taylor & Francis, Boca Raton, 2006, 311–324 (*marine lipids, nutrition*)
Gunstone, F.D. *et al*, *The Lipid Handbook with CD-ROM*, 3rd edn, Chapman & Hall/CRC Press, Boca Raton, 2007

1.2.2 Oxylipins (VA6150)

Three C_{20} acids, 20:3 (*n*-6), 20:4 (*n*-6), and 20:5 (*n*-3) are precursors of prostaglandins and of many other C_{20} metabolites. These are known collectively as eicosanoids and are products of the eicosanoid cascade.

The term oxylipin has been coined relatively recently to describe the class of natural product, of which prostaglandins are the most widespread. They are produced from C_{20} and in some cases C_{18} fatty acid precursors in at least one stage of mono- or dioxygenase-dependent oxidation. Since it is now known that C_{20} precursors are not universal, the term oxylipin is to be preferred to the previous term eicosanoid.

A wide variety of structural types is found in marine organisms where ring formation may produce three, (e.g. **Constanolactones**), five (e.g. **Ecklonialactone A**) or six- (e.g. **Manzamenone A**) membered rings.

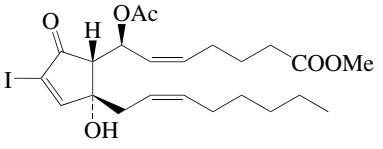


Manzamenone A

Gerwick, W.H., *Chem. Rev*., 1993, **93**, 1807–1823 (*marine oxylipins*)
Gerwick, W.H., *Adv. Exp. Med. Biol*., 1999, **447**, 211 (*biosynth*)
Pohnert, G. *et al, Nat. Prod. Rep*., 2002, **19**, 108–122 (*brown algal oxylipins*)

1.2.3 **Prostaglandins** (VA6100)

The eicosanoid or arachidonic acid cascade produces prostaglandins. **Prostaglandins $F_{2\alpha}$** and **E_2** are encountered in marine algae and invertebrates. In corals, it has been demonstrated that these arise via the cyclooxygenase from the arachidonic acid pathway involved in arachidonic acid metabolism. Other compounds in this group are the **Clavulones** and the **Punaglandins**. An example is **Iodopunaglandin 8**.



Iodopunaglandin 8

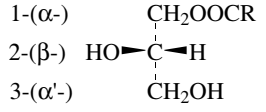
Bentley, P.H., *Chem. Soc. Rev*., 1973, **2**, 29–48 (*synth*)
Lai, S.M.F. *et al*, *Nat. Prod. Rep*., 1984, **1**, 409–441(*rev*)
Newton, R.F. *et al*, *Synthesis*, 1984, 449–478 (*synth*)
Hart, T.W., *Nat. Prod. Rep*., 1988, **5**, 1–45 (*synth*)
Lands, W.E.M., *Annu. Rev. Nutr*., 1991, **11**, 41–60 (*biosynth*)
Smith, W.L., *Am. J. Physiol*., 1992, **263**, F181 (*biosynth, action*)
Collins, P.W. *et al*, *Chem. Rev*., 1993, **93**, 1533–1564 (*synth*)
Moore, B.S. *et al*, *Nat. Prod. Rep*., 2006, **23**, 615–629 (*biosynth*)

1.2.4 **Glycerides** (VA6700, VA6800, VA6900)

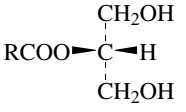
Fatty acids occur naturally as esters of **Glycerol** or of some other hydroxy compound or as amides of long-chain amines such as **Sphingenine**. The less common long-chain alcohols occur as esters or as ethers. Triacylglycerols are major storage lipids whilst phospholipids (see below) are important membrane constituents.

Acylglycerols are esters of glycerol and fatty acids. Partial glycerides are important intermediates in metabolism and triacylglycerols are the major constituents of natural fats and oils. In this Dictionary, glycerides are named as glycerol triesters, e.g. entry name = **Glycerol tri-9-octadecenoate**.

Monoacylglycerols (monoglycerides) (VA6700) are fatty acid monoesters. See the major Dictionary entries for **Glycerol 1-alkanoates** and **Glycerol 2-alkanoates**.



1-Monoacyl-*sn*-glycerol
(chiral)



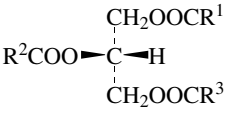
2-Monoacyl-*sn*-glycerol
(achiral)

Diacylglycerols (diglycerides) (VA6800) are fatty acid diesters of glycerol. See the major Dictionary entries for **Glycerol 1,2-dialkanoates** and **Glycerol 2,3-dialkanoates**.

1,2-Diacyl-*sn*-glycerol (α,β-isomer)

1,3-Diacyl-*sn*-glycerol (α,α'-isomer)

Triacylglycerols (triglycerides) (VA6900) are fatty acid triesters of glycerol. The fatty acids may be all different, two different, or all alike. See the major Dictionary entries for **Glycerol trialkanoates (diacid, symmetrical)**, **Glycerol trialkanoates (diacid, unsymmetrical)** and **Glycerol trialkanoates (triacid)**. The common monoacid triesters have separate entries.



Triacyl-*sn*-glycerol

Particular fatty acids may be concentrated in or excluded from particular positions in the glycerol ester.

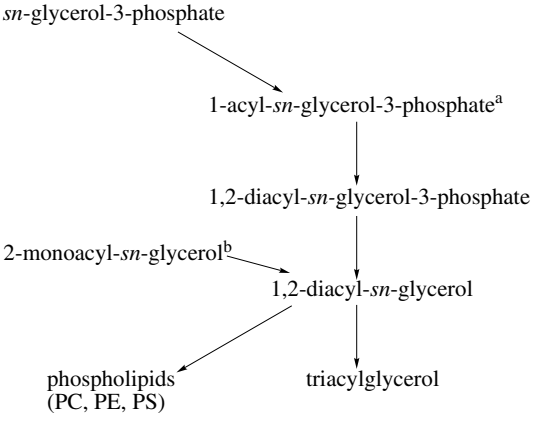


FIGURE 2. Biosynthesis of the major lipid classes

In plants glycerolipids are produced by wholly endogenous pathways but in animals there are additional routes by which dietary lipids are modified. The lipid composition of animals is influenced by dietary intake but is not completely defined by it.

1,2-Diacyl-*sn*-glycerols (Figure 2) are key intermediates in the biosynthesis of both triacylglycerols and phospholipids and are produced mainly from *sn*-glycerol-3-phosphate (a product of carbohydrate metabolism) by acylation of both free hydroxyl groups in separate stages followed by dephosphorylation. Further acylation of the *sn*-3 hydroxyl group gives triacylglycerols.

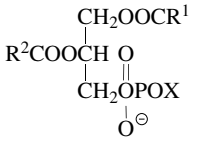
Gunstone, F.D. *et al*, *The Lipid Handbook with CD-ROM*, 3rd edn, Chapman & Hall/CRC Press, Boca Raton, 2007

1.2.5 Phospholipids and sphingolipids (VA7000, VA7200)

Phospholipids and sphingolipids are constituents of cell membranes and they play an essential role in the synthesis of plasma lipoproteins and in the transduction of messages from cell surfaces to second messengers that control cellular processes. **Phosphatidylcholine** (Lecithin) is the most abundant phospholipid (see Figure 3).

Sphingosine (4-Sphingenine) – the most common of the long-chain bases – is produced from Palmitic acid (as its CoA derivative) and Serine as shown in Figure 4. Such compounds are then acylated at the NH_2 group to give

ceramides and further modified at the primary hydroxyl group to give sphingolipids (Figure 5). In this Dictionary, most ceramides are reported as acyl derivatives of the various amino bases. A variety of unusual odd-carbon and branched-chain amines have been reported from marine organisms.



X	Name of class	Abbreviation
H	phosphatidic acid	PA
$CH_2CH_2N^{\oplus}H_3$	phosphatidylethanolamine	PE
$CH_2CH_2N^{\oplus}Me_3$	phosphatidylcholine	PC
$CH_2CH(N^{\oplus}H_3)COOH$	phosphatidylserine	PS
$CH_2CH(OH)CH_2OH$	phosphatidylglycerol	PG
$C_6H_{11}O_6$	phosphatidylinositol	PI

FIGURE 3. Structures of the major phospholipids

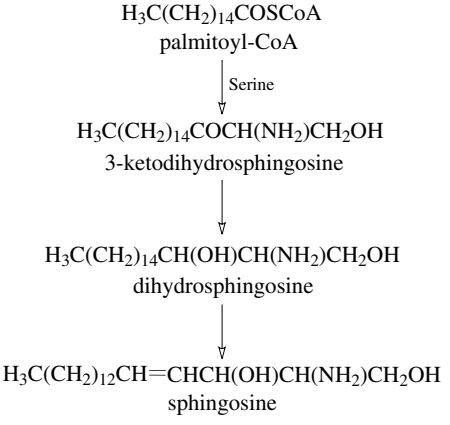
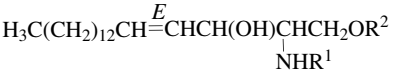


FIGURE 4. Biosynthesis of Sphingosine

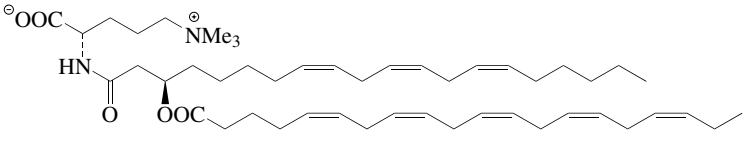


sphingosine	($R^1 = R^2 = H$)
ceramides	($R^1 = COR$, $R^2 = H$)
cerebrosides	($R^1 = COR$, R^2 = sugar residue)
sphingomyelin	($R^1 = COR$, $R^2 = PO_3^{\ominus}CH_2CH_2N^{\oplus}Me_3$)

FIGURE 5. Structures of sphingolipids

Alternatively the free hydroxyl group is converted to an appropriate phosphate ester to produce a phospholipid. Dietary triacylglycerols can be hydrolysed to 2-monoacyl-*sn*-glycerols and then reacylated to diacylglycerols and triacylglycerols.

Typical compounds in these classes are the **Acanthacerebrosides**, **Plakosides**, **Stellettacholine A** and **Yendolipin**.



Yendolipin

Djerassi, C. *et al, Acc. Chem. Res*., 1991, **24**, 69–75 (*sponge phospholipids*)
Gunstone, F.D., *Fatty Acid and Lipid Chemistry*, Blackie, London, 1996
Carballeira, N.M. *et al, Recent Res. Dev. Lipids Res*., 1997, **1**, 9–17 (*brominated phospholipids*)
Fattorusso, E. *et al, Progress in the Chemistry of Organic Natural Products*, (eds. Hertz, W. *et al*), SpringerWien, New York, 1997, **72**, 215–301 (*rev, glycolipids*)
Jie, M.S.F.L.K. *et al*, *Nat. Prod*. Rep., 1997, **14**, 163–189 (*rev*)
Carbohydr. Res., 1998, **312**, 167–175 (*glycolipid nomenclature*)
Tan, R.X. *et al*, *Nat. Prod. Rep*., 2003, **20**, 509–534 (*cerebrosides*)
Gunstone, F.D. *et al*, *The Lipid Handbook with CD-ROM*, 3rd edn, Chapman & Hall/CRC Press, Boca Raton, 2007

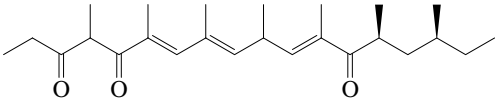
2. POLYKETIDES (VC)

Many organisms have the ability to produce a very wide range of structural types of metabolite which are derived from a poly-β-ketomethylene chain. This chain is formed by condensation of an acetyl unit (or other acyl unit) with malonyl or methylmalonyl units, with concomitant decarboxylation as in fatty acid biosynthesis but without the reduction of the intermediate β-dicarbonyl system. The resulting polyketide chain can take part in internal aldol-type condensations to give aromatic systems characterised by an alternating oxygenation pattern. Alternatively reduction or partial reduction of the carbonyls during biosynthesis can give rise to nonaromatic metabolites. One method of classifying polyketides is by the number of acetate (or propionate) units in a metabolite; however, this has the disadvantage of separating structurally similar types. The vast array of polyketides is treated in DMNP according to a mixture of structural, biosynthetic and functional criteria. The advantage of this approach is that related compounds are listed together. Aromatic polyketides are classified under the appropriate aromatic grouping (see section VG below).

Simpson, T.J., *Nat. Prod. Rep*., 1985, **2**, 321–347; 1987 **4**, 339–376; 1991, **8**, 573–602 (*biosynth*)
Herbert, R.B., *The Biosynthesis of Secondary Metabolites*, 2nd edn, Chapman & Hall, London, 1989
O'Hagan, D., *The Polyketide Metabolites*, Ellis Horwood, New York, 1991
O'Hagan, D., *Nat. Prod. Rep*., 1992, **9**, 447–479; 1995, **12**, 1–32 (*biosynth*)
Hopwood, D.A., *Chem. Rev*., 1997, **97**, 2465–2498 and refs therein (*biosynth*)
Davies-Coleman, M.T. *et al*, *Nat. Prod. Rep*., 1998, **15**, 477–493 (*marine polypropionates*)
Rawlings, B.J., *Nat. Prod. Rep*., 2001, **18**, 231–281 (*bacterial polyketides*)
Staunton, J. *et al*, *Nat. Prod. Rep*., 2001, **18**, 380–416 (*biosynth*)
Moore, B.S. *et al*, *Nat. Prod. Rep*., 2002, **19**, 70–99 (*bacterial starter units*)

2.1.1 Linear polyketides (VC0050)

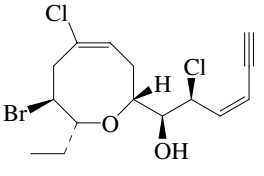
This section contains polyketides that do not contain carbocyclic or macrolide ring systems but may contain tetrahydrofuran or tetrahydropyran rings. An example is **Aglajne 1**.



Aglajne 1

2.1.2 Marine halogenated acetogenins (VC0070)

Marine metabolites include a series of halogenated polyketides particularly from red algae (*Laurencia* spp.). The metabolites contain, along with bromine and chlorine substituents, oxygen heterocycles, acetylenes and allenes. A typical example is **Bermudenynol**.

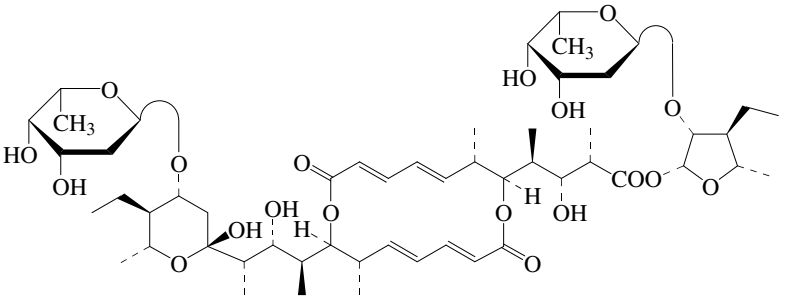


Bermudenynol

Faulkner, D.J., *Nat. Prod. Rep*., 1996, **13**, 75–125 (*rev*)
Butler, A. *et al*, *Nat. Prod. Rep*., 2004, **21**, 180–188 (*biosynth*)

2.1.3 Macrolides and lactone polyketides (VC0100, VC0150)

Structurally, macrolides are a class of complex lactones; normally containing a 12–16 membered macrocyclic ring, often with ether bridges forming further 3-, 4-, 5-, or 6-membered rings, and one to three neutral or aminosugar residues that are linked to the macrocycle via ether linkages. Examples in this class are the **Bryostatins**, **Amphidinolides**, **Macrolactins**, **Oscillatoxins** and **Halichoblelide**.

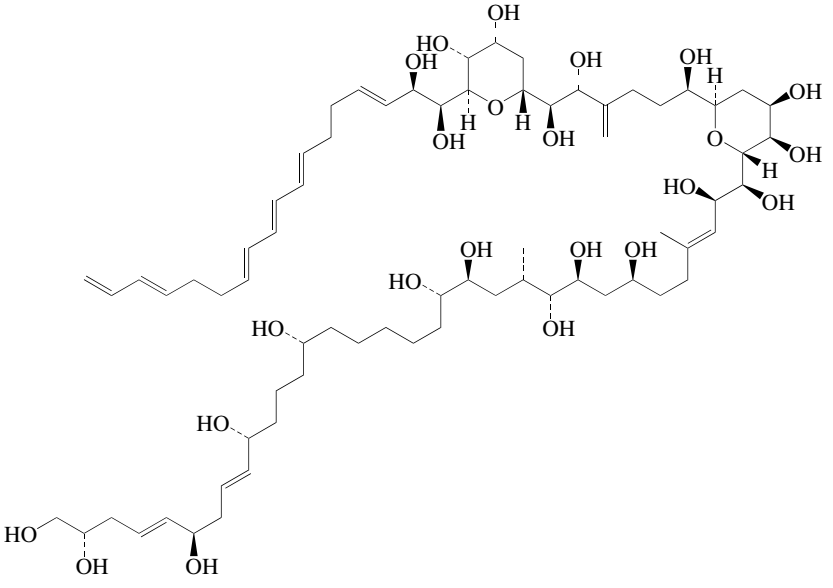


Halichoblelide

Omura, S., *Macrolide Antibiotics, Chemistry, Biology and Practice*, Academic Press, London, 1984 (*general*)
Paterson, I. *et al*, *Tetrahedron*, 1985, **41**, 3569–3624 (*synth*)
Omura, S., *Biotechnology*, (ed. Page, H.), VCH, Weinheim, 1986, **Vol. 4**, 359 (*general*)
Tatsuta, K., *Recent Prog. Chem. Synth. Antibiot*., 1990, 1–38 (*synth, rev*)
Nakata, M. *et al*, *Studies in Natural Product Chemistry*, (ed. Atta-ur-Rahman), Amsterdam, Elsevier, 1993, **Vol. 12**, 35 (*synth*)
O'Hagan, D., *Nat. Prod. Rep*., 1989, **6**, 205–219 (*biosynth*)
Hale, K.J. *et al*, *Nat. Prod. Rep*., 2002, **19**, 413–453 (*Bryostatins*)

2.1.4 Polyenes (VC0300)

The group of compounds, known collectively as polyenes, are compounds containing a series of conjugated double bonds. This leads to the sub-division of the group into trienes, tetraenes etc. The **Amphidinols** are built up with five regular C2-elongation sequences, which are separated by continuous acetate-methyl derived carbons. An example of this group is **Amphidinol 3**.



Amphidinol 3

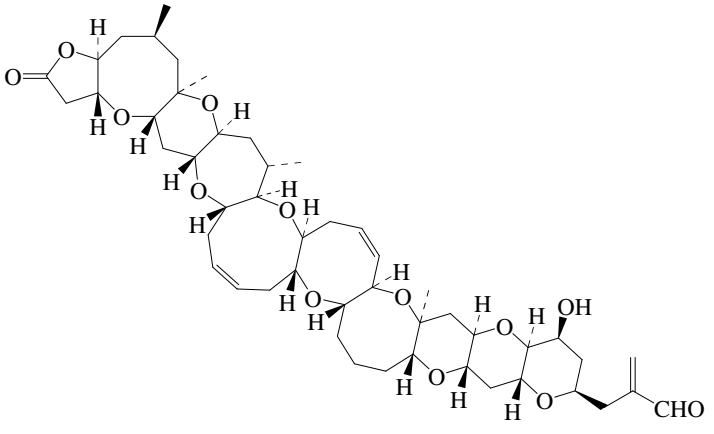
Rinehart, K.L., *Bio/Technology*, 1983, **1**, 581–588 (*ms*)
Omura, S., *Macrolide Antibiotics, Chemistry, Biology and Practice*, Academic Press, London, 1984
Thomas, A.H., *J. Antimicrob. Chemother*., 1986, **17**, 269–279 (*action*)
Rychnovsky, S.D., *Acta Pharm. Nord*., 1990, **2**, 155–160 (*synth, rev*)
Beau, J.M., *Recent Prog. Chem. Synth. Antibiot*., 1990, 135–182 (*synth, rev*)
Houdai, T. *et al*, *Tetrahedron*, 2001, **57**, 5551–5557 (*biosynth*)

2.1.5 Polyether antibiotics (VC0500)

The majority of polyethers are characterised by a linear series of tetrahydrofuran and tetrahydropyran residues, frequently linked by spiroketal systems. They are metabolites of marine microoganisms that are often symbiotic with sponges. Polyethers are generally produced as a series of closely related compounds, e.g. the major component may possess methyl substituents on each of the cyclic ether units, but in addition small amounts of ethyl homologues may also be present. Chemical subdivision can be based on the number of spiroketal functionalities, and the presence or absence of a sugar residue.

Polyethers possess the ability to bind and transport certain ions, and each antibiotic has its own ion specificity. The antibiotics show a wide range of activities, being active against gram-positive organisms and mycobacteria, fungi and yeasts, but because of their toxicity, these properties have found little application. Polyether compounds of this type, however, are now much more than antibiotics, e.g. **Halichondrins** are potent antimitotic agents, analogues of which are being developed through clinical trials.

Biosynthetically, the polyethers are polyketide in origin. The major building blocks are acetate, propanoate, and butyrate. There is evidence to suggest the intermediacy of an epoxide in the formation of the tetrahydrofuran and tetrahydropyran systems. **Brevetoxin** A is a typical polyether compound.



Brevetoxin A

Wieranga, W., *Total Synthesis of Natural Products* (ed. Ap'Simon, J.), Wiley, New York, 1981
Westley, J.W. (ed.), *Polyether Antibiotics*, Marcel Dekker, NY, 1982
Westley, J.W., *J. Nat. Prod*., 1986, **49**, 35–47 (*biosynth*)
Berdy, J., *Biotechnology*, (ed. Page, H.) VCH, Weinheim, Ger., 1986, **Vol 4**, 494
Crandall, L.W. *et al*, *The Bacteria*, (eds. Queener, S.W. *et al*.), Academic Press, Orlando, 1986, **Vol IX**, 385
Siegel, M.M. *et al, Biomed. Environ. Mass Spectrom*., 1987, **14**, 29–38 (*ms*)
Yonemitsu, O. *et al, Recent Prog. Chem. Synth. Antibiot*., 1990, 447–466 (*synth*)
Robinson, J.A., *Progress in the Chemistry of Organic Natural Products*, (eds. Herz, W. *et al*), SpringerWien, New York, 1991, **Vol. 58**, 1–81 (*biosynth*)
Dutton, C.J. *et al*, *Nat. Prod. Rep*., 1995, **12**, 165–181 (*rev*)
Rein, K.S. *et al, Comp. Biochem. Physiol., B: Comp. Biochem. Mol. Biol*., 1999, **124**, 117–131 (*dinoflagellate metabolites, pharmacol, biosynth*)
Fernandez, J.J. *et al, Recent Res. Dev. Org. Chem*., 2000, **4**, 188–189 (*diarrhetic shellfish poisons, biosynth*)
Nicholson, G.M. *et al*, *Mar. Drugs*, 2006, **4**, 82–118 (*Ciguatoxins, activity*)
Satake, M., *Top. Heterocyclic Chem*., (ed. Kiyota, H.), Springer, Berlin, 2006, **Vol. 5**, 21–51 (*rev*)

3. CARBOHYDRATES (VE)

This is an abbreviated account dealing only with aspects of carbohydrate chemistry relevant to marine natural products. Although carbohydrates are important components of the tissues of marine bacteria and algae, and of marine animal tissues (e.g. **chitin**), their marine chemistry presents few aspects that have not already been documented among terrestrial organisms. For a fuller coverage including synthetic carbohydrates, see the companion publication *Dictionary of Carbohydrates*.

Carbohydrates comprise a family of polyhydroxy aldehydes, ketones and acids, together with linear and cyclic polyols. They are diverse because they exist as a wide range of stereoisomers. These compounds are the most abundant and widespread organic substances in nature and are essential constituents of all living matter. Of the 36 possible stereoisomeric pentoses, pentuloses, hexoses and hexuloses only D-glucose, D-fructose, D-galactose, D-mannose and L-arabinose occur naturally in the free state, and only the first two are found in large amounts. However, modified sugar residues belonging to many of the stereoisomeric series are crucial components of, and precursors to, a wide range of important biologically active molecules.

Photosynthesis is the means by which plants produce sugars from carbon dioxide and water. In brief, it occurs by carbon dioxide being transferred to D-*erythro*-pentulose-1,5-diphosphate to give, via an unstable β-keto-6-carbon acid, two molecules of D-glyceric acid-3-phosphate, from which hexoses, for example, D-fructose 1,6-diphosphate and D-glucose 1-phosphate can be formed. Animals, on the other hand, use the reverse of the glycolysis metabolic pathway to produce glucose from proteins and fats utilising phosphoenolpyruvate as an intermediate. Most of the routes used by nature to interconvert sugars occur by way of enzymic reactions on nucleoside diphosphate sugars, particularly **Uridine diphosphate glucose** (UDPG) which gives D-galactose on epimerisation at *C*-4, D-glucuronic acid by oxidation at *C*-6 and D-xylose by decarboxylation of this acid. Deoxygenation at *C*-6 and configuration changes at *C*-4 and *C*-5 give L-rhamnose and by similar means the commonly occurring D-sugars may be transformed into members of the L-series.

3.1.1 Fundamental aldoses and ketoses (VE0100–VE2200)

In the Type of Compound classification the simple sugars are classified into their various stereoisomeric subgroups.

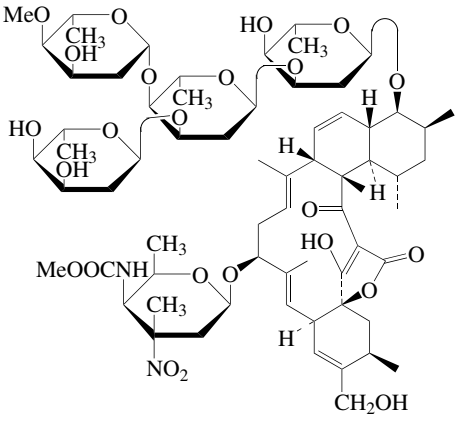
3.1.2 Modified aldoses and ketoses (VE2600–VE8400)

The number of natural sugars increases when modified forms of the 36 fundamental sugars are considered. Thus in addition to the common occurrence of combined forms of the five sugars mentioned above, D-allose, D-talose, D-arabinose, D-ribose, D-xylose, L-lyxose, D-psicose, L-sorbose and D-tagatose are also found as their derivatives in varying quantities. It is rather surprising that the vast number of naturally occurring carbohydrate compounds is derived from so few sugars in this pool. The shortfall is made up by the occurrence of so called modified sugars such as deoxy-, amino-, thio-, branched chain, and higher sugars in addition to various alditols, cyclitols and sugar acids.

Bacteria contain several sugars that are unique to their constitution. **Muramic acid**, glycosidically linked to ***N*-Acetylglucosamine**, is the disaccharide repeating unit that forms the peptidoglycan of gram-negative bacterial cell walls. In gram-positive bacteria, teichoic acids, which are large polymers of the phosphates of D-ribitol or glycerol, form up to 50% of the cell wall.

3.1.3 Branched-chain sugars (VE7200)

Carbon chain branching in sugars can arise biogenetically in two ways; either *C*-bonded hydrogen atoms are replaced to give *C*-substituted derivatives of the normal straight-chain compounds (CHOH → CROH), or else hydroxyl functions are replaced (CHOH →CHR). In the naming of the latter class, the 'deoxy' prefix is included to denote the absence of the hydroxyl substituent at the branching carbon atom, and members can be described as belonging to the 'deoxy' group of branched chain sugars (e.g. 3-*C*-methyl-D-glucose and 3-deoxy-3-*C*-methyl-D-glucose are the respective names of compounds obtained by replacing in glucose either the hydrogen at *C*-3 or the hydroxyl at *C*-3 by methyl). **Kijanimicin** produced by an actinomycete isolated from the alga *Lobophora variegata* contains a 3-*C*-methyl sugar residue.



Kijanimicin

3.1.4 Carbohydrate acids (VE7900, VE8000, VE8100, VE8200)

The following four types of carbohydrate acids occur in nature for which named examples are given for compounds derived from glucose: aldonic acids (VE7900) (**D-Gluconic acid**) which are formed when the aldehydic function in an aldose is oxidised; aldaric acids (VE8100) (**D-Glucaric acid**) which are dicarboxylic acids formed by oxidation of the aldehydic groups and hydroxymethyl groups in aldoses; uronic acids (VE8000) (**D-Glucuronic acid**) and ketoaldonic acids (VE8200) (**D-*arabino*-Hex-2-ulosonic acid**) which are formed by oxidation of the hydroxymethyl groups in aldoses and ketoses respectively.

3.1.5 Alditols (VE8600–VE8900)

The polyols, obtained by reduction of the aldehyde function of an aldose, are known as alditols. An example is **Mannitol**. They are named by a straightforward extension of the rules used for aldoses. The alditol corresponding to a chiral sugar may be *meso*-, e.g. **Galactitol**.

3.1.6 Cyclitols (VE9000)

The polyhydroxycycloalkanes, known as cyclitols, are a group of natural products closely related to the carbohydrates proper, of which the most important are the inositols (1,2,3,4,5,6-cyclohexanehexols). Trivial names are often used but systematic rules have been introduced to assign configurations at each enumerated ring carbon atom and this requires the application of a recommended numbering convention. Further information on the various descriptions of stereochemistry for these compounds can be obtained by the inspection of the individual Dictionary entries. It should be noted that some *meso*-isomers in the series can have optically active derivatives.

Angyal, S.J. *et al*, *Adv. Carbohydr. Chem*., 1959, **14**, 135–212 (*rev*)
Posternak, T., *The Cyclitols*, Holden-Day, San Francisco, 1965
Percival, E., *Oceanography and Marine Biology: An Annual Review*, CRC Press, Boca Raton, FL, 1968, **6**, 137–161 (*marine algal carbohydrates*)
Anderson, L., *The Carbohydrates*, (eds. Pigman, W. and Horton, D.), Academic Press, 1972, **IA**, 519
Pure Appl. Chem., 1974, **37**, 285–297 (*cyclitol nomenclature*)
Reitz, A.B., *Inositol Phosphates and Derivatives*, ACS Symposium Series, Washington, DC, 1991
Trefzer, A. *et al, Nat. Prod. Rep*., 1999, **16**, 283–314 (*deoxy sugars, biosynth*)
Collins, P.M., *Dictionary of Carbohydrates*, 2nd edn, Chapman & Hall/CRC, Boca Raton, 2006

3.1.7 Oligosaccharides and polysaccharides (VE9300, VE9400)

Oligosaccharides are most often found as glycosides in, for example, plants, antibiotics and some glycoproteins. Polysaccharides are the most abundant form of carbohydrates. **Cellulose** is the principal constituent of plant cell walls providing their structural strength. **Starch** and **Glycogen** are found preponderantly in plants and animals respectively where they serve as energy reserves. Whereas glucose is the building unit for the previous three polymers, **Chitin**, which is found in the shells of arthropods, is a polymer of 2-acetamido-2-deoxyglucose. **Carrageenan** and **Agar** are structural polysaccharides of the red algae. These polymers are derivatives of linear galactans.

Glycosidic bonds in naturally occurring oligosaccharides and glycosides are formed in natural glycosylations which take place primarily by way of the nucleoside diphosphate sugars as follows:

$$\text{nucleoside}-\text{DP}-\ \text{sugar}+\text{ROH}\rightarrow\text{sugar}-\text{OR}+\text{nucleoside}-\text{DPH}$$

Disaccharides or their phosphates are produced when ROH is a sugar or a sugar phosphate. Polysaccharide biosynthesis is basically similar but requires an oligomer primer as an acceptor; glycogen synthesis follows the course:

$$\text{primer}+\text{UDPG}\rightarrow\text{G}\alpha\text{-primer}+\text{UDP}$$

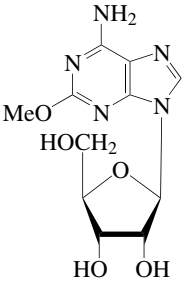
there being one enzyme present which catalyses the formation of 1,4-bonds and another responsible for glycosylations at position 6. The biosynthesis of cellulose and other polysaccharides is basically similar, UDP being the nucleoside diphosphate used predominantly. However, starch synthesis depends rather on adenosine diphosphate.

Guiry, M.D., *Trop. Sci.* 1979, **21**, 183–185 (*red algal polysaccharides*)
Ziener, M. *et al, Carbohydr. Res*., 2000, **328**, 209–216 (*polysaccharides, sponges*)
Duarte, M.E.R. *et al, Carbohydr. Res*., 2001, **333**, 281–293 (*sulfated polysaccharides*)
Aquino, R.S. *et al*, *Glycobiology*, 2005, **15**, 11–20 (*sulfated galactans*)
Nichols, C.A.M. *et al, Mar. Biotech*., 2005, **7**, 253–271 (*marine microbial exopolysaccharides*)

3.1.8 Nucleosides (VE9900)

These are glycosides of purines, pyrimidines and other heterocyclic bases. The well-known quartet of **Adenosine**, **Guanosine**, **Cytidine** and **Thymidine** are fundamental biomolecules essential to life through their participation in the structure of DNA and RNA. A number of 'hypermodified' nucleosides occur in bacterial nucleic acids.

Another group of nucleosides consist of a sugar linked to a base either via a ring nitrogen or through a ring C atom (the latter are designated *C*-nucleosides). Structurally they are rather diverse but a subclassification is given by Isono. A typical example is **Spongosine**.



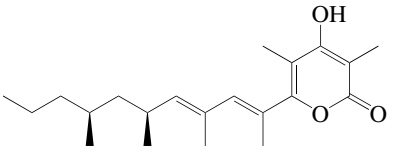
Spongosine

Suhadolnik, R.J., *Nucleosides as Biological Probes*, Wiley, New York, 1979
Suhadolnik, R.J., *Antibiotics* (N.Y.), 1981, **4**, 353–370 (*biosynth*)
Buchanan, J.G., *Progress in the Chemistry of Organic Natural Products*, (eds. Herz, W. *et al*), SpringerWien, New York, 1983, **Vol. 44**, 243–299 (*C-nucleosides*)
Isono, K., *J. Antibiot*., 1988, **41**, 1711–1739 (*biosynth, struct, rev*)
Townsend, L.B., *Chem. of Nucleosides and Nucleotides*, Plenum Press, New York, 1988, **Vol. 1**
Garner, P., *Studies in Natural Products Chemistry*, (ed. Atta-ur-Rahman), Elsevier, Amsterdam, 1988, **Vol. 1**, 397–434 (*synth, rev*)
Secrist, J.A. *et al* (eds.), *Nucleosides Nucleotides*, 1989, **8**, parts 5 and 6 (*rev*)
Brown, E.G., *Methods in Plant Biochemistry*, (ed. Roger, L.J.), Academic Press, New York, 1991, **5**, 53–90 (*rev*)
McCloskey, J.A., *Methods in Enzymology: Mass Spectrometry*, (ed. McCloskey, J.A.), Academic Press, San Diego, 1990, **Vol. 193**, 771–781 (*anal, ms*)
Hobbs, J.B., *The Chemistry of Natural Products*, 2nd edn (ed. Thomson, R.H.), Blackie, Glasgow, 1993, 259

4. OXYGEN HETEROCYCLES (VF)

Many simple natural products contain basic oxygen heterocycles - although most can be seen to be derived from polyketides or carbohydrates, some have unknown biosynthetic origins. The oxygen heterocycles are listed under

the headings: β-Lactones (VF1000), Furans (VF2000), Butanolides (VF3000), Pyrans (VF4000), Pentanolides (VF5000), 2-Pyrones (VF6000) and 4-Pyrones (VF7000). Natural products that contain these substructures in terpenoid, steroid or alkaloid skeletons are not listed here. An example of this group is **Diemenensin A**, which is clearly a polyketide and also coded as such.



Diemenensin A

Turner, W.B. *et al*, *Fungal Metabolites II*, Academic Press, London, 1983
Davies-Coleman, M.T. *et al*, *Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 1989, **Vol. 55**, 1–98 (*rev*)
Ley, S.V., *Heterocycles in Bioorganic Chemistry*, (eds. J. Bergman *et al*), RSC, London, 1991
Dickinson, J.M., *Nat. Prod. Rep*., 1993, **10**, 71–98 (*microbial 2-pyrones*)
Davies-Coleman, M.T. *et al*, *Nat. Prod. Rep*., 1998, **15**, 477–493 (*2- and 4-pyrones, biosynth*)
McGlacken, G.P. *et al, Nat. Prod. Rep*., 2005, **22**, 369–385 (*2-pyrones*)

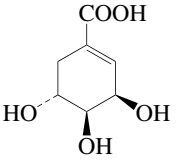
5. SIMPLE AROMATIC NATURAL PRODUCTS (VG)

5.1.1 Simple benzene derivatives (VG0005)

These may be of terpenoid, polyketide or shikimate origin. Those of terpenoid origin, such as the aromatic *p*-menthanes are coded as such and are described below. Fungi are a prolific source of simple benzoquinones which in the main arise by the polyketide route.

Thomson, R.H., *Naturally Occurring Quinones*, 2nd edn, Academic Press, London, 1971
Tyman, J.H.P., *Chem. Soc. Rev*., 1979, **8**, 499–537 (*long chain phenols*)
Turner, W.B. *et al*, *Fungal Metabolites II*, Academic Press, London, 1983
Simpson, T.J., *The Chemistry of Natural Products*, (ed. Thomson, R.H.), Blackie, Glasgow, 1985, 107
Thomson, R.H., *Naturally Occurring Quinones III*, Chapman & Hall, London, 1987
Herbert, R.B., *The Biosynthesis of Secondary Metabolites*, 2nd edn, Chapman & Hall, London, 1989
Simpson, T.J., *Nat. Prod. Rep*., 1991, **8**, 573–602 (*biosynth*)
Gill, M., *The Chemistry of Natural Products*, 2nd edn (ed. Thomson, R.H.), Blackie, Glasgow, 1993, 60

Shikimic acid is derived from glucose in plants *via* the shikimate pathway, which feeds many biosynthetic pathways including those involving the aromatic amino acids **Phenylalanine**, **Tyrosine**, **Tryptophan** and also **p-Aminobenzoic acid**, **Anthranilic acid**, **Cinnamic acid** and other phenylpropanoids. **4-Hydroxybenzoic acid** is the precursor of **2,4,6-Tribromophenol** in the green alga *Ulva lactuca*.

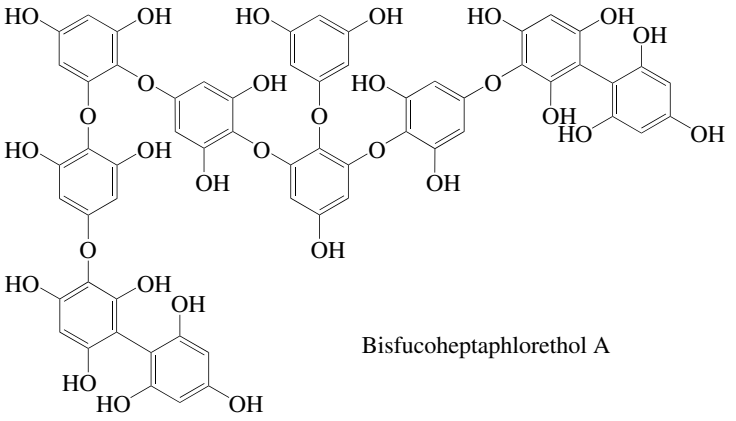


Shikimic acid

Floss, H.G., *Recent Adv. Phytochem*., 1979, **12**, 59–89 (*shikimate pathway*)
Bentley, R., *Crit. Rev. Biochem. Mol. Biol*., 1990, **25**, 307–384 (*shikimate pathway*)
Dewick, P.M., *Nat. Prod. Rep*., 1992, **9**, 153–181 (*biosynth*)
Haslam, E., *Shikimic Acid*, Wiley, Chichester, 1993
Campbell, M.M. *et al*, *Synthesis*, 1993, 179–193 (*shikimate derivs, synth*)
Dewick, P.M., *Nat. Prod. Rep*., 1995, **12**, 101–133; 579–607 (*shikimate metabolites*)
Flodin, C. *et al, Phytochemistry*, 1999, **51**, 249–255 (*tribromophenol biosynth*)
Knaggs, A.R., *Nat. Prod. Rep*., 2001, **18**, 334–355; 2003, **20**, 119–136 (*shikimate metabolites*)

5.1.2 Diphenyl ethers, biphenyls, dibenzyls and phlorotannins (VG1000, VG2000, VG3000, VG2500)

Diphenyl ethers and biphenyls probably arise by radical coupling mechanisms whereas dibenzyl derivatives may be derived from a mixed shikimate-polyketide pathway. Phlorotannins from brown algae are produced by the polymerisation of **Phloroglucinol**. An example is **Bisfucoheptaphlorethol A**.



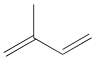
Bisfucoheptaphlorethol A

Turner, W.B. *et al*, *Fungal Metabolites II*, Academic Press, London, 1983
Ragan, M.A. *et al*, *Prog. Phycol. Res*., 1986, **4**, 129–241 (*phlorotannins*)
Gill, M. *et al*, *Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 1987, **Vol. 51**, 1–286 (*fungal phenolics*)
Bringmann, G. *et al, Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 2001, **Vol. 82**, 1–249 (*biaryls*)
Singh, I.P. *et al, Nat. Prod. Rep*., 2006, **23**, 558–591 (*phloroglucinols, phlorotannins*)

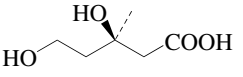
6. TERPENOIDS (VS)

6.1 Classification of terpenoids

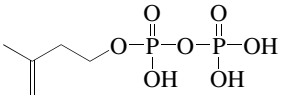
The immense variety of structural types found in the terpenoids was rationalised by the isoprene rule of Ruzicka. However, the number of exceptions to the regular arrangement of isoprene units led to the biogenetic isoprene rule which encompassed the possibility of rearrangements during biosynthesis. Terpenoids are thus seen as being formed from linear arrangements of isoprene units followed by various cyclisations and rearrangements of the carbon skeleton. They can also be biosynthetically modified by the loss or addition of carbon atoms. It is useful to classify terpenoids according to the number of isoprene units from which they are biogenetically derived, even though some carbons may have been added or lost. (This sometimes causes some uncertainty if it is believed that more than five carbons have been lost; only a biosynthetic study can resolve this issue). The biogenetic isoprene rule implies the involvement of a branched five-carbon unit in the biosynthesis of terpenoids. The biosynthetic origin of this five-carbon unit is well established; isoprene iself, although a natural product, is not a precursor of the terpenoids. There are two pathways to the common precursors, isopentenyl diphosphate and dimethylallyl diphosphate. One pathway involves mevalonic acid whereas the more recently discovered pathway involves 1-deoxyxylulose 5-phosphate and is known as the non-mevalonate pathway. The mevalonate pathway is found in animals, the cytoplasm of higher plants, fungi and some bacteria whereas the deoxyxylulose phosphate pathway is found in chloroplasts, algae, cyanobacteria, eubacteria and apicomplexan parasites.



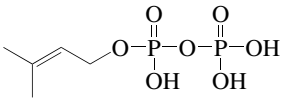
Isoprene



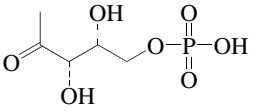
Mevalonic acid



Isopentenyl diphosphate



Dimethylallyl diphosphate



1-Deoxyxylulose 5-phosphate

Ruzicka, L. *et al*, *Experientia*, 1953, **9**, 357–367 (*Isoprene rule*)
Ruzicka, L., *Proc. Chem. Soc.*, 1959, 341–360 (*Isoprene rule)*
Loomis, W.D. *et al*, *Recent Adv. Phytochem.*, 1973, **6**, 147–185 (*biochem*)
Chappell, J., *Ann. Rev. Plant Physiol. Plant Mol. Biol*., 1995, **46**, 521–547 (*biosynth*)
Ramos-Valdivia, A.C. *et al, Nat. Prod. Rep*., 1997, **14**, 591–603 (*Isopentenyl diphosphate isomerase*)
Dewick, P.M., *Nat. Prod. Rep.*, 2002, **19**, 181–222 (*biosynth*)
Hunter, W.N. *et al, Biochem. Soc. Trans*., 2003, **31**, 537–542 (*non-mevalonate pathway*)
Dubey, V.S. *et al*, *J. Biosci*., 2003, **28**, 637–646 (*non-mevalonate pathway*)
Tomohisa, K. *et al*, *Nat. Prod. Rep*., 2003, **20**, 171–183 (*biosynth*)
Eisenreich, W. *et al, Cell. Mol. Life Sci*., 2004, **61**, 1401–1426 (*non-mevalonate pathway*)
Kashman, Y. *et al*, *Phytochem. Rev*., 2004, **3**, 309–323 (*biosynth*)

6.1.1 Nomenclature

The systems used for the nomenclature of terpenoids have evolved over a long period. For many terpenoid classes more than one name has been proposed for the carbon skeleton and in a large number of cases, including many recently discovered marine terpenoid skeletons, several numbering systems are in use. This Dictionary has used the most accepted numbering system for most skeletal types. In cases for which no numbering system has been proposed or where several are in use, preference has been given to the biogenetic system. Many higher terpenoids are named as formal variants of steroid structures and their nomenclature and numbering therefore follows on from that of steroids, which is described more fully in section VT below.

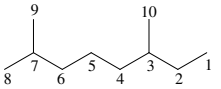
6.2 Monoterpenoids (VS0100–VS1200)

Monoterpenoids are found in many marine organisms, where they are generally halogenated, and as insect pheromones and defence secretions. The biosynthetic pathways of the main classes of monoterpenes have been well studied.

Banthorpe, D.V. *et al*, *Chem. Rev*., 1972, **72**, 115–155 (*monoterpene biosynth*)
Naylor, S. *et al, Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 1983, **Vol. 44**, 189–241 (*marine monoterpenoids*)
Croteau, R., *Chem. Rev*., 1987, **87**, 929–954 (*monoterpene biosynthesis*)
Grayson, D.H. *et al*, *Nat. Prod. Rep*., 2000, **17**, 385–419 (*monoterpenoids*)

6.2.1 Acyclic monoterpenoids (VS0100)

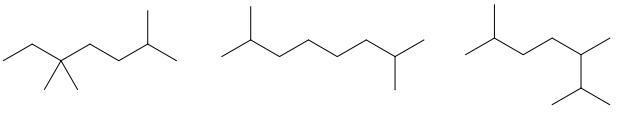
In this section are grouped the regular linear monoterpenoids, that is those formed by a head to tail arrangement of the isoprene units. No semisystematic name has been ascribed to this carbon skeleton because the systematic 2,6-dimethyloctane naming is straightforward. The numbering system shown below is in line with that used with other acyclic terpenoids.



Regular acyclic monoterpenoid skeleton
2,6-Dimethyloctane, 9Cl, 8Cl

6.2.2 Irregular acyclic monoterpenoids (VS0150)

Some acyclic monoterpenoids arise from other arrangements of the isoprene units. These may arise by alternative linkages of the units, e.g. head to head, by rearrangement of regular acyclic monoterpenoids or by cleavage of cyclic monoterpenoids.



Irregular acylic monoterpenoid skeletons

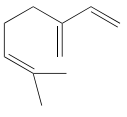
6.2.3 Halogenated dimethyloctane monoterpenoids (VS0200)

This group is obtained principally from marine organisms. They are all regular acyclic monoterpenoids and the numbering system follows the accepted pattern.

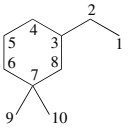
Naylor, S. *et al, Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 1983, **Vol. 44**, 189–241 (*marine terpenoids*)

6.2.4 Ochtodane monoterpenoids (VS0220)

The ochtodanes are also principally from marine organisms particularly *Ochtodes* spp. and presumably arise by cyclisation of myrcene.



Myrcene

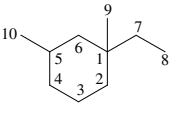


Ochtodane
3-Ethyl-1,1-dimethylcyclohexane, 9Cl

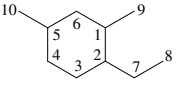
Naylor, S. *et al, Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 1983, **Vol. 44**, 189–241 (*marine terpenoids*)

6.2.5 1-Ethyl-1,3-dimethylcyclohexane and 1-ethyl-2,4-dimethylcyclohexane monoterpenoids (VS0240, VS0260)

These two terpenoid skeletons are only found in marine organisms and presumably arise by cyclisation of a regular acyclic monoterpene skeleton followed in the latter case by an ethyl migration. The numbering systems reflect their probable biogenetic relationship.



1-Ethyl-1,3-dimethyl-
cyclohexane



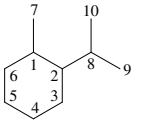
1-Ethyl-2,4-dimethyl-
cyclohexane

Naylor, S. *et al, Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 1983, **Vol. 44**, 189–241 (*marine terpenoids*)

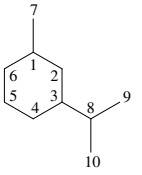
6.2.6 Menthane monoterpenoids (VS0500, VS0520, VS0540)

The menthane group comprises three isomeric types, *o*-, *m*- and *p*-menthanes. The *p*-menthanes are the most widespread and arise by a cyclisation of a regular acyclic monoterpenoid. The *o*- and *m*-menthanes are much rarer, and presumably arise by alkyl migration of *p*-menthanes. The numbering systems of the menthanes reflect

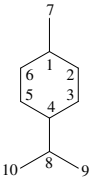
their biogenetic relationship. Since *p*-menthane has a plane of symmetry the numbering of ring substituents is chosen to give the lowest numbers consistent with the avoidance of compound locants for double bonds when possible. For example the name *p*-menth-1-en-6-one is preferred to *p*-menth-1(6)-en-2-one. They are mostly plant products and are thinly scattered in the marine environment.



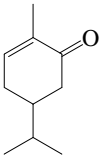
o-Menthane



m-Menthane



p-Menthane, 8Cl
1-Methyl-4-(1-methylethyl)-cyclohexane, 9Cl



p-Menth-1-en-6-one

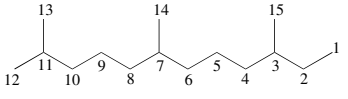
6.3 Sesquiterpenoids (VS1300–VS5320)

The sesquiterpenoids are C_{15} compounds formed by the assembly of three isoprenoid units. There is a large number of sesquiterpenoid carbon skeletons, which all however arise from the common precursor, farnesyl pyrophosphate, by various modes of cyclisations followed, in many cases, by skeletal rearrangement.

Cordell, G.A., *Chem. Rev*., 1976, **76**, 425–460 (*biosynth*)
Dewick, P.M., *Nat. Prod. Rep*., 2002, **19**, 181–222 (*biosynth*)
Fraga, B.M., *Nat. Prod. Rep*., 2004, **21**, 669–693 (*sesquiterpenoids*)

6.3.1 Simple farnesane sesquiterpenoids (VS1300)

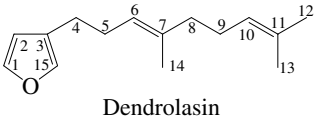
The simple farnesanes are named semi-systematically in this Dictionary although the systematic trimethyldodecane naming is also used extensively in the literature and often leads to numbering from the other end of the chain. The farnesane numbering system is used as a biogenetic numbering system for many sesquiterpenoid skeletons.



Farnesane
2,6,10-Trimethyldodecane, 9Cl

6.3.2 Furanoid farnesane sesquiterpenoids (VS1320)

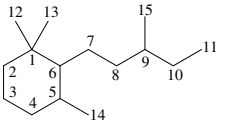
Although many numbering systems have been used for furanoid farnesanes, such as **Dendrolasin**, it is logical to use the farnesane numbering system for this group.



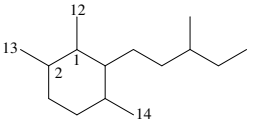
Dendrolasin

6.3.3 Cyclofarnesane and rearranged cyclofarnesane sesquiterpenoids (VS1450, VS1460, VS1470)

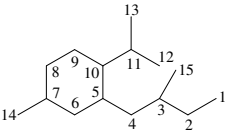
Cyclofarnesanes arise by formation of a six-membered ring between carbons 6 and 11 of farnesane, e.g. Aplysistatin. Methyl group migration gives the rearranged cyclofarnesane skeleton. The herbertianes, included in this group, (not to be confused with herbertanes) are 5,10-cyclofarnesanes.



Cyclofarnesane
1,1,3-Trimethyl-2-(3-methyl-pentyl)cyclohexane



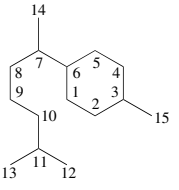
Rearranged cyclofarnesane skeleton
1,2,4-Trimethyl-3-(3-methyl-pentyl)cyclohexane



Herbertiane
4-Methyl-2-(2-methylbutyl)-1-(1-methylethyl)cyclohexane

6.3.4 Bisabolane sesquiterpenoids (VS1500)

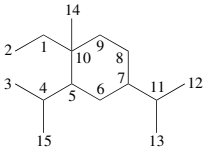
The bisabolanes are a fairly large group mainly found as constituents of higher plants, with some marine occurrences. The numbering system used for bisabolanes is the same as the farnesane system. Since the cyclohexane ring has a plane of symmetry, substituents in this ring should be numbered where possible avoiding the compound locant, 1(6), for a double bond and keeping the numbers for the substituents in the cyclohexane ring as low as possible.



Bisabolane
1-(1,5-Dimethylhexyl)-4-methylcyclohexane, 9Cl

6.3.5 Elemane sesquiterpenoids (VS1600)

Elemanes are numbered consistently with eudesmanes (see below) and germacranes. They are rapidly formed *in vitro* by Cope rearrangement of the corresponding 1(10),4-germacradienes and it is possible that they are artifacts produced during the isolation procedures.

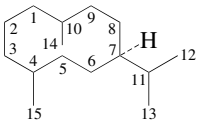


Elemane
1-Ethyl-1-methyl-2,4-bis-(1-methylethyl)cyclohexane, 9CI

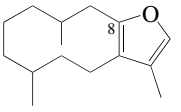
6.3.6 Germacranes (VS1650–VS1700)

These are extremely common as higher plant products but are scarce among marine algae. The numbering of the germacrane skeleton poses a problem since there is a plane of symmetry through carbons 2 and 7. Germacranes are normally drawn in a conventional way as shown below with *H*-7 in the α-configuration. Care should be taken with the small number of germacranes with a double bond at *C*-7 as the ring can be numbered in either direction. Germacranes frequently have double bonds in the 1(10) and 4 positions. A further problem with the representation of germacranes arises from substituents at carbons drawn as reentrant angles. Wherever possible germacranes should be drawn without substituents at reentrant centres as in this Dictionary, and care should be exercised when reading the literature.

The germacrane group is divided into simple germacranes, which is those without a lactone or furan ring (VS1650), 12,6-germacranolides (VS1660), 12,8-germacranolides and furanogermacranes (VS1670), nor- and homo-germacranes (VS1680), secogermacranes (VS1690) and cyclogermacranes (VS1700).



Germacrane
1,7-Dimethyl-4-(1-methyl-ethyl)cyclodecane, 9Cl

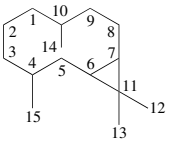


Furanogermacrane
4,5,6,7,8,9,10,11-Octahydro-3,6,10-trimethylcyclodeca[*b*]-furan, 9Cl

Fischer, N.H. *et al, Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 1979, **Vol. 38**, 47–390 (*sesquiterpene lactones*)
Fischer, N.H., *Recent Adv. Phytochem*., 1990, **24**, 161–201 (*biogenesis*)
Tashkhodzhaev, B. *et al*, *Chem. Nat. Compd*., 1997, **33**, 382–388 (*germacranes*)

6.3.7 Lepidozanes and bicyclogermacrane sesquiterpenoids (VS1710)

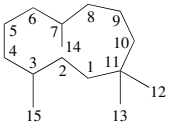
Bicyclogermacranes, found largely in higher plants, have a *cis*-fused cyclopropane ring junction whereas the stereoisomeric lepidozanes from liverworts and marine organisms have a *trans*-fused ring junction.



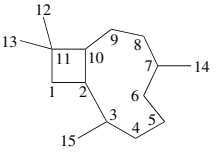
Bicyclogermacrane
3,7,11,11-Tetramethylbicyclo[8.1.0]undecane, 9Cl

6.3.8 Caryophyllane sesquiterpenoids (VS1730)

Cyclisation of the humulane skeleton between carbons 2 and 10 produces the caryophyllane skeleton. Several numbering systems are in use for caryophyllanes; the one chosen for this Dictionary is that based on farnesane.



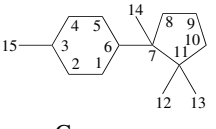
Humulane
1,1,4,8-Tetramethylcycloundecane, 9Cl



Caryophyllane
2,6,10,10-Tetramethylbicyclo[7.2.0]undecane, 9Cl

6.3.9 Cuparane sesquiterpenoids (VS1750)

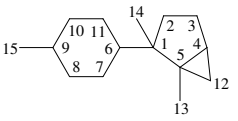
Cuparane is formed by cyclisation between carbons 6 and 11 of the bisabolane skeleton and the numbering system used here takes account of this fact. Cuparanes are found in liverworts, higher plants and marine organisms.



Cuparane
(Most have an aromatic ring and are named in CA as substituted benzenes)

6.3.10 Cyclolaurane sesquiterpenoids (VS1760)

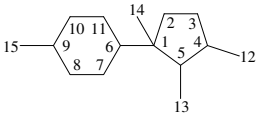
Cyclolauranes found in marine organisms may be considered as cyclocuparanes but as they co-occur with lauranes, the numbering system has been chosen to agree with the accepted laurane system.



Cyclolaurane
1,2-Dimethyl-2-(4-methylcyclohexyl)bicyclo[3.1.0]hexane, 9Cl

6.3.11 Laurane sesquiterpenoids (VS1850)

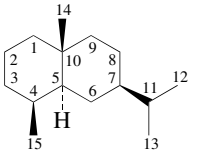
Lauranes are found in marine organisms, particularly *Laurencia* spp.



Laurane
(Mostly named as substituted benzenes in 9Cl)

6.3.12 Eudesmane sesquiterpenoids (VS1950–VS2000)

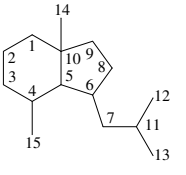
Eudesmanes are called selinanes in the older literature. As with the germacrane group, the eudesmanes are divided into groups comprising simple eudesmanes (VS1950), eudesman-12,6-olides (VS1970), eudesman-12,8-olides and furanoeudesmanes (VS1975), secoeudesmanes (VS1990), and noreudesmanes (VS2000). Within the eudesmane group there is some confusion concerning the numbering of carbons 14 and 15. The numbering given here should be adopted. Like the germacranes, they are common as higher plant products but only a few have been characterised from marine sources.



Eudesmane
Decahydro-1,4*a*-dimethyl-
7-(1-methylethyl)-
naphthalene, 9Cl

6.3.13 Oppositane sesquiterpenoids (VS2020)

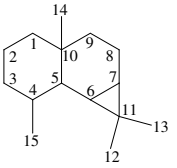
The oppositanes are 8(7 → 6)-abeoeudesmanes and are found in plants and marine organisms.



Oppositane
Octahydro-3*a*,7-dimethyl-1-(2-methylpropyl)-1*H*-indene, 9Cl

6.3.14 Cycloeudesmane sesquiterpenoids (VS2050)

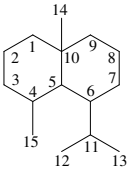
Various cycloeudesmanes are included in this section including the maalianes from marine organisms.



Maaliane
Decahydro-1,1,3*a*,7-tetramethyl-
1*H*-cyclopropa[*a*]naphthalene, 9CI

6.3.15 Gorgonane sesquiterpenoids (VS2060)

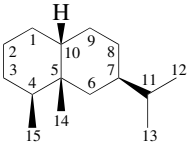
The gorgonanes are derived from eudesmanes by isopropyl group migration to C-6.



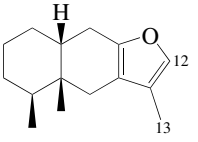
Gorgonane
Decahydro-1,4*a*-dimethyl-8-(1-methylethyl)naphthalene, 9Cl

6.3.16 Eremophilane sesquiterpenoids (VS2100–VS2130)

The eremophilanes have been shown to be derived from eudesmanes by migration of the methyl group at *C*-10 to *C*-5. There is confusion in the literature about the numbering of carbons 14 and 15; the biogenetic numbering given below should be used. The normal stereochemistry is shown, although there are several exceptions to this.



Eremophilane
Decahydro-1,8*a*-dimethyl-
7-(1-methylethyl)-
naphthalene, 9Cl

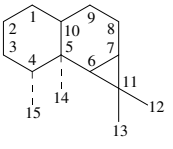


Furanoeremophilane
4,4*a*,5,6,7,8,8*a*,9-Octahydro-
3,4*a*,5-trimethylnaphtho-
[2,3-*b*]furan, 9Cl

Pinder, A.R., *Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 1977, **Vol. 34**, 81–186 (*eremophilanes*)

6.3.17 Aristolane sesquiterpenoids (VS2150)

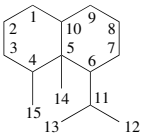
The aristolanes are 6,11-cycloeremophilanes.



Aristolane
Decahydro-1,1,7,7*a*-tetramethyl-1*H*-cyclopropa-
[*a*]naphthalene, 9Cl

6.3.18 Nardosinane sesquiterpenoids (VS2160)

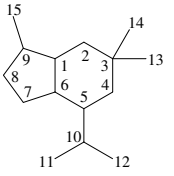
The nardosinanes, isolated from marine organisms, are eremophilanes in which the isopropyl group has migrated to carbon 6.



Nardosinane
Decahydro-1,8*a*-dimethyl-8-(1-methylethyl)naphthalene

6.3.19 Brasilane sesquiterpenoids (VS2170)

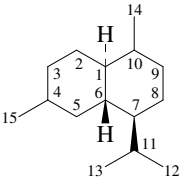
The brasilanes are rearranged sesquiterpenoids largely from *Laurencia* and *Aplysia* species.



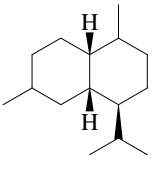
Brasilane
Octahydro-1,6,6-trimethyl-4-(1-methylethyl)-1*H*-indene

6.3.20 Cadinane sesquiterpenoids (VS2250, VS2260)

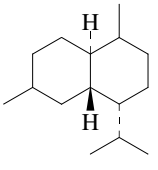
The nomenclature, numbering and absolute stereochemistry of this group is somewhat confused. Biogenetic (germacrane) numbering is used here, but many other numbering systems have been used in the literature. Historically, the names of the skeletons depended on the relative stereochemistries at carbons 1, 6 and 7 as indicated, but in this Dictionary the various stereoisomeric forms are merged into the same entry with these obsolescent names given as synonyms. The aromatised skeletons have also in the past been given different names, calamenene and cadalene, and these have often been given different numbering systems. Nor-and seco-cadinanes are grouped separately (VS2260).



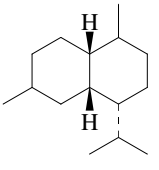
Cadinane
Decahydro-1,6-dimethyl-
4-(1-methylethyl)naphthalene, 9Cl



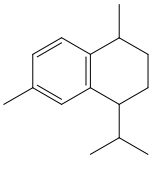
Muurolane



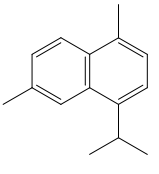
Bulgarane



Amorphane



Calamenene

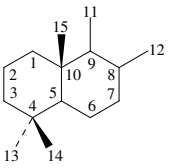


Cadalene

Bordoloi, M. *et al*, *Phytochemistry*, 1989, **28**, 2007–2037 (*cadinanes*)

6.3.21 Drimane sesquiterpenoids (VS2300)

The drimanes, mainly from terrestrial fungi and higher plants but also from marine organisms, arise by direct cyclisation of a farnesane derivative. The accepted numbering system is shown.

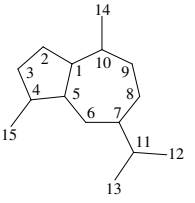


Drimane
Decahydro-1,1,4*a*,5,6-pentamethylnaphthalene

Vlad, P.F. *et al*, *Russ. Chem. Bull*., 1997, **46**, 855–873 (*synth*)

6.3.22 Guaiane sesquiterpenoids (VS2400–VS2440)

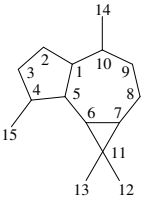
This large group is divided into simple guaianes (VS2400), 12,6-guaianolides (VS2410), 12,8-guaianolides (VS2420), guaiane dimers (VS2430), and seco-, cyclo- and abeo- and norguaianes (VS2440). They are very common in higher plants but are also found in marine organisms.



Guaiane
Decahydro-1,4-dimethyl-7-(1-methylethyl)azulene, 9Cl

6.3.23 Aromadendrane sesquiterpenoids (VS2500)

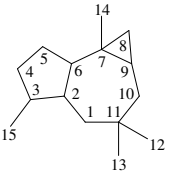
The aromadendranes are 6,11-cycloguaianes.



Aromadendrane
Decahydro-1,1,4,7-tetramethyl-1*H*-cycloprop[*e*]azulene, 9Cl

6.3.24 Africanane sesquiterpenoids (VS2750)

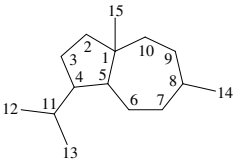
The farnesane numbering system is used for the africanane skeleton although the biosynthesis has not been established conclusively. Some compounds (e.g. **Africanone**) have been named as africananes but have since been shown to have a different skeleton.



Africanane
Decahydro-3,3,5,7*b*-tetramethyl-1*H*-cycloprop[*e*]azulene

6.3.25 Daucane sesquiterpenoids (VS3180)

Many numbering systems have been used for the daucanes; that chosen here is related to the guaiane system. They are mostly from terrestrial organisms but some are from marine sources.

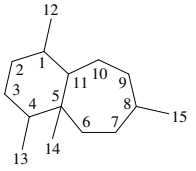


Daucane
Decahydro-3*a*,6-dimethyl-1-(1-methylethyl)azulene

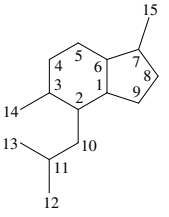
Ghisalberti, E.L., *Phytochemistry*, 1994, **37**, 597–623 (*daucanes*)

6.3.26 Perforane and pacifigorgiane sesquiterpenoids (VS3200, VS3350)

The perforanes form a small group found in *Laurencia* spp. Pacifigorgianes are found in liverworts, higher plants and marine organisms.



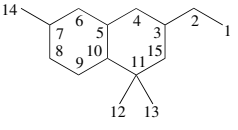
Perforane
Decahydro-1,4,7,9*a*-tetramethyl-1*H*-benzocycloheptane



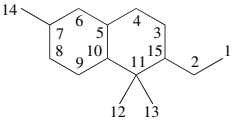
Pacifigorgiane
Octahydro-1,5-dimethyl-4-(2-methylpropyl)-1*H*-indene

6.3.27 Furodysin and furodysinin sesquiterpenoids (VS3550, VS3560)

A farnesane numbering system is used for the furodysin and the rearranged furodysinin groups from *Dysidea* spp.



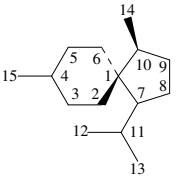
Furodysin skeleton
3-Ethyldecahydro-1,1,6-trimethylnaphthalene



Furodysinin skeleton
2-Ethyldecahydro-1,1,6-trimethylnaphthalene

6.3.28 Acorane sesquiterpenoids (VS3750)

The acoranes and the enantiomeric alaskanes have a symmetrical six-membered ring. It has been suggested that *C*-2 should be chosen to be *syn*- to *C*-14.

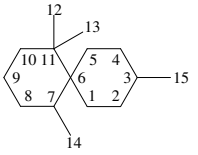


Acorane
1,8-Dimethyl-4-(1-methylethyl)spiro[4.5]decane, 9Cl

Marshall, J.A. *et al*, *Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 1974, **Vol. 31**, 283–376 (*acoranes*)

6.3.29 Chamigrane sesquiterpenoids (VS3800)

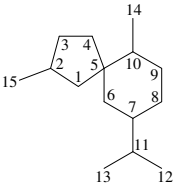
The chamigranes are a group of mainly marine natural products, mostly from *Laurencia* and *Aplysia* spp. The numbering system is based on farnesane. There are also some secochamigranes known (VS3810).



Chamigrane
1,1,5,9-Tetramethylspiro[5.5]undecane, 9Cl

6.3.30 Spiroaxane sesquiterpenoids (VS3820)

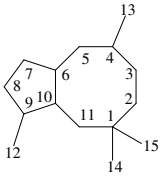
The spiroaxanes are marine natural products that appear to be rearranged cadinane derivatives.



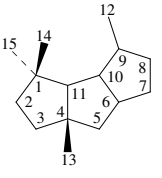
Spiroaxane
2,6-Dimethyl-9-(1-methylethyl)spiro[4.5]decane

6.3.31 Precapnellane and capnellane sesquiterpenoids (VS4200, VS4250)

Precapnellanes and capnellanes are of marine origin. Capnellanes are 4,11-cycloprecapnellanes.



Precapnellane
Decahydro-1,5,8,8-tetramethyl-1*H*-cyclopentacyclooctene



Capnellane
Decahydro-3,3,4,7*a*-tetramethyl-1*H*-cyclopenta[*a*]pentalene, 9Cl

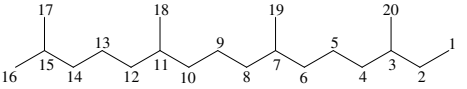
6.4 Diterpenoids (VS5350–VS7340)

The diterpenoids constitute a large group of compounds derived from geranylgeranyl pyrophosphate. They are found in higher plants, fungi, insects and marine organisms.

Hanson, J.R., *Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 1971, **Vol. 29**, 395–419 (*biosynth*)
West, C.A., *Biosynthesis of Isoprenoid Compounds*, (eds. Porter, J.W. *et al*), Wiley, New York, 1981, **Vol. 1**, 375
Dewick, P.M., *Nat. Prod. Rep*., 2002, **19**, 181–222 (*biosynth*)
Hanson, J.R., *Nat. Prod. Rep*., 2005, **22**, 594–602 (*diterpenoids*)

6.4.1 Phytane diterpenoids (VS5350)

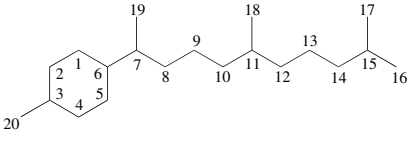
Phytanes are regular acyclic diterpenoids. The phytane numbering system is shown here.



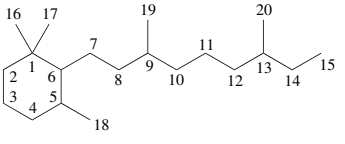
Phytane
2,6,10,14-Tetramethylhexadecane

6.4.2 Prenylbisabolane and 10,15-cyclophytane diterpenoids (VS5380, VS5390)

The prenylbisabolanes arise by cyclisation between carbons 1 and 6 of the phytane skeleton. They retain their phytane numbering system. The 10,15-cyclophytanes are important compounds including the retinal group. Since 10,15-cyclophytanes resemble carotenoids, a carotenoid-like numbering system has usually been adopted. It is possible to view 10,15-cyclophytanes as 9,10-secolabdanes and some are named and numbered as such in the literature.



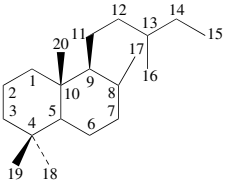
Prenylbisabolane
1-Methyl-4-(1,5,9-trimethyldecyl)cyclohexane



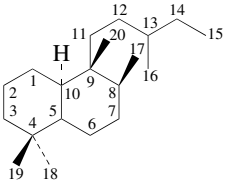
10,15-Cyclophytane
1,1,3-Trimethyl-2-(3,7-dimethylnonyl)cyclohexane

6.4.3 Labdane and halimane diterpenoids (VS5400–VS5470)

Labdanes form a large group and occur in both enantiomeric series. The halimanes are derived from labdanes by migration of the *C*-20 methyl group to *C*-9. Nor-, seco- and rearranged labdanes are given separate codes.



Labdane
Decahydro-1,1,4*a*,6-tetramethyl-5-(3-methylpentyl)naphthalene, 9Cl

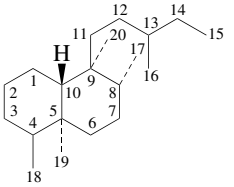


Halimane
Decahydro-1,1,5,6-tetramethyl-5-(3-methylpentyl)naphthalene

Singh, M. *et al*, *Planta Med*., 1999, **65**, 2–8 (*activity*)

6.4.4 Clerodane diterpenoids (VS5500–VS5530)

Clerodanes arise from labdanes by two methyl migrations. They are abundant in terrestrial plants, particularly in *Teucrium* spp., but are also found in marine species. In the past *ent*-clerodanes have been named as neoclerodanes and kolavanes but these names are not widely used. There is some confusion in the literature concerning the numbering of *C*-18 and *C*-19 in clerodanes.

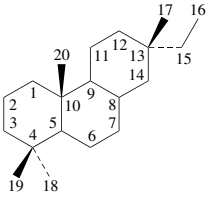


ent-Clerodane
Decahydro-1,2,4*a*,5-tetramethyl-1-(3-methylpentyl)naphthalene, 9Cl

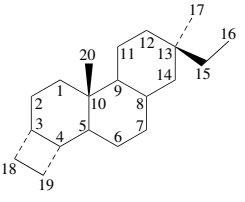
Merritt, A.T. *et al*, *Nat. Prod. Rep*., 1992, **9**, 243–287 (*clerodanes*)
Tokoroyama, T., *Synthesis*, 2000, 611–633 (*synth*)

6.4.5 Parguerane, isoparguerane and isopimarane diterpenoids (VS5730–VS5750)

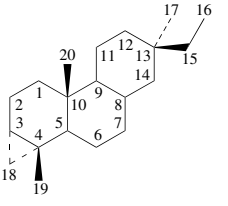
The isopimaranes (VS5750) (formerly called sandaracopimaranes) arise by further cyclisation of the labdane skeleton. The isopimaranes are largely of terrestrial origin but do occur in some marine species. Parguerenes (VS5730) and Isoparguerenes (VS5735), mainly from *Laurencia* and *Aplysia* species, are derived from the isomeric pimarane skeleton.



Isopimarane
7-Ethyltetradecahydro-1,1,4*a*,7-tetramethylphenanthrene



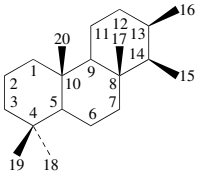
Isoparguerane
6-Ethyltetradecahydro-6,8*b*-dimethylcyclobuta[*a*]-phenanthrene



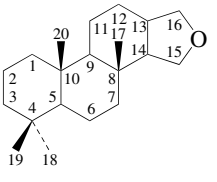
Parguerane
5-Ethyltetradecahydro-1*a*,5,7*b*-trimethyl-1*H*-cyclopropa[*a*]phenanthrene

6.4.6 Isocopalane and spongiane diterpenoids (VS5950)

Isocopalanes and spongianes are of marine origin and both have the same carbon skeleton. A spongiane or spongian is a 15,16-epoxyisocopalane.



Isocopalane
Tetradecahydro-1,1,4*a*,7,8,8*a*-hexamethylphenanthrene

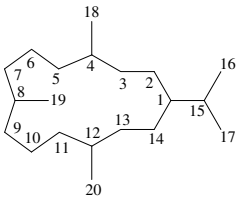


Spongiane skeleton

Keyzers, R.A. *et al*, *Nat. Prod. Rep*., 2006, **23**, 321–334 (*spongianes*)

6.4.7 Cembrane diterpenoids (VS6400–VS6410)

The cembranes form a large group of diterpenoids found in higher plants, insects and marine organisms. The cembrane nucleus has a plane of symmetry and is conventionally drawn with *C*-7 at the top as defined by the *C*-1, *C*-8 axis, *C*-7 being chosen as bearing a double bond or equivalent. The numbering system shown is generally accepted. Many polycyclic diterpenoids can be regarded as formally arising by cyclisation of the cembrane skeleton. Care is necessary in interpreting published configurations at centres involving reentrant angles.

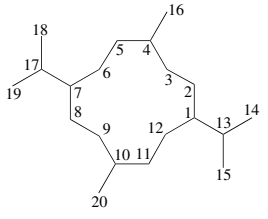


Cembrane
1,7,11-Trimethyl-4-(1-methylethyl)cyclotetradecane, 9Cl

Weinheimer, A.J. *et al*, *Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 1979, **Vol. 36**, 285–387 (*cembranoids*)
Tius, M.A., *Chem. Rev*., 1988, **88**, 719–732 (*synth*)
Marshall, J.A., *Studies in Natural Products Chemistry*, (ed. Atta-ur-Rahman), Elsevier, Amsterdam, 1992, **Vol. 10**, 3–42 (*synth*)
Wahlberg, I. *et al*, *Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 1992, **Vol. 59**, 141–294; **Vol. 60**, 1–141 (*cembranoids*)
Bernardelli, P. *et al*, *Heterocycles*, 1998, **49**, 531–556 (*marine cembranoids*)
Sung, P.-J. *et al*, *Heterocycles*, 2002, **57**, 1705–1715 (*gorgonian cembranoids*)

6.4.8 Rearranged cembrane diterpenoids (VS6420) and pseudopterane diterpenoids (VS6425)

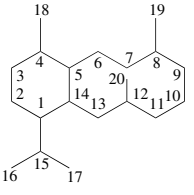
Various rearranged cembranes are found in marine organisms including the pseudopteranes from *Pseudopterogorgia* species.



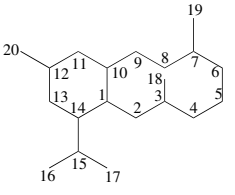
Pseudopterane
1,7-Dimethyl-4,10-bis(1-methylethyl)-
cyclododecane

6.4.9 Eunicellane and asbestinane diterpenoids (VS6440, VS6450)

These are marine natural products. The eunicellane (cladiellane) skeleton is formally a 5,14-cyclocembrane and the cembrane numbering system is preferred. The closely related asbestinane group has been assigned a different numbering system.



Eunicellane
Tetradecahydro-4,7,11-
trimethyl-1-(1-methylethyl)-
benzocyclodecene, 9CI

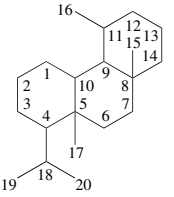


Asbestinane
Tetradecahydro-3,7,11-
trimethyl-1-(1-methylethyl)-
benzocyclodecene

Sung, P.-J. *et al, Heterocycles*, 2002, **57**, 1705–1715 (*eunicellanes, asbestinanes*)

6.4.10 Sphaerane diterpenoids (VS6460)

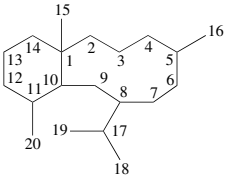
The bromosphaerol group of marine natural products contains an unusual carbon skeleton. The numbering system is as shown. Bicyclic (lacking the 1,10-bond) and tetracyclic (with a 2,17-bond) derivatives are known. (N.B. Sphaeranes are not to be confused with sphaeroanes, see below).



Sphaerane
Tetradecahydro-5,8*a*,10*a*-trimethyl-1-(1-methylethyl)-
phenanthrene

6.4.11 Briarane diterpenoids (VS6470)

The briaranes are a large group of marine diterpenoids with the numbering system as shown. The carbon skeleton is formerly a 3,8-cyclocembrane.

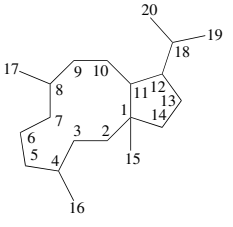


Briarane
Tetradecahydro-1,4*a*,8-trimethyl-
11-(1-methylethyl)benzocyclodecene

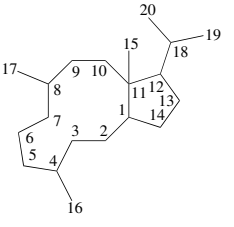
Sung, P.-J. *et al*, *Heterocycles*, 2002, **57**, 535–579; 2005, **65**, 195–204 (*briaranes*)

6.4.12 Dolabellane and modified dolabellane diterpenoids (VS6500, VS6510)

Dolabellanes are found in marine organisms and in liverworts. Several numbering systems have been used in the literature. We have used the one shown. The modified dolabellane group includes the neodolabellanes in which a methyl has migrated from *C*-1 to *C*-11.



Dolabellane
Tetradecahydro-3*a*,6,10-
trimethyl-1-(1-methylethyl)-
cyclopentacycloundecene

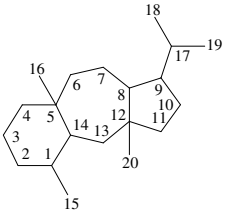


Neodolabellane
Tetradecahydro-6,10,12*a*-
trimethyl-1-(1-methylethyl)-
cyclopentacycloundecene

Rodriguez, A.D. *et al*, *Tetrahedron*, 1998, **54**, 11683–11729 (*dolabellanes*)
Hiersemann, M. *et al*, *Topics in Current Chemistry*, (ed. Mulzer, J.), Springer, Berlin, 2005, **Vol. 243**, 73–136 (*synth*)

6.4.13 Dolastane and modified dolastane diterpenoids (VS6540, VS6550)

The name clavularane was originally used for this group of marine natural products but now dolastane appears to be widely accepted. Dolastane is a 3,8-cyclododolabellane but a different numbering system is used. The modified dolastane group contains 8,9-secodolastanes and a chromophycane, a skeletal type related to dolastane by migration of the methyl *C*-20 to *C*-13.

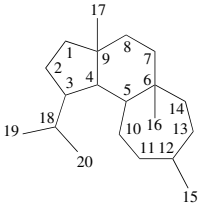


Dolastane
Tetradecahydro-3*a*,5,8*a*-trimethyl-1-(1-methylethyl)-
benz[*f*]azulene, 9Cl

Hiersemann, M. *et al*, *Topics in Current Chemistry*, (ed. Mulzer, J.), Springer, Berlin, 2005, **Vol. 243**, 73–136 (*synth*)

6.4.14 Cyathane diterpenoids (VS6560)

The cyathanes found in marine sponges are also fungal metabolites. The biosynthesis of this unusual skeleton has been studied. The accepted numbering system is as shown.

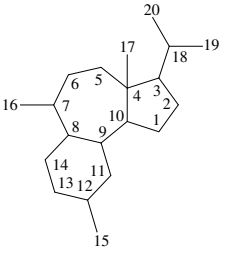


Cyathane
Tetradecahydro-3*a*,5*a*,8-trimethyl-1-(1-methylethyl)-
cyclohept[*e*]indene

Turner, W.B. *et al*, *Fungal Metabolites II*, Academic Press, London, 1983

6.4.15 Sphaeroane diterpenoids (VS6570)

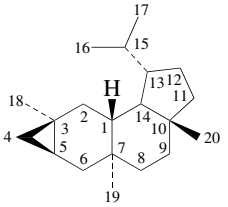
The sphaeroanes are marine algal products with a skeleton which is formally a 2,7-cyclodolabellane though the numbering system is different from that of dolabellanes.



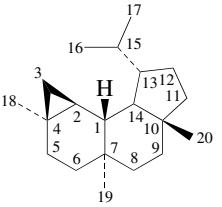
Sphaeroane
Dodecahydro-3*a*,6,9-trimethyl-3-(1-methylethyl)-
benz[*e*]azulene, 9Cl

6.4.16 Verrucosane and modified verrucosane diterpenoids (VS6580, VS6590)

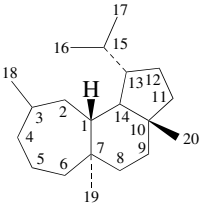
Verrucosanes and their modifications, including neoverrucosanes and 3,5-secoverrucanes, are constituents of marine sponges. The tetracyclic verrucosane skeleton is formally related to dolabellane by 4,10- and 6,8-bond formation. A different numbering system from that of dolabellane is used. The isomeric neoverrucosane has the cyclopropane bridging *C*-2 and *C*-3.



Verrucosane
Tetradecahydro-3*a*,5*a*,7*a*-trimethyl-
1-(1-methylethyl)cyclopenta-
[*a*]cyclopropa[*g*]naphthalene, 9Cl



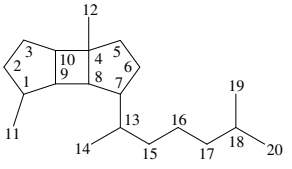
Neoverrucosane
Tetradecahydro-1*a*,3*a*,5*a*-trimethyl-
8-(1-methylethyl)cyclopenta-
[*a*]cyclopropa[*h*]naphthalene



3,5-Secoverrucane
Tetradecahydro-3*a*,5*a*,9-trimethyl-
1-(1-methylethyl)cyclohept[*e*]indene

6.4.17 Spatane diterpenoids (VS6800, VS6810)

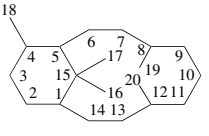
The spatane skeleton is formally derived from a prenylgermacrane by 1,5- and 6,10-cyclisation. The numbering system unfortunately does not reflect this derivation. Spatanes and the related 4,10-secospatanes are marine natural products.



Spatane
Decahydro-3*a*,6-dimethyl-1-(1,5-dimethylhexyl)cyclo-
buta[1,2:3,4]dicyclopentene, 9Cl

6.4.18 Verticillane diterpenoids (VS6880)

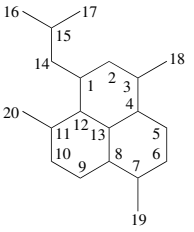
The verticillane group is formally derivable from cembrane by an 11,15-cyclisation. A non-cembrane numbering system is used. The Cespitularins from a soft coral are verticillane derivatives.



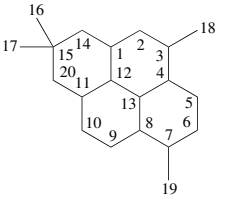
Verticillane
4,8,12,15,15-Pentamethylbicyclo[9.3.1]pentadecane, 9Cl

6.4.19 Amphilectane, cycloamphilectane, adociane and neoamphilectane diterpenoids (VS7020, VS7030, VS7040)

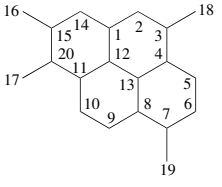
The amphilectanes (including the pseudopterosins), the cycloamphilectanes and adocianes (also called is isocycloamphilectanes) and neoamphilectanes are marine products. They are found with serrulatane derivatives from which amphilectanes are derived by cyclisation. Cycloamphilectanes represent a further cyclisation and adocianes have undergone a methyl migration. Neoamphilectanes are 2(1→12)-abeoamphilectanes. Many marine natural products from these groups contain isocyanate, isothiocyanate and isonitrile functional groups.



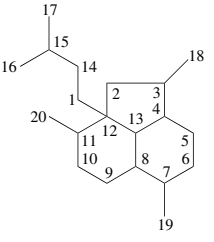
Amphilectane
Dodecahydro-1,4,7-trimethyl-3-(2-methylpropyl)-1*H*-phenalene, 9Cl



Cycloamphilectane
Hexadecahydro-1,4,7,7-tetramethylpyrene



Adociane
Hexadecahydro-1,2,5,8-tetramethylpyrene, 9Cl

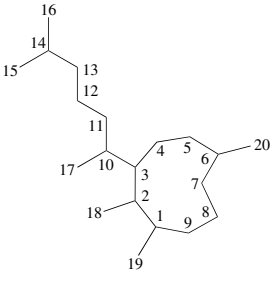


Neoamphilectane
Dodecahydro-1,3,6-trimethyl-2*a*-(3-methylbutyl)-acenaphthylene

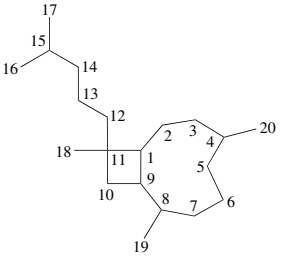
König, G.M., *J. Org. Chem*, 1996, **61**, 3259–3267 (*isocyanates, isothiocyanates, isonitriles*)
Kohl, A.C. *et al, J. Ind. Microbiol. Biotechnol*., 2003, **30**, 495–499 (*biosynth*)
Gross, H. *et al*, *Phytochem. Rev*., 2006, **5**, 115–141 (*rev*)

6.4.20 Xenicane and xeniaphyllane diterpenoids (VS7100, VS7110, VS7150)

Xenicanes and xeniaphyllanes are marine natural products. Xeniaphyllanes are the diterpenoid equivalent of the caryophyllane skeleton. Xenicanes are cleaved xeniaphyllanes.



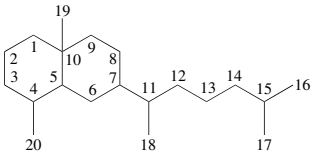
Xenicane
1,2,6-Trimethyl-3-(1,5-dimethylhexyl)-cyclononane



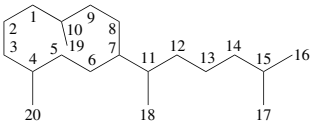
Xeniaphyllane
2,6,10-Trimethyl-10-(4-methylpentyl)-bicyclo[7.2.0]undecane

6.4.21 Prenyleudesmane, prenylgermacrane and prenylbicyclogermacrane diterpenoids (VS7190, VS7200, VS7210)

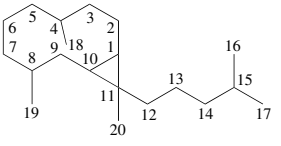
These three groups of 'extended' sesquiterpenoid skeletons are largely of marine origin.



Prenyleudesmane
Decahydro-7-(1,5-dimethylhexyl)-1,4*a*-dimethylnaphthalene



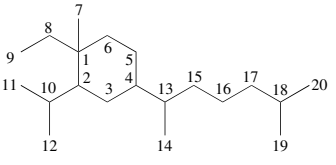
Prenylgermacrane
4-(1,5-Dimethylhexyl)-1,7-dimethylcyclodecane



Prenylbicyclogermacrane
3,7,11-Trimethyl-11-(4-methylpentyl)bicyclo-
[8.1.0]undecane

6.4.22 Lobane diterpenoids (VS7220)

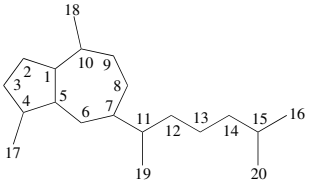
Lobanes are of marine origin and are 'extended' elemanes. A most unusual non-standard numbering system is used in the literature.



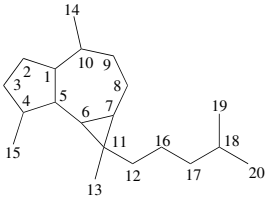
Lobane
4-(1,5-Dimethylhexyl)-1-ethyl-1-methyl-2-
(1-methylethyl)cyclohexane

6.4.23 Pachydictyane and cneorubine diterpenoids (VS7230, VS7240)

These two groups are also 'extended' sesquiterpenoids. The pachydictyanes are prenylguaianes from marine organisms and the cneorubine group are prenylaromadendranes found in marine species as well as leaves of *Cneorum tricoccon*.



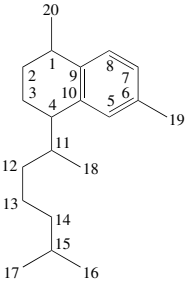
Pachydictyane
Decahydro-7-(1,5-dimethyl-
hexyl)-1,4-dimethyl-
azulene



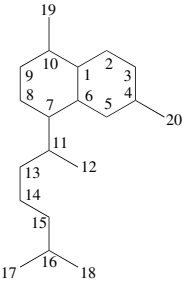
Cneorubine skeleton
Decahydro-1,4,7-trimethyl-1-
(4-methylpentyl)-1*H*-
cycloprop[*e*]azulene

6.4.24 Serrulatane and biflorane diterpenoids (VS7250)

The biflorane skeleton is found in marine organisms, insects and *Eremophila* spp. The skeleton is an 'extended' cadinane. The serrulatane name is given to the aromatic analogue. Unfortunately different numbering systems have been given to serrulatanes and bifloranes.



Serrulatane
4-(1,5-Dimethylhexyl-
1,2,3,4-tetrahydro-1,6-
dimethylnaphthalene

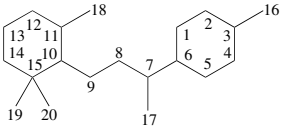


Biflorane
Decahydro-4-(1,5-dimethyl-
hexyl)-1,6-dimethyl-
naphthalene

Hechrodt, T.J. *et al*, *Topics in Current Chemistry*, (ed. Mulzer, J.), Springer, Berlin, 2005, **Vol. 244**, 1–41 (*serrulatanes*)

6.4.25 Obtusane diterpenoids (VS7280)

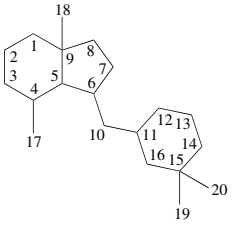
The obtusanes, of marine origin, are bicyclic phytanes. The numbering system is almost the same as for phytane (Note that the terpenoid **Obtusane** itself is a chamigrane).



Obtusane
1,1,3-Trimethyl-2-[3-(4-methylcyclohexyl)butyl]-
cyclohexane

6.4.26 Irieol diterpenoids (VS7290)

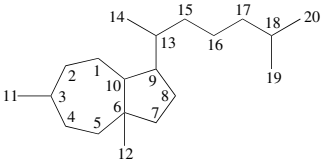
The irieol group, also of marine origin, represents an unusual diterpenoid skeleton.



Irieol skeleton
Octahydro-1-[(3,3-dimethylcyclohexyl)methyl]-
3*a*,7-dimethyl-1*H*-indene

6.4.27 Sphenolobane diterpenoids (VS7300)

The sphenolobane skeleton is an 'extended' daucane skeleton.



Sphenolobane
Decahydro-1-(1,5-dimethylhexyl)-3*a*,6-dimethylazulene

6.4.28 Miscellaneous diterpenoids (VS7310–VS7340)

Diterpenoids that do not easily fit into the other categories are collected here. Mono-, bi-, tri- and tetracyclic diterpenoids are given separate codes.

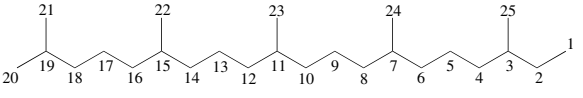
6.5 Sesterterpenoids (VS7400–VS7580)

Sesterterpenoids are a group of natural products that arise from five isoprene units. Although sesterterpenoids strictly have 25 carbons, there are many nor- and alkylated members. Also included here are the C_{21} acyclic terpenoids although their biosynthetic relationship with the sesterterpenoids has not been established with certainty. Sesterterpenoids are found in fungi, higher plants, insects and particularly in marine organisms.

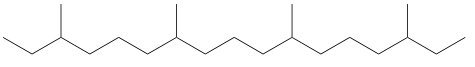
Cordell, G.A., *Progress in Phytochemistry*, (eds. Reinhold, L. *et al*), Pergamon Press, Oxford, 1977, **Vol. 4**, 209–256 (*sesterterpenoids*)
Crews, P. *et al, Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SprigerWien, New York, 1985, **Vol. 48**, 203–269 (*sesterterpenoids*)
Hanson, J.R. *et al*, *Nat. Prod. Rep*., 1996, **13**, 529–535 (*sesterterpenoids*)
Dewick, P.M., *Nat. Prod. Rep*., 2002, **19**, 181–222 (*biosynth*)

6.5.1 Acyclic and noracyclic sesterterpenoids (VS7400, VS7410)

The acyclic sesterterpenoids arise by a head to tail fusion of isoprene units. The accepted numbering system is used here. The noracyclic sesterterpenoids (VS7410) are numbered in a similar way; however, a problem arises with the symmetry of the C_{21} compounds as they may be numbered from either end. The acyclic sesterterpenoids frequently contain furanoid rings.



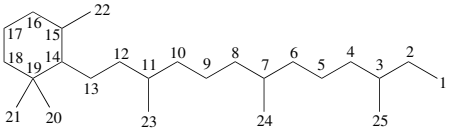
Acyclic sesterterpenoid skeleton
2,6,10,14,18-Pentamethyleicosane



C_{21} sesterterpenoid skeleton
3,7,11,15-Tetramethylheptadecane

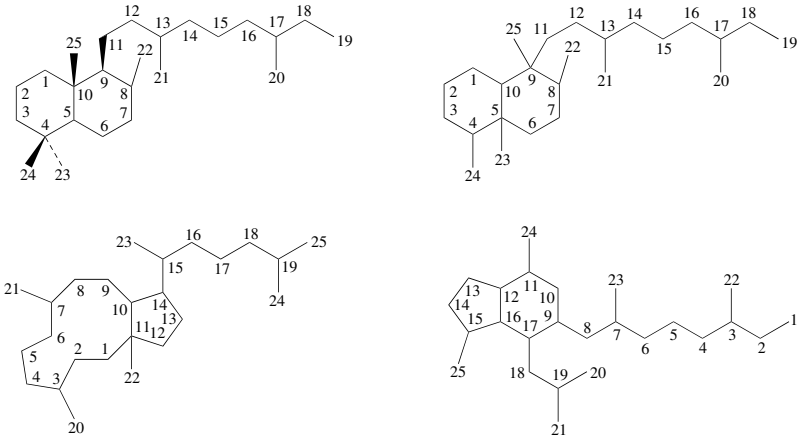
6.5.2 Cyclohexane sesterterpenoids (VS7420)

Most of the cyclohexane sesterterpenoids arise by cyclisation of the acyclic skeleton between carbons 14 and 19.



6.5.3 Bicyclic sesterterpenoids (VS7460)

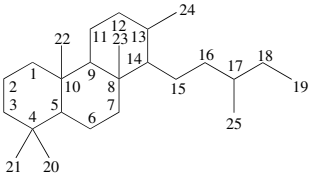
Various bicyclic sesterterpenoids are known. Some are prenylated analogues of diterpene skeletons and the numbering systems are related to the corresponding diterpenoid systems. Others have biogenetic numbering systems.



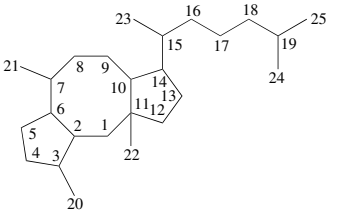
Some bicyclic sesterterpenoid skeletons

6.5.4 Cheilanthane and ophiobolane sesterterpenoids (VS7500, VS7520)

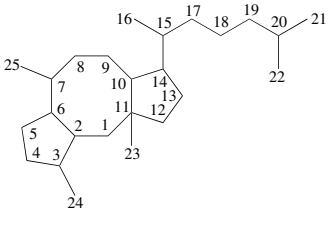
The accepted numbering systems for the cheilanthanes and ophiobolanes are shown here. *Chemical Abstracts* uses ophiobolane as a stereoparent; however it uses a different numbering system for the non-ring carbons.



Cheilanthane
4,4,8-Trimethyl-*D*(15),24-dinor-13,17-secocholane, 9Cl



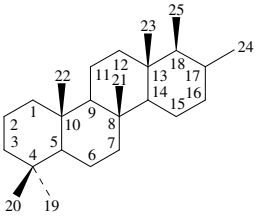
Ophiobolane



Ophiobolane, CA numbering

6.5.5 Scalarane sesterterpenoids (VS7540, VS7550)

The scalarane numbering system is shown here. Carbons 12, 24 and 25 are generally oxygenated in this skeleton. Several methyl and dimethylscalaranes are found in marine organisms. The additional methyl groups attached to *C*-24 and *C*-20 are numbered 26 and 27 respectively.

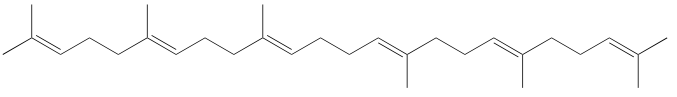


Scalarane
4,4,8,17,17*a*-Pentamethyl-*D*-homoandrostane, 9Cl

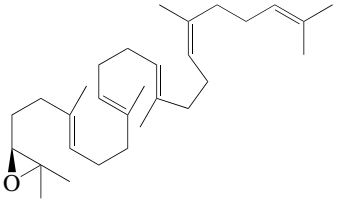
Ungur, N. *et al, Recent Res. Dev. Org. Chem*., 2003, **7**, 241–258 (*synth*)

6.6 Triterpenoids (VS7600–VS9450)

The triterpenoids constitute a large diverse group of natural products derived from squalene or, in the case of 3β-hydroxytriterpenoids, the 3*S*-isomer of squalene 2,3-epoxide. The conformation that *all-trans*-squalene 2,3-epoxide adopts when the initial cyclisation takes place determines the stereochemistry of the ring junctions in the triterpenoid produced. Thus cyclisation of the chair-boat-chair-boat conformation gives the protostane cation and cyclisation of the chair-chair-chair-boat conformation leads to the dammarane cation. The initially formed cation intermediate may undergo a series of 1,2-hydride and methyl migrations, commonly called backbone rearrangements, to give a variety of skeletal types.

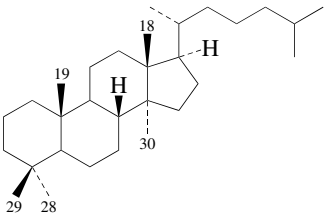


Squalene

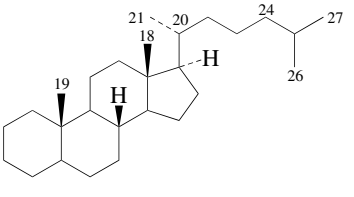


Squalene 2,3-epoxide

Backbone rearrangement of the protostane cation gives the lanostane skeleton; **Lanosterol** is the biogenetic precursor of the steroids in animals. The methyl groups at carbons 4 and 14 are removed during steroid biosynthesis. The steroid numbering system is adopted for lanostane and related tetracyclic triterpenoids. The three methyl groups that were removed during the biosynthesis of steroids are currently numbered 28, 29 and 30 as shown. However, older literature uses the numbers 31, 30 and 32, respectively. This was based on the assignment of carbon numbers 28 and 29 to the stigmastane ethyl group, even though most lanostanes do not have such an ethyl group. The numbering used here follows the currently accepted convention. (See also Steroid section following).



Lanostane numbering



Steroid numbering

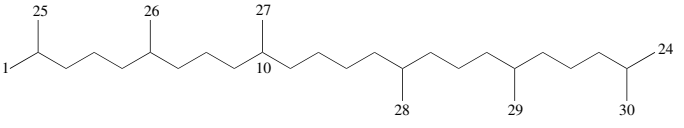
Abe, I. *et al*, *Chem. Rev*., 1993, **93**, 2189–2206 (*biosynth*)
Spencer, T.A., *Acc. Chem. Res*., 1994, **27**, 83–90 (*biosynth*)
Mahato, S.B., *Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 1998, **Vol. 74**, 1–96 (*saponins*)
Brown, G.D., *Nat. Prod. Rep*., 1998, **15**, 653–696 (*biosynth*)
Connolly, J.D. *et al*, *Nat. Prod. Rep*., 2005, **22**, 487–503 (*triterpenoids*)

The main tetracyclic triterpenoid skeletons have the steroid numbering for the skeleton including the side chain and only the methyl groups will be numbered in the structures that follow. As a general rule the methyls which migrate during terpenoid biosynthesis retain their numbering.

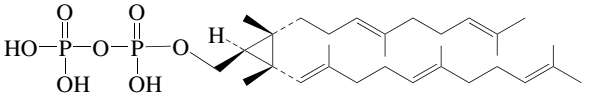
CA names most tetracyclic triterpenoids as derivatives of the steroid stereoparents. This has the disadvantage that some are assigned different names from those commonly used.

6.6.1 Linear triterpenoids (VS7600)

This group contains simple derivatives of squalene. The preferred numbering system is shown and is used for the related polyether derivatives found in marine algae, e.g. *Laurencia* spp. Also included are C_{30} polyprenols, and some homo- and nor-squalenes. Squalene is formed biosynthetically from farnesyl pyrophosphate *via* presqualene pyrophosphate.



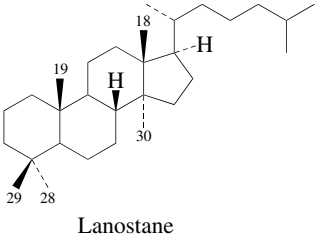
Squalane
2,6,10,15,19,23-Hexamethyltetracosane, 9Cl



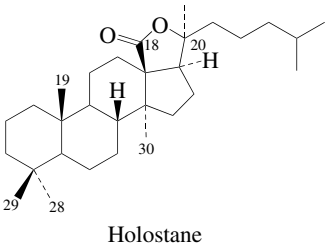
Presqualene pyrophosphate

6.6.2 Lanostane triterpenoids (VS7750)

The lanostanes are very common in higher plants and fungi. **Lanosterol** is a key intermediate in steroid biosynthesis. The metabolites of sea cucumbers or holothurians are characterised by lanostane glycosides with most aglycones possessing the 18,20-lactone of the holostane skeleton. Many of the glycosides of these metabolites are sulfated.



Lanostane

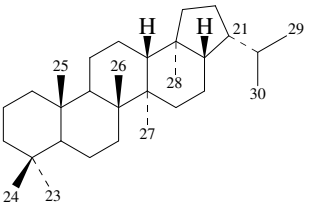


Holostane

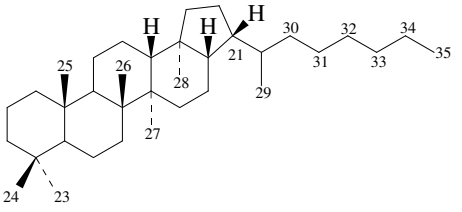
Stonik, V.A. *et al*, *J. Nat. Toxins*, 1999, **8**, 235–248 (*holothuroids*)
Chludil, H.G. *et al, Studies in Natural Products Chemistry*, (ed. Atta-ur-Rahman), Elsevier, Amsterdam, 2003, **Vol. 28**, 587–616 (*holothurian glycosides*)
Kalinin, V.I. *et al, Phytochem. Rev*., 2005, **4**, 221–236 (*holothurian glycosides*)

6.6.3 Hopane triterpenoids (VS8720, VS8730)

Cyclisation of squalene in the chair-chair-chair-chair-chair conformation affords the hopane skeleton. Degraded and extended hopanes, the bacteriohopanoids, occur widely in natural sediments and the latter are important components of archaeal lipid membranes and have been identified in marine sponges.



Hopane
A' -Neogammacerane, 9Cl

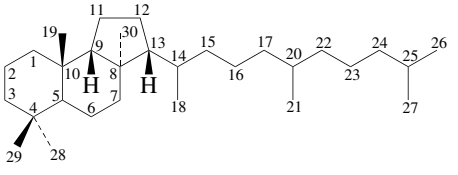


Bacteriohopane

Ourisson, G. *et al*, *Acc. Chem. Res*., 1992, **25**, 398–402 (*geohopanoids*)
Ourisson, G. *et al*, *Acc. Chem. Res*., 1992, **25**, 403–408 (*bacteriohopanoids*)
Kannenberg, E.L. *et al*, *Naturwissenschaften*, 1999, **86**, 168–176 (*biosynth*)
Costantino, V. *et al, Tetrahedron*, 2001, **57**, 4045–4048 (*sponge bacteriohopanoids*)

6.6.4 Isomalabaricane triterpenoids (VS9100)

Partial cyclisation of squalene 2,3-epoxide from one end leads to the isomalabaricane skeleton of marine triterpenoids. The 8,9-diepimeric malabaricane skeleton is found in terrestrial triterpenoids.

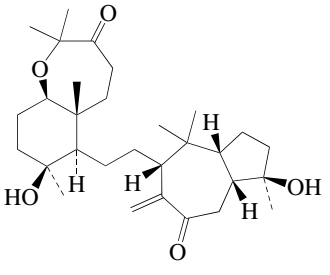


Isomalabaricane
Dodecahydro-3*a*,6,6,9*a*-tetramethyl-
3-(1,5,9-trimethyldecyl)-
1*H*-benz[*e*]indene

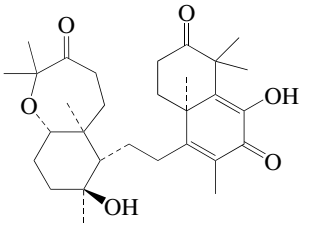
Fouad, M. *et al*, *J. Nat. Prod*., 2006, **69**, 211–218 (*bibl*)

6.6.5 Miscellaneous triterpenoids (VS9300)

This group contains assorted triterpenoid skeletons which are less easily classified. It includes intriguing group of compounds, such as **Sipholenone C**, from the sponge *Siphochalina siphonella* and **Sodwanone A** from *Axinella weltneri*.



Sipholenone C

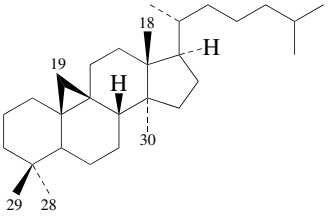


Sodwanone A

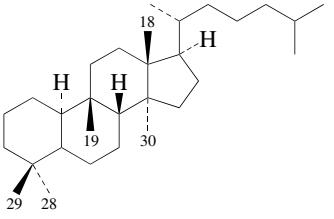
Kashman, Y. *et al Phytochem. Rev*., 2004, **3**, 309–323 (*bibl*)

6.6.6 Other marine triterpenoids

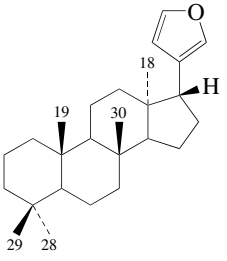
Triterpenoids are characteristic metabolites of terrestrial higher plants and are rare in the marine environment apart from the groups listed above. Many triterpenoids are important biomarkers in marine sediments. The triterpenoid groups are listed below for reference.



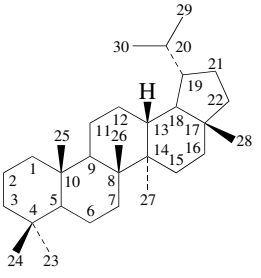
Cycloartane



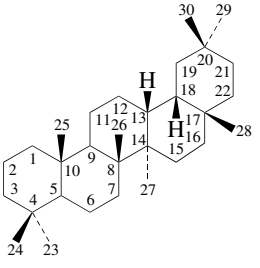
Cucurbitane



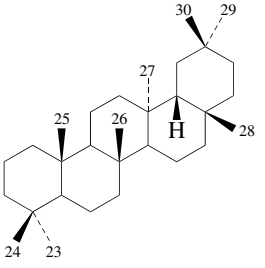
Tetranortriterpenoid skeleton



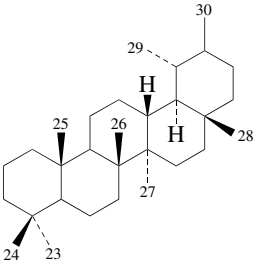
Lupane, 9Cl
(23/24 substituents specified in CA as (4α)23- and (4β)23- respectively)



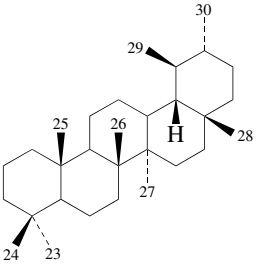
Oleanane, 9Cl
(23/24 substituents specified in CA as (4α)23- and (4β)23- respectively; and 29/30 substituents as (20α)29- and (20β)29- respectively)



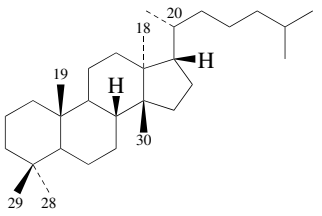
Taraxerane
D -Friedooleanane, 9Cl



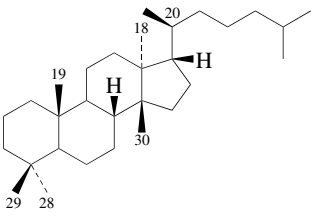
Taraxastane



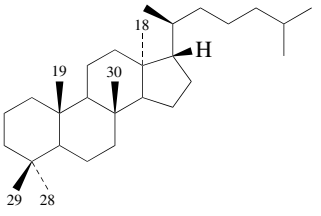
Ursane, 9Cl



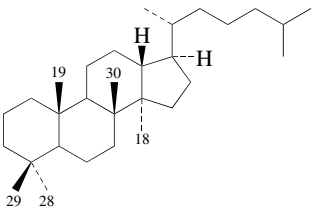
Euphane



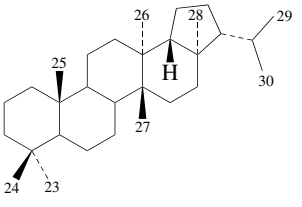
Tirucallane



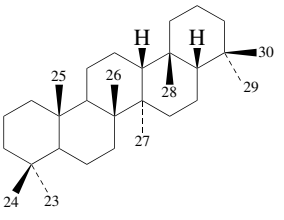
Apotirucallane



Dammarane



Fernane
D : *C* -Friedo-*B*' : *A*'-neogammacerane, 9Cl

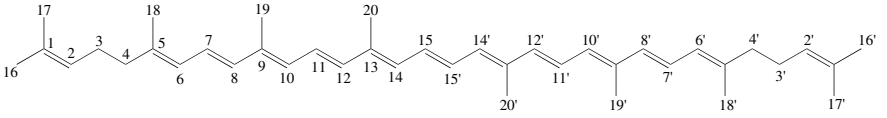


Gammacerane, 9Cl

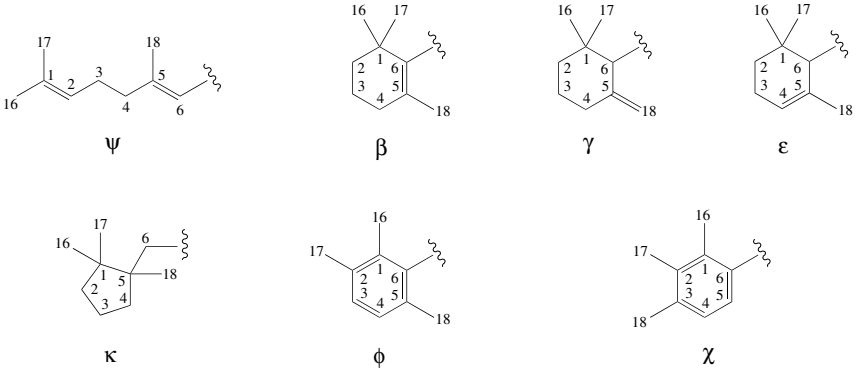
Minale, L. *et al, Advances in Experimental Medicine and Biology*, (eds, Waller, G.R. *et al*) Springer, 1996, **Vol. 404**, 335–356 (*marine triterpenoids*)

6.7 Tetraterpenoids (VS9400)

The tetraterpenes arise by head to head coupling of two geranylgeranyl diphosphate molecules.



ψψ-Carotene



ψ β γ ε

κ ϕ χ

Carotenoid end-groups

Spurgeon, S.L. *et al*, *Biosynthesis of Isoprenoid Compounds*, (eds. Porter, J.W. *et al*), Wiley, New York, 1981, **Vol. 2**, 1

6.7.1 Carotenoids

These include the hydrocarbons (carotenes) and their oxygenated derivatives (xanthophylls). Carotenoid nomenclature is based on a stem name, carotene, and two Greek letters as prefixes to define the two end groups. The numbering system and end groups are given below.

IUPAC treats 'hydro' prefixes in carotenoid names as non-detachable. This Dictionary follows IUPAC recommendations for nomenclature except that the 'hydro' prefix is treated as detachable and is placed alphabetically with the other prefixes. CA also uses a detachable 'hydro' prefix but it does not use hypothetical parents such as β-caroten-6-ols which are incapable of existence (see current *Chemical Abstracts Index Guide*). The following examples illustrate this point.

IUPAC name	**Chemical Abstracts name**
5,6-Dihydro-β,β-caroten-3-ol	5,6-Dihydro-β,β-caroten-3-ol
5,6-Dihydro-β,β-caroten-6-ol	5,6-Dihydro-6-hydroxy-β,β-carotene

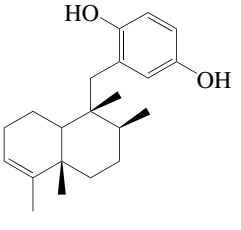
IUPAC, *Pure Appl. Chem*., 1975, **41**, 407–431 (*nomenclature*)
Goodwin, T.W., *Biochemistry of the Carotenoids*, 2nd edn, Chapman & Hall, London, 1980
Matsuno, T., *Pure Appl. Chem*., 1985, **57**, 659–666 (*marine animal carotenoids*)
Britton, G., *Nat. Prod. Rep*., 1991, **8**, 223–249 (*carotenoids*)
Liaaen-Jensen, S., *Pure Appl. Chem*., 1991, **63**, 1–12 (*marine carotenoids*)
Sandmann, G., *Eur. J. Biochem*., 1994, **223**, 7–24 (*biosynth*)
Mercadante, A.Z., *Pure Appl. Chem*., 1999, **71**, 2263–2272 (*carotenoids*)
Miki, W., *Food Style* 21, 2000, **4**, 67–70 (*marine carotenoids in food*)
Matsuno, T., *Fish. Sci*., 2001, **67**, 771–783 (*aquatic animal carotenoids*)
Carotenoids Handbook, (eds. Britton, G. *et al*) Birkhäuser, Basel, 2004

6.7.2 Apocarotenoids (VS9700)

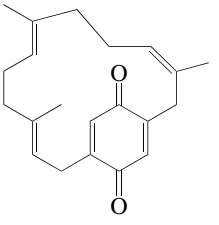
Apocarotenoids are carotenoids in which the carbon skeleton has been shortened by the formal removal of fragments from one or both ends. A locant is used to indicate that all of the molecule beyond the carbon with that locant has been removed. It is not necessary to give a Greek-letter end group designation if the apo-locant is greater than 5.

6.8 Meroterpenoids (VS9900)

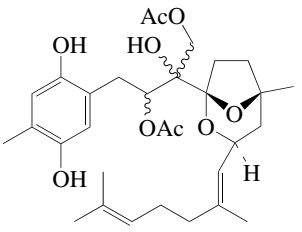
Meroterpenoids are of mixed biogenesis containing terpenoid and non-terpenoid derived fragments. This broad definition could include the vast number of simple prenylated phenolics but is normally reserved for compounds where the terpenoid fragment comprises a large part of the molecule. Many marine meroterpenoids have interesting biological activities such as **Avarol**, with a rearranged drimane terpenoid moiety, from the sponge *Dysidea avara*. The tunicate *Aplidium longithorax* contains a range of meroterpenoids such as **Longithorone B** with a sesquiterpenoid chain in paracyclophane arrangement. Meroditerpenoid and merotriterpenoid representatives include the tetraprenyltoluquinol **Sindurol** from the soft coral *Sinularia dura* and **Toxiusol** from the sponge *Toxiclona toxius*.



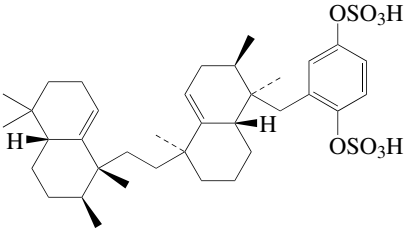
Avarol



Longithorone B



Sindurol



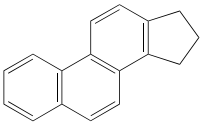
Toxiusol

Koren-Goldshlager, G. *et al*, *J. Nat. Prod*., 1996, **59**, 262–266 (*tetraprenyltoluquinols*)
Braekman, J.-C. *et al*, *Phytochem. Rev*., 2004, **3**, 275–283 (*sponge meroterpenoids*)
Zubia, E. *et al, Mini-Rev. Org. Chem*., 2005, **2**, 389–399 (*Aplidium meroterpenoids*)
Sladic, D. *et al*, *Molecules*, 2006, **11**, 1–33 (*avarol group*)

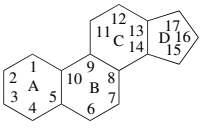
7. STEROIDS (VT)

For general information on the biogenesis of steroids, see the preceding terpenoid section.

The steroid structure is based on four carbocyclic rings arranged as in cyclopenta[*a*]phenanthrene, which is normally fully or partially reduced so that only limited unsaturation, if any, is present. The four steroid rings are labelled, and their carbon atoms are numbered according to the universal convention illustrated.

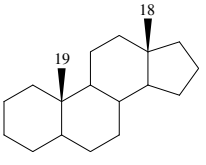


Cyclopenta[*a*]phenanthrene



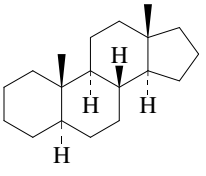
Basic steroid structure

The great majority of steroids also have one or two methyl groups present at the bridgehead positions *C*-10 and *C*-13; the methyl carbon atoms are numbered *C*-19 and *C*-18, respectively.



Methyl groups, hydrogen atoms, or substituents at the bridgehead positions *C*-8, 9, 10, 13, and 14 are assumed to have the 8β, 9α, 10β, 13β, 14α configurations unless otherwise specified. *C*-5 is a special case, as there are many steroids of each of the 5α and 5β configurations, and it is therefore necessary to specify the *C*-5 configuration for any steroid which is saturated at *C*-5 (e.g. 5α-Androstane or 5β-Androstane).

It is worth noting here some changes in *Chemical Abstracts* indexing policy. Prior to the 8th Collective Index (1967), the indexing of steroid stereoisomers gave priority to the *C*-5 configuration which effectively led to a separation of 5α- and 5β-steroids. Users should be alert to this when searching the literature before 1967.

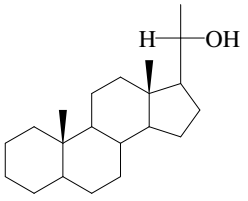


5α-Androstane

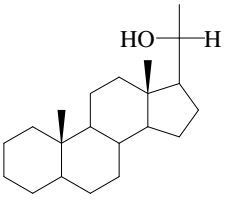
The hydrogen atoms at *C*-8, 9 and 14 are generally omitted from formulae if they have the natural configurations shown here.

Any side-chain at *C*-17 is assumed to have the 17β-configuration unless otherwise indicated. This is shown either by using a wedge bond or, where there is any possibility of uncertainty owing to substitution at *C*-20, by drawing in the *C*-17 α-hydrogen atom.

Configurations of substituents in the side chain were formerly also indicated by α or β, (Fieser convention), whereby the side-chain is drawn in Fischer projection, with the highest numbered locant at the top.



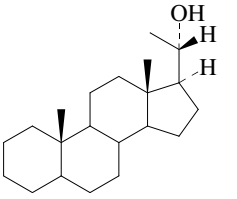
20α-form



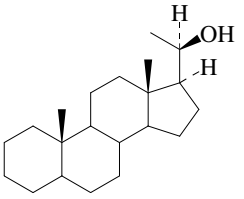
20β-form

The Fieser convention for pregnan-20-ols

The unambiguous Cahn-Ingold-Prelog sequence rule descriptors (*R* or *S*) are now recommended for side-chain configurations.

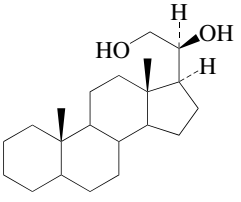


20*S* (= 20α)

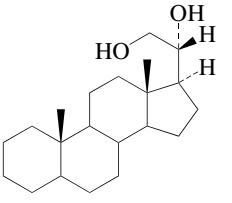


20*R* (= 20β)

The presence of substituents at *C*-17 or *C*-21 may change the priority of groups so that 20*S* is no longer equivalent to 20α. This happens for example in the pregnane-20,21-diols.

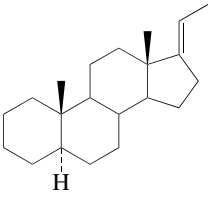


20*S* (= 20β)

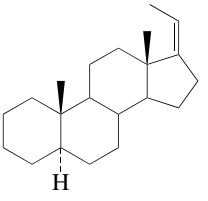


20*R* (= 20α)

The sequence rule descriptors (*E*-) and (*Z*-) are required for defining side-chain double bond configurations. The configuration of additional side-chain methyl or other alkyl groups, which are common in steroids produced by sponges and other marine organisms, are denoted by *R*- and *S*- (or ξ if unknown).



5α-Pregn-17(20)*E*-ene



5α-Pregn-17(20)*Z*-ene

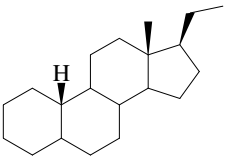
(Note that both locants for unsaturation are required when the numbers are non-consecutive)

Steroids, (eds. Fieser, L.F. *et al*) Reinhold, New York, 1959
Bernstein, S. *et al*, *Physical Properties of Steroid Conjugates*, Springer-Verlag, Berlin, 1968
Atlas of Steroid Structure, (eds. Duax, W.L. *et al*) Plenum, New York, 1975, **Vol. 1**; 1984, **Vol. 2**
Biochemistry of Steroid Hormones, 2nd edn, (ed. Makin, H.L.J.), Blackwell, Oxford, 1984
Danielsson, H. and Sjövall, J., *Sterols and Bile Acids*, Elsevier, Amsterdam, 1985
Zeelen, F.J., *Medicinal Chemistry of Steroids*, Elsevier, Amsterdam, 1990
Dictionary of Steroids, (eds. Hill, R.A. *et al*) Chapman & Hall, London, 1991
Zeelen, F.J., *Nat. Prod. Rep*., 1994, **11**, 607–612 (*total synth*)
Analysis of Sterols, (eds. Goad, L.J. *et al*), Blackie, London, 1997
Brown G.D., *Nat. Prod. Rep*., 1998, **15**, 653–696 (*biosynth*)
Hanson, J.R., *Nat. Prod. Rep*., 2006, **23**, 100–107 (*synth*)

7.1 Steroid classes

7.1.1 C_{20} steroids (VT0400)

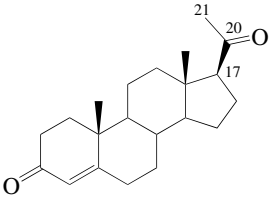
These are scarce among natural products. A few 19-norpregnanes, with the pregnane skeleton (see below) but lacking the bridgehead methyl group (*C*-19) occur in marine organisms. Alternative names based upon 17-ethylestrane are also often used for this series of compounds (see pregnanes).



19-Norpregnane

7.1.2 Pregnane steroids (C_{21}) (VT0450)

Pregnane is the parent hydrocarbon of the pregnancy hormone progesterone (pregn-4-ene-3,20-dione), and of the great majority of the corticosteroids and many other natural products, which together make the pregnanes the largest single group of steroids. Many pregnane derivatives have hydroxyl or a related group at *C*-17. To avoid any ambiguity as to the configuration, epimeric forms of 17-substituted pregnanes are specified as 17αOH or 17βOH.



Pregn-4-ene-3,20-dione (Progesterone)

7.2 The sterols

The sterols comprise several major groups of steroids characterised by having a hydroxyl group at *C*-3, normally in the β-configuration, and branching side chains of from eight to ten or more carbon atoms at *C*-17. They occur widely throughout the animal and particularly the plant kingdoms. They have both structural roles, as membrane constituents, and a key place in the biosynthetic sequences which lead to the steroid hormones and other biologically active steroidal species.

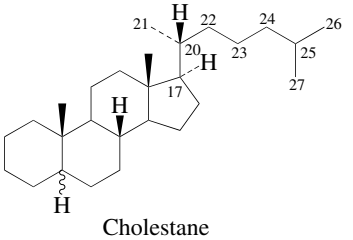
The following sections detail the main features of the various parent hydrocarbons which provide the structural basis and classification of the sterols.

Kerr, R.G. *et al*, *Nat. Prod. Rep*., 1991, **8**, 465–497 (*marine sterols*)
Baker, B.J. *et al*, *Topics in Current Chemistry*, (ed. Scheuer, P.J.), Springer, Berlin, 1993, **Vol. 167**, 1–31 (*biosynth*)
D'Auria, M.V. *et al*, *Chem. Rev*., 1993, **93**, 1839–1895 (*marine steroids*)
Giner, J.L. *et al*, *Chem. Rev*., 1993, **93**, 1735–1752 (*biosynth*)

Minale, L., *Progress in the Chemistry of Organic Natural Products*, (eds, Herz, W. *et al*), SpringerWien, New York, 1993, **Vol. 62**, 75–308 (*echinoderm sterols*)
Stonik, V.A., *Russ. Chem. Rev*., 2001, **70**, 673–715 (*marine steroids*)
Sica, D. *et al*, *Steroids*, 2004, **69**, 743–756 (*marine secosteroids*)
Sarma, N.S. *et al*, *Mar. Drugs*, 2005, **3**, 84–111 (*sponge sterols*)

7.2.1 Cholestane steroids (C_{27}) (VT1050, VT1100)

The cholestane skeleton, which derives its name from the longest-known and most familiar compound of its class, **Cholesterol**, can be regarded as the parent from which almost all other sterols are derived. This is true structurally, if not necessarily in terms of the detailed biosynthetic pathway.



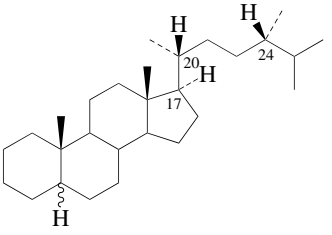
Cholestane

Other classes of sterols are derived from cholestane by the addition of one or more carbon atoms at side-chain positions, most commonly *C*-24 (see ergostanes, stigmastanes, etc, below).

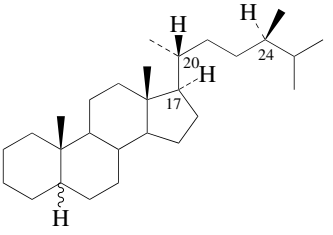
Alkylated cholestanes of many types occur widely in plants, fungi, and marine organisms. The very large classes of 24-methylcholestanes (ergostanes and campestanes) and 24-ethylcholestanes (stigmastanes and poriferastanes) are sufficiently important that their parent hydrocarbons have been assigned these special systematic names (not used in *Chemical Abstracts* however). They are treated in separate sections below. The 4,4,14-trimethylcholestanes (lanostanes) are covered in the preceding terpenoid section. Many alkylcholestane derivatives, however, fall outside these major groups, and have not been signified by special class names. They can be named as derivatives of cholestane, or alternatively if they contain a 24-methyl or 24-ethyl group can be named as substituted ergostanes or stigmastanes respectively. Both forms are usually given in the Dictionary to aid location. Others are homocholestanes, in which additional carbon atoms lengthen the side-chain, rather than branching off it. Many of these unusual sterols are best known by trivial names that reflect their biological origins.

7.2.2 Ergostane steroids (VT1300)

The 24-methylcholestane structure is termed ergostane. While the saturated and Δ^{25}-unsaturated ergostane side-chains have the 24*S* configuration, the altered priorities of groups around *C*-24 give ergost-22-ene the 24*R* configuration.

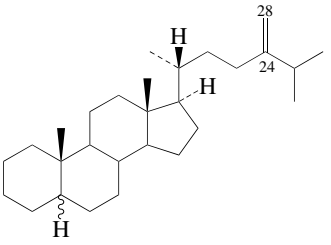


Ergostane

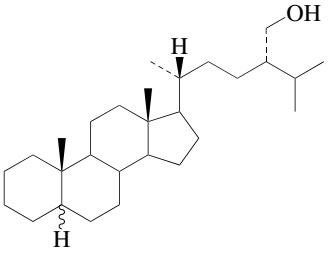


Campestane

A further complication, firmly rooted in historical precedent, is the use of the locant *C*-28 for the carbon atom of the 24-methyl group. The latest IUPAC-IUB recommendation is that the locant *C*-28 be reserved for the 4α-methyl group in lanostanes, and in other 4,4-dimethylsterols of terpenoid type, with *C*-29 and *C*-30 allocated, respectively, to the 4β- and 14α-methyl groups. The locant *C*-28 has therefore acquired two distinct meanings, according to context. In this Dictionary the *C*-24 methyl group in ergostanes and campestanes retains its original locant as *C*-28, allowing the use of derivative names containing such expressions as ergost-24(28)-ene (for 24-methylenecholestanes) or ergostan-28-ol (for 24-hydroxymethylcholestanes). The cholestane-based synonyms favoured by IUPAC-IUB are also given, where necessary, for clarity.



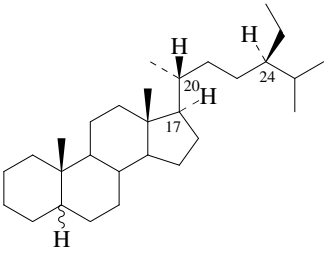
24-Methylenecholestane
[Ergost-24(28)-ene]



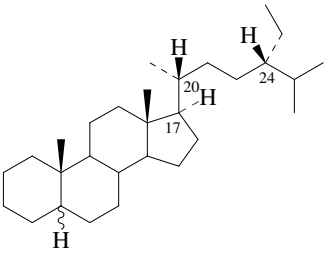
24-Hydroxymethylcholestane
(Ergostan-28-ol)

7.2.3 Stigmastane steroids (C_{29}) (VT1550)

These are the 24-ethylcholestanes, stigmastanes and poriferastanes being epimeric at *C*-24. The long history of stigmastane-based nomenclature, derived from the common plant sterol Stigmasterol, has ensured that this is by far the more widely used of the two names. In the Fieser system, stigmastanes have the 24α configuration, and poriferastanes are 24β. Again the sequence rule is now preferred, with 24*R* or 24*S* depending upon local substitution and/or unsaturation.

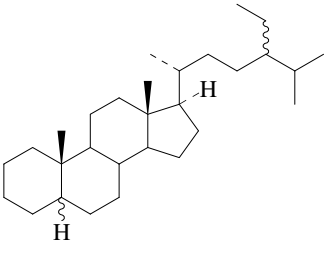


Stigmastane

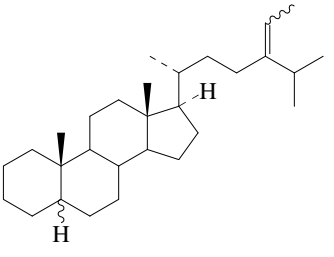


Poriferastane

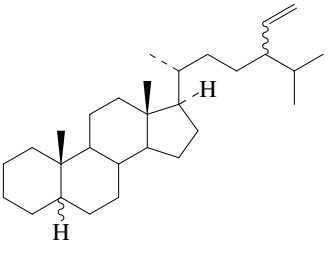
As with ergostanes, common usage over several decades has favoured the locants *C*-28 and *C*-29 for the two ethyl carbon atoms, and these are used here. The IUPAC-IUB recommendation is that the two ethyl carbon atoms be designated 24^1 and 24^2 whenever locants are needed. Synonyms based upon 24-ethylcholestane, 24-ethylidenecholestane, or 24-vinylcholestane are given in the Dictionary where suitable.



24-Ethylcholestane



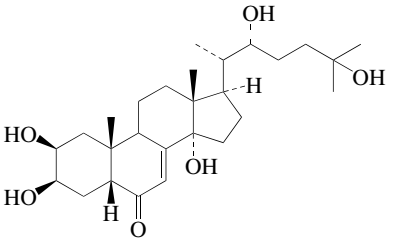
24-Ethylidenecholestane



24-Vinylcholestane

7.2.4 Ecdysteroids (C_{27}) (VT1150)

Ecdysteroids or ecdysones are moulting hormones of insects and crustaceans. They have also been isolated from many plants. The first ecdysone to be isolated was α-Ecdysone from the silkworm (*Bombyx mori*). Most ecdysteroids have a 2β,3β,14α,20,22-pentahydroxy-5β-cholest-7-en-6-one skeleton with further hydroxylation.

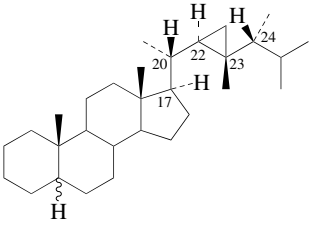


α-Ecdysone

Dauphin-Villemant, C., *Ann. NY Acad. Sci*., 1998, **839**, 306–310 (*biosynth*)
Subramoniam, T., *Comp. Biochem. Physiol*., 2000, **125C**, 135–156 (*crustacean ecdysteroids*)
Suksamrarn, A. *et al*, *J. Nat. Prod*., 2002, **65**, 1194–1197 (*bibl*)
Hopkins, P.M., *Recent Advances in Marine Biotechnology*, (eds. Fingerman, N. *et al*), Science Publishers, USA, 2003, **Vol. 10**, 263–278 (*crustacean ecdysteroids*)
Lafont, R. *et al*, *Comprehensive Molecular Insect Science*, (eds. Gilbert. L. *et al*), Elsevier, 2005, **Vol. 3**, 125–195 (*ecdysteroids*)

7.2.5 Gorgostane and other cyclopropacholestane steroids (C_{30}) (VT1700)

Gorgostane is the parent hydrocarbon of a widely-occurring group of sterols in marine organisms. Its skeleton comprises ergostane with an additional methyl group at *C*-23, and a methylene bridge between *C*-22 and *C*-23, forming a cyclopropane ring. Configurations in the side chain are as illustrated unless otherwise specified.



Gorgostane

A wide variety of at least 100 diverse C_{30} and C_{31} marine sterols in the gorgostane and related structural classes are known. Sponges are the most prolific source. Sponge sterols are characterised by multiply alkylated side chains, frequent presence of cyclopropane/cyclopropene functionality in the side chain, and wide variation in the steroid A-D ring skeleton, including many examples of A-nor and 19-nor variants.

Djerassi, C. *et al*, *Acc. Chem. Res*., 1991, **24**, 371–378 (*biosynth*)
Djerassi, C., *Studies in Natural Products Chemistry*, (ed. Atta-ur-Rahman), Elsevier, Amsterdam, 1991, **Vol. 9**, 25–50 (*marine cyclopropane sterols*)

8. AMINO ACIDS AND PEPTIDES (VV)

8.1 Amino acids (VV0050–VV0140)

8.1.1 Protein α-amino acids (VV0050)

The common α-amino acids are characterised by the structure $RCH(NH_2)COOH$, where R is an aliphatic (including hydrogen), aromatic or heterocyclic group. The exception is **Proline**, strictly an iminoacid, in which the N atom is incorporated into a 5-membered pyrrolidine ring.

They are the primary products of nitrogen anabolism in plants, where they are produced from ammonia (derived *ab initio* by nitrate reduction or nitrogen fixation) by a process called the glutamate synthetase cycle. This produces glutamate which is then transformed into the other amino acids by a variety of processes.

The amino acids thus represent the most important nitrogenous component (in terms of volume and accessibility) of the chiral pool produced by living organisms and are of great importance in chiral synthesis.

Several hundred natural amino acids are known. Of these, only 20 (known as the primary protein amino acids) are incorporated by all organisms into peptides and proteins (not all of these 20 amino acids can be biosynthesised by animals). This protein synthesis occurs in the ribosomes by a process involving ribonucleic acid (RNA), the nucleoside chain of which transmits the template instructions of the DNA genetic material to the protein sequences, each primary amino acid in the chain being coded for by one or more nucleoside base triplets or codons.

There is an IUPAC-IUB standard 3-letter code for each of the protein amino acids (as well as for the common non-protein amino acids). For ease of computerised documentation of large peptide structures, one-letter codes have more recently been introduced.

8.1.2 IUPAC-IUB abbreviations

Amino acids and their corresponding 3-letter and 1-letter codes

1.	Alanine	Ala	A
2.	Arginine	Arg	R
3.	Asparagine	Asn	N
4.	Aspartic acid	Asp	D
5.	Cysteine	Cys	C
6.	Glutamic acid	Glu	E
7.	Glutamine	Gln	Q
8.	Glycine	Gly	G
9.	Histidine	His	H
10.	Isoleucine	Ile	I
11.	Leucine	Leu	L
12.	Lysine	Lys	K
13.	Methionine	Met	M
14.	Phenylalanine	Phe	F
15.	Proline	Pro	P
16.	Serine	Ser	S
17.	Threonine	Thr	T
18.	Tryptophan	Trp	W
19.	Tyrosine	Tyr	Y
20.	Valine	Val	V

Various posttranslational protein amino acids, known as secondary amino acids, may then arise in the protein by various processes such as conjugation of OH, SH or NH groups, *N*-methylation or hydroxylation (especially to produce **4-Hydroxyproline**). A special case of posttranslational change is the reversible oxidation of cysteine residues to produce the disulfide, **Cystine**, thus linking different parts of the peptide chain by disulfide bridges as part of the secondary structure of the protein.

With the exception of **Glycine**, all of the genetically coded protein amino acids are chiral and belong to the L-series. In all cases, except Cysteine, this corresponds to the *S*-form according to the Cahn-Ingold-Prelog convention. In Cysteine, the higher priority of the CH_2SH group over the COOH group means that L- corresponds to the *R*-form.

Amino acids of the opposite D-series can be detected in hydrolysates of aged proteins in which they arise by slow racemisation (they are also produced as artifacts of racemisation during acid or especially alkaline hydrolysis of polypeptides). D-Amino acids are common constituents of antibiotics and bacterial proteins.

Chemistry and Biochemistry of the Amino Acids, (ed. Barrett, G.C.) Chapman & Hall, London, 1985
Asymmetric Synthesis: Construction of Chiral Molecules Using Amino Acids, (ed. Coppola, G.M. *et al*) Wiley, New York, 1987
Synthesis of Optically Active α-Amino Acids, (ed. Williams, R.M.), Pergamon, Oxford, 1989
Hunt, S., *Methods in Plant Biochemistry*, (ed. Rogers, L.J.), Academic Press, New York, 1991, **Vol. 5**, 1–52

8.1.2 Non-protein α-amino acids (VV0100)

In addition to the proteinaceous amino acids, there are several hundred known natural non-protein amino acids which arise by a variety of metabolic routes. Some of these have demonstrated functions, for example as defence chemicals; the plant amino acids probably perform a generalised nitrogen storage function.

A considerable number of atypical α-amino acids have been isolated from microbial sources. They inhibit the growth of a range of microorganisms but their effects can be readily reversed by supplementing the growth medium by the requisite principal amino acid.

Atypical amino acids are encountered in the hydrolysates of microbial peptide antibiotics. These do not always occur in the free state but a number have been included in DMNP since a given amino acid may be present in a range of different peptides.

Scannell, J.P. *et al*, *Chemistry and Biochemistry of Amino Acids Peptides and Proteins*, Dekker, New York, 1974 (*antimetabolites*)
Hatanaka, S.I. *et al*, *Progress in the Chemistry of Organic Natural Products*, (eds. Hertz, W. *et al*), SpringerWien, New York, 1992, **59**, 1 (*fungi amino acids*)

8.1.3 β-Amino acids (VV0120)

A small number of β-amino acids occur in the marine environment, especially in sponges. Of these the most widespread is 2-(aminomethyl)-2-propenoic acid and associated amides.

Drey, C.N.C., *Chemistry and Biochemistry of the α-Amino Acids*, (ed. Barrett, G.C.), Chapman & Hall, London, 1985

8.2 Peptides (VV0150–VV0500)

Peptides are oligomers and polymers notionally derived from amino acids by condensation to produce amide linkages. The boundary between oligopeptides and polypeptides is arbitrary and in DMNP has been set at 10 amino acid residues. The configuration of amino acid residues in polypeptides is assumed to be L- when not indicated otherwise.

There is evidence that in higher organisms small peptides (hormones) can arise only by cleavage of protein prohormones.

A large number of biologically-active atypical peptides have been isolated from bacteria, actinomycetes, cyanobacteria, fungi and higher animals. Structurally they represent an extremely diverse group, encompassing those metabolites containing two or more amino acid residues linked by a peptide bond, but possessing some additional features not characteristic of proteins. These may include unusual amino acid residues, protein amino acids with D-configuration or increased to a higher oxidation level, or non-peptide linkages between residues (e.g. ester, lactone or a γ-glutamyl amide). In addition, the molecules may be linear or cyclic, contain one or a combination of the above mentioned features, be modified by further interactions between the side chains of amino acid units within the peptide, or conjugated with either lipids or sugar units. They can possess a wide range of biological activities, e.g. the neuropeptides **Carcinustatins**, the hormone **Salcatonin**, and the enzyme inhibitor **Cyclotheonamide A**. Also worthy of note are the **Conotoxins**, a group of marine venoms isolated from snails with interesting biological properties, as well as many other toxins isolated from higher marine animals.

8.2.1 Diketopiperazines (dipeptide anhydrides) (VV0150)

These are among the most numerous of all naturally occurring peptides. They range from simple cyclic dipeptides, e.g. **Dysamide A**, to highly complex fused ring systems such as the cytotoxic **Leptosins** and related compounds. Nomenclature of the simple diketopiperazines is complicated by the proliferation of different ways of naming them. In this Dictionary, systematic *Chemical Abstracts* names are usually used as their entry names, but the entries contain a full range of possible synonyms.

8.2.2 Cyclic oligo- and polypeptides (VV0500)

No cyclic homodetic tripeptides with or without biological activity have been observed to date. Cyclic peptides derived from 4–11 amino acid residues linked by peptide bonds have been isolated from a variety of microorganisms, particularly those associated with sponges and algae, e.g. **Phakellistatins**. Their biological properties are diverse, ranging from antitumour/cytotoxic activities and antifungal and antibacterial properties.

8.2.3 Depsipeptides (VV0600, VV0610)

Cyclic heterodetic peptides or peptide lactones are those in which one or more of the peptide bonds have been replaced by ester linkages, examples include **Dolastatin 11** and **Aplidine** which has been used in clinical trials.

8.2.4 Large peptides and proteins (VV1000, VV2000)

Entries are given in DMNP for the majority of bioactive peptides secreted by marine plants and animals for which reasonable structural information exists, including many neuropeptides which are an active field of research. Entries are presented for the most important non-enzyme proteins and for some enzymes (VV1000), but full structures are not given in individual entries, the structures where known can be assessed *via* the cited references.

The Peptides, (ed. Gross, E.), Academic Press, New York, 1983 (*general*)
Bladon, C., *The Chemistry of Natural Products*, 2nd edn (ed. Thomson, R.H.), Blackie, Glasgow, 1993, 183 (*rev*)
Fusetani, N. *et al*, *Chem. Rev*., 1993, **93**, 1793–1806 (*sponge peptides*)

8.3 Glycopeptides and glycoproteins (VV3000)

This is a relatively small and structurally self-evident category of peptides predominantly consisting of proteinaceous toxins such as **Dolabellanins** and **Verrucotoxin**.

Fattorusso, E. *et al, Marine Natural Products: Chemical and Biological Perspectives*, (ed. Scheuer, P.J.), Academic Press, New York, 1980, **Vol. 3**, 95–140 (*amino acids from algae*)
Ireland, C.M. *et al, Bioorganic Marine Chemistry*, (ed. Scheuer, P.J.), Springer-Verlag, New York, 1989, **Vol. 3**, 1–46 (*peptides from marine organisms*)
Suzuki, N., *Bioorganic Marine Chemistry*, (ed. Scheuer, P.J.), Springer-Verlag, New York, 1989, **Vol. 3**, 47–70 (*peptides from sea urchins*)
Bernheimer, A.W., *ACS Symp. Ser*., 1990, **418**, 304–311 (*marine toxins*)
Sharma, G.M. *et al, Mar. Technol*., 1993, **1**, 153–180 (*marine proteins in clinical chem*)
Wipf, P., *Chem. Rev*., 1995, **95**, 2115–2134 (*cyclic peptides, synth*)
Gulavita, N.K. *et al, J. Nat. Toxins*, 1996, **5**, 225–234 (*peptides from sponges*)
Norton, R.S., *J. Toxicol. Toxin Rev*., 1998, **17**, 99–130 (*toxins in marine organisms*)
Fields, P.A., *Comp. Biochem. Physiol., A: Mol. Integr. Physiol*., 2001, **129**, 417–431 (*proteins in marine environment*)
O'Keefe, B.R., *J. Nat. Prod*., 2001, **64**, 1373–1381 (*proteins; activity*)
Anderluh, G. *et al, Toxicon*, 2002, **40**, 111–124 (*toxins from sea anemones*)
Massilia, G.R. *et al, Recent Res. Dev. Biochem*., 2002, **3**, 113–128 (*conopeptides*)
Matsunaga, S. *et al, Curr. Org. Chem*., 2003, **7**, 945–966 (*non-ribosomal peptides from sponges*)
Lehrer, R.I. *et al, Integr. Comp. Biol*., 2003, **43**, 313–322 (*peptide antibiotics from tunicates*)
Aneiros, A. *et al, J. Chromatogr. B*, 2004, **803**, 41–53 (*bioactive peptides, isol, pharmacol*)
Terlau, H. *et al, Physiol. Rev*., 2004, **84**, 41–68 (*Conus venoms*)
Tincu, J.A. *et al, Antimicrob. Agents Chemother*., 2004, **48**, 3645–3654 (*antimicrobial peptides from invertebrates*)
Gowd, K.H. *et al*, *Ann. NY Acad. Sci*., 2005, **1056**, 462–473 (*Conus peptides*)
Ma, D. *et al, Pept. Sci*., 2004, **41**, 71–74 (*cyclic peptides, synth*)
Hamada, Y. *et al*, *Chem. Rev*., 2005, **105**, 4441–4482 (*cyclic peptides, synth*)
Honma, T. *et al, Mar. Biotechnol*., 2006, **8**, 1–10 (*sea anemone toxins*)
Rawat, D.S. *et al, Anti-Cancer Agents Med. Chem*., 2006, **6**, 33–40 (*peptides in clinical trials*)
Layer, R.T. *et al*, *Mar. Drugs*, 2006, **4**, 119–142 (*Conotoxins*)

9. ALKALOIDS (VX)

Alkaloids are a large group of nitrogen-containing secondary metabolites of plant, microbial or animal origin. Biogenetically and structurally the alkaloids are diverse, and because of the structural complexity of many marine alkaloids, some of them are classified here under more than one heading.

In general, less is known about the biogenesis of marine alkaloids than their terrestrial counterparts because of experimental difficulties and the complexity of the ecosystems. There are many synthetic studies, but comparatively few biosynthetic ones. Few characteristic key intermediates have been identified in the later stages of marine alkaloid biosynthesis; an exception is Oroidine. Some types of marine alkaloid are of mixed biogenesis, different stages of the biosynthesis being affected by different organisms.

Where structural similarities exist between certain marine alkaloids and their terrestrial counterparts, this is frequently indicated in the following sections, but this should not be taken to imply that their biosynthesis takes place by identical routes. There may be cases of biochemical parallelism arising from convergent evolution. In many cases the relevant information is just not available for the marine alkaloids.

The order of the following sections, and the accompanying Type of Compound codes that can be used for searching the electronic version of the database, follows that of the parent *Dictionary of Natural Products* database, which is loosely based on biogenetic considerations (for example, ornithine-derived alkaloids precede those derived from lysine). However, in considering marine alkaloids, these considerations may not necessarily apply and the order is more arbitrary. Sections dealing with structurally related types of alkaloid are, though, usually close together. Some types have been extensively studied biosynthetically, for others there is currently no, or only fragmentary, information. In addition, details are now being uncovered about formerly unsuspected enzyme systems present in marine organisms, which superpose new biosynthetic possibilities on top of the traditional routes, thus blurring the traditional alkaloid subtypes. Foremost among these are the 'Diels-Alderases' (not confined to alkaloids) which are capable of catalysing the formation of new carbon skeletons from known types. The Type of Compound categories in the database are therefore subject to future revision in the light of new research results.

The term alkaloid originally implied pharmacologically active bases, but the definition has subsequently been broadened so that it is now generally considered to include the majority of nitrogen-containing natural products with the exception of the simple amino acids, proteins and nitrogen-containing substances of polyketide origin such as aminoglycosides. Basic properties may be weak or absent as in the various types of amide alkaloids. The term 'imperfect alkaloid' has been used for miscellaneous nitrogenous natural products, including amides that do not fall into one of the well-defined traditional alkaloid types. Nitrogenous compounds of novel structural type are of obvious medicinal interest.

Garson, M.J., *Chem. Rev*., 1993, **93**, 1699–1733 (*rev, biosynth*)
Oikawa, H. *et al, Nat. Prod. Rep*., 2004, **21**, 321–352 (*rev, Diels-Alder enzymes*)
Newman, D.J. *et al, J. Nat. Prod*., 2004, **67**, 1216–1238 (*rev, marine compounds in clinical trial*)
Moore, B.S., *Nat. Prod. Rep*., 2005, **22**, 580–593; 2006, **23**, 615–629 (*rev, biosynth*)

The following codes occur at the beginning of the sequence and refer to simple and miscellaneous amines, amides and related compounds;

9.1.1 Simple acyclic amine alkaloids with one N (VX0100)

These include simple amines of mostly widespread biological occurrence such as choline and ethylamine.

9.1.2 Simple acyclic amine alkaloids with two N (VX0120)

These include a variety of linear diamines such as the **Clathculines** and **Calyxoside**.

9.1.3 Simple guanidines (VX0150)

This heading covers low MW guanidinoid bases. The guanidine or modified guanidine group is common as a structural component of higher MW alkaloids, including hybrid polyketide alkaloids and peptide-alkaloids which have been classified elsewhere as polyketides or peptides.

Berlinck, R.G.S. *et al, Nat. Prod. Rep*., 2002, **19**, 617–649; 2005, **22**, 516–550 (*rev*)
Nagasawa, K. *et al, Chem. Rec*., 2003, **3**, 201–211 (*rev, synth*)

9.1.4 Nitriles, isonitriles and related compounds (VX0200)

Compounds containing the -NC, -NCS and -NHCHO groups frequently occur together and are biogenetically related. They are usually included in the same entry. It now appears that the thiocyanates are central in their biosynthesis.

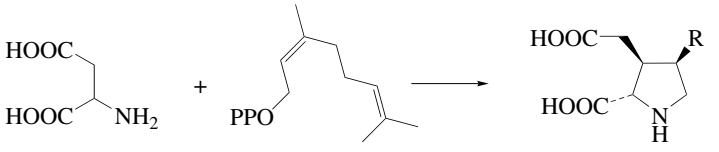
Garson, M.J. *et al, Nat. Prod. Rep*., 2004, **21**, 164–179 (*rev*)

9.1.5 Simple amide alkaloids (VX0250)

These include a variety of simple amides such as the **Variceramides**.

9.1.6 Pyrrolidine alkaloids (VX0300, VX0380)

These may arise by different biosynthetic pathways. The kainoids, e.g. **α-Kainic acid**, **Domoic acid**, are a group of non-proteinogenic pyrrolidinedicarboxylic acids. α-Kainic acid was first isolated from a rhodophyte alga but has since been found in terrestrial organisms. The kainoids are biosynthesised from glutamate and geranyl pyrophosphate. Other marine pyrrolidines such as the **Sarcotrines** are degraded pyrrolosesterterpenes, while many others are presumably proline-derived.



e.g. Domoic acid, R = $C(CH_3)$=CHCH=CHCH(CH_3)COOH

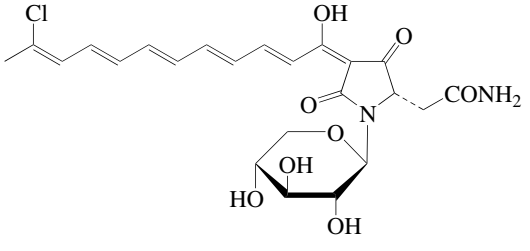
Parsons, A.F., *Tetrahedron*, 1996, **52**, 4149–4174 (*kainoids, rev*)

9.1.7 Chromone alkaloids (VX0340)

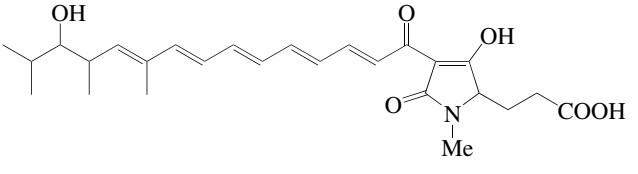
Chromone alkaloids, moderately common in higher plants, are currently represented only by **Tubastraine**, which appears doubtful.

9.1.8 Tetramic acids (VX0390)

These are longer-chain pyrrolidines exemplified among marine examples by the halogenated **Aurantosides** and **Rubrosides** from sponges (microbial products). They are polyketide in origin and are most closely related to nonhalogenated tetramic acids from terrestrial microorganisms such as Erythroskyrin and the Lipomycins.



Aurantoside G

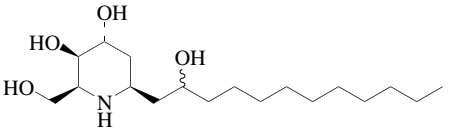


β-Lipomycin
(terrestrial)

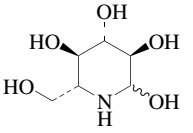
9.1.9 Piperidine alkaloids (VX0620, VX0680, VX0700)

The majority of the alkaloids in this group are plant-derived, but **Anabaseine** and several related alkaloids have been isolated from a hoplonemertean worm. Like the pyrrolidines, these alkaloids may arise by different biosynthetic routes, so the class is structural rather than biosynthetic. They may be derived from lysine, acetate, acetoacetate, etc. but the longer-chain **Batzellasides**, present in sponges, are iminoglycosides structurally related to the intensively-studied terrestrial iminosugars such as **Nojirimycin**, evidently with the incorporation of a fatty-acid derived fragment.

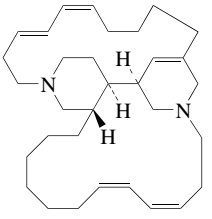
Other piperidine alkaloids included here include the **Halicyclamines** and relations, which are classified under miscellaneous piperidine alkaloids (VX0700), but which are the first of several types of alkaloids including the Xestospongins and the Manzamines below, which appear to be closely related and are based on elaboration of a macrocycle-linked 1,3-linked bispiperidine theme.



Batzellaside A



Nojirimycin
(terrestrial)

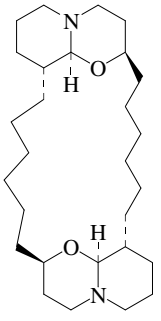


Halicyclamine A

Jaspars, M. *et al, J. Org. Chem*., 1994, **59**, 3253–3255 (*Halicyclamines, biosynth*)
Andersen, R.J. *et al, Alkaloids: Chemical and Biological Perspectives*, (ed. Pelletier, S.W.), Elsevier, Amsterdam, 1996, **10**, 301 (*rev, 3-alkylpiperidines*)

9.1.10 **Xestospongins** (VX0690)

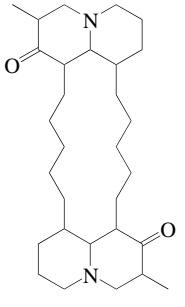
These are a group of exclusively marine elaborated piperidines. Their biosynthesis would appear to imply the involvement of a C_{10} dialdehyde equivalent as hypothesised for the Manzamine group (VX2250) below, and they appear closely related to intermediates postulated in the Baldwin scheme.



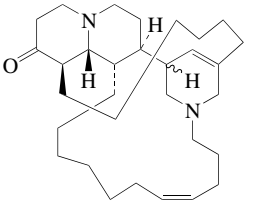
Xestospongin A

9.1.11 **Quinolizidine alkaloids** (VX0900, VX0980)

A few relatively simple marine quinolizidine alkaloids are known such as **Pictamine** and the **Clavepictines**. The **Saraines** are more complex sponge products classified under miscellaneous quinolizidines (VX0980), together with Halichlorine, a popular synthetic target, and the **Petrosines**, further examples of dimeric alkaloids in which the units are linked in a medium-sized aliphatic ring as in the Xestospongins.



Petrosines
(various stereoisomers)

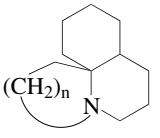


Saraine 1

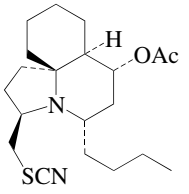
Michael, J.P., *Nat. Prod. Rep*., 2002, **19**, 719–741; 2004, **21**, 625–649 (*revs*)

9.1.12 **Cylindricines** (VX0960)

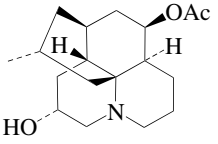
This small group of alkaloids is based on the perhydrobenzo[*i*]quinolizine and perhydrocyclopenta[*i*]quinoline skeletons. There are structural similarities to some of the terrestrial *Lycopodium* alkaloids such as **Paniculine**. The isolation of both thiocyanates and isothiocyanates is noteworthy.



n = 2-3



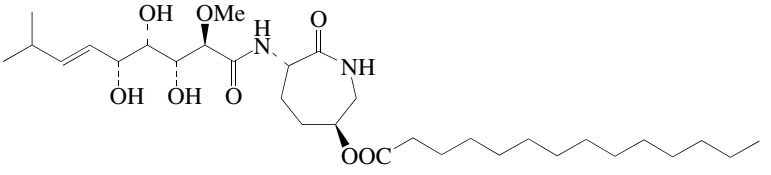
Cylindricine H



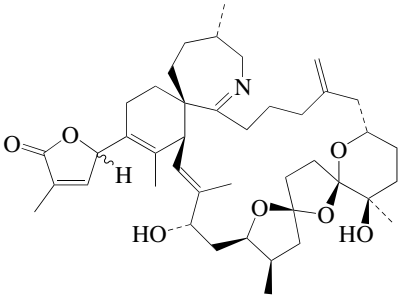
Paniculine (terrestrial)

9.1.13 **Azepine alkaloids** (VX1000)

These include the **Bengamides** and the **Spirolides**. The former are thought to be symbiotic products deriving from bacterial fatty acids, cyclised lysine and a 4-carbon diketide. The spirolides are shellfish toxins related to the Pinnatoxins (which are classified under VC0550, polyketides; the division is arbitrary) and like them presumably arising by a Diels-Alder process from a long-chain polyketides precursor.



Bengamide A



Spirolide A

9.1.14 **Pyridine alkaloids** (VX1040)

As well as some simple nicotinic acid-related bases (VX1040), a considerable number of pyridines carrying a long-chain substituent at *C*-3 have been isolated mostly from sponges. Examples include the **Xestamines**, **Ikimines** and **Niphatesines**. Small pyridinium betaine alkaloids such as **Trigonelline** are widespread in marine plants and animals as well as terrestrial organisms.

Almeida, A.M.P. *et al, Quim. Nova, 1997*, **20**, 170 (*rev, alkylpyridines from sponges*)
Sepčić, K., *J. Toxicol., Toxin Rev*., 2000, **19**, 139–160 (*rev, alkylpyridinium compounds from sponges*)

9.1.15 Cytochalasan alkaloids (VX1300)

Cytochalasins are metabolites of several different and unrelated fungi. They are characterised structurally by the presence of a perhydroisoindolone system fused to a macrocyclic ring of 11, 13 or 14 atoms. The macrocycle may be a carbocycle, a lactone or a carbonate. In addition the isoindole ring carries either a phenyl or an indolyl substituent at position 10; the latter group includes the Chaetoglobosins.

Biosynthetically, cytochalasins arise from phenylalanine or tryptophan and a polyketide derived from acetate and methionine. Cytochalasins possess a range of distinctive biological properties. These include inhibition of cytoplasmic cleavage leading to polynucleate cells, nuclear extrusion and the inhibition of cell mobility.

Some members of this important class of metabolites have been obtained from marine ascomycetes. It can be anticipated that other members of the series will be found in marine fungal cultures in future.

9.1.16 Indolizidine alkaloids (VX1360)

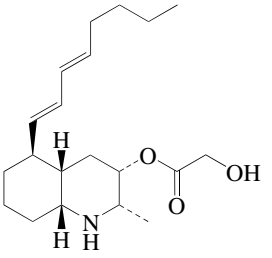
A few simple indolizidines (e.g. the **Stelletamides**) have been isolated from sponges. Indolizidines of a different structural type are commoner in terrestrial animals, esp. as frog toxins.

Michael, J.P., *Nat. Prod. Rep*., 2004, **21**, 625–649; 2005, **22**, 603–626 (*revs*)

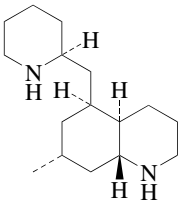
9.1.17 Quinoline alkaloids (VX1480, VX1580)

The majority of these are from higher plants, but a variety of simple heteroaromatic quinolines (VX1480) have been isolated from various marine sources including **2-Heptyl-4-hydroxyquinoline** from a marine pseudomonad, and **4,8-Quinolinediol** from cephalopod ink. There are also more elaborated hydrogenated quinolines (VX1580), especially the **Lepadins** from tunicates and flatworms. Bryozoans contain a number of simple quinolinequinone pigments and there are also the **Trididemnic acids** from ascidians. **Halitulin** from a sponge has been the subject of a recent major collaborative synthesis effort.

Quinoline alkaloids occur across a wide range of organisms and there are some structural similarities between marine octahydroquinolines such as **Lepadin A** and terrestrial alkaloids such as Phlegmarine from *Lycopodium* spp.



Lepadin A

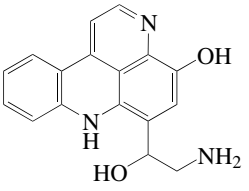


Phlegmarine
(terrestrial)

Michael, J.P., *Nat. Prod. Rep*., 2004, **21**, 650–668; 2005, **22**, 627–646 (*revs*)

9.1.18 Pyrido[2,3,4-*kl*]acridines (VX1700)

This is a group of exclusively marine alkaloids which includes the **Kuanoniamines**, the **Ascididemins**, the **Cystodytins**, the **Styelsamines**, the **Varamines** and others. The isolation of some of them from a variety of organisms argues for a microbial origin, but it could alternatively be a case of convergent evolution. They are biosynthesised from common amino acids.



Styelsamine A

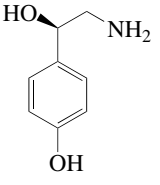
Ding, Q. *et al, Curr. Med. Chem*., 1999, **6**, 1–28 (*rev*)
Salomon, C.E. *et al, Mar. Biol*., 2001, **139**, 313–319 (*biosynth*)
Moore, B.S., *Nat. Prod. Rep*., 2006, **23**, 615–629 (*rev*)

9.1.19 Benzodiazepine alkaloids (VX1760)

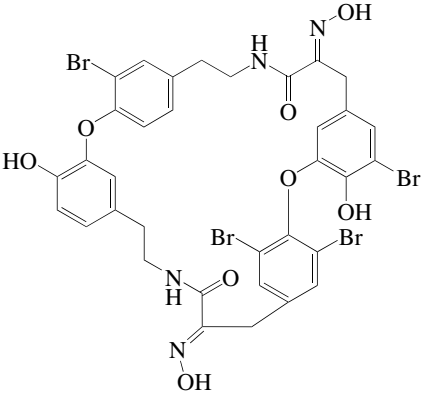
These are rare and among non-microbial products are currently limited to **Aplysepine** and **Diazepinomicin**. They are clearly derived from anthranilic acid and phenylalanine.

9.1.20 Phenethylamine alkaloids (VX2000–VX2015)

The simplest derivatives of phenylalanine or tyrosine are the β-phenylethylamines resulting from decarboxylation and obvious oxidation/alkylation, which are widespread among marine natural products. Compounds showing side-chain hydroxylation (VX2005), common among higher plants, are rare (e.g. **Octopamine**, which is an endometabolic neurotransmitter of molluscs); the majority of marine representatives are brominated compounds (VX2008) such as the **Purpuramines** and the **Bastadins** (including macrocyclic oligomers), produced by Verongid sponges. These are biosynthesised from the simple brominated tyrosines.



Octopamine



Bastadin 9

Bentley, K.W., *Nat. Prod. Rep*., 2004, **21**, 395–424; 2005, **22**, 249–268; 2006, **23**, 444–463 (*revs*)

9.1.21 Cinnamic acid amides (VX2020)

Simple cinnamate residues are scarcer among marine alkaloids than among terrestrial plant products. Examples are found for example in the **Tunichromes**, for which phenylalanine can function as a biosynthetic precursor.

Taylor, S.W. *et al, Chem. Rev*., 1997, **97**, 333–346 (*rev, tunichromes*)

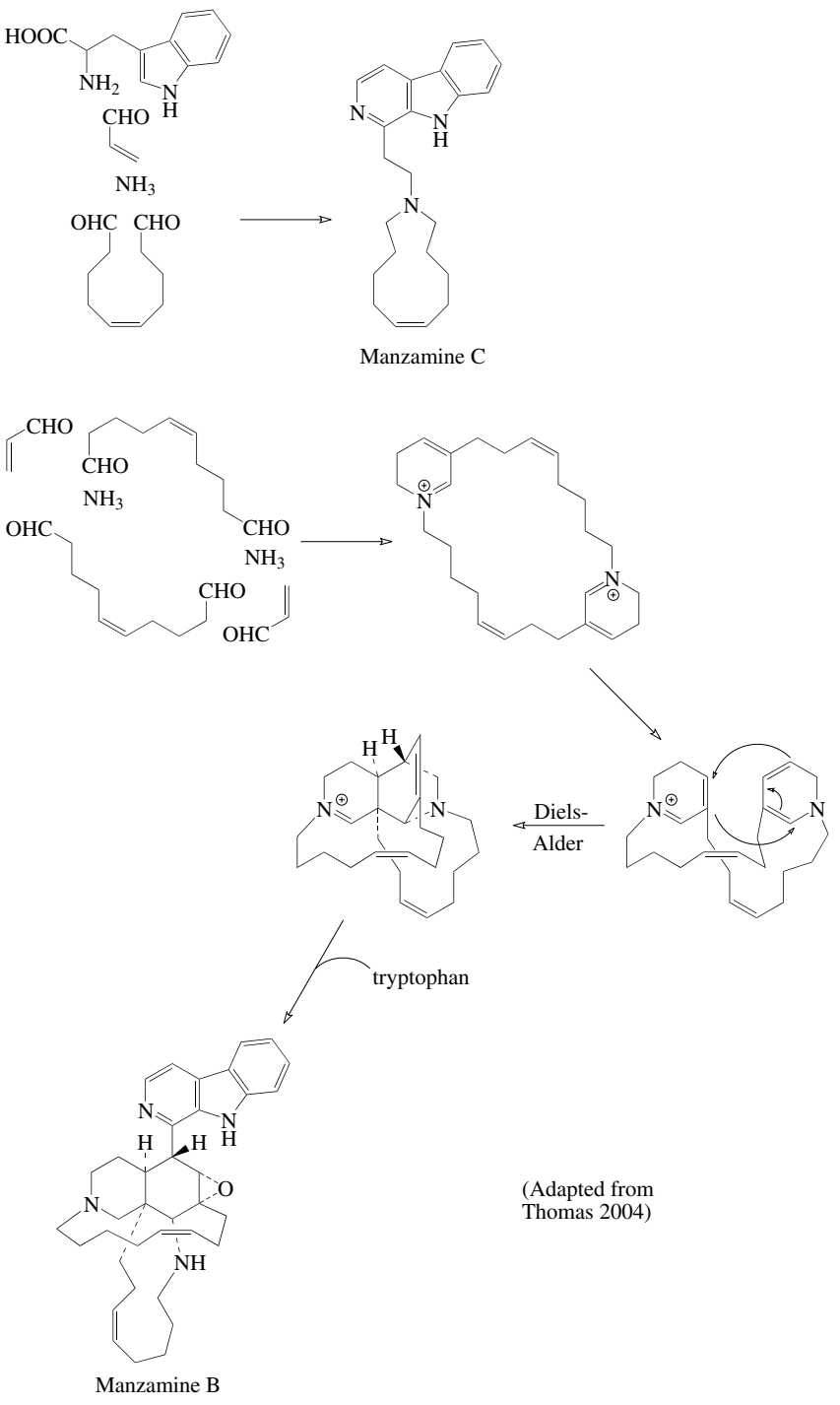
9.1.22 Simple isoquinoline alkaloids (VX2200)

These too are less widespread than in terrestrial sources, and isolated examples are restricted to some bases related to **Reneirol** and the **Cribrostatins**. However the isolation of one or two marine benzylisoquinoline alkaloids (VX2320) (**Imbricatine**; **Theoneberine**) is noteworthy.

Baker, B.J., *Alkaloid: Chemical and Biological Perspectives*, (ed. Pelletier, S.W.), Elsevier, Amsterdam, 1996, **10**, 357 (*rev, marine isoquinolines*)
Bentley, K.W., *Nat. Prod. Rep*., 2004, **21**, 395–424: 2005, **22**, 249–268; 2006, **23**, 444–463 (*revs*)

9.1.23 Manzamine alkaloids (VX2250)

This fairly extensive group is exclusively marine and represents the most structurally complex and characteristic type of marine alkaloid for which a biosynthetic scheme has been proposed. Their biosynthesis has been postulated to involve the condensation of tryptamine with one or more C_3 units and one or more straight-chain C_{10} dialdehyde equivalents, followed by an enzyme-assisted Diels-Alder cyclisation. The origin of the C_3 and C_{10} units is uncertain but it has been suggested that they could arise by oxidative fission of a hydroxylated fatty acid.



Manzamine C

Manzamine B

(Adapted from Thomas 2004)

Tsuda, M. *et al, Heterocycles*, 1997, **46**, 765–794 (*rev*)
Baldwin, J. *et al*, *Chem. Eur. J.*, 1999, **5**, 3154–3161 (*biosynth*)
Thomas, R., *Nat. Prod. Rep.*, 2004, **21**, 224–248 (*rev, biosynth*)

9.1.24 Indole alkaloids (VX4000-VX5950)

Indole alkaloids are numerous in marine organisms but the range of structural types differs from those found in terrestrial counterparts, and many of the 'traditional' indole alkaloid types produced by land plants have not been found. Halogenation is common.

Pindur, U. *et al, Curr. Med. Chem.*, 2001, **8**, 1681–1698 (*rev*)

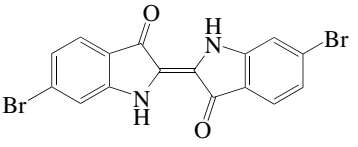
9.1.25 Simple indole alkaloids (VX4000)

Under this heading appear various halogenated indoles together with some higher MW alkaloids containing unsubstituted indole ring systems, such as **Aplysinopsin** and its relatives (which are also imidazoles).

Somei, M. *et al, Nat. Prod. Rep*., 2004, **21**, 278–311; Kawasaki, T. *et al*, *ibid*, 2005, **22**, 761–793 (*revs*)

9.1.26 Simple biindoles (VX4020)

This category includes **Indirubin**, **6,6′-Dibromoindigotin** and other biindoles, mostly polybrominated.

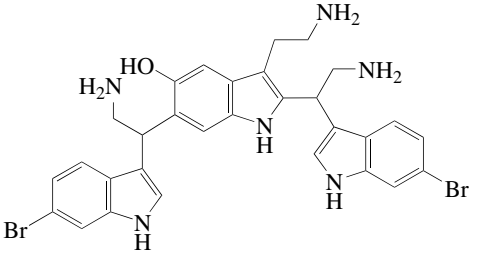


6,6'-Dibromoindigotin

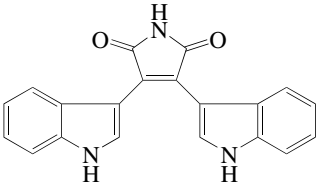
Yang, C.-G. *et al, Curr. Org. Chem*., 2004, **8**, 1691–1720 (rev, bisindole alkaloids from sponges)

9.1.27 Simple tryptamines (VX4040, VX4140, VX4160)

Tryptamine itself and some simple relatives have been isolated from marine tissues, and it noteworthy that **Bufotenine**, long known as an amphibian product, has more recently been detected in a gorgonian. More highly elaborated marine alkaloids containing a (dehydro)tryptamine residue include the **Kottamides**. There are also some simple tryptamine dimers (VX4140) and oligomers (VX4160) such as the **Gelliusines**. The bisindolylmaleimides such as the **Arcyriarubins** listed here are closely related to the indolo[2,3-*a*]carbazoles (VX4350) below.



Gelliusines A-B



Arcyriarubin A

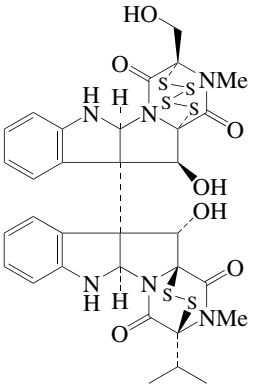
Somei, M. *et al*, *Nat. Prod. Rep*., 2004, **21**, 278–311; Kawasaki, T. *et al*, *ibid*, 2005, **22**, 761–793 (*revs*)

9.1.28 Physostigmine-like alkaloids (VX4100)

Physostigmine itself was originally isolated from a land plant, and has also been isolated from microorganisms. Alkaloids sharing the physostigmine (hexahydropyrrolo[2,3-*b*]indole) nucleus such as the **Flustramines** have however been isolated from marine animals, as well as from land animals, especially amphibians.

9.1.29 Chaetocin-like alkaloids (VX4110)

Also called Epipolythiodioxopiperazines, although some members of the series lack the polysulfur bridge. These are microbial products, but a considerable number, including Chaetocin itself and the extensive series of **Leptosins**, have been isolated from marine sources. They are thought to be biosynthesised from diketopiperazines (VV0150).

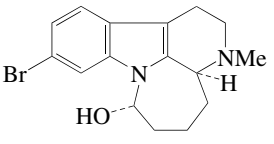


Leptosin A

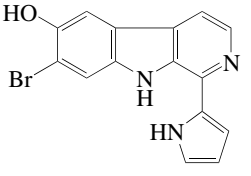
Somei, M. *et al, Nat. Prod. Rep*., 2004, **21**, 278–311; Kawasaki, T. *et al*, *ibid*, 2005, **22**, 761–793 (*revs*)
Gardiner, D.M. *et al*, *Microbiology*, 2005, **151**, 1021–1032 (*biosynth*)

9.1.30 β-Carboline alkaloids (VX4240)

Long known as terrestrial alkaloids, these are also widespread in marine organisms. β-Carboline (Norharman) itself has been found in an ascidian and in dinoflagellates, and examples of simple brominated analogues include the **Eudistomins** and some of the **Arborescidines**. Another group of β-carboline derivatives, presumably derived from tryptophan and cysteine, have been isolated from *Eudistoma olivaceum*, a Caribbean tunicate. The β-carboline nucleus is also found in some of the **Manzamines** and other more complex alkaloids.



Arborescidine C

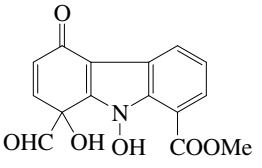


Eudistomin A

Baker, B.J., *Alkaloids: Chemical and Biological Perspective*, (ed. Pelletier, S.W.), Elsevier, Amsterdam, 1996, **Vol. 10**, 357 (*rev, marine β-carbolines*)
Somei, M. *et al, Nat. Prod. Rep*., 2004, **21**, 278–311; Kawasaki, T. *et al*, *ibid*, 2005, **22**, 761–793 (*revs*)
Fresneda, P.M. *et al*, *Synlett*, 2004, 1–17 (*rev, synth*)

9.1.31 Carbazole alkaloids (VX4300)

A few simple halogenated carbazoles have been isolated such as **3,6-dibromo-** and **3,6-diiodocarbazoles**. **Coproverdine** exemplifies a small number of unhalogenated carbazoles so far isolated.

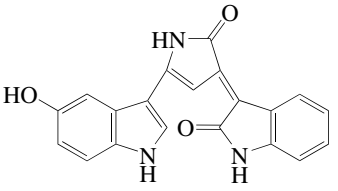


Coproverdine

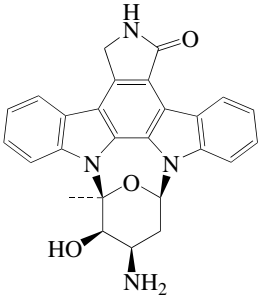
Knölker, H.-J. *et al, Chem. Rev*., 2002, **102**, 4303–4428 (*rev*)
Somei, M. *et al, Nat. Prod. Rep*., 2004, **21**, 278–311; Kawasaki, T. *et al*, *ibid*, 2005, **22**, 761–793 (*revs*)
Knölker, H.-J., *Curr. Org. Synth*, 2004, **1**, 309–331 (*rev, synth*)

9.1.32 Indolo[2,3-*a*]carbazole alkaloids (VX4350)

These are a class of alkaloids exemplified by **Staurosporine**, which was first isolated in 1977 from a terrestrial microorganism but which has since been found to be widely distributed. They are essentially microbial metabolites from a variety of organisms (field-collected or cultured), and show a wide range of biological activities. The isolation of **4′-*N*,*O*-Didemethylstaurosporine** from a flatworm *Pseudoceros* sp. is noteworthy. Their biosynthesis has been intensively studied; they are produced from diindolyl precursors resembling **Violacein**; the indolyl residues are derived from tryptophan *via* 7-chlorotryptophan followed by an oxidative ring closure.



Violacein

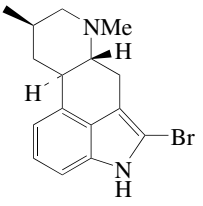


4'-*N*,*O*-Didemethylstaurosporine

Sánchez, C. *et al, Nat. Prod. Rep*., 2006, **23**, 1007–1045 (*rev, biosynth*)
Walsh, C.T. *et al, Nat. Prod. Rep*., 2006, **23**, 517–531 (*rev, biosynth*)

9.1.33 Ergot alkaloids (VX4460)

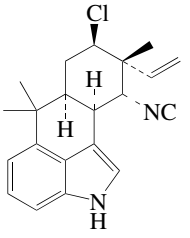
These have been considered exclusively the metabolites of terrestrial fungi and microorganisms, but the recent isolation of the **Pibocines**, simple brominated analogues of Festuclavine, from *Eudistoma* ascidians, have provided a first marine occurrence. In terrestrial fungi these bases are derived from 4-prenyltryptophan by cyclisation. The presence of the bromine substituent in the Pibocines argues for their being genuine ascidian products, and this is presumably a case of biochemical parallelism.



Pibocine A

9.1.34 Hapalindoles (VX5950)

The extensive series of hapalindoles, from *Hapalosiphon* and other cyanophytes, have mostly been characterised from freshwater species but are included in the Dictionary for completeness. They are mostly based on the naphth[1,2,3-*cd*]indole skeleton as shown by **Hapalindole A**.

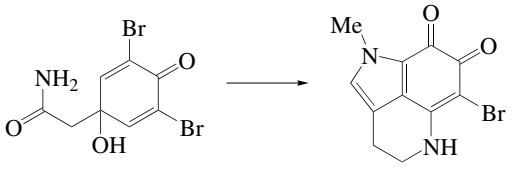


Hapalindole A

Somei, M. *et al, Nat. Prod. Rep*., 2004, **21**, 278–311; Kawasaki, T. *et al*, *ibid*, 2005, **22**, 761–793 (*revs*)

9.1.35 Pyrrolo[4,3,2-*de*]quinoline alkaloids (VX6070)

This skeleton is characteristic of and almost exclusive to marine (sponge) alkaloids. Major subgroups include the simple **Batzellines**, **Makaluvamines** and **Damirones**, and those in which the pyrroloquinoline nucleus forms part of a larger skeleton such as in the **Discorhabdins** and the closely related **Epinardines**. They are thought to be biosynthesised from tyrosine via **3,5-Dibromoverongiaquinol**.



3,5-Dibromoverongiaquinol Makaluvone

Ding, Q. *et al, Curr. Med. Chem*., 1999, **6**, 1–28 (*rev*)

9.1.36 Miscellaneous indole alkaloids (VX6100)

Under this heading are listed a large number of miscellaneous types of marine indole alkaloids for which a classification remains premature, either because they currently belong to a very limited subtype, and/or because there has been no work on their biosynthesis. Many of them probably represent minor branches on the biosynthetic pathways to the larger groups; for example the **Rhopaladins** are probably biosynthetically close to the indolo[2,3-*a*]carbazole alkaloids (VX4350), but this is not yet established experimentally. **Granulatimide** may represent a lower benzologue of these alkaloids incorporating a histamine residue in place of one tryptamine.

Somei, M. *et al, Nat. Prod. Rep*., 2004, **21**, 278–311; Kawasaki, T. *et al*, *ibid*, 2005, **22**, 761–793 (*revs*)

9.1.37 Sesquiterpene alkaloids (VX6300)

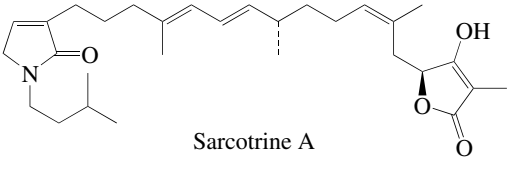
A variety of sesquiterpene alkaloids have been isolated which are nearly all relatively simple amine or amide derivatives of well-known sesquiterpenoid skeletons. These may be acyclic (e.g. **Axinyssimides**), monocyclic (**Siphonodictidine**) or bicyclic (**Nakijiquinones**). The relevant alkaloids are also coded with to the appropriate sesquiterpene (VS) code.

9.1.38 Miscellaneous diterpene alkaloids (VX6480)

There are few reported diterpenoid alkaloids (as opposed to nonalkaloidal diterpenes) reported from marine species. The **Agelasines**, **Agelasimines** and related compounds are a series of guanidinoid- or purinoid-substituted simple acyclic, mono- or bi-cyclic terpenoids, and there are one or two simple amino-substituted cembranoids.

9.1.39 Sesterterpene alkaloids (VX6490)

The number of nitrogen-containing sesterterpenoids so far isolated is relatively low by comparison with the number of nitrogen-free tetracyclic sesterterpenes known. The **Spongidines** and the **Molliorins**, in which a ring-E pyridine or pyrrole ring, respectively, is fused to one of the common tetracyclic skeletons, are the main types. There are also linear pyrrolic compounds including the **Sarcotrines** and **Sarcotragins** which are considered to have a common biosynthetic origin, the latter being degraded norsesterterpenoids.

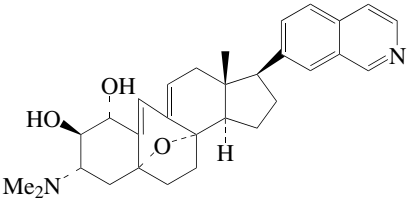


Sarcotrine A

Liu, Y. *et al, Nat. Prod. Rep*., 2006, **23**, 630–651 (*rev*)

9.1.40 Steroidal alkaloids (Buxus type) (VX6760)

Few steroidal alkaloids (as opposed to nitrogen-free steroids) have been isolated from marine organisms. The recent characterisation of the **Cortistatin** alkaloids from a *Corticium* sponge, represent a new development in marine natural products. Structurally their 9(10 →19)-abeosteroid moiety resembles that of one subgroup of the terrestrial *Buxus* alkaloids, but the presence of an isoquinoline ring system at the other end of the molecule is without precedent among terrestrial alkaloids



Cortistatin A

9.1.41 Miscellaneous steroidal alkaloids (VX6790)

This heading covers a small number of marine steroidal alkaloids of novel type such as the **Plakinamines**.

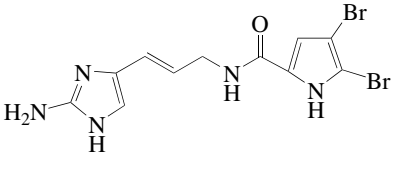
9.1.42 Pyrazole alkaloids (VX6900)

Pyrazole alkaloids are rare in general and there is only one marine example, **1-Methyl-1*H*-pyrazole-5-carboxylic acid**, from a gorgonian.

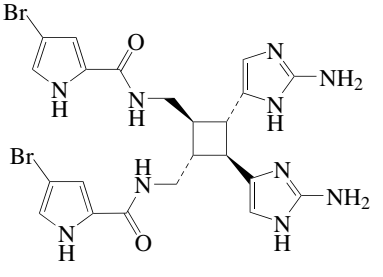
9.1.43 Imidazole alkaloids (VX6920)

This group, obviously derived from histidine, contains many structurally diverse marine examples, for example **Aplysinopsin** and related alkaloids, **Odiline** and the **Rhopaladins**. They show a range of biological activities and considerable pharmaceutical potential.

One of the most important subtypes is the pyrrole-imidazole alkaloids exemplified by **Oroidine** which with various relatives (e.g. the dimeric **Sceptrine**) appears to be a genuine sponge product. A recent biogenetically-based classification (see Hoffmann) recognises a class of nearly 100 pyrrole-imidazole alkaloids arising in various ways from this key intermediate and containing 0-4 further rings, additional to the pyrrole and imidazole rings already present. Future organisation of this database may recognise this category; at present, many of them are placed in the miscellaneous categories VX9000–VX9400.



Oroidine

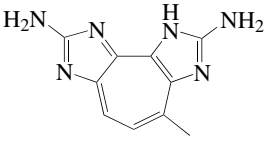


Sceptrine

Hoffmann, H. *et al, Synthesis*, 2003, 1753–1783 (*pyrrole-imidazole alkaloids*)
Jin, Z. *et al, Nat. Prod. Rep.*, 2005, **22**, 196–229; 2006, **23**, 464–496 (*revs*)

9.1.44 Cycloheptadiimidazoles (Zoanthoxanthins) (VX6925)

These are a group of marine alkaloids which are condensed imidazoles closely related in structure, and which in this Dictionary are grouped under just two entries; those for **Pseudozoanthoxanthin A** and **Parazoanthoxanthin A**. Their biosynthesis does not appear to have been studied in detail but they are condensed imidazoles presumably derived from histidine.



Pseudozoanthoxanthin A
(one tautomer)

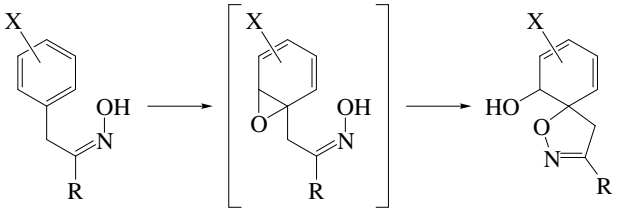
9.1.45 Oxazole and benzoxazole alkaloids (VX6930)

Numerous naturally occurring oxazoles are currently known, isolated from various marine (and terrestrial) sources – nudibranch egg masses (**Ulapualides**), algae and microorganisms. The marine and bacterial oxazoles appear to have been formed from peptides of aliphatic amino acids. Structurally they are diverse and may be open-chain (e.g. **Bengazoles**) or macrocyclic (e.g. **Patellamides**). Like the imidazoles, they show considerable drug potential.

Pattenden, G., *J. Heterocycl. Chem*., 1992, **29**, 607–618 (*rev, synth*)
Yeh, V.S.C., *Tetrahedron*, 2004, **60**, 11995–12042 (*rev, synth*)
Jin, Z. *et al, Nat. Prod. Rep*., 2005, **22**, 196–229; 2006, **23**, 464–496 (*revs*)

9.1.46 Spirobenzoxazoline alkaloids (VX6934)

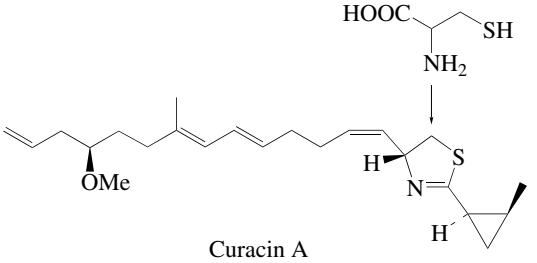
These exclusively marine alkaloids such as the **Psammaplysins** are derived by cyclisation of open-chain halogenated tyrosinoid oxime precursors (see VX2008 above). This is probably via the intermediary of an arene oxide, although attempts to replicate this chemically have given only low yields.



Okamoto, K.T. *et al*, *Tetrahedron Lett*., 1987, **28**, 4969–4972 (*biosynth*)

9.1.47 Thiazole alkaloids (VX6935, VX6937)

More than 100 naturally occurring compounds that incorporate the thiazole ring system have been isolated to date from marine organisms. These alkaloids are a heterogeneous group ranging in complexity from small molecules such as **Herbamide A** (isolated from a sponge) to open-chain or macrocyclic compounds such as the **Lyngbyapeptins**, **Dysidenin** and its relatives. These appear to be essentially microbial products, from cyanobacteria or other microorganisms, although some such as the **Patellamides** were actually isolated from tunicates. The **Latrunculins** (VX6936) are a subclass of mostly macrocyclic tetrahydrothiazoles isolated from sponges. Marine thiazoles show a range of interesting drug activities. The biosynthesis of the thiazole ring in the highly bioactive **Curacin A** has been shown to be from cysteine, with the rest of the carbon chain including the cyclopropane functionality acetate-derived.

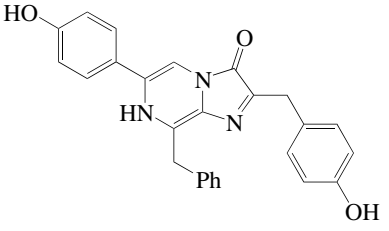


Curacin A

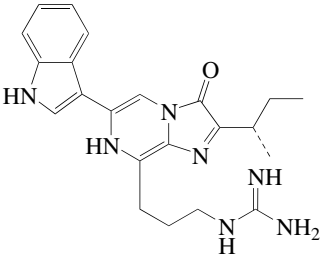
Pattenden, G., *J. Heterocycl. Chem*., 1992, **29**, 607–618 (*rev, synth*)
Jin, Z. *et al*, *Nat. Prod. Rep*., 2005, **22**, 196–229; 2006, **23**, 464–496 (*revs*)

9.1.48 Pyrazine and quinoxaline alkaloids (VX6940)

Pyrazines have been isolated from widely differing biological sources including marine organisms, where some of them are the actual light emitters in bioluminescence processes. Bioluminescence emitters are found scattered throughout different types of organism, which implies multiple independent origins during the course of evolution. The imidazopyrazine **Coelenterazine** and closely related compounds though account for the great majority of observed bioluminescence. There is evidence for Coelenterazine's *de novo* biosynthesis in shrimps. ***Cypridina* Luciferin** is biosynthesised from arginine and tryptophan.



Coelenterazine



Cypridina Luciferin

Rees, J.F. *et al, J. Exp. Biol*., 1998, **201**, 1211–1221 (*rev, bioluminescence*)

9.1.49 Morpholines (VX6955)

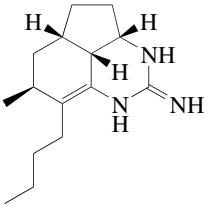
These are relatively few in number, e.g. **Chelonins A**, **B** and **C** and the **Oxazinines**.

9.1.50 Pyrimidines (VX6960)

Simple thymine-derived bases such as **Thyminol** are found in marine organisms together with some more highly elaborated substances such as the **Meridianins**.

9.1.51 Ptilocaulins (VX6970)

This group is based on the (partially hydrogenated) cyclopenta[*de*]quinazoline skeleton, which contains a pyrimidine nucleus. It comprises **Ptilocaulin** and relatives, the **Mirabilins** and a few other related alkaloids, mostly isolated from sponges, but which may be symbiont metabolites. It has been suggested that these arise by a late-stage addition of guanidine to a polyketide precursor.

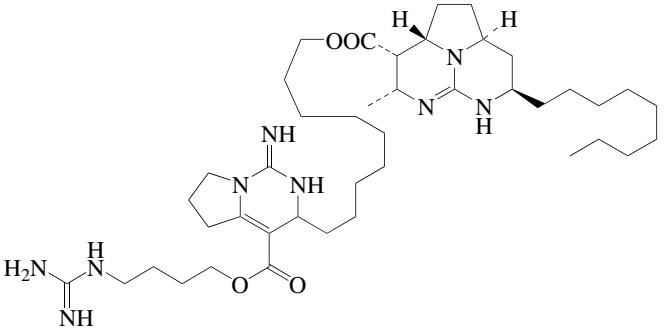


Ptilocaulin

Snider, B.B. *et al, J. Org. Chem*., 1993, **58**, 3828–3839 (*biosynth*)

9.1.52 Triazaacenaphthylene alkaloids (VX6980)

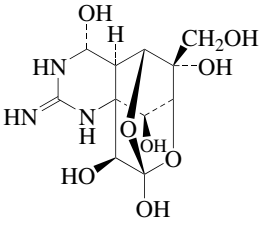
These are another group based on a tricyclic pyrimidine-related nucleus, and include the **Batzelladines** and the **Crambescidins** from sponges and echinoderms. Their biosynthesis does not appear to have been studied in detail, but they are formally composed of a guanidine unit, with which the biological activity is associated, embedded in a linear unbranched perimeter, presumably derived from a lipid precursor.



Batzelladine A

9.1.53 **Tetrodotoxins** (VX6990)

Tetrodotoxin and its homologues are well-known and important causes of human poisoning and are known principally from certain tissues of the Japanese puffer fish, but also found in other organisms and are thought to be *Pseudomonas* products. They have been extensively reviewed. The carbocycle ring in tetrodotoxins may be of isoprenoid origin.



Tetrodotoxin

Miyazawa, K. *et al, Toxin Rev*., 2001, **20**, 11–33 (*rev*)
Yotsu-Yamashita, M., *Toxin Rev*., 2001, **20**, 51–66 (*rev*)
Daly, J.W., *J. Nat. Prod*., 2004, **67**, 1211–1215 (*rev, occur*)

9.1.54 **Phenazine and phenoxazine alkaloids** (VX7000, VX7005)

A limited number of simple phenazines and phenoxazines have been reported from microorganisms, some of them from marine sources.

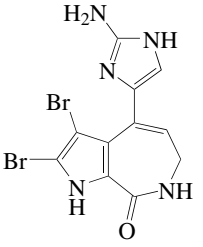
9.1.55 **Pyrrole alkaloids** (VX7010)

The pyrrole alkaloids are a heterogeneous group ranging in complexity from the very simple brominated pyrroles (e.g. **2,3-Dibromo-1*H*-pyrrole**) and peptides to the lipophilic **Malyngamides**, porphyrins and other tetrapyrrole pigments (see following section). Compounds that incorporate the pyrrole nucleus have been isolated from a variety of marine sources (sponges, microorganisms and algae). Further examples are the dimeric **Tambjamines** and a range of alkaloids in which halogenated pyrrole residues are linked to indolic and other heterocyclic nuclei, e.g. **Ageliferin** and its relatives. The pyrrole nucleus is of course a component of the indole alkaloids, but whereas these are tryptophan-derived, the polypyrroles are biosynthesised from 5-Amino-4-oxopentanoic acid (5-aminolaevulinic acid, ALA). Lower-MW alkaloids may arise from either route, or from proline/ornithine pathways via pyrrolidines (see above under VX0300); in the **Prodigiosins**, each of the three pyrrole residues is biosynthesised differently. The process of biohalogenation differs between Cl and Br. Chlorination takes place oxidatively by a combination of chloride ion, dioxygen and reduced FAD producing a Cl^+ equivalent, whilst bromination is mediated by vanadium bromoperoxidases.

Hoffmann, H. *et al, Synthesis*, 2003, 1753–1783 (*pyrrole-imidazole alkaloids*)
Walsh, C.T. *et al, Nat. Prod. Rep*., 2006, **23**, 517–531 (*rev, biosynth*)

9.1.56 Pyrroloazepines (VX7015)

These form a numerically limited but well-defined group consisting of **Hymenialdisine**, **Odiline** and related alkaloids, all with an additional imidazole ring system attached to a pyrrolo[2,3-*c*]azepine residue. Odiline (Stevensine) has been postulated to arise by cyclisation of the open-chain pyrrolic precursor Oroidine (see above).



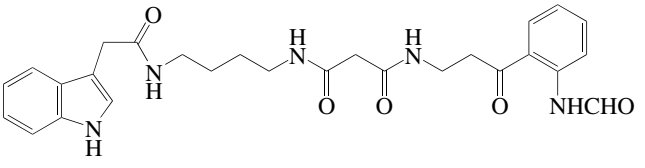
Odiline

Walsh, C.T. *et al*, *Nat. Prod. Rep*., 2006, **23**, 517–531 (*rev, biosynth*)

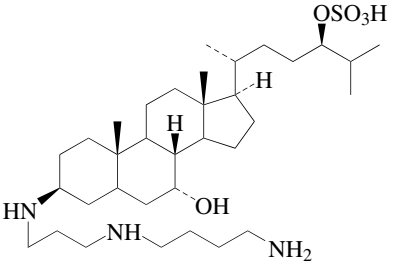
9.1.57 Polyamine alkaloids (VX7020, VX7030, VX7040, VX7050, VX7060, VX7070)

These categories cover the various types of alkaloid containing one or more -N$(CH_2)_n$N- groups, with *n* usually 3 or 4, less often 2 or 5. They show markedly different properties (reactivity, basicity, complexing ability, mass spectrometry) from monobasic amines. Alkaloids based on the ornithine-derived putrescine (*n*=4, classified as PA 4 alkaloids) are common in terrestrial plants but only a few have so far been characterised from marine organisms, such as the **Monodontamides** from gastropods. A number of alkaloids are derived from **Spermine** (PA 343) or **Spermidine**, (PA 34) themselves derived (in plants, certainly) from ornithine *via* putrescine, but again, the number currently characterised is much lower than those known from terrestrial organisms. See for example the **Penaramides** and the unusual medium-ring azaaliphatic **Motuporamines**. Classes PA 33, PA 35, PA 44 and PA 33433 have also been found in nature, but less frequently. The largest number is arachnid toxins, not marine alkaloids. In terrestrial plants it is well established that these alkaloids derive from decarboxylation and coupling of amino acids such as ornithine.

PA structures also occur in more complex alkaloids such as **Crambescidin 816** (PA 34 substructure) and as steroidal conjugates, in **Squalamine** and related compounds from fish livers (PA 34 and PA 343 substructures).



Monodontamide D



Squalamine

Bienz, S. *et al*, *Alkaloids* (N.Y.), 2002, **58**, 83–338 (*rev*)
Bienz, S., *Nat. Prod. Rep*., 2005, **22**, 647–658 (*rev*)

9.1.58 Peptide alkaloids (VX7100)

Several hundred peptide alkaloids are known, many macrocyclic, which by definition are composed of a number of amino acids, among which phenylalanine or tyrosine is frequently found. The boundaries between compounds classified under this heading and those classified under peptides (VV) or macrolide polyketides (VC) are vague and subjective, and these categories should also be scanned when browsing. They occur in both terrestrial and marine organisms, but most peptide alkaloids isolated from higher plants form a relatively homogenous group based on a medium-sized ring incorporating an *ansa*- aromatic ring. The marine peptide alkaloids are much more heterogenous, incorporating unusual, often halogenated, amino acid residues (e.g. the **Dysidenins**, **Geodiamolides**) and/or thiazole and oxazole rings, either open-chain or macrocyclic (**Dolastatins**, **Bistratamides**, **Lissoclinamides**, etc). The **Patellamides** are widely distributed in the tissues and are suspected to be of cyanobacterial origin, but this is by no means established. Peptides play an important role in invertebrate defence mechanisms.

Tincu, J.A. *et al, Antimicr. Agents Chemother*., 2004, **48**, 3645–3654 (*rev, biochem*)
Aneiros, A. *et al, J. Chromatog., B*., 2004, **803**, 41–53 (*rev, isol, pharmacol*)

9.1.59 Pyrrolo[2,3-*d*]pyrimidines (VX7200)

This is a numerically limited group consisting of the nucleosides **Tubercidin**, **Mycalisine B** and related bases and some simple halogenated pyrrolopyrimidines as well as the **Rigidins**. These appear to be microbial products. It has been shown that the pyrimidine ring is derived intact from a purine base precursor which undergoes ring opening and reformation with the incorporation of a C_2 fragment to form the pyrrole ring.

9.1.60 Purines (VX7300)

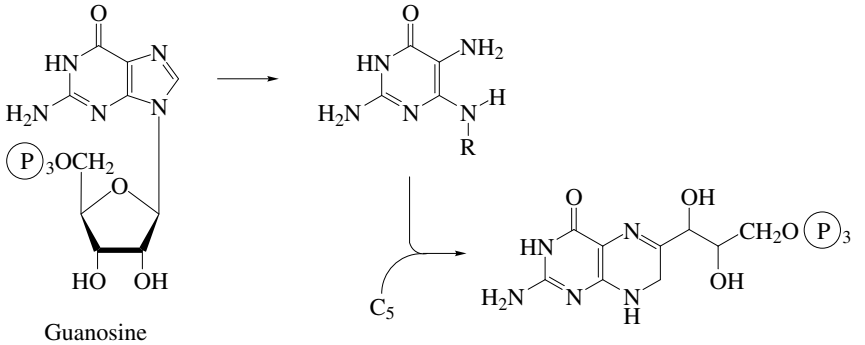
Purines are involved along with pyrimidines as bases in DNA and RNA. The well-known purine bases **Xanthine**, **Inosine**, **Theobromine** and **Theophylline** have been found in marine organisms along with substituted purines (e.g. **Phidolopin**) and terpenoid-purine alkaloid bases (**Agelines** and others).

Rosemeyer, H., *Chem. Biodiversity*, 2004, **1**, 361–401 (*rev*)

9.1.61 Pteridines and analogues (VX7350)

Pteridines are a widely distributed class of naturally occurring compounds. They owe their exceptional position in the field of heterocyclic chemistry mainly to their unusual chemical properties, their conspicuous fluorescence and their importance in metabolism. Pteridine bases were characterised as pigments originally from butterfly wings, but more recently from fish and other marine organisms (see **Isoxanthopterin**). Marine pteridines are also represented by **Leucettidine** and **Urochordamines**, and the pteridine nucleus is also present in the **Pseudoanchynazines**.

The biosynthesis of pteridines pigments has been well studied in terrestrial organisms; as in the case of the pyrrolopyrimidines above, the imidazole ring is derived unchanged from a purine precursor, in this case guanosine triphosphate, and the pyrazine ring is built by ring fission and incorporation of two carbons derived from a ribose fragment. The biosynthesis in marine organisms need not necessarily be the same.

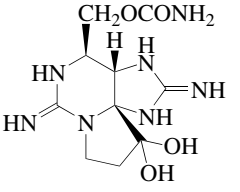


Guanosine triphosphate

Pfleiderer, W., *J. Heterocycl. Chem*., 1992, **29**, 583–605 (*rev*)

9.1.62 **Saxitoxins** (VX7400)

The saxitoxins are a group of over 30 highly important modified purinoid toxins known as Paralytic Shellfish Toxins or PSTs. Originally characterised as a cause of dangerous shellfish poisoning, they are now known definitely to be biosynthesised only by dinoflagellates (and some freshwater cyanobacteria), although it is possible that the red alga *Jania* does so also. Their presence in shellfish tissues probably results by diffusion according to a yet unknown mechanism. Their exact biosynthesis is not yet known but it appears from radiolabelling experiments that the two guanidine groups derive from arginine and the carbamoyl side-chain from methionine.



Saxitoxin

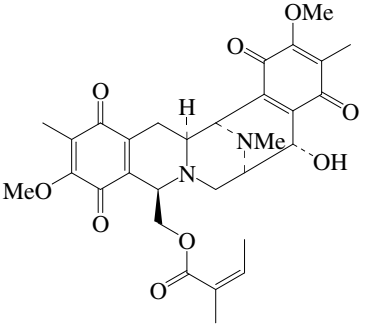
Garson, M.J., *Chem. Rev*., 1993, **93**, 1699–1733 (*rev, biosynth*)
Llewellyn, L.E., *Nat. Prod. Rep*., 2006, **23**, 200–222 (*rev*)

9.1.63 **Naphthyridinomycins** (VX7700)

These are a class of microbial products. Only a handful, so far, have been isolated from marine bacteria.

9.1.64 **Saframycins** (VX7800)

These are representative of the group known as the tetrahydroisoquinoline antitumour antibiotics (also including among terrestrial products some having slightly different skeletons, such as Lemonomycin). The saframycins themselves are microbial products produced by *Streptomyces* spp. of terrestrial origin. Close analogues such as the **Renieramycins** and the **Ecteinascidins** were isolated from marine organisms (sponges or tunicates) and are all presumably microbial products. The skeleton (studied for Saframycin A) is derived from two tyrosine molecules and the methyl groups from methionine.



Renieramycin A

Mikami, Y. *et al*, *J. Biol. Chem*., 1985, **260**, 344–348 (*biosynth*)

9.1.65 **Miscellaneous alkaloids with 0-4+ rings** (VX9000, VX9100, VX9200, VX9300, VX9400)

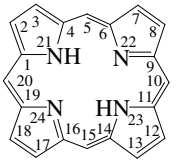
These categories are self-explanatory, and include some fairly well-defined structural groups where the small number of representatives currently known does not appear to justify the creation of individual categories at the present time.

10. POLYPYRROLES (VY)

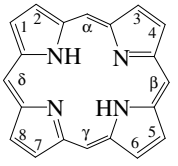
The polypyrroles (tetrapyrroles) are a numerically limited class of natural products that are mostly strictly functional. The main examples are haems, chlorophylls, bilins and Vitamin B_{12}. Only a few polypyrroles included under the miscellaneous category (VY0945) can be considered truly characteristic of marine organisms - the

chlorophylls for example are found in all types of photosynthetic organism, although there are important differences between the chlorophylls present in different phyla of marine plants. For a full description of the different polypyrrole types and their nomenclature and numbering, refer to the *Dictionary of Natural Products on DVD*. All types of organism use tetrapyrroles of one or more of these classes and all the functional tetrapyrroles derive from one common tetrapyrrolic intermediate, Uroporphyrinogen III (Uro'gen III). Uro'gen III is derived entirely from eight molecules of 5-Aminolaevulinic acid (ALA) by the action of three enzymes, *via* Porphobilinogen (PBG) and Hydroxymethylbilane (HMB) as intermediates. A particularly important feature in Uro'gen III is the fact that ring D has been inverted and so the acetate and propionate side-chains are not in the same order as on the other three pyrrolic rings, A to C. This feature can be found in virtually all naturally occurring tetrapyrroles.

The main system of nomenclature used in this Dictionary is that recommended by the IUPAC-IUB Joint Commission on Biochemical Nomenclature. For the cyclic tetrapyrroles this is based on the porphyrin with the carbon atoms numbered 1 to 20 and the nitrogen atoms numbered 21 to 24. This has superseded the older 'Fischer' numbering which numbered only the eight β-positions of the five-membered pyrrole rings and labelled the four bridging *meso*-carbons α, β, γ and δ.

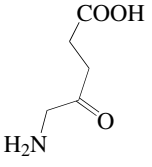


Porphyrin; IUPAC-IUB numbering

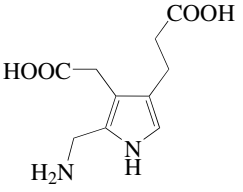


Porphyrin; Fischer numbering

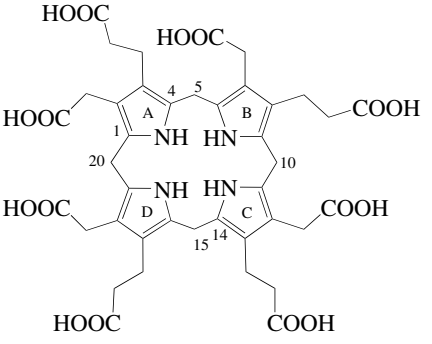
For natural porphyrins the IUPAC-IUB numbering starts on ring A and continues to rings B, C, and D, as shown below for Uro'gen III (ring D is always the inverted ring, see above). *Chemical Abstracts* on the other hand, though it uses the same 1 to 20 numbering for the carbon atoms, starts the numbering at such a position and in such a direction that the propionate side-chains get the lowest possible locants (thus for Uro'gen III the numbering would start at the position shown as 14 and proceed anticlockwise).



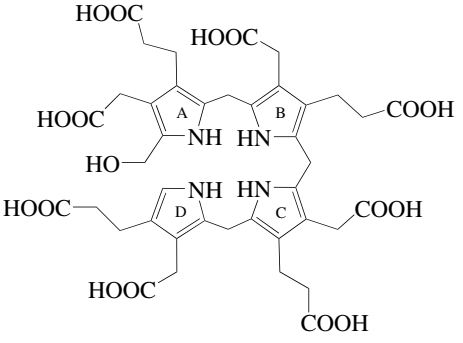
ALA



PBG



Uro'gen III



HMB

10.1.1 Porphyrins and porphyrinogens (VY0905)

The main biosynthetic pathway from Uro'gen III starts with the stepwise decarboxylation of each of the four acetate side-chains to give Coproporphyrinogen III, then oxidative decarboxylation of two of the propionate side-chains to give Protoporphyrinogen. These porphyrinogens and the partly decarboxylated intermediates are always isolated after aerial oxidation to give the corresponding porphyrin which is much more stable. Enzymic oxidation of Protoporphyrinogen gives **Protoporphyrin**, which is the branch point in the pathways to the haems and bilins and to the chlorophylls. Protoporphyrin has been isolated from the cnidarian *Atolla wyvillei*. Other porphyrins that can be found are mostly bacterial degradation products of Protoporphyrin with modification of the vinyl groups, e.g. **Haematoporphyrin**.

10.1.2 Bile pigments (bilins) (VY0915)

In animals the degradative pathway for haem is *via* an oxidative ring cleavage to give **Biliverdin** (Biliverdin IXα). This is then reduced to Bilirubin (10,23-dihydrobiliverdin) and excreted, as a bis-glucuronide ester, through the bile duct into the gut, where further reduction of double bonds by bacteria occurs. The same oxidative cleavage of haem can be affected non-enzymically by the coupled action of oxygen and a reducing agent such as ascorbic acid. In this reaction, cleavage can occur at any one of the four *meso* positions (*C*-5, 10, 15 and 20) and thus four isomeric Biliverdins (IXα, β, γ and δ) are produced.

In plants, the same oxidative cleavage of haem leads to the photoresponsive pigment Phytochromobilin and, in algae, to the light-harvesting pigments such as **Phycocyanobilin**. Both of these are found *in vivo* covalently attached to proteins by thioether links, and their presence or absence is an important taxonomic marker for different types of marine algae (see under the organism descriptions below).

10.1.3 Chlorophylls and derivatives (VY0920)

Insertion of Mg^{2+} is the start of the pathway that leads to the chlorophylls. A key intermediate in this pathway is **Protochlorophyllide**, in which the carbocyclic ring E, found in all chlorophylls and bacteriochlorophylls, has been formed in an oxidative cyclisation reaction. The chlorophyll c family, found in phytoplankton, have a porphyrin skeleton derived from Protochlorophyllide by insertion of a double bond into the propionate side-chain but the plant chlorophylls are all chlorins, having the *C*-17/18 double bond reduced in a photochemical, NADPH-dependent reduction of Protochlorophyllide giving **Chlorophyllide a**. Esterification with phytol gives **Chlorophyll a**.

10.1.4 Bacteriochlorophylls and derivatives (VY0925)

Photosynthetic bacteria rely on a slightly more diverse range of tetrapyrrole pigments. Purple photosynthetic bacteria contain **Bacteriochlorophyll a**, which is a bacteriochlorin, having two opposite pyrrole rings reduced. Green sulfur bacteria on the other hand contain Bacteriochlorophylls c, d and e, which are in fact chlorins, not bacteriochlorins, and are each a family of pigments with varying numbers of extra methyl groups introduced onto the *C*-8 and *C*-12 side-chains.

Bacteriochlorophylls also have a wider range of esterifying groups than do the chlorophylls. Thus, whereas Bacteriochlorophyll a usually has the normal phytyl ester, Bacteriochlorophylls c, d and e commonly have a farnesyl group. Geranylgeranyl and straight-chain hydrocarbon esters are also found in some organisms.

10.1.5 Miscellaneous polypyrroles (VY0945)

Although the majority of tetrapyrroles found in organisms are the ones described above, widely-distributed and having specific well understood catalytic functions, there are a few that are found in individual organisms and have more obscure or unusual functions. Some are present purely as pigments. Among the unusual functions are those of **Bonellin**, produced as a hormone by the females of the annelid worm *Bonella viridis* to determine the ender of the offspring. Other examples, such as **Corallistin A** from a sponge or **Chlorophyllone a** from various molluscs, do not have any recognised function.

Smith, K.M. (ed.), *Porphyrins and Metalloporphyrins*, Elsevier, Amsterdam, 1975
Dolphin, D. (ed.), *The Porphyrins*, Academic Press, New York, 1978–79, **Vols 1–7**
Leeper, F.J., *Nat. Prod. Rep.*, 1985, **2**, 19, 561–580; 1987 **4**, 441–469; 1989, **6**, 171–203 (*biosynth*)
Scheer, H. (ed.), *Chlorophylls*, CRC Press, Boca Raton, 1991

Jordan, P.M. (ed.), *Biosynthesis of Tetrapyrroles*, Elsevier, Amsterdam, 1991
The Biosynthesis of the Tetrapyrrole Pigments, Ciba Foundation Symposium, Wiley, Chichester, 1994, **180**
Battersby, A.R., *Nat. Prod. Rep*., 2000, **17**, 507–526 (*tetrapyrroles*, *rev*)
Montforts, F.-P. *et al, Progress in the Chemistry of Organic Natural Products*, (eds. Herz, W. *et al*.), SpringerWien, New York, 2002, **84**, 1–51 (*rev*)
Bandaranayake, W.M., *Nat. Prod. Rep*., 2006, **23**, 223–255 (*pigments rev*)
Walsh, C.T. *et al*, *Nat. Prod. Rep*., 2006, **23**, 517–531 (*biosynth*)

Classification of Organisms

1. GENERAL

This introduction gives only a very general overview of the different organism types. The natural products with names given in **heavy type** are only typical representatives of those found. This is particularly true of the prolific groups such as cyanobacteria and sponges, where this introduction can only give general pointers and should not attempt to displace the function of the main body of the Dictionary. To obtain a more comprehensive overview of the natural products present in particular types of organism, it is necessary either (a) to browse the entries given in the main section of the book, or (b) to search the CD-ROM version. This is most effectively done by using the **Type of Organism codes**, which are given in each section below (and above). These can be used alone or combined with other types of search parameter to restrict the result to certain broad classes of organism.

Many natural products pass up the food chain, and what may have been isolated for example from a sponge, may in fact be a cyanobacterial metabolite. This phenomenon reflects the large range of signalling roles (in the widest sense, to include defence chemical and anti-predator substances) that the marine environment involves, and the complexity of the alimentary chains which leads to frequent metabolic modification of molecules taken up from prey organisms.

Wherever possible, the Dictionary carries codes for both types of organism in the entry, but this cannot always be guaranteed. Other marine natural products such as the commoner steroids are just widespread, not necessarily as part of the food-chain.

Kornprobst, J.-M. (ed.), *Substances Naturelles d'Origine Marine*, Lavoisier, Paris, 2005

This recent two-volume work gives much background information on all aspects of marine natural products, including more detailed schemes for correlation of natural product type with taxonomic position of the organism. It was consulted extensively in preparing this introduction.

Tringali, C. (ed.), *Bioactive Compounds from Natural Sources*, Taylor & Francis, 2001

2. TAXONOMIC CONSIDERATIONS

The nineteenth century high-level classification of organisms into plant and animal kingdoms has been abandoned since about the 1960s with the development of cladistic analysis. Since then it has become increasingly clear that certain groups of organisms, some of them previously little studied, such as the cyanobacteria or cyanophytes (so-called blue-green algae; more closely related to bacteria), the chromista (including the brown algae) and the archaebacteria or archaea, show greater differences in both fundamental biochemistry and genetics from each other and from the so-called higher organisms, than higher plants and animals show from each other. Whittaker (1959) proposed that the most fundamental division should be between the prokaryotes and the eukaryotes, a classification that has now been generally accepted, but subsequently modified to include the discovery of the archaea in the 1970s.

Further studies of the genome might in principle lead to a classification scheme of all organisms that can be considered 'absolute', but many ecologists consider this view as essentially simplistic; for example, it does not take into account the possibility of convergent evolution in the genome. Evolutionary pressures are exerted through the phenotype, not the genotype.

Genus names in this Dictionary have, wherever possible, been validated using the *Species 2000/ITIS Catalogue of Life*, with which the Chapman & Hall/CRC chemical database has established a reciprocal relationship. The Catalogue of Life (COL) must be considered the most authoritative resource across the whole of taxonomy in respect of taxa which it currently covers. COL is a cooperative integration and standardisation of the information contained in many of the world's authoritative databases. At the time of finalisation of the dataset for this Dictionary, COL gave a taxonomic view of over half the world's reported species, and is planned to achieve completion in terms of published taxa by 2011. Where the name reported in the primary literature is not yet in COL, the genus name was cross-checked with other internet resources. If a genus name appears unreliable, this is noted in the entry.

There are many different schemes for taxonomic higher-level organisation. The discussion which follows is largely based on schemes given in Kornprobst (2005). Users should be aware, however, that the classification of genera into phyla, classes, subclasses, etc. given in Kornprobst is only one view. In some groups of organism (e.g. molluscs) there is reasonable agreement among biologists; in others (e.g. protozoa) there are huge differences between different schemes. Since most users of this Dictionary are likely to want to search using broad parameters (e.g. 'Find all pyridines in echinoderms', 'find all compounds with MW 300-310 in ascomycetes'), the Type of Organism categories have been kept broad, (largely phyla) and the uncertainties concerning organisation between the level of phylum and the level of genus should not affect the results. Where there are major taxonomic uncertainties, as with protozoa, the phylum is not subdivided; all organisms that can reasonably be considered as protozoa are grouped under the same code heading (**ZD**). Future development of the database may involve some further subdivision of these large categories.

Whittaker, R.H., *Quart. Rev. Biol*., 1959, **34**, 210–226 (*organism classification*)
Cimino, G. *et al, Marine Chemical Ecology*, (eds. McClintock, J.B. *et al*), CRC Press, Boca Raton, 2001, **115** (*rev, taxonomy*)

2.1 Archaea (Archaebacteria) (ZA)

The archaea are prokaryotic organisms inhabiting extreme environments, both marine and terrestrial, such as hydrothermal vents, and also highly saline regions. There are three generally recognised groups; thermophiles (heat-tolerant), halophiles (tolerant of highly saline media such as the Dead Sea; some species are also extremely alkali tolerant, growing in media up to pH 12) and methanogens (some species of which are also highly thermotolerant). It is also convenient to recognise a group of 'psychrophiles' tolerant of cold arctic and antarctic conditions. Although only discovered in the 1970s, it now appears that the archaea are in fact the most numerous bacteria in the marine environment. They show major differences from other prokaryotes in their genome, and these are carried through into fundamental differences in their membrane structure and biochemistry. Their cell walls do not contain the glycopeptides found in the eubacteria. Stabilisation of the membrane structure is affected by esters of glycerol with characteristic branched-chain terpenoid fatty acids, a role which in prokaryotes is performed by carotenoids and/or hopanoids and in eukaryotes by sterols. **Archaeol** is considered the prototype of this type of lipid; there are some unusual structural variations; for example the presence of lipids based on **Calditol** is noteworthy. A number of prenylated naphthoquinones related to vitamin K_1 have also been isolated, and sulfur bacteria contain a range of prenylated and aliphatic sulfur compounds.

2.2 Eubacteria (ZB)

The eubacteria are characterised by their cell wall structure, which is based on a glycoprotein formed of (1→4) linked *N*-acetylglucosamine and *N*-acetylmuramic acid, cross-linked by peptide side chains containing unusual amino acids which render different bacterial strains biochemically and immunologically distinct. In Gram-positive bacteria the glycoprotein coat forms the outermost layer; in Gram-negative bacteria there is an outer membrane coat which prevents this layer being stained by the reagent.

The classification of bacteria is a complex and specialised subject, and there is no official classification scheme. The nearest equivalent is the scheme being evolved for Bergey's Manual (Garrity *et al*), which is work in progress available for inspection online.

Bacteria may be photosynthetic or nonphotosynthetic, and the photosynthetic bacteria may be anaerobic (sulfur bacteria) or aerobic (which includes the cyanobacteria). The former group utilises the bacteriochlorophylls as photosynthetic pigments. Further major subdivisions such as alpha, beta-, gamma- and deltaproteobacteria have been delineated according to various schemes, but the overall picture is complex. Fortunately, within the context of natural products, the majority of investigations have been into two major bacterial subcategories, the actinomycetes and the cyanobacteria. The code ZB0001 is used in this Dictionary for all eubacteria which do not fall into one of these two major groups.

It is possible that some isolations from eubacteria, including actinomycetes, that have not been prominently flagged in the literature as being of marine origin, do not appear in this Dictionary. To search all bacterial isolations, consult the Dictionary of Natural Products on DVD. The coverage of cyanophyte products should be complete.

Lepage, S.P. *et al, International Code of Nomenclature of Bacteria*, American Soc. for Microbiol, Washington D.C., 1992
Austin, B., *Recent Advances in Marine Biotechnology*, (eds. Fingerman, N. *et al*), Science Publishers, USA, 2001, **Vol. 6**, 1–28 (*rev*)
Piel, J., *Nat. Prod. Rep.*, 2004, **21**, 519–538 (*rev, symbiotic bacteria*)
Garrity, G.M. *et al, Taxonomic Outline of the Prokaryotes, Bergey's Manual of Systematic Bacteriology*, 2nd edn, version 5.0, May 2004 http://141.150.157.80/bergeysoutline/outline/bergeysoutline_5_2004.pdf
Moore, B.S., *Nat. Prod. Rep*., 2005, **22**, 580–593 (*rev*)
König, G.M. *et al, ChemBioChem*, 2006, **7**, 229–238 (*rev, natural products from associated microbes*)

2.3 Cyanobacteria (ZB1000) (cyanophytes, blue-green algae, Myxophyceae)

The older term blue-green alga is now considered a misnomer, and the cyanobacteria are considered a subdivision of the photosynthetic eubacteria. They are unicellular organisms which are both marine and terrestrial; some marine species also inhabit fresh water. Some are truly monocellular, but when found unassociated with other organisms, many species adhere via their mucilaginous coats into filaments or tufts visible to the naked eye, and are sometimes found as large colonies known as stromatolites. These are well documented in the precambrian fossil record and thus place the cyanobacteria among the earliest known organisms. Schemes for the subclassification of cyanobacteria are based on their mode and degree of such association, or alternatively by the type of spores formed. Attempts have also been made to classify them chemotaxonomically. About 7500 species have currently been described. According to one view as few as 200 of these may be taxonomically distinct, but conversely according to recent chemical studies, a colony appearing to consist of a single species may comprise many genetically distinct strains. Cyanobacteria are responsible for frequent algal blooms, the toxicity of which is associated with their high level of secondary metabolites.

Their cell wall structures contain some sterols, but more characteristically conjugated hopanoids such as **Bacteriohopanetetrol**. The fundamental chemotaxonomic distinction between prochlorophytes and cyanobacteria lies in their photosynthetic pigments; in cyanobacteria there is **Chlorophyll a** but no chlorophyll b, which is replaced by the phycobilins, **Phycoerythrobilin** and **Phycocyanobilin**. These pigments are also found in the red algae, which show other chemical similarities to the cyanobacteria, notably in their polysaccharides. Cyanobacteria contain characteristic xanthophylls such as **Myxoxanthophyll**.

Cyanobacteria are present in the tissues of many sponges, often as a major component of the biomass. In an extreme case, the species *Terpios hoshinota* has been characterised as a 'Cyanobacteriosponge', in which the cyanobacterial cell mass constitutes over 50%. Some of the sponge-associated cyanobacteria are of unique type and have even been assigned to new genera. DNA sequence analysis has shown that different species of *Dysidea* sponge are associated with a different cyanobacterium, which may account for the wide range of different secondary metabolites isolated from them, while mass spectral analysis of colonies of *Microcystis* and *Planktothrix* cyanobacteria has demonstrated the presence in a single colony of multiple strains showing great diversity in their metabolites. Attempts to separately culture these cyanobacterial cells have proved unsuccessful, and evidence as to the true origin of the secondary metabolites is based on cell separation experiments. Peptides such as **13-Demethylisodysidenin** and chlorinated diketopiperazines, such as **Dihydrodysamide C**, were exclusively found in the cyanobacterial cells, whereas several terpenoids, such as **Spirodysin**, were found in the sponge cells. Halogenated aromatics are also associated with the cyanobacterial fraction of *Dysidea* sponges, and resemble metabolites such as **Ambigols** from cultured cyanobacteria.

The most characteristic secondary metabolites of the cyanobacteria, free or associated, however, are nitrogenous. The known metabolites are also characterised by a high degree of halogenation. See for example the extensive series of **Malyngamides**. A high degree of halogenation (notably terminal -CCl_3 groups) is shown by **Dysidenin** and its relatives isolated from sponge-cyanobacterial symbionts. An extensive series of brominated indoles typified by the **Hapalindoles** have been isolated.

Cyanobacteria produce an extensive range of modified depsipeptides, largely cyclic. Examples include the **Lyngbyabellins** and **Majusculamide C**. Acyclic peptides include the **Tasiamides** and the **Microcolins**.

Burja, A.M. *et al*, *Tetrahedron*, 2001, **57**, 9347–9377 (*rev*)
Gerwick, W.H. *et al*, Alkaloids, 2001, **57**, 75–184 (*rev*)
Van Wagoner, R.M. *et al*, *Adv, Appl. Microbiol*., 2007, **61**, 89–217 (rev)

2.4 Actinomycetes (ZB5000)

These are a particular class of Gram-positive eubacteria showing filamentous growth, and some similarities to fungi. (In the past they have often been classified as filamentous fungi and are sometimes called 'higher bacteria'). They also merit special treatment biochemically speaking because of their vast production of different types of natural product, many of them with strong antibiotic or other pharmacological activity. The most important genera by far in terms of natural products are *Streptomyces* and *Actinomyces;* according to which definition is used, the actinomycetes can also include the important pathogenic genera *Nocardia* and *Mycobacterium*.

Actinomycetes occur in marine sediments, and probably as endophytes in many marine organisms, but evidence is fragmentary. As a group they tolerate a wide range of salinities. A typical situation is that of the indolocarbazole alkaloids (VX4350), the Staurosporines. Staurosporine itself is produced by various actinomycetes, both terrestrial and marine, but close homologues have been obtained from ascidians *Eudistoma*, from planarians *Pseudoceros* that prey on them, and from prosiobranch molluscs *Coriocella.* The Holyrines, isolated from actinomycetes present in marine sediments, are probable precursors of these compounds and support the idea that they are all of ultimate actinomycete origin.

Moore, B.S., *Nat. Prod. Rep*., 2005, **22**, 580–593 (*microorganism biosynth*)
König, G.M. *et al, ChemBioChem*, 2006, **7**, 229–238 (*rev, natural products from associated microbes*)

2.5 Protozoa (ZD)

The term 'protozoa' is difficult to define taxonomically and is subject to ongoing modification in the light of biochemical studies, which are leading to the reclassification of many groups. It was formerly used as a blanket term to describe almost any kind of unicellular organism, but it is now known, for example, that the dinoflagellates (see ZH7000) are more closely related to the brown algae than to other unicellular organisms. In this Dictionary the code ZD0001 is used for all unicellular organisms that cannot be placed elsewhere*. The ciliate organisms, for example *Paramecium*, can be placed here, although it now appears that they are biochemically closest to the dinoflagellates. It is convenient to recognise four subdivisions; flagellates, amoebae, sporozoans and ciliates, but the reservations expressed above concerning their fundamental dissimilarities must be borne in mind, and a proper classification remains premature. Genera studied chemically include *Euplotes, Tetrahymena, Litonotus and Pseudokeronopsis*. The ciliates are nonphotosynthetic organisms but can often harbour photosynthetic algae as symbionts.

Chemical studies have been fairly limited, but a range of sesquiterpenoids, and some highly unusual triterpenes, the **Vannusals**, have been isolated.

* Some genera considered dinoflagellates are currently classified in the Dictionary under ZD0001, protozoa, but they are being reclassified under dinoflagellates, ZH7000, for future releases of the database

3. MARINE ALGAE; GENERAL CONSIDERATIONS

The algae considered in their totality, can be described as lower, mostly multicellular plants of a simple body plan, lacking well-defined differentiation into roots, stems and leaves. The higher plants, which show such differentiation, are virtually absent from the oceans, although some species (mangroves; several different spp. of higher plant) are important components of the estuarine saltmarsh environment.

The classification of algae has undergone a number of changes in recent decades and there is no definitive overall plan that takes care of every subgroup. The most fundamental division is between the Brown algal branch and the Green algal branch, two groupings which show large biochemical differences from each other. The 'Green' branch comprises not only the green algae proper (Chlorophyta), but also the red algae (Rhodophyta), which are now considered more closely related to the green algae than either of them are to the brown algae and their relatives. The taxonomic classification codes used here recognise only these major subdivisions, although one scheme for the Chlorophyta for example subdivides them into fourteen orders.

Red and brown algae are of commercial significance, but the commercial exploitation of green algae is very limited. The use of whole plants as food products is mostly confined to Japan, but the extraction of the algal polysaccharides for use in food and medicines is a major industry.

3.1 Chlorophya (green algae) (ZE)

About 7000 species are recognised, of which 1000 are marine, inhabiting mostly surface waters of the calmer seas. Of these, about 20% have so far been investigated chemically, principally in the orders Broypsidales and Ulvales. In their fundamental biochemistry (photosynthetic pigments, storage polysaccharides etc.) they resemble the higher plants. Some members are unicellular, sometimes as endophytes in other species of green algae.

Green algae photosynthesise using the common carotenoids **α- and β-Carotenes**, and contain a range of relatively common xanthophylls such as **Lutein**. The most common storage polysaccharides are amylose and amylopectin, and the commonest structural polysaccharide is cellulose, although some groups also secrete β-1,3-xylan and β-1,4-mannan. The most widespread sterols are Cholesterol, Brassicasterol, Sitosterol and their close relatives, although some rarer sterols such as **Saringosterol** have been characterised from certain classes of green algae. Studies have not always distinguished between sterols involved in the algal membrane structure and those present in the cytoplasm.

The known secondary metabolites of the green algae are rather limited in structural range and are mostly confined to terpenoids of relatively common skeleton, and a range of aromatics including meroterpenoids. Halogenation is uncommon, and the terpenoids are so far limited to sesqui- and diterpenes and a few triterpenes (acyclic and pentacyclic cycloartanes, e.g. **Capisterone B**). Many of the terpenoids contain enoloid functionality, for example **Caulerpenyne** and/or furan rings formed biogenetically by the cyclisation of the related unsaturated aldehydes, such as **Furocaulerpin**. Some of these metabolites have also been isolated from species that feed on green algae, such as molluscs. **Halimedatrial** is the only terpenoid so far isolated from green algae containing a carbon skeleton that has not been found elsewhere. The brominated aromatics are exemplified by **Rawsonol**, and the meroterpenoids by **Cymopol** and related compounds.

Nitrogenous compounds found in green algae tend to be low molecular-weight amines related to the amino acids, such as Agmatine, or peptides and modified peptides such as the **Kahalalides**. There are few more highly elaborated alkaloids except for purines and an unusual 1,3,5-triazine, **Halimedin**. Exceptions to this generalisation are the five-ring nitrogenous pigments **Caulerpin** and **Caulersin** isolated from the structurally atypical algae of the *Caulerpa* genus.

3.2 Rhodophyta (red algae) (ZF)

The red algae are characterised by a unique and complex reproductive cycle involving three alternating generations. The great majority of the 4000 species known are marine, sometimes inhabiting deep water. They may be mono- or multicellular with a complete absence of flagellae. The chloroplasts have a double membrane similar to those of cyanobacteria and presumably arose by endosymbiosis with these organisms. There is no general agreement about the subclassification of red algae. Several schemes have been suggested, and the taxonomy is fluid, for example the genus *Plocamium* has now been moved to a separate order, the Plocamiales. At the highest level, a division into two unequal subclasses is usually recognised. The Bangiophyceae, considered the more primitive group, is the smaller and consists of either unicellular or very simple multicellular organisms. The most studied genus chemically in the Bangiophyceae is *Porphyra.* The larger subgroup is the Florideophyceae, comprising the better-known more highly differentiated macroscopic plants.

An important biochemical similarity between the red algae and the cyanobacteria is the presence of the phycobilins, **Phycocyanobilin** (blue-green) and **Phycoerythrobilin** (red). It is the latter that is responsible for the red colour of the tissues, but the colour may be modified or masked by the presence of phycocyanobilin and/or chlorophylls. The red algae contain chlorophyll a and the characteristic pigment **Chlorophyll d**. The isolation of **Isochlorin e_4** from *Dasya pedicellata* is also noteworthy. The range of carotenoids is rather limited but includes the furanoid cyclised xanthophylls **Aurochrome** and **Auroxanthin** which are also widespread in terrestrial plants.

The storage saccharides consist not only of highly branched amylopectins but of the osmoregulatory galactoglycerols **Floridoside** and **Isofloridoside**. There is some cellulose content but the most abundant and characteristic polysaccharides are the commercially significant **Carrageenan** and **Agar**. These are rarely present in the same species. Red algae have a relatively high content of polyunsaturated fatty acids and phospholipids, as well as some unusual acids such as the cyclopentanoid **Dihydrochaulmoogric acid**. Derived from these unsaturated C_{18} and C_{20} acids are a large number of oxylipins, for example the **Constanolactones** and **Peyssonenynes**.
The range of sterols so far characterised is rather narrow and confined to relatively simple hydroxylated cholestanes such as the **Liagosterols** and **Pinnasterol**. Side-chain methylated steroids are rare; see **11,20-Dihydroxy-23-methylcholesta-1,22-dien-7-one**.

The secondary metabolites of the red algae are characterised by a high proportion of halogenated terpenoids and aromatics, particularly in the intensively studied genus *Laurencia.* The terpene skeletons are strongly

weighted towards the lower MW members of the series (especially sesquiterpenes), and there are many representatives of unique terpene skeletons not found in higher plants or elsewhere in the algae. Kornprobst [Kornprobst, 2005; **1**, 329] attempts a correlation of natural products with taxonomic subgroup (order), but in view of the taxonomic uncertainties referred to above and to the fact that several groups have hardly been investigated chemically, this must be considered tentative; the classification of red algae into orders given by Kornprobst and given here does not correspond with that found in the Catalogue of Life. The Ceramiales (e.g. *Ceramium, Delesseria, Chondria, Laurencia, Polysiphonia*) contain many halogenated sesquiterpenes and brominated aromatics, plus a range of halogenated C_{15} acetogenins which are characteristic of the order. The Gigartinales (e.g. *Chondrococcus*, *Plocamium, Ochtodes, Sphaerococcus*) also contain many halogenated terpenes, mostly monoterpenes such as **Halomon** and **Violacene** but in the case of *Sphaerococcus* some (often brominated) diterpenes based on sphaerane, presphaerane and related carbon skeletons, such as **Sphaerococcenol A** and **Presphaerol**. On the other hand, the Nemaliales (e.g. *Asparagopsis, Bonnemaisonia, Rhodymenia*) and others yield halogenated aliphatic compounds of low molecular weight such as halogenated acetones. The genus *Ochtodes* (Cryptonemiales) yielded a range of halogenated monoterpenoids based on the unusual ochtodane skeleton, such as **Ochtodene**; other genera in this order did not contain terpenoids. Other orders have either not been extensively investigated, or yielded only a limited range of natural products.

The order Ceramiales, especially the genus *Laurencia*, is a rich source of natural products with over 500 compounds so far isolated. The sesquiterpenes of *Laurencia* are based on more than 20 different carbon skeletons, some of them 'traditional' and found also terrestrial organisms, others novel. Many of these have also been isolated from molluscs and other animals that feed on red algae. Using chemotaxonomic evidence, the species in this genus can in fact be divided into three subgenera. The first group contains only halogenated terpenes, the second only acetogenins and the third group both. However, the situation is complex and there may be interbreeding between different chemotypes. [Kornprobst 2005; **1**, 346–347]. There is also a wide range of halogenated (mostly brominated) diterpenes, many derived from the common (marine and terrestrial) skeleton labdane and other skeletons closely related to it. The parguerane skeleton, as found in **Parguerene** and related compounds, is however unique to marine organisms. There is also a series of **Irieols** based on the irieane skeleton. Certain *Laurencia* and *Chondria* species have also yielded a series of triterpenoid polyethers derived from squalene, for example **Thyrsiferol, Enshuol** and the **Armatols**.

The most characteristic class of natural product isolated from these genera, however, is the extensive series of mostly halogenated compounds based on a linear C_{15} skeleton, the first of which to be discovered was **Laurencin** in 1968. A wide variety of structure based on ether formations is founded on this basic skeleton (for example **Obtusenyne**; **Microcladallenes**), which probably arise by loss of a C_1 fragment from a C_{16} precursor. The isolation of **Laurediol** supports this hypothesis. The Ceramiales also contain a range of halogenated phenolics such as **Lanosol**.

Nitrogenous natural products are relatively scarce in the majority of red algae, and mostly limited to widely-distributed small molecules such as **Homarine**, and cyclic peptides such as **Ceratospongamide** (isolated from a red algal-sponge symbiont). A range of simple halogenated indoles was isolated from *Rhodophyllis membranacea.* Once again, it is the Ceramiales that show a much greater range. A characteristic amino acid is **Kainic acid**, together with its homologue **Domoic acid** and other analogues. The range of indoloids is also greater, including some of greater elaboration such as the **Almazoles**.

The chemotaxonomic unpredictability of this group of organisms is shown by studies of *Chondria californica*, which yielded a range of polysulfur compounds such as **Lenthionine**. These were unaccompanied by terpenes, and were not found in apparently closely related species.

3.3 Phaeophyta (brown algae) (ZH1000)

About 1500 species of brown algae are known, almost exclusively marine. The term Phaeophyta is to be preferred, since modern studies have shown that they are only very distantly related to the other algae and the term 'brown alga' is therefore a misnomer, although it remains in widespread use. Together with the diatoms and the chrysophytes, they constitute the Stramenopiles. Whereas the other two subgroups are entirely monocellular, the vast majority of brown algae are multicellular and macroscopic, sometimes attaining very large size. Most species inhabit cold and temperate, often rough, seas, and are sessile, demonstrating a well-defined differentiation into a foot (holdfast), stem (stipe) and frond, and growing in surface or relatively shallow waters. The exception is the brown algae of the Sargasso Sea, which are two free-floating *Sargassum* species inhabiting tropical waters.

Two superorders are recognised, based on life-cycle criteria. The Fucales do not show generational alternation, producing haploid gametes which reproduce the diploid stage (cf. higher plants and animals). The other brown algae show generational alternation between a haploid gametophyte and a diploid sporophyte (cf.

ferns). In some families the two forms are both macroscopic and may be indistinguishable to the naked eye; in others, the gametophyte is microscopic. Kornprobst [Kornprobst, 2005; **1**, 420–421; *ibid*., 481] gives a classification scheme into 11 orders (the Fucales being one), but as with the red algae, there have been several different views of the taxonomy in recent years, with much ongoing research having chemotaxonomic implications. For example, it has been shown that the much-studied *Dictyota dichotoma* must be considered a complex in which several endophytic species can be distinguished.

The photosynthetic pigments of all organisms of the Stramenopiles are **Chlorophylls a, c_1** and **c_2**. (characteristic absence of chlorophyll b). The carotenoid content is limited to **Fucoxanthin** and lesser amounts of **Violaxanthin**; **Diatoxanthin** and **Diadinoxanthins** have also been reported, but may be the result of diatomaceous contamination of samples. Some Fucales have yielded pseudomonoterpenoids related to **Loliolide**, which in other types of organism are known to be degradation products of xanthophylls.

Both the structural and the storage carbohydrates of the phaeophytes differ from those present in other classes of algae. The main storage polysaccharide is **Laminarin**, accompanied by **Mannitol** and **Laminitol** which perform osmoregulatory functions. The matrix polysaccharides are based on **Alginic acid** in which the anions are carboxylate groups rather than the sulfates found in carageenans and agar. Phaeophytes in the orders Fucales and Laminariales also contain smaller amounts of the pharmacologically interesting **Fucoidin**.

As in the red algae, the range of sterols found is limited and mostly based on minor modifications of the **Fucosterol** structure, which is the major steroid. There is a wide range of unusual oxylipins, for example the rare oxa compounds given in the entry for **12-Hydroxy-6,9,11-dodecatrienoic acid**, bridged epoxy compounds such as the **Cymathere ethers**, and prostanoid-like cyclopentanoids such as the **Ecklonialactones**.

Brown algae contain a wide range of terpenoids, phenolics and meroterpenoids, but a striking and somewhat unexpected feature is the paucity of halogenated compounds, and those that are found in small amounts are bromo- and iodo-, rather than chloro-substituted. They are unique in their ability to concentrate iodine (and also arsenic; see below) to concentrations of up to 1% dry weight, and although 99% of the iodine in the tissues is inorganic, the other 1% finds its way into **Thyroxine** and other iodinated tyrosines, and a small number of miscellaneous phenolics. There are also few alkaloids, nitrogen compounds being represented only by compounds of low molecular weight, some peptides such as **Fastigiatine** and one or two other compounds such as the terpenoid amide **Joalin**. However, studies have so far been confined to two orders, the commercially important Fucales and the Dictyotales. No lower terpenoids have been isolated from the former group, and mostly only linear diterpenes such as **Crinitol**, although the presence of the rare cyclobutanoid norditerpene **1-(2-Isopropyl-1-methylcyclobutyl)-4-methyl-4-nonene-1,8-dione** in *Cystophora moniliformis* is noteworthy. On the other hand the Dictyotales contain some sesquiterpenes such as **Zonarene**.

The diterpenoids of the Dictyotales include many examples of prenylogues of well-known sesquiterpenoid skeletons, for example **Dilophol** (prenylgermacrane), **Dictyotin A** (prenylcadinane = biflorane) **Dictyotetraene** (a dictyotane) and other elaborations on this theme (for a tabulation in chart form, see Kornprobst, 2005, **1**, 442-3). Other characteristic skeletons are xenicane and its relatives (pachydictyane, crenulane and others), and dolabellane and dolastane.

The major secondary metabolite content of brown algae is represented by phenols and phenolic meroterpenoids, many of them sulfated and/or halogenated. The content of these in the tissues may reach 20% by weight and they may play a role in the prevention of larval fixation by marine animals and for protection against bacteria. A major series is represented by the phlorotannins (see for example **Trifucol**, **Trifuhalols**, **Eckol** and their numerous homologues) which are radical-induced oligomers of Phlorotannin containing C-C or C-O-C linkages. The genus *Cytoseira* has been much investigated and has yielded a large range of structurally diverse meroterpenoids; for example, **Strictaketal**, the **Cystoseirols** and the **Mediterraneols**.

The reproductive cycle of brown algae is mediated by a range of hydrocarbon pheromones secreted by the female gametes, and which act as attractants for the male cells. In some orders of brown algae the gametes are both mobile and may be either of similar (microscopic) size, or with the female gamete larger. The most advanced form of reproduction is shown by the Fucales, where the female gamete is large and immobile, and the male gamete is attracted to it solely by the very low concentrations (nanomolar to picomolar) of the attractants. These molecules modulate the navigation of the male gametophytes in the marine environment over the very short ranges (~1mm) required for fertilisation. They are small, non-halogenated aliphatic molecules, the secretion of which is a unique feature of phaeophyte biochemistry. The majority are C_{11} compounds which appear to be derived by degradation of unsaturated acids such as eicosahexaenoic, of a type not found in terrestrial plants. They may be acyclic (e.g. **Cystophorene**) or containing 3-, 5-, 6-, 7- or 8-membered rings (e.g. **Dictyopterenes A-B, Multifidene**, **Aucantene**, **Ectocarpene** and **7-(1-Propenyl)-1,4-cyclooctadiene** respectively). Some *Fucus* and

Sargassum species employ the smaller molecule **1,3,5-Octatriene** (various stereoisomers). Unexpectedly, Ectocarpene was also found in terrestrial *Sencecio* spp.

The tissues of brown algae uniquely concentrate inorganic arsenic at concentrations of up to 40ppm and some of this is converted via biomethylation to dimethylarsinate and thence into a range of ribosides such as **2,3-Dihydroxypropyl[5-deoxy-5-(dimethylarsino)]ribofuranoside**.

3.4 Bacillariophytes (diatoms), Chrysophytes (golden algae) and Haptophytes (ZH5000)

These three groups of unicellular organisms belong to the 'brown' major biochemical line and together with the brown algae (mostly multicellular) constitute the Stramenopiles. The term 'algae' formerly applied to some of these groups is now considered on biochemical and submicrostructural studies to be a misnomer (cf. brown algae). Although these organism types are linked together in the classification scheme used here, this is tentative as they may be rather unrelated and biochemically distinct.

These organisms have been relatively little studied chemically by comparison with the brown algae. The diatoms and haptophytes secrete hard exoskeletons of aluminosilicates and calcium salts respectively, while the golden algae do not, though they may contain silica microspicules. There are roughly 200 known species of marine golden algae and 500 of haptophytes, but the number of marine diatom species may be as high at 50,000, constituting the bulk of the phytoplankton at certain times of the year, and therefore of crucial importance to marine ecosystems.

The storage polysaccharide of diatoms and Chrysophyceae is **Chrysolaminarin**. Photosynthetic pigments resemble those of the brown algae, with no phycobilins but with chlorophylls c including the more recently discovered **Chlorophyll c_3**. A number of minor xanthophylls have been detected and *Phaeodactylum triconutum* has yielded some degraded carotenoids such as **Apo-13′-fucoxanthinone**. There have been extensive studies on their lipids on account of their biotechnological importance (cf. algae). The content of sulfur glycerides, especially **1,2-Diacylglycerol 6-sulfoquinovosides** (also found in other classes of organism) is relatively high. The range of known steroids resembles that of the brown algae in being based on limited side-chain modification of the cholestane skeleton, up to C_{30} in the case of **24-Propylidenecholesterol**, with some sulfation, e.g. **Hymenosulfate**. The **Bacillariolides** appear to be oxylipins produced by the arachidonate pathway. The **Prymnesins** are toxic polyethers produced by a haptophyte.

The range of terpenoids isolated is very narrow and limited so far to simple phytanes. It is noteworthy that in two studied diatom species, the biosynthesis of these (in the chloroplasts) is by a non-mevalonate pathway while the steroids, produced in the cytoplasm, are mevalonate-derived.

Nitrogenous compounds are similarly few in number, but the toxic pyrrolidine **Domoic acid**, also found in red algae, was isolated as a shellfish toxin resulting from *Nitzschia* infection.

Moore, B.S., *Nat. Prod. Rep*., 2005, **22**, 580–593 (*diatoms*)

3.5 Dinoflagellates (ZH7000)

Note; Many shellfish toxins are now known to be dinoflagellate metabolites but may not currently be classified as such in the database

These monocellular organisms are economically important as the causative agents of toxic 'red tides'. Biochemical and other studies have shown clearly that they are more closely related to the ciliates and to certain other groups than they are to other flagellate organisms. (Kornprobst 2005 describes them as 'Mesocaryotic', i.e. intermediate between the eukaryotes and the Stramenopiles). About 200 species are known, predominately marine. Only just over half are photosynthetic; some are carnivorous. Their main anatomical characteristic is the possession of two flagellae, one equatorial and one longitudinal. Most are unicellular but some are filamentous. They participate in a range of symbiotic associations, especially with corals and with molluscs.

Those organisms which are photosynthetic contain **chlorophylls a** and **c**. They contain a range of xanthophylls, most characteristically the C_{37} trisnortriterpenoid pigment **Peridinin** and also the structurally unusual **Gyroxanthin**. The characteristic steroids are a range of 4α- methyl compounds such as **Amphisterol** and **Peridinosterol** representing an intermediate stage between the tetracyclic triterpenoids and the cholestane/ergostane type predominant in the brown algae and relatives. **Gorgosterol**, originally isolated from a gorgonian, was found later to be produced by a dinoflagellate symbiont.

The known toxins of dinoflagellates fall into two main groups, though the exact type of toxin produced is genus-specific. The first main group is polyketide-derived, either long-chain with some cyclic ether formation

(**Amphidinols**, **Luteophanols**, **Colopsinols**, **Zooxanthellatoxins**) or with multiple ether rings ('polyether ladders') (**Brevetoxins**, **Ciguatoxins**, **Yessotoxin** and their analogues, together with the giant C_{164} molecule **Maitotoxin**). Another structural subtype is shown by **Okadaic acid**, while other polyketides are macrolides such as the **Amphidinolides**. The **Prorocentrolides**, **Pinnatoxins** and **Spirolides** are cyclic nitrogenous polyketides which have been isolated from shellfish but are known to be dinoflagellate produced. It is notable that in known cases the biosynthesis of polyketides in dinoflagellates is by a totally different pathway from that in other organisms.
The other main class is composed of nitrogenous guanidinoid toxins of which **Saxitoxin** is the prototype.

Moore, B.S., *Nat. Prod. Rep*., 2005, **22**, 580–593

3.6 Fungi (ZG)

Fungi are now considered part of the Eukaryote kingdom, and are characterised by the lack of a photosynthetic mechanism and by a mode of life which is saprophytic, parasitic or symbiotic. Another major biochemical difference from algae lies in their cell wall structure usually based on chitin rather than cellulose. Fungi are found throughout a wide range of terrestrial and marine environments and it is not possible to produce a meaningful definition of 'marine fungi', only to refer to a range of halotolerance among the various fungal species that are widely distributed. Thus marine sediments and marine invertebrate tissues yield fungal species from genera also found terrestrially, but which have developed a preference for growing in saline environments. Of the approximately 100,000 fungal species so far described, about 500 have been found in marine environments, but this figure is certain to increase in the light of further research. Many metabolites, such as **Gliotoxin**, have been isolated from both terrestrial and marine fungi, and when the identical compound has not yet been found in a terrestrial fungus, there are often close relatives. One basidiomycete species, *Coriolus consors* (preferred name *Irpex consors*) has been cultivated in both seawater and freshwater and yielded the same natural products. Since fungi are invariably cultivated on a medium which is then extracted, cross-contamination of cultures by terrestrial fungi or bacteria is a possibility that must be guarded against.

The lower fungi or Chytridiomycotes (ZG1000) are found only to a very limited extent. They are taxonomically difficult to classify, resembling the higher fungi in their lack of photosynthesis, but resembling the monocellular algae in having a cellulosic cell wall structure and a flagellate stage, sometimes with alternation of generations. There are different views as to how they should classified vis-à-vis the simpler Stramenopiles, and several classes of organisms formerly considered to be lower fungi have now been reclassified on biochemical grounds. Chemical studies are limited.

The majority of fungi fall into the category of higher fungi or Eumycetes having typical fungal biochemistry, and which can be subdivided into the four main classes of Zygomycetes (ZG2000), Ascomycetes (ZG3000), Basidiomycetes (ZG4000) and Deuteromycetes (ZG5000). These groups are distinguished by their method of spore formation (zygospores, asci and basidia respectively for the first three groups). The Deuteromycetes are an ill-defined group roughly corresponding with the term fungi imperfecti (the terms Mycelia sterilia and Hyphomycetes are also found according to various schemes). These are fungi in which no reproduction is observable and which are therefore extremely difficult to identify. Spore formation can be induced in some of them under laboratory conditions, work which shows that they are a loose collection of unrelated fungi rather than a true taxonomic group, and can lead to reclassification into one of the other classes. This can lead to taxonomic duplication, with the organism allotted a new name based on the reproductive form (which should take priority) while still retaining its old name.

The Ascomycetes and the Deuteromycetes are the most represented in the marine environment and been the most investigated chemically.

The great majority of fungal secondary metabolites have been isolated from fungi associated with other organisms. Examples of natural products isolated from non-associated marine fungi include the simple polyketide **Phomoxin**, the carotenoid **Neurosporaxanthin** and some indolopeptides from surface waters or marine sediments.

Marine algae (green, red and brown), like higher plants, harbour a wide variety of endophytic fungal species; for example, 116 different fungal strains were cultivated from a single specimen of *Fucus serratus*. It is not in general known whether any particular relationship should be considered as symbiotic, benign or pathogenic. There are usually strong structural similarities between the natural products from these epiphytic marine fungi and their terrestrial equivalents.

Fungal mycelia are also found in marine animal tissues. Evidence for their presence is based entirely on culturing experiments and as yet there is no evidence from direct microscopic examination or other techniques.

Their role is unknown. In general, compounds produced by fungi associated with marine animals are structurally related to other fungal metabolites and are distinct from natural products produced by the animal organisms themselves. It does not appear that fungi are the biogenetic source of natural products isolated from marine invertebrates, unlike the situation found with bacteria. An example of a natural product isolated from a sponge-associated fungus is **Ulocladol**, while **Epicoccamide** is an example of a substance isolated from a fungus associated with a cnidarian (a jellyfish). Other series of characteristic fungal products have been isolated from fungi associated with all other classes of marine invertebrates, as well as from fungi parasitic on fish.

The most characteristic sterols of all fungi are **Ergosterol** and related ergostanes. Reports of 5,7-dienic steroids from other marine species are suggestive of fungal contamination. Other steroids isolated include **Fusidic acid**, and the **Gymnasterones** from an ascomycete-sponge association.

There are very few reports of the incorporation of halogens. Most fungal secondary metabolites are based on a polyketide biogenesis, but some terpenoids are found, for example the unusual nitrobenzoyl esters of **6,7,14-Trihydroxy-8-drimen-12,11-olide** and the **Hirsutanols** from a sponge-associated fungus. The alkaloids obtained from marine fungi are dominated by diketopiperazines/indoles, as is the case with terrestrial fungi.

Very few biosynthetic studies have been reported for natural products specifically from marine fungi.

Dictionary of the Fungi, 9th edn, (eds. Kirk, P.M. *et al*), CABI publishing, 2001
Bugni, T.S. *et al, Nat Prod. Rep*., 2004, **21**, 143–163 (*rev*)
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Ebel, R., *Frontiers in Marine Biotechnology*, (eds. Proksch, P. *et al*), Horizon Bioscience, 2006, 73–143 (*secondary metabolites from marine fungi*)

3.7 Porifera (sponges) (ZS)

The sponges are considered as the most primitive of the multicellular organisms, providing an evolutionary bridge between the monocellular eukaryotes and the rest of the animal kingdom. They are multicellular organisms lacking all organ differentiation (including gonads) and some can uniquely reconstitute themselves after passing through a sieve. They are almost exclusively marine. Sponges are found at all marine depths but the proportion of calcareous sponges diminishes with depth owing to the physicochemical effect of pressure on the ability of the organisms to secrete calcium.

The taxonomy of sponges is particularly difficult owing to the paucity of well-marked morphological feature by which they can be distinguished. Many species have been synonymised and genera renamed (e.g. *Aplysina* = *Verongia*), and there are numerous views on their classification at higher levels; a recent multi-volume treatise (Hooper *et al*, 2002) proposes many changes. Three main subdivisions have been generally recognised, depending on the nature of the skeletons that they secrete; calcareous (ZS1000), siliceous or askeletal. The largest group is the demosponges, about 95% of known species, in which the skeleton is of spongine, a proteinaceous polymer similar to keratin. The Hexactinellida sponges, characterised by silica spicules of 6-fold symmetry, are found only at great depth and have been little studied chemically.

In this database a simple classification into four groups is used, which is based on Hooper (2002) as summarised in tabular form by Kornprobst (2005). This divides sponges into; Calcareous sponges (ZS1000), Homoscleromorphous demosponges (e.g. *Plakortis*) (ZS3000), Tetractinomorphous demosponges (e.g. *Stelletta*) (ZS4000) and Ceractinomorphous demosponges, (e.g. *Agelas*) (ZS5000).

Sponges participate in a wide range of symbiotic/commensal relationships, and a large number of the isolations of natural products earlier reported from them are in fact owing to the presence of cyanophytes in particular. It is estimated that the biomass represented globally by sponge-cyanophyte symbionts is greater than that of the sponges themselves. Given the extent of these associations, it is not surprising that the diversity of natural products reported from sponges and sponge aggregates covers the whole range of known types. Other natural products reported may be true metabolites of the symbionts.

A wide variety of cell membrane components have been isolated, not only extensive series of both straight-chain, branched and methylenic (cyclopropanoid) fatty acids but alkylglycerols (e.g. **Raspailynes**) and hopanoids based on **Bacteriohopanetetrol** and relatives as well as a vast range of steroids. There are also numerous brominated and α-hydroxyacids. Certain linear terpenoids such as the **Furospongins** have also been postulated to play a role in membrane structure. Associated with the membrane structure is a wide variety of glycolipids, many of them of unique structural type. The simpler *N*-containing parents are the **Sphingosines**, the Dictionary entries for which include their *N*-acyl derivatives collectively known as ceramides, and their glycosides, known as

glycosphingolipids or cerebrosides. More complex types of sphingosine such as the **Plakosides** (containing cyclopropa fatty acids) have individual entries. The nitrogen-free glycolipid content also includes some structural types not found elsewhere, such as the **Crasserides** (ether glycerides of a 5-membered cyclitol), which as a class have been suggested to be uniquely diagnostic of the Porifera and found in all species examined. A unique class of compounds so far discovered only in sponges is the range of carotenoids aromatised in one or both rings such as **Renieratene** and **Tethyanin**.

Among calcareous sponges the most investigated genera are *Clathrina* and *Leucetta*. These genera have yielded in particular long-chain unsaturated aminoalcohols such as the **Leucettamols**, a range of imidazole (e.g. the **Naamines**) and other alkaloids, and cyclic peptides, (e.g. **Leucamide A**).

By far the most studied have been the demosponges, reflecting their numerical preponderance and shallow-water accessibility. Demosponges contain a very wide range of steroids, which encompasses not only the conservatively modified structures biogenetically not far removed from cholesterol (ergostanes, stigmastanes) found in the algae, but also a large number showing more profound modification. These include 19-norsteroids such as **Hapaioside** and a range of A-ring abeosteroids (3-hydroxymethyl-A-norsteroids). The most common type of modification, however, is further side-chain methylation which leads to an extensive series of steroids having various branching patterns up to C_{32}, (e.g.; C_{29}, **Aplysterol**; C_{30}, **Stelliferasterol**; C_{31} **Axinyssasterol**; C_{32} (**26,27-Dimethyl-26-methylenestigmast-7-en-3-ol**). Side-chain cyclopropasterols such as **Calysterol** and **Aragusterol A** occur in the range C_{27}-C_{31} and there are also many secosterols with fission at 5,6- (e.g. **Hipposterol**), 8,9- (**Jereisterol A**), 8,14- (**Jereisterol B**) and 9,11- (**Blancasterol**). There are also many polyhydroxylated and sulfated sterols of the type found also in many other marine organisms, and many steroidal glycosides. Halogenated steroids (e.g. **Aragusterol C**) and steroidal alkaloids (e.g. **Plakinamines**) are rare.

Demosponges of the genera *Plakortis* and *Plakinastrella* (order Homosclerophorida) contain a wide range of oxylipins, including many cyclic peroxides such as the **Plakortides**.

Another group of unusual natural products found in sponges are the terpenic isocyanides R-NC such as **7,20-Diisocyanoisocycloamphilectane**, together with their related isothiocyanates R-NCS, isocyanates R-NCO and formamides R-NHCHO. In the appropriate DMNP entries these are grouped as derivatives under the parent isocyanide, reflecting the fact that they have a common biogenetic origin, the isothiocyanates and formamides apparently being derived *in vivo* from the isocyanides (and not the other way round as was formerly proposed). However the biogenetic origin of the isocyanides themselves has not yet been completely solved.

A wide range of alkaloids and terpenoids are found in demosponges. Indole alkaloids range from simple halogenated indoles such as the **Plakohypaphorines** to polycyclics such as the pentacyclic pyridoacridines (e.g. **Meridine**). Demosponges are the most prolific of all marine organisms in terms of the secondary metabolites that have been isolated from (but not necessarily produced by) them. In order to get a good overview, the best route is to search the CD-ROM version of the Dictionary using the search term **ZS*** (all sponges), but further information can also be obtained from the introductory sections dealing with terpenoid and alkaloid types, and of course by perusing the pages of the printed Dictionary.

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3.8 Cnidaria (medusae, sea anemones, hydroids and corals) (ZT)

This class of organisms represents the first major development in body-plan over the undifferentiated sponges, showing cellular differentiation into cells with different functions, but in general no well-defined organs. The term Cnidarian replaces the older 'Coelenterate'. This is a class of organisms typified by a carnivorous lifestyle, the presence of specialised stinging cells (cnidocysts) used in the capture of prey and defensively, and a digestive system consisting of a sac with only one opening. They have a basically radial body plan, which may be modified either in the direction of a fixed polyp with a central gastric cavity (hydras), or a free-swimming medusa form (jellyfish) in which the gastric cavity is underneath. Reproduction is sexual, producing a free-swimming larval

planula which develops into a free-swimming followed by a polyp form, although in some species only one of these is formed.

About 10,000 species are documented, classified into two subphyla. The first subphylum (Anthozoa) comprises the sea-anemones, gorgonians, crinoids and corals which have no free-floating phase, and a skeletal structure consisting either of secreted calcareous minerals, or of proteinaceous material (gorgonine, analogous to the spongine found in the sponges). The anthozoa are divided into two groups depending on their symmetry; eightfold in the octocorals, (alcyonians or soft corals and gorgonians) (ZT1000) or sixfold or a multiple of sixfold (hexacorals, including the sea anemones and hard corals) (ZT2000). The former subphylum is the most studied group of the cnidarians chemically.

In general, relatively few nitrogenous secondary metabolites have been isolated. The proportion of halogenated metabolites is also relatively low, except for halogenated briaranes from *Briareum* spp., such as the **Briareins**. Some sea anemones owe their colour to carotenoids including **Peridinin** and **Actinoerythrin**. The former in particular is produced by dinoflagellates, and these carotenoids work their way up the food chain to molluscs. Octocorals are rich in prostanoids, steroids, terpenoids (but only sesqui- and diterpenes) and aromatics. The prostanoids include a number identical with those found in higher organisms of the **Prostaglandin** series (A, B, E and F), but also halogenated prostanoids containing Cl, Br and I such as the **Chlorovulones**, especially from *Clavularia*. Further oxylipins are now being found in other cnidarians and it appears that their presence may be ubiquitous. Series of furanoid compounds similar to **Ancepsenolide** elsewhere in the phylum support this hypothesis. The hexacorals contain a range of polyunsaturated long-chain acids such as **Leiopathic acid** and the **Montiporynes**.

Like the sponges, cnidarians contain a wide range of sterols, both typical cholesterol-related, and those with modified side-chains. An important class is the side-chain cyclopropanoid steroids based around **Gorgosterol**, although it has been shown that these are in fact produced by symbiotic dinoflagellates. **Yonarasterol I** is an example of this group showing halogenation at *C*-6. There are many polyhydroxylated steroids, often showing side-chain epoxidation, for example the **Hippuristerols**, and a considerable number of secosteroids, some of unusual type such as **Nicobarsterol**. Also are encountered pregnane glycosides (**Verrucoside**, **Pregnediosides** and others). In contrast to the sponges, however, *O*-sulfation is absent. The hexacorals produce polyhydroxylated ecdysteroids such as **Zoanthusterone** which are thought to protect the organism against crustacean larvae.

The sesqui- and diterpenes found in the octocorals are diverse and include some skeletons unique to them (nardosinanes, capnellanes, sterpuranes and some others), which in most cases are unique to certain families. In contrast, terpenoids are almost absent from the hexacorals. The sesquiterpene hydrocarbon content of octocoral tissues may be exceptionally high and they are thought to play an ecological role as predator and larval implantation repellents. An important feature is the frequent occurrence of common terpenoids of the enantiomeric series to that familiar from terrestrial plants, as shown for example by **γ-Maaliene** and **α-Copaene**. There is a complete absence of the isocyanides characteristic of the sponges, and only a limited range of terpenoid alkaloids such as **Clavulinin**. The well-known skeletons represented include many furanoterpenes. The hexacorals have yielded only a few sesquiterpenes; some lepidozanes and secolepidozanes, e.g. **Anthoplalone**.

The octocorals are very rich in diterpenoids, with over 1500 belonging to 50 skeletal types isolated. As with the sesquiterpenes, some skeletons are widespread throughout the phylum, while others are restricted to a single family and can be considered as chemotaxonomic markers. Particularly widespread skeletons include cembrane (including norcembranes and some dimers such as **Sinuflexlin**), xenicanes, lobanes, briaranes, cladiellanes, dolabellanes and amphilectanes. As with the sponges, many skeletons are prenylogues of widespread sesquiterpenoid skeletons. The briaranes are particularly numerous and unlike most other skeletons, frequently halogenated (chlorine only).

Some diterpene alkaloids have been found such as the **Sarcodictyins** (imidazoles containing the eunicellane skeleton, closely related to briarane). The hexacorals produce a range of ceramides, often containing unusual sphingosines, and some other acyclic amides such as **Sinulamide**. Their range of cyclic alkaloids is restricted, e.g. the **Villagorgins**, **Calliactine**, but includes the unique class of fluorescent pigments based on the cycloheptadiimidazole skeletons of **Parazoanthoxanthin A** and **Pseudozoanthoxanthin A**.

Hexacorals of the order Zoantharia (genus *Zoanthus*) have yielded a range of polyketide alkaloids similar to **Zooxanthellamine**. Chemically and pharmacologically, the most significant natural product isolated from cnidarians is probably **Palytoxin**. Hexacorals inhabiting surface waters also contain a range of mycosporins such as **Mycosporin-Gly** which are closely related to analogues found in fungi and appear to perform a photoprotective function. They also contain a range of small nitrogenous betaines and other amines, some purines such as **Caissarone**, and some simple indole-imidazole alkaloids centred on **Aplysinopsin**.

The other subphylum of cnidarians (Medusozoa) comprises the Cubozoa (box jellies, ZT5000), Hydrozoa (hydras, ZT6000) and Scyphozoa (true jellyfish, ZT7000). Chemical studies have been mostly confined to their venoms, which are peptides. (See for example the entry for ***Anemonia sulcata* Toxin**). One difficulty associated with studying their secondary metabolites is the large amount of water in the tissues, which can reach 98%. Some steroids have been identified, plus a small range of polyketides e.g. **Solandelactones**, **Lytophilipines**, and some anthracenoids, e.g. **Garvins**, and simple alkaloids, e.g. **Corydendramines**, **Tridentatols**. There are also the nitrogenous compounds associated with the bioluminescence of some species; ***Cypridina* Luciferin** and **Coelenterazine**.

Faith, F.M.Y. *et al, Recent Advances in Marine Biotechnology*, (eds. Fingerman, N. *et al*), Science Publishers, USA, 2001, **Vol. 6**, 85–100; Venkateswarlu, Y., *ibid*, 101–143 (*revs, coral*)
Anderluh, G. *et al*, *Toxicon*, 2002, **40**, 111–124 (*rev, anemone toxins*)

3.9 Platyhelminthes (flukes, tapeworms and free-living flatworms) (ZU1000)

These are the flatworms, characterised by a bilateral body plan and the complete absence of a digestive cavity. About 18,000 species are known. They may be terrestrial, freshwater or marine and many belong to orders which are exclusively parasitic (e.g. flukes). The majority of marine species belong to the class of planarians (turbellarians). These are mobile, carnivorous animals having no physical means of defence and relying entirely on substances absorbed or modified from the diet, or produced by symbiotic organisms, as chemical antifeedants. The most studied genus is *Amphiscolops*. These worms are protected by **Amphidinolides** produced by symbiotic dinoflagellates and contain other dinoflagellate products such as **Luteophanols**. Other planarians feeding on ascidians have yielded alkaloids (e.g. **Lepadins**, **Villatamines**).

3.10 Annelida (trueworms) (ZU3000)

These are the segmented worms, having an alimentary canal. They include the polychaetes, oligochaetes (earthworms; mostly terrestrial), hirudineans (leeches; mostly freshwater), echiurians and Vestimentifera. They locomote by means of bristles which can be irritant or venomous. The best-known genus among the echiurians is the spoonworm *Bonellia viridis*, most studied on account of its tetrapyrrole pigment **Bonellin** which also plays a role in inducing sexual differentiation in the larva. The Vestimentifera include the recently-discovered giant hydrothermal vent dwellers *Riftia* which coexist with sulfur bacteria, and store elemental sulfur in the tissues.

There has so far been little study of lipid or steroid content. Their carotenoid pigments appear to be mainstream components such as **Astaxanthin**, derived dietetically. Other annelid pigments are anthracenes and anthraquinones, such as **Hallachrome**. Annelids also contain brominated phenols (e.g. **2,6-Dibromophenol**) and derived aromatics such as **Thelepin**, which protect them against bacteria.

Certain annelids bioluminesce and in *Odontosyllis* spp. this is based on pteridines such as **6-Propionyllumazine**. **Nereistoxin** is a simple aminodithiolane with powerful cytotoxic properties produced by *Lumbriconereis* sp. Some annelids contain large amounts of **Hypotaurine** and **Thiotaurine**.

3.11 Other vermiform groups (ZU5000)

The ribbon-worms or nemerteans have yielded the powerful nicotinic receptor agonist **Anabaseine**, used as a venom by the worm, together with several related oligopyridines. Toxins of the tetrodotoxin series are also found in the tissues, and also some peptide toxins, which have only been investigated fully for one species, *Cerebratulus lacteus* (see **Neurotoxin B-IV**)

The unsegmented phoronidian worms *Phoronopsis* have yielded antibacterial bromophenols like those obtained from the annelids.

3.12 Bryozoa (ZU6000)

These colonial organisms are entirely aquatic and mostly marine. They are distinguished by their unique form of gastric cavity, which is surrounded by tentacles forming an organ called the lophophore. The colonies are produced by budding and therefore consist of genetically identical individuals, each of which is surrounded by a bilayered exoskeleton, the inner layer calcareous (not always continuous) and the outer layer chitinous. They are suspension feeders, feeding on plankton and bacteria, and are found at all depths.

Bryozoans have so far been less studied than the number of known species (5700) would justify given the range of interesting natural products already isolated from them. This is probably a consequence of the difficulty of harvesting them.

Terpenoids and steroids have been little studied. A number of common mono-, di- and triterpenes (e.g. Cuminol, Neoabietic acid, Ursolic acid or a stereoisomer) were reported from *Conopeum* sp., but this work needs confirmation. The single diterpenoid **Murrayanolide** that has been obtained apart from this work has a unique skeleton which implies that many more unusual terpenoids may exist on other bryozoans. The similarly limited studies of steroid content have yielded only relatively common types based on cholestane methylated in the side chain and/or hydroxylated. One or two anthraquinone pigments have been characterised, of which the most unusual is **Bryoanthrathiophene**.

The most numerous metabolites from bryozoans are defence chemicals, which comprise numerous alkaloids, and the **Bryostatins**, an important series of polyether polyketide toxins with anticancer properties, some of which have also been found in other marine organisms. The ultimate source of these may be *Candidatus* bacteria.

The range of alkaloids is extensive taking into account the limited amount of work that has so far been done. There are simple halogenated phenethylamines (**Convolutamines**, **Volutamides**). Pyrroles and pyrrolidines include **Tambjamines** (originally isolated from animals higher up the food chain, and which could be tetrapyrrole degradation products), **Amathamides**, **Amathaspiramides** and **Convolutamides**. Indoles are mostly brominated simple indoles (**Flusrabromine**, **Alternatamides**) but *Flustra foliacea* yielded a series of **Flustramines** and related alkaloids of the physostigmine type (VX4100) unique in the marine environment. The **Securamines**, **Chartellines** and **Chartellamides** represent a further elaboration of this structural type up to a maximum of seven rings. There are also a number of quinolinequinones, halogenated or bearing thioether substituents (**Perfragilins**, **Caulibugulones**). The presence of nitro groups in a few alkaloids including the purinoid **Phidolopin** is notable.

Kerr, R.G. *et al, Recent Advances in Marine Biotechnology*, (eds. Fingerman, N. *et al*), Science Publishers, USA, 2001, **Vol. 6**, 149–164; Prinsep, M.R., *ibid*, 165–186; Kem, W.R., *ibid*, 187 (*revs*)

3.13 Mollusca (ZV)

This is a diverse and widely distributed phylum of organisms. The body plan is basically nonsegmented and bilateral, although in some molluscs (the gastropods) it is often modified by torsion into a spiral surrounded by a shell. There are well- developed organs inside a more or less thickened outer layer, the mantle, which secretes a shell formed of calcareous matter and protein. This shell may be external, as in the gastropods, internal as in squids, or may be totally lacking (octopuses and nudibranchs). There is generally a muscular foot and a cephalic region which may be highly developed into tentacles and other organs, as in the cephalopods. The alimentary canal is well developed and furnished with a rasping radula used in feeding. Different classes of molluscs show variation in this general body plan, for example the bivalves have a hinged shell, no cephalic region and no radula, and some of them also lack the foot. Many species of mollusc are known, present in marine, freshwater and terrestrial environments, ranging in size from microscopic to very large. They show a wide range of dietary behaviour (carnivores, herbivores, filter feeders and detritus feeders) and undergo a wide range of symbiotic relationship. In particular, in some molluscs the mantle incorporates symbiotic algae providing toxic antipredator substances.

The phylum is usually divided taxonomically into seven unequal classes, but of these four (including Chitons, ZV1000) are numerically limited and have been studied chemically little or not at all. The most important classes both in terms of number of species, economic importance and chemical studies are the gastropods (ZV2000, ZV3000, ZV4000), the bivalves (ZV6000) and the cephalopods (ZV8000). However, the bivalves with their well-developed physical protective mechanism of the double shell, appear to have less need for chemical defence mechanisms and their secondary metabolites are less profuse. They have mostly been studied in terms of their economically important shellfish toxins, which are in fact microbial/dinoflagellates products. The cephalopods too have been rather little studied; their most characteristic metabolites are **Adenochromines**. The most studied organisms chemically have been various types of gastropod which have little or no physical defence and rely almost entirely on chemical defence against predators.

The numerous gastropods are sometimes further divided into three subclasses, the Prosobranchia (ZV2000) the Opisthobranchia (ZV3000) and the Pulmonata (ZV4000). (This division is not recognised by the Catalogue of Life, but since it is a convenient subdivision of a large group of natural product-producing organisms it is followed here). A table of these subdivisions is given in Kornprobst (2005), Chapter 23, which also gives a more detailed description of the secondary metabolites of gastropods organised by class and subclass.

Terpenoids are numerous. The genus *Planaxis* (Gastropoda, Prosobranchia) has provided a series of cembranoids such as **Jeunicin** and **Planaxool**. Among the opisthobranchs, the sea hares or aplysians, which are herbivorous, feed on cyanobacteria and algae, and their digestive systems and mantles contain a wide variety of unchanged and metabolised secondary metabolites which perform an antifeedant function. These alimentary chains are complex and have been much studied. The two most studied genera are *Aplysia* and *Dolabella;* the former feed mostly on red algae and contain many halogenated and nonhalogenated terpenoids (**Kurodainol**, **Aplysin 20**, **Brasilenol**, **Punctatol** and many others), cyclic halogenated ethers (**Dactylyne**, **Aplyparvunin**, etc.), lactones (e.g. **Aplyolides**, **Aplyronines**), and both peptide and nonpeptidal alkaloids (**Aplaminone**). *Dolabella* spp. feed on brown algae, and in accordance with the terpenoid profile shown by these, contain mostly nonhalogenated diterpenoids (**Auriculol**, **Dolatriol**) as well as lactones (**Dolabelides**), peptides (notably the extensive range of highly cytotoxic **Dolastatins**, from cyanobacterial symbiosis) and alkaloids. A few *Aplysia* spp. feed on brown algae and also contain nonhalogenated diterpenes, e.g. **4-Hydroxycrenulide**. Other products isolated from this type of mollusc appear to derive from symbiotic/commensal green algae (**Aplyolides**) and even fungi (**Aplysiatoxin**).

The shell-less nudibranchs can incorporate cnidocysts obtained from cnidarians into their mantle, and also rely heavily on compounds, especially terpenes, ingested in the diet as a means of defence. A wide range of skeletal types have been isolated, and include sponge-derived terpenoid isocyanides and compounds derived metabolically from them, such as the **Acanthenes**, and sponge-derived scalarane sesterterpenoids such as **Deoxoscalarin**. However, nudibranchs also synthesise terpenoids *de novo via* the mevalonate pathway. Many terpenoids are present as glyceryl esters such as the **Anisodorins** and the **Verrucosins**. In general it is possible to predict with a fair degree of accuracy what types of compound (though not necessarily the exact compounds) that will be isolable from nudibranch tissues by studying the prey of the different species. The sacoglossan gastropods also contain a range of terpenoids, but these animals are herbivorous and the terpenoids derive from commensal green algae entering into the tissues (e.g. **Ascobullins**). A number of degraded chlorophylls such as **Chlorophyllone a** have been isolated from bivalve molluscs, which have also yielded modified carotenoids (**Pectenoxanthin**, **Crassostreaxanthins**)

Nudibranchs contain a narrow range of carotenoids (e.g. **Hopkinsiaxanthin**) and steroids (**Lovenone**, a secosteroid, for example). Other defence allomones include quinonoid and related meroterpenoids, and macrocyclic lactones (**Laulimalide**, **Sphinxolides**, the isoxazolide lactone **Kabiramides** and others, some of these at least probably cyanobacterially derived). Also noteworthy is the isolation of prostanoid lactones from *Tethys fimbria*.

The distribution of polyketides in molluscs is patchy. They are found only in some classes of the gastropods, for example the **Auripyrones** (strictly, polypropionates) from *Dolabella*, the **Aglajnes** from *Bulla* spp. which are preyed upon by carnivorous molluscs *Aglaja*, and **Tridachiapyrones** from the herbivourous sacoglossans. Pulmonarians have afforded a number such as **Muamvatin, Maurapyrone C** and the **Onchitriols**.

Long chain aromatic and heteroaromatic metabolites, which do not appear to be derived from the diet, are found in *Navanax* spp. (**Navenones**, which play a role as alarm pheromones), *Haminoea* spp. (**Haminols**) and other genera.

Peptides, especially cyclic oligopeptides often containing unusual amino acid residues, are probably widely distributed and show structural resemblances to similar compounds found further down the food chain, e.g. in sponges. See for example the **Kulolides** from *Philinopsis* spp. Peptides such as the **Kahalalides** have also been isolated from sacoglossans, and **Onchidin** is an example of a cyclic oligopeptide isolated from a pulmonarian. Nudibranchs also contain some characteristic nucleosides such as **Doridosine**.

Among other nitrogenous metabolites, the best-known from gastropods is the dyestuff **6,6'-Dibromoindigotin**, known since ancient times. The genus *Lamellaria* (Gastropoda; Prosobranchia) yielded a wide range of the pyrrole alkaloids. The **Lamellarins**, which, however, are also found in ascidians on which the molluscs feed and in sponges, are probably biosynthesised symbiotically. Other gastropods (nudibranchs) prey on bryozoans, and yield the **Tambjamines**, which are also pyrroles. There are also guanidine alkaloids, e.g. **Triophamine**.

Similarly, the **Kuanoniamines** from *Chelynotus* (Gastropoda; Mesogastropoda) are closely similar to, though not identical with, **Dercitine** and similar alkaloids isolated from sponges. Other compounds isolated bearing a close structural relationship to sponge products include **Jorumycin**, which closely resembles the **Renieramycins** from sponges.

Carnivorous gastropods of the genus *Conus* produce a vast series (there appear to be tens of thousands of chemically distinct compounds) of highly toxic peptides the **Conotoxins**, which are delivered to the prey by means of a highly specialised injecting organ. Other toxic molluscs lack this specialised delivery system and administer

toxins through the radula. Such toxins are complex alkaloids related to **Tetrodotoxin** and **Surugatoxin** and are bacterial products (see also under fish, below).

The bivalve toxins (**Yessotoxins**, **Pectenotoxins**, **Pinnatoxins**, **Azaspiracids**, **Saxitoxins**) responsible for various kinds of shellfish poisoning are mostly produced by commensal dinoflagellates and have been mentioned above. There are differences in the distribution of different members of the saxitoxin series between the tissues of the bivalves and the originating dinoflagellates.

The kidneys of the giant clam *Tridacna maxima* concentrate up to 0.1% of arsenic, the function of which is unknown. It is stored as various dimethylarsinoylribosides.

Cimino, G. *et al, Curr. Org. Chem*., 1999, **3**, 327–372 (*rev, opisthobranchs*)
Molluscs: From Chemico-ecological Study to Biotechnological Application; Progress in Molecular and Submolecular Biology, (eds. Cimino, G. *et al*), Springer, 2006, **Vol. 43** (*book*)

3.14 Echinodermata (ZW)

These organisms are characterised by a radially symmetrical body plan, (which is acquired in the adult stage, the larvae being bilaterally symmetrical) and a unique system of respiration through water-filled tube feet which also provide locomotion. There is a calcareous endoskeleton. This is the largest phylum of exclusively marine animals, with about 7000 species known. They may be herbivores, suspensivores, detritivores, carnivores or necrophages, and the carnivorous species may prey for example on corals or other echinoderms. There are many examples of commensalism and parasitism between echinoderms and other organisms.

Although various classification schemes for echinoderms differ in detail, five main groups are generally recognised. The taxonomy used in this Dictionary follows the Catalogue of Life scheme. The most primitive, widely represented in the fossil record, are the Crinoids (ZW1000) in which the mouth and anus are on the same surface. They have a planktonic larval form followed by an adult form which may be sessile (sea lilies) or mobile (feather stars). The other four groups, in which the mouth and anus are on opposing faces, are the starfish (Asteriodea) (ZW2000), sea urchins (Echinoidea) (ZW3000), sea cucumbers (Holothuroidea) (ZW4000) and brittle stars (Ophiurioidea) (ZW5000).

The presence of steroidal saponins of different types in the starfish and in the sea urchins is unique in the animal kingdom, and serves to delineate them from the other echinoderms and from each other. Other characteristic markers are the dominance of 3α-hydroxylated steroids in the ophiurians, and of quinonoid pigments of different types in the crinoids and in the sea urchins.

The various types of echinoderm produce a variety of specialised polysaccharides, the study of which is still in its infancy. One which has been characterised is **Frondecaside**. The lipid content of sea urchins and ophiurians is high in polyunsaturates. The starfish have been relatively little investigated but appear to follow the same pattern, with some prostanoid precursors. A high proportion of branched-chain acids have been isolated from sea cucumbers, but these are probably of bacterial origin. Phospholipids and glycosphingolipids appear to be universally present in echinoderms and a wide range of structural types of ceramides and cerebrosides have been isolated from starfish (see **Acanthacerebrosides**, **Astrocerebrosides** and similar compounds) and holothuroids.
About 30 different carotenoids have been characterised from sea urchins, mostly from the gonads, including the apocarotenoid **Paracentrone**, and others from ophiuroids (**Ophioxanthin**). The starfish are pigmented by carotenoids derived from the food chain and often modified by the introduction of oxo functions to give pigments of bluer colour, such as **Adonixanthin**.

Throughout the echinoderms, halogenation is rare and found only in a few anthraquinone pigments such as the **Gymnochromes** (from crinoids). There are also few alkaloids of greater complexity than a range of aliphatic amines. The few exceptions to this generalisation are very probably derived from organisms such as dinoflagellates present in the food chain. **Asterina 330** is a mycosporin analogue related to such compounds found in cnidarians. The identification of some unusual sulfur compounds is also noteworthy, for example the **Hedathiosulfonic acids**.

As noted above, the type and extent of steroid content is a major distinguishing feature of different types of echinoderm. The crinoids and echinoids have been little studied, but appear to contain exclusively 'classical' steroid types closely related structurally to cholesterol. The ophiurians, which in some respects are intermediate between the primitive crinoids and the more highly evolved echinoderms, contain many 3α-hydroxysteroids with only one or two glycosides. In the starfish, the range of glycosides and of steroid sulfates is extensive, derived from a wide range of side-chain modified parent steroids, which, however, are mostly 3β-hydroxylated. The side chain may be degraded (e.g. **Asterosterol**, **Hermaphrodiol**) or cyclopropanated (**Acanthasterol**). Polyhydroxylation/

O-sulfation of the steroid nucleus, which is widespread in marine organisms, is at its most extensive here. The glycosides, such as the **Asterosaponins** play a role in chemical defence through their surface-active properties. Both pentose and hexose residues are found.

The holothurians contain many steroids, some biosynthesised *de novo* from acetate via lanostane triterpenes, others apparently derived from the diet. In *Holothuria*, it has been shown that two biosynthetic routes operate, one via **Lanosterol** and the other via **Parkeol**. These biosynthetic routes provide steroids with all combinations of presence or absence of the methyl groups at *C*-4 and *C*-14, as well as side chain variations (cholestane, ergostane and further additional carbons). The chief distinguishing feature of the holothurians, however, is the exclusive occurrence of specialised triterpenoid glycosides of the holostane type, the prototype for which is **Holothurinogenin** but with well over 100 currently known. These appear to be derived biogenetically via Parkeol. A smaller group showing (19→16) lactonisation is based on **Posietogenin**.

Examples of the anthraquinonoid pigments that are readily extracted from crinoids include **Ptilometric acid**. Some of these are O-sulfates, e.g. **Comantherin sulfate**. The sea urchin pigments however are exclusively naphthoquinonoid, e.g. the **Spinochromes**. The number of alkaloid-like compounds isolated from echinoderms is extremely limited, e.g. **Asterina 330** (a palytoxin analogue).

Stonik, V.A. *et al, J. Nat. Toxins*, 1999, **8**, 235-238 (*rev, holothuroid toxins*)
Moore, B.S., *Nat. Prod. Rep*., 2006, **23**, 615-629

3.15 Crustacea (ZX8000)

The crustaceans, including the decapods, are the only type of animals in the vast arthropod phylum (ZX) that occur to any extent in the sea. (There is also the horseshoe crab *Limulus*, an ancient animal related to the arachnids, and which has a few mentions in this Dictionary, and a few saline-tolerant millipedes living in shore environments). In the past the crustaceans have been considered a separate phylum, but they are now often considered a major subphylum of the arthropods having in common the hard chitinous exoskeleton and the body divided into head, thorax and abdomen. About 60,000 species are known, some of them (ostracods, e.g. *Cypridina*, and copepods, e.g. *Calanus*) very small planktonic organisms. The best-known large species are the decapods (crabs and lobsters). **Chitin**, derived industrially from crab shells, is an important industrial material.

Chemical studies on crustaceans have been fragmentary and are mostly confined to their carotenoid pigments, some of which have also been obtained from other marine organisms but which were originally characterised as crustacean products. These are mostly derived by a variety of oxygenations of the terminal rings of the carotenes, and include **Astaxanthin**, **Crustaxanthin**, **Zeaxanthin** and various others.

The moulting hormones of crustaceans are terpenoid (**Methylfarnesate**) and steroidal (**Ecdysone/Crustecdysone**), the latter being common to insects also. Steroid studies have been fragmentary and have indicated a preponderance of cholesterol and closely related compounds. Various endohormones such as testosterone, similar to their mammalian equivalents, have been shown to be present in crustaceans but these are mostly not included in the Dictionary.

The simple pyridine **Homarine** and the arsenical **Arsenobetaine** are widespread in nature but were first isolated from crustaceans.

3.16 Hemichordata (ZY1000)

This is a numerically limited class of animal (about 100 species recorded), consisting of two surviving types of organism; the acorn worms (Enteropneusts) inhabiting temperate and tropical waters, and the pterobranchs, colonial animals inhabiting chitinous tube galleries and found in polar waters. There is differentiation of the body into three well-defined zones, and they have some but not all of the morphological characters that define the chordates. Two types of natural product have been identified from them. The first is a range of toxic cyclohexanes (e.g. **Bromoxone**), halogenated phenols (e.g. **2,4-Dibromophenol**) and halogenated indoles (**Glossobalol**) isolated from *Ptychodera, Balanoglossus* and *Glossobalanus* spp. respectively. These are used by the worms as defence chemicals, and are of environmental significance. Of greater biochemical interest are the highly cytotoxic disteroidal metabolites the **Cephalostatins** from *Cephalodiscus gilchristi.* Owing to the difficulty of culturing hemichordate species, there is no information currently available concerning their possible distribution elsewhere in the phylum, or on their biosynthesis.

3.17 Protochordata (ZY5000)

These simplest chordate animals are generally divided into two unequal groups; the urochordates (tunicates) and the cephalochordates which are free-swimming bilaterally symmetrical animals (*Amphioxus*). Protochordates are the most developed of the invertebrates and have a notochord which is the evolutionary precursor of the spinal column characteristic of the vertebrates. They are exclusively marine. The larger group of urochordates is divided into three classes. Of these, two, including the free-floating salps, have been little investigated.

Most chemical studies have been on the third group, the sessile ascidians or sea squirts. These are filter feeders, often harbouring commensal cyanobacteria and other organisms which may be the true source of some of the reported natural products. Their chemistry is dominated by the presence of an extraordinary range of mostly biologically potent nitrogen compounds. The ascidians also famously accumulate vanadium to a very high concentration in specialised cells, and some have highly acidic tissues (down to pH 1). Other metals are also accumulated, as shown by the presence of **Tunichlorin**, probably the product of metabolism of a commensal organism.

The epidermis of ascidians contains a range of sulfated glycans, including some unusual residues such as L-Iduronic acid, and the unusual polysulfated polymannose **Kakelokelose**. The membrane lipids have been little studied, and presumably are close to those of other higher organisms in structure. A few oxylipins have been isolated, such as **Didemnilactone** and **Lissoclinolide**. Ceramides and cerebrosides appear to be widespread as in the echinoderms, with some unusual types such as **Didemniserinolipids** isolated. Ascidians contain a range of carotenoids, both common ones and some rarer ones such as **Halocynthiaxanthin** and **Amarouciaxanthins** probably derived from metabolic alteration of commoner carotenoids present in the filtered plankton. The steroids so far identified lack the wide structural range shown by the echinoderms and are mostly straightforward cholestanes and ergostanes, with some 5,8-epidioxysteroids and secosteroids, e.g. **Aplidiasterols**. The **Ritterazines** from *Ritterella* have disteroid structures linked by a central pyrazine ring, showing close structural similarity to the cephalostatins from hemichordates.

Non-nitrogenous secondary metabolites are few in number. These include some small acetogenins such as the **Didemnenones**. Terpenoids are rare; the **Haterumaimides** are unusual not only in being diterpenes but also in being chlorinated; however, they may derive from *Prochloron* symbionts. *Ritterella* spp. provided some furanoterpenoids related to Dendrolasin such as **8-Hydroxydendrolasin** but Dendrolasin itself was not present, and the depth of dredging would rule out a sponge symbionts, so their origin is obscure. Several series of meroterpenoids have been isolated, especially from the Polyclinidae, such as the **Verapliquinones** and the structurally complex ansa-compounds the **Longithorones** from *Aplidium*.

Among the nitrogenous metabolites, many of which doubtless also spring from commensal organisms, there is a very wide range of structure including some with, and some without, analogies in other phyla.

Firstly, there is an extensive range of modified peptides and depsipeptides. Several series of these are macrocyclic thiazoles and oxazoles, for example the **Comoramides**, the **Bistratamides**, the **Lissoclinamides** and the **Patellamides**. Other cyclic depsipeptides are more strictly peptide-related, although containing a range of unusual amino acids. The most studied have been the **Didemnins** and their relatives.

Heterocyclic alkaloids are numerous and include the extensive range of pyrroloisoquinolines the **Lamellarins** which were first isolated from molluscs but which are the products of ascidians on which they prey, or possibly of a symbiotic association involving sponges. These, like the **Ningalins**, are probably derived biosynthetically from **DOPA**. Quinoline alkaloids are represented by the **Trididemnic acids** and the basic quinoline ring system is further elaborated into pyridoacridines, e.g. **Ascididemin** and other polycycles. These too are also found in other marine organism classes. In the ascidians they fulfil the role of pigmentation, and are also mostly cytotoxic.

Indole alkaloids are also numerous, again known mostly as polycyclic condensed systems, e.g. **Fascaplysin**. For a fuller count of the numerous ascidian alkaloids, it is necessary to search the main body of the Dictionary.
Ascidians also contain a wide range of sulfur compounds, both sulfur-heterocycles and polysulfides, such as the aromatic **Lissoclinotoxins**.

Davidson, B.S., *Chem. Rev.,* 1993, **93**, 1771–1791 (*rev*)

3.18 Pisces (fish) (ZZ1000)

The fish represent the most numerous of marine vertebrates. They are well studied taxonomically and extensively documented in the online database *Fishbase* (a contributor database to the Catalogue of Life). They can be divided into cartilaginous fishes (e.g. sharks), and the larger category of bony fishes, considered to be the more highly evolved. Their commercially important lipids have been extensively studied; see for example **Squalene**.

The cartilaginous fishes contain a wide range of polyhydroxylated nitrogenous and non-nitrogenous sterols, based on 5β-cholestane. Examples are **Chimaerol** and the important drug **Squalamine**. The colour of different fish is due to the presence of various carotenoids and xanthophylls, including **Astaxanthin**, **Salmoxanthin**, **Idoxanthin** and **Tunaxanthins**.

The sexual development of many species of fish is determined by the presence of steroids in the water. Many of the studies have been on freshwater species such as the goldfish, but 17α,20β-Dihydroxypregn-4-en-3-one as its 20-sulfate is known to be a hormone of the male Atlantic salmon together with Testosterone.

The fish products that have received the most chemical attention, apart from the lipids, are the toxins produced by various species. These may be steroidal (e.g. **Pavoninins**), peptide (**Grammistins**) or alkaloid-like, such as the much-studied **Tetrodotoxin** and its relatives from fugu fish (various species of the Tetraodontidae). The latter, however, are metabolites of *Pseudomonas* bacteria or dinoflagellates in the fish, and are also found in other marine organisms and even terrestrial ones.

Some fish secrete peptide venoms in specialised spines to deter prey. An example is the powerful poison **Stonustoxin** from the stonefish.

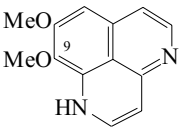
A2 1 A-1

Glycoprotein. Isol. from *Chlorella* sp. Shows antitumour activity. Poorly sol. hexane.

Japan. Pat., 1982, 82 32 224; *CA*, **96**, 223259z (*isol*)

Aaptamine A-2

*8,9-Dimethoxy-1*H-*benzo[*de*][1,6]naphthyridine, 9CI*
[85547-22-4]



$C_{13}H_{12}N_2O_2$ 228.25
Alkaloid from the marine sponge *Aaptos aaptos*. α-Adrenoreceptor blocker. Antineoplastic agent. Brilliant green cryst; bright yellow cryst. (MeOH/Me_2CO) (as hydrochloride). Sol. MeOH, $CHCl_3$.
Mp 110-113° (107°) (hydrochloride). λ_{max} 215 (ϵ 13700); 236 (ϵ 14700); 255 (ϵ 17900); 309 (ϵ 3640); 350 (ϵ 3750); 380 (ϵ 5000); 394 (ϵ 4570) (H_2O) (Derep). λ_{max} 220 (ϵ 8900); 239 (ϵ 11750); 257 (ϵ 13200); 274 (ϵ 9700); 312 (ϵ 3160); 354 (ϵ 3300); 384 (ϵ 5620) (MeOH) (Berdy).

▶ DI2410500

N^4-*Me:* **N^4-*Methylaaptamine***
$C_{14}H_{14}N_2O_2$ 242.277
Alkaloid from *Aaptos* sp. Pale yellow oil. λ_{max} 216 (ϵ 1318); 239 (ϵ 13356); 258 (ϵ 11025); 269 (sh) (ϵ 9522); 277 (sh) (ϵ 8654); 314 (ϵ 2420); 360 (ϵ 2939); 394 (sh) (ϵ 2780) (MeOH).

O^9-*De-Me:* ***Demethylaaptamine***
[88839-98-9]
$C_{12}H_{10}N_2O_2$ 214.223
Alkaloid from *Aaptos aaptos*. Cytotoxic and antimicrobial agent. Greenish-yellow powder + $1.5H_2O$ (as hydrochloride).
Mp 248-251° (dec., sealed tube) (hydrochloride). λ_{max} 241 (ϵ 18300); 313 (ϵ 3890); 370 (ϵ 4470); 400 (ϵ 4130) (H_2O) (Derep).

O^9-*De-Me,* N^1-*Me:* ***Isoaaptamine****. Demethyl-*N-*methylaaptamine*
[117173-75-8]
$C_{13}H_{12}N_2O_2$ 228.25
Alkaloid from the sponges *Aaptos aaptos*, *Hymeniacidon* sp. and *Suberites* sp. Antineoplastic agent and β-glucanase inhibitor.
Amorph. yellow powder.
Mp 200-205° dec.

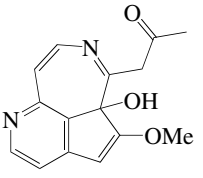
*Di-*O*-de-Me:* ***Dide*-O-*methylaaptamine***
$C_{11}H_8N_2O_2$ 200.196
Isol. from *Aaptos* sp. Yellow solid (as TFA salt). λ_{max} 241 (log ϵ 4.43); 267 (log ϵ 4.19); 313 (log ϵ 3.63); 363 (log ϵ 3.67); 402 (log ϵ 3.58) (no solvent reported).

*Di-*O*-de-Me, 9-sulfate: Dide-*O*-methylaaptamine 9-sulfate*
$C_{11}H_8N_2O_5S$ 280.261
Isol. from *Aaptos* sp. Pale yellow solid (as TFA salt). λ_{max} 216 (log ϵ 4.14); 236 (log ϵ 4.12); 257 (log ϵ 4.18); 310 (log ϵ 3.49); 373 (log ϵ 3.63) (no solvent reported).

Nakamura, H. *et al., Tet. Lett.*, 1982, 5555 (*isol, uv, pmr, cmr, struct*)
Pelletier, J.C. *et al., Tet. Lett.*, 1985, **26**, 1259 (*synth, uv, pmr*)
Kelly, T.R. *et al., Tetrahedron*, 1985, **41**, 3033 (*synth*)
Sakamoto, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 2760 (*synth*)
Bassoli, A. *et al., Chem. Comm.*, 1987, 150 (*synth*)
Nakamura, H. *et al., J.C.S. Perkin 1*, 1987, 173 (*deriv*)
Pelletier, J.C. *et al., J.O.C.*, 1987, **52**, 616 (*synth, ir, pmr*)
Andrew, R.G. *et al., Tetrahedron*, 1987, **43**, 4803 (*synth, uv, ir, pmr, ms*)
Hibino, S. *et al., J.C.S. Perkin 1*, 1988, 2429 (*synth, pmr*)
Fedoreev, S.A. *et al., Khim.-Farm. Zh.*, 1988, **22**, 943-946 (*isol*)
Sova, V.V. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 420-422 (*Demethyl-N-methylaaptamine*)
Balczewski, P. *et al., J.C.S. Perkin 1*, 1990, **31**, 3193 (*synth*)
Molina, P. *et al., Synthesis*, 1996, 1199 (*synth*)
Sugino, E. *et al., Heterocycles*, 1999, **50**, 543-559 (*rev, synth*)
Walz, A.J. *et al., J.O.C.*, 2000, **65**, 8001-8010 (*Isoaaptamine, synth*)
Coutinho, A.F. *et al., Heterocycles*, 2002, **57**, 1265-1272 (N^4-*Methylaaptamine*)
Calcul, L. *et al., Tetrahedron*, 2003, **59**, 6539-6544 (*isol, pmr, cmr*)
Pettit, G.R. *et al., J. Nat. Prod.*, 2004, **67**, 506-509 (*Isoaaptamine, pmr, cmr, cryst struct*)
Pettit, G.R. *et al., J.O.C.*, 2004, **69**, 2251-2256 (*Isoaaptamine, synth*)
Herlt, A. *et al., Tetrahedron*, 2004, **60**, 6101-6104 (*Didemethylaaptamines*)

Aaptosamine A-3

[219642-41-8]

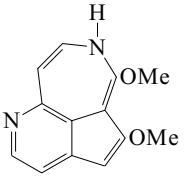


$C_{15}H_{14}N_2O_3$ 270.287
Alkaloid from the sponge *Aaptos aaptos*. Orange gum. λ_{max} 240 (log ϵ 4.01); 336 (log ϵ 3.93) (MeOH).

Tinto, W.F. *et al., Heterocycles*, 1998, **48**, 2089-2093 (*isol, uv, ir, pmr, cmr, ms*)

Aaptosine A-4

*1,9-Dimethoxy-8*H-*5,8-diazabenz*[cd]*azulene, 9CI*
[151041-63-3]

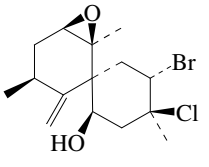


$C_{13}H_{12}N_2O_2$ 228.25
Trace alkaloid from the Red Sea sponge *Aaptos aaptos*. Cytotoxic agent. Yellow oil. λ_{max} 377 (ϵ) (MeOH/HCl) (Derep). λ_{max} 225 (ϵ 9700); 346 (ϵ 3800) (MeOH) (Derep).

Rudi, A. *et al., Tet. Lett.*, 1993, **34**, 4683 (*isol, uv, ir, pmr, cmr, ms, struct*)

12(11 →10)-Abeo-4-bromo-3-chloro-7,8-epoxy-11(13)-chamigren-1-ol A-5

[116498-63-6]



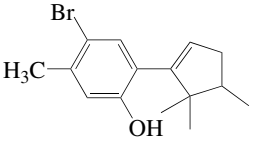
$C_{15}H_{22}BrClO_2$ 349.694
Constit. of a *Laurencia* sp.
$[\alpha]_D$ +67 (c, 0.5 in $CHCl_3$).

Ac: ***Pinnatifate***
[124019-98-3]
$C_{17}H_{24}BrClO_3$ 391.731
Constit. of *Laurencia pinnatifida*.
$[\alpha]_D^{25}$ +61 (c, 0.6 in $CHCl_3$).

Bittner, M.L. *et al., Phytochemistry*, 1985, **24**, 987 (*isol, pmr, cmr*)
Atta-ur-Rahman, *et al., Pure Appl. Chem.*, 1989, **61**, 453 (*Pinnatifate*)

14(7 →10)-Abeo-4-bromo-1,3,5,7-cuparatetraen-1-ol A-6

4-Bromo-5-methyl-2-(4,5,5-trimethylcyclopentenyl)phenol. 1-(5-Bromo-2-hydroxy-4-methylphenyl)-4,5,5-trimethylcyclopentene
[864956-88-7]

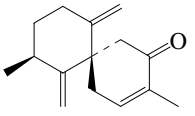


$C_{15}H_{19}BrO$ 295.219
Constit. of *Laurencia microcladia*. Oil. $[\alpha]_D^{20}$ +5 (c, 0.06 in CH_2Cl_2). λ_{max} 237 (log ϵ 3.19); 290 (log ϵ 2.92) (CH_2Cl_2).

Kladi, M. *et al., Tet. Lett.*, 2005, **46**, 5723-5726 (*Laurencia microcladia constit*)

13(11 →10)-Abeo-2,7(14),11-chamigratrien-4-one A-7

3,10-Dimethyl-7,11-dimethylidenespiro[5.5]undec-2-en-4-one
[269075-36-7]

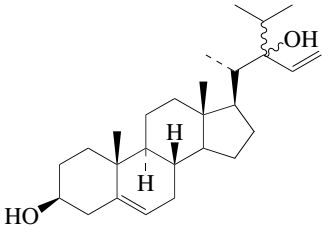


$C_{15}H_{20}O$ 216.322
Constit. of an *Aplysia* sp. Oil. $[\alpha]_D^{20}$ +15 (c, 0.1 in EtOH).

Fedorov, S.N. *et al., Tet. Lett.*, 2000, **41**, 1979-1982 (*isol, pmr, cmr*)

25(24 →22)-Abeocholesta-5,23-diene-3,22-diol A-8

22-Isopropylchola-5,23-diene-3,22-diol (incorr.)
[96386-53-7]

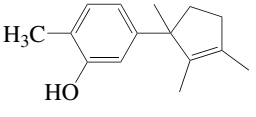


$C_{27}H_{44}O_2$ 400.643
Constit. of the brown alga *Desmarestia aculeata*. Cryst. Mp 127-130°.

Findlay, J.A. *et al., Phytochemistry*, 1985, **24**, 366-367 (*isol, pmr, ms*)

12(11 →10)-Abeo-1,3,5,10-cuparatetraen-2-ol A-9

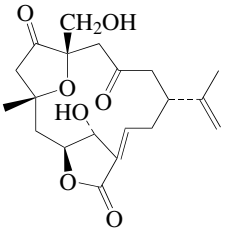
2-Methyl-5-(1,2,3-trimethyl-2-cyclopentenyl)phenol. 3-(3-Hydroxy-4-methylphenyl)-1,2,3-trimethylcyclopentene
[864956-89-8]



$C_{15}H_{20}O$ 216.322
Constit. of *Laurencia microcladia*. Oil. $[\alpha]_D^{20}$ +40 (c, 0.07 in CH_2Cl_2). λ_{max} 235 (log ϵ 2.88); 274 (log ϵ 2.67); 280 (log ϵ 2.55) (CH_2Cl_2).

Kladi, M. *et al., Tet. Lett.*, 2005, **46**, 5723-5726 (*Laurencia microcladia constit*)

18(4 →5)-Abeo-5,8-epoxy-11,18-dihydroxy-3,6-dioxo-12,15-cembradien-20,10-olide A-10

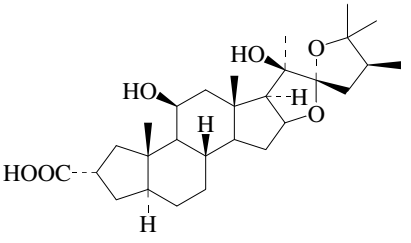


$C_{20}H_{26}O_7$ 378.421

(1R,5R,8R,10S,11R,12Z)-form
Sinulochmodin B
[864685-95-0]
Constit. of *Sinularia lochmodes*. Cryst. Mp 165-166°. $[\alpha]_D^{25}$ -91 (c, 1.5 in Py).

Tseng, Y.-J. *et al., Org. Lett.*, 2005, **7**, 3813-3816 (*Sinulochmodin B, cryst struct*)

4(3 →2)-Abeo-22,25-epoxy-11,20-dihydroxy-24-methylfurostan-3-oic acid A-11

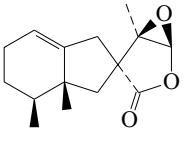


$C_{28}H_{44}O_6$ 476.652

(2α,5α,11β,20R,22S,24S)-form
A-*Nor-22-epihippurin-2-carboxylic acid*
[761430-26-6]
Constit. of *Isis hippuris*. Cryst. Mp 263-264°. $[\alpha]_D^{25}$ -20 (c, 1.04 in MeOH).

Sheu, J.-H. *et al., Tet. Lett.*, 2004, **45**, 6413-6416 (*Isis hippuris constit, cryst struct*)

7(8 →9)-Abeo-11,12-epoxy-1(10)-eremophilen-8,12-olide A-12

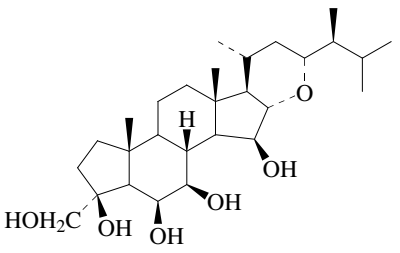


$C_{15}H_{20}O_3$ 248.321

(7α,11β,12β)-form
Palmosalide C
[128255-38-9]
Constit. of *Coelogorgia palmosa*. Cryst. Mp 147-149°.

Weimer, D.F. *et al., Tet. Lett.*, 1990, **31**, 1973 (*cryst struct*)
Hartmann, B. *et al., Tet. Lett.*, 1993, **34**, 1487 (*synth*)
Brocksom, T.J. *et al., J.A.C.S.*, 2002, **124**, 15313-15325 (*synth*)

5(4 →3)-Abeo-16,23-epoxyergostane-3,4,6,7,15-pentol A-13

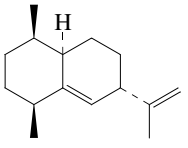


$C_{28}H_{48}O_6$ 480.684

(3β,5α,6β,7β,15β,16α,23*R*,24*S*)-*form*

15-(Methylphosphate), 3-sulfate: [346589-24-0]
$C_{29}H_{51}O_{12}PS$ 654.755
Constit. of a *Cribrochalina* sp. Powder. $[\alpha]_D^{24}$ -18 (c, 0.5 in MeOH).
Fujita, M. *et al., Tetrahedron*, 2001, **57**, 3885-3890 (*isol, pmr, cmr*)

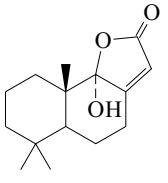
14(10 →1)-Abeo-5,11-eudesmadiene A-14



$C_{15}H_{24}$ 204.355

(1β,4β,7α,10α)-*form* [860641-45-8]
Constit. of *Nephthea hainansis.*
Oil. $[\alpha]_D^{25}$ +9.71 (c, 0.27 in $CHCl_3$).
Li, G.Q. *et al., Chin. Chem. Lett.*, 2005, **16**, 494-496 (*Nephthea hainansis constit*)

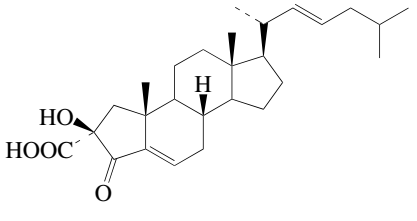
11(9 →12)-Abeo-9-hydroxy-8(12)drimen-11,9-olide A-15



$C_{15}H_{22}O_3$ 250.337

9α-*form* [174720-20-8]
Constit. of *Dysidea fragilis* from the lagoon of Venice.
Aiello, A. *et al., Biochem. Syst. Ecol.*, 1996, **24**, 37-42 (*isol, pmr, cmr*)

4(3 →2)-Abeo-2-hydroxy-4-oxocholesta-5,22-dien-3-oic acid A-16
2-Carboxy-2-hydroxy-A-*norcholesta-5,22-dien-4-one*



$C_{27}H_{40}O_4$ 428.611

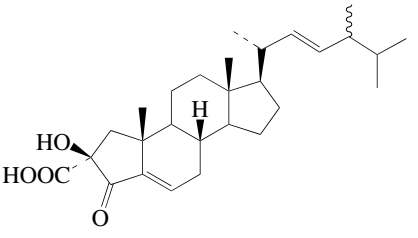
(2β*OH*,22*E*)-*form*

Et ester: [848123-88-6]
$C_{29}H_{44}O_4$ 456.664
Constit. of a *Dendronephthya* sp. Amorph. solid. $[\alpha]_D^{25}$ -17.4 (c, 0.4 in $CHCl_3$).

22,23-Dihydro: 4(3 →2)-Abeo-2-hydroxy-4-oxocholesta-5-en-3-oic acid. 2-Carboxy-2-hydroxy-A-*norcholest-5-en-4-one*
$C_{27}H_{42}O_4$ 430.626

22,23-Dihydro, Et ester: [848123-86-4]
$C_{29}H_{46}O_4$ 458.68
Constit. of a *Dendronephthya* sp. Amorph. solid. $[\alpha]_D^{25}$ -20.8 (c, 0.8 in $CHCl_3$).
Li, G. *et al., Steroids*, 2005, **70**, 13-18 (*Dendronephthya constits*)

4(3 →2)-Abeo-2-hydroxy-4-oxoergosta-5,22-dien-3-oic acid A-17
2-Carboxy-2-hydroxy-A-*norergosta-5,22-dien-4-one*

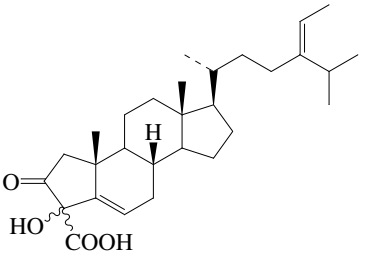


$C_{28}H_{42}O_4$ 442.637

(2β*OH*,22*E*,24ξ)-*form*

Et ester: [848137-19-9]
$C_{30}H_{46}O_4$ 470.691
Constit. of a *Dendronephthya* sp. Amorph. solid. $[\alpha]_D^{25}$ -16.3 (c, 0.6 in $CHCl_3$).
Li, G. *et al., Steroids*, 2005, **70**, 13-18 (*Dendronephthya constit*)

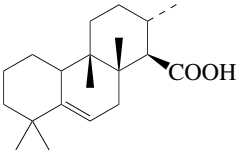
4(3 →2)-Abeo-4-hydroxy-2-oxostigmasta-5,24(28)-dien-3-oic acid A-18



$C_{29}H_{44}O_4$ 456.664

Et ester: [677758-18-8]
$C_{31}H_{48}O_4$ 484.718
Constit. of *Sargassum carpophyllum.*
Tang, H. *et al., Zhongguo Haiyang Yaowu*, 2003, **22**, 28-30; *CA*, **140**, 318008h (*isol, pmr, cmr*)

20(10 →9)-Abeo-5-isocopalen-15-oic acid A-19



$C_{20}H_{32}O_2$ 304.472

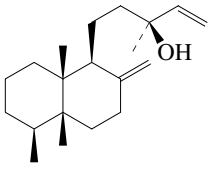
*(3-Acetoxy-2-hydroxypropyl) ester (*S-*):* ***Verrucosin A***
[115713-02-5]
$C_{25}H_{40}O_5$ 420.588
Isol. from the dorid nudibranch *Doris verrucosa*. Ichthyotoxic agent. Sol. MeOH, Me_2CO, Et_2O. $[\alpha]_D$ +37.3 (c, 1,1 in $CHCl_3$).

*(2-Acetoxy-3-hydroxypropyl) ester (*R-*):* ***Verrucosin B***
[115712-99-7]
$C_{25}H_{40}O_5$ 420.588
Constit. of *Doris verrucosa*. Ichthyotoxic agent. Cryst. (Et_2O/hexane). Sol. MeOH, Me_2CO, Et_2O.
Mp 118-120°. $[\alpha]_D$ +19.2 (c, 0.5 in $CHCl_3$).

Cimino, G. *et al., Tetrahedron*, 1988, **44**, 2301-2310 (*isol, pmr, cmr, cryst struct*)
Gavagnin, M. *et al., Tet. Lett.*, 1990, **31**, 6093-6094 (*stereochem*)
Fontana, A. *et al., Eur. J. Org. Chem.*, 2003, 3104-3108 (*biosynth*)

19(4 →5)-Abeo-8(17),14-labdadien-13-ol A-20

8(17),14-Thelopogadien-13-ol

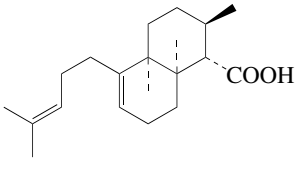


$C_{20}H_{34}O$ 290.488

(4β,13S)-form
Nakamurol A
[174756-40-2]
Constit. of *Agelas nakamurai*.
Oil. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{25}$ +39.1 (c, 1.6 in $CHCl_3$).

Shoji, N. *et al., J. Nat. Prod.*, 1996, **59**, 448-450 (*isol, pmr, cmr*)
Bonjoch, J. *et al., Tet. Lett.*, 2000, **41**, 5669-5672 (*synth*)
Díaz, S. *et al., J.O.C.*, 2003, **68**, 7400-7406 (*synth, abs config*)

20(10 →9)-Abeo-4,5-seco-3,5(10)-isocopaladien-15-oic acid A-21



$C_{20}H_{32}O_2$ 304.472

(ent-13βH)-form

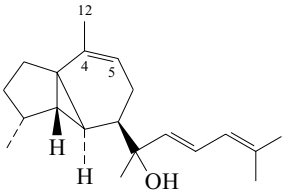
*(2-Acetoxy-3-hydroxypropyl)ester (*S-*):* ***Verrucosin 8***
[183239-53-4]
$C_{25}H_{40}O_5$ 420.588
Constit. of *Doris verrucosa*. Protein kinase C activator. Morphogenetic hydra tentacle regeneration agent. $[\alpha]_D$ +41.5 (c, 0.05 in $CHCl_3$).

*(3-Acetoxy-2-hydroxypropyl)ester (*S-*):* ***Verrucosin 3***
[183239-55-6]
$C_{25}H_{40}O_5$ 420.588
Constit. of *Doris verrucosa*. Protein kinase C activator. Morphogenetic hydra tentacle regeneration agent. Tumour promoter. $[\alpha]_D$ +46.8 (c, 2.4 in $CHCl_3$).

De Petrocellis, L. *et al., Experientia*, 1996, **52**, 874-877 (*isol*)
Gavagnin, M. *et al., Tetrahedron*, 1997, **53**, 1491-1504 (*isol, pmr, cmr*)

8(4 →10)-Abeo-4,15,17-spatatrien-13-ol A-22

[117928-75-3]

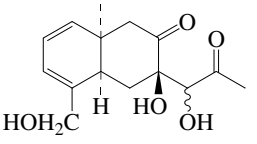


$C_{20}H_{30}O$ 286.456
Compds. not named by the authors. Metab. of *Dilophus okamurai*. Antifeedant. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ -8.13 (c, 1.15 in $CHCl_3$). λ_{max} 232 (ϵ 31000); 247 (ϵ 23000) (EtOH) (Berdy).

$\Delta^{4,12}$-Isomer: ***8(4 →10)-Abeo-4(12),15,17-spatatrien-13-ol***
[132216-17-2]
$C_{20}H_{30}O$ 286.456
Metab. of *Dilophus okamurai*. Antifeedant. Oil. $[\alpha]_D$ +50.7 (c, 0.025 in $CHCl_3$).

Kurata, K. *et al., Chem. Lett.*, 1988, 1629-1632 (*isol, pmr, cmr*)
Kurata, K. *et al., Phytochemistry*, 1990, **29**, 3453-3455 (*isol, pmr, cmr*)

13(11 →12)-Abeo-7,11,15-trihydroxy-1,3-eudesmadiene-8,12-dione A-23



$C_{15}H_{20}O_5$ 280.32

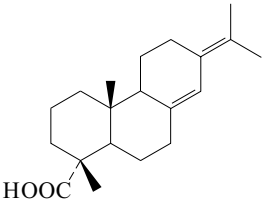
(5α,7βOH,10α,11ξ)-form

15-Ac: ***Tubiporone***
[385793-38-4]
$C_{17}H_{22}O_6$ 322.357
Constit. of *Tubipora musica*. Oil. $[\alpha]_D^{25}$ +3.4 (c, 0.03 in $CHCl_3$). λ_{max} 262 (log ϵ 3.26) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2001, **64**, 1430-1433 (*isol, pmr, cmr*)

8(14),13(15)-Abietadien-18-oic acid A-24

Neoabietic acid
[471-77-2]



$C_{20}H_{30}O_2$ 302.456
Isol. from resins of *Pinus* spp., *Abies* spp. and *Agathis microstachya*. Also detected in the Black Sea bryozoan *Conopeum seuratum*. Cryst. (EtOH aq.).
Mp 173-173.5° (167-169°) (sealed tube under N_2). $[\alpha]_D^{25}$ +161.6 (c, 2.5 in 95% EtOH). Air-sensitive. Dextrosapinic acid was a mixt. of Abietic and Neoabietic acids.

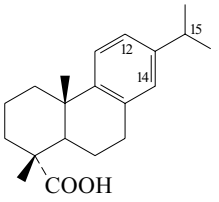
► TP8740000

Harris, G.C. *et al., J.A.C.S.*, 1948, **70**, 334; 339
Schuller, W. *et al., J.A.C.S.*, 1961, **83**, 2563 (*isol, props, struct*)
Carman, R.M. *et al., Aust. J. Chem.*, 1966, **19**, 2403 (*isol*)

Hadjieva, P. *et al., Z. Naturforsch., C*, 1987, **42**, 1019-1022 (*occur, Conopeum*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NBU800

8,11,13-Abietatrien-18-oic acid A-25

Dehydroabietic acid
[1740-19-8]



$C_{20}H_{28}O_2$ 300.44
Constit. of *Pinus* and *Cedrus* spp. Also from *Abies sachalinensis* and *Cistus labdaniferus*. EBV-EA activation inhibitor. Cryst. (EtOH aq.).
Mp 172-173°. $[\alpha]_D^{20}$ +62 (EtOH). λ_{max} 218; 243; 252; 270; 278 (EtOH) (Berdy).

▶ TP8710000

Me ester: [1235-74-1]
$C_{21}H_{30}O_2$ 314.467
Constit. of *Cistus labdaniferus* and *Pinus* spp. Also detected in the Black Sea bryozoan *Conopeum seuratum*. Cryst. (EtOH).
Mp 62-63°. $Bp_{0.2}$ 152-154°. $[\alpha]_D^{20}$ +60 (EtOH).

Et ester:
$C_{22}H_{32}O_2$ 328.494
Isol. from *Bugula turrita*.

Propyl or isopropyl ester:
$C_{23}H_{34}O_2$ 342.52
Detected in bryozoan *Conopeum seuratum*.

15-Hydroxy: See 8,11,13-Abietatriene-15,18-diol in *The Combined Chemical Dictionary.*

15-Hydroperoxy: 15-Hydroperoxy-8,11,13-abietatrien-18-oic acid. 15-Hydroperoxydehydroabietic acid
$C_{20}H_{28}O_4$ 332.439
Constit. of *Pinus* spp.

12-Chloro: 12-Chloro-8,11,13-abietatrien-18-oic acid. 12-Chloro-dehydroabietic acid
[65310-45-4]
$C_{20}H_{27}ClO_2$ 334.885
Found in kraft papermill effluent. Fish poison. Cryst. (hexane).
Mp 178-180°.

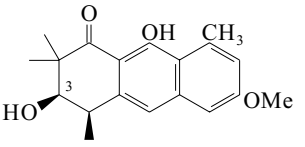
14-Chloro: 14-Chloro-8,11,13-abietatrien-18-oic acid. 14-Chloro-dehydroabietic acid
[65281-76-7]
$C_{20}H_{27}ClO_2$ 334.885
Found in kraft papermill effluent. Fish toxicant. Cryst. (pentane).
Mp 159-160°.

12,14-Dichloro: 12,14-Dichloro-8,11,13-abietatrien-18-oic acid. 12,14-Dichlorodehydroabietic acid
[65281-77-8]
$C_{20}H_{26}Cl_2O_2$ 369.33
Found in kraft papermill effluent. Fish toxin. Cryst. (hexane).
Mp 219-220°.

Tabacik-Wlotzka, C. *et al., Bull. Soc. Chim. Fr.*, 1964, 618 (*isol*)
Ireland, R.E. *et al., J.O.C.*, 1966, **31**, 2543 (*synth*)
Narayanan, C.R. *et al., Tet. Lett.*, 1968, 1565 (*pmr*)
Welch, S.C. *et al., Synth. Commun.*, 1976, **6**, 27 (*synth*)
Meyer, W.L. *et al., J.O.C.*, 1977, **42**, 2769 (*synth*)
Kutney, J.P. *et al., Helv. Chim. Acta*, 1982, **65**, 1343; 1351 (*Chlorodehydroabietic acids*)
Hadijeva, P. *et al., Z. Naturforsch., C*, 1987, **42**, 1019-1022 (*Me ester, propyl ester, occur, Conopeum*)
Shao, L.P. *et al., Phytochemistry*, 1995, **38**, 853 (*15-Hydroperoxydehydroabietic acid*)
Anderson, K.B. *et al., Synth. Commun.*, 1998, **28**, 1375-1380 (*synth*)
Kinouchi, Y. *et al., J. Nat. Prod.*, 2000, **63**, 817-820 (*activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DAK400

Abietinarin A A-26

[127476-27-1]

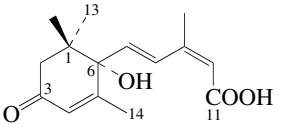


$C_{19}H_{22}O_4$ 314.38
Metab. of an *Abietinaria* sp. Cytotoxic. Yellow amorph. solid.

3-Epimer: ***Abietinarin B***
[128571-56-2]
$C_{19}H_{22}O_4$ 314.38
Metab. of an *Abietinaria* sp. Cytotoxic. Yellow amorph. solid.
Pathirana, C. *et al., Can. J. Chem.*, 1990, **68**, 394 (*isol, pmr*)

Abscisic acid A-27

5-(1-Hydroxy-2,6,6-trimethyl-4-oxo-2-cyclohexen-1-yl)-3-methyl-2,4-pentadienoic acid, 9CI. Abscisin II. Dormin
[7773-56-0]
[2228-72-0, 52392-36-6]



(*S*)-*form*

$C_{15}H_{20}O_4$ 264.321
Terpenoid (cyclofarnesane) numbering shown. Other schemes freq. encountered. λ_{max} 252 (ϵ 25200) (no solvent reported) (Derep). λ_{max} 244 (ϵ 25000) (EtOH/NaOH) (Derep). λ_{max} 245 (sh); 260 (ϵ 21300) (EtOH) (Derep).

▶ RZ2475100

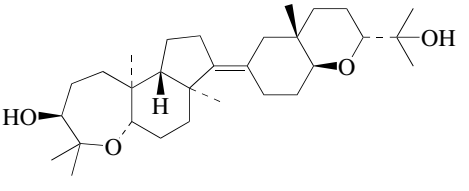
(S)-form [21293-29-8]
[72029-68-6, 72029-69-7]
Constit. of sycamore, birch, rose, cabbage, potato, lemon etc. Also from the fungus *Curvularia lunata* isol. from the marine sponge *Niphates olemda*. Used to regulate fruit ripening. Abscission-accelerating substance. Plays a role in plant signal transduction and pest resistance of plants. Antagonist of plant growth hormones. Cryst. ($CHCl_3$/petrol).
Mp 160-161°. $[\alpha]_D$ +430. The incorrect abs. config. was formerly assigned.

[6735-04-2, 6755-41-5, 14398-53-9, 14674-85-2, 40331-02-0, 58801-55-1, 69350-43-2, 69350-44-3, 78340-30-4, 79199-48-7, 97806-70-7]

Jadulco, R. *et al., J. Nat. Prod.*, 2002, **65**, 730-733 (*Niphates olemda constit*)

Abudinol A-28

[205750-26-1]

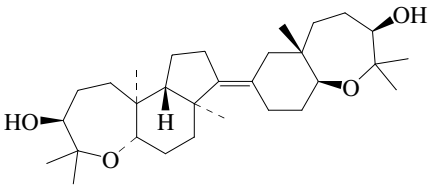


$C_{30}H_{50}O_4$ 474.723
Constit. of *Ptilocaulis spiculifer*.

Rudi, A. *et al., Tet. Lett.*, 1998, **39**, 1445-1448 (*isol, pmr, cmr, cryst struct*)

Abudinol B A-29

[233607-64-2]

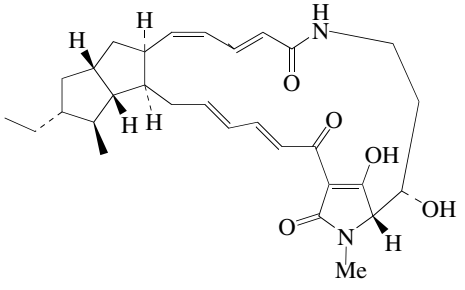


$C_{30}H_{50}O_4$ 474.723
Constit. of *Ptilocaulis spiculifer*. Oil. $[\alpha]_D$ -5 (c, 0.05 in MeOH).

Rudi, A. *et al., Tetrahedron*, 1999, **55**, 5555-5566 (*isol, pmr, cmr*)

Aburatubolactam A A-30

[170894-24-3]



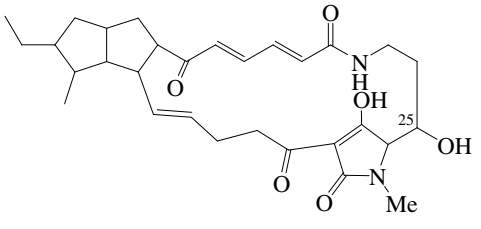
$C_{30}H_{40}N_2O_5$ 508.656

Tetramic acid deriv. Closely related to Alteramide A, A-217. Prod. by *Streptomyces* sp. SCRC-A20 from a marine mollusc. Cytotoxic agent, apoptosis inducer. Inhibitor of superoxide anion generation.

Japan. Pat., 1995, 95 228 583; *CA*, **123**, 337551v (*isol*)
Bae, M.-A *et al., Heterocycl. Commun.*, 1996, **2**, 315-318 (*isol, pmr, struct*)

Aburatubolactam B A-31

[170894-25-4]

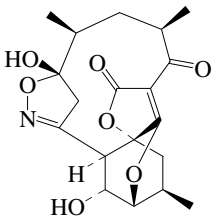


$C_{30}H_{40}N_2O_6$ 524.656
Prod. by *Streptomyces* sp. SCRC A-20. Antiinflammatory and cytotoxic agent. Cryst. $[\alpha]_D$ +197 (Py).

25-Deoxy: ***Aburatubolactam C***
[170894-26-5]
$C_{30}H_{40}N_2O_5$ 508.656
Prod. by *Streptomyces* sp. SCRC A-20. Apoptosis-inducing substance. Antiinflammatory and cytotoxic agent. Powder. $[\alpha]_D$ +136 (Py).

Japan. Pat., 1995, 95 228 583; *CA*, **123**, 337551v
Bae, M.-A. *et al., J. Microb. Biotechnol.*, 1998, **8**, 455-460

Abyssomicin B A-32

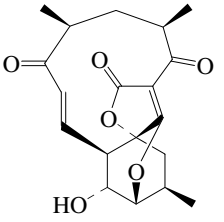


Absolute Configuration

$C_{19}H_{23}NO_7$ 377.393
Prod. by *Verrucosispora* sp. AB 18-032. Powder.

Bister, B. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 2574-2576 (*struct*)
Riedlinger, J. *et al., J. Antibiot.*, 2004, **57**, 271-279 (*isol, activity*)

Abyssomicin C A-33

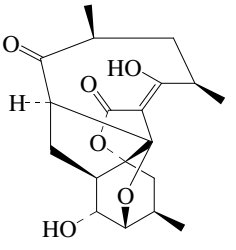


Absolute Configuration

$C_{19}H_{22}O_6$ 346.379
Prod. by *Verrucosispora* sp. AB 18-032. Inhibitor of the *p*-Aminobenzoic acid/tetrahydrofolate biosynthetic pathway. Antibacterial agent. Powder.

Bister, B. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 2574-2576 (*pmr, cmr, ms*)
Riedlinger, J. *et al., J. Antibiot.*, 2004, **57**, 271-279 (*isol, activity*)
Nicolaou, K.C. *et al., Angew. Chem., Int. Ed.*, 2006, **45**, 3256-3260 (*synth*)
Couladouros, E.A. *et al., Tetrahedron*, 2006, **62**, 5272-5279 (*synth*)

Abyssomicin D A-34

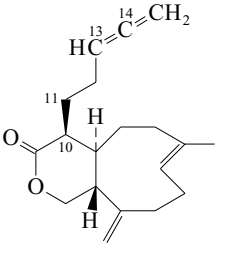


$C_{19}H_{24}O_6$ 348.395
Prod. by *Verrucosispora* sp. AB 18-032. Powder.

Bister, B. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 2574-2576 (*struct*)
Riedlinger, J. *et al., J. Antibiot.*, 2004, **57**, 271-279 (*isol, activity*)

Acalycixeniolide B A-35

[113021-56-0]



$C_{19}H_{26}O_2$ 286.413

Constit. of gorgonian *Acalycigorgia inermis*. Inhibits cell division in fertilised starfish eggs. λ_{max} 225 (ϵ 10000) (MeOH) (Derep).

13,14-Dihydro: ***Acalycixeniolide A***
[113021-55-9]
$C_{19}H_{28}O_2$ 288.429
Isol. from *Acalycigorgia inermis*. Inhibitor of starfish egg division. Amorph. powder. $[\alpha]_D$ +143 (c, 0.31 in $CHCl_3$). λ_{max} 225 (ϵ 10000) (MeOH) (Derep).

*10,11*E*-Didehydro:* ***Acalycixeniolide C***†
[121769-80-0]
$C_{19}H_{24}O_2$ 284.397
From *Acalycigorgia* sp. Cytotoxic inhibitor of starfish egg division. Oil. $[\alpha]_D$ +208 (c, 0.20 in $CHCl_3$). λ_{max} 206 (ϵ 1100) (EtOH) (Berdy).

6α,7α-Epoxide: ***Acalycixeniolide C***†
[259657-90-4]
$C_{19}H_{26}O_3$ 302.413
Constit. of *Acalycigorgia inermis*. Amorph. solid.
Mp 91-93°. $[\alpha]_D^{25}$ +43.2 (c, 0.4 in MeOH).

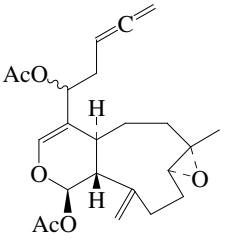
*6α,7α-Epoxide, 10,11*E*-didehydro:* ***Acalycixeniolide D***
[259658-04-3]
$C_{19}H_{24}O_3$ 300.397
Constit. of *Acalycigorgia inermis*. Amorph. solid.
Mp 87-90°. $[\alpha]_D^{25}$ +162.7 (c, 0.1 in MeOH). λ_{max} 220 (log ϵ 3.75) (MeOH).

10-Epimer: ***Acalycixeniolide B′***
[121842-78-2]
$C_{19}H_{26}O_2$ 286.413
Constit. of *Acalycigorgia* sp. Oil. $[\alpha]_D$ +15 (c, 0.25 in $CHCl_3$).

Fusetani, Y. *et al., Tet. Lett.*, 1987, **28**, 5837
Fusetani, Y. *et al., Tetrahedron*, 1989, **45**, 1647
Rho, J.-R. *et al., J. Nat. Prod.*, 2000, **63**, 254-257 (*Acalycixeniolides C and D*)

Acalycixeniolide E A-36

[259658-05-4]

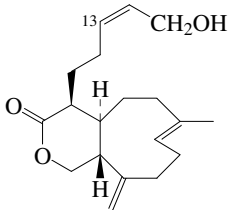


$C_{23}H_{30}O_6$ 402.486
Constit. of *Acalycigorgia inermis*. Gum. $[\alpha]_D^{25}$ +41.5 (c, 0.3 in MeOH).

Rho, J.-R. *et al., J. Nat. Prod.*, 2000, **63**, 254-257 (*isol, pmr, cmr*)

Acalycixeniolide K A-37

[340156-19-6]



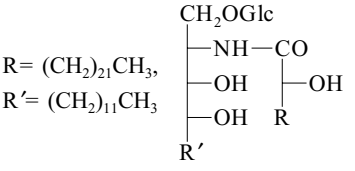
$C_{19}H_{28}O_3$ 304.428
Constit. of *Acalycigorgia inermis*. Amorph. solid.
Mp 127-129°. $[\alpha]_D^{25}$ +36.8 (c, 0.1 in MeOH).

*13*E*-Isomer:* ***Acalycixeniolide L***
[340156-20-9]
$C_{19}H_{28}O_3$ 304.428
Constit. of *Acalycigorgia inermis*. Amorph. solid.
Mp 137-140°. $[\alpha]_D^{25}$ +47 (c, 0.12 in MeOH).

Rho, J.-R. *et al., J. Nat. Prod.*, 2001, **64**, 540-543 (*isol, pmr, cmr*)

Acanthacerebroside A A-38

1-Glucopyranosyl-2-(2-hydroxytetracosanoylamino)-1,3,4-hexadecanetriol
[110744-71-3]



$C_{46}H_{91}NO_{10}$ 818.226
Cerebroside from the starfish *Acanthaster planci*. Needles + $3H_2O$ (MeOH). Poorly sol. H_2O, Me_2CO.
Mp 209-210°. $[\alpha]_D$ +2.4 (c, 0.81 in propanol).

Kawano, Y. *et al., Annalen*, 1988, 19-24 (*isol, pmr, cmr, struct*)
Sugiyama, S. *et al., Annalen*, 1988, 619-625; 1990, 1063-1068 (*abs config, synth*)

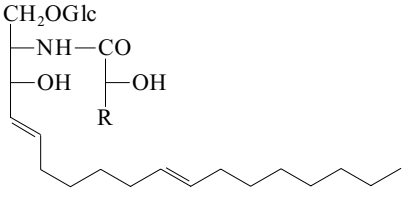
Acanthacerebroside C A-39

1-Glucopyranosyl-2-(2-hydroxyhexadecanoylamino)-13-docosene-1,3,4-triol
[110744-73-5]
As Acanthacerebroside A, A-38 with
R = $(CH_2)_{13}CH_3$, R′ = $-(CH_2)_8CH{=}CH(CH_2)_7CH_3$ (*Z*-)
$C_{44}H_{85}NO_{10}$ 788.156
Cerebroside from the starfish *Acanthaster planci*. Needles (MeOH). Poorly sol. H_2O, Me_2CO.
Mp 203-204°. $[\alpha]_D$ +18.3 (c, 1.24 in propanol).

Kawano, Y. *et al., Annalen*, 1988, 19-24 (*isol, pmr, cmr, struct*)
Sugiyama, S. *et al., Annalen*, 1988, 619-625 (*abs config*)

Acanthacerebroside D A-40

[110744-74-6]



R = $-(CH_2)_{19}CH_3$

$C_{46}H_{87}NO_9$ 798.195
Cerebroside from the starfish *Acanthaster planci*. Needles + $2H_2O$ (MeOH). Poorly sol. H_2O, Me_2CO.
Mp 198-199°. $[\alpha]_D$ +1.1 (c, 0.3 in propanol).

Kawano, Y. *et al., Annalen*, 1988, 19-24 (*isol, pmr, cmr, struct*)
Sugiyama, S. *et al., Annalen*, 1988, 619-625 (*abs config*)

Acanthacerebroside E A-41

[110744-75-7]
As Acanthacerebroside D, A-40 with
R = $-(CH_2)_{20}CH_3$
$C_{47}H_{89}NO_9$ 812.221
Cerebroside from the starfish *Acanthaster planci*. Needles + $3H_2O$ (MeOH). Poorly sol. H_2O, Me_2CO.
Mp 194-195°. $[\alpha]_D$ +1 (c, 0.3 in propanol).

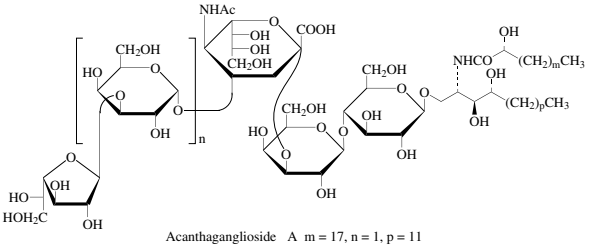
Kawano, Y. *et al., Annalen*, 1988, 19-24 (*isol, pmr, cmr, struct*)
Sugiyama, S. *et al., Annalen*, 1988, 619-625 (*abs config*)

Acanthacerebroside F A-42

[110744-76-8]
As Acanthacerebroside D, A-40 with
R = $(CH_2)_{21}CH_3$
$C_{48}H_{91}NO_9$ 826.248
Cerebroside from the starfish *Acanthaster planci*. Needles + $2H_2O$ (MeOH). Poorly sol. H_2O, Me_2CO.
Mp 193-194°. $[\alpha]_D$ +1.2 (c, 0.5 in propanol).

Kawano, Y. *et al., Annalen*, 1988, 19-24 (*isol, pmr, cmr, struct*)
Sugiyama, S. *et al., Annalen*, 1988, 619-625 (*abs config*)

Acanthagangliosides A-H A-43



Acanthaganglioside A m = 17, n = 1, p = 11
B m = 13, n = 1, p = 17
C m = 21, n = 1, p = 11
D m = 13, n = 2, p = 17
E m = 21, n = 2, p = 11
F m = 18, n = 1, p = 11
G m = 20, n = 1, p = 11
H m = 21, n = 1, p = 12

Glycosphingolipid complex. Struct. revised in 1997. Constit. of the water soluble lipid fraction of the starfish *Acanthaster planci*.

Acanthaganglioside A [121038-38-8]
$C_{71}H_{130}N_2O_{33}$ 1539.802
Needles (MeOH aq.). Mp 156-158°. $[\alpha]_D^{25}$ +27.9 (c, 0.2 in MeOH aq.).

Acanthaganglioside B [121038-37-7]
$C_{73}H_{134}N_2O_{33}$ 1567.855
Needles (MeOH aq.). Mp 155-157°. $[\alpha]_D^{25}$ +16.7 (c, 0.2 in MeOH aq.).

Acanthaganglioside C [121038-31-1]
$C_{75}H_{138}N_2O_{33}$ 1595.909
Needles (MeOH aq.). Mp 157-159°. $[\alpha]_D^{25}$ +19.4 (c, 0.2 in MeOH aq.).

Acanthaganglioside D [121038-32-2]
$C_{79}H_{144}N_2O_{38}$ 1729.997
Needles (MeOH aq.). Mp 161-163°. $[\alpha]_D^{25}$ +10.3 (c, 0.2 in MeOH aq.).

Acanthaganglioside E [121038-33-3]
$C_{81}H_{148}N_2O_{38}$ 1758.051
Needles (MeOH aq.). Mp 164-166°. $[\alpha]_D^{25}$ +8.1 (c, 0.2 in MeOH aq.).

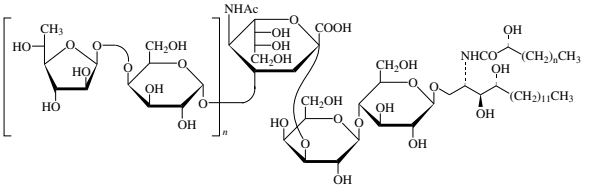
Acanthaganglioside F
$C_{72}H_{132}N_2O_{33}$ 1553.828
Amorph. powder. Mp 160-162° dec. $[\alpha]_D^{27}$ +10 (c, 0.08 in $CHCl_3$/MeOH).

Acanthaganglioside G
$C_{74}H_{136}N_2O_{33}$ 1581.882
Amorph. powder. Mp 163-165° dec. $[\alpha]_D^{27}$ +16.8 (c, 0.3 in $CHCl_3$/MeOH).

Acanthaganglioside H
$C_{76}H_{140}N_2O_{33}$ 1609.936
Amorph. powder. Mp 163-165° dec. $[\alpha]_D^{27}$ +15.5 (c, 0.5 in $CHCl_3$/MeOH).

Kawano, Y. *et al., Annalen*, 1990, 43 (*isol*)
Miyamoto, T. *et al., Liebigs Ann./Recl.*, 1997, 931-936 (*isol, pmr, ms, struct*)

Acanthagangliosides I-J A-44



Acanthaganglioside I, n = 19
J, n = 21

Differ from Acanthagangliosides A-H, A-43 in having a terminal 4-fucofuranosyl residue in place of 3-galactofuranosyl. Isol. from lipid fraction of the starfish *Acanthaster planci*.

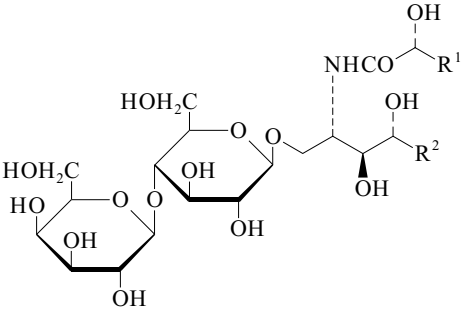
Acanthaganglioside I
Amorph. powder. Mp 159-161° dec. $[\alpha]_D^{24}$ +33 (c, 0.024 in $CHCl_3$).

Acanthaganglioside J
Amorph. powder. Mp 170-172° dec. $[\alpha]_D^{24}$ +40.8 (c, 0.015 in $CHCl_3$/MeOH 1:1).

Miyamoto, T. *et al., Eur. J. Org. Chem.*, 2000, 2295-2301 (*isol, pmr, cmr, struct*)

Acanthalactoside A A-45

[116635-90-6]



R^1 = $(CH_2)_{21}CH_3$, R^2 = $(CH_2)_{11}CH_3$

$C_{52}H_{101}NO_{15}$ 980.368
Constit. of the starfish *Acanthaster planci*. Needles + $2H_2O$ (MeOH).
Mp 196-198°. $[\alpha]_D$ +5.3 (c, 0.8 in $CHCl_3$/MeOH).

Kawano, Y. *et al., Annalen*, 1988, 1181-1183 (*isol, struct*)
Sugiyama, S. *et al., Annalen*, 1991, 349-356 (*synth*)

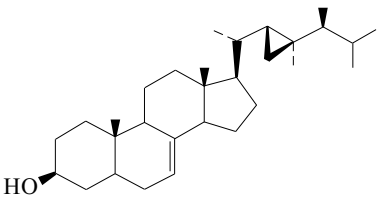
Acanthalactoside B A-46

[116635-91-7]
As Acanthalactoside A, A-45 with
R^1 = $-(CH_2)_{13}CH_3$, R^2 = $-(CH_2)_8CH{=}CH(CH_2)_7CH_3$(*Z*-)
$C_{50}H_{95}NO_{15}$ 950.298
Constit. of the starfish *Acanthaster planci*. Needles + $1H_2O$ (MeOH).
Mp 188-190°. $[\alpha]_D$ +8.5 (c, 0.5 in $CHCl_3$/MeOH).

Kawano, Y. *et al., Annalen*, 1988, 1181-1183 (*isol, struct*)

Acanthasterol A-47

Acansterol
[31653-84-6]

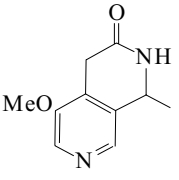


$C_{30}H_{50}O$ 426.724
Constit. of *Acanthaster planci*. Cryst.
Mp 179-180°. $[\alpha]_D^{21}$ +5 ($CHCl_3$).

Gupta, K.C. *et al., Tetrahedron*, 1968, **24**, 5831 (*isol*)
Sheikh, Y.M. *et al., Chem. Comm.*, 1971, 217 (*isol*)

Acanthicifoline A-48

[76193-60-7]

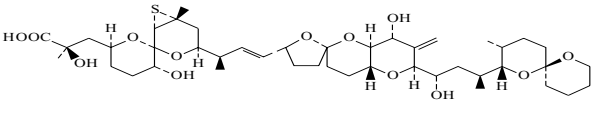


$C_{10}H_{12}N_2O_2$ 192.217
Alkaloid from *Acanthus ilicifolius* (Acanthaceae).
Mp 168-170°. $[\alpha]_D^{24}$ -31.6 ($CHCl_3$).

Tiwara, K.P. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1980, **54**, 857 (*isol, uv, ir, pmr, ms, struct*)

Acanthifolicin A-49

Acanthifolic acid
[77739-71-0]

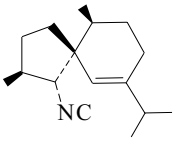


$C_{44}H_{68}O_{13}S$ 837.079
Polyether antibiotic. From *Pandaros acanthifolium*, prob. a metab. of a symbiotic bacterium. Shows cytotoxic and antitumour activity. Useful as growth stimulant or in treatment of coccidiosis. Ichthyotoxin. Phycotoxin. Protein phosphatase inhibitor. Smooth muscle contractor. Ionophoric agent. Cryst. ($CHCl_3/C_6H_6$). Sol. MeOH, hexane; poorly sol. H_2O, hexane. Mp 167-169°. $[\alpha]_D$ +25.3 (c, 0.08 in $CHCl_3$).
▶ LD_{50} (mus, ivn) 0.14 mg/kg.

Schmitz, F.J. *et al., J.A.C.S.*, 1981, **103**, 2467 (*isol, cryst struct, spectra*)
U.S. Pat., 1981, 4 302 470; *CA*, **96**, 74612 (*isol, props*)

Acanthisonitrile 3 A-50

[112766-99-1]



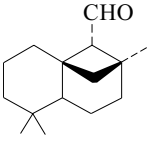
$C_{16}H_{25}N$ 231.38
Metab. of marine sponge *Acanthella acuta*. Oil. $[\alpha]_D$ -31.5 (c, 1.2 in $CHCl_3$).

Isothiocyanate: ***Acanthisothiocyanate 3***
[112767-00-7]
$C_{16}H_{25}NS$ 263.446
Metab. of *Acanthella acuta*. Oil. $[\alpha]_D$ -12.9 (c, 0.3 in $CHCl_3$). Has -NCS replacing -NC.

Mayol, L. *et al., Tetrahedron*, 1987, **43**, 5381-5388

Acanthodoral A-51

[90857-63-9]



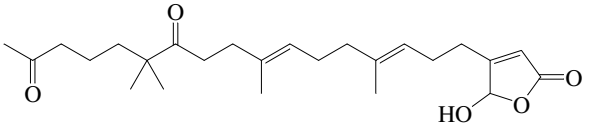
$C_{15}H_{24}O$ 220.354
Constit. of *Acanthodoris nanaimoensis.*
$[\alpha]_D^{22}$ +15.2 (c, 0.23 in $CHCl_3$). Optical rotation of natural product not detd., rotation refers to synthetic material.

4-Bromophenylurethane:
Cryst. (hexane). Mp 109-110°.

Ayer, S.W. *et al., J.O.C.*, 1984, **49**, 2653-2654 (*isol*)
Zhang, L. *et al., Org. Lett.*, 2004, **6**, 537-540 (*synth*)

Acantholide C A-52

[799808-30-3]

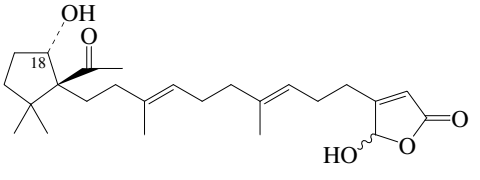


$C_{25}H_{38}O_5$ 418.572
Constit. of an *Acanthodendrilla* sp. Oil. $[\alpha]_D$ -58.2 (c, 1 in $CHCl_3$). λ_{max} 210 (MeOH).

Elkhayat, E. *et al., J. Nat. Prod.*, 2004, **67**, 1809-1817 (*isol, pmr, cmr*)

Acantholide D A-53

[799808-32-5]



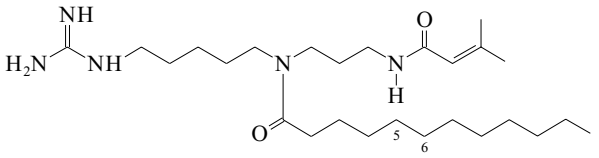
$C_{25}H_{38}O_5$ 418.572
Constit. of an *Acanthodendrilla* sp. Oil. $[\alpha]_D$ -21.6 (c, 1 in $CHCl_3$). λ_{max} 213 (MeOH).

18-Epimer: ***Acantholide E***
[799808-34-7]
$C_{25}H_{38}O_5$ 418.572
Constit. of an *Acanthodendrilla* sp. Oil. $[\alpha]_D$ -41.2 (c, 1 in $CHCl_3$). λ_{max} 212 (MeOH).

Elkhayat, E. *et al., J. Nat. Prod.*, 2004, **67**, 1809-1817 (*isol, pmr, cmr*)

3,5-Acarnidine A-54

$C_{12:0}$-Acarnidine
[67534-25-2]



$C_{26}H_{51}N_5O_2$ 465.721
Isol. from the sponge *Acarnus erithacus* as part of an inseparable mixt. Possesses broad antimicrobial activity and modest antiviral activity.

5,6Z-Didehydro: ***$C_{12:1}$-Acarnidine***
[67534-26-3]
$C_{26}H_{49}N_5O_2$ 463.705
Component of *Acarnus erithacus* acarnidine mixt. λ_{max} 218 (ϵ 17000) (no solvent reported) (Derep).

N-*Dedodecanoyl,* N-*(5Z,8Z,11Z-tetradecatrienoyl):* ***$C_{14:3}$-Acarnidine***
[67534-27-4]
$C_{28}H_{49}N_5O_2$ 487.727
Isol. from *Acarnus erithacus.*

Carter, G.T. *et al., J.A.C.S.*, 1978, **100**, 4302-4304 (*isol, ir, pmr, cmr, ms, struct*)
Yorke, S.C. *et al., Aust. J. Chem.*, 1986, **39**, 447-455 (*synth*)

ACE inhibitor peptide C 105 A-55

C 105
[144357-25-5]
H-Ser-Val-Ala-Lys-Leu-Glu-Lys-OH
$C_{34}H_{63}N_9O_{11}$ 773.925
Isol. from the intestine of the bonito fish. Angiotensin I-converting enzyme inhibitor.

Matsumura, N. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1743 (*isol, struct*)

ACE inhibitor peptide C 107 A-56

C 107
[143936-45-2]
H-Ala-Leu-Pro-His-Ala-OH
$C_{23}H_{37}N_7O_6$ 507.589
Isol. from the intestine of the bonito fish. Angiotensin I-converting enzyme inhibitor.

Matsumura, N. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1743 (*isol, struct*)

ACE inhibitor peptide C 111 A-57

C 111
[146935-77-5]
H-Gly-Val-Tyr-Pro-His-Lys-OH
$C_{33}H_{49}N_9O_8$ 699.806
Isol. from the liver of the bonito fish. Angiotensin I-converting enzyme inhibitor. Sol. H_2O.

Matsumura, N. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1743 (*isol, struct*)

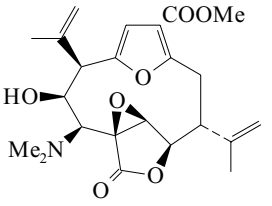
ACE inhibitor peptide C 112 A-58

C 112
[148162-36-1]
H-Ile-Arg-Pro-Val-Gln-OH
$C_{27}H_{49}N_9O_7$ 611.74
Isol. from the intestine of the bonito fish. Angiotensin I-converting enzyme inhibitor.

Matsumura, N. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1743 (*isol, struct*)

Aceropterine A-59

[176227-10-4]



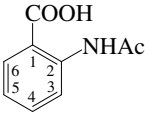
Relative configuration

$C_{23}H_{29}NO_7$ 431.485
Alkaloid from the Caribbean sea plume *Pseudopterogorgia acerosa*.
$[\alpha]_D$ +0.44 (c, 2.0 in $CHCl_3$). Closely related to Tobagolide, T-347 and Pseudopterolide, P-680. λ_{max} 258 (ϵ 3750) (MeOH) (Berdy).

Rodríguez, A.D. *et al., Tet. Lett.*, 1996, **37**, 2687 (*isol, pmr, cmr, ms, struct*)

2-Acetamidobenzoic acid A-60

2-(Acetylamino)benzoic acid, 9CI. N-*Acetylanthranilic acid. Lappaconitic acid*
[89-52-1]



$C_9H_9NO_3$ 179.175
Needles (AcOH). Mp 185°. pK_a 5.64.
▶ LD_{50} (mus, orl) 1114 mg/kg. CB2455000

Me ester: [2719-08-6]
$C_{10}H_{11}NO_3$ 193.202
Needles (EtOH). Mp 101°.

Et ester: [20628-20-0]
$C_{11}H_{13}NO_3$ 207.229
Needles (EtOH). Mp 64-65°.

Amide: 2-Acetamidobenzamide. 2-(Acetylamino)benzamide. ***Antibiotic NP 101A****. NP 101A*
[33809-77-7]
$C_9H_{10}N_2O_2$ 178.19
Prod. by *Streptomyces aurantiogriseus* and *Cytophaga marinoflava* sp. AM13.1. Antifungal agent. Needles (EtOH). Sol. MeOH, EtOH, EtOAc, C_6H_6, DMSO, Py; poorly sol. H_2O.
Mp 177°. Exists in two cryst. forms, accounting for unreliable melting point determinations. λ_{max} 219 (log ϵ 3.56); 252 (log ϵ 3.31); 299 (log ϵ 2.72) (MeOH). λ_{max} 219 (ϵ 3630); 252 (ϵ 2042); 299 (ϵ 550) (MeOH) (Berdy).
▶ CU8702020

N-*Ac: Diacetylanthranilic acid*
$C_{11}H_{11}NO_4$ 221.212
Prisms (EtOH). Mp 180°.

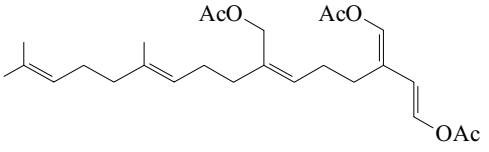
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 356D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1362B (*nmr*)
Matsuo, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 990 (*nmr*)
Erikson, J. *et al., J. Chem. Educ.*, 1972, **49**, 688 (*synth*)
Matsuda, V. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 430 (*synth*)
Ger. Pat., 1976, 2 556 590; *CA*, **85**, 160115 (*synth*)
Errede, L.A. *et al., J.C.S. Perkin 2*, 1981, 233-238 (*Acetamidobenzamide*)
Phay, N. *et al., J. Antibiot.*, 1996, **49**, 703-705 (*Acetamidobenzamide*)
Shaaban, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*Cytophaga marinoflava isol*)

2-[(2-Acetamidopropanoyl)amino]benzamide A-61

N^2-*[2-(Acetylamino)propanoyl]anthranilamide.* N^2-*Acetylalanylanthranilamide*
$C_{12}H_{15}N_3O_3$ 249.269

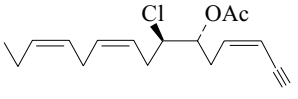
(S)-form
Antibiotic NI 15501A. *NI 15501A*
[208345-44-2]
Prod. by the marine fungus *Penicillium* sp. NI15501.
Solid. Sol. MeOH, butanol; poorly sol. H_2O. $[\alpha]_D^{30}$ -62.8 (c, 0.15 in MeOH). λ_{max} 216 (ϵ 12000); 253 (ϵ 6100); 290 (ϵ 1800) (MeOH).
Onuki, H. *et al., J. Antibiot.*, 1998, **51**, 442-444 (*isol, uv, ir, pmr, cmr, ms*)

1-Acetoxy-7-acetoxymethyl-3-acetoxymethylene-11,15-dimethyl-1,6,10,14-hexadecatetraene **A-62**



$C_{26}H_{38}O_6$ 446.583
Compd. not named in the paper, not indexed by*CA*. Metab. of *Penicillus dumetosus*. Antibacterial and antifungal. Oil. $[\alpha]_D^{25}$ +17 (c, 1.3 in $CHCl_3$).
Paul, V.J. *et al., Tetrahedron*, 1984, **40**, 2913

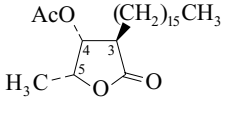
6-Acetoxy-7-chloro-3,9,12-pentadecatrien-1-yne **A-63**



$C_{17}H_{23}ClO_2$ 294.82

(3Z,6R,7R,9Z,12Z)-form
Metab. of *Laurencia pinnatifida*.
Oil. $[\alpha]_D^{25}$ +4.54 (c, 11.0 in $CHCl_3$).
Gonzalez, A.G. *et al., Tetrahedron*, 1982, **38**, 1009

4-Acetoxy-3-hexadecyldihydro-5-methyl-2(3*H*)-furanone **A-64**
3-Acetoxy-2-hexadecyl-4-pentanolide



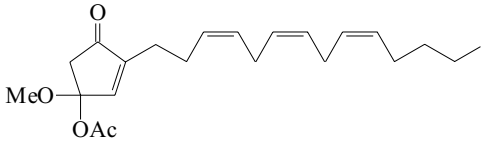
(3*R**,4*R**,5*R**)–*form*

$C_{23}H_{42}O_4$ 382.582

(3R*,4R*,5R*)-form [81601-89-0]
Constit. of the gorgonian *Plexaura flava*.
Oil. $[\alpha]_D$ +31.9 (c, 1.3 in CH_2Cl_2).

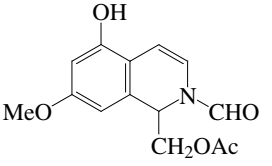
(3R*,4S*,5R*)-form [81601-90-3]
Constit. of *Plexaura flava*.
$[\alpha]_D^{20}$ -32.5 (c, 1.6 in CH_2Cl_2).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 105 (*isol, ir, pmr, ms*)
Sibi, M.P. *et al., J.O.C.*, 1996, **61**, 7848 (*synth*)

4-Acetoxy-4-methoxy-2-(3,6,9-tetradecatrienyl)-2-cyclopenten-1-one **A-65**
[156992-93-7]



$C_{22}H_{32}O_4$ 360.492
Constit. of the sea pen *Virgularia* sp. Unstable oil. $[\alpha]_D$ +12.05 (c, 0.9 in $CHCl_3$). Incorrect MF and name in CA.
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 55 (*isol, ir, pmr, cmr*)

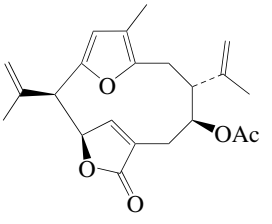
1-(Acetoxymethyl)-2-formyl-1,2-dihydro-5-hydroxy-7-methoxyisoquinoline **A-66**



$C_{14}H_{15}NO_5$ 277.276

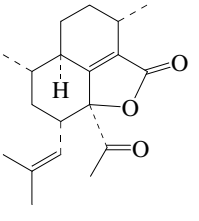
(+)-form
Alkaloid from the sponge *Petrosia similis*.
Amorph. solid. $[\alpha]_D^{25}$ +208 (c, 0.72 in $CHCl_3$). λ_{max} 224 (ϵ 6660); 228 (ϵ 6680); 231 (ϵ 6650); 299 (ϵ 4790) (MeOH).
Ramesh, P. *et al., J. Nat. Prod.*, 1999, **62**, 780-781 (*isol, uv, pmr, cmr, ms*)

12-Acetoxypseudopterolide **A-67**
[264268-02-2]



$C_{22}H_{26}O_5$ 370.444
Constit. of *Pseudopterogorgia elisabethae*. Yellow gum. $[\alpha]_D^{20}$ +18 (c, 0.9 in $CHCl_3$). Trivial name is misleading. λ_{max} 246 (log ϵ 2.68) (MeOH).
Ata, A. *et al., Heterocycles*, 2000, **53**, 717-722 (*isol*)

4-Acetylamphilectolide **A-68**
[325691-49-4]

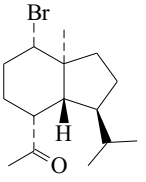


$C_{19}H_{26}O_3$ 302.413
Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{25}$ -277 (c, 0.3 in $CHCl_3$). λ_{max} 206 (ϵ 9100); 232 (ϵ 10500) (MeOH).
Rodríguez, A.D. *et al., Tetrahedron*, 2000, **56**, 9015-9023 (*isol, pmr, cmr*)

7-Acetyl-4-bromo-1-isopropyl-3*a*-methylindane A-69

*1-(7-Bromo-7*a*-methyl-3-(1-methylethyl)octahydro-1*H*-inden-4-yl)ethanone*

[149492-40-0]



$C_{15}H_{25}BrO$ 301.266

Constit. of *Laurencia marianensis*. Cryst.

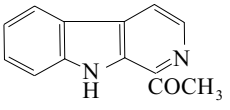
Mp 49-53°. $[\alpha]_D$ -13 (c, 0.1 in $CHCl_3$).

de Nys, R. *et al., Aust. J. Chem.*, 1993, **46**, 933 (*isol, pmr, cmr*)

1-Acetyl-β-carboline A-70

*1-(9*H*-Pyrido[3,4-*b*]indol-1-yl)ethanone, 9CI*

[50892-83-6]



$C_{13}H_{10}N_2O$ 210.235

The compd. lycii Alkaloid I, isol. from several plant spp. and erroneously assigned the struct. N^9-Formylharman, has now been shown by Bracher *et al* to be identical with 1-Acetyl-β-carboline. Alkaloid from the bark of *Ailanthus malabarica* (Simaroubaceae). Also isol. from the sponge *Tedania ignis*.

Light yellow solid.

Mp 203-205°.

N^2-*Oxide:*

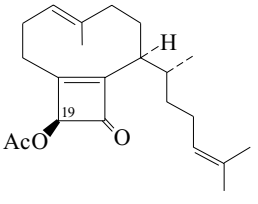
$C_{13}H_{10}N_2O_2$ 226.234

Mp 180°.

Joshi, B.S. *et al., Heterocycles*, 1977, **7**, 193 (*isol, uv, ir, pmr, ms, struct*)
Dillman, R.L. *et al., J. Nat. Prod.*, 1991, **54**, 1056-1061; 1141 (*isol, sponge, ir, pmr, cmr, ms*)
Bracher, F. *et al., Annalen*, 1993, 837; 1335 (*synth, pmr, cmr, lycii Alkaloid I*)
Bracher, F. *et al., Synth. Commun.*, 1995, **25**, 1557 (*synth*)
Zhou, T.-S. *et al., Phytochemistry*, 1998, **49**, 1807-1809 (*isol, uv, ir, pmr, cmr*)
Kast, O. *et al., Synth. Commun.*, 2003, **33**, 3843-3850 (N^2-*oxide*)

Acetylcoriacenone A-71

[85612-73-3]



$C_{22}H_{32}O_3$ 344.493

Constit. of *Pachydictyon coriaceum*. Oil. λ_{max} 229 (ε 6500) (EtOH) (Berdy).

19-Epimer: ***Isoacetylcoriacenone***

$C_{22}H_{32}O_3$ 344.493

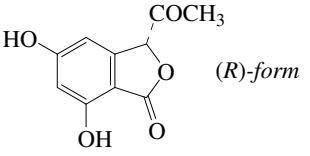
Constit. of *Pachydictyon coriaceum*. Oil. λ_{max} 229 (ε 6500) (EtOH) (Berdy).

Ishitsuka, M. *et al., J.O.C.*, 1983, **48**, 1937

3-Acetyl-5,7-dihydroxy-1(3*H*)-isobenzofuranone A-72

Acetophthalidin

[71089-07-1]



$C_{10}H_8O_5$ 208.17

Readily isomerises to 3,4-Dihydro-3,4,6,8-tetrahydroxy-3-methyl-1*H*-2-benzopyran-1-one, D-585. λ_{max} 223 (ε 14130); 225 (sh) (ε 13680); 258 (ε 10580); 294 (ε 4305) (MeOH). λ_{max} 223 (ε 14130); 258 (ε 10580); 294 (ε 4305) (MeOH) (Berdy).

(*R*)-*form* [205056-68-4]

Powder. Mp 189-201° dec. $[\alpha]_D^{20}$ +23 (c, 0.89 in EtOAc).

(*S*)-*form* [205056-72-0]

Synthetic.

Powder. Mp 190-201° dec. $[\alpha]_D^{20}$ -27 (c, 0.72 in EtOAc).

(±)-*form*

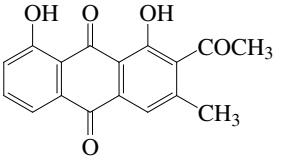
Prod. by a fungus isol. from a marine sediment. Inhibitor of mammalian cell cycle. Powder.

Mp 213-215° dec.(195°-205°).

Grove, J.F. *et al., J.C.S. Perkin 1*, 1979, 337 (*synth*)
Cui, C.-B. *et al., J. Antibiot.*, 1996, **49**, 216 (*isol, uv, ir, pmr, cmr*)
Watanabe, H. *et al., Heterocycles*, 1997, **46**, 45-48 (*synth*)
Nomoto, S. *et al., Liebigs Ann./Recl.*, 1997, 721 (*synth, ir, pmr, cmr*)
Uchida, K. *et al., Heterocycles*, 1998, **48**, 2049-2060 (*synth*)

2-Acetyl-1,8-dihydroxy-3-methylanthraquinone A-73

2-Acetyl-1,8-dihydroxy-3-methyl-9,10-anthracenedione, 9CI. ***2-Acetylchrysophanol***



$C_{17}H_{12}O_5$ 296.279

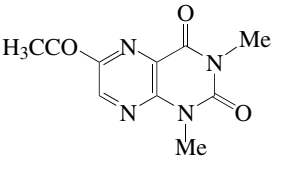
Prod. by the marine-derived *Streptomyces* sp. Mei 6-1,2.

Laatsch, H. *et al., Dissertation*, Univ. of Göttingen, 2005,

6-Acetyl-1,3-dimethyl-2,4(1*H*,3*H*)-pteridinedione, 9CI A-74

6-Acetyl-1,3-dimethyllumazine

[94591-18-1]



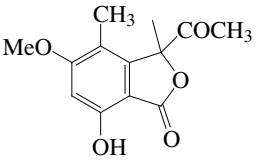
$C_{10}H_{10}N_4O_3$ 234.214

Isol. from the marine polychaete worm *Odontosyllis undecimdonta*. Needles (MeOH).

Mp 177-178° (173°).

Kakoi, H. *et al., Heterocycles*, 1995, **41**, 789-797 (*isol, synth, pmr, cmr*)

3-Acetyl-7-hydroxy-5-methoxy-3,4-dimethyl-1(3*H*)-isobenzofuranone A-75



$C_{13}H_{14}O_5$ 250.251

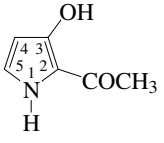
(+)-*form*

Prod. by *Halorosellinia oceanica* BCC 5149.
Needles. $[\alpha]_D^{29}$ +200 (c, 0.05 in EtOH). λ_{max} 216; 260; 303 (EtOH).

Chinworrungsee, M. *et al., J.C.S. Perkin 1*, 2002, 2473-2476 (*isol, pmr, cmr*)

2-Acetyl-3-hydroxy-1*H*-pyrrole A-76

*1-(3-Hydroxy-1*H*-pyrrol-2-yl)ethanone*



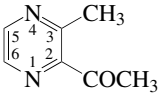
$C_6H_7NO_2$ 125.127

O-*[β-D-Fucopyranosyl-(1→3)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranoside]:*
$C_{30}H_{47}NO_{18}$ 709.697
Alkaloid from the starfish *Asterina pectinifera*. Amorph. powder.
Mp 240-245°. $[\alpha]_D^{18}$ +0.2 (c, 0.3 in MeOH).

Zhang, L.-X. *et al., Nat. Prod. Res.*, 2006, **20**, 229-233 (*isol, pmr, cmr, ms*)

2-Acetyl-3-methylpyrazine A-77

1-(3-Methylpyrazinyl)ethanone, 9CI. Methyl (3-methylpyrazinyl) ketone, 8CI
[23787-80-6]

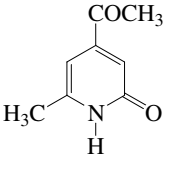


$C_7H_8N_2O$ 136.153
Present in spiny lobster *Panulirus argus*. Liq. with burnt, popcorn-like odour. d 1.11. $Bp_{0.5}$ 56°. n_D^{20} 1.5216. Odour threshold 2×10^{-2} ppm in H_2O.

Mookherjee, B.D. *et al., J.O.C.*, 1972, **37**, 511-513 (*synth, ir, pmr, ms*)
Wolt, J. *et al., J.O.C.*, 1975, **40**, 1178-1179 (*synth, pmr, ms*)
Mihara, S. *et al., J. Agric. Food Chem.*, 1988, **36**, 1242-1247 (*props*)
Nakamura, S. *et al., Agric. Biol. Chem.*, 1989, **53**, 1891-1899 (*glc, occur*)
Cadwallader, K.R. *et al., J. Agric. Food Chem.*, 1995, **43**, 2432-2437 (*detn, occur*)

4-Acetyl-6-methyl-2(1*H*)-pyridinone A-78

4-Acetyl-2-hydroxy-6-methylpyridine. ***Streptokordin***



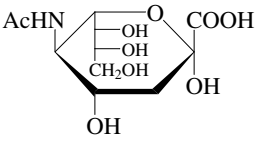
$C_8H_9NO_2$ 151.165

Prod. by a marine-derived *Streptomyces* sp. KORDI-3238.
Cytotoxic. Amorph. powder. λ_{max} 217 (ε 10500) (MeOH).

Jeong, S.-Y. *et al., J. Antibiot.*, 2006, **59**, 234-240 (*isol, pmr, cmr*)

N-Acetylneuraminic acid A-79

*5-(Acetylamino)-3,5-dideoxy-D-*glycero-*D-*galacto-*2-nonulosonic acid, 9CI.* O-*Sialic acid.* ***Aceneuramic acid, INN****. Lactaminic acid. Gynaminic acid. Serolactaminic acid. KI 111. NANA. Neu5Ac. Neu5NAc*
[131-48-6]



α-D-Pyranose-*form*

$C_{11}H_{19}NO_9$ 309.272

See also Sialic acids, S-172. Isol. from eggs, milk, colostrum, submaxillary mucin and meconium by acid or enzymic hydrol. of the constit. sialoproteins and oligosaccharides. Present in urine of patients with sialuria. Most abundant source is Collocalia mucoid, the nest cementing glycoprotein substance of the Chinese Swiftlet. Occurs in sialic acids of the starfish *Asterias rubens*. Chiral synthon. Antiinflammatory, antiviral and antitussive agent. Involved with blood protein half-life regulation, bacterial adhesion, toxin neutralisation, glycoprotein lytic protection.
Mp 185-187° dec. $[\alpha]_D^{22}$ -32 (H_2O). The only sialic acid formed in human tissues. Store below 0° in the dark.

α-Pyranose-*form*

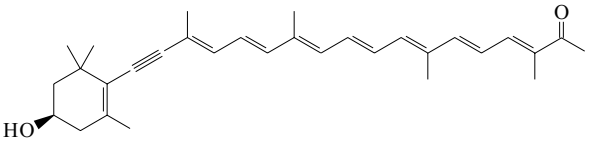
8-Me ether: [41341-17-7]
$C_{12}H_{21}NO_9$ 323.299
Occurs in gangliosides of the starfish *Distolasterias nipon* and *Patiria pectinifera*.

8-Me ether, 9-Ac: [141364-03-6]
$C_{14}H_{23}NO_{10}$ 365.336
Occurs in sialic acids of the starfish *Asterias rubens.*

[19342-33-7, 126934-33-6]

Kochetkov, N.K. *et al., Carbohydr. Res.*, 1973, **27**, 5-10 (*8-Me ether, occur*)
Kochetkov, N.K. *et al., Biochim. Biophys. Acta*, 1983, **759**, 192-198 (*8-Me ether, occur*)
Bergwerff, A.A. *et al., Biochimie*, 1992, **74**, 25-37 (*occur, 8-Me ether, 8-Me ether 9-Ac*)

12-(Acetyloxy)-10-[(acetyloxy)methylene]-6-methyl-2-(4-methyl-3-pentenyl)-2,6,11-dodecatrienal, 9CI A-80



$C_{24}H_{34}O_5$ 402.53

(2*E*)-*form*

Metab. of *Penicillus dumetosus.*
Oil.

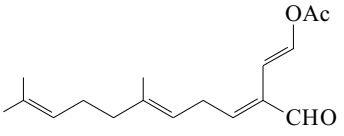
(2*Z*)-*form*

Metab. of *Penicillus dumetosus.*
Oil.

Paul, V.J. *et al., Tetrahedron*, 1984, **40**, 2913

2-[2-(Acetyloxy)ethenyl]-6,10-dimethyl-2,5,9-undecatrienal, 9CI A-81

[93888-67-6]

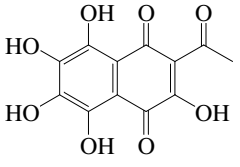


$C_{17}H_{24}O_3$ 276.375
Metab. of algae *Penicillus capitatus* and *Udotea cyathiformis*. Antibacterial and ichthyotoxin. Oil.

Paul, V.J. *et al., Tetrahedron*, 1984, **40**, 2913

2-Acetyl-3,5,6,7,8-pentahydroxy-1,4-naphthoquinone A-82

2-Acetyl-3,5,6,7,8-pentahydroxy-1,4-naphthalenedione, 9CI. Spinochrome C. Spinochrome F1. Spinone A. Isoechinochrome
[3468-83-5]



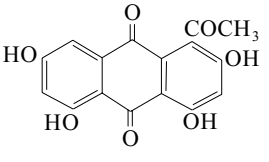
$C_{12}H_8O_8$ 280.19
Isol. from sea urchins *Paracentrotus (Strongylocentrotus) lividus, Echinometra oblonga, Hemicentrotus* and *Acacia* spp. Red cryst. (MeOH).
Mp 246-248°. λ_{max} 240 (ϵ 13200); 285 (ϵ 16300); 463 (ϵ 5900); 504 (ϵ 4600) (EtOH) (Berdy).

3,6,7-Tri-Me ether:
$C_{15}H_{14}O_8$ 322.271
Cryst. Mp 116-117°.

Kuhn, R. *et al., Ber.*, 1939, **72**, 1407; 1941, **74**, 1594-1598 (*isol*)
Lederer, E. *et al., Biochim. Biophys. Acta*, 1952, **9**, 92-101 (*isol*)
Singh, I. *et al., J.A.C.S.*, 1965, **87**, 4023-4024 (*synth*)
Singh, I. *et al., Tetrahedron*, 1968, **24**, 2969-2978 (*synth*)
Miyauchi, T. *et al., Proc. Jpn. Acad.*, 1970, **46**, 1032-1035 (*isol*)

1-Acetyl-2,4,5,7-tetrahydroxyanthraquinone A-83

Rhodolamprometrin
[37850-99-0]



$C_{16}H_{10}O_7$ 314.251
Constit. of the crinoids *Lamprometra klunzingeri* and *Comatula solaris*, also from cultures of *Trichoderma* sp. Red solid (MeOH) or red prisms.
Mp 327° dec. (224-226°). λ_{max} 224 (ϵ 51280); 255 (ϵ 41690); 263 (ϵ 43650); 294 (ϵ 20900); 316 (ϵ 7940); 365 (ϵ 5250); 457 (ϵ 4070) (MeOH) (Berdy).

Tetra-Me ether:
$C_{20}H_{18}O_7$ 370.358
Cryst. (MeOH). Mp 260.5-261°.

Erdman, T.R. *et al., J.C.S. Perkin 1*, 1972, 1291-1292 (*isol*)
Banville, J. *et al., J.C.S. Perkin 1*, 1976, 1852-1856 (*synth*)
Francesconi, K.A. *et al., Aust. J. Chem.*, 1980, **33**, 2781-2784 (*isol*)

2-Acetyl-1,3,6,8-tetrahydroxyanthraquinone A-84

Haematommone
[133362-56-8]

$C_{16}H_{10}O_7$ 314.251
Constit. of *Haematomma puniceum* and *Melanotheca cruenta*. Red needles (Me_2CO).
Mp 300° dec. λ_{max} 205 (log ϵ 4.67); 235 (log ϵ 4.71); 269 (log ϵ 4.43); 281 (log ϵ 4.43); 310 (log ϵ 4.63); 464 (log ϵ 4.18) (MeOH).

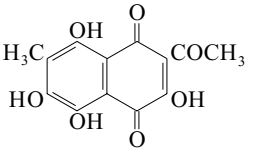
*1′*R-*Alcohol:* ***1,3,6,8-Tetrahydroxy-2-(1-hydroxyethyl)anthraquinone***
[274696-75-2]
$C_{16}H_{12}O_7$ 316.267
Prod. by a *Microsphaeropsis* sp. isol from the sponge *Aplysia aerophoba*. Inhibitor of protein kinases. Orange-yellow powder. $[\alpha]_D$ +151.5 (c, 0.1 in EtOH). λ_{max} 224; 291; 430 (MeOH).

*1′*R-*Alcohol, 1′-Me ether:* ***1,3,6,8-Tetrahydroxy-2-(1-methoxyethyl)anthraquinone***
[274696-76-3]
$C_{17}H_{14}O_7$ 330.293
Prod. by a *Microsphaeropsis* sp. isol from the sponge *Aplysia aerophoba*. Inhibitor of protein kinases. Orange-yellow powder. $[\alpha]_D$ -193.8 (c, 0.1 in EtOH). λ_{max} 224; 292; 453 (MeOH).

Hunek, S. *et al., Phytochemistry*, 1991, **30**, 706-707 (*isol, uv, pmr*)
Couturier, M. *et al., Synthesis*, 1994, 703-708 (*synth, ir, uv*)
Brauers, G. *et al., J. Nat. Prod.*, 2000, **63**, 739-745 (*1′-alcohol*)
Mathey, A. *et al., Z. Naturforsch., C*, 2002, **57**, 565-567 (*isol, pmr*)

2-Acetyl-3,5,6,8-tetrahydroxy-7-methyl-1,4-naphthoquinone A-85

3-Acetyl-2,7-dihydroxy-6-methylnaphthazarin
[64000-80-2]

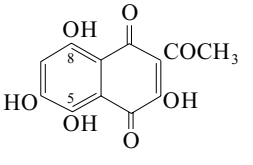


$C_{13}H_{10}O_7$ 278.218
Isol. from the sea urchin *Strongylocentrotus nudus*. Red needles. Mp 179-181°.

Kol'tsova, E.A. *et al., Khim. Prir. Soedin.*, 1977, 202 (*isol, uv, ir, pmr, ms, struct*)

2-Acetyl-3,5,6,8-tetrahydroxy-1,4-naphthoquinone A-86

2-Acetyl-3,5,6,8-tetrahydroxy-1,4-naphthalenedione, 9CI. Spinochrome A. Spinochrome M
[3718-80-7]



$C_{12}H_8O_7$ 264.191
In equilib. with the isomeric 5,8-quinone. Isol. from the sea urchins *Echinometra oblonga*, *Colobocentrotus atratus* and *Strongylocentrotus purpuratus*; also from *Anthocidaris crassispina*, *Ophiocoma erinaceus*, *Ophiocoma insularia*, *Tetrapygus niger*, *Diadema paucispinum*, *Echinothrix calamaris*, *Echinothrix diadema* and *Tripneustes gratilla*. Purple needles (MeOH).
Mp 182-183° (MeOH solvate) Mp 192-193° (anhyd.). λ_{max} 287 (sh) (ϵ 16200); 328 (ϵ 19050); 443 (ϵ 3090); 469 (ϵ 3090); 569 (ϵ 6310) (MeOH/NaOH) (Derep). λ_{max} 251 (ϵ 14450); 270 (sh) (ϵ 12590); 317 (ϵ 12590); 514 (ϵ 4677) (MeOH) (Derep).

Goodwin, T.W. *et al., Biochem. J.*, 1950, **47**, 69-76 (*isol, bibl*)
Goodwin, T.W. *et al., Experientia*, 1951, **7**, 375-376 (*isol*)
Chang, C.W.J. *et al., J.A.C.S.*, 1964, **86**, 2959-2961 (*isol*)
Singh, I. *et al., J.A.C.S.*, 1965, **87**, 4023-4024 (*synth*)
Moore, R.E. *et al., J.O.C.*, 1966, **31**, 3645-3650 (*isol*)
Singh, H. *et al., Experientia*, 1967, **23**, 624-625 (*isol*)
Singh, I. *et al., Tetrahedron*, 1968, **24**, 2969-2978 (*synth*)
Farina, F. *et al., An. Quim.*, 1969, **65**, 713-715 (*isol*)

3-Acetyl-2,5,6,7-tetrahydroxy-1,4-naphthoquinone A-87

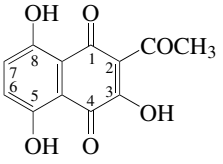
Spinochrome S
[16241-90-0]

$C_{12}H_8O_7$ 264.191
Pigment from the echinoid *Salmacis sphaeroides*. Dark-brown cryst. (MeOH).
Mp 275-280° dec.

Gough, J.H. *et al., Aust. J. Chem.*, 1967, **20**, 1693-1697 (*isol, struct, uv*)

2-Acetyl-3,5,8-trihydroxy-1,4-naphthoquinone A-88

2-Acetyl-3-hydroxynaphthazarin
[5111-33-1]



$C_{12}H_8O_6$ 248.192
Isol. from *Echinothrix calamaris* and *Echinothrix diadema*. Red needles (2,2,4-trimethylpentane). Sol. $CHCl_3$, butanol, MeOH, EtOH, C_6H_6, Me_2CO; poorly sol. H_2O, Et_2O, hexane.
Mp 163-164°. λ_{max} 250 (sh) (ϵ 9210); 296 (ϵ 10500); 490 (ϵ 4490); 525 (sh) (ϵ 3980); 568 (sh) (ϵ 1950) ($CHCl_3$).

Moore, R.E. *et al., J.O.C.*, 1966, **31**, 3638; 1996, 3645; 3650 (*isol, uv, pmr, ms*)
Farina, F. *et al., Tetrahedron*, 1982, **38**, 1531 (*synth*)

6-Acetyl-2,5,7-trihydroxy-1,4-naphthoquinone A-89

6-Acetyl-2,7-dihydroxyjuglone
[13378-89-7]

$C_{12}H_8O_6$ 248.192
Isol. from *Echinothrix calamaris* and *Echinothrix diadema*. Small orange needles ($CHCl_3$).
Mp 215° (dec.). λ_{max} 241 (ϵ 28100); 307 (ϵ 14600); 374 (ϵ 2850); 469 (ϵ 2960) ($CHCl_3$).

Moore, R.E. *et al., J.O.C.*, 1966, **31**, 3638; 3645; 3650 (*isol, uv, pmr, ms*)

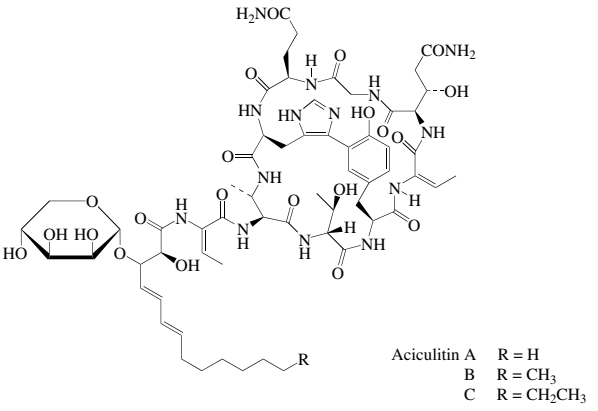
6-Acetyl-2,5,8-trihydroxy-1,4-naphthoquinone A-90

6-Acetyl-2-hydroxynaphthazarin
[13379-24-3]

$C_{12}H_8O_6$ 248.192
Isol. from *Echinothrix calamaris* and *Echinothrix diadema*. Black needles ($CHCl_3$/2,2,4-trimethylpentane).
Mp 179-180° (dec.). λ_{max} 236 (ϵ 16500); 297 (ϵ 7930); 507 (ϵ 6450) ($CHCl_3$).

Moore, R.E. *et al., J.O.C.*, 1966, **31**, 3645; 3650 (*isol, uv, pmr, ms*)
Farina, F. *et al., Tetrahedron*, 1982, **38**, 1531 (*synth, pmr*)

Aciculitin A-91



Cyclic peptide antibiotic complex. Isol. from the sponge *Aciculites orientalis*. Antifungal and cytotoxic agent.

Aciculitin A [176330-16-8]
$C_{61}H_{86}N_{14}O_{21}$ 1351.432
Pale yellow powder. $[\alpha]_D$ -35 (c, 0.3 in MeCN aq.). λ_{max} 210 (ϵ 12100); 270 (ϵ 12700); 310 (ϵ 1300); 330 (ϵ 1100) (MeOH).

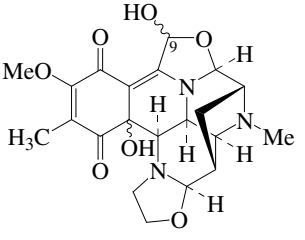
Aciculitin B [176330-15-7]
$C_{62}H_{88}N_{14}O_{21}$ 1365.458
Pale yellow powder. $[\alpha]_D$ -37 (c, 0.3 in MeCN aq.).

Aciculitin C [176330-17-9]
$C_{63}H_{90}N_{14}O_{21}$ 1379.485
Pale yellow powder. $[\alpha]_D$ -34 (c, 0.3 in MeCN aq.).

Bewley, C.A. *et al., J.A.C.S.*, 1996, **118**, 4314-4321 (*isol, pmr, cmr*)

Aclidinomycin B A-92

[342814-66-8]



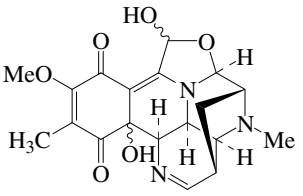
$C_{21}H_{25}N_3O_7$ 431.444
Related to Naphthyridinomycin A. Prod. by *Streptomyces halstedi* KB012 and a marine-derived *Streptomyces* sp.
$[\alpha]_D$ +188 (c, 0.16 in MeOH). λ_{max} 286 (ϵ 21500); 398 (ϵ 5000) (MeOH).

N-*De-Me:* ***Aclidinomycin D***
$C_{20}H_{23}N_3O_7$ 417.418
Prod. by a marine-derived *Streptomyces* sp.

9-Deoxy: ***Aclidinomycin A***
[342814-65-7]
$C_{21}H_{25}N_3O_6$ 415.445
Prod. by *Streptomyces halstedi* KB012.
$[\alpha]_D$ 0 (MeOH). λ_{max} 282 (ϵ 19000); 403 (ϵ 3500) (MeOH).

Thorwest, M. *et al., Dissertation*, Univ. of Göttingen, 2001, (*marine, isol*)
Cang, S. *et al., J. Antibiot.*, 2001, **54**, 304-307 (*isol, pmr, cmr*)

Aclidinomycin C A-93

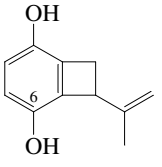


$C_{19}H_{21}N_3O_6$ 387.391
Prod. by a marine-derived *Streptomyces* sp.

Thorwest, M. *et al., Dissertation*, Univ. of Göttingen, 2001,

Acremonin A A-94

7-(1-Methylethenyl)bicyclo[4.2.0]octa-1,3,5-triene-2,5-diol. 1-Isopropenyl-3,6-benzocyclobutenediol. 1-(1-Methylethenyl)-3,6-benzocyclobutenediol



$C_{11}H_{12}O_2$ 176.215

(+)-*form*
Prod. by a marine-derived *Acremonium* sp. Antioxidant. Yellow-brown viscous oil. $[\alpha]_D^{23}$ +93 (c, 1.4 in Me_2CO). λ_{max} 205 (log ϵ 4.4); 286 (log ϵ 3.6) (MeOH).

6-O-β-D-Glucopyranoside:
$C_{17}H_{22}O_7$ 338.357
Prod. by an *Acremonium* sp. Amorph. powder. $[\alpha]_D^{23}$ +4.3 (c, 2 in Me_2CO). λ_{max} 205 (log ϵ 4.3); 280 (log ϵ 3.2) (MeOH).

Abdel-Lateff, A. *et al., J. Nat. Prod.*, 2002, **65**, 1605-1611 (*isol, pmr, cmr, ms*)

Actinine A-95

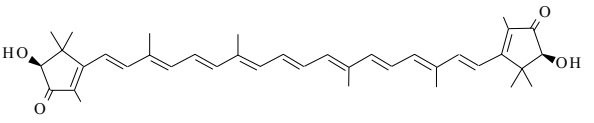
3-Carboxy-N,N,N-*trimethyl-1-propanaminium hydroxide inner salt, 9CI. Tri*-N-*methyl-γ-butyrobetaine. 4-Aminobutanoic acid betaine. γ-Butyrobetaine. Butyrobetaine. 4-Aminobutanoic acid trimethylbetaine*
[407-64-7]
$Me_3N^{\oplus}CH_2CH_2CH_2COO^{\ominus}$
$C_7H_{15}NO_2$ 145.201
Inner salt. Occurs in the sea-rose *Actinia equina*, in muscles of various snakes and in urine in cases of pernicious anaemia. Isol. from brain tissue. Also from *Polyporus sulphureus*. Biosynthetic intermed. in synth. of Carnitine. Plates + $3H_2O$ ($EtOH/Et_2O$ aq.). Sol. EtOH. Dec. at 220°.
▶ BP3930000

Hydrochloride: [6249-56-5]
Mp 203° Mp 214-219°.
▶ BP3850000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 681A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 878B (*nmr*)
Engeland, R. *et al., Ber.*, 1921, **54**, 2212 (*derivs*)
Linneweh, W. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1928, **175**, 95; **176**, 220; 1929, **181**, 48; **182**, 9 (*isol*)
List, P.H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1959, **292**, 260 (*isol*)
Hosein, E.A. *et al., Nature (London)*, 1960, **187**, 321 (*isol*)
Cox, R.A. *et al., Biochem. J.*, 1973, **136**, 1083 (*biosynth*)
Anderson, L. *et al., Synthesis*, 1981, 468 (*synth*)

Actinioerythrol A-96

[22453-07-2]



$C_{38}H_{48}O_4$ 568.795
Constit. of *Actinia equina*. Red cryst. (MeOH).

Diacyl: ***Actinoerythrin***
[69020-32-2]
Isol. from *Actinia equina* and *Tealia felina*.
Red cryst.
Mp 91°. Nature of acylating residues not yet identified.

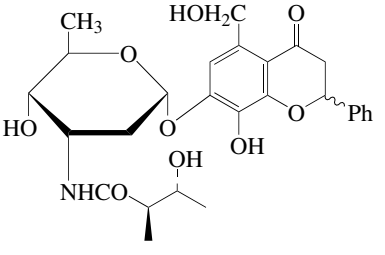
Diketone: 2,2′-Dinor-β,β-carotene-3,3′,4,4′-tetrone. Violerythrin
[22453-06-1]
$C_{38}H_{44}O_4$ 564.763
Obt. by alkaline hydrol. of Actinoerythrin. First known blue carotenoid. Blue cryst. ($CHCl_3$/hexane).
Mp 243° (236-238°). λ_{max} 544 (Me_2CO).

Dialcohol: 2,2′-Dinor-β,β-carotene-3,3′,4,4′-tetrol. Violerythrol
[22467-23-8]
$C_{38}H_{52}O_4$ 572.826
Cryst. (Et_2O). Mp 138°. Obt. as a mix of diastereoisomers.

Hertzberg, S. *et al., Acta Chem. Scand.*, 1968, **22**, 1714; 1969, **23**, 3290 (*isol, struct*)
Andrewes, A.G. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 730 (*struct*)
Coman, R. *et al., J.C.S. Perkin 1*, 1976, 2140 (*synth*)
Kienzle, F. *et al., Helv. Chim. Acta*, 1978, **61**, 242 (*synth*)
Müller, R.K. *et al., Helv. Chim. Acta*, 1978, **61**, 2881 (*abs config*)
Kummer, M. *et al., Angew. Chem., Int. Ed.*, 1986, **25**, 1018 (*uv, pe, Violerythirin*)

Actinoflavoside A-97

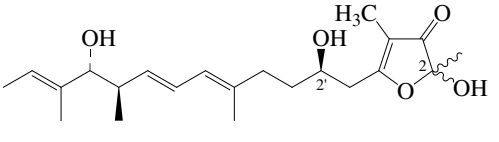
[194873-80-8]



$C_{27}H_{33}NO_9$ 515.559
Prod. by a marine *Streptomyces* sp. Non-cryst. solid. $[\alpha]_D$ -110 (c, 1.3 in MeOH). λ_{max} 232 (ϵ 19000); 282 (ϵ 18000); 325 (ϵ 4500) (MeOH).

Jiang, Z.-D. *et al., Tet. Lett.*, 1997, **38**, 5065-5068 (*isol, uv, ir, pmr, cmr*)

Actinofuranone A A-98



$C_{22}H_{34}O_5$ 378.508
1:1 Mixt. of C-2 epimers. Prod. by a marine-derived *Streptomyces* sp. (strain CNQ766). Yellow oil. $[\alpha]_D$ -20 (c, 0.1 in MeOH). λ_{max} 241 (log ϵ 4); 282 (log ϵ 3.8) (MeOH).

*2′-Deoxy, 2′,3′-didehydro(*E-*):* ***Actinofuranone B***
$C_{22}H_{32}O_4$ 360.492

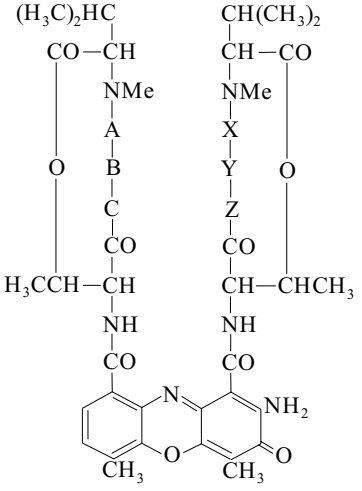
Prod. by *Streptomyces* sp. (strain CNQ766). Yellow oil. $[\alpha]_D$ -37 (c, 0.07 in MeOH). λ_{max} 241 (log ϵ 4); 317 (log ϵ 3.7) (MeOH).

Cho, J.Y. *et al., J. Nat. Prod.*, 2006, **69**, 425-428 (*isol, pmr, cmr*)

Actinomycin D, 9CI, 8CI, JAN A-99

Dactinomycin, BAN, INN. *Actinomycin IV. Actinomycin A_{IV}. Actinomycin Au_3. Actinomycin B_1†. Actinomycin B_{IV}. Actinomycin C_1. Actinomycin D_{IV}. Actinomycin Fo. Actinomycin I_1. Actinomycin S_2. Actinomycin X_1. Auranthin A 3. Auranthin C. Cosmegen. Cosmogen. Meractinomycin. Oncostatin K. NSC 3053. Chuoungwamycin B*

[50-76-0]



A = X = Sar,
B = Y = L–Pro
C = Z = D–Val

$C_{62}H_{86}N_{12}O_{16}$ 1255.432

Depsipeptide antibiotic. Isol. from *Streptomyces parvulus* and other *Streptomyces* spp. Active against gram-positive bacteria and malignant neoplasms. Red rhomboids + $3H_2O$ (EtOH). Mp 246-247°. $[\alpha]_D^{28}$ -315 (c, 0.25 in MeOH). Log P 7.32 (uncertain value) (calc). Intercalates DNA and can cause single strand breaks in DNA. λ_{max} 288 (ϵ 12500); 342 (ϵ 21200); 445 (ϵ 5770) (pH 13/5 h) (Derep). λ_{max} 240 (ϵ 30000); 426 (ϵ 21000); 427 (sh) (ϵ); 442 (ϵ 22300) (MeOH) (Derep).

▶ Skin irritant. Dermatitis, gastrointestinal effects and bone-marrow depression reported when used therapeutically. LD_{50} (rat, orl) 7.2 mg/kg. Exp. carcinogenic, reprod. and teratogenic effects. AU1575000

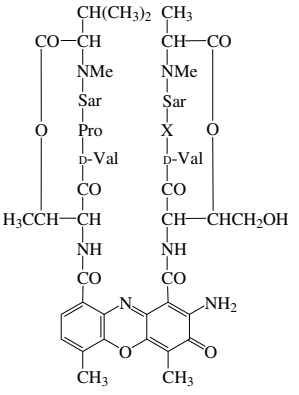
N,N′-*Di-de-Me:* **N,N′-*Didemethylactinomycin D.*** *Auranthin 3B*
$C_{60}H_{82}N_{12}O_{16}$ 1227.379
Prod. by *Streptomyces* sp. Orange-yellow powder. Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane. λ_{max} 240; 442 (MeOH).

[1402-43-3, 1402-51-3, 1402-58-0, 54650-01-0]

Bullock, E. *et al., J.C.S.*, 1957, 3280 (*struct, uv*)
Brockmann, H. *et al., Naturwissenschaften*, 1964, **51**, 382; 384 (*synth*)
Meienhofer, J. *et al., J.A.C.S.*, 1970, **92**, 3771 (*synth*)
Lackner, H. *et al., Chem. Ber.*, 1971, **104**, 3653 (*synth, ir, ms, nmr*)
Lackner, H. *et al., Tet. Lett.*, 1971, 2221 (*struct, pmr, conformn*)
Hollstein, U. *et al., J.A.C.S.*, 1974, **96**, 8036 (*cmr, struct*)
IARC Monog., 1976, **10**, 29; *Suppl.* 6, 32; *Suppl.* 7, 80 (*rev, tox*)
Gottschewski, G.H.M. *et al., Arzneim.-Forsch.*, 1980, **30**, 236 (*rev, pharmacol*)
Goldman, D. *et al., Cancer Treat. Rep.*, 1981, **65**, 43 (*rev*)
Nakajima, K. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 3237 (*synth*)
Terent'eva, T.G. *et al., Antibiot. Med. Biotekhnol.*, 1985, **30**, 619 (*rev, pharmacol*)
Mauger, A.B. *et al., J.A.C.S.*, 1985, **107**, 7154 (*synth, struct*)
Martin, D.G. *et al., J. Antibiot.*, 1986, **39**, 721 (*purifn*)
Katz, E. *et al., J. Antibiot.*, 1990, **43**, 731 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **3**, 288 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 473
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AEB000

Actinomycin HKI 0155 A-100

Antibiotic HKI 0155. HKI 0155



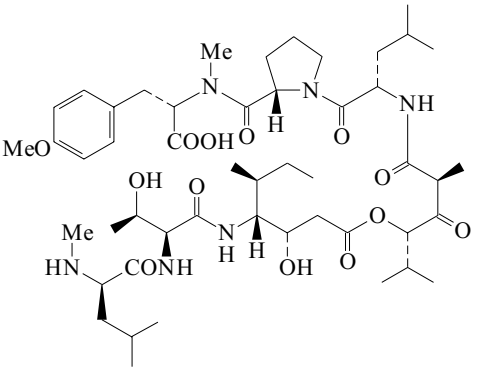
X = 3-hydroxy-5-methyl-L-Pro

$C_{61}H_{84}N_{12}O_{18}$ 1273.404
Prod. by *Streptomyces* sp. HKI 0155 and marine *Streptomyces* sp. B8335. Yellow cryst. $[\alpha]_D$ +226 (MeOH). λ_{max} 443 (ϵ 24500) (MeOH).

Lackner, H. *et al., J. Antibiot.*, 2000, **53**, 84-87 (*isol*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)

Acyclodidemnin A A-101

[155569-78-1]



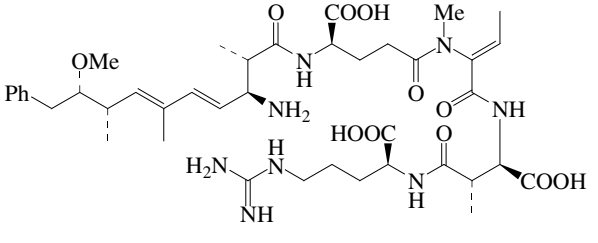
$C_{49}H_{80}N_6O_{13}$ 961.203

Peptide antibiotic. Ring-opened form of Didemnin A, D-396. Isol. from *Tridemnum solidum*. Weak cytotoxic agent. Powder. Mp 126-130°. $[\alpha]_D^{26}$ -71 (c, 0.06 in $CHCl_3$). λ_{max} 206 (ϵ 63100); 230 (ϵ 32360) (MeOH).

Sakai, R. *et al., J.A.C.S.*, 1995, **117**, 3734-3748 (*isol, uv, ir, pmr, cmr*)
Sakai, R. *et al., J. Med. Chem.*, 1996, **39**, 2819-2834 (*activity*)

Acyclonodularin A-102

[154093-28-4]



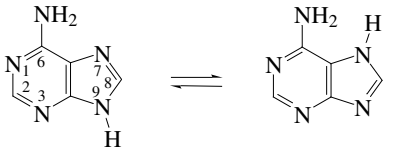
$C_{41}H_{62}N_8O_{11}$ 842.988

Ring-opened form of Nodularin, N-136. Isol. from marine cyanobacterium *Nodularia spumigena*. Biosynthetic precursor of Nodularin N-136. $[\alpha]_D^{25}$ -58.2 (c, 0.001 in MeOH).

Choi, B.W. *et al., Tet. Lett.*, 1993, **34**, 7881-7884 (*isol, struct*)
Namikoshi, M. *et al., J.O.C.*, 1994, **59**, 2349-2357 (*isol*)

Adenine, JAN, USAN A-103

*1*H-*Purin-6-amine, 9CI. 6-Aminopurine. Vitamin* B_4. *Angustmycin B*
[73-24-5]



9H-form *7H-form*

$C_5H_5N_5$ 135.128

9*H*-form is favoured in free base. CAS refers mainly to 1*H* struct. which is not in reality a favoured tautomer. Widespread throughout animal and plant tissue, purine components of DNA, RNA, and coenzymes and biosynthetic intermediates. Antiviral agent, granulocyte antagonist.Vitamin. Pharmaceutical aid used to extend storage life of whole blood. Needles + $3H_2O$ (H_2O).

Mp 360-365° (anhyd.) dec. pK_{a1} 4.12; pK_{a2} 9.83 (25°).

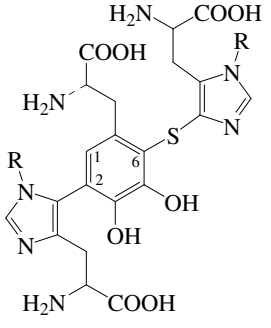
▶ Exp. reprod. and teratogenic effects. LD_{50} (rat, orl) 745 mg/kg. AU6125000

Hydrochloride: [2922-28-3]
Cryst. + $0.5H_2O$. Mp 285°.

[2312-73-4, 6055-72-7]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 589C; 589D; 590C (*pmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 708A; 713C; 713D; 714D (*ir*)
Traube, W. *et al., Annalen*, 1904, **331**, 64-88 (*synth*)
Richter, E. *et al., J.A.C.S.*, 1960, **82**, 3144-3146 (*synth*)
Chenon, M.T. *et al., J.A.C.S.*, 1975, **97**, 4636-4642 (*cmr, tautom*)
Kos, N.J. *et al., J.O.C.*, 1979, **44**, 3140-3143 (*synth, nmr*)
Lin, J. *et al., J.A.C.S.*, 1980, **102**, 4627-4631 (*pe, tautom*)
Gonella, N.C. *et al., J.A.C.S.*, 1983, **105**, 2050-2055 (*nmr*)
Mathlouth, M. *et al., Carbohydr. Res.*, 1984, **131**, 1-15 (*ir, Raman*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1331
Merck Index, 13th edn., 2001, No. 152 (*props, bibl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AEH000; AEH250

Adenochrome A-104



R = H or Me
Adenochromine A

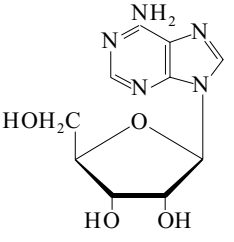
Iron containing compd. which has been isolated as its deferri-deriv. Consists of a mixture of peptides derived from glycine and 3 isomeric amino acids Adenochromines A, B and C. Struct. of Adenochromine A shown. B and C have ortho- and meta- arrangements respectively of the two (histidinylthio) groups. Pigment from the branchial heart of *Octopus vulgaris*. Violet.

[63026-38-0, 63026-40-4, 64925-68-4]

Ito, S. *et al., J.C.S. Perkin 1*, 1979, 2617-2623 (*isol, struct*)
Michael, J.P. *et al., Angew. Chem., Int. Ed.*, 1993, **32**, 1

Adenosine, 9CI, 8CI, BAN, USAN A-105

*9-β-D-Ribofuranosyl-9*H-*purin-6-amine, 9CI. 9-β-D-Ribofuranosyladenine, 8CI. 6-Amino-9-β-D-ribofuranosyl-9*H-*purine. Adenocard. Adenocor. Adenoscan. SR 96225*
[58-61-7]



$C_{10}H_{13}N_5O_4$ 267.244
Widely distributed in nature. One of the four principal nucleosides of nucleic acid. Antiarrhythmic agent. Cardiac depressant. Launched 1989. Cryst. (H_2O). Sol. H_2O, MeOH; poorly sol. Me_2CO, hexane.
Mp 234-236°. $[\alpha]_D^{11}$ -61.7 (c, 0.7 in H_2O). pK_{a1} 3.6; pK_{a2} 12.4 (25°). Log P -2.88 (calc). Component of numerous preparations. λ_{max} 259 (ε 15400) (H_2O). λ_{max} 260 (ε 15100) (H_2O) (Berdy).

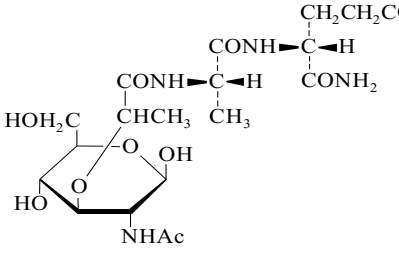
▶ LD_{50} (mus, ipr) 500 mg/kg. AU7175000

[3080-29-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 719C; 720A; 721A; 722C; 725B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 222A; 224A; 227B; 229B (*nmr*)
Davoll, J. *et al., J.C.S.*, 1948, 967-969 (*synth*)
Brown, D.M. *et al., J.C.S.*, 1950, 3299-3304 (*synth*)
Biemann, K. *et al., J.A.C.S.*, 1962, **84**, 2005-2007 (*ms*)
Shikata, K. *et al., Acta Cryst. B*, 1973, **29**, 31-38 (*cryst struct*)
Sarma, R.H. *et al., J.A.C.S.*, 1974, **96**, 7337-7348 (*pmr, conformn*)
Mathlouth, M. *et al., Carbohydr. Res.*, 1984, **131**, 1-15 (*ir, Raman*)
Puech, P. *et al., Handb. Exp. Pharmacol.*, 1989, **89**, 453-460 (*rev, metab, props, use*)
Adenosine and Adenosine Receptors, Williams, M., ed., Chapman and Hall, 1990, (*book*)
Reddy, A.M. *et al., J. Het. Chem.*, 1990, **27**, 1297-1305 (*ms*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 57
Mahler, G.S. *et al., Anal. Profiles Drug Subst.*, 1998, **25**, 1-37 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AEH750

Adjuvant peptide A-106

N^2-*[*N-*(*N-*Acetylmuramoyl)-L-alanyl]-D-α-glutamine, 9CI.* N-*Acetylmuramyl-L-alanyl-D-isoglutamine. Muramyl dipeptide. MDP*
[53678-77-6]



$C_{19}H_{32}N_4O_{11}$ 492.482

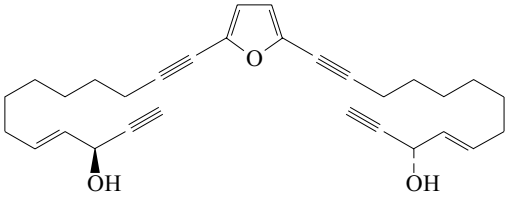
Identified as the minimum structural constit. of the mycobacterial cell wall component of Freund's complete adjuvant which is necessary for adjuvant activity. It and many of its analogues have been investigated as adjuvants in the immunisation of animals. Immunomodulator. Somnogenic and pyrogenic agent.
Mp 190-194°. $[\alpha]_D^{25}$ +44 (c, 1 in AcOH).

▶ MA2275260

LeFrancier, P. *et al., Int. J. Pept. Protein Res.*, 1977, **9**, 249; 1978, **11**, 289 (*synth*)
Nebelin, E. *et al., FEBS Lett.*, 1979, **107**, 254 (*ms*)
LeFrancier, P. *et al., Prog. Chem. Org. Nat. Prod.*, 1981, **40**, 1 (*rev*)
Chapman, B.E. *et al., Aust. J. Chem.*, 1982, **35**, 489 (*pmr*)
Fogler, W.E. *et al., Immunol. Ser.*, 1984, **25**, 499 (*rev*)
Masek, K. *et al., Int. J. Immunother.*, 1985, **1**, 177 (*rev, pharmacol*)
Ivanov, V.T. *et al., Pure Appl. Chem.*, 1987, **59**, 317 (*synth, pharmacol*)
LeFrancier, P. *et al., Pure Appl. Chem.*, 1987, **59**, 449 (*rev, pharmacol*)
Misra, P.K. *et al., J. Chem. Res., Synop.*, 1988, 374 (*bibl, synth*)
Boulanger, Y. *et al., Tetrahedron*, 1992, **48**, 8855 (*bibl, conformn, pmr*)

Adociacetylene B A-107

13,13′-(2,5-Furandiyl)bis[4-tridecene-1,12-diyn-3-ol], 9CI. 14,17-Epoxy-4,14,16,26-tricontatetraene-1,12,18,29-tetrayne-3,28-diol
[176182-13-1]

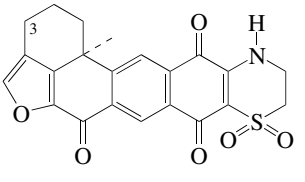


$C_{30}H_{36}O_3$ 444.613
Constit. of the sponge *Adocia* sp. Endothelial cell-neutrophil leukocyte adhesion inhibitor. Oil. $[\alpha]_D$ +21.7 (c, 0.4 in $CHCl_3$). Related to Petrosynol, P-292. λ_{max} 275 (ϵ 27100); 279 (ϵ 27900); 285 (ϵ 25800); 293 (ϵ 26300) (MeOH).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 720 (*isol, uv, ir, pmr, cmr*)
Gung, B.W. *et al., Tet. Lett.*, 2001, **42**, 4761-4763 (*synth*)
Trost, B.M. *et al., Org. Lett.*, 2006, **8**, 4461-4464 (*synth*)

Adociaquinone A A-108

[113830-99-2]



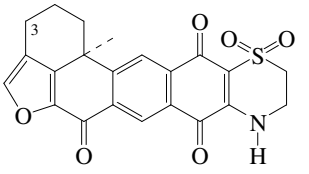
$C_{22}H_{17}NO_6S$ 423.445
Isol. from the sponge *Adocia* sp. Topoisomerase II inhibitor. Yellow solid. Fairly sol. DMSO; poorly sol. $CHCl_3$, hexane. $[\alpha]_D$ +25. Slowly dec. >300°. λ_{max} 249 (ϵ 29200); 294 (ϵ 16800) (EtOH) (Derep). λ_{max} 272 (ϵ 11400) (MeOH) (Berdy). λ_{max} 288 (ϵ 3600); 340 (ϵ 12000) (EtOH) (Berdy).

3-Oxo: ***3-Oxoadociaquinone A****. 3-Ketoadociaquinone A*
[113831-01-9]
$C_{22}H_{15}NO_7S$ 437.429
Isol. from *Adocia* sp. Yellow solid. $[\alpha]_D$ +65.4. Slowly dec. >300°. λ_{max} 238 (ϵ 26200); 288 (ϵ 26000) (EtOH) (Derep).

Schmitz, F.J. *et al., J.O.C.*, 1988, **53**, 3922-3925 (*isol, pmr, cmr*)
Harada, N. *et al., Tetrahedron: Asymmetry*, 1995, **6**, 375-376 (*synth, abs config*)

Adociaquinone B A-109

[113831-00-8]



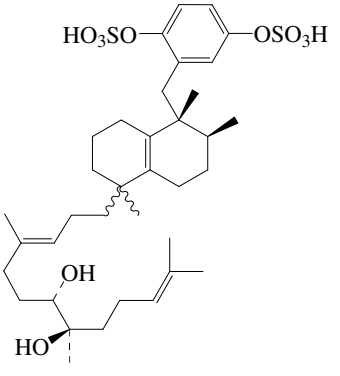
$C_{22}H_{17}NO_6S$ 423.445
Isol. from the sponges *Adocia* and *Xestospongia*spp. Mildly cytotoxic. Topoisomerase inhibitor. Yellow solid. $[\alpha]_D$ +22. Slowly dec. >300°. λ_{max} 288 (ϵ 36000); 340 (ϵ 12000) (EtOH) (Derep). λ_{max} 294 (ϵ 14400) (MeOH) (Berdy).

3-Oxo: ***3-Oxoadociaquinone B****. 3-Ketoadociaquinone B*
$C_{22}H_{15}NO_7S$ 437.429
Isol. from a *Xestospongia* sp. Yellowish powder. $[\alpha]_D^{23}$ +13 (c, 0.12 in MeOH). λ_{max} 273 (log ϵ 3.6) (MeOH).

Schmitz, F.J. *et al., J.O.C.*, 1988, **53**, 3922-3925 (*isol, pmr, cmr*)
Harada, N. *et al., Tetrahedron: Asymmetry*, 1995, **6**, 375-376 (*synth, abs config*)
Cao, S. *et al., Bioorg. Med. Chem.*, 2005, **13**, 999-1003 (*3-Oxoadociaquinone B*)

Adociasulfate 3 A-110

[242459-63-8]

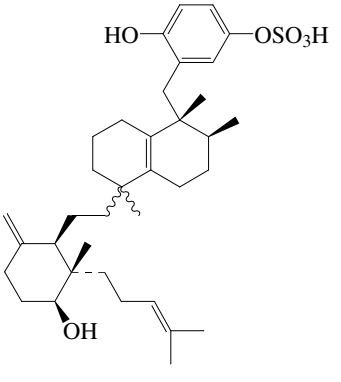


$C_{36}H_{56}O_{10}S_2$ 712.964
Constit. of a *Haliclona* (*Adocia*) sp. Glass. $[\alpha]_D$ -6.25 (c, 0.08 in MeOH). λ_{max} 270 (ϵ 868) (MeOH).

Blackburn, C.L. *et al., J.O.C.*, 1999, **64**, 5565-5570 (*isol, pmr, cmr*)

Adociasulfate 4 A-111

[242459-65-0]



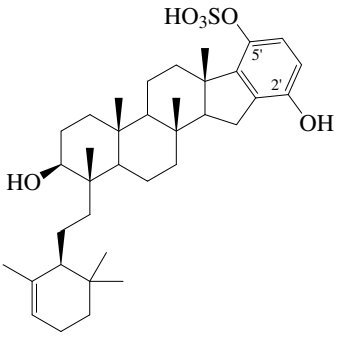
$C_{36}H_{54}O_6S$ 614.885

Constit. of a *Haliclona* (*Adocia*) sp. Amorph. solid. $[\alpha]_D$ -12.1 (c, 1.2 in MeOH). λ_{max} 281 (ϵ 1730) (MeOH).

Blackburn, C.L. *et al., J.O.C.*, 1999, **64**, 5565-5570 (*isol, pmr, cmr*)

Adociasulfate 5 **A-112**

[242459-67-2]



$C_{36}H_{54}O_6S$ 614.885
Constit. of a *Haliclona* (*Adocia*) sp. Amorph. solid. $[\alpha]_D$ -10.9 (c, 0.15 in MeOH). λ_{max} 265 (ϵ 415) (MeOH).

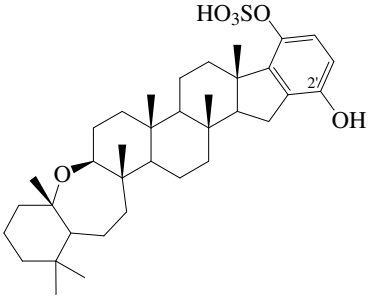
2′-Sulfate: ***Adociasulfate 1***
[230631-38-6]
$C_{36}H_{54}O_9S_2$ 694.949
Constit. of a *Haliclona* (*Adocia*) sp. Amorph. solid. $[\alpha]_D$ -15 (c, 0.1 in MeOH). $[\alpha]_D^{26}$ -34 (c, 0.1 in MeOH). λ_{max} 265 (ϵ 540) (MeOH).

5′-Desulfo, 2′-sulfate: ***Adociasulfate 7***
[242486-89-1]
$C_{36}H_{54}O_6S$ 614.885
Constit. of an *Adocia* sp. Amorph. powder. $[\alpha]_D^{26}$ +5 (c, 0.17 in MeOH). λ_{max} 276 (ϵ 336) (MeOH).

Kalaitzis, J.A. *et al., J. Nat. Prod.*, 1999, **62**, 1682-1684 (*Adociasulfate 5*)
Blackburn, C.L. *et al., J.O.C.*, 1999, **64**, 5565-5570 (*isol, pmr, cmr*)
Kalaitzis, J.A. *et al., J.O.C.*, 1999, **64**, 5571-5574 (*isol, pmr, cmr*)

Adociasulfate 6 **A-113**

[242459-69-4]



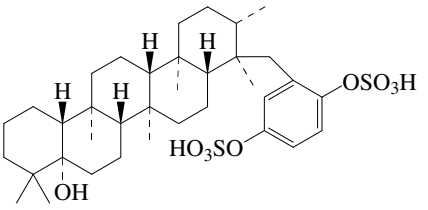
$C_{36}H_{54}O_6S$ 614.885
Constit. of a *Haliclona* (*Adocia*) sp. Amorph. solid. $[\alpha]_D$ -12.3 (c, 0.76 in MeOH). λ_{max} 276 (ϵ 2525) (MeOH).

2′-Sulfate: ***Adociasulfate 2***
[208181-29-7]
$C_{36}H_{54}O_9S_2$ 694.949
Constit. of a *Haliclona* (*Adocia*) sp. Amorph. solid. $[\alpha]_D$ -10.9 (c, 0.15 in MeOH). λ_{max} 265 (ϵ 415) (MeOH).

Blackburn, C.L. *et al., J.O.C.*, 1999, **64**, 5565-5570 (*isol, pmr, cmr*)

Adociasulfate 8 **A-114**

[242486-90-4]

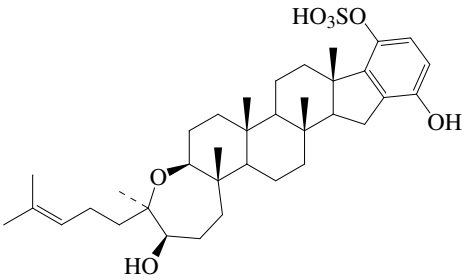


$C_{36}H_{56}O_9S_2$ 696.965
Constit. of an *Adocia* sp. Amorph. powder. $[\alpha]_D^{26}$ +18 (c, 0.19 in MeOH). λ_{max} 296 (ϵ 982) (MeOH).

Kalaitzis, J.A. *et al., J.O.C.*, 1999, **64**, 5571-5574 (*isol, pmr, cmr*)

Adociasulfate 9 **A-115**

[252034-37-0]

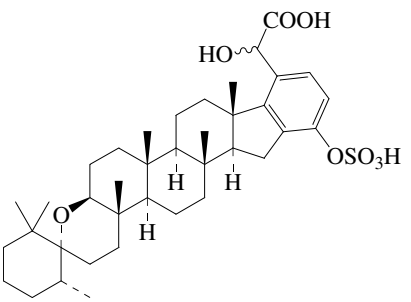


$C_{36}H_{54}O_7S$ 630.884
Constit. of *Adocia aculeata*. Powder. $[\alpha]_D^{25}$ +6.9 (c, 0.14 in MeOH). λ_{max} 216 (log ϵ 8.45); 272 (log ϵ 7.24) (no solvent reported).

Kalaitzis, J.A. *et al., J. Nat. Prod.*, 1999, **62**, 1682-1684 (*isol, pmr, cmr*)

Adociasulfate 10 **A-116**

[313503-82-1]



$C_{38}H_{56}O_8S$ 672.922
Constit. of a *Haliclona* (*Adocia*) sponge. Solid. $[\alpha]_D$ -30.2 (c, 0.57 in MeOH). λ_{max} 265 (ϵ 978) (MeOH).

Blackburn, C.L. *et al., Tetrahedron*, 2000, **56**, 8429-8432 (*isol, pmr, cmr*)

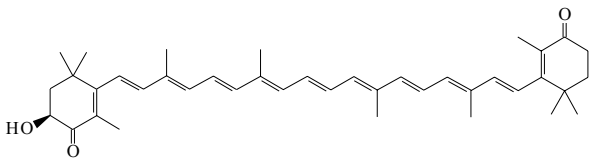
Adociavirin **A-117**

Homodimeric protein. Isol. from the New Zealand sponge *Adocia* sp. Shows anti-HIV activity.

O'Keefe, B.R. *et al., FEBS Lett.*, 1998, **431**, 85-90 (*isol*)

Adonirubin A-118

3-Hydroxy-β,β-carotene-4,4′-dione. Phoenicoxanthin
[4418-72-8]

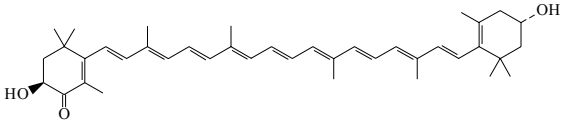


$C_{40}H_{52}O_3$ 580.849
Red pigment from feathers of flamingos (e.g. *Phoenicopterus ruber*) and from flowers of *Adonis annua*. Constit. of various crustaceans and sea urchins. Serves as prosthetic group for carotenoprotein alloporin. Red-violet plates (CH_2Cl_2/MeOH). Mp 214-216°. λ_{max} 478 (C_6H_6).

Englert, G. *et al., Helv. Chim. Acta*, 1975, **58**, 2367 (*cmr*)
Cooper, R.D.G. *et al., J.C.S. Perkin 1*, 1975, 2195
Bernhard, K. *et al., Helv. Chim. Acta*, 1981, **64**, 2469 (*synth*)
Berger, H. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **71**, 253 (*biochem*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 391 (*bibl*)

Adonixanthin A-119

3,3′-Dihydroxy-β,β-caroten-4-one. β-Doradexanthin. 3,3′-Dihydroxyechinenone. 4-Ketozeaxanthin
[80183-56-8]



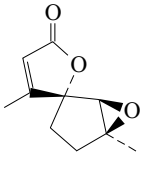
$C_{40}H_{54}O_3$ 582.865
Synth. by Wittig reaction. Isol. from green algae, red flowers of *Adonis annua*, various crustaceans and sponges. Red-violet cryst. (CH_2Cl_2/MeOH).
Mp 180-181°. λ_{max} 304, 481 nm ($CHCl_3$); 296, 458 nm (hexane); 474 nm (C_6H_6); 299, 468 nm (EtOH).

3-O-β-D-Glucopyranoside:
$C_{46}H_{64}O_8$ 745.007
Constit. of *Agrobacterium aurantiacum*. λ_{max} 476 nm (C_6H_6).

Egger, K. *et al., Phytochemistry*, 1965, **4**, 609 (*isol*)
Bernhard, K. *et al., Helv. Chim. Acta*, 1981, **64**, 2469 (*synth*)
Czeczuga, B. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1984, **78**, 259 (*occur*)
Yokoyama, A. *et al., J. Nat. Prod.*, 1995, **58**, 1929 (*glucoside*)

Adriadysiolide A-120

[113540-73-1]

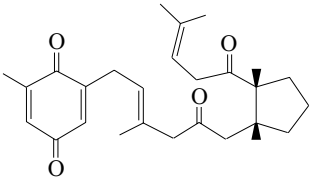


$C_{10}H_{12}O_3$ 180.203
Constit. of a *Dysidea* sp. of the Adriatic Sea. Powder.
Mp 76-77°. $[\alpha]_{435}^{20}$ +2.1 (c, 0.625 in MeOH).

Mancini, I. *et al., Helv. Chim. Acta*, 1987, **70**, 2011

Adriaticone A-121

2-[6-[1,2-Dimethyl-2-(4-methyl-1-oxo-3-pentenyl)cyclopentyl]-3-methyl-5-oxo-2-hexenyl]-6-methyl-2,5-cyclohexadiene-1,4-dione, 9CI
[97730-90-0]

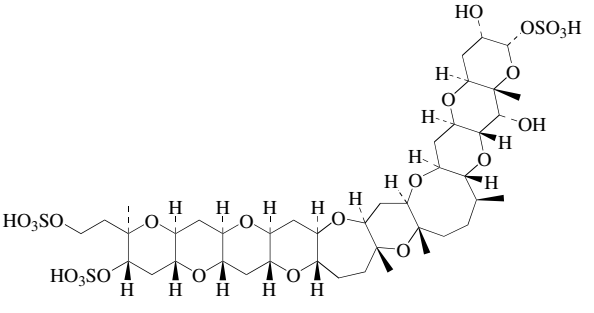


$C_{27}H_{36}O_4$ 424.579
Found in the brown alga *Cystoseira jabukae* and *Cystoseira adriatica*. Yellow oil. $[\alpha]_D^{20}$ +9.7 (c, 0.9 in EtOH). Poss. artifact.

Hydroquinone: ***Dihydroadriaticone****. 6-(2,5-Dihydroxy-3-methylphenyl)-1-[1,2-dimethyl-2-(4-methyl-1-oxo-3-pentenyl)cyclopentyl]-4-methyl-4-hexen-2-one, 9CI*
[97743-94-7]
$C_{27}H_{38}O_4$ 426.595
From *Cystoseira jabukae* and *Cystoseira adriatica*. Oil. $[\alpha]_D^{20}$ +8.5 (c, 2 in EtOH).

Amico, V. *et al., Phytochemistry*, 1985, **24**, 1047 (*isol, uv, ir, pmr, cmr, ms*)

Adriatoxin A-122



$C_{42}H_{66}O_{24}S_3$ 1051.167
Toxic constit. of the mussel *Mytilus galloprovincialis* from northern Adriatic Sea. λ_{max} 230 (MeOH) (Berdy).

Ciminiello, P. *et al., Tet. Lett.*, 1998, **39**, 8897-8900 (*isol, pmr*)

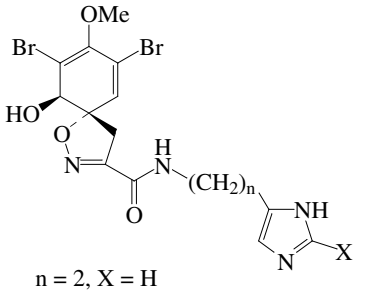
Aequorin A-123

Photoprotein, MW *ca.* 19500, containing 189 amino acid residues. Isol. from the jellyfish *Aequorea victoria*. Used in luminoassay of $Ca^{2\oplus}$ in biol. systems.

Shimomura, O. *et al., J. Cell. Comp. Physiol.*, 1962, **59**, 223-229 (*isol*)
Charbonneau, H. *et al., Biochemistry*, 1985, **24**, 6762-6771 (*struct*)
Shimomura, O. *et al., Biochem. J.*, 1986, **234**, 271-277 (*isol, struct*)
Kendall, J.M. *et al., Trends Biotechnol.*, 1998, **16**, 216-224 (*rev*)
Head, J.F. *et al., Nature (London)*, 2000, **405**, 291-293 (*cryst struct*)
Vysotski, E.S. *et al., Acc. Chem. Res.*, 2004, **37**, 405-415 (*rev*)

Aerophobin 1 A-124

[87075-24-9]



n = 2, X = H

$C_{15}H_{16}Br_2N_4O_4$ 476.124
Isol. from the sponges *Verongia aerophoba* and *Verongula rigida*. Also from *Tylodina perversa*.
Mp 164-167° (Ac). $[\alpha]_D$ +187 (c, 2.0 in MeOH).

Cimino, G. *et al., Tet. Lett.*, 1983, **24**, 3029 (*isol, pmr, cmr, ms, struct*)
Nishiyama, S. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 3453 (*synth*)
Gunasekera, M. *et al., J. Nat. Prod.*, 1989, **52**, 753 (*isol, uv, ir, pmr, cmr, ms*)
Teeyapant, R. *et al., Z. Naturforsch., C*, 1993, **48**, 640-644 (*isol*)

Aerophobin 2 A-125

[87075-23-8]
As Aerophobin 1, A-124 with
n = 3, X = NH_2
$C_{16}H_{19}Br_2N_5O_4$ 505.165
Isol. from the sponges *Verongia aerophoba* and *Aiolochroia crassa*.
$[\alpha]_D$ +139 (c, 1.9 in MeOH).

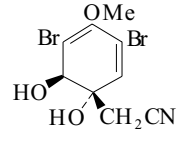
N-*Me (X = NHMe):* **N-*Methylaerophobin 2***
[209472-96-8]
$C_{17}H_{21}Br_2N_5O_4$ 519.192
Alkaloid from the sponge *Aiolochroia crassa*.

13,14-Dihydro, 14-oxo: ***14-Oxoaerophobin 2***
[232259-26-6]
$C_{16}H_{19}Br_2N_5O_5$ 521.165
Isol. from *Aplysina insularis.*

Cimino, G. *et al., Tet. Lett.*, 1983, **24**, 3029 (*Aerophobin 2*)
Assmann, M. *et al., Z. Naturforsch., C*, 1998, **53**, 398-401 (*N-Methylaerophobin 2*)
Fendert, T. *et al., Z. Naturforsch., C*, 1999, **54**, 246-251 (*14-Oxoaerophobin 2*)

Aeroplysinin 1 A-126

3,5-Dibromo-1,6-dihydroxy-4-methoxy-2,4-cyclohexadiene-1-acetonitrile, 9CI. 3,5-Dibromo-1-cyanomethyl-4-methoxy-3,5-cyclohexadiene-1,2-diol



(+)–*form*

$C_9H_9Br_2NO_3$ 338.983

(+)-*form* [28656-91-9]
Constit. of the sponges *Aplysina aerophoba (Verongia aerophoba*), *Aplysina archeri*, *Aiolochroia crassa*, *Verongula rigida*, *Psammaplysilla purpurea*, *Ianthella* sp. and others. Cytotoxic. Protein-tyrosine kinase inhibitor. Algicide, molluscicide. Sol. MeOH, Et_2O, Me_2CO; poorly sol. hexane.
Mp 120-121° (112-113°). $[\alpha]_D$ +193 (c, 0.63 in Me_2CO). $[\alpha]_D^{20}$ +185 (c, 0.17 in MeOH). λ_{max} 284 (ϵ 4910) (MeOH) (Derep). λ_{max} 231 (ϵ 3220); 284 (ϵ 4910) (MeOH) (Berdy).
▶ GU4735000

Di-Ac:
Cryst. (C_6H_6/petrol). Mp 114°. $[\alpha]_D$ +218 ($CHCl_3$).

(-)-*form*
Constit. of the sponges *Ianthella ardis*, *Verongula gigantea*, *Suberea creba*, *Psammaplysilla arabica* and *Pseudoceratina crassa*.
Mp 116-117°. $[\alpha]_D^{20}$ -176 (c, 0.125 in MeOH). $[\alpha]_D$ -198 (c, 0.5 in Me_2CO). λ_{max} 284 (ϵ 4910) (MeOH) (Derep).

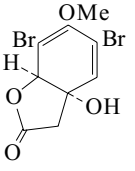
(±)-*form*
Constit. of *Verongula gigantea* and *Aiolochroia crassa*.
Mp 153-154°. λ_{max} 284 (ϵ 4910) (MeOH) (Derep).

[30951-40-7, 55057-73-3, 55057-74-4, 66141-25-1]

Fulmor, W. *et al., Tet. Lett.*, 1970, 4551 (*ir, pmr, cd, abs config*)
Cosulich, D.B. *et al., Chem. Comm.*, 1971, 397 (*cryst struct, abs config*)
Mazzarella, L. *et al., Gazz. Chim. Ital.*, 1972, **102**, 391 (*cryst struct, abs config*)
Fattorusso, E. *et al., J.C.S. Perkin 1*, 1972, 16 (*isol, uv, ir, pmr, ms, struct*)
Andersen, R.J. *et al., J.A.C.S.*, 1975, **97**, 936 (*synth*)
Chang, C.W.J. *et al., Tet. Lett.*, 1977, 4005 (*isol*)
Makarieva, T.N. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1981, **68**, 481 (*isol, uv, ir, ms*)
Koulman, A. *et al., J. Nat. Prod.*, 1996, **59**, 591 (*activity*)

Aeroplysinin 2 A-127

*5,7-Dibromo-3*a,*7*a*-dihydro-3*a*-hydroxy-6-methoxy-2(3*H*)-benzofuranone, 9CI*
[37694-12-5]



$C_9H_8Br_2O_4$ 339.968
Sol. MeOH.
▶ LD_{50} (mus, ipr) 202 mg/kg.

(+)-*form*
Constit. of the sponge *Aplysina aerophoba*.
Mp 106-108°. $[\alpha]_D$ +22 (c, 3 in MeOH). λ_{max} 284 (ϵ 4900) (MeOH) (Derep).

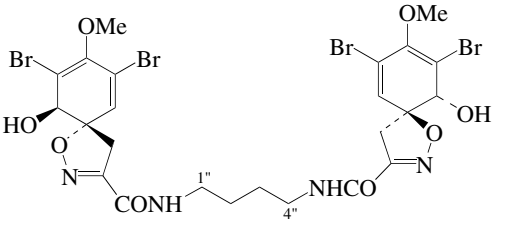
(±)-*form*
Constit. of the sponges *Aplysina cauliformis, Aplysina archeri, Psammaplysilla purpurea* and *Ianthella* sp.
Mp 127-128° (110-111°). λ_{max} 284 (ϵ 4900) (MeOH) (Derep).

[37676-85-0, 41841-33-2]

Minale, L. *et al., Chem. Comm.*, 1972, 674 (*uv, ir, pmr, ms, struct*)
Chang, C.W.J. *et al., Tet. Lett.*, 1977, 4005 (*isol*)
Makarieva, T.N. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1981, **68**, 481 (*isol*)

Aerothionin A-128

[28714-26-3]



$C_{24}H_{26}Br_4N_4O_8$ 818.107
Metab. from the sponges *Aplysina aerophoba* (*Verongia aerophoba*), *Aplysina fistularis* and *Aplysina thiona*, also from *Pseudoceratina durissima* and *Psammaplysilla purpurea*. Plates (Me_2CO/C_6H_6).
Mp 134-137° dec. $[\alpha]_D$ +252 (Me_2CO). λ_{max} 234 (ϵ 14450); 284 (ϵ 13490) (EtOH) (Derep). λ_{max} 284 (ϵ 12660) (MeOH) (Berdy).

Di-Ac:
Needles (Me_2CO). Mp 206-208°. $[\alpha]_D$ +236 ($CHCl_3$).

2′′-Hydroxy: ***11-Hydroxyaerothionin***
[73622-27-2]
$C_{24}H_{26}Br_4N_4O_9$ 834.107
Metab. from the verongid sponge *Pseudoceratina durissima* and by *Aplysina lacunosa*. Glass. $[\alpha]_D$ +189 (c, 0.15 in MeOH). λ_{max} 233 (ϵ 19780); 284 (ϵ 11100); 295 (ϵ 18900) (MeOH) (Berdy).

2′′,3′′-Dihydroxy: ***Dihydroxyaerothionin***
[122759-72-2]
$C_{24}H_{26}Br_4N_4O_{10}$ 850.106
Metab. of *Verongula rigida*. Powder.
Mp 162-164°. $[\alpha]_D^{25}$ -64.2 (c, 0.1 in MeOH).

2′′-Oxo: ***11-Oxoaerothionin***
[73622-23-8]
$C_{24}H_{24}Br_4N_4O_9$ 832.091
Metab. from the Caribbean sponge *Aplysina lacunosa* and from *Verongia cavernicola*. Exhibits pronounced and selective antitumour activity against human colon (HCT116) cell line. Powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 174.6-176.6° dec. $[\alpha]_D^{25}$ +181.15 (c, 2.17 in DMSO). λ_{max} 262 (ϵ 11600); 284 (ϵ 11500) (MeOH) (Berdy).

*2′′-Oxo, 3′′*R*-hydroxy:* ***12R-Hydroxy-11-oxoaerothionin***
[157544-68-8]
$C_{24}H_{24}Br_4N_4O_{10}$ 848.09
Metab. from the Caribbean sponge *Aplysina fistularis* forma *fulva*. $[\alpha]_D^{25}$ +160.7.

*2′′-Oxo, 3′′*S*-hydroxy:* ***12S-Hydroxy-11-oxoaerothionin***
[157497-57-9]
$C_{24}H_{24}Br_4N_4O_{10}$ 848.09
Metab. from the sponge *Aplysina fistularis* forma *fulva*. $[\alpha]_D^{25}$ +152.5.

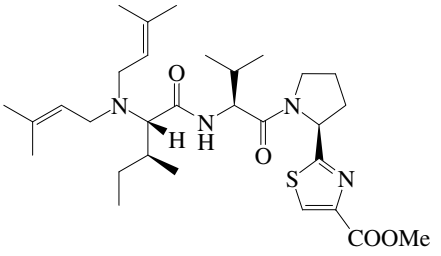
Homologue: ***Homoaerothionin***
[34232-66-1]
[35036-48-7]
$C_{25}H_{28}Br_4N_4O_8$ 832.134
Constit. of the sponges *Aplysina aerophoba*, *Verongia thiona* and *Verongia cavernicola*. Amorph. solid.
Mp 166-167° (as di-Ac). $[\alpha]_D$ +191.5 ($CHCl_3$) (di-Ac). Has a C_5 bridging chain instead of C_4. λ_{max} 289 (ϵ 13348) (MeOH) (Berdy).

Homologue, 2′′-oxo: 11-Oxohomoaerothionin
[191112-17-1]
$C_{25}H_{26}Br_4N_4O_9$ 846.118
Constit. of *Aplysina cavernicola*. Has a C_5 bridging chain instead of C_4. λ_{max} 232 (ϵ 19000); 284 (10500) (MeOH).

Fattorusso, E. *et al., Chem. Comm.*, 1970, 752-753 (*uv, ir, pmr, struct*)
Fattorusso, E. *et al., Gazz. Chim. Ital.*, 1971, **101**, 61-63 (*Homoaerothionin*)
Moody, K. *et al., J.C.S. Perkin 1*, 1972, 18-24 (*isol, uv, ir, pmr, struct, Homoaerothionin*)
Forrester, A.R. *et al., Annalen*, 1978, 66-73 (*synth*)
McMillan, J.A. *et al., Tet. Lett.*, 1981, **22**, 39-42 (*cryst struct, uv, pmr, cd, abs config*)
Nishiyama, S. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 3453-3456 (*synth*)
Gunasekera, M. *et al., J. Nat. Prod.*, 1989, **52**, 753-756 (*Dihydroxyaerothionin*)
Kernan, M.R. *et al., J. Nat. Prod.*, 1990, **53**, 615-622 (*11-Hydroxyaerothionin*)
Acosta, A.L. *et al., J. Nat. Prod.*, 1992, **55**, 1007-1012 (*11-Oxoaerothionin*)
Ciminiello, P. *et al., J. Nat. Prod.*, 1994, **57**, 705-712 (*12-Hydroxy-11-oxoaerothionin*)
Ciminiello, P. *et al., Tetrahedron*, 1997, **53**, 6565-6572 (*11-Oxohomoaerothionin*)
Wasserman, H.H. *et al., J.O.C.*, 1998, **63**, 5581-5586 (*synth*)
Ogamino, T. *et al., Tet. Lett.*, 2006, **47**, 727-731 (*synth, abs config*)

Aeruginosamide A-129

[241483-64-7]

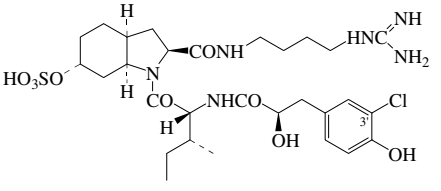


$C_{30}H_{48}N_4O_4S$ 560.8
Modified peptide antibiotic. Isol. from *Microcystis aeruginosa*. Moderate cytotoxic agent. Pale green oil. $[\alpha]_D$ -71.4 (c, 0.01 in $CHCl_3$).

Lawton, L.A. *et al., J.O.C.*, 1999, **64**, 5329-5332 (*isol, pmr, cmr, ir, ms*)

Aeruginosin 98A A-130

[167172-80-7]



Absolute Configuration

$C_{29}H_{45}ClN_6O_9S$ 689.228
Isol. from the blue-green alga *Microcystis aeruginosa* NIES98. Inhibitor of trypsin, thrombin and serine proteases. Amorph. powder. Sol. MeOH, H_2O. $[\alpha]_D$ -7.6 (c, 0.2 in H_2O). λ_{max} 279 (ϵ 1472) (H_2O) (Berdy).

5′-Chloro: ***Aeruginosin 101***
$C_{29}H_{44}Cl_2N_6O_9S$ 723.673
Isol. from *Microcystis aeruginosa*. Protease inhibitor. $[\alpha]_D$ -11 (c, 0.5 in MeOH aq.). λ_{max} 290 (ϵ 1810) (MeOH).

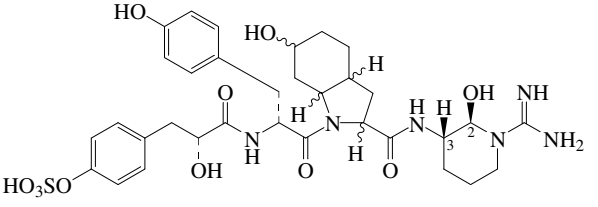
3′-Dechloro: ***Aeruginosin 98B***
[167228-01-5]
$C_{29}H_{46}N_6O_9S$ 654.783
Isol. from *Microcystis aeruginosa* NIES98. Inhibitor of trypsin, thrombin, plasmin and serine proteases. Amorph. powder. Sol. MeOH, H_2O. $[\alpha]_D$ -5.2 (c, 0.2 in H_2O). λ_{max} 276 (ϵ 1177) (H_2O) (Berdy).

3′-Dechloro, 3′-bromo: ***Aeruginosin 98C***
[167172-73-8]
$C_{29}H_{45}BrN_6O_9S$ 733.679
Isol. from *Microcystis aeruginosa* NIES98. Serine protease inhibitor. Powder. Sol. MeOH, H_2O. $[\alpha]_D$ -13 (c, 0.25 in H_2O). λ_{max} 281 (ϵ 860) (H_2O).

Murakami, M. *et al., Tet. Lett.*, 1995, **36**, 2785-2788 (*isol, pmr, cmr*)
Ishida, K. *et al., Tetrahedron*, 1999, **55**, 10971-10988 (*isol, abs config*)

Aeruginosin 102A A-131

[173357-14-7]



$C_{33}H_{44}N_6O_{11}S$ 732.81

Isol. from the cyanobacterium *Microcystis aeruginosa* NEIS 102. Thrombin inhibitor. Amorph. powder. λ_{max} 275 (ϵ 1500) (MeOH).

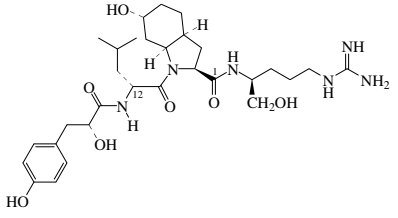
2-Et ether, O-*desulfo:* ***Aeruginosin 103A***
[211428-63-6]
$C_{35}H_{48}N_6O_8$ 680.8
Isol. from *Microcystis viridis* NEIS 102. Thrombin inhibitor. Amorph. powder. $[\alpha]_D$ -7.6 (c, 0.1 in MeOH). λ_{max} 224 (ϵ 11600); 274 (ϵ 2100) (H_2O).

3-Epimer: ***Aeruginosin 102B***
[173401-69-9]
$C_{33}H_{44}N_6O_{11}S$ 732.81
Isol. from *Microcystis viridis* NEIS 102. Thrombin inhibitor. Amorph. powder. λ_{max} 275 (ϵ 2300) (MeOH).

Matsuda, H. *et al., Tetrahedron*, 1996, **52**, 14501-14506 (*Aeruginosins 102A, 102B*)
Kodani, S. *et al., J. Nat. Prod.*, 1998, **61**, 1046-1048 (*Aeruginosin 103A*)

Aeruginosin 298A A-132

[156312-05-9]



Absolute Configuration

$C_{30}H_{48}N_6O_7$ 604.745
Abs. config. finally confirmed in 2001 after synth. Isol. from the freshwater blue-green alga *Microcystis aeruginosa* (NIES-298). Thrombin and trypsin inhibitor. Amorph. powder. Sol. H_2O, butanol, MeOH; poorly sol. Et_2O. $[\alpha]_D$ +22.3 (c, 0.36 in H_2O). λ_{max} 275 (ϵ 1166) (H_2O) (Berdy).

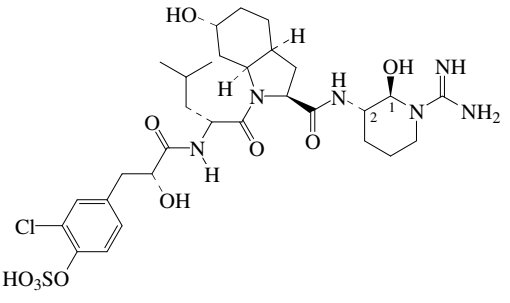
N^1-*De(argininolyl):* ***Aeruginosin 298B***
[249282-92-6]
$C_{24}H_{35}N_3O_6$ 461.557
Isol. from *Microcystis aeruginosa* (NIES-298). Obt. as a C-12 epimeric mixt. λ_{max} 277 (ϵ 2030) (MeOH).

N^1-*De(argininolyl), stereoisomer:* ***Aeruginosin EI 461***
$C_{24}H_{35}N_3O_6$ 461.557
Isol. from *Microcystis aeruginosa*. Oil. $[\alpha]_D^{25}$ +5 (c, 0.006 in MeOH).

Murakami, M. *et al., Tet. Lett.*, 1994, **35**, 3129-3132 (*isol, uv, pmr, cmr, struct*)
Ishida, K. *et al., Tetrahedron*, 1999, **55**, 10971-10988 (*isol*)
Wipf, P. *et al., Org. Lett.*, 2000, **2**, 4213-4216 (*synth, abs config*)
Valls, N. *et al., Chem. Eur. J.*, 2001, **7**, 3446-3460 (*synth, abs config*)
Ploutno, A. *et al., J. Nat. Prod.*, 2002, **65**, 973-978 (*EI 461*)
Valls, N. *et al., Org. Lett.*, 2003, **5**, 447-450 (*EI 461, synth, struct*)
Ohshima, T. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1031-1052 (*rev, synth*)
Fukuta, Y. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2004, **101**, 5433-5438 (*synth*)

Aeruginosin 89B A-133

[249298-28-0]



$C_{30}H_{45}ClN_6O_{10}S$ 717.238
Isol. from *Microcystis aeruginosa*. Protease inhibitor. $[\alpha]_D^{23}$ +9.4 (c, 0.1 in MeOH). λ_{max} 283 (ϵ 1660) (MeOH).

Diastereoisomer: ***Aeruginosin 89A***
[249282-93-7]
$C_{30}H_{45}ClN_6O_{10}S$ 717.238
Isol. from *Microcystis aeruginosa*. Epimeric with Aeruginosin 89B at C-2. C-1 config. not determined.

Ishida, K. *et al., Tetrahedron*, 1999, **55**, 10971-10988

AF Toxin A-134

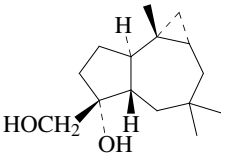
Anthopleura fuscoviridis *Toxin*
[109020-92-0]
Complex of two peptides designated AFT-I and AFT-II which consist of 47 and 48 amino acid residues respectively, and are crosslinked with 3 disulfide bridges. The sequences have high homology to those of toxins I and II from *Anemonia sulcata* and Anthopleurins A and B from *Anthopleura xanthogrammica*. Isol. from the sea urchin *Anthopleura fuscoviridis*. Not related to AF Toxin II.

[109020-93-1]

Sunahara, S. *et al., Toxicon*, 1987, **25**, 211-219 (*isol, struct*)

3,15-Africananediol A-135

9,15-Africananediol



3α-*form*

$C_{15}H_{26}O_2$ 238.369

3α-form [251453-75-5]
Constit. of *Sinularia intacta*.
Cryst. (Me_2CO/hexane).
Mp 122-125°. $[\alpha]_D^{25}$ +15.3 (c, 1.2 in $CHCl_3$).

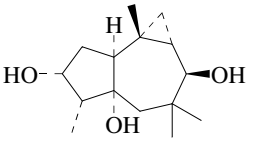
3-Me ether: 3-Methoxy-15-africananol
[251453-76-6]
$C_{16}H_{28}O_2$ 252.396
Constit. of *Sinularia intacta*. Cryst. (Me_2CO/hexane).
Mp 118-120°. $[\alpha]_D^{25}$ -22 (c, 1.2 in $CHCl_3$).

3β-form [236126-36-6]
Constit. of *Sinularia dissecta*.
Cryst.
Mp 113°. $[\alpha]_D^{25}$ +13.8 (c, 1.25 in $CHCl_3$).

15-Ac: [251453-77-7]
$C_{17}H_{28}O_3$ 280.406
Constit. of *Sinularia intacta*. Oil. $[\alpha]_D^{25}$ -26 (c, 1.5 in $CHCl_3$).

Ramesh, P. *et al., J. Nat. Prod.*, 1999, **62**, 1019-1021 (*isol, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 1999, **62**, 1600-1604 (*Sinularia intacta constits*)

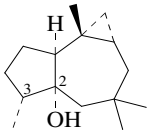
2,4,10-Africananetriol A-136



$C_{15}H_{26}O_3$ 254.369

(2α,3α,4α,6α,10β)-*form*
Africantriol
Prod. by the marine-derived *Streptomyces* sp. strain HKI0297 and from the octocoral *Lemnalia africana*.
Cryst. ($CHCl_3$/MeOH).
Mp 189-190°. $[\alpha]_D$ +63.9 (c, 0.44 in MeOH).
Jurek, J. *et al., J. Nat. Prod.*, 1993, **56**, 508-513 (*isol*)
Hu, J.-F. *et al., J. Antibiot.*, 2003, **56**, 747-754 (*isol, pmr, cmr*)

2-Africananol A-137



(2α,3α,6α)-*form*

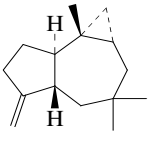
$C_{15}H_{26}O$ 222.37

(2α,3α,6α)-*form*
Isoafricanol
[104975-19-1]
Constit. of fungus *Leptographium lundbergii*.
Oil. $[\alpha]_D^{23}$ +11.4 (c, 0.59 in $CHCl_3$).

(2α,3β,6α)-*form*
Africanol
[53823-07-7]
Constit. of *Lemnalia africana*.
Cryst.
Mp 58-60°. $[\alpha]_D$ +59.5 (c, 0.5 in $CHCl_3$).
Tursch, B. *et al., Tet. Lett.*, 1974, 747 (*Africanol*)
Karlsson, R. *et al., Acta Cryst. B*, 1976, **32**, 2609 (*cryst struct*)
Abraham, W.R. *et al., Tetrahedron*, 1986, **42**, 4475 (*Isoafricanol*)
Fan, W. *et al., J.O.C.*, 1993, **58**, 3557 (*synth*)
Marques, F. de A. *et al., J. Braz. Chem. Soc.*, 2000, **11**, 502-511 (*synth*)

3(15)-Africanene A-138

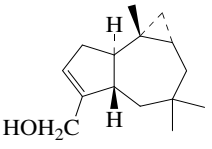
9(15)-Africanene
[74016-87-8]



$C_{15}H_{24}$ 204.355
Constit. of *Sinularia erecta* and *Sinularia leptoclados*. Cytotoxic. Shows hypertensive and antiinflammatory activity. Oil. $[\alpha]_D^{24}$ +86 (c, 3.7 in $CHCl_3$).
3β,15-Epoxide: ***3,15-Epoxyafricanene****. 9,15-Epoxyafricanene*
[236126-35-5]
$C_{15}H_{24}O$ 220.354
Constit. of *Sinularia dissecta*. Amorph. solid.
Mp 125°. $[\alpha]_D^{25}$ +16.2 (c, 1.1 in $CHCl_3$).
Kashman, Y. *et al., Experientia*, 1980, **36**, 891
Rao, T.S. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 1356 (*isol, pmr, ms*)
Reddy, B.S.G. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1214-1220 (*activity*)
Ramesh, P. *et al., J. Nat. Prod.*, 1999, **62**, 1019-1021 (*epoxide*)

3-Africanen-15-ol A-139

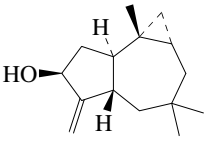
9-Africanen-15-ol
[376597-20-5]



$C_{15}H_{24}O$ 220.354
Constit. of *Sinularia dissecta*. Oil. $[\alpha]_D$ +6.43 (c, 0.45 in $CHCl_3$).
Ramesh, P. *et al., Indian J. Chem., Sect. B*, 2001, **40**, 867-868 (*isol, pmr, cmr*)

3(15)-Africanen-4-ol A-140

9(15)-Africanen-10-ol



$C_{15}H_{24}O$ 220.354

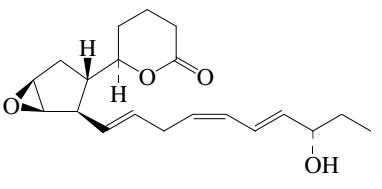
4β-*form* [236126-34-4]
Constit. of *Sinularia dissecta*.
Cryst. (hexane).
Mp 98°. $[\alpha]_D^{25}$ +19.1 (c, 1.2 in $CHCl_3$).
Ramesh, P. *et al., J. Nat. Prod.*, 1999, **62**, 1019-1021 (*isol, pmr, cmr*)

Agar A-141

Agar-agar. Gum agar. Gelose. Japan agar. Bengal isinglass. Ceylon isinglass. Chinese isinglass. Japan isinglass. FEMA 2012. E406
[9002-18-0]
See also Agarose, A-144. Consists of a mixt. of 2 polysaccharides, Agarose A-144 and Agaropectin, which has essentially the same struct. except that a variable proportion of the sugars in the polymer are replaced by 4,6-*O*-(1-carboxyethylidene)galactose or by sulfated or methylated sugar residues such as to retain the alternating sequence of 3-linked β-D- and 4-linked α-L- units. Distinguished from Carrageenan, C-140 by the presence of L-galacto residues and by the generally lower MW (mean ca. 120kDa but with a range of approx. 70-700). Mucilaginous substance extracted from red marine algae (Rhodophyceae); *Gelidiella acerosa*, various *Gelidium* spp. *Gracilaria confervoides*, *Pterocladia capillacea* and *Pterocladia lucida* are used in various parts of the world. There is some species variation in gel structure and strength. An important thickener, stabiliser and gelling agent in the food industry. Also used as protective colloid in photometric detn. of Sn, Mg, Si, $SO_4^{2\ominus}$. Solid medium for the cultivation of bacteria. Laxative-cathartic. Strips or fine powder. Sl. sol. in hot H_2O.
▶ AW7950000
Clark, R.E. *et al., Analyst (London)*, 1937, **62**, 661 (*detn, Sn*)
Bogan, E.J. *et al., Ind. Eng. Chem., Anal. Ed.*, 1942, **14**, 849 (*detn, $SO_4^{2\ominus}$*)
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, New York, 1948, **4**, (*use*)
BeMiller, J.N. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 65 (*purifn*)
Duckworth, M. *et al., Carbohydr. Res.*, 1971, **18**, 1 (*struct, bibl*)
Davidson, R.L. *et al., Handb. Water-Soluble Gums Resins*, McGraw-Hill, N.Y., 1980, 7/1 (*rev*)
Glickmann, M. *et al., Food Hydrocolloids*, CRC Press, Boca Raton, Florida, 1983, **2**, 73 (*rev*)
Rochas, C. *et al., Carbohydr. Res.*, 1994, **253**, 69 (*bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 53-56 (*use, props*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1470
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AEX250

Agardhilactone A-142

[178949-88-7]



Absolute Configuration

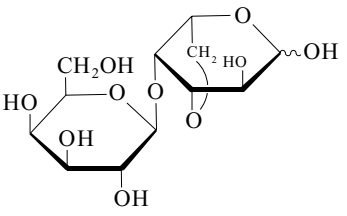
$C_{20}H_{28}O_4$ 332.439

Stereochem. revised in 2005. Isol. from the red alga *Agardhiella subulata*. Oil. λ_{max} 236 (ϵ 39000) (MeOH) (as Ac).

Graber, M.A. *et al., Tet. Lett.*, 1996, **37**, 4635-4638 (*isol, pmr, cmr*)
Miyaoka, H. *et al., Tet. Lett.*, 2005, **46**, 7945-7949 (*synth, config*)

Agarobiose, 9CI A-143

3,6-Anhydro-4-O-β-D-galactopyranosyl-L-galactose, 9CI. β-D-Galactopyranosyl-(1→4)-3,6-anhydro-L-galactose
[5627-25-8]



$C_{12}H_{20}O_{10}$ 324.284
Obt. from agar by partial acid hydrol. and from the polysaccharide of the red seaweed *Gloiopeltis furcata*. Amorph. solid. $[\alpha]_D^{15}$ -15.9 (c, 0.82 in H_2O).

Phenylosazone: Mp 220-221°. $[\alpha]_D^{16}$ +136.2 → -109.2 (c, 0.42 in 3:2 MeOH/Py).

Di-Me acetal: Mp 162-164°. $[\alpha]_D$ -36 (MeOH).

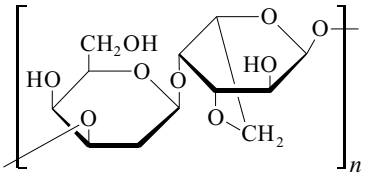
Diethyldithioacetal: Mp 171-172°.

1,2-O-Isopropylidene:
$C_{15}H_{24}O_{10}$ 364.349
Cryst. (MeOH). Mp 163-165°. $[\alpha]_D^{16}$ -29.4 (c, 1.2 in H_2O).

Hirase, S. *et al., Bull. Chem. Soc. Jpn.*, 1958, **31**, 428; 1968, **41**, 626 (*isol, synth*)
BeMiller, J.N. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 65 (*synth*)

Agarose A-144

Neutral agarose. Indubiose A4
[9012-36-6]
[9036-61-7]



See also Agar, A-141. Composed of repeating units of β-D-Gal*p*-(1→4)-3,6-anhydro-α-L-Gal*p*-(1→3). Has a domain struct. of double helixes aggregating into a three-dimensional framework holding water molecules. Isol. from red seaweed agar (*Gelidium* spp.). Gives gels of high strength at low concs. in water which are nearly transparent. These are used commercially as gelling agents and for biomedical applications, e.g. electrophoresis media, chromatography and immunology assays.
There are two other polysaccharides in agar, one is similar to agarose but with 4,6-acetals of pyruvic acid at some of the D-galactose units. The other contains fewer 3,6-anhydro-L-galactose units and is sulfated.

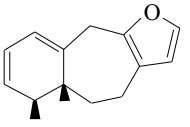
Poly(6-aminohexyl) ether: Agarose (6-aminohexyl)carbamimidate. Sepharose AH
[58856-73-8]
Intermed. for the prepn. of affinity chromatog. absorbents. Non-stoichiometric.

Poly(5-carboxypentyl) ether: [55128-01-3]
Intermed. for the prepn. of affinity chromatog. absorbents. Non-stoichiometric.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 201C; 201D (*ir*)
Hegenauer, J.C. *et al., Biochim. Biophys. Acta*, 1965, **111**, 334 (*isol*)
BeMiller, J.N. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 65 (*purifn*)
Percival, E. *et al., The Carbohydrates*, 1970, **2B**, 553
Batey, J.F. *et al., Carbohydr. Res.*, 1975, **43**, 133
Turvey, J.R. *et al., Carbohydr. Res.*, 1976, **49**, 419
Rees, D. *et al., Angew. Chem., Int. Ed.*, 1977, **16**, 214
Taylor, J.L. *et al., J. Chromatogr.*, 1983, **257**, 275-284 (*5-carboxypentyl ether*)
Szewezyk, A. *et al., Biochim. Biophys. Acta*, 1987, **89**, 252-260 (*6-aminohexyl ether*)
Kiwitt-Haschemie, K. *et al., Carbohydr. Res.*, 1993, **248**, 267
Arndt, E.R. *et al., Carbohydr. Res.*, 1997, **303**, 73-78 (*cd, struct*)
Gamini, A. *et al., Carbohydr. Res.*, 1997, **304**, 293-302 (*pmr, cmr, conformn*)

Agassizin A-145

[79827-32-0]

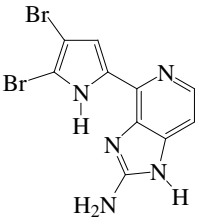


$C_{15}H_{18}O$ 214.307
Constit. of the nudibranch *Hypselodoris agassizi* spp. and sponge *Pleraplysilla spinifera*. Oil. $[\alpha]_D$ -94 (c, 1.2 in MeOH). λ_{max} 220 (ϵ 10300); 268 (ϵ 7000) (MeOH) (Derep). λ_{max} 225 (ϵ 9250); 266 (ϵ 3500) (MeOH) (Berdy). λ_{max} 223 (ϵ 9430); 258 (ϵ 3510) (Et_2O) (Berdy).

Hochlowski, J.E. *et al., J.O.C.*, 1982, **47**, 88-91 (*isol*)

Ageladine A A-146

[643020-13-7]

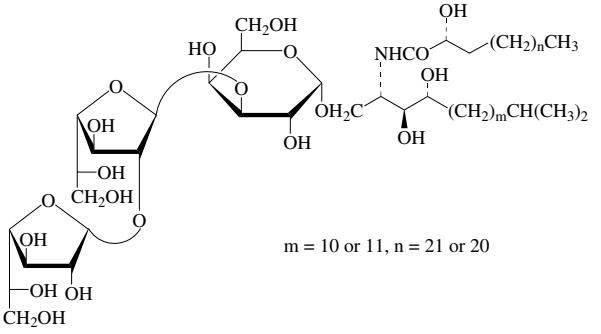


$C_{10}H_7Br_2N_5$ 357.007
Isol. from *Agelas nakamurai*. Antiangiogenic matrixmetalloproteinase inhibitor. Yellow powder (as di-TFA salt). λ_{max} 227 (ϵ 15400); 250 (ϵ 9960); 381 (ϵ 12200) (MeOH) (di-TFA salt).

Fujita, M. *et al., J.A.C.S.*, 2003, **125**, 15700-15701 (*Ageladine A*)
Meketa, M.L. *et al., Org. Lett.*, 2006, **8**, 1443-1446 (*synth*)
Shengule, S.R. *et al., Org. Lett.*, 2006, **8**, 4083-4084 (*synth*)

Agelagalastatin A-147

[233608-55-4]



m = 10 or 11, n = 21 or 20

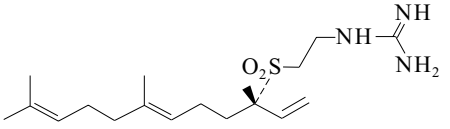
$C_{60}H_{115}NO_{20}$ 1170.563
Isol. from the marine sponge *Agelas* sp. Antineoplastic agent. Amorph. powder. $[\alpha]_D$ +59 (c, 0.65 in MeOH).

Pettit, G.R. *et al., Chem. Comm.*, 1999, 915-916 (*isol, pmr, cmr, activity*)
Lee, Y.J. *et al., Org. Lett.*, 2006, **8**, 3971-3974 (*synth*)

Agelasidine A A-148

2-[[(1-Ethenyl-1,5,9-trimethyl-4,8-decadienyl)sulfonyl]ethyl]guanidine, 9CI

[87853-53-0]



$C_{18}H_{33}N_3O_2S$ 355.544

Isol. from the Okinawan sea sponge *Agelas nakamurai* and from a Pacific sponge *Agelas* sp. Shows antispasmodic and antibacterial activity. Unstable yellow oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 227 (ϵ 5400); 265 (ϵ 1800) (EtOH) (Berdy). λ_{max} 226 (ϵ 4000); 270 (ϵ 2000) (EtOH/HCl) (Berdy).

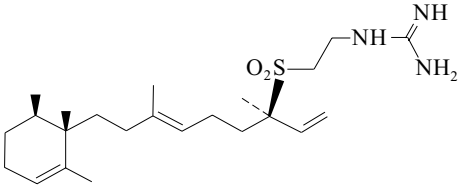
Hydrochloride:

Cryst. + ⅓ H_2O (EtOAc). Mp 108-108.5°. $[\alpha]_D^{25}$ +19.1 (c, 1 in MeOH).

Capon, R.J. *et al., J.A.C.S.*, 1984, **106**, 1819 (*isol, uv, ir, pmr, cmr, ms*)
Nakamura, H. *et al., J.O.C.*, 1985, **50**, 2494 (*isol, uv, ir, pmr, cmr*)
Ichikawa, Y. *et al., J.C.S. Perkin 1*, 1992, 1497 (*synth*)

Agelasidine B A-149

[96617-50-4]

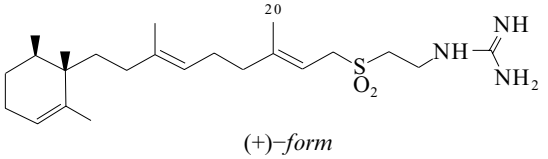


$C_{23}H_{41}N_3O_2S$ 423.662

Isol. from the Okinawan sea sponge *Agelas nakamurai*. Shows antispasmodic and antibacterial activity. Syrup (as hydrochloride). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{25}$ -2.5 (c, 0.43 in MeOH).

Nakamura, H. *et al., J.O.C.*, 1985, **50**, 2494 (*isol, uv, ir, pmr, cmr, struct*)

Agelasidine C A-150



(+)–form

$C_{23}H_{41}N_3O_2S$ 423.662

(+)-*form* [96617-52-6]

Isol. from the sponges *Agelas nakamurai* and *Agelas dispar*. Shows antispasmodic and antibacterial activity. Syrup (as hydrochloride). Sol. MeOH, $CHCl_3$. $[\alpha]_D^{25}$ +8.5 (c, 2.0 in MeOH) (hydrochloride).

(-)-*form* [139757-42-9]

Isol. from *Agelas clathrodes*.

Oil. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{29}$ -5.6 (c, 7.2 in MeOH).

20-Hydroxy: ***Agelasidine D***

[139680-61-8]

$C_{23}H_{41}N_3O_3S$ 439.661

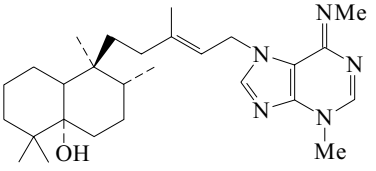
Isol. from *Agelas clathrodes*. Oil. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{29}$ -3.6 (c, 2.75 in MeOH).

[96617-52-6]

Nakamura, H. *et al., J.O.C.*, 1985, **50**, 2494-2498 (*isol, uv, ir, pmr, cmr, struct*)
Asao, K. *et al., Chem. Lett.*, 1989, 1813-1814 (*synth*)
Morales, J.J. *et al., J. Nat. Prod.*, 1992, **55**, 389-394 (*isol*)

Agelasimine A A-151

[114216-85-2]



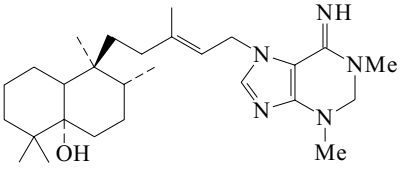
$C_{27}H_{43}N_5O$ 453.67

Metab. from the marine sponge *Agelas mauritiana*. Exhibits cytotoxicity, inhibition of adenosine transfer into rabbit erythrocytes, $Ca^{2\oplus}$-channel antagonistic action and α_1 adrenergic blockade. Yellowish oil. Sol. MeOH, EtOH, $CHCl_3$. $[\alpha]_D^{25}$ +2.3 (MeOH). λ_{max} 223 (ϵ 9700); 287 (ϵ 14700) (MeOH) (Berdy).

Fathi-Afshar, R. *et al., Can. J. Chem.*, 1988, **66**, 45 (*isol, uv, ir, pmr, cmr, ms, struct*)
Ohba, M. *et al., J.A.C.S.*, 1996, **118**, 8250 (*synth*)
Ohba, M. *et al., Tetrahedron*, 1997, **53**, 16977-16986 (*synth, abs config*)

Agelasimine B A-152

[114216-87-4]



$C_{27}H_{45}N_5O$ 455.685

Metab. from the marine sponge *Agelas mauritiana*. Exhibits cytotoxicity, inhibition of adenosine transfer into rabbit erythrocytes, $Ca^{2\oplus}$-channel antagonistic action and α_1 adrenergic blockade. Viscous yellowish oil. Sol. MeOH, $CHCl_3$, EtOH. $[\alpha]_D^{25}$ +2.46 (MeOH). λ_{max} 245 (ϵ 7100); 327 (ϵ 5400) (MeOH) (Berdy).

Fathi-Afshar, R. *et al., Can. J. Chem.*, 1988, **66**, 45 (*isol, uv, ir, pmr, cmr, ms, struct*)
Ohba, M. *et al., J.A.C.S.*, 1996, **118**, 8250 (*synth*)
Ohba, M. *et al., Tetrahedron*, 1997, **53**, 16977-16986 (*synth, abs config*)

Agelasine† A-153

Struct. unknown

$C_{26}H_{40}N_5^{\oplus}$ 422.635

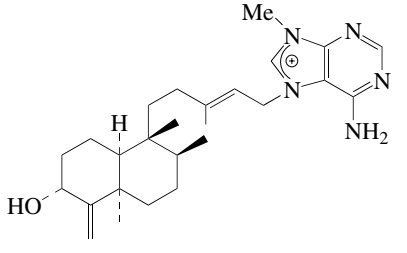
Quaternary 9-methyladenine deriv. of an unidentified bicyclic diterpene. Isol. from the sponge *Agelas dispar*. Cryst. (butanone/THF) (as chloride).

Mp 197-200° dec. (chloride). Mp of chloride does not appear to correspond with any of the Agelasines of known struct. λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH) (Derep).

Cullen, E. *et al., Can. J. Chem.*, 1975, **53**, 1690 (*isol, uv, ir, pmr, ms*)

Agelasine I A-154

[205382-10-1]



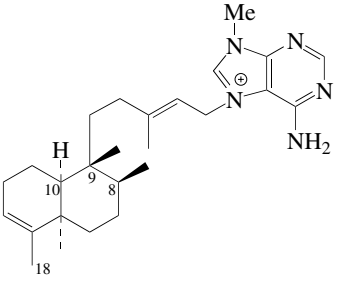
$C_{26}H_{40}N_5O^{\oplus}$ 438.635

Isol. from a sponge *Agelas* sp. Amorph. solid (as chloride). $[\alpha]_D$ -2.5 (c, 0.2 in MeOH). λ_{max} 272 (ϵ 8230) (MeOH).

Fu, X. *et al., J. Nat. Prod.*, 1998, **61**, 548-550 (*isol, uv, ir, pmr, cmr*)

Agelasine A† A-155

[56271-74-0]



$C_{26}H_{40}N_5^{\oplus}$ 422.635

Constit. of the Okinawan sponge *Agelas nakamurai*. ATPase inhibitor, spasmolytic agent, smooth muscle contractant. Cryst. (as chloride). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 173-174° (chloride). $[\alpha]_D^{25}$ -31.3 (c, 0.59 in MeOH). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH) (Derep).

18-Hydroxy: ***Agelasine H***

[205382-09-8]

$C_{26}H_{40}N_5O^{\oplus}$ 438.635

Constit. of an *Agelas* sp. Amorph. solid (as chloride). $[\alpha]_D$ -63.9 (c, 0.36 in MeOH). λ_{max} 272 (ϵ 9015) (MeOH).

8,9,10-Triepimer: ***Agelasine B***

[92664-76-1]

$C_{26}H_{40}N_5^{\oplus}$ 422.635

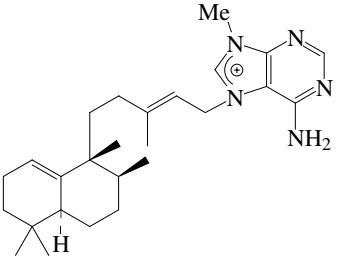
Constit. of *Agelas nakamurai*. ATPase inhibitor, spasmolyic agent. Cryst. (as chloride). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 167-170° (chloride). $[\alpha]_D^{25}$ -21.5 (c, 1.00 in MeOH). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH) (Derep). λ_{max} 272 (ϵ 8240) (MeOH) (Berdy).

Nakamura, H. *et al., Tet. Lett.*, 1984, **25**, 2989 (*uv, pmr, cmr, struct*)
Piers, E. *et al., J.C.S. Perkin 1*, 1995, 963 (*synth*)
Fu, X. *et al., J. Nat. Prod.*, 1998, **61**, 518-550 (*Agelasine H*)

Agelasine C A-156

[92664-78-3]

[92664-79-4 (chloride)]



$C_{26}H_{40}N_5^{\oplus}$ 422.635

Stereochem. revised in 2005. Isol. from the sponge *Agelas nakamurai*. Shows antimicrobial activity. ATP-ase inhibitor. Spasmolytic agent. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 176-179° (as chloride). $[\alpha]_D^{25}$ -55.1 (c, 2.04 in MeOH) (chloride). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH) (Derep).

5,9-Diepimer: ***Epiagelasine C***

$C_{26}H_{40}N_5^{\oplus}$ 422.636

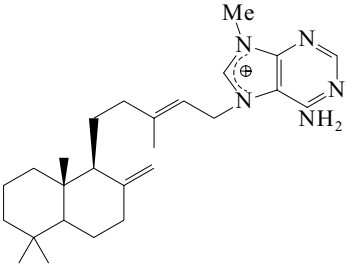
Constit. of sponge *Agelas mauritiana*. Antifouling substance against macroalgae. Powder (as chloride). $[\alpha]_D^{25}$ +33.9 (c, 0.056 in MeOH) (chloride). Stereochem. revised in 2005. λ_{max} 273 (ϵ 8140) (MeOH).

Nakamura, H. *et al., Tet. Lett.*, 1984, **25**, 2989-2992 (*isol, uv, pmr, cmr*)
Hattori, T. *et al., J. Nat. Prod.*, 1997, **60**, 411-413 (*5-epimer*)
Marcos, I. *et al., Tetrahedron*, 2005, **61**, 11672-11678 (*synth, abs config*)

Agelasine D A-157

[92664-80-7]

[92664-81-8 (chloride)]



$C_{26}H_{40}N_5^{\oplus}$ 422.635

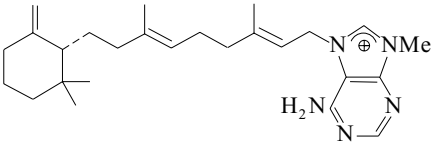
Isol. from the Okinawan sea sponge *Agelas nakamurai*. Shows antimicrobial activity. Spasmolytic agent. Na/K ATP-ase inhibitor. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 175-176° (as chloride). $[\alpha]_D^{25}$ +10.4 (c, 1.1 in MeOH) (chloride). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH) (Derep).

Nakamura, H. *et al., Tet. Lett.*, 1984, **25**, 2989 (*uv, pmr, cmr, struct*)
Utenova, B.T. *et al., Tet. Lett.*, 2004, **45**, 4233-4235 (*synth*)
Vik, A. *et al., J. Nat. Prod.*, 2006, **69**, 381-386 (*synth, activity*)

Agelasine E A-158

[92599-00-3]

[92599-01-4 (chloride)]



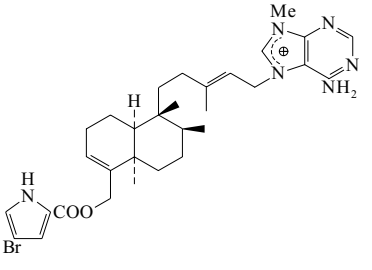
$C_{26}H_{40}N_5^{\oplus}$ 422.635

Isol. from the Okinawan sea sponge *Agelas nakamurai*. ATP-ase inhibitor, spasmolytic agent. Powder (as chloride). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 180-182° (chloride). $[\alpha]_D^{23}$ -17.1 (c, 1.88 in MeOH) (chloride). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH) (Derep).

Wu, H. *et al., Tet. Lett.*, 1984, **25**, 3719 (*uv, pmr, cmr, ms, struct*)
Bakkestuen, A.K. *et al., Org. Biomol. Chem.*, 2005, **3**, 1025-1033 (*synth*)

Agelasine G A-159

[142808-37-5]



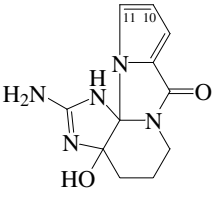
$C_{31}H_{42}BrN_6O_2^{\oplus}$ 610.616

Isol. from the Okinawan marine sponge *Agelas* sp. Exhibits cytotoxicity against murine lymphoma L1210 cells *in vitro*. $[\alpha]_D^{27}$ -85 (c, 0.02 in $CHCl_3$) (as chloride). λ_{max} 212 (ϵ 24000); 272 (ϵ 19000) (MeOH) (Berdy).

Ishida, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 766 (*isol, uv, ir, pmr, cmr, ms, struct*)

Agelaspongin A-160

[122893-39-4]



$C_{11}H_{13}N_5O_2$ 247.256

CA numbering shown. Synthetic. Cryst. (MeOH). Mp 220° dec.

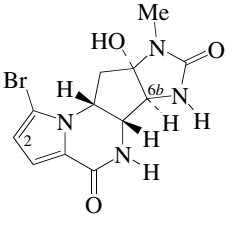
Hydrochloride:
Cryst. (EtOH). Mp 250° dec.

10,11-Dibromo: ***Dibromoagelaspongin***
[122893-38-3]
$C_{11}H_{11}Br_2N_5O_2$ 405.048
Glucanase inhibitor. Yellow-green cryst. (MeOH/Me_2CO) (as hydrochloride). Mp 233-235° dec. (hydrochloride). λ_{max} 235 (ϵ 11250); 290 (ϵ 7420) (MeOH) (Berdy).

Fedoreyev, S.A. *et al., Tetrahedron*, 1989, **45**, 3487 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)

Agelastatin A A-161

[152406-28-5]



Absolute Configuration

$C_{12}H_{13}BrN_4O_3$ 341.164
Alkaloid from the sponge *Agelas dendromorpha* and *Cymbastela* sp. Exhibits marked cytotoxicity; insecticide. $[\alpha]_D^{20}$ -84.3 (c, 0.3 in EtOH) (as *N,N,O*-tri-Me). Not obt. completely pure. λ_{max} 203 (ϵ 12400); 232 (ϵ 8400); 279 (ϵ 11900) (EtOH) (Derep).

N-*De-Me:* ***Agelastatin D***
$C_{11}H_{11}BrN_4O_3$ 327.137
Alkaloid from the sponge *Cymbastela* sp. Insecticide. Solid. λ_{max} 227 (ϵ 7900); 277 (ϵ 10800) (MeOH).

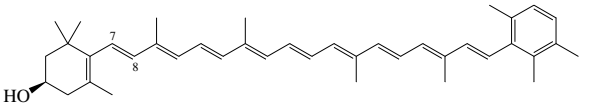
2-Bromo: ***Agelastatin B***
[159903-65-8]
$C_{12}H_{12}Br_2N_4O_3$ 420.06
Minor alkaloid from *Agelas dendromorpha*.
$[\alpha]_D$ -84.4 (c, 0.49 in EtOH) (as *N,N,O*-tri-Me). Obt. as insep. mixt. with Agelastatin A but characterised as the tri-Me deriv.

*6*b-*Hydroxy:* ***Agelastatin C***
$C_{12}H_{13}BrN_4O_4$ 357.163
Alkaloid from the sponge *Cymbastela* sp. Cytotoxic; insecticide. Solid. $[\alpha]_D$ -5 (c, 0.06 in MeOH). λ_{max} 228 (ϵ 7900); 278 (ϵ 11000) (MeOH).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1994, **77**, 1895; 1996, **79**, 727 (*Agelastatins A,B*)
Hong, T.W. *et al., J. Nat. Prod.*, 1998, **61**, 158-161 (*Agelastatins C,D*)
Stien, D. *et al., J.A.C.S.*, 1999, **121**, 9574-9579 (*synth*)
Feldman, K.S. *et al., J.O.C.*, 2002, **67**, 7096-7109 (*synth*)
Hale, K.J. *et al., Org. Lett.*, 2003, **5**, 2927-2930 (*synth*)
Domostoj, M.M. *et al., Org. Lett.*, 2004, **6**, 2615-2618 (*synth*)
Davis, F.A. *et al., Org. Lett.*, 2005, **7**, 621-623 (*synth*)
Trost, B.M. *et al., J.A.C.S.*, 2006, **128**, 6054-6055 (*synth*)

Agelaxanthin A A-162

β,ϕ-Caroten-3-ol. β-Isorenieratane
[65634-07-3]



$[C_{40}H_{52}O]$Constit. of *Agelas schmidtii*. Also found in sediments. Cryst. (Et_2O/hexane).

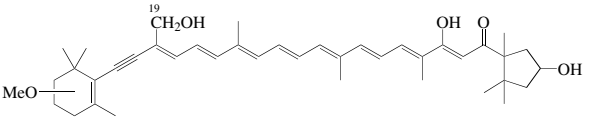
Deoxy: ***β-Isorenieratene****. β,ϕ-Carotene*
[4382-02-9]
$C_{40}H_{52}$ 532.851
Isol. from photosynthetic brown bacteria *Phaeobium* spp. Red cryst. (C_6H_6/EtOH).
Mp 128°. λ_{max} 430 (sh); 453; 480 (Me_2CO). λ_{max} 456; 487; 508 (CS_2).

7,8-Didehydro: 7,8-Didehydro-β,ϕ-caroten-3-ol, 9CI. ***Isotedaniaxanthin***
[73954-32-2]
$C_{40}H_{50}O$ 546.834
Isol. from the sponge *Tedania digitata*.

Cooper, R.D.G. *et al., J.C.S.*, 1963, 5637 (*synth*)
Jensen, S.L. *et al., Acta Chem. Scand.*, 1965, **19**, 1025 (*β-Isorenieratene*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1977, **60**, 2780 (*isol*)
Tanaka, Y. *et al., Nippon Suisan Gakkaishi*, 1980, **46**, 381-383 (*Isotedaniaxanthin*)
Shimada, A. *et al., Tet. Lett.*, 1981, 773 (*synth*)
Schaeffer, P. *et al., Tet. Lett.*, 1997, **38**, 8413-8416 (*isol, pmr, ms*)

Agelaxanthin C A-163

[65684-23-3]



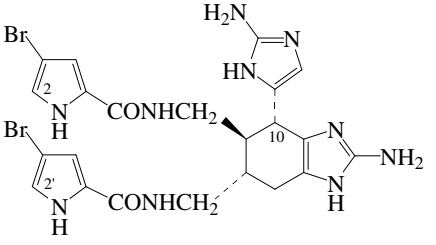
$C_{41}H_{56}O_5$ 628.89
Constit. of *Agelas schmidtii*. Cryst. (Et_2O/hexane).

19-Me ether: ***Agelaxanthin B***
[65497-25-8]
$C_{42}H_{58}O_5$ 642.917
Constit. of *Agelas schmidtii*. Tentative struct. assigned.

Buchecker, R. *et al., Helv. Chim. Acta*, 1977, **60**, 2780

Ageliferin A-164

[117417-64-8]



$C_{22}H_{24}Br_2N_{10}O_2$ 620.305
Alkaloid from the marine sponges *Agelas conifera*, *Agelas novaecaledoniae*, *Agelas* cf. *mauritiana* and *Xestospongia* sp. Potent actomyosin ATPase activator. Antifouling agent. Somatostatin antagonist. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O.

$[\alpha]_D^{33}$ +15.5 (c, 0.11 in MeOH). λ_{max} 204 (ϵ 25500); 220 (ϵ 27100); 267
(ϵ 25900); 393 (ϵ 300) (MeOH) (Derep).

1′-N-*Me:* ***1′*-N-*Methylageliferin***
[175861-97-9]
$C_{23}H_{26}Br_2N_{10}O_2$ 634.332
Alkaloid from the sponge *Astrosclera willeyana*. Pale yellow glass (as bis(trifluoroacetate)). $[\alpha]_D$ +40 (c, 0.01 in MeOH).

1,1′-Di-N-*Me:* ***N*^{1},N$^{1′}$-*Dimethylageliferin***
[175861-98-0]
$C_{24}H_{28}Br_2N_{10}O_2$ 648.359
Alkaloid from the sponge *Astrosclera willeyana*. Pale buff glass (as dihydrochloride). $[\alpha]_D$ +40 (c, 0.01 in MeOH).

2-Bromo: ***Bromoageliferin***
[117417-67-1]
$C_{22}H_{23}Br_3N_{10}O_2$ 699.201
Alkaloid from the sponges *Agelas conifera*, *Agelas* cf. *mauritiana* and *Astrosclera willeyana*. Potent actomyosin ATPase activator. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{33}$ +8.8 (c, 0.08 in MeOH). λ_{max} 203 (ϵ 30600); 220 (ϵ 26300); 270 (ϵ 24500); 396 (ϵ 700) (MeOH) (Derep). λ_{max} 204 (ϵ 15000); 222 (ϵ 12200); 274 (ϵ 12500); 396 (ϵ 700) (EtOH) (Berdy).

2-Bromo, 1′-N-*Me:* ***1′*-N-*Methyl-2-bromoageliferin***
[175862-01-8]
$C_{23}H_{25}Br_3N_{10}O_2$ 713.228
Alkaloid from the sponge *Astrosclera willeyana*. Off-white glass (as bis(trifluoroacetate)). $[\alpha]_D$ +50 (c, 0.01 in MeOH).

2′-Bromo, 1′-N-*Me:* ***1′*-N-*Methyl-2′-bromoageliferin***
[175862-02-9]
$C_{23}H_{25}Br_3N_{10}O_2$ 713.228
Alkaloid from the sponge *Astrosclera willeyana*. Off-white glass (as bis(trifluoroacetate)). $[\alpha]_D$ +40 (c, 0.01 in MeOH).

2,2′-Dibromo: ***Dibromoageliferin***
[117417-69-3]
$C_{22}H_{22}Br_4N_{10}O_2$ 778.098
Alkaloid from the sponges *Agelas conifera*, *Agelas* cf. *mauritiana* and *Astrosclera willeyana*. Potent actomyosin ATPase activator. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{33}$ +3 (c, 0.1 in MeOH). λ_{max} 204 (ϵ 12200); 220 (ϵ 9100); 278 (ϵ 8200); 394 (ϵ 300) (no solvent reported) (Derep). λ_{max} 202 (ϵ 24300); 214 (ϵ 24500); 274 (ϵ 25000) (MeOH) (Derep). λ_{max} 204 (ϵ 12200); 220 (ϵ 9100); 278 (ϵ 8200); 394 (ϵ 300) (EtOH) (Berdy).

2,2′-Dibromo, 1′-N-*Me:* ***1′*-N-*Methyl-2,2′-dibromoageliferin***
[175862-03-0]
$C_{23}H_{24}Br_4N_{10}O_2$ 792.124
Alkaloid from the sponge *Astrosclera willeyana*. Off-white glass (as bis(trifluoroacetate)). $[\alpha]_D$ +30 (c, 0.01 in MeOH).

3′-Debromo, 2′-bromo, 1′-N-*Me:* ***1′*-N-*Methylisoageliferin***
[175861-99-1]
$C_{23}H_{26}Br_2N_{10}O_2$ 634.332
Alkaloid from the sponge *Astrosclera willeyana*. Pale yellow glass (as bis(trifluoroacetate)). $[\alpha]_D$ +40 (c, 0.01 in MeOH).

3′-Debromo, 2′-bromo, 1,1′-di-N-*Me:* ***N*^{1},N$^{1′}$-*Dimethylisoageliferin***
[175862-00-7]
$C_{24}H_{28}Br_2N_{10}O_2$ 648.359
Alkaloid from the sponge *Astrosclera willeyana*. Off-white glass (as dihydrochloride). $[\alpha]_D$ +40 (c, 0.01 in MeOH).

10-Epimer: ***Nagelamide E***
[690627-58-8]
$C_{22}H_{24}Br_2N_{10}O_2$ 620.305
Alkaloid from an *Agelas* sp. Amorph. solid. $[\alpha]_D^{17}$ -11.3 (c, 1 in MeOH). λ_{max} 202 (ϵ 32000); 215 (sh) (ϵ 18000); 272 (ϵ 17200) (MeOH).

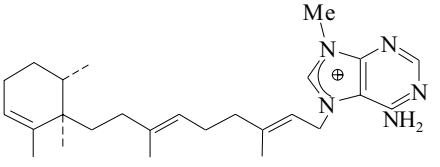
10-Epimer, 2-bromo: ***Nagelamide F***
[690627-59-9]
$C_{22}H_{23}Br_3N_{10}O_2$ 699.202
Alkaloid from an *Agelas* sp. Amorph. solid. $[\alpha]_D^{17}$ -14.1 (c, 1 in $CHCl_3$). λ_{max} 202 (ϵ 24000); 216 (sh) (ϵ 20100); 272 (ϵ 17700) (MeOH).

10-Epimer, 2,2′-dibromo: ***Nagelamide G***
[690627-60-2]
$C_{22}H_{22}Br_4N_{10}O_2$ 778.098
Alkaloid from an *Agelas* sp. Inhibitor of protein phosphatase 2A. Amorph. solid. $[\alpha]_D^{17}$ +6.7 (c, 1 in MeOH). λ_{max} 202 (ϵ 32000); 215 (sh) (ϵ 28900); 277 (ϵ 27400) (MeOH).

Kobayashi, J. *et al., Tetrahedron*, 1990, **46**, 5579-5586 (*isol, pmr, cmr, struct*)
Keifer, P.A. *et al., J.O.C.*, 1991, **56**, 2965-2975; 6728 (*isol*)
Vassas, A. *et al., Planta Med.*, 1996, **62**, 28-30 (*isol, activity*)
Williams, D.H. *et al., Tetrahedron*, 1996, **52**, 5381-5390 (*N-Methylageliferins*)
Kawasaki, I. *et al., Tet. Lett.*, 2002, **43**, 4377-4380 (*deriv, synth*)
Endo, T. *et al., J. Nat. Prod.*, 2004, **67**, 1262-1267 (*Nagelamides*)
Baran, P.S. *et al., Angew. Chem., Int. Ed.*, 2006, **45**, 249-252 (*synth*)

Ageline A A-165

Agelasine F
[88929-28-6]
[8885-51-6]

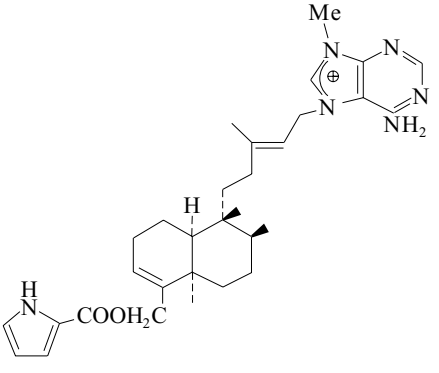


$C_{26}H_{40}N_5^{\oplus}$ 422.635
Constit. of sponge *Agelas* sp. Active against gram-positive bacteria and fungi. ATPase inhibitor, weak ichthyotoxin. Active against *Mycobacterium tuberculosis*. Plates (MeCN) or powder (as chloride).
Mp 178-180° (chloride). $[\alpha]_D^{25}$ -5.5 (c, 2.5 in MeOH). $[\alpha]_D$ -8.4 (c, 3 in $CHCl_3$). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH) (Derep).

Capon, R.J. *et al., J.A.C.S.*, 1984, **106**, 1819
Wu, H. *et al., Tet. Lett.*, 1984, **25**, 3719 (*isol, struct, nmr*)
Mangalindan, G.C. *et al., Planta Med.*, 2000, **66**, 364-365 (*activity*)

Ageline B A-166

[88874-28-6]



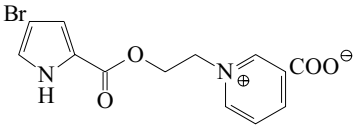
$C_{31}H_{43}N_6O_2^{\oplus}$ 531.72
Constit. of sponge *Agelas* sp. Active against gram-positive bacteria. ATPase inhibitor. Smooth muscle contractor. Phytotoxin. Weak ichthyotoxin. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 210 (ϵ); 274 (ϵ) (EtOH) (Derep). λ_{max} 268 (ϵ 8320) (MeOH) (Berdy). λ_{max} 212 (ϵ 18100); 272 (ϵ 10111) (EtOH) (Berdy). λ_{max} 212 (ϵ 18100); 272 (ϵ 10000) (EtOH-HCl) (Berdy).

[88855-18-9, 88855-19-0]

Capon, R.J. *et al., J.A.C.S.*, 1984, **106**, 1819

Agelongine A-167

[163564-84-9]



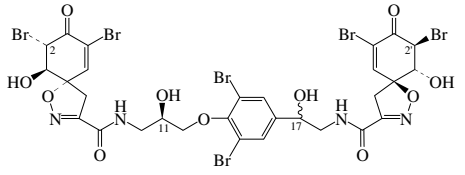
$C_{13}H_{11}BrN_2O_4$ 339.145
Alkaloid from *Agelas longissima* and *Axinella damicornis*. Exhibits antiserotonergic activity. Amorph. solid. Sol. MeOH, butanol. λ_{max} 262 (log ϵ 4.2) (MeOH).

Debromo: ***Daminine***
[862288-76-4]
$C_{13}H_{12}N_2O_4$ 260.249
Alkaloid from *Axinella damicornis*. Amorph. solid.
Mp 193° dec.

Cafieri, F. *et al., Bioorg. Med. Chem. Lett.*, 1995, **5**, 799-804 (*isol, uv, pmr, cmr*)
Aiello, A. *et al., Tetrahedron*, 2005, **61**, 7266-7270 (*Daminine*)

Agelorin A A-168

[149998-47-0]



Absolute Configuration

$C_{29}H_{26}Br_6N_4O_{11}$ 1085.969
Hydrol. prod. of Fistularin 3, F-43 on standing. Metab. from the tropical marine sponge *Agelas oroides*. Shows antibacterial activity. Amorph. off-white powder. $[\alpha]_D^{25}$ -17.1 (c, 1.26 in Me_2CO). λ_{max} 220 (ϵ 12600); 250 (ϵ 7740) (EtOH) (Berdy).

11,17-Dideoxy: ***11,17-Dideoxyagelorin A***
$C_{29}H_{26}Br_6N_4O_9$ 1053.97
Isol. from the sponge *Suberea* aff. *praetensa*.

2,2′-Diepimer: ***Agelorin B***
[150133-30-5]
$C_{29}H_{26}Br_6N_4O_{11}$ 1085.969
Isol. from *Agelas oroides*. Shows antibacterial activity. Amorph. powder. $[\alpha]_D^{25}$ +50 (c, 0.27 in Me_2CO). λ_{max} 215 (ϵ 12570); 250 (ϵ 7940) (EtOH) (Berdy).

2,2′-Diepimer, 11,17-dideoxy: ***11,17-Dideoxyagelorin B***
$C_{29}H_{26}Br_6N_4O_9$ 1053.97
Isol. from the sponge *Suberea* aff. *praetensa*.

König, G.M. *et al., Heterocycles*, 1993, **36**, 1351 (*isol, uv, ir, pmr, cmr, ms*)
Kijjoa, A. *et al., Z. Naturforsch., C*, 2001, **56**, 1116-1119 (*11,17-Dideoxyagelorins*)
Rogers, E.W. *et al., J. Nat. Prod.*, 2005, **68**, 891-896 (*stereochem*)
Bardhan, S. *et al., Org. Lett.*, 2006, **8**, 927-930 (*stereochem*)

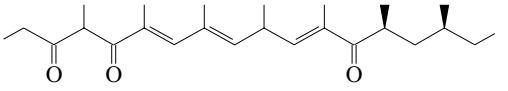
Saxidomus purpuratus Agglutinin A-169

SPA
Protein; can be separated into at least 7 components of which SPA-I and SPA-III are the major ones. Isol. from the shellfish *Saxidomus purpuratus*. Lectin.

Tatsumi, M. *et al., J. Biochem. (Tokyo)*, 1982, **91**, 1139-1146 (*isol*)

Aglajne 1 A-170

4,6,8,10,12,14,16-Heptamethyl-6,8,11-octadecatriene-3,5,13-trione, 9CI
[98571-24-5]



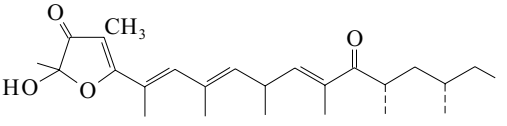
$C_{25}H_{40}O_3$ 388.589
Metab. of mollusc *Aglaja depicta* and its prey *Bulla striata*. Oil. $[\alpha]_D$ +72 (c, 2.6 in $CHCl_3$). λ_{max} 232 (ϵ); 310 (ϵ) (MeOH/KOH) (Derep). λ_{max} 232 (ϵ 13000); 284 (ϵ 14000) (MeOH) (Derep).

*14,15*E*-Didehydro: 4,6,8,10,12,14,16-Heptamethyl-6,8,11,14-octadecatetraene-3,5,13-trione. Niuhinone B*
[99624-11-0]
$C_{25}H_{38}O_3$ 386.573
Metab. of molluscs *Philinopsis speciosa*, *Bulla gouldiana* and *Navanax inermis*. Toxic to brine shrimp. $[\alpha]_D$ +72 (c, 0.47 in hexane). λ_{max} 238 (ϵ); 312 (ϵ) (EtOH/NaOH) (Derep). λ_{max} 238 (ϵ 10500); 285 (ϵ 10400) (EtOH) (Derep). λ_{max} 236 (ϵ 10800); 282 (ϵ 4800) (EtOH) (Berdy).

Coval, S.J. *et al., Tet. Lett.*, 1985, **26**, 5359-5362 (*Niuhinone B*)
Cimino, G. *et al., J.O.C.*, 1987, **52**, 5326 (*Aglajne 1*)
Spinella, A. *et al., Tetrahedron*, 1993, **49**, 3203 (*Niuhinone B*)
Fontana, A. *et al., Tet. Lett.*, 2004, **45**, 6847-6850 (*biosynth*)

Aglajne 2 A-171

[110848-77-6]



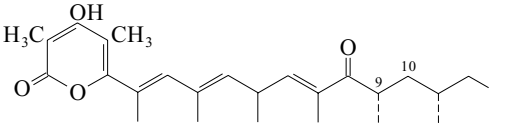
$C_{25}H_{38}O_4$ 402.573
Constit. of the mollusc *Aglaja depicta* and its prey *Bulla striata*. λ_{max} 234 (ϵ 19200); 310 (ϵ 12400) (MeOH) (Derep).

Ac:
Oil. $[\alpha]_D^{20}$ +46 (c, 1.3 in $CHCl_3$).

Cimino, G. *et al., J.O.C.*, 1987, **52**, 5326-5331 (*isol*)
Fontana, A. *et al., Tet. Lett.*, 2004, **45**, 6847-6850 (*biosynth*)

Aglajne 3 A-172

[110744-65-5]



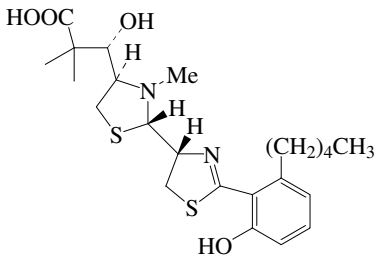
$C_{26}H_{38}O_4$ 414.584
Constit. of the mollusc *Aglaja depicta* and its prey *Bulla striata*. Oil. $[\alpha]_D^{20}$ +105 (c, 0.8 in $CHCl_3$). λ_{max} 234 (ϵ 19200); 310 (ϵ 12400) (MeOH) (Derep).

*9,10-Didehydro(*E*)-:* ***5,6-Dehydroaglajne 3***
[149155-22-6]
$C_{26}H_{36}O_4$ 412.568
Isol. from the molluscs *Navanax inermis*, *Bulla striata* and *Bulla gouldiana*. Sol. MeOH. $[\alpha]_D$ +53 (c, 0.1 in $CHCl_3$). λ_{max} 240 (ϵ 19000); 310 (ϵ 7700) (MeOH) (Berdy).

Cimino, G. *et al., J.O.C.*, 1987, **52**, 5326-5331 (*isol*)
Spinella, A. *et al., Tetrahedron*, 1993, **49**, 3203 (*Dehydroaglajne 3*)
Fontana, A. *et al., Tet. Lett.*, 2004, **45**, 6847-6850 (*biosynth*)

Agrochelin A-173

[247115-74-8]



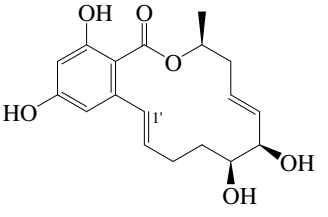
Relative Configuration

$C_{23}H_{34}N_2O_4S_2$ 466.665

Alkaloid from a marine *Agrobacterium* sp. Cytotoxic agent. Siderophore. Pale yellow oil. $[\alpha]_D^{25}$ -20.5 (c, 0.2 in $CHCl_3$). Chelates $Zn^{2\oplus}$ ion. λ_{max} 210 (log ϵ 5.18); 264 (log ϵ 4.8) (MeOH).

Acebal, C. *et al., J. Antibiot.*, 1999, **52**, 983-987 (*isol*)
Canedo, L.M. *et al., Tet. Lett.*, 1999, **40**, 6841-6844 (*isol, uv, cd, pmr, cmr*)

Aigialomycin D A-174



Absolute Configuration

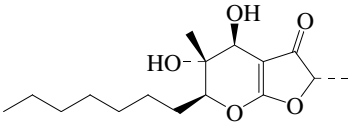
$C_{18}H_{22}O_6$ 334.368

Macrolide antibiotic. Related to Hypothemycin, in A-552. Prod. by the marine mangrove fungus *Aigialus parvus* BCC 5311. Antimalarial. Cryst.
Mp 83-85°. $[\alpha]_D^{24}$ -19 (c, 0.24 in MeOH). λ_{max} 238 (log ϵ 4.42); 275 (log ϵ 4.05); 314 (log ϵ 3.71) (MeOH).

(1′Z)-Isomer: ***Aigialomycin E***
$C_{18}H_{22}O_6$ 334.368
Prod. by *Aigialus parvus* BCC 5311. Amorph. solid.
Mp 91-94°. $[\alpha]_D^{24}$ +14 (c, 0.28 in MeOH). λ_{max} 226 (log ϵ 4.31); 268 (log ϵ 4); 307 (log ϵ 3.69) (MeOH).

Isaka, M. *et al., J.O.C.*, 2002, **67**, 1561-1566 (*isol, uv, pmr, cmr, ms*)
Geng, X. *et al., Org. Lett.*, 2004, **6**, 413-416 (*synth*)
Barluenga, S. *et al., Angew. Chem., Int. Ed.*, 2006, **45**, 3951-3954 (*synth*)

Aigialone A-175



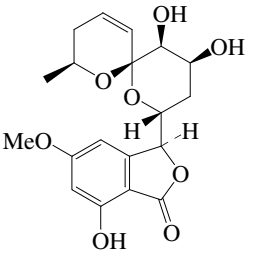
Relative Configuration

$C_{16}H_{26}O_5$ 298.378

Prod. by the mangrove fungus *Aigialus parvus* BCC 5311. Cryst. (EtOAc/hexane).
Mp 132.5-133°. $[\alpha]_D^{26}$ -193 (c, 0.65 in $CHCl_3$). λ_{max} 254 (log ϵ 4.35) (MeOH).

Vongvilai, P. *et al., J. Nat. Prod.*, 2004, **67**, 457-460 (*isol, pmr, cmr, cryst struct*)

Aigialospirol A-176



Relative Configuration

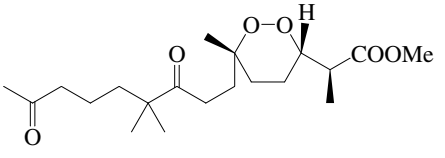
$C_{19}H_{22}O_8$ 378.378

Prod. by the mangrove fungus *Aigialus parvus* BCC 5311. Pale yellow amorph. solid.
Mp 85-89°. $[\alpha]_D^{25}$ +47 (c, 0.5 in $CHCl_3$). λ_{max} 217 (log ϵ 4.29); 257 (log ϵ 3.92); 292 (log ϵ 3.51) (MeOH).

Vongvilai, P. *et al., J. Nat. Prod.*, 2004, **67**, 457-460 (*isol, pmr, cmr*)

Aikupikoxide C A-177

[377088-40-9]



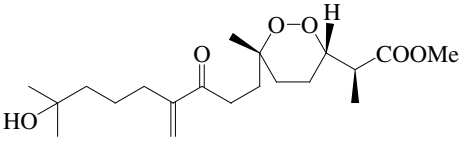
$C_{20}H_{34}O_6$ 370.485

Constit. of a Red Sea sponge *Diacarnus erythraenus*. Oil. $[\alpha]_D$ +88 (c, 2.0 in CH_2Cl_2).

Youssef, D.T.A. *et al., J. Nat. Prod.*, 2001, **64**, 1332-1335 (*isol, pmr, cmr*)

Aikupikoxide D A-178

[377088-41-0]



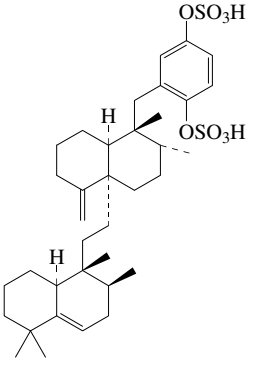
$C_{20}H_{34}O_6$ 370.485

Constit. of Red Sea sponge *Diacarnus erythraenus*. Oil. $[\alpha]_D$ +69 (c, 0.45 in CH_2Cl_2).

Youssef, D.T.A. *et al., J. Nat. Prod.*, 2001, **64**, 1332-1335 (*isol, pmr, cmr*)

Akaterpin A-179

[188576-24-1]



$C_{36}H_{54}O_8S_2$ 678.95

Constit. of a *Callyspongia* sponge. Inhibits phospholipase C. Solid.
Mp >240°. $[\alpha]_D^{24}$ +15 (c, 0.59 in MeOH). λ_{max} 207 (ϵ 16800); 275 (ϵ 1070) (MeOH).

Fukami, A. *et al., Tet. Lett.*, 1997, **38**, 1201 (*isol, pmr, cmr*)
Kawai, N. *et al., Tet. Lett.*, 1999, **40**, 4193-4196 (*stereochem*)

AKFFL amide **A-180**

[152247-52-4]
Ala-Lys-Phe-Phe-Leu-NH_2
$C_{33}H_{49}N_7O_5$ 623.794
Isol. from the echiuroid worm *Urechis unicinctus*.

Ikeda, T. *et al., Pept. Chem.*, 1992, **30**, 583-585 (*isol*)

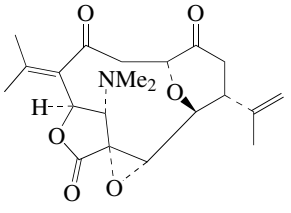
AKYFL amide **A-181**

[152247-50-2]
Ala-Lys-Tyr-Phe-Leu-NH_2
$C_{33}H_{49}N_7O_6$ 639.793
Isol. from the echiuroid worm *Urechis unicinctus*.

Ikeda, T. *et al., Pept. Chem.*, 1992, **30**, 583-585 (*isol*)

Alanolide **A-182**

[177715-26-3]



$C_{21}H_{27}NO_6$ 389.447
Constit. of *Pseudopterogorgia acerosa*. Oil. $[\alpha]_D^{25}$ -84.5 (c, 2 in $CHCl_3$). λ_{max} 260 (ϵ 11300) (no solvent reported).

Rodríguez, A.D. *et al., J.O.C.*, 1996, **61**, 4487-4490 (*isol, pmr, cmr*)

β-Alanopine dehydrogenase **A-183**

E.C. 1.5.1.26. N-*(D-1-Carboxyethyl)-β-alanine:NAD⊕ oxidoreductase (β-alanine-forming)*
[113573-64-1]
Oxidoreductase enzyme. Isol. from *Scapharca broughtonii*. Catalyses the reaction of 2,3′-Iminobispropanoic acid, I-34 with $NAD^⊕$ and H_2O to give 3-Aminopropanoic acid, pyruvate and NADH.

Sato, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1987, **88**, 803-806

Alanopine dehydrogenase **A-184**

E.C. 1.5.1.17. 2,2′-Diiminodipropanoate:NAD⊕ oxidoreductase (L-alanine-forming)
[71343-07-2]
Oxidoreductase enzyme. Isol. from *Crassostrea* and *Mytilus* spp. Catalyses the reversible reaction of 2,2′-Iminobispropanoic acid, I-33 with $NAD^⊕$ and H_2O to give Alanine, pyruvate and NADH.

Dando, P.R. *et al., Biochem. Soc. Trans.*, 1981, **9**, 297-298 (*Mytilus edulis*)
Fields, J.H.A. *et al., Eur. J. Biochem.*, 1981, **114**, 615-621 (*Crassostrea gigas*)

Alanylprolylglutamylalanylserylprolylphenylalanylisoleucylarginylphenylalaninamide, 9CI **A-185**

CF9. Peptide CF9
[188563-26-0]
H-Ala-Pro-Glu-Ala-Ser-Pro-Phe-Ile-Arg-Phe-NH_2
$C_{54}H_{80}N_{14}O_{13}$ 1133.312

Isol. from the nematode *Caenorhabditis elegans*. Myoactive neuropeptide.

Marks, N.J. *et al., Biochem. Biophys. Res. Commun.*, 1997, **231**, 591-595 (*isol*)

Alanylprolylglycyltryptophan **A-186**

H-Ala-Pro-Gly-Trp-OH
$C_{21}H_{27}N_5O_5$ 429.475

Amide: [126675-52-3]
$C_{21}H_{28}N_6O_4$ 428.49
Isol. from the ganglia of the molluscs *Fusinus ferrugineus* and *Lymnaea stagnalis*. Molluscan neuropeptide hormone.

Minakata, H. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1991, **100**, 565-571 (*activity*)
Smit, A.B. *et al., J. Neurosci.*, 1992, **12**, 1709-1715 (*isol, struct*)

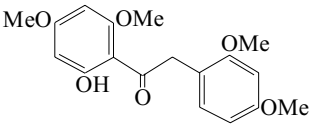
Alanylthreonyltryptophylleucylaspartylthreonine **A-187**

[157724-16-8]
H-Ala-Thr-Trp-Leu-Asp-Thr-OH
$C_{32}H_{47}N_7O_{11}$ 705.764
Isol. from the annelid *Perinereis vancaurica*.

Takahashi, T. *et al., Pept. Chem.*, 1993, **31**, 169-174 (*isol, struct*)
Takahashi, T. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1995, **110**, 297-304 (*isol, struct*)

Albizoin **A-188**

1-(2-Hydroxy-4,6-dimethoxyphenyl)-2-(2,4-dimethoxyphenyl)ethanone
[39604-69-8]

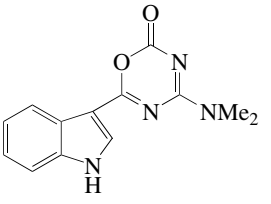


$C_{18}H_{20}O_6$ 332.352
Constit. of marine mollusc *Nerita albicilla*. Light-yellow needles (C_6H_6).
Mp 140°.

Sanduja, R. *et al., J. Chem. Res., Synop.*, 1985, 56-57

Alboinone **A-189**

*4-(Dimethylamino)-6-(1*H*-indol-3-yl)-2*H*-1,3,5-oxadiazin-2-one, 9CI*
[188547-40-2]

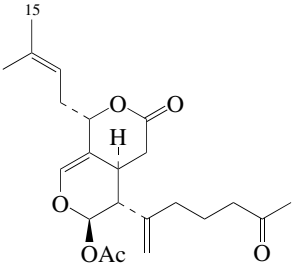


$C_{13}H_{12}N_4O_2$ 256.263
First naturally occurring oxadiazinone. Alkaloid from the ascidian *Dendrodoa grossularia*. λ_{max} 210; 252; 270; 334 (MeOH).

Bergmann, T. *et al., Tetrahedron*, 1997, **53**, 2055-2060 (*isol, uv, ir, pmr, cmr, ms, struct, synth*)

Alcyonolide A-190

[81134-49-8]



Absolute Configuration

$C_{22}H_{30}O_6$ 390.475

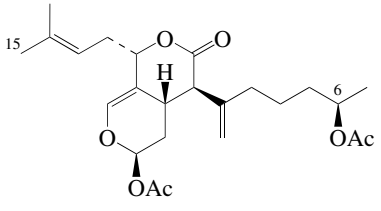
A secoxenicane. Constit. of an *Alcyonium* spp. Oil. $[\alpha]_D^{24}$ -20 ($CHCl_3$).

15-Acetoxy: ***Alcyonolide 2***
[88924-73-6]
$C_{24}H_{32}O_8$ 448.512
Constit. of a *Efflatounaria* sp. Cryst.
Mp 90-91°. $[\alpha]_D$ -20.8 (c, 0.2 in $CHCl_3$).

Kobayashi, M. *et al., Tet. Lett.*, 1981, **22**, 4445 (*Alcyonolide*)
Bawden, B.F. *et al., Aust. J. Chem.*, 1983, **36**, 2279-2288 (*Alcyonolide 2*)
Coll, J.C. *et al., J. Nat. Prod.*, 1998, **61**, 835-837 (*nomencl*)

Alcyonolide 3 A-191

[88924-74-7]



$C_{24}H_{34}O_7$ 434.528
Constit. of *Efflatounaria* spp. Cryst. (Et_2O/petrol).
Mp 63-65°. $[\alpha]_D$ +114 (c, 0.4 in $CHCl_3$).

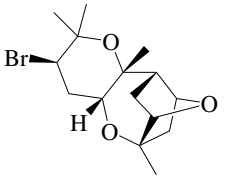
6-Ketone, 6-de-Ac: ***Alcyonolide 4***
[88924-75-8]
$C_{22}H_{30}O_6$ 390.475
Constit. of *Efflatounaria* spp. Oil. $[\alpha]_D$ +113 (c, 4.9 in $CHCl_3$).

15-Acetoxy: ***Alcyonolide 5***
[209673-91-6]
$C_{26}H_{36}O_9$ 492.565
Constit. of two soft corals (Alcyonacea). Pale yellow gum. $[\alpha]_D^{25}$ +92.6 (c, 0.0074 in $CHCl_3$). Stereochemistry at C-6 is uncertain. λ_{max} 200 (log ϵ 4.3); 236 (log ϵ 3.5) (EtOH).

Bowden, B.F. *et al., Aust. J. Chem.*, 1983, **36**, 2279-2288 (*Alcyonolides 3 and 4, cryst struct*)
Coll, J.C. *et al., J. Nat. Prod.*, 1998, **61**, 835-837 (*Alcyonolide 5*)

Aldingenin A A-192

[577705-26-1]



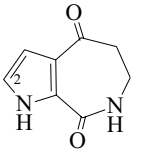
$C_{15}H_{23}BrO_3$ 331.249

Constit. of *Laurencia aldingensis*. Cryst. (MeOH).
Mp 169-171°. $[\alpha]_D^{25}$ -10 (c, 0.05 in $CHCl_3$).

De Carvalho, L.R. *et al., Tet. Lett.*, 2003, **44**, 2637-2640 (*isol, pmr, cmr*)

Aldisine A-193

6,7-Dihydropyrrolo[2,3-c]azepine-4,8(1H,5H)-dione, 9CI
[72908-87-3]



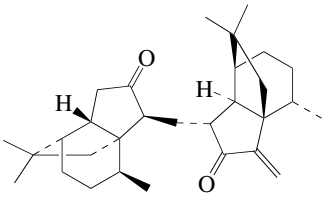
$C_8H_8N_2O_2$ 164.163
Isol. from the marine sponges *Hymeniacidon aldis*, *Axinella carteri* and *Pseudaxinyssa cantharella*.
Mp 275-277° (269° dec.). $[\alpha]_D$ -6 (c, 0.12 in MeOH). λ_{max} 216 (ϵ 19100); 245 (ϵ 8370); 295 (ϵ 6770) (MeOH) (Derep).

2-Bromo: ***2-Bromoaldisine***
[96562-96-8]
$C_8H_7BrN_2O_2$ 243.059
Isol. from *Hymeniacidon aldis*, an unidentified sponge from Fiji, a *Lissodendoryx* sp. of sponge from Sri Lanka and from *Pseudaxinyssa cantharella*. Cryst. (MeOH).
Mp 265° (243°). $[\alpha]_D$ +5 (c, 0.47 in MeOH). λ_{max} 220 (ϵ 29600); 244 (sh) (ϵ 12100); 303 (ϵ 8130) (MeOH) (Derep).

Sharma, G.M. *et al., Chem. Comm.*, 1980, 435 (*synth, uv, pmr, cmr*)
Schmitz, F.J. *et al., J. Nat. Prod.*, 1985, **48**, 47 (*isol, uv, ir, pmr, cmr, ms, struct, deriv*)
Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1985, **21**, 578; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 547 (*isol*)
De Nanteuil, G. *et al., Tetrahedron*, 1985, **41**, 6019 (*isol, uv, ir, pmr, cmr, ms, cd, deriv*)
Xu, X.-H. *et al., J. Struct. Chem. (Engl. Transl.)*, 2001, **20**, 173-175 (*cryst struct*)

Alertenone A-194

[222735-88-8]



$C_{30}H_{44}O_2$ 436.676
Constit. of an *Alertigorgia* sp.
$[\alpha]_D$ +15.4 (c, 0.23 in $CHCl_3$). Dimer of Suberosenone, in S-529. λ_{max} 231 (ϵ 3500) (hexane).

Bokesch, H.R. *et al., J. Nat. Prod.*, 1999, **62**, 633-635 (*isol, pmr, cmr*)

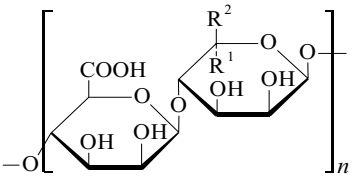
Alginate synthase A-195

E.C. 2.4.1.33. GDP-D-mannuronate:alginate D-mannuronyltransferase. Mannuronosyl transferase
[37257-31-1]
Hexosyltransferase enzyme. Isol. from the marine brown alga *Fucus gardneri*. Catalyses the reaction of GDP-D-mannuronate with $(alginate)_n$ to give GDP and $(alginate)_{n+1}$.

Lin, T.-Y. *et al., J. Biol. Chem.*, 1966, **241**, 5284-5297

Alginic acid, BAN A-196

Gum levan. Levan gum. Kelacid. Norgine. Sazio. E400
[9005-32-7]



R^1 = H, R^2 = COOH
or R^1 = COOH, R^2 = H

$[C_6H_8O_6]$

A polymer consisting of various proportions of β-D-Mannuronic acid and α-L-Guluronic acid linked 1 →4 and arranged in a block fashion. To a first approximation there are poly-M , poly-G and $(M\text{-}G)_n$ blocks of about 20 units with an overall degree of polymerisation of 1000-10,0000. Occurs as the major matrix polysaccharide in brown seaweed (Phaeophyceae) as an insol. complex of K, Na, Ca and Mg alginates. Extracted commerically from various genera incl. *Laminaria* (Europe and Japan), *Macrocystis* (N. America pacific coast), *Ascophyllum* (Europe) and *Ecklonia* (S. Africa). Alginates are used to improve food texture, e.g. in ice cream, pie fillings. Used in tablet disintegrants and paper coatings. Food additive: emulsifier, stabiliser, thickener. Pharmaceutical aid for preparation of water-miscible pastes, creams and gels. Co-administered with antacid or H_2-receptor agonist for management of gastro-oesophageal reflux. $[\alpha]_D$ -120 (as Na salt in H_2O). Approx. 200 grades of the acid and its salts (ammonium, Ca, K, Na) comly. available. Alginates with the highest guluronic acid content display the strongest gel-forming activity.

▶ AZ5775000

Na salt: Sodium alginate. Algin. E401
[9005-38-3]
Stabiliser, emulsifier, thickener, formulation aid; used in food processing.
Pale yellow-brown powder. Sol. H_2O; poorly sol. EtOH, hexane. λ_{max} 260 (H_2O) (Berdy).

▶ AZ5820000

K salt: Potassium alginate. E402
[9005-36-1]
Stabiliser, emulsifier, thickener, formulation aid; used in food processing. Insol. EtOH, Et_2O.

Ca salt: Calcium alginate. E404
[9005-35-0]
Stabiliser, emulsifier, thickener, formulation aid; used in food processing. Sl. sol. EtOH; insol. H_2O, Et_2O.

NH_4 salt: Ammonium alginate. E403
[9005-34-9]
Stabiliser, emulsifier, thickener, formulation aid; used in food processing. Insol. EtOH, Et_2O.

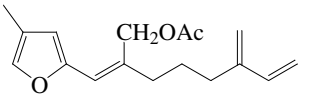
2-Hydroxypropyl ester: Propylene glycol alginate. Colloid 602. Dricoid. Kelcoloid. FEMA 2941. E405. Many other trade names
[39306-87-1, 51374-11-9, 52441-26-6, 57762-73-9, 59125-52-9, 95328-14-6]
Manuf. by reaction of alginic acid with propylene oxide.
White to yellowish fibrous or granular powder. Sol. H_2O.
Composition varies acc. to the degree of esterification.

[9005-31-6, 9019-42-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1225B (*ir*)
Hirst, E. *et al., Chem. Ind. (London)*, 1963, 257
Haug, A. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 69 (*synth*)
Percival, E. *et al., The Carbohydrates*, (Pigman, W., Ed.), Academic Press, 1970, **2B**, 545
Ger. Pat., 1971, 2 046 966; *CA*, **75**, 22923d (*2-hydroxypropyl ester, manuf*)
Rees, D.A. *et al., Angew. Chem., Int. Ed.*, 1977, **16**, 214 (*struct, rev*)
Grasdalen, H. *et al., Carbohydr. Res.*, 1977, **56**, C11; 1981, **89**, 179 (*nmr, cmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **12**, 45 (*use*)
Cottrell, I.W. *et al., Handb. Water-Soluble Gums Resins*, McGraw-Hill, N.Y., 1980, 2/1-2/43 (*rev*)
Fed. Regist., 1982, **47**, 29946-29952 (*propylene glycol alginate*)
Martin, G. *et al., Sci. Aliments*, 1986, **6**, 473 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AFL000
Beale, J.M. *et al., Environ. Sci. Res.*, 1992, **44**, 209 (*rev, biosynth, struct*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 10-11; 428-430
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1535
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 71-74; 2349-2352 (*props, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AFL000; SEH000; CAM200; PKU700

Algoafuran A-197

[369380-50-7]

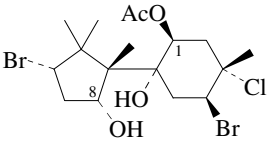


$C_{17}H_{22}O_3$ 274.359
Constit. of *Leminda millecra*. Oil.

McPhail, K.L. *et al., J. Nat. Prod.*, 2001, **64**, 1183-1190 (*isol, pmr, cmr*)

Algoane A-198

[251455-23-9]



$C_{17}H_{27}Br_2ClO_4$ 490.659
Constit. of *Aplysia dactylomela*. Cryst. (EtOAc/hexane).
Mp 188-192°. $[\alpha]_D^{22}$ +51.1 (c, 0.6 in $CHCl_3$).

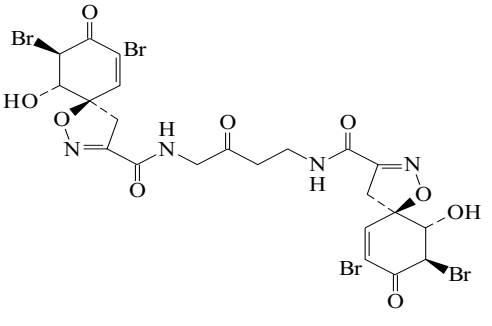
1-Deacetoxy: ***1-Deacetoxyalgoane***
[251450-53-0]
$C_{15}H_{25}Br_2ClO_2$ 432.622
Constit. of *Aplysia dactylomela*. Cryst. (EtOAc/hexane).
Mp 152-155°. $[\alpha]_D^{22}$ +18 (c, 0.4 in $CHCl_3$).

1-Deacetoxy, 8-deoxy: ***Deacetoxy-8-deoxyalgoane***
[251450-54-1]
$C_{15}H_{25}Br_2ClO$ 416.623
Constit. of *Aplysia dactylomela*. Cryst. (EtOAc/hexane).
Mp 138-142°. $[\alpha]_D^{22}$ +22.5 (c, 1.15 in $CHCl_3$).

McPhail, K.L. *et al., J. Nat. Prod.*, 1999, **62**, 1618-1623 (*isol, pmr, cmr, cryst struct*)

Aplysina archeri Alkaloid A-199

[179523-37-6]

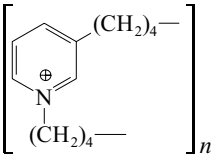


$C_{22}H_{20}Br_4N_4O_9$ 804.037

Probable abs. config. illus. Metab. from the Caribbean sponge *Aplysina archeri*. Shows antifungal activity. λ_{max} 252 (ϵ 7850) (MeOH).

Ciminiello, P. *et al., Tetrahedron*, 1996, **52**, 9863 (*isol, uv, ir, pmr, cmr, cd, struct*)

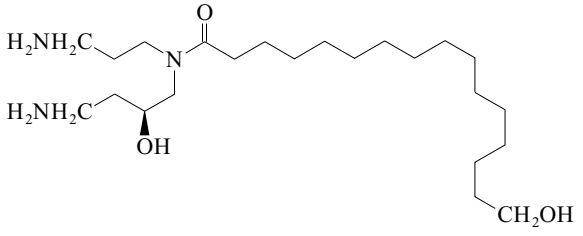
Callyspongia fibrosa Alkaloid A-200



High molecular weight oligomer or polymer. Alkaloid from the Micronesian sponge *Callyspongia fibrosa*. Inhibitor of the epidermal growth factor receptor.

Davies-Coleman, M.T. *et al., J.O.C.*, 1993, **58**, 5925

Fromia monilis Alkaloid A-201



$C_{23}H_{49}N_3O_3$ 415.658

(*S*)-*form* [162340-03-6]

Alkaloid from the New Caledonian starfish *Fromia monilis*. Cytotoxic agent. $[\alpha]_D$ +3.5.

Palagiano, E. *et al., Tetrahedron*, 1995, **51**, 3675 (*isol, pmr, cmr, struct*)

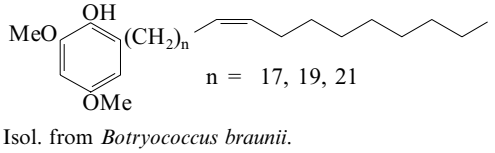
Pseudaxinyssa Alkaloid A-202

$C_9H_{14}BrN_5O$ 288.146

Struct. unknown. Isol. from the marine sponge *Pseudaxinyssa cantharella*. Amorph. $[\alpha]_D$ +15.

De Nanteuil, G. *et al., Tetrahedron*, 1985, **41**, 6019

2-Alkenyl-4,6-dimethoxyphenols A-203



Isol. from *Botryococcus braunii*.

2-(18-Heptacosenyl)-4,6-dimethoxyphenol [123219-94-3]

$C_{35}H_{62}O_3$ 530.873
n = 17.

2,4-Dimethoxy-6-(20-nacosenyl)phenol [123219-95-4]

$C_{37}H_{66}O_3$ 558.927
n = 19.

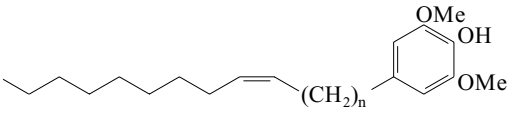
2-(22-Hentriacontenyl)-4,6-dimethoxyphenol [123219-96-5]

$C_{39}H_{70}O_3$ 586.98
n = 21.

[132210-27-6, 132210-28-7, 132210-29-8]

Metzger, P. *et al., Phytochemistry*, 1989, **28**, 2097; 1995, **40**, 543 (*isol*)

4-Alkenyl-2,6-dimethoxyphenols A-204



Isol. from *Botryococcus braunii*.

2,6-Dimethoxy-4-(16-pentacosenyl)phenol [168981-76-8]

$C_{33}H_{58}O_3$ 502.819
n = 15.

4-(18-Heptacosenyl)-2,6-dimethoxyphenol [168981-77-9]

$C_{35}H_{62}O_3$ 530.873
n = 17.

2,6-Dimethoxy-4-(20-nonacosenyl)phenol [168981-78-0]

$C_{37}H_{66}O_3$ 558.927
n = 19.

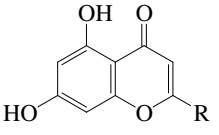
4-(22-Hentriacontenyl)-2,6-dimethoxyphenol [168981-79-1]

$C_{39}H_{70}O_3$ 586.98
n = 21.

Metzger, P. *et al., Phytochemistry*, 1995, **40**, 543-554 (*isol, ms*)

2-Alkyl-5,7-dihydroxy-4*H*-1-benzopyran-4-ones A-205

2-Alkyl-5,7-dihydroxychromones



5,7-Dihydroxy-2-pentadecyl-4*H*-1-benzopyran-4-one
5,7-Dihydroxy-2-pentadecylchromone
[82513-78-8]

$C_{24}H_{36}O_4$ 388.546
Isol. from the brown alga *Zonaria tournefortii*.
Mp 79-80°.

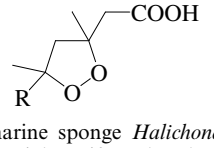
5,7-Dihydroxy-2-nonadecyl-4*H*-1-benzopyran-4-one
5,7-Dihydroxy-2-nonadecylchromone
[82513-79-9]

$C_{28}H_{44}O_4$ 444.653
Constit. of *Antidesma membranaceum*.

*4′,5′Z,7′,8′Z,10′,11′Z,13′,14′Z,16′,17′Z-Decakisdehydro: 5,7-Dihydroxy-2-(4,7,10,13,16-nonadecapentaenyl)-4*H*-1-benzopyran-4-one. 5,7-Dihydroxy-2-(4,7,10,13,16-nonadecapentaenyl)chromone*
[82513-77-7]
$C_{28}H_{34}O_4$ 434.574
Constit. of the brown alga *Zonaria tournefortii*.
Mp 53-54°.

Tringali, C. *et al., Tet. Lett.*, 1982, **23**, 1509-1512 (*Zonaria constits*)
Blackman, A.J. *et al., J. Nat. Prod.*, 1988, **51**, 158-160 (*nonadecapentaenyl, isol*)

5-Alkyl-3,5-dimethyl-1,2-dioxolane-3-acetic acids A-206



Isol. from a marine sponge *Halichondria* sp. Cytotoxic agents. Exhibit antibacterial, antifungal and antitumour activities.

3,5-Dimethyl-5-tridecyl-1,2-dioxolane-3-acetic acid, 9CI [115082-90-1]
$C_{20}H_{38}O_4$ 342.518
R = -$(CH_2)_{12}CH_3$.

3,5-Dimethyl-5-tetradecyl-1,2-dioxolane-3-acetic acid [115082-91-2]
$C_{21}H_{40}O_4$ 356.545
R = -$(CH_2)_{13}CH_3$.

3,5-Dimethyl-5-pentadecyl-1,2-dioxolane-3-acetic acid, 9CI [115102-78-8]
[175410-41-0, 175410-46-5]
$C_{22}H_{42}O_4$ 370.571
R = -$(CH_2)_{14}CH_3$.

5-Hexadecyl-3,5-dimethyl-1,2-dioxolane-3-acetic acid, 9CI [115082-92-3]
$C_{23}H_{44}O_4$ 384.598
R = -$(CH_2)_{15}CH_3$.

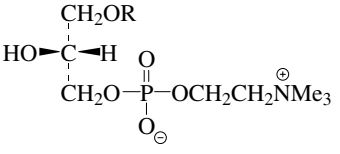
5-Heptadecyl-3,5-dimethyl-1,2-dioxolane-3-acetic acid, 9CI [115082-93-4]
$C_{24}H_{46}O_4$ 398.625
R = -$(CH_2)_{16}CH_3$.

[175410-23-8, 175410-28-3, 175410-32-9, 175410-37-4]

Pat. Coop. Treaty (WIPO), 1987, 87 04 708; *CA*, **109**, 17027f (*isol*)
Bloodworth, A.J. *et al., Tet. Lett.*, 1996, **37**, 1885-1888 (*synth*)
Dussault, P.H. *et al., Org. Lett.*, 1999, **1**, 1391-1393 (*synth*)

1-*O*-Alkylglycero-3-phosphocholines A-207

Lyso-PAF



The biol. significant compds. have the *R*-config. illus.

1-Hexadecylglycero-3-phosphocholine [78119-19-4]
[52691-62-0, 77249-80-0]
$C_{24}H_{52}NO_6P$ 481.652
Isol. from *Solanderia secunda* and *Spirastrella abata*. Powder. Mp 250° dec. $[\alpha]_D^{25}$ -6.09 (c, 1.04 in $CHCl_3$/MeOH).

*2-Ac: 2-*O*-Acetyl-1-*O*-hexadecylglycero-3-phosphocholine. 1-*O*-Hexadecyl-PAF. PAF(C-16)*
[74389-68-7]
$C_{26}H_{54}NO_7P$ 523.689
Powerful mediator in physiological processes such as anaphylaxis and inflammation. Amorph. solid. Mp 247° dec. $[\alpha]_D^{20}$ -3.3 (c, 0.53 in $CHCl_3$/MeOH). Major molecular form of Platelet activating factor.

*2-*O*-(N-Methylcarbamoyl): 1-*O*-Hexadecyl-2-*N*-methylcarbamoylglycero-3-phosphocholine. C-PAF*
[110406-02-5]
$C_{26}H_{55}N_2O_7P$ 538.703
Biologically potent non-metabolisable PAF analogue. Stimulates human neutrophils to synthesise PAF. No phys. props. reported.

*2-Me ether: 1-*O*-Hexadecyl-2-*O*-methylglycero-3-phosphocholine. 2-*O*-Methyl PAF (C-16)*
[78858-44-3]
$C_{25}H_{54}NO_6P$ 495.678
Potential antineoplastic agent. Cryst. $[\alpha]_D^{20}$ -5.41 (c, 0.95 in $CHCl_3$/MeOH).

*2-Et ether: 1-*O*-Hexadecyl-2-*O*-ethylglycero-3-phosphocholine. 7-Ethoxy-4-hydroxy-*N,N,N*-trimethyl-3,5,9-trioxa-4-phosphapentacosan-1-aminium hydroxide inner salt 4-oxide, 9CI. AEGPC. E-PAF*
[78858-42-1]
$C_{26}H_{56}NO_6P$ 509.705
Degranulates human neutrophils and desensitises neutrophils to PAF. $[\alpha]_D^{23}$ -0.19 (c, 1.3 in MeOH/$CHCl_3$). PAF-analogue.

*2-Benzyl ether: 2-*O*-Benzyl-1-*O*-hexadecylglycero-3-phosphocholine. 2-*O*-Benzyl PAF (C-16)*
[91326-84-0]
$C_{31}H_{58}NO_6P$ 571.776
Amorph. solid. Mp 200°. $[\alpha]_D^{20}$ +2.41 (c, 2.32 in MeOH). Stable PAF analogue.

1-Octadecylglycero-3-phosphocholine
*4,7-Dihydroxy-*N,N,N*-trimethyl-3,5,9-trioxa-4-phosphaheptacosan-1-aminium hydroxide inner salt 4-oxide. Lyso-PAF (C-18). 1-Octadecyl-*sn*-glycero-3-phosphocholine*
[74430-89-0]
$C_{26}H_{56}NO_6P$ 509.705
Mp 240° dec. $[\alpha]_D^{20}$ -4.65 (c, 1.00 in $CHCl_3$/MeOH).

*2-Ac: 2-Acetyl-1-octadecyl-sn-glycero-3-phosphocholine. PAF (C-18). 1-*O*-Octadecyl-PAF*
[74389-69-8]
$C_{28}H_{58}NO_7P$ 551.742
Powerful mediator in physiological processes such as anaphylaxis and inflammation. Mp 260° (214-215° dec.). $[\alpha]_D^{20}$ -3.46 (c, 0.90 in $CHCl_3$/MeOH). Major molecular form of PAF.

► YK0715000

2-Me ether: See Edelfosine in *The Combined Chemical Dictionary.*

*2-Benzyl ether: 2-Benzyl-1-octadecyl-sn-glycero-3-phosphocholine. 2-*O*-Benzyl PAF (C-18)*
[80483-86-9]
$C_{33}H_{62}NO_6P$ 599.83
Mp 220° dec. $[\alpha]_D^{20}$ +2.24 (c, 2.18 in MeOH).

1-(9*Z*-Octadecenyl)glycero-3-phosphocholine
$C_{26}H_{54}NO_6P$ 507.69

*2-Ac: 2-*O*-Acetyl-1-*O*-oleyl-sn-glycero-3-phosphocholine. 2-*O*-Acetyl-1-*O*-(9-octadecenyl)-sn-glycero-3-phosphocholine. Oleyl-PAF*
[85966-90-1]
$C_{28}H_{56}NO_7P$ 549.727
$[\alpha]_D^{20}$ -0.25 (c, 5.0 in MeOH/$CHCl_3$).

1-(11*Z*-Octadecenyl)glycero-3-phosphocholine [153534-79-3]
$C_{26}H_{54}NO_6P$ 507.689
Isol. from the sea cucumber *Cucumaria frondosa* and sponge *Spirastrella abata*. Oil. $[\alpha]_D^{20}$ -2.9 (c, 0.1 in $CHCl_3$/MeOH).

1-Tetradecylglycero-3-phosphocholine [93824-39-6]
[102268-55-3 (*R*)]
$C_{22}H_{48}NO_6P$ 453.598
Isol. from the hydroid *Solanderia secunda*.

1-(15-Methylhexadecyl)glycero-3-phosphocholine [147163-19-7]
Isol. from the sponge *Spirastrella abata*.
Amorph. solid.

1-(3*Z*-Hexadecenyl)glycero-3-phosphocholine [339984-37-1]
$C_{24}H_{50}NO_6P$ 479.636
Constit. of *Spirastrella abata*.

1-(4*Z*-Hexadecenyl)glycero-3-phosphocholine [339984-36-0]
Constit. of *Spirastrella abata*.

1-(2-Methoxyhexadecyl)glycero-3-phosphocholine [340023-96-3]
Constit. of *Spirastrella abata*.

1-(2-Methoxy-4*Z*-hexadecenyl)glycero-3-phosphocholine [340023-97-4]
$C_{25}H_{52}NO_7P$ 509.662
Constit. of *Spirastrella abata*.

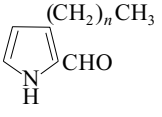
1-(3*Z*-Octadecenyl)glycero-3-phosphocholine [251092-28-1]
$C_{26}H_{54}NO_6P$ 507.69
Isol. from *Spirastrella abata*. Amorph. solid.

1-(4*Z*-Octadecenyl)glycero-3-phosphocholine [251092-29-2]
$C_{26}H_{54}NO_6P$ 507.69
Isol. from *Spirastrella abata*. Amorph. solid.

Wykle, R.L. *et al., Biochem. Biophys. Res. Commun.*, 1981, **100**, 1651 (*synth, biochem*)
Lartigue-Mattel, C. *et al., Agents Actions*, 1982, **12**, 703 (*pharmacokin*)
Tsushima, S. *et al., Chem. Pharm. Bull.*, 1982, **30**, 3260 (*synth, Me ether*)
Berchtold, R. *et al., Chem. Phys. Lipids*, 1982, **30**, 389 (*synth, Me ether*)
Hirth, G. *et al., Helv. Chim. Acta*, 1982, **65**, 1059; 1983, **66**, 1210 (*synth, ir, pmr, oleyl PAF*)
Keraly, C. *et al., Br. J. Haematol*, 1983, **53**, 513 (*biochem, struct*)
Hadvary, P. *et al., Thromb. Res.*, 1983, **30**, 143 (*biochem*)
Kasuya, Y. *et al., Can. J. Physiol. Pharmacol.*, 1984, **62**, 457 (*deriv*)
Ohno, M. *et al., Chem. Pharm. Bull.*, 1985, **33**, 572 (*synth, pmr, ir, biochem*)
Robinson, M. *et al., J. Biol. Chem.*, 1985, **260**, 7889 (*biosynth, derivs*)
Sturk, A. *et al., Thromb. Res.*, 1985, **40**, 359 (*biochem*)
Fusetani, N. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **83**, 511-513 (*Solanderia secunda constits*)
Kertscher, H.P. *et al., Pharmazie*, 1986, **41**, 596 (*synth, lyso PAF*)
Cimetiere, B. *et al., Tet. Lett.*, 1986, **27**, 6329 (*synth, PAF*)
O'Flaherty, J.T. *et al., Biochem. Biophys. Res. Commun.*, 1987, **147**, 18 (*synth, biochem*)
Kramer, R.M. *et al., Biochim. Biophys. Acta*, 1988, **959**, 269 (*synth, biochem, acyl derivs*)
Bhatia, S.K. *et al., J.O.C.*, 1988, **53**, 5034 (*synth, ir, pmr*)
Wolfgang, J. *et al., Synform*, 1988, **6**, 115; 1990, **8**, 313 (*rev, synth*)
Hofmann, B. *et al., Thromb. Res.*, 1988, **49**, 415 (*biochem*)
Benveniste, J. *et al., Adv. Prostaglandin, Thromboxane, Leukotriene Res.*, 1989, **19**, 355 (*rev, props*)
Ostermann, G. *et al., Biochim. Biophys. Acta*, 1989, **47**, 5233 (*biochem*)
Tessner, T.G. *et al., J. Biol. Chem.*, 1989, **264**, 4794 (*biochem*)
Guivisdalsky, P.N. *et al., J.O.C.*, 1989, **54**, 4637; 4643 (*synth, ir, pmr*)
Murari, M.P. *et al., Lipids*, 1990, **25**, P606 (*synth, lyso PAF*)
Jeong, B.Y. *et al., Lipids*, 1990, **25**, 624 (*isol, acyl derivs*)
Leslie, C.C. *et al., Methods Enzymol.*, 1990, **187**, 216 (*synth, props, acyl derivs*)
Nakamura, N. *et al., Tet. Lett.*, 1990, **31**, 699 (*synth*)
Kumar, A. *et al., Synth. Commun.*, 1991, **21**, 1763 (*synth, enantio-PAF, pmr*)
Yayli, N. *et al., J. Nat. Prod.*, 1994, **57**, 84 (*isol, sea cucumber*)
Shin, B.A. *et al., J. Nat. Prod.*, 1999, **62**, 1554-1557 (*Spirastrella abata constits*)
Alam, N. *et al., J. Nat. Prod.*, 2001, **64**, 533-535 (*Spirastrella abata constits*)
Hong, J. *et al., Rapid Commun. Mass Spectrom.*, 2001, **15**, 120-1126 (*isol, ms*)

3-Alkyl-1*H*-pyrrole-2-carboxaldehydes A-208

3-Alkyl-2-formylpyrroles



Isol. as a mixt. of 3.3% n = 18, 12.5% n = 19, 49% n = 20, 25% n = 21, and 10.2% n = 22. The substitution pattern of these constits. has been questioned (Stierle *et al*). Metabs. of the marine sponge *Oscarella lobularis*.

3-Nonadecyl-1*H*-pyrrole-2-carboxaldehyde [57992-51-5]
$C_{24}H_{43}NO$ 361.61
n = 18.

3-Eicosyl-1*H*-pyrrole-2-carboxaldehyde
*3-Icosyl-1*H*-pyrrole-2-carboxaldehyde*
[57992-52-6]
$C_{25}H_{45}NO$ 375.637
n = 19.

3-Heneicosyl-1*H*-pyrrole-2-carboxaldehyde [57992-53-7]
$C_{26}H_{47}NO$ 389.663
n = 20.

*12′,13′-Didehydro (*E*-): 13-(12-Heneicosenyl)-1*H*-pyrrole-2-carboxaldehyde, 9CI*
[57992-57-1]
$C_{26}H_{45}NO$ 387.648
Isol. from the marine sponge *Oscarella lobularis*.

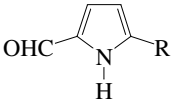
3-Docosyl-1*H*-pyrrole-2-carboxaldehyde [57992-54-8]
$C_{27}H_{49}NO$ 403.69
n = 21.

3-Tricosyl-1*H*-pyrrole-2-carboxaldehyde [57992-55-9]
$C_{28}H_{51}NO$ 417.717
n = 22.

Cimino, G. *et al., Experientia*, 1975, **31**, 1387 (*isol, uv, ir, pmr, ms, struct*)
Stierle, D.B. *et al., J.O.C.*, 1980, **45**, 4980

5-Alkyl-1*H*-pyrrole-2-carboxaldehydes A-209

2-Alkyl-5-formylpyrroles



5-Nonyl-1*H*-pyrrole-2-carboxaldehyde [89631-84-5]
$C_{14}H_{23}NO$ 221.342
Isol. from a soft coral, *Telesto* sp., and its associated, but unidentified, demosponge. Yellow oil. Not possible to identify the exact source of the natural product since it perfused both organisms.

5-Pentadecyl-1*H*-pyrrole-2-carboxaldehyde [75233-97-5]
$C_{20}H_{35}NO$ 305.503
Metab. from a marine sponge *Laxosuberites* sp. Isol. in admixture (46%) with the hexadecyl (12%), heptadecyl (23%) and nonadecyl (19%) homologues. λ_{max} 297 (ϵ 16000) (MeCN) (Derep).

*6′,7′*E*-Didehydro: 5-(6-Pentadecenyl)-1*H*-pyrrole-2-carboxaldehyde*
$C_{20}H_{33}NO$ 303.487
Metab. of the sponge *Mycale tenuispiculata*. Pale yellow solid. Mp 42-44°. λ_{max} 297 (ϵ 15400) (MeCN).

5-(13-Methyltetradecyl)-1*H*-pyrrole-2-carboxaldehyde [233744-63-3]
$C_{20}H_{35}NO$ 305.503
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

5-Hexadecyl-1*H*-pyrrole-2-carboxaldehyde [75233-98-6]
$C_{21}H_{37}NO$ 319.529
Metab. from *Laxosuberites* sp. See note under pentadecyl above.

5-(14-Methylpentadecyl)-1*H*-pyrrole-2-carboxaldehyde [233744-64-4]
$C_{21}H_{37}NO$ 319.529
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

5-Heptadecyl-1*H*-pyrrole-2-carboxaldehyde [75233-99-7]
$C_{22}H_{39}NO$ 333.556
Metab. from *Laxosuberites* sp. See note under pentadecyl above.

*9,10*Z*-Didehydro: 5-(9*Z*-Heptadecenyl)-1*H*-pyrrole-2-carboxaldehyde*
[233744-73-5]
$C_{22}H_{37}NO$ 331.54
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

5-Octadecyl-1*H*-pyrrole-2-carboxaldehyde [262351-87-1]
$C_{23}H_{41}NO$ 347.583
Isol. from *Mycale mytilorum*. Pale yellow flakes. Mp 56-58°. λ_{max} 302 (ϵ 16000) (EtOH).

5-(16-Methylheptadecyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 6
[705973-02-0]
$C_{23}H_{41}NO$ 347.583
Isol. from the sponge *Mycale cecilia*. Amorph. powder. λ_{max} 203 (ϵ 6260); 249 (ϵ 2080); 300 (ϵ 9790) (MeOH).

5-Nonadecyl-1*H*-pyrrole-2-carboxaldehyde [75234-00-3]
$C_{24}H_{43}NO$ 361.61
Metab. from *Laxosuberites* sp. See note under pentadecyl above.

*9,10*Z*-Didehydro: 5-(9*Z*-Nonadecenyl)-1*H*-pyrrole-2-carboxaldehyde*
[233744-74-6]
$C_{24}H_{41}NO$ 359.594

Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

*12,13Z-Didehydro: 5-(12Z-Nonadecenyl)-1*H*-pyrrole-2-carboxaldehyde.* ***Mycalazal 4***
[705972-97-0]
$C_{24}H_{41}NO$ 359.594
Isol. from the sponge *Mycale cecilia*. Amorph. powder. λ_{max} 202 (ϵ 7585); 249 (ϵ 2340); 300 (ϵ 11760) (MeOH).

5-Eicosyl-1*H*-pyrrole-2-carboxaldehyde [233744-67-7]
$C_{25}H_{45}NO$ 375.637
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

5-(9*Z*-Heneicosenyl)-1*H*-pyrrole-2-carboxaldehyde [233744-65-5]
$C_{26}H_{45}NO$ 387.648
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

5-(14*Z*-Heneicosenyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 8
[705973-25-7]
Isol. from the sponge *Mycale cecilia*.
Amorph. powder. λ_{max} 202 (ϵ 7800); 248 (ϵ 2320); 300 (ϵ 11290) (MeOH).

5-(12*Z*,15*Z*-Heneicosadienyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 5
[705972-98-1]
$C_{26}H_{43}NO$ 385.632
Isol. from the sponge *Mycale cecilia*. Oil. λ_{max} 204 (ϵ 9250); 248 (ϵ 2390); 300 (ϵ 11150) (MeOH).

5-(12*Z*,15*Z*,18*Z*-Heneicosatrienyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 3
[705972-95-8]
$C_{26}H_{41}NO$ 383.616
Isol. from the sponge *Mycale cecilia*. Oil. λ_{max} 204 (ϵ 14690); 248 (ϵ 3440); 300 (ϵ 15400) (MeOH).

5-(12*Z*-Docosenyl)-1*H*-pyrrole-2-carboxaldehyde [233744-66-6]
$C_{27}H_{47}NO$ 401.674
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*. Indexed as the Δ^{11}-isomer in CAS.

5-Tricosyl-1*H*-pyrrole-2-carboxaldehyde [233744-70-2]
$C_{28}H_{51}NO$ 417.717
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

*9,10Z-Didehydro: 5-(9Z-Tricosenyl)-1*H*-pyrrole-2-carboxaldehyde*
[233744-68-8]
$C_{28}H_{49}NO$ 415.701
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

*14,15Z-Didehydro: 5-(14Z-Tricosenyl)-1*H*-pyrrole-2-carboxaldehyde*
[233744-69-9]
$C_{28}H_{49}NO$ 415.701
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

*14,15Z,17,18Z-Tetradehydro: 5-(14Z,17Z-Tricosadienyl)-1*H*-pyrrole-2-carboxaldehyde.* ***Mycalazal 9***
[705973-27-9]
$C_{28}H_{47}NO$ 413.685
Isol. from the sponge *Mycale cecilia*. Oil. λ_{max} 201 (ϵ 14170); 248 (ϵ 4060); 300 (ϵ 21160) (MeOH).

*14,15Z,17,18Z,20,21Z-Hexadehydro: 5-(14Z,17Z,20Z-Tricosatrienyl)-1*H*-pyrrole-2-carboxaldehyde.* ***Mycalazal 7***
[705973-15-5]
$C_{28}H_{45}NO$ 411.67
Isol. from the sponge *Mycale cecilia*. Oil. λ_{max} 204 (ϵ 9250); 248 (ϵ 2390); 300 (ϵ 11150) (MeOH).

5-(11*Z*-Pentacosenyl)-1*H*-pyrrole-2-carboxaldehyde [233744-71-3]
$C_{30}H_{53}NO$ 443.755
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

5-(15*Z*-Pentacosenyl)-1*H*-pyrrole-2-carboxaldehyde [233744-72-4]
$C_{30}H_{53}NO$ 443.755
Isol. from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*.

5-(16*Z*-Pentacosenyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 12
[705973-36-0]
$C_{30}H_{53}NO$ 443.755
Isol. from the sponge *Mycale cecilia*.

5-(18*Z*-Pentacosenyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 13
[705973-38-2]
$C_{30}H_{53}NO$ 443.755
Isol. form the sponge *Mycale cecilia*.

5-(16*Z*,19*Z*-Pentacosadienyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 11
[705973-35-9]
Isol. from the sponge *Mycale cecilia*.
Oil. λ_{max} 202 (ϵ 6040); 248 (ϵ 1800); 301 (ϵ 7630) (MeOH).

5-(16*Z*,19*Z*,22*Z*-Pentacosatrienyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 10
[705973-28-0]
Isol. from the sponge *Mycale cecilia*.
Oil. λ_{max} 204 (ϵ 11920); 248 (ϵ 3690); 300 (ϵ 16900) (MeOH).

5-(10*Z*,13*Z*,16*Z*,19*Z*,22*Z*-Pentacosapentaenyl)-1*H*-pyrrole-2-carboxaldehyde, 9CI
Mycalazal 2
[185389-83-7]
$C_{30}H_{45}NO$ 435.692
Metab. from *Mycale micracanthoxea*. Cytotoxic agent. Oil.

5-(7*Z*,10*Z*,13*Z*,16*Z*,19*Z*,22*Z*-Pentacosahexaenyl)-1*H*-pyrrole-2-carboxaldehyde
Mycalazal 1
[185389-71-3]
Metab. of the sponge *Mycale micracanthoxea*.
Oil.

Stierle, D.B. *et al., J.O.C.*, 1980, **45**, 4980 (*isol, uv, ir, pmr, cmr, ms, struct*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1984, **37**, 227 (*isol, uv, ir, pmr, cmr, ms, struct, synth*)
Ortega, M.J. *et al., Tetrahedron*, 1997, **53**, 331-340; 2004, **60**, 2517-2524 (*Mycalazals 1-13*)
Compagnone, R.S. *et al., Nat. Prod. Lett.*, 1999, **13**, 203-211 (*alkenyls, branched-chain alkyls*)
Reddy, G.B.S. *et al., Bioorg. Med. Chem.*, 2000, **8**, 27-36 (*octadecyl*)
Venkatesham, U. *et al., J. Nat. Prod.*, 2000, **63**, 1318-1320 (*6-pentadecenyl*)
Hansen, T.V. *et al., Tet. Lett.*, 2004, **45**, 2809-2811 (*Mycalazal 2, synth*)

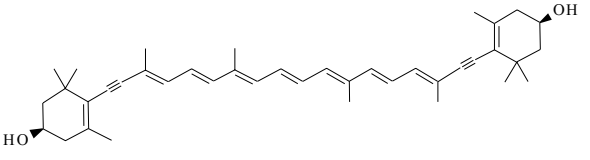
Allophycocyanin A-210

Complex large protein. Isol. from the red alga *Porphyra yezoensis*. Photopigment.

Liu, J.-Y. *et al., J. Biol. Chem.*, 1999, **274**, 16945-16952 (*cryst struct*)

Alloxanthin A-211

7,7′,8,8′-Tetradehydro-β,β-carotene-3,3′-diol. Cynthiaxanthin. Cryptomonaxanthin. Manixanthin. Pectenoxanthin
[28380-31-6]



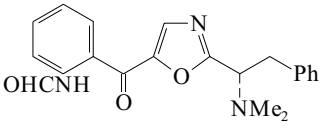
$C_{40}H_{52}O_2$ 564.85
Constit. of many shellfish including the giant scallop (*Pecten maximus*) and edible mussel (*Mytilus edulis*); constit. of Cryptophyceae. Also occurs in sponges. Reddish needles (Me_2CO/petrol). Mp 188-190° (186-188°).

Enantiomer, di-Me ether: 7,7′,8,8′-Tetradehydro-3,3′-dimethoxy-β,β-carotene. ***Suberixanthin***
[166774-49-8]
$C_{42}H_{56}O_2$ 592.903
Isol. from the sponge *Suberites massa*. λ_{max} 428 (sh); 452; 480 (Et_2O).

[26666-93-3, 95343-66-1]

Chapman, D.J. *et al., Phytochemistry*, 1966, **5**, 1331 (*isol*)
Davies, A.J. *et al., Chem. Comm.*, 1967, 941-942 (*isol*)
De Ville, T.E. *et al., Chem. Comm.*, 1969, 1311 (*struct*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97 (*cmr*)
Liaaen-Jensen, S. *et al., Biochem. Syst. Ecol.*, 1982, **10**, 167-174 (*occur, sponges*)
Davies, A.J. *et al., J.C.S. Perkin 1*, 1984, 2147 (*synth*)
Pennington, F.C. *et al., Biochem. Syst. Ecol.*, 1985, **13**, 215 (*isol, cd*)
Matsuno, T *et al., J. Nat. Prod.*, 1985, **48**, 606 (*isol*)
Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495 (*isol, pmr, uv*)
Aiello, A. *et al., J. Prakt. Chem.*, 1995, **337**, 397-400 (*Suberixanthin, cd, pmr, cmr*)

Almazole A A-212



$C_{21}H_{21}N_3O_3$ 363.415

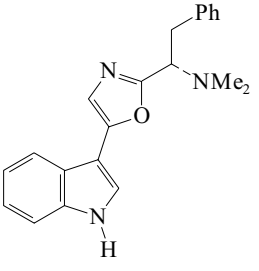
(S)-form [157382-33-7]
Alkaloid from the red alga *Haraldiophyllum* sp.
Semisolid. $[\alpha]_D^{20}$ +103 (c, 0.155 in MeOH). λ_{max} 204 (ϵ 36700); 237 (ϵ 26400); 278 (ϵ 18200); 320 (ϵ 6000) (MeOH) (Derep).

Deformyl: ***Almazole B***
[157382-34-8]
$C_{20}H_{21}N_3O_2$ 335.405
Alkaloid from *Haraldiophyllum* sp. Yellow semisolid. $[\alpha]_D^{20}$ +92 (c, 0.05 in MeOH). λ_{max} 203 (ϵ 40300); 234 (ϵ 22600); 260 (ϵ 16500); 396 (ϵ 6300) (MeOH) (Derep).

N'Diaye, I. *et al., Tet. Lett.*, 1994, **35**, 4827-4830 (*isol, uv, cd, pmr, cmr, ms*)
Khalafy, J. *et al., Aust. J. Chem.*, 1999, **52**, 31-36 (*synth*)

Almazole C A-213

[161068-69-5]

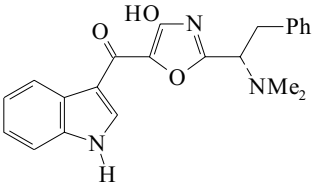


$C_{21}H_{21}N_3O$ 331.416
Alkaloid from the red alga *Haraldiophyllum* sp. CNS active. $[\alpha]_D^{20}$ +168 (c, 1.08 in MeOH). λ_{max} 222 (ϵ 26000); 271 (ϵ 15100); 282 (ϵ 14500); 300 (ϵ 12900) (MeOH) (Berdy).

Guella, G. *et al., Helv. Chim. Acta*, 1994, **77**, 1999-2006 (*isol, synth, cd, uv, pmr, cmr, ms*)

Almazole D A-214

[176739-66-5]



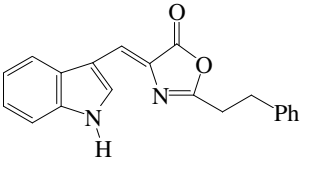
$C_{22}H_{21}N_3O_3$ 375.426
Alkaloid from the red alga *Haraldiophyllum* sp. Shows antifungal activity. Powder. $[\alpha]_D^{20}$ +20 (c, 0.07 in MeOH).

Me ether:
Powder. $[\alpha]_D^{20}$ +70 (c, 0.1 in MeOH).

N'Diaye, I. *et al., Tet. Lett.*, 1996, **37**, 3049-3050 (*isol, uv, pmr, cmr, ms*)

Almazolone A-215

[878143-16-9]
[878143-13-6 (*E*–form), 878143-15-8 (*Z*-form)]

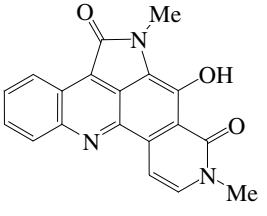


(*Z*)-*form*

$C_{20}H_{16}N_2O_2$ 316.359
Isol. from the red alga *Haraldiophyllum* sp. Yellow powder. Mp 245-247°. Isol. as an 80:20 mixt. of (*Z*/*E*)-isomers to which data refers.

Guella, G. *et al., Tetrahedron*, 2006, **62**, 1165-1170 (*isol, synth, pmr, cmr, ms*)

Alpkinidine A-216

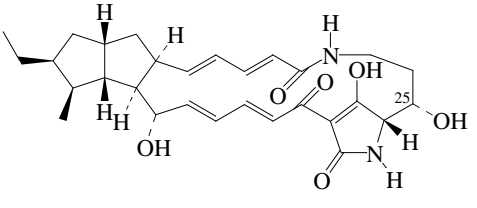


$C_{19}H_{13}N_3O_3$ 331.33
Alkaloid from *Xestospongia* cf. *carbonaria*. Purple solid.

Thale, Z. *et al., J.O.C.*, 2002, **67**, 9384-9391 (*isol, pmr, cmr, cryst struct*)

Alteramide A A-217

[142131-06-4]



$C_{29}H_{38}N_2O_6$ 510.629

Macrocylic lactam antibiotic. Isol. from an *Alteromonas* sp. associated with the sponge *Halichondria okadai*. Exhibits cytotoxicity against murine leukaemia P388 cells, murine lymphoma L1210 cells and the human epidermoid carcinoma KB cells *in vitro*. Yellow powder. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O.
Mp 200° (dec.). $[\alpha]_D^{22}$ +36.2 (c, 0.1 in MeOH). λ_{max} 268 (ϵ 30300); 347 (ϵ 11000) (MeOH) (Derep).

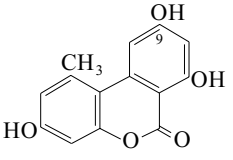
25-Deoxy: ***Alteramide B***
$C_{29}H_{38}N_2O_5$ 494.63
From an *Alteromonas* sp. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O. λ_{max} 268; 347 (MeOH) (Berdy).

[142131-07-5]

Shigemori, H. *et al., J.O.C.*, 1992, **57**, 4317-4320 (*isol, ir, uv, pmr, cmr, struct*)

Alternariol A-218

*3,7,9-Trihydroxy-1-methyl-6*H*-dibenzo[*b,d*]pyran-6-one, 9CI.*
3,4′,5-Trihydroxy-6′-methyldibenzo-α-pyrone
[641-38-3]



$C_{14}H_{10}O_5$ 258.23
Occurs in mycelium of *Alternaria tenuis* responsible for alternaria cone disorder in hops and fruit spot on papaya (*Carica papaya*) and *Passiflora* spp. Also from marine *Alternaria* spp. Phytotoxic, DNA-intercalating mycotoxin. Needles (EtOH aq.). Sol. MeOH, bases, Et_2O; poorly sol. C_6H_6, hexane, H_2O.
Mp 350° dec. Subl. 250° *in vacuo*. λ_{max} 213 (ϵ 21900); 258 (ϵ 41700); 290 (ϵ 10500); 303 (ϵ 11200); 336 (ϵ 11500) (MeOH).

▶ Exp. reprod. and teratogenic effects. HP8757000

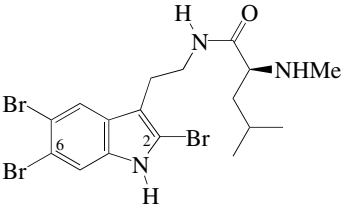
Tri-Ac:
Cryst. (EtOH). Mp 167-169°.

*9-Me ether: 9-*O*-Methylalternariol.* ***Djalonensone***
[26894-49-5]
$C_{15}H_{12}O_5$ 272.257
Metab. of *Alternaria* spp. incl. marine spp. Also from *Anthocleista djalonensis*. Needles (EtOH or dioxan).
Mp 266-268° dec.

Raistrick, H. *et al., Biochem. J.*, 1953, **55**, 421 (*isol*)
Thomas, R. *et al., Proc. Chem. Soc., London*, 1959, 88 (*biosynth*)
Gatenbeck, S. *et al., Acta Chem. Scand.*, 1965, **19**, 65 (*synth*)
Sóti, F. *et al., Chem. Ber.*, 1977, **110**, 979 (*synth*)
Harris, T.M. *et al., J.A.C.S.*, 1977, **99**, 1631 (*synth*)
Abell, C. *et al., Chem. Comm.*, 1982, 1011 (*biosynth*)
Leeper, F.J. *et al., J.C.S. Perkin 1*, 1984, 1053 (*synth*)
DiCosimo, F. *et al., Experientia*, 1985, **41**, 1188
Stinson, E.E. *et al., Can. J. Chem.*, 1986, **64**, 1590 (*biosynth*)
Abell, C. *et al., Chem. Comm.*, 1986, 15 (*synth*)
Dasenbrock, J. *et al., Chem. Comm.*, 1987, 1235 (*biosynth*)
Kanakam, C.C. *et al., J.C.S. Perkin 1*, 1990, 2233 (*synth*)
Onocha, P.A. *et al., Phytochemistry*, 1995, **40**, 1183 (*Djalonensone*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)
Koch, K. *et al., J.O.C.*, 2005, **70**, 3275-3276 (*synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 615; 623
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGW476

Alternatamide B A-219

[191212-58-5]



$C_{17}H_{22}Br_3N_3O$ 524.092
Alkaloid from the marine bryozoan *Amathia alternata*. Moderate antibacterial agent. Amorph. powder.

N^1*-Me:* ***Alternatamide A***
[191212-57-4]
$C_{18}H_{24}Br_3N_3O$ 538.119
Alkaloid from *Amathia alternata*. Amorph. powder.

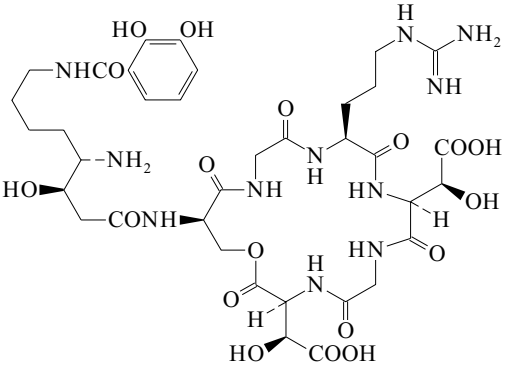
2-Debromo: ***Alternatamide D***
[191212-60-9]
$C_{17}H_{23}Br_2N_3O$ 445.196
Alkaloid from *Amathia alternata*. Amorph. powder.

6-Debromo: ***Alternatamide C***
[191212-59-6]
$C_{17}H_{23}Br_2N_3O$ 445.196
Alkaloid from *Amathia alternata*. Amorph. powder.

Lee, N.-K. *et al., J. Nat. Prod.*, 1997, **60**, 697-699 (*isol, uv, cd, ir, pmr, cmr, ms*)

Alterobactin A A-220

[153888-52-9]

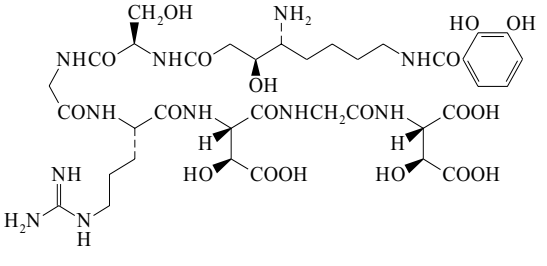


$C_{36}H_{53}N_{11}O_{18}$ 927.878
Depsipeptide antibiotic. Isol. from the marine bacterium *Alteromonas luteoviolacea*. Siderophore. λ_{max} 480 (MeOH) (Berdy).

Reid, R.T. *et al., Nature (London)*, 1993, **366**, 455-458 (*Alterobactin A*)
Deng, J. *et al., Synthesis*, 1998, 627-638 (*synth*)

Alterobactin B A-221

[153888-53-0]



$C_{36}H_{55}N_{11}O_{19}$ 945.893

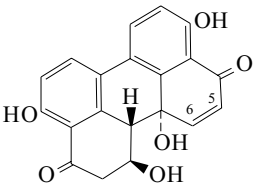
Ring-opened form of Alterobactin A, A-220. Isol. from the marine bacterium *Alteromonas luteoviolacea*. Siderophore. λ_{max} 480 (MeOH) (Berdy).

Reid, R.T. *et al., Nature (London)*, 1993, **366**, 455-458 (*Alterobactin B*)

Alterperylenol A-222

*1,2,12*a,*12*b-*Tetrahydro-1,4,9,12*a-*tetrahydroxy-3,10-perylenedione, 9CI. Alteichin*

[88899-62-1]



$C_{20}H_{14}O_6$ 350.327

Same struct. detd. crystallographically for Alterperylenol and Alteichin but widely differing phys. consts. reported. Pigment from *Alternaria* spp. incl. a marine sp. Antifungal and phytotoxic agent. Cryst. (MeOH/$CHCl_3$).
Mp 182-185° Mp 350°. $[\alpha]_D$ +90. λ_{max} 230 (ϵ); 252 (ϵ); 290 (ϵ); 380 (ϵ) (MeOH) (Derep).

5,6-Dihydro: ***Dihydroalterperylenol****. Altertoxin I. ATX 1*
[88899-63-2]
$C_{20}H_{16}O_6$ 352.343
Constit. of *Alternaria alternata* and a marine *Alternaria* sp. Antifungal and cytotoxic. Cryst. (MeOH/$CHCl_3$).
Mp 180° dec.(147-150°). $[\alpha]_D^{26}$ +380 (c, 0.20 in Me_2CO). $[\alpha]_D$ +484 (c, 0.002 in $CHCl_3$). λ_{max} 213 (ϵ); 257 (ϵ); 285 (ϵ); 355 (ϵ) (MeOH) (Derep).

*5,6-Dihydro, 6*α*-hydroxy:* ***Stemphytriol***
$C_{20}H_{16}O_7$ 368.342
Isol. from *Monodictys fluctuata*. Yellow solid.
Mp 180-182° (150-152°). $[\alpha]_D^{20}$ +451 (c, 0.07 in MeOH). Two different Mps stated in ref. λ_{max} 254 (ϵ 25000); 285 (ϵ 12000); 353 (ϵ 4200) (MeOH).

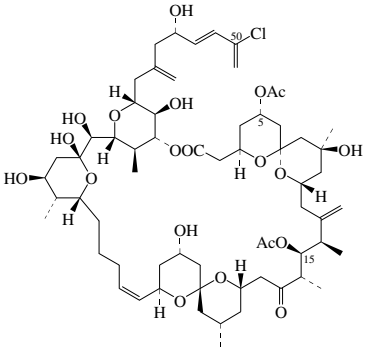
[56258-32-3, 95781-70-7]

Stinson, E.E. *et al., J.O.C.*, 1982, **47**, 4111 (*struct*)
Okuno, T. *et al., Tet. Lett.*, 1983, **24**, 5653 (*cryst struct*)
Robeson, D. *et al., Experientia*, 1984, **40**, 1248 (*isol, cryst struct*)
Stack, M.E. *et al., J. Nat. Prod.*, 1986, **49**, 866 (*isol, bibl*)
Arnone, A. *et al., J.C.S. Perkin 1*, 1986, 525 (*struct*)
Hradil, C.M. *et al., Phytochemistry*, 1988, **28**, 73 (*isol*)
Krohn, K. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 31-34 (*Stemphytriol*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 635

Altohyrtin A A-223

Spongistatin 1

[149715-96-8]



Absolute configuration

$C_{63}H_{95}ClO_{21}$ 1223.884

Macrocyclic lactone antibiotic. Altohyrtin A and Spongistatin 1 have same gross struct. Stereochem. shown here is for Altohyrtin A. Isol. from marine sponges *Spongia* sp. and *Hyrtios altum*. Antitumour agent. Amorph. powder (as Na salt).
Mp 161-162° (Na salt). $[\alpha]_D^{22}$ +26.2 (c, 0.32 in MeOH) (Na salt). λ_{max} 216 (ϵ 8490) (MeOH) (Derep). λ_{max} 227 (ϵ 19000) (MeOH) (Derep).

50-Bromo analogue: ***Altohyrtin B***
[151656-54-1]
$C_{63}H_{95}BrO_{21}$ 1268.335
Isol. from *Hyrtios altum*. Antitumour agent. Amorph. solid.
$[\alpha]_D$ +45 (c, 0.2 in MeOH). λ_{max} 228 (ϵ 20000) (MeOH) (Derep).

50-Dechloro: ***Altohyrtin C****. Spongistatin 2*
[151717-16-7]
$C_{63}H_{96}O_{21}$ 1189.439
Isol. from *Hyrtios altum* and *Spongia* sp. Cytotoxic agent. Amorph. solid.
Mp 140-141°. $[\alpha]_D$ +24.5 (c, 0.39 in MeOH). λ_{max} 220 (ϵ 16200); 273 (ϵ 891) (MeOH) (Derep). λ_{max} 226 (ϵ 17000) (MeOH) (Derep).

*5-*O*-De-Ac:* ***Spongistatin 3****. 5-De-*O*-acetylaltohyrtin A*
[150642-07-2]
$C_{61}H_{93}ClO_{20}$ 1181.846
Isol. from *Hyrtios altum* and *Spongia* sp. Cytotoxic agent. Powder.
Mp 148-149°. $[\alpha]_D$ +28.1 (c, 0.15 in MeOH). λ_{max} 227 (ϵ 13800); 268 (ϵ 1740) (MeOH) (Derep). λ_{max} 227 (ϵ 20000) (MeOH) (Derep).

*15-*O*-De-Ac: 15-De-*O*-acetylaltohyrtin A*. ***Spongistatin 4****. Cinachyrolide A*
[153745-94-9]
[148439-44-5]
$C_{61}H_{93}ClO_{20}$ 1181.846
Isol. from the sponges *Spirastrella spinispirulifera* (Porifera) and *Cinachyra* sp. Cytotoxic agent. Solid.
Mp 153-154°. $[\alpha]_D^{22}$ +23 (c, 0.2 in MeOH). λ_{max} 227 (ϵ 13800); 268 (ϵ 1740) (MeOH) (Derep).

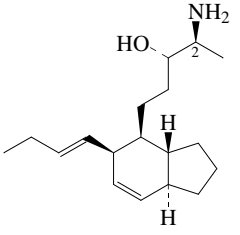
*50-Dechloro, 15-de-*O*-Ac:* ***Spongistatin 6***
[158080-65-0]
$C_{61}H_{94}O_{20}$ 1147.402
Isol. from *Spirastrella spinispirulifera* (Porifera). λ_{max} 223 (ϵ 18621) (MeOH) (Berdy).

[148179-94-6, 150624-44-5]

Ireland, C.M. *et al., J.A.C.S.*, 1980, **102**, 5688
Pettit, G.R. *et al., Chem. Comm.*, 1993, 1166; 1805 (*Spongistatins*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1993, **41**, 989; 1996, **44**, 2142 (*Altohyrtins, isol, uv, pmr, cmr, ms, abs config*)
Fusetani, N. *et al., J.A.C.S.*, 1993, **115**, 3977 (*Cinachyrolide A*)
Pettit, G.R. *et al., J.O.C.*, 1993, **58**, 1302 (*Spongistatin 1*)
Pettit, G.R. *et al., Nat. Prod. Lett.*, 1993, **3**, 239 (*Spongistatin 6*)
Evans, D.A. *et al., Tetrahedron*, 1999, **55**, 8671-8726 (*Altohyrtin C, synth*)
Smith, A.B. *et al., Angew. Chem., Int. Ed.*, 2001, **40**, 191-195; 196-199 (*synth*)
Aoki, S. *et al., Tetrahedron*, 2001, **57**, 2289-2292 (*struct, config*)
Crimmins, M.T. *et al., J.A.C.S.*, 2002, **124**, 5661-5663 (*synth*)
Heathcock, C.H. *et al., J.A.C.S.*, 2003, **125**, 12844-12849 (*synth*)
Smith, A.B. *et al., Org. Lett.*, 2003, **5**, 761-764 (*synth*)
Terauchi, T. *et al., Tet. Lett.*, 2003, **44**, 7741-7745; 7747-7751 (*synth*)
Paterson, I. *et al., Org. Biomol. Chem.*, 2005, **3**, 2399-2409; 2410-2419; 2420-2430 (*synth*)

Amaminol A A-224

[261622-18-8]



Absolute Configuration

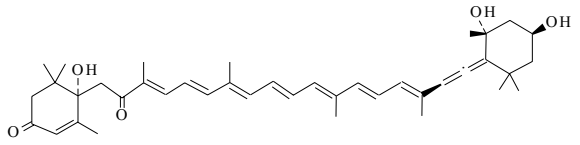
$C_{18}H_{31}NO$ 277.449

Isol. from an unidentified tunicate of the family Polyclinidae. Cytotoxic agent. Pale yellow oil. $[\alpha]_D^{24}$ -170.8 (c, 0.2 in MeOH).

2-Epimer: ***Amaminol B***
[261622-22-4]
$C_{18}H_{31}NO$ 277.449
Isol. from an unidentified tunicate of the family Polyclinidae. Cytotoxic agent. Pale yellow oil. $[\alpha]_D^{24}$ -112.4 (c, 0.2 in MeOH).
Sata, N.U. *et al., Tet. Lett.*, 2000, **41**, 489-492 (*isol, pmr, cmr*)

Amarouciaxanthin A A-225

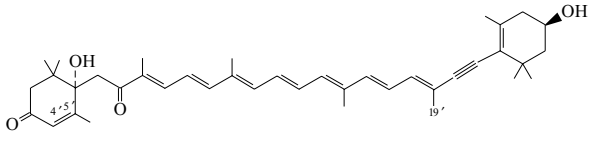
6,7-Didehydro-5,6,7′,8′-tetrahydro-3,5,6′-trihydroxy-β,ϵ-carotene-3′,8′-dione
[100667-78-5]



$C_{40}H_{54}O_5$ 614.864
Constit. of *Amaroucium pliciferum*. Red needles (petrol). Sol. MeOH, hexane; poorly sol. H_2O.
Mp 160°. λ_{max} 230; 269; 457 (Et_2O) (Berdy).
Matsuno, T. *et al., J. Nat. Prod.*, 1985, **48**, 606

Amarouciaxanthin B A-226

7,8-Didehydro-7′,8′-dihydro-3,6′-dihydroxy-β,ϵ-carotene-3′,8′-dione. Sidnyaxanthin
[92121-55-6]



$C_{40}H_{52}O_4$ 596.848
Constit. of the tunicates *Sidnyum argus* and *Amaroucium pliciferum*. Shows weak cytotoxic activity. Dark reddish cryst. (Et_2O); reddish needles (petrol/Et_2O). Sol. MeOH, hexane; poorly sol. H_2O.
Mp 88-89° Mp 154°. $[\alpha]_D$ +1.6 (c, 0.9 in $CHCl_3$). λ_{max} 230; 281; 463 (Et_2O) (Berdy).

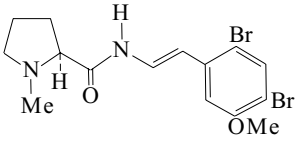
4,5β-Dihydro: 7,8-Didehydro-5′,6′,7′,8′-tetrahydro-3,6′-dihydroxy-β,β-carotene-3,8-dione. ***Isomytiloxanthin***
[50906-60-0]
$C_{40}H_{54}O_4$ 598.864
Isol. from the edible mussel (*Mytilus edulis*). Red gum. Tentative abs. config. λ_{max} 451 (no solvent reported).

19′-Hexanoyloxy, 4,5β-dihydro: ***19′-Hexanoyloxymytiloxanthin***
$C_{46}H_{64}O_6$ 713.008
Isol. from the edible mussel (*Mytilus edulis*).

Khare, A. *et al., Tet. Lett.*, 1973, 3921-3924 (*isol*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97 (*cmr*)
Belaud, C. *et al., Tet. Lett.*, 1984, **25**, 3087 (*isol, struct*)
Matsuno, T. *et al., J. Nat. Prod.*, 1985, **48**, 606 (*isol, struct*)
Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495 (*19′-Hexanoyloxymytiloxanthin*)
Khare, A. *et al., J.C.S. Perkin 1*, 1988, 1389 (*isol, struct*)

Amathamide A A-227

[99615-75-5]

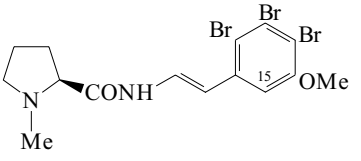


$C_{15}H_{18}Br_2N_2O_2$ 418.127
Alkaloid from the marine bryozoan *Amathia wilsoni*.
Mp 189-190.5°.

(Z)-Isomer: ***Amathamide B***
[99615-76-6]
Alkaloid from *Amathia wilsoni*.
Oil.
Blackman, A.J. *et al., Heterocycles*, 1985, **23**, 2829-2833 (*isol, ir, pmr, cmr, ms, cd, struct, abs config*)

Amathamide E A-228

[112515-28-3]



$C_{15}H_{17}Br_3N_2O_2$ 497.023
Alkaloid from the bryozoan *Amathia wilsoni*. Light yellow oil.

N-*Me:* ***Amathamide C***
[112515-26-1]
$C_{16}H_{19}Br_3N_2O_2$ 511.05
Alkaloid from *Amathia wilsoni* and *Amathia pinnata*. Pale yellow oil.

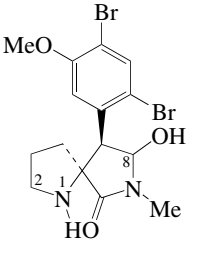
Dihydro: ***Amathamide D***
[112515-27-2]
$C_{15}H_{19}Br_3N_2O_2$ 499.039
Alkaloid from *Amathia wilsoni*. Light green oil.

(Z)-Isomer: ***Amathamide F***
[112515-29-4]
$C_{15}H_{17}Br_3N_2O_2$ 497.023
Alkaloid from *Amathia wilsoni*. Oil.

N-*Me, 15-methoxy:* ***Amathamide G***
[149355-72-6]
$C_{17}H_{21}Br_3N_2O_3$ 541.076
Alkaloid from *Amathia convoluta*. Oil.
Blackman, A.J. *et al., Aust. J. Chem.*, 1987, **40**, 1655-1662 (*isol, ir, pmr, cmr, ms, struct*)
Blackman, A.J. *et al., Aust. J. Chem.*, 1993, **46**, 401-405 (*Amathamide G*)

Amathaspiramide C A-229

[226993-86-8]



$C_{15}H_{18}Br_2N_2O_3$ 434.127

Alkaloid from the marine bryozoan *Amathia wilsoni*. Amorph. solid. $[\alpha]_D^{25}$ -2 (c, 0.005 in MeOH). λ_{max} 215 (log ϵ 4.16); 289 (log ϵ 3.15); 294 (log ϵ 3.15) (MeOH).

N^1-*Me:* ***Amathaspiramide A***
[226993-84-6]
$C_{16}H_{20}Br_2N_2O_3$ 448.154
Alkaloid from *Amathia wilsoni*. Amorph. solid. $[\alpha]_D^{25}$ -3 (c, 0.004 in MeOH). λ_{max} 216 (log ϵ 4.2); 289 (log ϵ 3.34); 295 (log ϵ 3.36) (MeOH).

1,2-Didehydro: ***Amathaspiramide E***
[226993-88-0]
$C_{15}H_{16}Br_2N_2O_3$ 432.111
Alkaloid from *Amathia wilsoni*. Amorph. solid. $[\alpha]_D^{25}$ -21 (c, 0.002 in MeOH). λ_{max} 220 (log ϵ 4.13); 289 (log ϵ 3.17); 295 (log ϵ 3.17) (MeOH).

2-Oxo: ***Amathaspiramide D***
[226993-87-9]
$C_{15}H_{16}Br_2N_2O_4$ 448.11
Alkaloid from *Amathia wilsoni*. Amorph. solid. $[\alpha]_D^{25}$ -44 (c, 0.002 in MeOH). λ_{max} 215 (log ϵ 4.03); 289 (log ϵ 3.22); 295 (log ϵ 3.22) (MeOH).

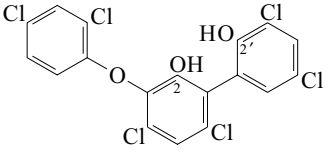
2-Oxo, N^1*-Me:* ***Amathaspiramide B***
[226993-85-7]
$C_{16}H_{18}Br_2N_2O_4$ 462.137
Alkaloid from *Amathia wilsoni*. Amorph. solid. $[\alpha]_D^{25}$ -13 (c, 0.002 in MeOH). λ_{max} 208 (log ϵ 4.5); 310 (log ϵ 4.38); 436 (log ϵ 4.6) (MeOH).

8-Epimer: ***Amathaspiramide F***
[226993-89-1]
$C_{15}H_{18}Br_2N_2O_3$ 434.127
Alkaloid from *Amathia wilsoni*. Amorph. solid. $[\alpha]_D$ -10 (c, 0.002 in MeOH). λ_{max} 214 (log ϵ 4.12); 290 (log ϵ 3.08); 296 (log ϵ 3.08) (MeOH).

Morris, B.D. *et al., J. Nat. Prod.*, 1999, **62**, 688-693 (*isol, uv, ir, pmr, cmr, ms*)
Hughes, C.C. *et al., Angew. Chem., Int. Ed.*, 2002, **41**, 4556-4559 (*Amathaspiramide F, synth*)

Ambigol A A-230

3′,4,5′,6-Tetrachloro-3-(2,4-dichlorophenoxy)-2,2′-biphenyldiol
[151487-20-6]

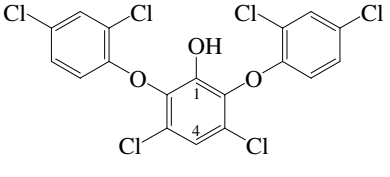


$C_{18}H_8Cl_6O_3$ 484.976
Isol. from the blue-green alga *Fischerella ambigua*. Exhibits antibacterial, antifungal and cytotoxic activity. Inhibits cyclooxygenase and HIV reverse transcriptase. Molluscicidal agent. Toxic to brine shrimp. Powder.
Mp 181.5-183.5°. $[\alpha]_D$ 0. λ_{max} 231 (ϵ 37300); 291 (ϵ 5700); 324 (ϵ 7700) (MeOH) (Derep).

Falch, B.S. *et al., J.O.C.*, 1993, **58**, 6570 (*isol, pmr, cmr, struct*)
Falch, B.S. *et al., Planta Med.*, 1995, **61**, 321 (*isol, activity*)

Ambigol B A-231

3,5-Dichloro-2,6-bis(2,4-dichlorophenoxy)phenol
[151515-56-9]



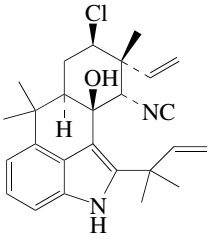
$C_{18}H_8Cl_6O_3$ 484.976
Metab. of *Fischerella ambigua*. Molluscicidal and antiinflammatory agent. HIV reverse transcriptase inhibitor. Toxic to brine shrimp . Exhibits antibacterial, antifungal and cytotoxic props. Pale yellow powder. λ_{max} 282 (6700); 288 (6640); 300 (4200); 340 (2740) (MeOH). λ_{max} 282 (ϵ 6700); 288 (ϵ 6640); 300 (ϵ 4200); 340 (ϵ 2740) (MeOH) (Derep). λ_{max} 232 (ϵ 26700); 288 (ϵ 6640); 300 (ϵ 4200); 340 (ϵ 2740) (MeOH) (Berdy).

1-Deoxy, 4-hydroxy: 2,6-Dichloro-3,5-bis(2,4-dichlorophenoxy)-phenol. ***Ambigol C***
$C_{18}H_8Cl_6O_3$ 484.976
Metab. of *Fischerella ambigua*. Amorph. powder.
Mp 197°. λ_{max} 285 (ϵ 8190); 294 (ϵ 9100); 308 (ϵ 7410) (EtOH).

Falch, B.S. *et al., J.O.C.*, 1993, **58**, 6570-6575 (*isol, uv, ir, pmr, cmr, ms*)
Falch, B.S. *et al., Planta Med.*, 1995, **61**, 321 (*isol, props*)
König, G.M. *et al., J. Nat. Prod.*, 2005, **68**, 459-461 (*Ambigol C*)

Ambiguine B isonitrile A-232

A 89271C. Antibiotic A 89271C
[138630-60-1]



Relative Configuration

$C_{26}H_{31}ClN_2O$ 422.996
Alkaloid from the terrestrial blue-green alga *Fischerella ambigua*. Amorph. solid. $[\alpha]_D$ -44.3 (c, 0.1 in MeOH). λ_{max} 223 (ϵ 40700); 281 (ϵ 9400); 291 (ϵ 7700) (MeOH).

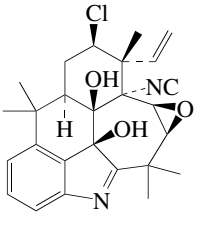
Deoxy: ***Ambiguine A isonitrile****. A 89271B. Antibiotic A 89271B*
[138630-59-8]
$C_{26}H_{31}ClN_2$ 406.997
From the terrestrial blue-green algae *Fischerella ambigua* and *Hapalosiphon hibernicus*. Needles (hexane/CH_2Cl_2). $[\alpha]_D$ -37 (c, 0.1 in MeOH). Mp >300° dec. λ_{max} 225 (ϵ 32400); 282 (ϵ 7600); 295 (sh) (ϵ 6500) (MeOH).

Dechloro: ***Ambiguine C isonitrile****. A 89271E. Antibiotic A89271E*
[138630-61-2]
$C_{26}H_{32}N_2O$ 388.552
From *Fischerella ambigua*. Amorph. solid. $[\alpha]_D$ -9.5 (c, 0.1 in MeOH). λ_{max} 223 (ϵ 36000); 281 (ϵ 8400); 291 (ϵ 6800) (MeOH).

Smitka, T.A. *et al., J.O.C.*, 1992, **57**, 857 (*isol, uv, ir, pmr, cmr, cd, struct*)

Ambiguine D isonitrile A-233

A 89271A. Antibiotic A89271A
[138666-15-6]



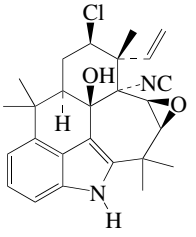
Relative Configuration

$C_{26}H_{29}ClN_2O_3$ 452.979
Alkaloid from the terrestrial blue-green algae *Fischerella ambigua* and *Westiellopsis prolifica*. Cryst. (MeOH aq.). $[\alpha]_D$ -30.3 (c, 0.1 in MeOH). Mp >300° dec. λ_{max} 227 (ϵ 13900); 301 (ϵ 2170) (MeOH).

Smitka, T.A. *et al., J.O.C.*, 1992, **57**, 857 (*isol, uv, ir, pmr, cmr, cd, cryst struct*)

Ambiguine E isonitrile A-234

A 89271D. Antibiotic A 89271D
[138666-16-7]



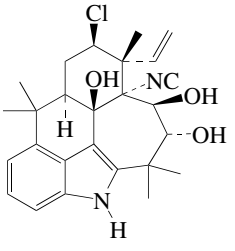
Relative Configuration

$C_{26}H_{29}ClN_2O_2$ 436.98
Alkaloid from the terrestrial blue-green algae *Fischerella ambigua*, *Hapalosiphon hibernicus* and *Westiellopsis prolifica*. Needles (hexane/CH_2Cl_2). $[\alpha]_D$ -59.7 (c, 0.1 in MeOH). Mp >300° dec. λ_{max} 223 (ϵ 36000); 272 (ϵ 7100); 279 (ϵ 6800) (MeOH).

Smitka, T.A. *et al., J.O.C.*, 1992, **57**, 857 (*isol, uv, ir, pmr, cmr, cd, struct*)

Ambiguine F isonitrile A-235

A 89271F. Antibiotic A 89271F
[138630-62-3]



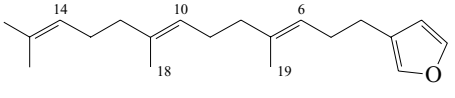
Relative Configuration

$C_{26}H_{31}ClN_2O_3$ 454.995
Alkaloid from the terrestrial blue-green alga *Fischerella ambigua*. Amorph. solid. $[\alpha]_D$ -18.2 (c, 0.1 in MeOH). λ_{max} 224 (ϵ 36000); 280 (ϵ 7200); 290 (ϵ 5500) (MeOH).

Smitka, T.A. *et al., J.O.C.*, 1992, **57**, 857 (*isol, uv, ir, pmr, cmr, cd, struct*)

Ambliofuran A-236

3-(4,8,12-Trimethyl-3,7,11-tridecatrienyl)furan, 9CI. 1,20-Epoxy-1,3(20),6,10,14-phytapentaene
[76215-29-7]



$C_{20}H_{30}O$ 286.456
Constit. of *Dysidea amblia*. Ichthyotoxin. Oil. Sol. MeOH, Et_2O; poorly sol. H_2O.

6,7,10,11,14,15-Hexahydro: 3-(4,8,12-Trimethyltridecyl)furan, 9CI. 1,20-Epoxy-1,3(20)-phytadiene. ***Phytofuran***
[54869-11-3]
$C_{20}H_{36}O$ 292.504
Constit. of Burley tobacco. Oil.

18,19-Dihydroxy: 1,20-Epoxy-1,3(20),6,10,14-phytapentaene-18,19-diol. ***Conypododiol***
[84765-52-6]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Conyza podocephala*. Gum.

12-Hydroxy: ***Furosolidagonol***
[101508-35-4]
$C_{20}H_{30}O_2$ 302.456
Isol. from *Solidago drummondi* and a *Spongia* sp. Oil. $[\alpha]_D^{24}$ -10 (c, 1 in $CHCl_3$). Isol. from *S.* sp. as a partial racemate.

12-Acetoxy: ***12-Acetoxyambliofuran***
$C_{22}H_{32}O_3$ 344.493
Constit. of a *Spongia* sp. Oil. $[\alpha]_D$ -10.2 (c, 2.8 in $CHCl_3$).

12-Oxo: ***Furosolidagonone***
[101508-36-5]
$C_{20}H_{28}O_2$ 300.44
Isol. from *Solidago drummondi*, *Solidago flexicaulis* and *Solidago racemosa*. Oil.

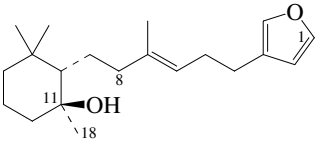
12-Oxo, 13-hydroxy: ***13-Hydroxyfurosolidagonone***
[101508-38-7]
$C_{20}H_{28}O_3$ 316.439
Isol. from *Solidago drummondi*. Oil. $[\alpha]_D^{24}$ +82 (c, 0.2 in $CHCl_3$).

*8,9*E*-Didehydro, 18-hydroxy:* ***1,20-Epoxy-1,3(20),6,8,10,14-phytahexaen-18-ol***
$C_{20}H_{28}O_2$ 300.44
Isol. from *Thorectandra choanoides*. Oil.

Dare, D.L. *et al., J.C.S. Perkin 1*, 1973, 1130
Fujimori, T. *et al., Agric. Biol. Chem.*, 1974, **38**, 2273
Demole, E. *et al., Helv. Chim. Acta*, 1978, **61**, 2318
Walker, R.P. *et al., J.O.C.*, 1981, **46**, 1098 (*Ambliofuran*)
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1693 (*Conypododiol*)
Bohlmann, F. *et al., Planta Med.*, 1985, **51**, 487 (*Furosolidagonol, Furosolidagonone, 13-Hydroxyfurosolidagonone*)
Searle, P.A. *et al., Tetrahedron*, 1994, **50**, 9893 (*12-Hydroxyambliofuran, 12-Acetoxyambliofuran*)
Urban, S. *et al., Aust. J. Chem.*, 1995, **48**, 1903 (*deriv*)

Ambliol A A-237

10,15-Cyclo-1,20-epoxy-1,3(20),6-phytatrien-11-ol
[76215-30-0]



$C_{20}H_{32}O_2$ 304.472
Constit. of *Dysidea amblia* and sponge *Oceanapia bartschi*. Ichthyotoxin, algicide. Oil. Sol. MeOH, Et_2O, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ -3.9 (c, 2.5 in $CHCl_3$). λ_{max} 213 (ϵ 7450) (MeOH) (Berdy).

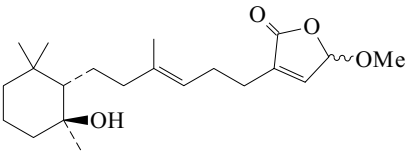
11-Deoxy, 11,18-didehydro: ***Dehydroambliol A****. 10,15-Cyclo-1,20-epoxy-1,3(20),6,11(18)-phytatetraene*
[76249-87-1]
$C_{20}H_{30}O$ 286.456
Isol. from *Dysidea*, *Chelonaplysilla* and *Dendrilla* spp. Ichthyotoxin. Oil. Sol. MeOH, Et_2O, hexane, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ -1.3 (c, 1.8 in $CHCl_3$). The name Dehydroambliol A is somewhat misleading. λ_{max} 223 (ϵ 6030) (hexane) (Berdy).

1-Bromo, 8-oxo, Ac: ***1-Bromo-8-ketoambliol A acetate****. 11-Acetoxy-1-bromo-10,15-cyclo-1,3(20),6-phytatrien-8-one*
[91178-22-2]
$C_{22}H_{31}BrO_4$ 439.388
Metab. of a *Dendrilla* sp. and a *Chelonaplysilla* sp. Oil. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{20}$ +18.2 (c, 1.2 in $CHCl_3$). λ_{max} 227 (ϵ 9000) (MeOH) (Derep).

Walker, R.P. *et al., J.O.C.*, 1981, **46**, 1098 (*isol*)
Sullivan, B. *et al., J.O.C.*, 1984, **49**, 3204 (*deriv*)
Magatti, C.V. *et al., J.O.C.*, 1991, **56**, 3102 (*synth*)
Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705 (*abs config*)
Cafieri, F. *et al., Z. Naturforsch., B*, 1992, **48**, 1408-1410 (*isol, sponge*)
Chakraborty, A. *et al., Tetrahedron*, 1997, **53**, 8513-8518 (*synth*)

Ambliolide A-238

[76215-28-6]

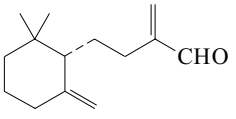


$C_{21}H_{34}O_4$ 350.497
Constit. of *Dysidea amblia*. Ichthyotoxin. Oil. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{20}$ -4 (c, 2.2 in $CHCl_3$).

Walker, R.P. *et al., J.O.C.*, 1981, **46**, 1098

Ambraaldehyde A-239

2,2-Dimethyl-α,6-bis(methylene)cyclohexanebutanal, 9CI. 4-(2,2-Dimethyl-6-methylenecyclohexyl)-2-methylenebutanal. γ-Coronal
[72905-10-3]



$C_{14}H_{22}O$ 206.327

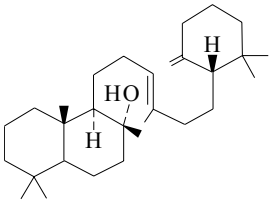
(*S*)-*form* [65716-62-3]
Isol. from sperm whale ambergris.
$[\alpha]_D$ +2.5 (c, 1.2 in $CHCl_3$).

[72892-63-8]

Ohloff, G. *et al., Helv. Chim. Acta*, 1977, **60**, 2763 (*ir, pmr, ms*)
Jegou, E. *et al., Nouv. J. Chim.*, 1977, **1**, 529 (*isol, struct, synth*)
Schulte-Elte, K.H. *et al., Nouv. J. Chim.*, 1978, **2**, 427 (*synth*)

Ambrein A-240

[473-03-0]

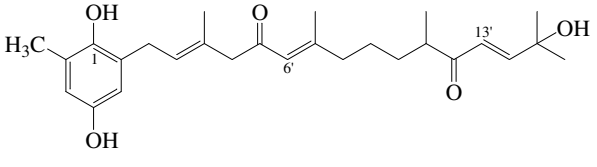


$C_{30}H_{52}O$ 428.74
Constit. of ambergris, an intestinal secretion of the sperm whale *Physeter catodon*. Coml. source of 8,12-Epoxy-13,14,15,16-tetranorlabdane, E-536. Cryst. Mp 82-83°. $[\alpha]_D$ +14.1 (c, 1 in C_6H_6). Dec. on exp. to air, forming 8,12-Epoxy-13,14,15,16-tetranorlabdane E-536.

▶ QK4240100

Oritani, T. *et al., Agric. Biol. Chem.*, 1970, **34**, 1244; 1990, **54**, 571 (*isol, synth, bibl*)
Mori, K. *et al., Annalen*, 1990, 361 (*synth*)
Tanimoto, H. *et al., Tetrahedron*, 1997, **53**, 3527 (*synth*)

Amentadione A-241



$C_{27}H_{38}O_5$ 442.594
Constit. of *Cystoseira stricta* var. *amentacea*. Oil. $[\alpha]_D$ -0.44 (c, 1.6 in EtOH).

1-Me ether:
$C_{28}H_{40}O_5$ 456.621
Constit. of *Cystoseira tamariscifolia* and *Cystoseira abies-marina*. Oil. $[\alpha]_D^{20}$ -2.4 (c, 2.4 in EtOH). λ_{max} 221 (ϵ 34560); 227 (ϵ 11000) (MeOH).

13′,14′-Dihydro, 1-Me ether: [128397-54-6]
$C_{28}H_{42}O_5$ 458.637
Constit. of *Cystoseira sauvageauana*.

13′,14′-Dihydro, 1,4-di-Me ether: [128443-58-3]
$C_{29}H_{44}O_5$ 472.664
Constit. of *Cystoseira dubia*. Oil. $[\alpha]_D^{20}$ +1.2 (c, 1 in EtOH). λ_{max} 224 (ϵ 13400); 242 (ϵ 12000); 282 (ϵ 2800) (EtOH).

6′Z-isomer, 1-Me ether:
$C_{28}H_{40}O_5$ 456.621
Constit. of *Cystoseira tamariscifolia* and *Cystoseira abies-marina*. Oil. $[\alpha]_D^{20}$ -1 (c, 3.9 in EtOH). λ_{max} 222 (ϵ 29690); 279 (ϵ 4600) (MeOH).

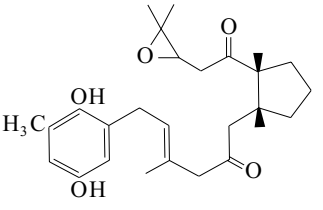
6Z-Isomer, 13′,14′-dihydro, 1-Me ether: [128397-53-5]
$C_{28}H_{42}O_5$ 458.637
Constit. of *Cystoseira sauvageauana*.

6Z-Isomer, 13′,14′-dihydro, 1,4-di-Me ether: [128443-57-2]
$C_{29}H_{44}O_5$ 472.664
Constit. of *Cystoseira dubia*. Oil. $[\alpha]_D^{20}$ +1 (c, 1 in EtOH). λ_{max} 222 (ϵ 13600); 244 (ϵ 11000); 283 (ϵ 3000) (EtOH).

Amico, V. *et al., Phytochemistry*, 1987, **26**, 1715 (*isol, pmr*)
Amico, V. *et al., Gazz. Chim. Ital.*, 1989, **119**, 467 (*isol, pmr, cmr*)
Amico, V. *et al., J. Nat. Prod.*, 1990, **53**, 517; 1991, **54**, 877 (*13′,14′-dihydro derivs*)
Basabe, P. *et al., Stud. Chem.*, 1992, **17**, 101; *CA*, **122**, 182858d (*isol, pmr, cmr*)

Amentaepoxide A-242

[110309-06-3]

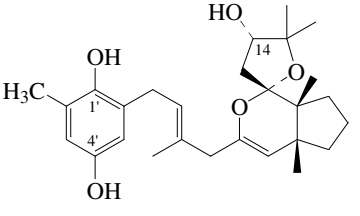


$C_{27}H_{38}O_5$ 442.594
Constit. of *Cystoseira stricta*. Oil. $[\alpha]_D^{20}$ +14.6 (c, 1.25 in EtOH).

Amico, V. *et al., Phytochemistry*, 1987, **26**, 1715

Amentol A-243

[111455-66-4]



$C_{27}H_{38}O_5$ 442.594
Constit. of brown alga *Cystoseira stricta*. Oil. $[\alpha]_D$ +7.3 (c, 1.6 in EtOH).

1′-Me ether: Amentol 1′-methyl ether
$C_{28}H_{40}O_5$ 456.621
Constit. of *Cystoseira stricta*. Oil. $[\alpha]_D^{20}$ +2.4 (c, 5.7 in EtOH).

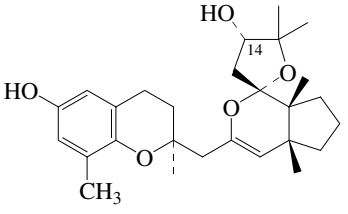
14-Epimer: ***14-Epiamentol***
[676339-99-4]
$C_{27}H_{38}O_5$ 442.594

Constit. of a *Cystoseira* sp. Oil (as tri-Ac). $[\alpha]_D^{25}$ -15.2 (c, 0.023 in $CHCl_3$) (tri-Ac). CAS no. refers to tri-Ac. λ_{max} 208 (log ε 4.08); 285 (log ε 3.4) (MeOH) (tri-Ac).

Amico, V. *et al., Tetrahedron*, 1986, **42**, 6015-6020 (*Amentol, 1′-Me ether*)
Navarro, G. *et al., J. Nat. Prod.*, 2004, **67**, 495-499 (*14-Epiamentol*)

Amentolchromane A-244

[676339-96-1]

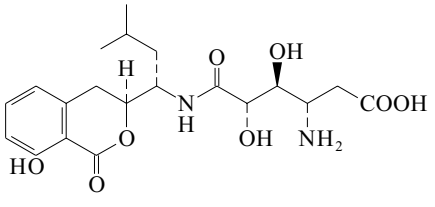


$C_{27}H_{38}O_5$ 442.594
Constit. of a *Cystoseira* sp. Oil (as di-Ac). $[\alpha]_D^{25}$ +6 (c, 0.19 in $CHCl_3$) (di-Ac). CAS no. refers to di-Ac. λ_{max} 220 (log ε 3.97); 280 (log ε 3.36) (MeOH) (as di-Ac).

14-Me ether: ***14-O-Methylamentolchromane****. 14-Methoxyamentolchromane (incorr.)*
[676340-00-4]
$C_{28}H_{40}O_5$ 456.621
Constit. of a *Cystoseira* sp. Oil. $[\alpha]_D^{25}$ +17.6 (c, 0.015 in $CHCl_3$).
Navarro, G. *et al., J. Nat. Prod.*, 2004, **67**, 495-499 (*isol, pmr, cmr*)

Amicoumacin B A-245

AI 77B. BN 103B. Antibiotic AI 77B. Antibiotic BN 103B
[82768-33-0]



$C_{20}H_{28}N_2O_8$ 424.45
Prod. by *Bacillus pumilus*, incl. strains associated with marine sponges *Dendrilla* sp. Also prod. by marine-derived *Alternaria tenuis* Sg17-1. Shows weak antibacterial activity and antiulcer props. Cryst. + H_2O. Mp 137-145° dec. $[\alpha]_D^{23}$ -106.1 (c, 0.5 in MeOH). λ_{max} 213; 247; 315 (MeOH).

Amide: ***Amicoumacin A***
[78654-44-1]
$C_{20}H_{29}N_3O_7$ 423.465
Prod. by *Bacillus pumilus*. Shows antibacterial, antiinflammatory and antiulcer props. Acts as an acaricide. Powder (as hydrochloride). Sol. H_2O, EtOH, Py, MeOH; fairly sol. Me_2CO; poorly sol. C_6H_6, hexane, $CHCl_3$, EtOAc.
Mp 132-135° dec. (hydrochloride). $[\alpha]_D^{23}$ -97.2 (c, 1.0 in MeOH) (hydrochloride). λ_{max} 298; 348 (0.1*N* NaOH) (Derep). λ_{max} 216 (ε 29000); 245 (ε 6050); 314 (ε 4900) (MeOH) (Derep). λ_{max} 208; 247; 315 (MeOH). λ_{max} 208 (ε 27300); 247 (ε 6400); 315 (ε 4380) (MeOH) (Berdy). λ_{max} 247 (E1%/1cm 140); 313 (E1%/1cm 85) (HCl) (Berdy). λ_{max} 245 (E1%/1cm 296); 296 (E1%/1cm 52); 345 (E1%/1cm 106) (NaOH) (Berdy).
▶ LD_{50} (mus, ivn) 25-75 mg/kg; LD_{50} (mus, orl) 132 mg/kg.
AU7802000

Amide, N-*Ac:* [78654-45-2]
Cryst. ($CHCl_3$). Mp 178-181°. $[\alpha]_D^{23}$ -79.8 (c, 0.5 in MeOH).

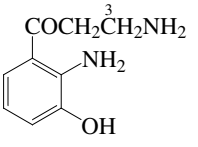
Amide, N,O,O,O-*tetra-Ac:* [78468-39-0]
Cryst. (Me_2CO). Mp 227-229°. $[\alpha]_D^{23}$ -79 (c, 0.5 in MeOH).

[77674-99-8]

Netherlands Pat., 1980, 80 3 985; *CA*, **95**, 78461 (*isol*)
Itoh, J. *et al., Agric. Biol. Chem.*, 1982, **46**, 1255; 2659 (*struct, spectra*)
Shimojima, Y. *et al., J. Med. Chem.*, 1983, **26**, 1370
Japan. Pat., 1983, 83 18 379; *CA*, **99**, 20906
Japan. Pat., 1983, 83 216 107; *CA*, **100**, 116494 (*props*)
Shojima, Y. *et al., Tetrahedron*, 1984, **40**, 2519 (*struct, config*)
Afiyatullov, S.S. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1991, **27**, 765-766 (*isol, sponge*)
Hamada, Y. *et al., Tetrahedron*, 1991, **47**, 8635 (*synth*)
Ward, R.A. *et al., Tet. Lett.*, 1992, **33**, 3359 (*synth*)
Durgnat, J.-M. *et al., Helv. Chim. Acta*, 1993, **76**, 222 (*synth*)
Ward, R.A. *et al., Tetrahedron*, 1995, **51**, 12301 (*synth, pmr*)
Broady, S.D. *et al., J.C.S. Perkin 1*, 1999, 1083-1094 (*synth*)
Kotsuki, H. *et al., Org. Lett.*, 1999, **1**, 499-502 (*synth*)
Ghosh, A.K. *et al., Org. Lett.*, 2001, **3**, 2677-2680 (*synth*)
Huang, Y.-F. *et al., J. Antibiot.*, 2006, **59**, 355-357 (*Alternaria, marine isol*)

3-Amino-1-(2-amino-3-hydroxyphenyl)-1-propanone A-246

2′,3-Diamino-3′-hydroxypropiophenone. 2-Amino-3-(3-aminopropanoyl)phenol. 3-Hydroxykynuramine

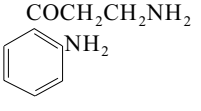


$C_9H_{12}N_2O_2$ 180.206

N^3-Ac: ***Erebusinone****. Eribusinone*
[325477-44-9]
[194615-13-9]
$C_{11}H_{14}N_2O_3$ 222.243
Isol. from the sponge *Isodictya erinacea*. Yellow solid. λ_{max} 238 (ε 1240); 372 (ε 180) (MeOH).
Moon, B. *et al., Tetrahedron*, 2000, **56**, 9057-9062 (*Erebusinone*)

3-Amino-1-(2-aminophenyl)-1-propanone, 9CI A-247

2′,3-Diaminopropiophenone. ***Kynuramine***
[363-36-0]



$C_9H_{12}N_2O$ 164.207
Found in rat brains, and derived from tryptophan. Liq.

Hydrochloride: Mp 185-187° dec.

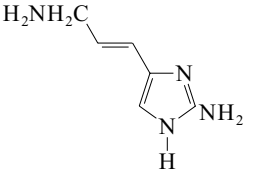
Picrate: Mp 176-177° dec.

N^3-Ac: ***N^3-Acetylkynuramine***
$C_{11}H_{14}N_2O_2$ 206.244
Prod. by the marine-derived *Janibacter limosus* Hel 1. Light yellow oil. λ_{max} 202 (log ε 4.21); 227 (log ε 4.31); 362 (log ε 3.61) (MeOH). λ_{max} 208 (log ε 4.3); 227 (log ε 4.31); 255 (log ε 3.77); 360 (log ε 3.68) (MeOH/NaOH).

Butenandt, A. *et al., Z. Naturforsch., B*, 1953, **86**, 454 (*synth, pharmacol*)
Seiler, N. *et al., CA*, 1971, **74**, 39005 (*ms*)
Gal, E.M. *et al., J. Neurochem.*, 1978, **30**, 607 (*occur*)
Asolkar, R.N. *et al., J. Antibiot.*, 2004, **57**, 17-23 (*N^3-Acetylkynuramine*)

2-Amino-4-(3-amino-1-propenyl)-1*H*-imidazole A-248

*4-(3-Amino-1-propenyl)-1*H*-imidazol-2-amine, 9CI. 3-(2-Amino-1*H*-imidazol-4-yl)-2-propen-1-amine. 3-Amino-1-(2-aminoimidazolyl)-1-propene*



$C_6H_{10}N_4$ 138.172

(E)-form [140381-65-3]

Alkaloid from the marine sponges *Ptilocaulis walpersi* and *Teichaxinella morchella*.

Light brown oil. λ_{max} 276 (ϵ 8790) (MeOH) (Derep).

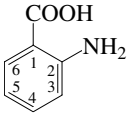
Wright, A.E. *et al., J. Nat. Prod.*, 1991, **54**, 1684 (*isol, uv, pmr, cmr, struct*)

2-Aminobenzoic acid, 9CI A-249

Anthranilic acid, 8CI. Vitamin L_1

[118-92-3]

[1321-11-5]



$C_7H_7NO_2$ 137.138

Prod. by bacteria and fungi. An important intermed. in the synth. of many compds., corrosion inhibitor for metals. Used as 3% aq. soln. of Na salt for gravimetric detn. of Co, Ni, Cu(*II*), Hg(*II*), Mn, Pb, Cd, U(*VI*), Zn. Inducer of fruiting body formation. Leaflets. Sol. hot H_2O, EtOH, Et_2O.

Mp 144-148°. pK_{a1} 1.97; pK_{a2} 4.79 (25°). pK_{a1} 2.17; pK_{a2} 4.85 (25°, 0.1*M* KCl). Sublimes, triboluminescent. λ_{max} 218 (ϵ 20200); 248 (ϵ 7000); 335 (ϵ 4700) (MeOH) (Berdy).

▶ LD_{50} (mus, orl) 1400 mg/kg. Exp. reprod. effects. CB2450000

Amide: 2-Aminobenzamide. Anthranilamide

[88-68-6]

$C_7H_8N_2O$ 136.153

Prod. by a marine *Cytophaga marinoflava* sp. AM13.1. Acetaldehyde scavenger for polyethylene beverage bottles. Fluorescent label for polysaccharides etc. Leaflets.

Mp 109-111.5° dec.

▶ CU8993000

N-*[3-(Methoxycarbonyl)propanoyl], Me ester:*

$C_{13}H_{15}NO_5$ 265.265

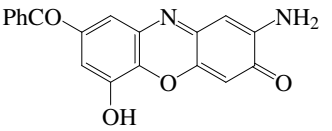
Constit. of the alga *Jolyna laminarioides*. Chymotrypsin inhibitor. Amorph. powder.

Mp 50°. λ_{max} 222; 251; 307 (MeOH).

[552-37-4, 99196-74-4, 99196-75-5, 99197-00-9, 117808-63-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 189A; 301D; 302A; 368D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1066B; 1262B; 1262C; 1390C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1371A; 1371B (*ir*)
Smith, P.A.S. *et al., J.A.C.S.*, 1954, **76**, 431 (*synth*)
Forbes, W.F. *et al., Can. J. Chem.*, 1958, **36**, 1371 (*uv*)
Evans, H.B. *et al., J. Phys. Chem.*, 1968, **72**, 2552 (*pmr*)
Dhaneshwar, N.N. *et al., Acta Cryst. B*, 1972, **28**, 647 (*cryst struct*)
Errede, L.A. *et al., J.O.C.*, 1976, **41**, 1763 (*synth*)
Boone, C.D.G. *et al., Acta Cryst. B*, 1977, **33**, 3205 (*cryst struct*)
Kashino, S. *et al., Acta Cryst. C*, 1991, **47**, 2236 (*cryst struct, amide*)
Atta-ur-Rahman, *et al., Phytochemistry*, 1997, **46**, 1215-1218 (*Jolyna ester*)
Osvath, R. *et al., Food Chem. News*, 2001, **43(26)**, 30 (*amide, use*)
Shaaban, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, API500; EGM000; APJ250

2-Amino-8-benzoyl-6-hydroxy-3*H*-phenoxazin-3-one A-250



$C_{19}H_{12}N_2O_4$ 332.315

Prod. by marine bacterium *Halomonas* sp. GWS-BW-H8hM. Moderately cytotoxic. Red solid. λ_{max} 257 (log ϵ 3.81); 309 (log ϵ 3.59); 432 (log ϵ 3.46) (MeOH). λ_{max} 254 (log ϵ 3.73); 305 (log ϵ 3.53); 454 (log ϵ 3.57) (MeOH/HCl). λ_{max} 243 (log ϵ 3.89); 438 (log ϵ 3.67) (MeOH/NaOH).

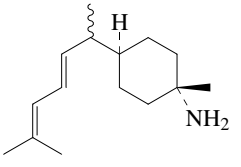
*4′-Hydroxy: 2-Amino-6-hydroxy-8-(4-hydroxybenzoyl)-3*H*-phenoxazin-3-one*

$C_{19}H_{12}N_2O_5$ 348.314

Prod. by *Halomonas* sp. GWS-BW-H8hM. Red solid. λ_{max} 266 (log ϵ 3.54); 300 (log ϵ 3.52); 428 (log ϵ 3.44); 434 (log ϵ 3.45) (MeOH). λ_{max} 249 (log ϵ 3.62); 304 (log ϵ 3.58); 465 (log ϵ 3.35) (MeOH/HCl). λ_{max} 239 (log ϵ 3.61); 346 (log ϵ 3.56); 445 (log ϵ 3.49) (MeOH/NaOH).

Bitzer, J. *et al., J. Antibiot.*, 2006, **59**, 86-92 (*isol, uv, pmr, cmr, ms*)

3-Amino-8,10-bisaboladiene A-251



$C_{15}H_{27}N$ 221.385

(3α,6β,7ξ,8E)-form

N-*Formyl:* ***3-Formamido-8,10-bisaboladiene***

[134781-22-9]

$C_{16}H_{27}NO$ 249.395

Isol. from the sponge *Halichondria* cf. *lendenfeldi*. Dec. on isol.

Isocyanide: ***3-Isocyano-8,10-bisaboladiene***

[134781-21-8]

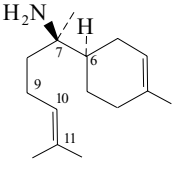
$C_{16}H_{25}N$ 231.38

Isol. from the sponge *Halichondria* cf. *lendenfeldi* and the mollusc *Phyllidia pustulosa*. Oil. $[\alpha]_D$ -5.6 (c, 0.2 in $CHCl_3$). Has -NC replacing NH_2. λ_{max} 230 (sh) (ϵ 14000); 237 (ϵ 15300); 246 (sh) (ϵ 11100) (no solvent reported).

Kassühlke, K.E. *et al., J.O.C.*, 1991, **56**, 3747-3750 (*isol, pmr, cmr*)

7-Amino-2,10-bisaboladiene A-252

7-Amino-7,8-dihydro-α-bisabolene. 7-Aminobisabolene



(6*R*,7*R*)–*form*

$C_{15}H_{27}N$ 221.385

(6R,7R)-form [105281-34-3]

Constit. of *Ciocalypta* sp.

Oil. $[\alpha]_D$ -15 (c, 0.4 in MeOH).

Hydrochloride: [105281-33-2]

Yellow oil. $[\alpha]_D^{23}$ -8.3 (c, 0.5 in MeOH).

(6R,7S)-form [105281-43-4]

Constit. of a *Halichondria* sp. and a sponge *Theonella* sp.

Oil. $[\alpha]_D$ +39 (MeOH). $[\alpha]_D^{20}$ +59.9 (c, 3 in $CHCl_3$).

Δ^9-Isomer, 11-hydroxy: 7-Amino-2,9-bisaboladien-11-ol. ***Aminobisabolenol***
[108384-61-8]
$C_{15}H_{27}NO$ 237.384
Constit. of *Theonella* sp. Oil. Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +29 (MeOH).

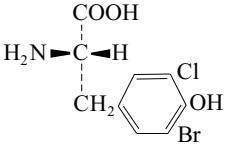
*Δ^{11}-Isomer, 10*R*-hydroxy: 7-Amino-2,11-bisaboladien-10*R*-ol.* ***Isoaminobisabolenol b***
[108384-62-9]
$C_{15}H_{27}NO$ 237.384
Constit. of *Theonella* sp. Oil. Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +40 (MeOH).

*Δ^{11}-Isomer, 10*S*-hydroxy: 7-Amino-2,11-bisaboladien-10*S*-ol.* ***Isoaminobisabolenol a***
[108449-15-6]
$C_{15}H_{27}NO$ 237.384
Constit. of *Theonella* sp. Oil. Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +34 (MeOH).

Sullivan, B.W. *et al., J.O.C.*, 1986, **51**, 5134-5136 (*Halichondria constits*)
Gulavita, N.K. *et al., J.O.C.*, 1986, **51**, 5136-5139 (*Ciocalypta constit*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1987, **35**, 928 (*Theonella constits, cryst struct*)

2-Amino-3-(3-bromo-5-chloro-4-hydroxyphenyl)-propanoic acid A-253

3-Bromo-5-chlorotyrosine, 9CI. 3-Chloro-5-bromotyrosine



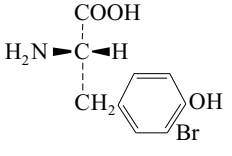
$C_9H_9BrClNO_3$ 294.532

(S)-form
L-form
Isol. from the operculum of *Buccinum undatum* and cuticle of *Limulus polyphemus.*

Hunt, S. *et al., Biochim. Biophys. Acta*, 1971, **252**, 401 (*isol*)
Welinder, B.S. *et al., Biochim. Biophys. Acta*, 1972, **279**, 491 (*isol, synth, ms*)

2-Amino-3-(3-bromo-4-hydroxyphenyl)propanoic acid A-254

3-Bromotyrosine. Monobromotyrosine



$C_9H_{10}BrNO_3$ 260.087

(S)-form
L-form
[38739-13-8]
Isol. from gorgonians and molluscs, may occur in blood serum.

N,N,N-*Tri-Me, betaine:* [153343-24-9]
[165329-91-9]
$C_{12}H_{16}BrNO_3$ 302.167
Isol. from *Pseudoceratina crassa*. Sol. H_2O, MeOH. $[\alpha]_D^{25}$ -15 (MeOH). λ_{max} 287 (ϵ 1260) (H_2O). λ_{max} 287 (ϵ 1275) (H_2O) (Berdy). λ_{max} 307 (ϵ 1994) (pH 10 buffer) (Berdy).

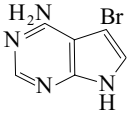
4-Me ether, N,N,N-*tri-Me, betaine:* [153343-23-8]
[165329-90-8]
$C_{13}H_{18}BrNO_3$ 316.194
Isol. from *Pseudoceratina crassa*. Sol. H_2O, MeOH. $[\alpha]_D$ -9 (MeOH). λ_{max} 277 (ϵ 1260) (H_2O). λ_{max} 277 (ϵ 1260) (H_2O) (Berdy).

(±)-form [54788-30-6]
Mp 245-246°.

Johnson, T.B. *et al., J.A.C.S.*, 1912, **34**, 1061 (*synth*)
Welinder, B.S. *et al., Biochim. Biophys. Acta*, 1972, **279**, 491 (*isol, ms, synth*)
Firnau, G. *et al., Bioinorg. Chem.*, 1973, **2**, 167; *CA*, **79**, 124178q
McCord, T.J. *et al., J. Med. Chem.*, 1975, **18**, 26 (*synth*)
Albrizio, S. *et al., Tetrahedron*, 1994, **50**, 783-788 (*isol, betaines*)
Gao, H. *et al., Tetrahedron*, 1999, **55**, 9717-9726 (*abs config*)

4-Amino-5-bromopyrrolo[2,3-*d*]pyrimidine A-255

*5-Bromo-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-amine, 9CI*
[22276-99-9]



$C_6H_5BrN_4$ 213.036
Isol. from a sponge *Echinodictyum* sp. Bronchodilator and hypotensive agent. Adenosine kinase inhibitor. Needles (EtOH aq.). Mp 240-241° (238-239°) dec. λ_{max} 232 (ϵ 16600); 282 (ϵ 8710) (pH 1) (Derep). λ_{max} 225 (ϵ 14800); 279 (ϵ 8910) (pH 11) (Derep).

Gerster, J.F. *et al., J. Het. Chem.*, 1969, **6**, 207-213 (*synth, uv*)
Kazlauskas, R. *et al., Aust. J. Chem.*, 1983, **36**, 165-170 (*isol, uv, pmr, cmr, ms*)

(4-Aminobutyl)guanidine, 9CI A-256

4-Guanidinobutylamine. 1-Amino-4-guanidinobutane. ***Agmatine***
[306-60-5]
$HN{=}^6C(NH_2)NH(CH_2)_3CH_2NH_2$
$C_5H_{14}N_4$ 130.192
Present in ergot, pollen of *Ambrosia artemisiifolia* (Compositae), the sea anemone *Anthopleura japonica* and herring semen. Metabolic intermediate for polyamines. Synth. in mammalian brain. Endogenous neurotransmitter. Inhibits hyperalgesia and tolerance to morphine. NMDA receptor antagonist and nitric oxide synthase inhibitor.
Mp 101.5-103°.

Sulfate: [2482-00-0]
Cryst. Mp 229° (224-225°).

N^1*-(4-Hydroxy-*E*-cinnamoyl):* **N^1-trans-p-*Coumaroylagmatine***
[47096-24-2]
[7295-86-5]
$C_{14}H_{20}N_4O_2$ 276.338
Alkaloid from barley seedlings, *Hordeum bulbosum, Hordeum distichon, Hordeum jubatum, Hordeum murinum* and *Hordeum spontaneum* (Gramineae). Exhibits weak antifungal activity. Sol. H_2O.
Mp 215-217° (as picrate). λ_{max} 229 (ϵ 33100); 300 (ϵ 26300) (H_2O) (Berdy).

N^1*-(4-Hydroxy-Z-cinnamoyl):* **N^1-cis-p-*Coumaroylagmatine***
[191330-81-1]
$C_{14}H_{20}N_4O_2$ 276.338
Constit. of *Albizzia julibrissin*. Leaf-opening factor. Syrup or powder. λ_{max} 278 (ϵ 2000) (H_2O).

N^1*-(4-Hydroxy-3-methoxy-*E*-cinnamoyl):* **N^1-trans-*Feruloylagmatine***
[188305-06-8]
$C_{15}H_{22}N_4O_3$ 306.364
Isol. from *Triticum aestivum* (wheat) exposed to low temps. Antifungal agent.

N^1*-(3,4-Dimethoxycinnamoyl):* **N^1-*(3,4-Dimethoxycinnamoyl)agmatine***
[128009-18-7]
[146072-40-4]
$C_{16}H_{24}N_4O_3$ 320.391
Alkaloid from *Verbesina caracasana.*

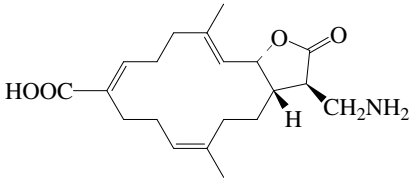
N^6*-Me:* N-*(4-Aminobutyl)*-N′-*methylguanidine.* **N^6-*Methylagmatine***
[77414-15-4]
$C_6H_{16}N_4$ 144.219
Constit. of *Glycine max* and *Medicago sativa.*

N^6-*(3-Methyl-2-butenyl):* N-*(4-Aminobutyl)*-N′-*prenylguanidine.* ***N^6-(3-Methyl-2-butenyl)agmatine.*** N^6-*Prenylagmatine*
[128009-17-6]
$C_{10}H_{22}N_4$ 198.311
Alkaloid from *Verbesina caracasana*. Antihypertensive.

N^6-*(3-Methyl-2-butenyl),* N^1-*(3,4-dimethoxycinnamoyl):* See Caracasanamide in *The Combined Chemical Dictionary.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 821B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1330A (*nmr*)
Kossel, A. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1910, **66**, 257; **68**, 170 (*isol, struct, synth*)
Heyl, F.W. *et al., J.A.C.S.*, 1919, **41**, 681 (*isol*)
Stoessl, A. *et al., Phytochemistry*, 1965, **4**, 973 (*isol, uv, struct, synth, N-coumaroyl*)
Boldt, A. *et al., Phytochemistry*, 1971, **10**, 731 (*biosynth*)
Smith, T.A. *et al., Phytochemistry*, 1978, **17**, 1093 (*occur, N-coumaroyl*)
Kowabata, T. *et al., CA*, 1979, **89**, 178349 (*isol*)
Bird, C.R. *et al., Phytochemistry*, 1981, **20**, 2345 (*biosynth, N-coumaroyl*)
Chandrasekhar, K. *et al., Acta Cryst. B*, 1982, **38**, 2538 (*cryst struct*)
Cho, Y.B. *et al., Anal. Biochem.*, 1987, **160**, 429 (N^6-*Methylagmatine*)
Matsuzaki, S. *et al., Phytochemistry*, 1990, **29**, 1313 (N^6-*Methylagmatine*)
Mitchinson, A. *et al., Chem. Comm.*, 1994, 2613 (*synth*)
Ueda, M. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 2133-2137 (*Z-coumaroyl*)
Reis, D.J. *et al., Ann. N.Y. Acad. Sci.*, 1999, **881**, 65-80 (*rev, activity*)
Monache, G.D. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 3249-3254 (*Prenylagmatine, Dimethoxycinnamoylagmatine*)
Jin, S. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1614-1617 (*Feruloylagmatine*)
Fairbanks, C.A. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2000, **97**, 10584-10589 (*pharmacol*)
Reis, D.J. *et al., Trends Pharmacol. Sci.*, 2000, **21**, 187-193 (*pharmacol, rev*)
Demady, D.R. *et al., Mol. Pharmacol.*, 2001, **59**, 24-29 (*pharmacol*)

17-Amino-3,7,11-cembratrien-16,2-olid-19-oic acid A-257

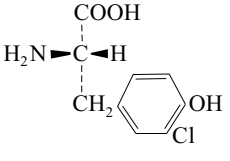


$C_{20}H_{29}NO_4$ 347.453

(1*S*,2*S*,3*E*,7*E*,11*E*,15*R*)-*form*
N,N-*Di-Me: 17-Dimethylaminolobohedleolide (incorr.)*
[267007-12-5]
$C_{22}H_{33}NO_4$ 375.507
Constit. of a *Lobophytum* sp. Shows moderate anti-HIV activity. Gum. $[\alpha]_D$ +13.1 (c, 0.25 in $CHCl_3$). λ_{max} 218 (log ϵ 3.6); 222 (log ϵ 3.56) (EtOH).
Rashid, M.A. *et al., J. Nat. Prod.*, 2000, **63**, 531-533 (*isol, pmr, cmr*)

2-Amino-3-(3-chloro-4-hydroxyphenyl)propanoic acid A-258

3-Chlorotyrosine. Monochlorotyrosine
[7298-90-0]



$C_9H_{10}ClNO_3$ 215.636
Isol. from hydrolysates of mollusc scleroproteins and insect cuticle.

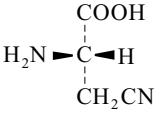
(*R*)-*form*
D-*form*
Mp 255-256° dec. $[\alpha]_D^{20}$ +26 (c, 0.9 in H_2O). $[\alpha]_D$ -12 (c, 3.05 in MeOH).

N-*(3-Methoxycarbonyl-2*E*-propenoyl):* ***Xylariamide A***
$C_{14}H_{14}ClNO_6$ 327.72
Isol. from *Xylaria* sp. (FRR 5657). Pale yellow gum. $[\alpha]_D^{24}$ -22 (c, 0.06 in MeOH). λ_{max} 202 (log ϵ 4.05); 217 (sh) (log ϵ 3.74); 278 (log ϵ 3.12) (MeOH).

(*S*)-*form*
L-*form*
$[\alpha]_D^{20}$ -26.2.
Dibbo, A. *et al., J.C.S.*, 1961, 2645 (*synth*)
Welinder, B.S. *et al., Biochim. Biophys. Acta*, 1972, **279**, 491 (*isol, ms*)
Hunt, S. *et al., FEBS Lett.*, 1972, **24**, 109 (*isol*)
Patel, V.F. *et al., J. Med. Chem.*, 1999, **42**, 2588-2603 (*synth, pmr, cmr*)
Davis, R.A. *et al., J. Nat. Prod.*, 2005, **68**, 769-772 (*Xylariamide A*)
Davis, R.A. *et al., Tet. Lett.*, 2005, **46**, 5199-5201 (*Xylariamide A, synth*)

2-Amino-3-cyanopropanoic acid A-259

3-Cyanoalanine, 9CI. β-Cyano-α-alanine. Aminosuccinic acid 4-mononitrile
[923-01-3]

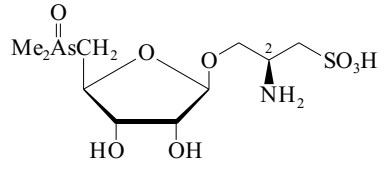


$C_4H_6N_2O_2$ 114.104
► AY4520000

(*S*)-*form*
L-*form*
[6232-19-5]
Isol. from seeds of *Vicia* spp., from *Lotus tenuis* and *Clitocybe acromelalga*. Prod. by *Vibrio* sp. C-979. Shows algicidal props. Active against cyanobacteria. Neurotoxin. Rectangular needles (dioxan aq.).
Mp 218-218.5°. $[\alpha]_D^{26}$ -2.9 (c, 1.4 in H_2O).
N-*Benzyloxycarbonyl:* [3309-41-9]
$C_{12}H_{12}N_2O_4$ 248.238
Mp 136°. $[\alpha]_D^{23}$ -46 (c, 0.47 in DMF).

(±)-*form*
Dendritic aggregates. Mp 213°.
N-*Ac, Me ester:* [204767-38-4]
$C_7H_{10}N_2O_3$ 170.168
Mp 72-75°.
N-*Benzoyl, Me ester:* [180311-33-5]
$C_{12}H_{12}N_2O_3$ 232.238
Cryst. (EtOAc/MeOH).
Mp 135-138°.
Bell, G.A. *et al., Biochem. J.*, 1965, **97**, 104-111 (*occur*)
Fowden, L. *et al., Nature (London)*, 1965, **208**, 1206-1207 (*biosynth*)
Floss, H.G. *et al., Nature (London)*, 1965, **208**, 1207-1208 (*biosynth*)
Liberek, B. *et al., Tetrahedron*, 1966, **22**, 2303-2306 (*synth*)
Ressler, C. *et al., J.O.C.*, 1971, **36**, 3960-3966 (*synth*)
Arnold, L.D. *et al., J.A.C.S.*, 1988, **110**, 2237-2241 (*synth, ir, pmr, ms*)
Pizzioli, L. *et al., Helv. Chim. Acta*, 1998, **81**, 231-235 (*acyl derivs, synth, pmr*)
Japan. Pat., 1999, 99 71 203; *CA*, **130**, 206271a (*activity, isol*)
Yoshikawa, K. *et al., Appl. Environ. Microbiol.*, 2000, **66**, 718-722 (*isol, activity*)

2-Amino-3-[[5-deoxy-5-(dimethylarsinoyl)ribofuranosyl]oxy]-1-propanesulfonic acid A-260



$C_{10}H_{22}AsNO_8S$ 391.273

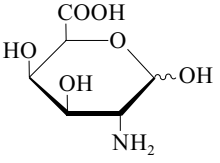
(2*S*)-β-D-*form* [138382-72-6]
Constit. of the seaweeds *Hizikia fusiforme, Sargassum lacerifolium* and *Sphaerotrichia divaricata*.

[109028-17-3]

Edmonds, J.S. *et al., J.C.S. Perkin 1*, 1987, 577-580 (*isol, pmr*)
Jin, K. *et al., Agric. Biol. Chem.*, 1988, **52**, 1965-1971 (*isol*)
Francesconi, K.A. *et al., J.C.S. Perkin 1*, 1991, 2707-2716 (*isol, pmr, cryst struct*)

2-Amino-2-deoxygalacturonic acid A-261

Galactosaminuronic acid



D–Pyranose–*form*

$C_6H_{11}NO_6$ 193.156

D-*form* [14307-17-6]
Prod. of hydrol. of Vi antigen from *Escherichia coli*. Amine component of the lipopolysaccharide of *Pseudomonas aeruginosa* NCTC 8505.
Mp 160° (blackens). $[\alpha]_D^{20}$ +84.5 (c, 1.0 in HCl, pH2).

N-*Formyl: 2-Deoxy-2-formamido-D-galacturonic acid*
[93772-80-6]
$C_7H_{11}NO_7$ 221.166
Component of *Pseudomonas aeruginosa* type 1 lipopolysaccharide.

N-*Ac: 2-Acetamido-2-deoxy-D-galacturonic acid*
$C_8H_{13}NO_7$ 235.193
Component of *Acinetobacter bowmannii*, *Pseudomonas fluorescens* and the marine *Pseudoalteromonas distincta* polysaccharides. Amorph. powder. $[\alpha]_D^{22}$ +29 (c, 1.4 in H_2O). Stored as Na salt.

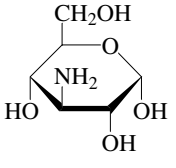
N-*Ac, amide: 2-Acetamido-2-deoxy-D-galacturonamide*
[93790-40-0]
$C_8H_{14}N_2O_6$ 234.208
Component of *Pseudomonas aeruginosa* type 1 lipopolysaccharide.

L-*form*
N-*Ac: 2-Acetamido-2-deoxy-L-galacturonic acid*
[82838-35-5]
$C_8H_{13}NO_7$ 235.193
Component of the O-specific polysaccharide chains of the two serotypes of *Pseudomonas aeruginosa*.

Heyns, K. *et al., Chem. Ber.*, 1957, **90**, 2443; 1959, **92**, 2435 (*isol, synth, D-form*)
Brownlee, S.T. *et al., Anal. Biochem.*, 1966, **14**, 414 (*anal*)
Wilkinson, S.G. *et al., Biochem. J.*, 1977, **161**, 103 (*occur*)
Dimitriev, B.A. *et al., Bioorg. Khim.*, 1979, **5**, 77 (*occur*)
Darakas, E. *et al., Carbohydr. Res.*, 1982, **103**, 176 (*synth, N-Ac*)
Knirel, Y.A. *et al., Carbohydr. Res.*, 1984, **133**, C12 (*occur, synth, derivs*)
Haseley, S.R. *et al., Eur. J. Biochem.*, 1996, **237**, 229 (*occur, N-Ac*)
Shashkov, A.S. *et al., Carbohydr. Res.*, 1998, **306**, 297-303 (*occur, N-Ac*)
Muldoon, J. *et al., Carbohydr. Res.*, 2001, **330**, 231-239 (*occur, N-Ac*)

3-Amino-3-deoxyglucose, 9CI, 8CI A-262

Kanosamine



α-D-Pyranose-*form*

$C_6H_{13}NO_5$ 179.172

D-*form* [576-44-3]
Isol. from the antibiotic Kanamycin. Occurs as the free sugar in fermentation broths of *Bacillus aminoglucosidicus*, a deep-sea strain of *Bacillus* sp. and *Streptomyces lansus*. Has bactericidal props. The only amino sugar antibiotic.

Hydrochloride:
Hygroscopic solid. Mp 132-137° Mp 150° dec. approx. $[\alpha]_D^{20}$ +47 (c, 1.0 in H_2O).

α-D-Pyranose-*form*

*Me glycoside, 4,6-*O*-benzylidene: Methyl 3-amino-4,6-*O*-benzylidene-3-deoxy-α-D-glucopyranoside*
[4603-89-8]
$C_{14}H_{19}NO_5$ 281.308
Cryst. (petrol/EtOH). Subl. 186. $[\alpha]_D^{22}$ +102 (c, 1.02 in $CHCl_3$).

*Me glycoside, 4,6-*O*-benzylidene,* N*-Ac: Methyl 3-acetamido-4,6-*O*-benzylidene-3-deoxy-α-D-glucopyranoside*
$C_{16}H_{21}NO_6$ 323.345
Cryst. (EtOH). Mp 283-286° dec.

*Me glycoside, 4,6-*O*-ethylidene,* N*-Ac: Methyl 3-acetamido-3-deoxy-4,6-*O*-ethylidene-α-D-glucopyranoside*
$C_{11}H_{19}NO_6$ 261.274
Cryst. (MeOH). Subl. 320.

Me glycoside, N*,2,4,6-tetra-Ac: Methyl 3-acetamido-2,4,6-tri-*O*-acetyl-3-deoxy-α-D-glucopyranoside*
[2595-38-2]
$C_{15}H_{23}NO_9$ 361.348
Cryst. (EtOH). Mp 182-184°. $[\alpha]_D^{20}$ +109 (c, 1.1 in $CHCl_3$).

β-D-Pyranose-*form*

N-*Ac: 3-Acetamido-3-deoxy-β-D-glucopyranose*
$C_8H_{15}NO_6$ 221.21
Needles (EtOH aq.). Mp 204-205° dec. $[\alpha]_D$ +37 (5 min.) → +50 (equilib.) (c, 2.5 in H_2O).

Me glycoside: Methyl 3-amino-3-deoxy-β-D-glucopyranoside
[14133-36-9]
$C_7H_{15}NO_5$ 193.199
Cryst. (EtOH). Mp 205-207° (201-202°). $[\alpha]_D^{20}$ -38 (c, 2 in H_2O).

Me glycoside, N*-Ac: Methyl 3-acetamido-3-deoxy-β-D-glucopyranoside*
$C_9H_{17}NO_6$ 235.236
Mp 214-215°. $[\alpha]_D$ -21 (H_2O).

*Me glycoside, 4,6-*O*-benzylidene,* N*-Ac: Methyl 3-acetamido-4,6-*O*-benzylidene-3-deoxy-β-D-glucopyranoside*
$C_{16}H_{21}NO_6$ 323.345
Subl. 277-278. $[\alpha]_D^{23}$ -80.8 (c, 0.5 in DMF).

*Me glycoside, 4,6-*O*-benzylidene,* N*,2-di-Ac: Methyl 3-acetamido-2-*O*-acetyl-4,6-*O*-benzylidene-3-deoxy-β-D-glucopyranoside*
$C_{18}H_{23}NO_7$ 365.382
Subl. 276. $[\alpha]_D^{21}$ -96.2 (c, 1.0 in $CHCl_3$).

Me glycoside, N*,2,4,6-tetra-Ac: Methyl 3-acetamido-2,4,6-tri-*O*-acetyl-3-deoxy-β-D-glucopyranoside*
[4338-42-5]
$C_{15}H_{23}NO_9$ 361.348
Cryst. (C_6H_6/petrol). Mp 156°. $[\alpha]_D^{22}$ -21.4 (c, 2.5 in $CHCl_3$).

α-D-Furanose-*form*

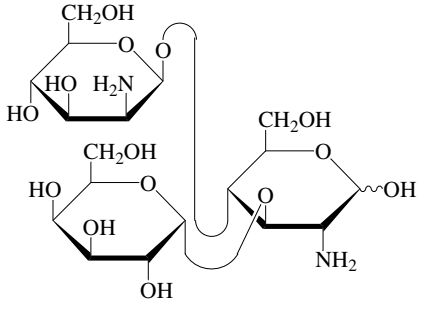
*1,2-*O*-Isopropylidene,* N*-Ac: 3-Acetamido-3-deoxy-1,2-*O*-isopropylidene-α-D-glucofuranose*
$C_{11}H_{19}NO_6$ 261.274
$[\alpha]_D^{24}$ -2 (c, 1.5 in $CHCl_3$).

*1,2:5,6-Di-*O*-Isopropylidene,* N*-Ac: 3-Acetamido-3-deoxy-1,2:5,6-di-*O*-isopropylidene-α-D-glucofuranose*
$C_{14}H_{23}NO_6$ 301.339
Mp 76-77° Mp 108-109° (double Mp). $[\alpha]_D$ -30 (c, 3.5 in $CHCl_3$).

Cron, M.J. *et al., J.A.C.S.*, 1958, **80**, 2342; 4115; 4741 (*isol, struct*)
Lindberg, B. *et al., Acta Chem. Scand.*, 1959, **13**, 1226 (*β-D-Me pyr, β-D-Me pyr tetra-Ac*)
Foster, A.B. *et al., Adv. Carbohydr. Chem.*, 1959, **14**, 213 (*rev*)
Baer, H.H. *et al., J.A.C.S.*, 1961, **83**, 1882 (*struct, β-D-N-Ac*)
Guthrie, R.D. *et al., J.C.S.*, 1961, 4166 (*α-D-Me pyr benzylidene, α-D-Me pyr benzylidene N-Ac, α-D-Me pyr tetra-Ac*)

Chittenden, G.J.F. *et al., Carbohydr. Res.*, 1965, **1**, 196 (*α-D-Me pyr benzylidene, α-D-Me pyr ethylidene N-Ac, β-D-Me pyr benzylidene di-Ac, β-D-Me pyr tetra-Ac*)
Meyer zu Reckendorf, W. *et al., Angew. Chem., Int. Ed.*, 1966, **5**, 967 (*D-N-Ac*)
Bishop, E.O. *et al., Carbohydr. Res.*, 1967, **5**, 477 (*α-D-Me pyr benzylidene N-Ac*)
Lichtenthaler, F.W. *et al., Chem. Ber.*, 1969, **102**, 994 (*β-D-Me pyr tetra-Ac, pmr*)
Horton, D. *et al., The Amino Sugars*, (Ed. Jeanloz, R.W.), Academic Press, 1969, **1A**, 1 (*rev*)
Richardson, A.C. *et al., Methods Carbohydr. Chem.*, 1972, **6**, 218 (*β-D-pyr-N-Ac, α-D-fur diisopropylidene N-Ac*)
Lichtenthaler, F.W. *et al., Methods Carbohydr. Chem.*, 1972, **6**, 250 (*β-D-Me pyr*)
Trnka, T. *et al., Coll. Czech. Chem. Comm.*, 1975, **40**, 3038 (*D-form, synth*)
Uchida, K. *et al., Tetrahedron*, 1975, **31**, 2315 (*cmr*)
Dolak, L.A. *et al., J. Antibiot.*, 1980, **33**, 900 (*isol*)
Horton, D. *et al., The Carbohydrates*, 2nd Ed., Academic Press, 1980, **1B**, 644 (*rev*)
Fusetani, N. *et al., Experientia*, 1987, **43**, 464 (*isol*)

2-Amino-2-deoxy-β-D-mannopyranosyl-(1→4)-[β-D-galactopyranosyl-(1→3)]-2-amino-2-deoxy-β-D-glucose A-263



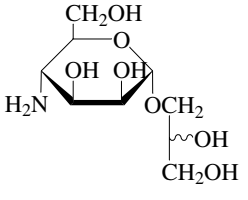
$C_{18}H_{34}N_2O_{14}$ 502.472

N,N′-Di-Ac:
$C_{22}H_{38}N_2O_{16}$ 586.546
Prod. by the marine bacterium *Alteromonas marinoglutinosa* NCIMB 1770.

Komandrova, N.A. *et al., Biokhimiya (Moscow)*, 2001, **66**, 894-897 (*isol*)

1-*O*-(4-Amino-4-deoxy-α-D-mannopyranosyl)glycerol A-264

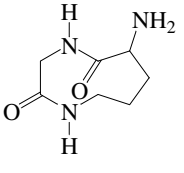
Glycerol 1-(4-amino-4-deoxy-α-D-mannopyranoside)
[205448-98-2]



$C_9H_{19}NO_7$ 253.252
Constit. of the red alga *Caloglossa leprieurii*.

Xu, X. *et al., CA*, 1998, **129**, 38766z (*isol*)

6-Amino-1,4-diazacyclononane-2,5-dione A-265



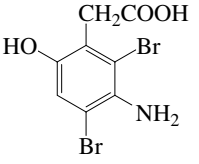
$C_7H_{13}N_3O_2$ 171.199

(-)-*form*
Prod. by a marine-derived *Streptomyces acrimycini*.
Glassy solid. $[\alpha]_D$ -6.8 (c, 0.08 in MeOH). CAS no. not found in CA 140 or 141.

Hernandez, I.L.C. *et al., J. Braz. Chem. Soc.*, 2004, **15**, 441-444 (*isol, pmr, cmr*)

2-(3-Amino-2,4-dibromo-6-hydroxyphenyl)acetic acid A-266

3-Amino-2,4-dibromo-6-hydroxybenzeneacetic acid, 9CI

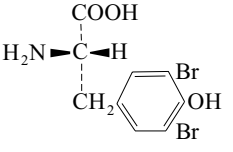


$C_8H_7Br_2NO_3$ 324.956
Isol. from *Aplysina cauliformis*. Antimycobacterial agent. Glassy solid. λ_{max} 228 (log ϵ 4.1); 304 (log ϵ 3.98) (MeOH).

De Oliveira, M.F. *et al., Planta Med.*, 2006, **72**, 437-441 (*isol, pmr, cmr, ms*)

2-Amino-3-(3,5-dibromo-4-hydroxyphenyl)propanoic acid A-267

3,5-Dibromotyrosine
[537-24-6]



$C_9H_9Br_2NO_3$ 338.983

(*S*)-*form*
L-form
[300-38-9]
Isol. from sponges and gorgonians. Mp 245°.

N-Ac:
$C_{11}H_{11}Br_2NO_4$ 381.02
Resolving agent. Cryst. + ½ H_2O (MeOH aq.). Mp 118°.
$[\alpha]_D^{25}$ +34.5 (c, 4 in MeOH).

4-Me ether:
$C_{10}H_{11}Br_2NO_3$ 353.01
Cryst. + H_2O (95% EtOH) (as hydrochloride). Mp 212-215° dec. (hydrochloride). $[\alpha]_D^{26}$ +4 (c, 1.0 in MeOH).

(±)-*form* [5741-93-5]
N-Ac: Mp 213-215° dec.

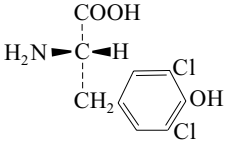
(ξ)-*form*
N,N,N-Tri-Me, betaine: [153343-21-6]
[165329-93-1]
$C_{12}H_{15}Br_2NO_3$ 381.063
Isol. from *Pseudoceratina crassa*. Sol. H_2O, MeOH. $[\alpha]_D^{25}$ -1.3 (MeOH). λ_{max} 287 (ϵ 1260) (H_2O). λ_{max} 307 (ϵ 1995) (pH 10 buffer) (Berdy).

4-Me ether, N,N,N-tri-Me, betaine: [153343-22-7]
[165329-92-0]
$C_{13}H_{17}Br_2NO_3$ 395.09
Isol. from *Pseudoceratina crassa*. Sol. H_2O, MeOH. $[\alpha]_D^{25}$ -8.3 (MeOH). λ_{max} 277 (ϵ 1260) (H_2O).

Mörner, C.T. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1913, **88**, 138 (*isol, synth*)
DeWitt, H.D. *et al., J.A.C.S.*, 1951, **73**, 5782 (*synth, use*)
Welinder, B.S. *et al., Biochim. Biophys. Acta*, 1972, **279**, 491 (*isol, ms*)
Albrizio, S. *et al., Tetrahedron*, 1994, **50**, 783-788 (*isol, betaines*)
Gao, H. *et al., Tetrahedron*, 1999, **55**, 9717-9726 (*synth, isol, derivs*)
Stewart, J. *et al., Synth. Commun.*, 2004, **34**, 547-555 (*4-Me ether*)

2-Amino-3-(3,5-dichloro-4-hydroxyphenyl)propanoic acid A-268

3,5-Dichlorotyrosine, 9CI



(*S*)–*form*

$C_9H_9Cl_2NO_3$ 250.08

Isol. from the cuticle of *Limulus polyphemus*.

(*S*)-*form*

L-form

Tablets + $2H_2O$. Mp 247-248° dec., 260°. $[\alpha]_D^{20}$ -2.8 (c, 5 in 4% HCl).

N-Ac:

$C_{11}H_{11}Cl_2NO_4$ 292.118

Cryst. (H_2O). Mp 136-139°. $[\alpha]_D^{20}$ +83 (c, 5.6 in doxan).

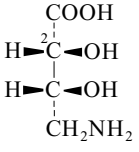
N-*Ac, Et ester:*

$C_{13}H_{15}Cl_2NO_4$ 320.171

Mp 140-141°.

Zeynek, R. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1921, **114**, 275 (*synth*)
Dibbo, L. *et al., J.C.S.*, 1961, 2645 (*synth*)
Welinder, B.S. *et al., Biochim. Biophys. Acta*, 1972, **279**, 491 (*isol, ms*)

4-Amino-2,3-dihydroxybutanoic acid, 9CI A-269



(2*R*,3*R*)–*form*

$C_4H_9NO_4$ 135.119

(2*R*,3*R*)-*form*

4-Amino-4-deoxy-D-erythronic acid

[27294-73-1]

Mp 217-219° dec. $[\alpha]_D^{20}$ +32.4 (c, 0.28 in H_2O).

(2*R*,3*S*)-*form*

4-Amino-4-deoxy-L-threonic acid

[40519-14-0]

Cryst. (2-propanol aq.). Mp 221-225° dec. $[\alpha]_D^{20}$ +4.6 (c, 0.64 in H_2O).

N,N,N-*Tri-Me, betaine: 3-Carboxy-2,3-dihydroxy*-N,N,N-*trimethyl-1-propanaminium(1+), 9CI.* ***Anthopleurine***

[56595-17-6]

$C_7H_{15}NO_4$ 177.2

Alarm pheromone from *Anthopleura elegantissima*. Sol. H_2O; poorly sol. Et_2O.

Mp 213-216° (as chloride). $[\alpha]_D^{20}$ -19.4 (c, 0.41 in H_2O).

(2*S*,3*R*)-*form*

4-Amino-4-deoxy-D-threonic acid

[67812-36-6]

Cryst. (2-propanol aq.). Mp 227-230° dec. $[\alpha]_D^{20}$ +14.5 (c, 0.72 in 1M HCl).

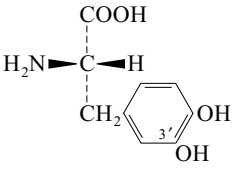
[67844-17-1, 67844-18-2]

Howe, N.R. *et al., Science (Washington, D.C.)*, 1975, **189**, 386 (*isol, deriv*)
Musich, J.A. *et al., J.A.C.S.*, 1978, **100**, 4865 (*synth, bibl*)
Tolstikov, A.G. *et al., Bioorg. Khim.*, 1991, **17**, 988 (*Anthopleurine, synth*)

2-Amino-3-(3,4-dihydroxyphenyl)propanoic acid A-270

3-Hydroxytyrosine, 9CI. 3,4-Dihydroxyphenylalanine. DOPA

[587-45-1]



(*S*)–*form*

$C_9H_{11}NO_4$ 197.19

Used in treatment of the Parkinsonian syndrome. The immediate precursor of the neurotransmitter dopamine. Usually administered with a peripheral DOPA decarboxylase inhibitor. Intermed. in biosynth. of various marine alkaloids, e.g. the Lamellarins. Log P -2.82 (uncertain value) (calc).

(*S*)-*form*

L-form. ***Levodopa, BAN, INN, JAN, USAN****. Bendopa. Brocadopa. Dopar. Larodopa. Levopa. Veldopa. Many other names*

[59-92-7]

Occurs in seedlings and pods of *Vicia faba*, in *Mucuna pruriens, Sarothamnus scoparius, Stizolobium deeringianum, Stizolobium hassjoo, Aristolochia clematitis* and other plants. Also prod. by *Bacillus* spp.

Prisms, needles (H_2O + SO_2) or plates (EtOH aq.).

Mp 285.5° dec. $[\alpha]_D^{20}$ -12.15 (c, 4 in 1*N* HCl). Pharmacol. active isomer. Rapidly turns green in air, aq. solns. darken in air. Green col. with $FeCl_3$. Reduces $AgNO_3$, NH_3 and acid $KMnO_4$.

Component of Sinemet. High-mol.-wt. polymers have been synth.

▶ Systemic (e.g. CNS) and adverse effects when used therapeutically. LD_{50} (rat, orl) 1780 mg/kg. Exp. reprod. and teratogenic effects. AY5600000

3′-O-Sulfate: 3-(Sulfooxy)tyrosine, 9CI

[96253-55-3]

$C_9H_{11}NO_7S$ 277.254

Constit. of the brown alga *Ascophyllum nodosum*.

3′-Me ether: 4-Hydroxy-3-methoxyphenylalanine. 3-Methoxytyrosine

[300-48-1]

$C_{10}H_{13}NO_4$ 211.217

Isol. from *Cortinarius brunneus, Pachymatisma johnstoni* and the blood of Parkinsonian patients. Cryst. (H_2O). $[\alpha]_D$ -34 (c, 0.39 in H_2O). $[\alpha]_D$ -15.4 (c, 0.36 in 0.1*M* HCl).

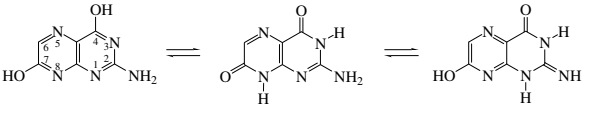
[57308-51-7, 127441-81-0]

Laycock, M.V. *et al., J. Nat. Prod.*, 1984, **47**, 1033 (*isol, sulfate*)
Behrman, E.J. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 351 (*synth, sulfate*)

2-Amino-4,7-dihydroxypteridine A-271

*2-Amino-4,7(1*H*,8*H*)-pteridinedione, 9CI.* ***Isoxanthopterin****. Ranachrome 4*

[529-69-1]



$C_6H_5N_5O_2$ 179.138

Widespread insect pigment found in amphibian and fish skin; normal constit. of urine.

Mp 300°. pK_{a1} 7.34; pK_{a2} 10.06 (20°,H_2O).

▶ UO3425000

1*H*,3*H*-*form*

Me ether, 1,3-di-Me: **N^1,N^3,O^7-*Trimethylisoxanthopterin***

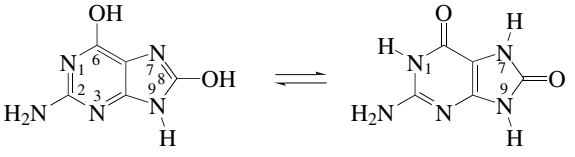
$C_9H_{11}N_5O_2$ 221.218

Isol. from a *Eudistoma* sp. Solid. λ_{max} 208 (sh) (log ε 4); 236 (sh) (log ε 3.7); 268 (log ε 3.4); 316 (log ε 3.6); 328 (sh) (log ε 3.6); 350 (sh) (log ε 3) (MeOH).

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 769A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 895D (*ir*)
Pfleiderer, W. *et al., Chem. Ber.*, 1961, **94**, 1 (*struct, bibl, uv*)
Konrad, G. *et al., Chem. Ber.*, 1970, **103**, 735 (*uv, props*)
Taylor, E.C. *et al., J.O.C.*, 1975, **40**, 2341 (*synth, bibl*)
Pfleiderer, W. *et al., J. Het. Chem.*, 1992, **29**, 583 (*rev*)
Van Wagoner, R.M. *et al., J. Nat. Prod.*, 2001, **64**, 1100-1101 (*N,N,O-trimethyl*)

2-Amino-6,8-dihydroxypurine A-272

*2-Amino-7,9-dihydro-1*H*-purine-6,8-dione, 9CI. 8-Oxoguanine. 7,8-Dihydro-8-oxoguanine. 2-Aminopurine-6,8-diol. 8-Hydroxyguanine*
[5614-64-2]



$C_5H_5N_5O_2$ 167.127

Other tautomers possible. 8-Oxo form predominates. Prod. *in vivo* by free radical hydroxylations of guanine radicals in DNA. Involved in base pair mismatches in mutagenesis. Crystalline powder. Mp 300°.

▶ Potent mutagen.

7-Me: 2-Amino-6,8-dihydroxy-7-methylpurine. 2-Amino-7-methyl-6,8-purinediol. 8-Hydroxy-7-methylguanine
[1688-85-3]
$C_6H_7N_5O_2$ 181.154
Platelets.

*9-Me: 2-Amino-6,8-dihydroxy-9-methylpurine. 2-Amino-9-methyl-6,8-purinediol. 8-Hydroxy-9-methylguanine. 9-Methylguanin-8(7*H*)-one*
[21823-84-7]
$C_6H_7N_5O_2$ 181.154
Cryst. + H_2O. Mp 400°.

*1,7-Di-Me: 1,7-Dimethyl-8-oxo-9*H*-guanine*
[65879-11-0]
$C_7H_9N_5O_2$ 195.18
Cryst. (H_2O). Gradual dec. >240°.

7,O^6-Di-Me: ***2-Amino-8-hydroxy-6-methoxy-7-methylpurine****. 2-Amino-7,9-dihydro-6-methoxy-7-methyl-8*H*-purin-8-one. 6-Methoxy-7-methyl-8-oxoguanine*
[247165-80-6]
$C_7H_9N_5O_2$ 195.18
Isol. from the ascidian *Symplegma rubra*. Solid. λ_{max} 210 (log ε 4.2); 246 (log ε 3.6); 284 (log ε 3.9) (MeOH).

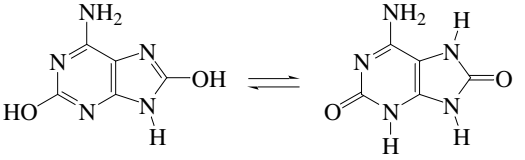
*9-Et: 2-Amino-9-ethyl-6,8-dihydroxypurine. 2-Amino-9-ethyl-6,8(1*H*,9*H*)-purinedione*
[21823-85-8]
$C_7H_9N_5O_2$ 195.18
Cryst. (KOH aq./AcOH). Mp 359-360°.

[112009-08-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 716D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 217C (*nmr*)
Fischer, E. *et al., Ber.*, 1897, **30**, 570 (*synth*)
Karrer, P. *et al., Helv. Chim. Acta*, 1948, **31**, 1214 (*isol*)
Cavalieri, L.F. *et al., J.A.C.S.*, 1950, **72**, 2587 (*synth, uv*)
Borowitz, I.J. *et al., Biochemistry*, 1965, **4**, 650 (*7-Me*)
Perini, F. *et al., J.O.C.*, 1970, **35**, 812 (*synth, uv, derivs*)
Brown, R. *et al., J.C.S. Perkin 1*, 1977, 1003 (*9-Me*)
Parham, J.C. *et al., J.O.C.*, 1978, **43**, 2325 (*di-Me*)
Dizdaroglu, M. *et al., Biochemistry*, 1985, **24**, 4476 (*formn*)
Kohda, K. *et al., Biochem. Biophys. Res. Commun.*, 1987, **149**, 1141 (*formn*)
Kasai, H. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 3799 (*cryst struct, 9-Et*)
Floyd, R.A. *et al., Carcinogenesis (London)*, 1990, **11**, 1447 (*rev*)
Doi, M. *et al., J.C.S. Perkin 1*, 1991, 55 (*cryst struct, 9-Et*)
Brown, T. *et al., Chem. Ber.*, 1993, 484 (*rev*)
Linday, B.S. *et al., J. Nat. Prod.*, 1999, **62**, 1573-1575 (*2-Amino-8-hydroxy-6-methoxy-7-methylpurine*)

6-Amino-2,8-dihydroxypurine A-273

*6-Amino-1*H*-purine-2,8(3*H*,7*H*)-dione, 9CI. 6-Amino-2,8-purinediol. 2,8-Dihydroxyadenine*
[30377-37-8]



$C_5H_5N_5O_2$ 167.127

Other tautomers possible. Prod. by *Alcaligenes aquamarinus*. Found in urine of humans with 2,8-dihydroxyadenine urolithiasis associated with adenine phosphoribosyltransferase deficiency. Xanthine oxidase inhibitor. Sol. bases; fairly sol. H_2O; poorly sol. MeOH, DMSO, hexane.
Mp 335-340° dec. λ_{max} 305 (ε 19950) (HCl) (Berdy). λ_{max} 300 (ε 14800) (NaOH) (Berdy).

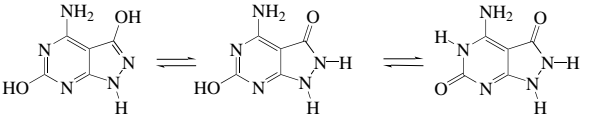
(1*H*,3*H*)-form

*1,3-Di-Me: 6-Amino-1,3-dimethyl-1*H*-purine-2,8(3*H*,8*H*)-dione. 1,3-Dimethyl-8-oxoisoguanine*
[683228-71-9]
$C_7H_9N_5O_2$ 195.18
Isol. from the ascidian *Pseudodistoma cereum* and from *Phestilla melanobtanchia* and a *Tubastrea* sp. Amorph. solid. λ_{max} 203 (log ε 3.89); 308 (log ε 3.57) (MeOH).

Bendich, A. *et al., J. Biol. Chem.*, 1950, **183**, 267-277 (*isol*)
Cavalieri, L.F. *et al., J.A.C.S.*, 1950, **72**, 2587-2594 (*synth*)
Klenow, H. *et al., Biochem. J.*, 1952, **50**, 404-407 (*isol*)
Stevens, M.A. *et al., J.A.C.S.*, 1960, **82**, 1148-1152 (*synth*)
Simmonds, H.A. *et al., Biochem. J.*, 1976, **157**, 485-487 (*isol*)
Sunahara, N. *et al., Agric. Biol. Chem.*, 1977, **41**, 1103-1109 (*isol*)
Simmonds, H.A. *et al., Clin. Chim. Acta*, 1986, **160**, 103-108 (*biochem, rev*)
Kamatani, N. *et al., Pharma Med.*, 1988, **6**, 39-42 (*rev*)
Kojima, T. *et al., Biomed. Chromatogr.*, 1991, **5**, 57-61 (*hplc*)
Simmonds, H.A. *et al., Lancet*, 1992, **ii**, 1295-1296 (*biochem*)
Sumi, S. *et al., J. Chromatogr., B: Biomed. Appl.*, 1995, **672**, 233-239 (*hplc*)
Sevcik, J. *et al., Clin. Chim. Acta*, 1996, **245**, 85-92 (*occur*)
Engle, S.J. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1996, **93**, 5307-5312 (*biochem*)
Appleton, D.R. *et al., Nat. Prod. Res.*, 2004, **18**, 39-42 (*1,3-di-Me*)

4-Amino-3,6-dihydroxy-1*H*-pyrazolo[3,4-*d*]pyrimidine A-274

*4-Amino-1*H*-pyrazolo[3,4-*d*]pyrimidine-3,6(2*H*,5*H*)-dione, 9CI.* ***Hydroxyakalone***
[182056-35-5]

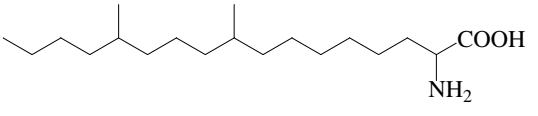


$C_5H_5N_5O_2$ 167.127
Prod. by the marine *Agrobacterium aurantiacum*. Xanthine oxidase inhibitor. Shows antigout activity. Powder. Sol. bases, DMSO; poorly sol. MeOH, hexane, $CHCl_3$. λ_{max} 298 (H_2O). λ_{max} 298 (pH12 buffer) (Berdy).

Izumida, H. *et al., J. Antibiot.*, 1997, **50**, 916-918 (*isol, pmr, cmr*)

2-Amino-9,13-dimethylheptadecanoic acid A-275

Antibiotic 1010-F1
[338420-14-7]



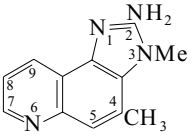
$C_{19}H_{39}NO_2$ 313.523

Prod. by a marine *Streptomyces* sp. 1010. Antibacterial agent.

Ivanova, V. *et al., Z. Naturforsch., C*, 2001, **56**, 1-5 (*isol, pmr, cmr*)

2-Amino-3,4-dimethylimidazo[4,5-*f*]quinoline A-276

Me-IQ
[77094-11-2]



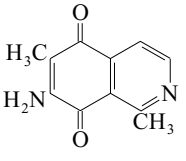
$C_{12}H_{12}N_4$ 212.254
Isol. from sardines.
Mp 296-298° (sealed tube). λ_{max} 219; 265; 332 (no solvent reported).

▶ Highly mutagenic. Exp. carcinogenic data. Possible human carcinogen (IARC 2B). NJ5907000

Kasai, H. *et al., Chem. Lett.*, 1980, 1391 (*struct, bibl*)
Kasai, H. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2233
Adolfsson, L. *et al., Acta Chem. Scand., Ser. B*, 1983, **37**, 157 (*synth*)
Ohgaki, H. *et al., Environ. Health Perspect.*, 1986, **67**, 129 (*carcinogenicity*)
IARC Monog. (Web), (*tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AJQ600

7-Amino-1,6-dimethyl-5,8-isoquinolinedione, 9CI A-277

Cribrostatin 1
[144279-35-6]

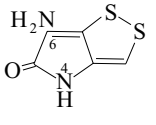


$C_{11}H_{10}N_2O_2$ 202.212
Alkaloid from the blue marine sponge *Cribrochalina* sp. Exhibits cytotoxicity against the P388 lymphocytic leukaemia cell line.
Red-orange cryst. (CH_2Cl_2/MeOH).
Mp 220-235° dec. λ_{max} 207 (ϵ 8730); 232 (ϵ 4700); 256 (ϵ 4170); 272 (ϵ 4160); 304 (ϵ 537) (MeOH) (Berdy).

Pettit, G.R. *et al., Can. J. Chem.*, 1992, **70**, 1170 (*isol, uv, ir, pmr, cmr, cryst struct*)

6-Amino-1,2-dithiolo[4,3-*b*]pyrrol-5(4*H*)-one, 9CI A-278

Holothin
[488-03-9]



$C_5H_4N_2OS_2$ 172.231
Hydrol. prod. of Holomycin. Greenish-black cryst. (as hydrochloride). Mp 300° (hydrochloride).

▶ AB7450000

N^6-*Ac:* ***Holomycin***. N-*(4,5-Dihydro-5-oxo-1,2-dithiolo[4,3-*b*]pyrrol-6-yl)acetamide, 9CI, 8CI*. N-*Demethylthiolutin. Antibiotic MM 21801. MM 21801*
[488-04-0]
$C_7H_6N_2O_2S_2$ 214.269
Prod. by *Streptomyces* sp. P6621 and *Streptomyces clavuligerus*. Shows antibiotic props. Orange-yellow flakes (MeOH/EtOAc). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 268-270° dec. λ_{max} 246 (ϵ 6460); 302 (ϵ 3090); 388 (ϵ 11200) (MeOH or EtOH) (Derep). λ_{max} 246 (ϵ 4665); 301 (ϵ 2354); 388 (ϵ 7918) (MeOH) (Berdy). λ_{max} 245 (ϵ 6310); 302 (ϵ 3310); 390 (ϵ 11750) (EtOH) (Berdy).

▶ AB7450000

N^6-*Propanoyl:* **N-*Propionylholothin***. N-*(4,5-Dihydro-5-oxo-1,2-dithiolo[4,3-*b*]-pyrrol-6-yl)propanamide, 9CI*
[4708-23-0]
$C_8H_8N_2O_2S_2$ 228.295
Isol. from *Streptomyces* P6621. Orange-yellow prisms. Sol. MeOH. Mp 255-264° dec. λ_{max} 246 (ϵ 6460); 302 (ϵ 3090); 388 (ϵ 11200) (MeOH or EtOH) (Derep). λ_{max} 246 (ϵ 7800); 302 (ϵ 4250); 388 (ϵ 14400) (MeOH) (Berdy).

N^6-*Hexanoyl:* ***Xenorhabdin 1***. N-*(4,5-Dihydro-5-oxo-1,2-dithiolo[4,3-*b*]pyrrol-6-yl)hexanamide, 9CI*
[92680-94-9]
$C_{11}H_{14}N_2O_2S_2$ 270.376
Prod. by *Xenorhabdus* spp. Possesses antimicrobial and insecticidal props. Sol. MeOH, EtOAc, DMSO; fairly sol. hexane; poorly sol. H_2O. Mp 192-193°. Related to Thiolutin, 4-Me, N^6-*Ac and Aureothricin, 4-Me,* N^6*-propanoyl. λ_{max} 243 (sh) (ϵ 6000); 300 (ϵ 3100); 387 (ϵ 11000) (MeOH) (Derep). λ_{max} 250; 310; 390 (MeOH) (Berdy).*

N^6-*Octanoyl:* ***Xenorhabdin 3***
[92680-91-6]
$C_{13}H_{18}N_2O_2S_2$ 298.429
Prod. by *Xenorhabdus* spp. Possesses antimicrobial and insecticidal props. Sol. MeOH, DMSO, EtOAc; fairly sol. hexane; poorly sol. H_2O. Mp 360°. λ_{max} 243 (sh) (ϵ 6000); 300 (ϵ 3100); 387 (ϵ 11000) (MeOH) (Derep). λ_{max} 250; 310; 390 (MeOH) (Berdy). λ_{max} 300; 387 (MeOH) (Berdy).

N^6-*Tetradecanoyl:* N-*Tetradecanoylholothin*
$C_{19}H_{30}N_2O_2S_2$ 382.59
Prod. by a marine-derived *Alteromonas* sp.

N^6-*(5-Methylhexanoyl):* ***Xenorhabdin 2***
[92680-90-5]
$C_{12}H_{16}N_2O_2S_2$ 284.403
Prod. by *Xenorhabdus* spp. Possesses antimicrobial and insecticidal props. Sol. MeOH, EtOAc, DMSO; fairly sol. hexane; poorly sol. H_2O. Mp 210-213°. λ_{max} 243 (sh) (ϵ 6000); 300 (ϵ 3100); 387 (ϵ 11000) (MeOH) (Derep). λ_{max} 244; 300; 387 (MeOH) (Berdy).

*4-Me: 6-Amino-4-methyl-1,2-dithiolo[4,3-*b*]pyrrol-5(4*H*)-one.* ***Pyrrothine***
[642-77-3]
$C_6H_6N_2OS_2$ 186.258
Isol. from a *Streptomyces* sp. Active against gram-positive and -negative bacteria. Amorph. yellow solid.
Mp 191-194° dec.

4-Me; hydrochloride:
Yellow prisms + $1H_2O$. Sinters at *ca.* 200°.

4-Me, N^6*-Ac:* ***Thiolutin***. N-*Acetylpyrrothine. Farcinicine. Acetopyrrothine*
[87-11-6]
$C_8H_8N_2O_2S_2$ 228.295
Prod. by *Streptomyces albus*, *Streptomyces pimprina*, *Streptomyces thioluteus* other *Streptomyces* spp. and *Saccharothrix* sp. SA 233. Antibiotic which inhibits microbiological growth in beer. Phytotoxic in high concentrations. Shows platelet aggregation props. Brilliant yellow needles (1-butanol). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, C_6H_6, Et_2O, hexane.
Mp 273-276° dec. $Bp_{0.1}$ 200° subl. λ_{max} 248 (ϵ 6300); 311 (ϵ 5700); 388 (ϵ 10800) (MeOH) (Derep). λ_{max} 250 (ϵ 6030); 311 (ϵ 5600); 388 (ϵ 10960) (MeOH) (Berdy).

▶ LD_{50} (mus, scu) 25 mg/kg. JP1355000

4-Me, N^6*-propanoyl:* ***Aureothricin***. *Propionylpyrrothine. Farcinicin*†
[574-95-8]
$C_9H_{10}N_2O_2S_2$ 242.322
Isol. from *Streptomyces celluloflavus* 39a , *Streptomyces cyanoflavus*, *Streptomyces kasugaensis* and *Streptomyces farcinicus*. Antibiotic and antifungal agent. Platelet aggregation inhibitor. Golden yellow cryst. (EtOAc). Sol. MeOH, $CHCl_3$; fairly sol. C_6H_6; poorly sol. Et_2O, H_2O, hexane.

Mp 260-270° dec. λ_{max} 246 (ϵ 6500); 313 (ϵ 4000); 390 (ϵ 11100) (EtOH) (Berdy).

▶ LD_{50} (mus, scu) 10 mg/kg.

4-Me, N^6*-butanoyl:* N-*(4,5-Dihydro-4-methyl-5-oxo-1,2-dithiolo[4,3-*b*]pyrrol-6-yl)butanamide.* **N-*Butanoylpyrrothine*.** *Antibiotic PSC$_2$. PSC$_2$*

[112843-01-3]

$C_{10}H_{12}N_2O_2S_2$ 256.349

Prod. by *Xenorhabdus bovienii* A2 and *Saccharothrix* sp. SA 233. Yellow powder. λ_{max} 308 (log ϵ 3.7); 389 (log ϵ 3.92) (MeOH).

4-Me, N^6*-(2-methylpropanoyl):* N-*(2-Methylpropanoyl)pyrrothine.* ***Isobutyropyrrothine.*** N-*Isobutyrylpyrrothine. Antibiotic PSC$_1$. PSC$_1$*

[39859-18-2]

$C_{10}H_{12}N_2O_2S_2$ 256.349

Prod. by *Streptomyces pimprina* and *Saccharothrix* sp. SA 233. Shows platelet aggregation props. Orange-red plates (C_6H_6). Sol. $CHCl_3$, EtOAc, Me_2CO; fairly sol. C_6H_6; poorly sol. H_2O, hexane.

Mp 228-229°. λ_{max} 245; 290; 310; 388 (MeOH) (Berdy). λ_{max} 246 (ϵ 5400); 302 (ϵ 3000); 386 (ϵ 11000) (MeOH) (Derep).

4-Me, N^6*-hexanoyl:* ***Xenorhabdin 4***. N-*Pentanoylpyrrothine*

[92680-92-7]

$C_{12}H_{16}N_2O_2S_2$ 284.403

From *Xenorhabdus* spp. Possesses antimicrobial and insecticidal props. Sol. MeOH, DMSO, EtOAc; fairly sol. hexane; poorly sol. H_2O.

Mp 165°. λ_{max} 246 (sh) (ϵ 6300); 308 (ϵ 5700); 388 (ϵ 11000) (MeOH) (Derep). λ_{max} 245; 310 (ϵ 1000); 312; 390 (ϵ 10000) (MeOH) (Berdy).

4-Me, N^6*-(3-methylbutanoyl):* N-*(4,5-Dihydro-4-methyl-5-oxo-1,2-dithiolo[4,3-*b*]pyrrol-6-yl)-3-methylbutanamide.* ***N-(3-Methylbutanoyl)pyrrothine***

[167559-98-0]

$C_{11}H_{14}N_2O_2S_2$ 270.376

Isol. from *Xenorhabdus bovienii* A2. Solid.

4-Me, N^6*-(5-methylhexanoyl): N-(5-Methylhexanoyl)pyrrothine.* ***Xenorhabdin 5***

[92680-93-8]

$C_{13}H_{18}N_2O_2S_2$ 298.429

From *Xenorhabdus* spp. Possesses antimicrobial and insecticidal props. Sol. MeOH, EtOAc, DMSO; fairly sol. hexane; poorly sol. H_2O. λ_{max} 246 (sh) (ϵ 6300); 308 (ϵ 5700); 388 (ϵ 11000) (MeOH) (Derep). λ_{max} 246; 250; 308; 310 (ϵ 1000); 388; 390 (ϵ 10000) (MeOH) (Berdy).

4-Me, N^6*-(3-methyl-2-butenoyl):* **N-*Senecioylpyrrothine*.** *PSA. Antibiotic PSA*

$C_{11}H_{12}N_2O_2S_2$ 268.36

Prod. by *Saccharothrix* sp. SA 233. Yellow-orange powder. λ_{max} 302 (log ϵ 3.87); 402 (log ϵ 3.97) (MeOH).

4-Me, N^6*-tigloyl:* **N-*Tigloylpyrrothine*.** *PSB. Antibiotic PSB*

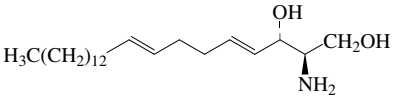
$C_{11}H_{12}N_2O_2S_2$ 268.36

Prod. by *Saccharothrix* sp. SA 233. Yellow-orange powder. λ_{max} 302 (log ϵ 3.85); 402 (log ϵ 3.96) (MeOH).

Celmer, W.D. *et al., J.A.C.S.*, 1952, **74**, 6304; 1955, **77**, 2861 (*Pyrrothine, Aureothricin, Thiolutin, isol, ir, uv, struct*)
Ettlinger, L. *et al., Helv. Chim. Acta*, 1959, **42**, 563 (*isol*)
Bhate, D.S. *et al., Experientia*, 1960, **16**, 504-505 (*Isobutyropyrrothine*)
Schmidt, U. *et al., Chem. Ber.*, 1964, **97**, 1511 (*synth, uv, ir*)
Büchi, G. *et al., J.A.C.S.*, 1964, **86**, 5654 (*synth*)
Yamagishi, S. *et al., Yakugaku Zasshi*, 1971, **91**, 351 (*Aureothicin, isol, struct, ir, pmr, ms*)
Hagio, K. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 1484 (*Holothin, Thiolutin, Aureothricin, synth, ir, uv, pmr*)
Okamura, K. *et al., J. Antibiot.*, 1977, **30**, 334-336 (*isol, ir, ms*)
Ellis, J.E. *et al., J.O.C.*, 1977, **42**, 2891-2893 (*synth, ir, uv, ms, nmr*)
Kenig, M. *et al., J. Antibiot.*, 1979, **32**, 549-554 (*MM 21801*)
Ninomiya, Y.T. *et al., Chem. Pharm. Bull.*, 1980, **28**, 3157-3162 (*Pyrrothine, Thiolutin, props, ms*)
Deb, P.R. *et al., Curr. Sci. (India)*, 1984, **53**, 659 (*Thiolutin, props*)
Pat. Coop. Treaty (WIPO), 1984, 01 775; *CA*, **101**, 189727 (*Xenorhabdins*)
McInerney, B.V. *et al., J. Nat. Prod.*, 1991, **54**, 774 (*Xenorhabdins*)
Dell, I. *et al., ACS Symp. Ser.*, 1992, **504**, 384 (*synth*)
Sato, A. *et al., Annu. Rep. Sankyo Res. Lab.*, 1995, **47**, 1-58 (*N-Tetradecanoylholothin*)
Li, J. *et al., J. Nat. Prod.*, 1995, **58**, 1081-1086 (*N-Butanoylpyrrothine, N-3-Methylbutanoylpyrrothine*)
Lamari, L. *et al., J. Antibiot.*, 2002, **55**, 696-701; 702-706 (*Saccharothrix pyrrothines*)

2-Amino-4,8-docosadiene-1,3-diol A-279

Docosasphinga-4,8-dienine



(2*R*,3*S*,4*E*,8*E*)-*form*

$C_{22}H_{43}NO_2$ 353.587

(2*R*,3*S*,4*E*,8*E*)-*form*

erythro-*form*

[129549-17-3]

N-*Dodecanoyl:* N-*Dodecanoyldocosasphinga-4,8-dienine.* N-*Lauroyldocosasphinga-4,8-dienine*

[129646-06-6]

$C_{34}H_{65}NO_3$ 535.892

Constit. of *Anemonia sulcata* and *Heteroxenia gardaquensis.* Cryst. (Me_2CO).

Mp 297-298°. $[\alpha]_D$ +2.94 ($CHCl_3$).

(2*RS*,3*SR*,4*E*,8*E*)-*form*

(±)-erythro-*form*

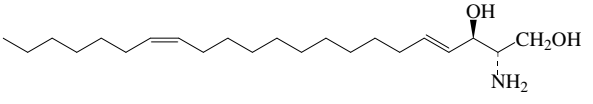
N-*Dodecanoyl:* [129549-11-7]

Mp 75.5°.

[102673-10-9, 129646-04-4]

Chebaane, K. *et al., Tet. Lett.*, 1986, **27**, 1495 (*isol, deriv*)
Hirsch, S. *et al., Tetrahedron*, 1989, **45**, 3897 (*isol, deriv*)
Nakagawa, M. *et al., Chem. Comm.*, 1990, 603 (*synth, abs config*)

2-Amino-4,15-docosadiene-1,3-diol A-280



$C_{22}H_{43}NO_2$ 353.587

(2*S*,3*R*,4*E*,15*Z*)-*form*

N-*(2*R-*Hydroxyhexadecanoyl), 1*-O-*β*-D-*glucopyranoside:*

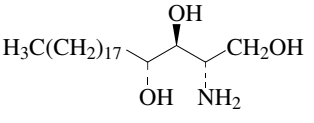
[457645-49-7]

$C_{44}H_{83}NO_9$ 770.141

Isol. from the starfish *Allostichaster inaequalis.* Amorph. solid. Mp 175°. $[\alpha]_D$ -31.2 (c, 0.2 in $CHCl_3$).

Diaz de Vivar, M.E. *et al., Lipids*, 2002, **37**, 597-603 (*isol, pmr, cmr*)

2-Amino-1,3,4-docosanetriol A-281



$C_{22}H_{47}NO_3$ 373.618

(2*S*,3*S*,4*R*)-*form*

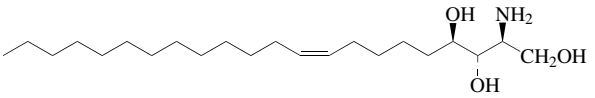
N-*Docosanoyl:* [636589-66-7]

$C_{44}H_{89}NO_4$ 696.191

Constit. of the sponge *Iotrochota baculifera.*

Muralidhar, P. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1193-1195 (*isol*)

2-Amino-9-docosene-1,3,4-triol A-282



$C_{22}H_{45}NO_3$ 371.602

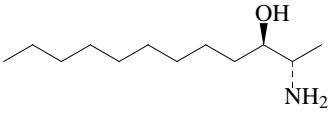
(2*S*,3*S*,4*R*,9*Z*)-*form*

N-*(2*R-*Hydroxyhexadecanoyl):* [202601-29-4]
$C_{38}H_{75}NO_5$ 626.014
Isol. from the starfish *Acanthaster planci*. Amorph. powder.
Mp 135-137°. $[\alpha]_D$ +11.5 (c, 1 in Py).

N-*(2*R-*Hydroxyhexadecanoyl), 1*-O-*[β-*D*-galactopyranosyl-(1→4)-β-*D*-glucopyranoside]:* ***Luidialactoside C***
$C_{50}H_{95}NO_{15}$ 950.298
Isol. from the starfish *Luidia maculata*. Amorph. powder.
Mp 217-220°. $[\alpha]_D^{27}$ +8.6 (c, 0.17 in $CHCl_3$/MeOH).

Inagaki, M. *et al., Eur. J. Org. Chem.*, 1998, 129-131 (*isol, pmr, cmr*)
Inagaki, M. *et al., Eur. J. Org. Chem.*, 2003, 325-331 (*Luidialactoside C*)

2-Amino-3-dodecanol A-283



$C_{12}H_{27}NO$ 201.351

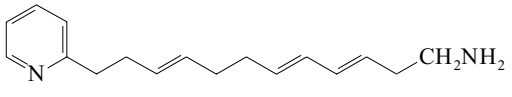
(2*S*,3*R*)-*form*

Isol. from the ascidian *Clavelina oblonga*. Antifungal agent.
Glassy solid. $[\alpha]_D^{29}$ +4.5 (c, 0.22 in MeOH).

Kossuga, M.H. *et al., J. Nat. Prod.*, 2004, **67**, 1879-1881 (*isol, pmr, cmr*)

2-(12-Amino-3,7,9-dodecatrienyl)pyridine A-284

12-(2-Pyridinyl)-3,5,9-dodecatrien-1-amine



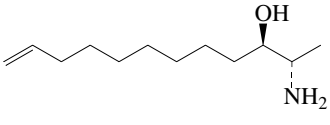
$C_{17}H_{24}N_2$ 256.39

(all-*E*)-*form*

Naloamine
[179118-58-2]
Alkaloid from the mollusc *Smaragdinella calyculata*.
Amorph. solid. λ_{max} 206 (ϵ 12000); 230 (ϵ 15000); 262 (ϵ 4300); 268 (ϵ 4200); 280 (ϵ 2700) (MeOH).

Szabo, C.M. *et al., Tetrahedron*, 1996, **52**, 9681 (*isol, uv, pmr, cmr, ms, struct*)

2-Amino-11-dodecen-3-ol A-285



$C_{12}H_{25}NO$ 199.336

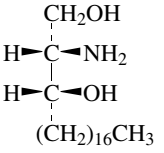
(2*S*,3*R*)-*form*

Halaminol B
[389125-59-1]
Isol. from a marine sponge *Haliclona* n. sp.
Oil. $[\alpha]_D$ +2.1 (c, 0.06 in CH_2Cl_2).

Clark, R.J. *et al., J. Nat. Prod.*, 2001, **64**, 1568-1571 (*Halaminol B, isol, pmr, cmr*)

2-Amino-1,3-eicosanediol A-286

Dihydro-C_{20}-sphingosine. Eicosasphinganine
[24028-07-7]
[3530-52-7, 24006-62-0, 91685-44-8, 98575-69-0]



(2*S*,3*R*)-*form*

$C_{20}H_{43}NO_2$ 329.565

(2*S*,3*R*)-*form*

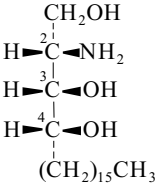
N-*Docosanoyl, 1*-O-*β-D*-glucopyranoside: ***Temnoside B***
[191731-31-4]
$C_{48}H_{95}NO_8$ 814.28
Isol. from the sea urchin *Temnopleurus toreumaticus*. Amorph. powder.
Mp 216-217°. $[\alpha]_D^{27}$ +8.1 (c, 0.01 in Py).

N-*(2*R-*Hydroxytricosanoyl), 1*-O-*β-D*-glucopyranoside: ***Temnoside A***
[191731-30-3]
$C_{49}H_{97}NO_9$ 844.307
Isol. from the sea urchin *Temnopleurus toreumaticus*. Amorph. powder.
Mp 205-207°. $[\alpha]_D^{27}$ +8.6 (c, 0.01 in Py).

Babu, U.V. *et al., J. Nat. Prod.*, 1997, **60**, 732-734 (*isol, ir, pmr, cmr*)

2-Amino-1,3,4-eicosanetriol A-287

2-Amino-1,3,4-icosanetriol. 4-Hydroxyeicosasphinganine. C_{20}-Phytosphingosine



(2*S*,3*S*,4*R*)−*form*

$C_{20}H_{43}NO_3$ 345.565

(2*S*,3*S*,4*R*)-*form*

D-ribo-*form*
[3530-53-8]
Isol. from yeast and fungal cerebrins. Constit. of mullet roe (*Mugil cephalus*) gangliosides.
Cryst. (MeCN).
Mp 97-99°. $[\alpha]_D^{17}$ +8.1 (c, 0.34 in $CHCl_3$).

N-*Hexadecanoyl:*
$C_{36}H_{73}NO_4$ 583.977
Isol. from the soft coral *Lobophytum crassum*. Antibacterial agent. Config. not confirmed.

N-*Docosanoyl:* [168212-28-0]
$C_{42}H_{85}NO_4$ 668.138
Constit. of the sponge *Iotrochota baculifera*.

N-*Benzoyl:*
Cryst. (EtOAc). Mp 136-137°. $[\alpha]_D$ +3.6 (c, 1 in Py).

N-*Benzoyl, tri*-O-*Ac:* Mp 81-82°. $[\alpha]_D$ +2 (c, 0.7 in $CHCl_3$).

(2*RS*,3*RS*,4*SR*)-*form*

(±)-ribo-*form*
[34506-41-7]
Cryst. (MeCN). Mp 95-105°.

(2*RS*,3*SR*,4*SR*)-*form*

(±)-xylo-*form*
Cryst. (MeCN). Mp 128-132°.

Gigg, J. *et al., J.C.S.(C)*, 1966, 1872-1876; 1876-1879; 1879-1882 (*synth*)
Kisic, A. *et al., Chem. Phys. Lipids*, 1971, **7**, 135-143 (*synth*)
Li, Y.-T. *et al., J. Biol. Chem.*, 1984, **259**, 8980-8985 (*occur*)

Vanisree, M. *et al., Asian J. Chem.*, 2002, **14**, 957-960 (*Lobophytum crassum constit*)
Muralidhar, P. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1193-1195 (*N-docosanoyl*)

2-Aminoethanesulfinic acid, 9CI A-288

Hypotaurine. *Cystaminesulfinic acid*
[300-84-5]
$H_2NCH_2CH_2SO_2H$
$C_2H_7NO_2S$ 109.149
Constit. of rat brain. Found in the marine vestimentiferan worm *Riftia pachyptila* and other marine invertebrates.
Mp 186-188°. pK_{a1} 2.16; pK_{a2} 9.56.

Chatagner, F. *et al., C. R. Hebd. Seances Acad. Sci.*, 1951, **232**, 448 (*isol*)
Biochem. Prep., 1963, **10**, 72-75 (*synth*)
Hope, D.B. *et al., J.C.S.(C)*, 1970, 270 (*synth*)
Fellman, J.H. *et al., J. Labelled Compd. Radiopharm.*, 1981, **18**, 765 (*synth*)
Stipanuk, M.H. *et al., Methods Enzymol.*, 1987, **143**, 155 (*hplc*)
Fugler-Domenico, L. *et al., Biol. Amines*, 1989, **6**, 289 (*conformn*)
Chaimbault, P. *et al., Anal. Biochem.*, 2004, **332**, 215-225 (*marine, occur*)

2-Aminoethanesulfonic acid, 9CI A-289

Taurine, 8CI, INN. *Aminoethylsulfonic acid. Ethylaminesulfonic acid. FEMA 3813*
[107-35-7]
$H_2NCH_2CH_2SO_3H$
$C_2H_7NO_3S$ 125.148
Occurs free in animal tissues, bacteria, sponges, red algae, e.g. isol. from *Macrocallista nimbosa*, *Turbo stenogyrus*, *Calyx nicaeensis*, *Geodia gigas*, *Mytilus edulis*. Also from green algae, e.g. *Caulerpa okamurai*, *Caulerpa racemosa*, *Chlorodesmis comosa*, *Codium adherens*, *Codium fragile* and *Enteromorpha linza*. Isol. from marine vestimentarian worm *Riftia pachyptila* and from higher plants, e.g. leguminous seedlings. A non-essential amino acid. Intermed. in metab. of cysteine. Used as an adjunct in treatment of hypercholesterolaemia. Metabolic regulator. Monoclinic prismatic rods with sharp taste. Sol. H_2O, insol. EtOH.
Mp 328° (320-325° dec.). pK_{a1} 1.5; pK_{a2} 8.74. Dec. at 300°.
▶ LD_{50} (mus, scu) 6000 mg/kg. WX0175000

Amide: [4378-70-5]
$C_2H_8N_2O_2S$ 124.163
Plates (EtOH) (as hydrochloride). Mp 133° (hydrochloride).

N-*Me:* [107-68-6]
$C_3H_9NO_3S$ 139.175
Widely distributed in marine algae including the red alga *Ptilota pectinata* and green alga *Chlorodesmis comosa*. Also found in sponges *Calyx nereis* and *Halichondria* sp. Prisms. V. sol. H_2O; insol. EtOH, Et_2O.
Mp 241-242°.

N,N-*Di-Me:* [637-95-6]
$C_4H_{11}NO_3S$ 153.202
Obt. from *Corallina officinalis*. Present in *Furcellaria fastigiata* and other red algae. Prisms (MeOH). V. sol. H_2O, AcOH, insol. EtOH, Et_2O.
Mp 315-316° dec.

N,N-*Bis(2-chloroethyl): Taumustine*
[98277-87-3]
$C_6H_{13}Cl_2NO_3S$ 250.145
Cryst. (H_2O). Mp 178-180°.

N-*(2,3-Dihydroxypropyl):* N-*Glyceryltaurine*
[65222-42-6]
$C_5H_{13}NO_5S$ 199.227
Isol. from the red alga *Gigartina leptorhynchos*. Cryst. (EtOH aq.). Mp 163-164°. $[\alpha]_D^{23}$ -21 (H_2O).

N-*(15-Methyl-9Z-hexadecenoyl):* **N-*(15-Methyl-9-hexadecenoyl)taurine***
[679834-30-1]
$C_{19}H_{37}NO_4S$ 375.572
Isol. from the sponge *Erylus nobilis*.

N-*(5Z,8Z,11Z,14Z-Eicosatetraenoyl):* N-*(5,8,11,14-Eicosatetraenoyl)taurine*
[679834-28-7]
$C_{22}H_{37}NO_4S$ 411.605
Isol. from the starfish *Certonardoa semiregularis*.

[4316-74-9, 7347-25-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 890A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1433C (*nmr*)
Org. Synth., Coll. Vol., 2, 1943, 563; 564 (*synth*)
Ishidate, M. *et al., Chem. Pharm. Bull.*, 1954, **2**, 275-279 (*synth*)
Lindberg, B. *et al., Acta Chem. Scand.*, 1955, **9**, 1093-1096; 1323-1326 (*isol, N-Me, N,N-di-Me*)
Wickberg, B. *et al., Acta Chem. Scand.*, 1956, **10**, 1097-1099 (*Glyceryltaurine*)
Sutherland, H.H. *et al., Acta Cryst.*, 1963, **16**, 897-901 (*cryst struct*)
Huxtable, R. *et al., Taurine, [Int. Symp.], 1st, 1975 (1976)*, (Eds.), Raven Press, New York, 1975, (*book*)
Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1984, 124-125; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 126-127 (*N-Me, occur*)
Hashem, K.M.E. *et al., Bull. Soc. Chim. Belg.*, 1985, **94**, 735-754 (*cmr*)
Taurine: Nutritional Value and Mechanisms of Action, (eds. Lombardini, J.B. *et al*), Plenum Press, 1992, (*book*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1419
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1665-1666 (*use, occur*)
Merck Index, 13th edn., 2001, No. 9163 (*bibl*)
Hibbs, D.E. *et al., Chem. Eur. J.*, 2003, **9**, 1075-1084 (*cryst struct*)
Wang, W. *et al., Nat. Prod. Sci.*, 2003, **9**, 241-244; *CA*, **140**, 335912 (*N-Methylhexadecenoyl, N-Eicosatetraenoyl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TAG750

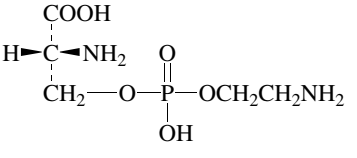
2-Aminoethanesulfonothioic acid, 9CI A-290

S-*(2-Aminoethyl) thiosulfate, 8CI*. ***Thiotaurine***
[2937-54-4]
[31999-89-0 (Na salt)]
$H_2NCH_2CH_2SO_2SH$
$C_2H_7NO_2S_2$ 141.215
Isol. from various marine invertebrates incl. *Bathymodiolus* spp., *Calyptogena magnifica* and *Riftia pachyptila*. Biomarker of sulfur-based symbiosis in deep-sea bivalves. Cryst. (EtOH aq.).
Mp 213° dec.

Sörbö, B.H. *et al., Acta Chem. Scand.*, 1958, **12**, 146 (*synth*)
Biochem. Prep., 1963, **10**, 72-75 (*synth*)
Pruski, A.M. *et al., J. Exp. Biol.*, 2003, **206**, 2923-2930 (*biosynth*)
Chaimbault, P. *et al., Anal. Biochem.*, 2004, **332**, 215-225 (*occur*)

2-Aminoethyl seryl phosphate A-291

Serine ethanolamine phosphodiester. SEP
[17871-37-3, 18635-48-8]



(R)-form

$C_5H_{13}N_2O_6P$ 228.141

(*R*)-*form*
D-*form*
[16106-04-0]
Isol. from the earthworms *Lumbricus terrestris* and *Megascolides cameroni*.
Cryst. (MeOH aq.).
Mp 143-144° (dec.). $[\alpha]_D^{23}$ +18.2 (c, 0.7 in H_2O).

(*S*)-*form*
L-*form*
[1186-34-1]
Isol. from numerous animals incl. chicken, fish and reptiles.
Needles (MeOH aq.).
Mp 142-143° (dec.). $[\alpha]_D^{23}$ -15 (c, 2 in H_2O).

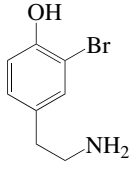
(±)-*form* [114760-94-0]
Prisms (EtOH aq.). Mp 193-194° (dec.).

Ennor, A.H. *et al., J. Biochem. (Tokyo)*, 1960, **75**, 179-182
Beatty, I.M. *et al., J.A.C.S.*, 1960, **82**, 4983-4989 (*synth*)

Rosenberg, H. *et al., J. Biochem. (Tokyo)*, 1961, **50**, 81-84 (*occur, biosynth*)
Allen, A.K. *et al., Biochim. Biophys. Acta*, 1968, **151**, 504-519; **152**, 208-210 (*biosynth*)
Euerby, M.R. *et al., J. Chem. Res., Synop.*, 1988, 394-395 (*synth, pmr, cmr, ms*)
Merchant, T.E. *et al., J. Lipid Res.*, 1990, **31**, 479-486 (*P-31 nmr*)

4-(2-Aminoethyl)-2-bromophenol, 9CI A-292

2-(3-Bromo-4-hydroxyphenyl)ethylamine. 3-Bromotyramine
[104616-74-2]



$C_8H_{10}BrNO$ 216.077
Isol. from the ascidian *Cnemidocarpa bicornuta*. Cryst.
Mp 162-164°. λ_{max} 203 (log ϵ 4.4); 283 (log ϵ 3.3) (MeOH).

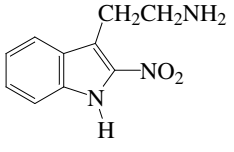
Hydrochloride:
Cryst. (MeOH/EtOAc). Mp 205.5-207°.

N,N,N-*Tri-Me: 3-Bromo-4-hydroxy*-N,N,N-*trimethylbenzeneethanaminium, 9CI. 3-Bromo*-N,N,N-*trimethyltyramine*
[259533-84-1]
$C_{11}H_{17}BrNO^{\oplus}$ 259.165
Isol. from the sponge *Verongula gigantea*. Isol. as trifluoroacetate salt. λ_{max} 281 (ϵ 1485) (MeOH).

Tolkachev, O.N. *et al., Zh. Obshch. Khim.*, 1958, **28**, 3320-3323; *J. Gen. Chem. USSR (Engl. Transl.)*, 1958, **28**, 3345-3348 (*synth*)
Lindsay, B.S. *et al., J. Nat. Prod.*, 1998, **61**, 857-858 (*isol, uv, ir, pmr, cmr, ms*)
Ciminiello, P. *et al., J. Nat. Prod.*, 2000, **63**, 263-266 (*N-tri-Me deriv*)

3-(2-Aminoethyl)-2-nitroindole A-293

*2-Nitro-1*H-*indole-3-ethanamine. 2-Nitrotryptamine*



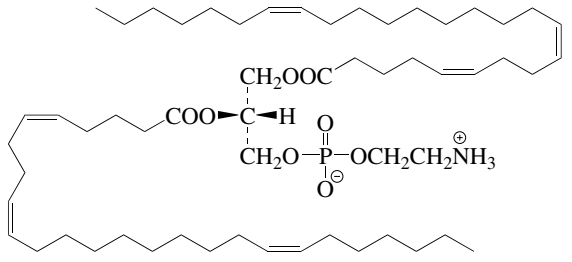
$C_{10}H_{11}N_3O_2$ 205.216

N^b-*Ac:* N^b-***Acetyl-2-nitrotryptamine***
$C_{12}H_{13}N_3O_3$ 247.253
Isol. from the marine-derived *Flavobacterium* sp. T436.

Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*Ac, isol*)

1-*O*-(2-Aminoethylphospho)-2,3-bis(5,9,19-hexacosatrienoyl)glycerol A-294

1,2-Di-(5,9,19-hexacosatrienoyl)-sn-*glycero-3-phosphocholine*



$C_{57}H_{102}NO_8P$ 960.409

(***R***)-(***all-Z***)-*form* [107447-10-9]
Isol. from the phospholipids of the sponge *Microciona prolifera*.

19,19′,20,20′-Tetrahydro: 1-O-*(2-Aminoethylphospho)-2,3-bis(5,9-hexacosadienoyl)glycerol*
[99824-60-9]
$C_{57}H_{106}NO_8P$ 964.44
Isol. from the sponges *Microciona prolifera* and *Paresperella psila*.

Mena, P.L. *et al., Chem. Phys. Lipids*, 1985, **37**, 257 (*synth, pmr, ms*)
Dasgupta, A. *et al., Chem. Phys. Lipids*, 1986, **41**, 335 (*isol, ms*)

(2-Aminoethyl)phosphonic acid, 9CI A-295

Ciliatine. *AEP*
[2041-14-7]
$H_2NCH_2CH_2P(O)(OH)_2$
$C_2H_8NO_3P$ 125.064
Constit. as glyceryl esters of rumen protozoan, *Tetrahymena pyriformis*, sea anemones, bovine brain, mycobacteria, and a fungus *Pythium prolatum*. Rhombic cryst. or needles (EtOH aq.). Mp 295-297° dec. pK_{a1} 2.45; pK_{a2} 7; pK_{a3} 10.8. pK_{a1} 1.3; pK_{a2} 6.51; pK_{a3} 11.5 (25°). The metastable rhombic form is difficult to prepare. First known natural compd. contg. the C–P bond.

Di-Et ester: [41468-36-4]
$C_6H_{16}NO_3P$ 181.171
Liq. $Bp_{0.025}$ 54-56°.

N-*Benzoyl: 2-(Benzoylamino)ethylphosphonic acid*
$C_9H_{12}NO_4P$ 229.172
Solid. Mp 191-192°.

N-*Me:* N-*Methylciliatine. 2-(Methylamino)ethylphosphonic acid*
[14596-55-5]
$C_3H_{10}NO_3P$ 139.091
Isol. from the sea anemone *Anthopleura xanthogrammica*. Needles (MeOH aq.).
Mp 291° dec.

N,N-*Di-Me: 2-Dimethylaminoethylphosphonic acid.* N,N-*Dimethylciliatine*
[14596-56-6]
$C_4H_{12}NO_3P$ 153.117
Isol. from *Anthopleura xanthogrammica*. Pale yellow cryst. (MeOH aq.).
Mp 249.5° dec.

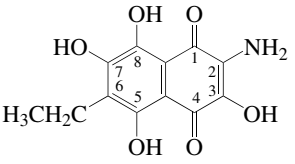
N,N-*Di-Me, Et ester:* [41948-36-1]
$C_6H_{16}NO_3P$ 181.171
Bp_1 100°.

N-*Phthalimide, di-Et ester: Diethyl (2-phthalimidoethyl)phosphonate*
$C_{14}H_{18}NO_5P$ 311.274
Cryst. (Et_2O/petrol). Mp 58°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1477A (*nmr*)
Kosolapoff, G.M. *et al., J.A.C.S.*, 1947, **69**, 2112 (*synth*)
Top. Phosphorus Chem., Interscience, 1966, **4**, 23: **11**; 297 (*rev*)
Barycki, J. *et al., Tet. Lett.*, 1970, 3147 (*synth*)
Isbell, A.F. *et al., J.O.C.*, 1972, **37**, 4399 (*synth, bibl*)
Harvey, D.J. *et al., J. Chromatogr.*, 1973, **79**, 65 (*ms*)
Lagrange, C.G. *et al., Can. J. Chem.*, 1978, **56**, 663 (*ir, Raman*)
Brigot, D. *et al., Tetrahedron*, 1979, **35**, 1345 (*synth, pmr, derivs*)
Fabre, G. *et al., Can. J. Chem.*, 1981, **59**, 2864 (*synth, di-Et ester, ir, pmr*)
Varlet, J.M. *et al., Tetrahedron*, 1981, **37**, 3713 (*dervis*)
Al-Rawi, J.M.A. *et al., Org. Magn. Reson.*, 1983, **21**, 75 (*di-Et ester, cmr*)
Appleton, T.G. *et al., Aust. J. Chem.*, 1984, **37**, 1833 (*props, cmr, P-31 nmr*)
Yamauchi, K. *et al., J.O.C.*, 1984, **49**, 1158 (*N-phthalimide deriv*)
Gubnitskaya, E.S. *et al., Zh. Obshch. Khim.*, 1986, **56**, 2017; *J. Gen. Chem. USSR (Engl. Transl.)*, 1986, **56**, 1779 (*esters, synth, ir*)
Osapay, G. *et al., Tetrahedron*, 1987, **43**, 2977 (*ir, pmr*)
Lazukina, L.A. *et al., Zh. Obshch. Khim.*, 1988, **58**, 939; *J. Gen. Chem. USSR (Engl. Transl.)*, 1988, **58**, 833 (*synth, P-31 nmr*)
Thayer, J.S. *et al., Appl. Organomet. Chem.*, 1989, **3**, 203 (*rev*)
Warielewski, C. *et al., J. Prakt. Chem.*, 1989, **331**, 507 (*synth, ir*)
Harris, R.K. *et al., Magn. Reson. Chem.*, 1989, **27**, 470 (*cmr, N-15 nmr, P-31 nmr*)
Glowacki, Z. *et al., Magn. Reson. Chem.*, 1989, **27**, 897 (*cmr*)
Warielewski, C. *et al., Synthesis*, 1989, 52 (*synth, ir, pmr*)
Ohashi, K. *et al., Tetrahedron*, 1989, **45**, 2557 (*N-Me, synth, ir*)
Hayashi, A. *et al., Chem. Phys. Lipids*, 1990, **52**, 57 (*fab-ms*)
Neidlein, R. *et al., Helv. Chim. Acta*, 1992, **75**, 2545 (*N-phthalimide deriv*)
Ohno, K. *et al., J. Mol. Struct.*, 1993, **298**, 1 (*ir, Raman, conformn*)Fields, S.C. *et al., Tetrahedron*, 1999, **55**, 12237-12273 (*rev, synth*)

2-Amino-6-ethyl-3,5,7,8-tetrahydroxy-1,4-naphthoquinone A-296

2-Amino-6-ethyl-3,7-dihydroxynaphthazarin. ***Echinamine A***



$C_{12}H_{11}NO_6$ 265.222
Isol. from the sea urchin *Scaphechinus mirabilis*. Dark brown powder (Me_2CO).
Mp 245-246°. λ_{max} 217 (log ϵ 4.33); 233 (log ϵ 4.41); 274 (log ϵ 4.11); 345 (log ϵ 3.29); 479 (log ϵ 3.3) (EtOH).

Mischenko, N.P. *et al., J. Nat. Prod.*, 2005, **68**, 1390-1393 (*isol, pmr, cmr, ms*)
Pokhilo, N.D. *et al., J. Nat. Prod.*, 2006, **69**, 1125-1129 (*synth*)
Pokhilo, N.D. *et al., Tet. Lett.*, 2006, **47**, 1385-1387 (*synth*)

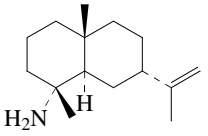
2-Amino-7-ethyl-3,5,6,8-tetrahydroxy-1,4-naphthoquinone A-297

2-Amino-7-ethyl-3,6-dihydroxynaphthazarin. ***Echinamine B***

$C_{12}H_{11}NO_6$ 265.222
Isol. from the sea urchin *Scaphechinus mirabilis*. Dark brown needles (Me_2CO).
Mp 265-267°. λ_{max} 217 (log ϵ 4.33); 275 (log ϵ 4.41); 343 (log ϵ 3.19); 480 (log ϵ 3.3) (EtOH).

Mischenko, N.P. *et al., J. Nat. Prod.*, 2005, **68**, 1390-1393 (*isol, pmr, cmr, ms*)
Pokhilo, N.D. *et al., J. Nat. Prod.*, 2006, **69**, 1125-1129 (*synth*)

4-Amino-11-eudesmene A-298



$C_{15}H_{27}N$ 221.385

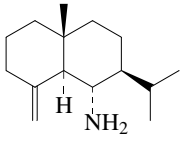
(4α,7α)-*form* [442851-12-9]
[442851-11-8]
Constit. of *Axinyssa ambrosia*.
Oil; cryst. (as hydrochloride).
Mp 210-220° (hydrochloride). $[\alpha]_D$ -17.5 (c, 0.9 in $CHCl_3$).

N-*Formyl:* ***4-Formamido-11-eudesmene***
[442851-14-1]
$C_{16}H_{27}NO$ 249.395
Constit. of *Axinyssa ambrosia*. Cryst.
Mp 104-107°. $[\alpha]_D$ -10 (c, 0.22 in $CHCl_3$).

4-Isocyanide: ***4-Isocyano-11-eudesmene***
[442851-13-0]
$C_{16}H_{25}N$ 231.38
Constit. of *Axinyssa ambrosia*. Oil. $[\alpha]_D$ -15 (c, 0.2 in $CHCl_3$).
Has -NC in place of NH_2.

Petrichtcheva, N.V. *et al., J. Nat. Prod.*, 2002, **65**, 851-855 (*isol, pmr, cmr*)

6-Amino-4(15)-eudesmene A-299



$C_{15}H_{27}N$ 221.385

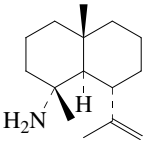
6α-*form*

Halichonadin D
[847605-79-2]
Constit. of a *Halichondria* sp.
Yellow oil. $[\alpha]_D^{27}$ +18 (c, 0.2 in $CHCl_3$).

N-*Methoxycarbonyl:* ***Halichonadin B***
[847605-77-0]
$C_{17}H_{29}NO_2$ 279.422
Constit. of a *Halichondria* sp. Amorph. solid. $[\alpha]_D^{24}$ -10 (c, 1 in $CHCl_3$).

Ishiyama, H. *et al., Tetrahedron*, 2005, **61**, 1101-1105 (*isol, pmr, cmr*)

4-Amino-11-gorgonene A-300



$C_{15}H_{27}N$ 221.385

(4α,6α)-*form*

N-*Formyl: 4-Formamido-11-gorgonene*
[134781-19-4]
$C_{16}H_{27}NO$ 249.395
Isol. from the molluscs *Phyllidia pustulosa* and *Phyllidia varicosa*.
Cryst. $[\alpha]_D$ -61.8 (c, 0.11 in $CHCl_3$). Mp >300° dec.

4-Isocyanide: ***4-Isocyano-11-gorgonene***
[134781-18-3]
$C_{16}H_{25}N$ 231.38
Isol. from the molluscs *Phyllidia pustulosa* and *Phyllidia varicosa*.
Oil. $[\alpha]_D$ -66.9 (c, 1.6 in $CHCl_3$).

4-Isothiocyanate: 4-Isothiocyanato-11-gorgonene
[134781-20-7]
$C_{16}H_{25}NS$ 263.446
Isol. from *Phyllidia pustulosa*. Oil. $[\alpha]_D$ -101.6 (c, 0.5 in $CHCl_3$).

Kassühlke, K.E. *et al., J.O.C.*, 1991, **56**, 3747-3750 (*isol, pmr, cmr, ms*)

2-Amino-1,3-heneicosanediol A-301

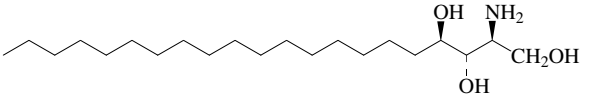
$H_3C(CH_2)_{17}CH(OH)CH(NH_2)CH_2OH$
$C_{21}H_{45}NO_2$ 343.592

(2ξ,3ξ)-*form*

N-*(2ξ,20ξ-Dihydroxyheneicosanoyl):* [851308-73-1]
$C_{42}H_{85}NO_5$ 684.137
Constit. of *Spongia zimocca* ssp. *irregularia*. Cryst. (Me_2CO).
Mp 111-112°.

Lin, C.-W. *et al., Youji Huaxue*, 2005, **25**, 225-228; *CA*, **142**, 444769m

2-Amino-1,3,4-heneicosanetriol A-302



$C_{21}H_{45}NO_3$ 359.591

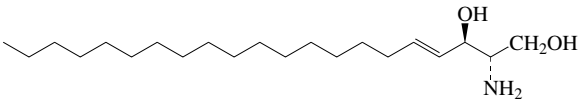
(2*S*,3*S*,4*R*)-*form*

N-*(2*R-*Hydroxyheneicosanoyl):* ***Hemisceramide***
$C_{42}H_{85}NO_5$ 684.137
Constit. of *Hemisteptia lyrata*. Cryst. (MeOH).
Mp 129-130°.

N-*Docosanoyl:*
$C_{43}H_{87}NO_4$ 682.165
Constit. of the sponge *Iotrochota baculifera*.

Ren, Y.-L. *et al., Yaoxue Xuebao*, 2002, **37**, 440-443 (*Hemisceramide*)
Muralidhar, P. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1193-1195 (*N-docosanoyl*)

2-Amino-4-heneicosene-1,3-diol A-303



$C_{21}H_{43}NO_2$ 341.576

(2*S*,3*R*,4*E*)-*form*

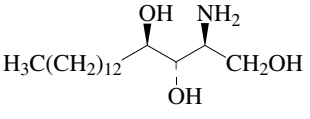
N-*Ac:* ***Tanacetamide B***
[787551-29-5]
$C_{23}H_{45}NO_3$ 383.613
Constit. of *Tanacetum artemisioides*. Oil. $[\alpha]_D^{23}$ -6.7 (c, 0.03 in $CHCl_3$/MeOH).

N-*Heneicosanoyl:* [262351-89-3]
$C_{42}H_{83}NO_3$ 650.123
Isol. from *Mycale mytilorum*. Amorph. solid.
Mp 75-77°. $[\alpha]_D^{28}$ -11 (c, 0.1 in $CHCl_3$).

N-*(2*R*-Hydroxy-3*E*-heneicosenoyl):* ***Tanacetamide A***
[787551-28-4]
$C_{42}H_{81}NO_4$ 664.106
Constit. of *Tanacetum artemisioides*. Oil. $[\alpha]_D^{23}$ -6 (c, 0.01 in $CHCl_3$/MeOH).

Reddy, G.B.S. *et al., Bioorg. Med. Chem.*, 2000, **8**, 27-36 (*N-heneicosanoyl*)
Ahmad, V.U. *et al., Z. Naturforsch., B*, 2004, **59**, 329-333 (*Tanacetamides A,B*)

2-Amino-1,3,4-heptadecanetriol A-304



$C_{17}H_{37}NO_3$ 303.484

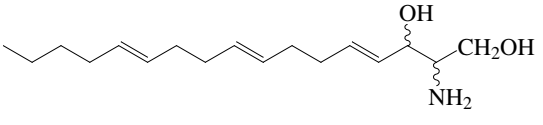
(2*S*,3*S*,4*R*)-*form*

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-α-D-*galactopyranoside:* ***Agelasphin 9a***
[148289-27-4]
$C_{47}H_{93}NO_{10}$ 832.252
Isol. from the sponge *Agelas mauritianus*. Immunostimulant.
Mp 201-203.5°. $[\alpha]_D^{24}$ +49.9 (c, 1 in Py).

N-*(2*R*-Hydroxy-23-methyltetracosanoyl):* [326597-32-4]
$C_{42}H_{85}NO_5$ 684.137
Constit. of the sex pheromone of the crab *Erimacrus isenbeckii*.

Natori, T. *et al., Tetrahedron*, 1994, **50**, 2771-2784 (*Agelasphin 9a*)
Asai, N. *et al., Tetrahedron*, 2000, **56**, 9895-9899 (*Erimacrus pheromone*)

2-Amino-4,8,12-heptadecatriene-1,3-diol A-305



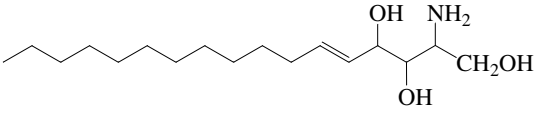
$C_{17}H_{31}NO_2$ 281.437

(2ξ,3ξ,4*E*,8*E*,12*E*)-*form*

N-*Hexadecanoyl:* ***Nephtixamide A***
$C_{33}H_{61}NO_3$ 519.85
Isol. from the soft coral *Nephthea tixierae verseveldt*. Cryst. (EtOAc).
Mp 92-93°.

Wang, G.Y.S. *et al., Chin. Chem. Lett.*, 1993, **4**, 499-500 (*Nephtixamide A*)

2-Amino-5-heptadecene-1,3,4-triol A-306



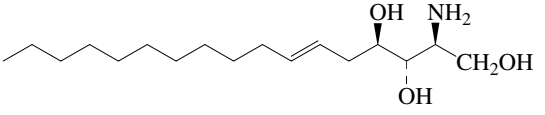
$C_{17}H_{35}NO_3$ 301.468

(2ξ,3ξ,4ξ,5*E*)-*form*

N-*(2-Hydroxyeicosanoyl):*
$C_{37}H_{73}NO_5$ 611.987
Isol. from *Sinularia gravis*. Cryst. ($CHCl_3$/MeOH).
Mp 145°. $[\alpha]_D^{25}$ +7.5 (c, 0.1 in MeOH).

Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 357-360

2-Amino-6-heptadecene-1,3,4-triol A-307



$C_{17}H_{35}NO_3$ 301.468

(2*S*,3*S*,4*R*,6*E*)-*form*

4-Sulfate: [443652-05-9]
$C_{17}H_{35}NO_6S$ 381.533
Isol. from the sponge *Spirastrella abata*. Amorph. solid. $[\alpha]_D^{19}$ +11.6 (c, 0.07 in $CHCl_3$).

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*[α-D-galactopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Amphimelibioside A_2***
$C_{51}H_{97}NO_{15}$ 964.325
Isol. from an *Amphimedon* sp. Powder. Isol. as a mixt. with Amphimelibioside A_1.

Alam, N. *et al., J. Nat. Prod.*, 2002, **65**, 944-945 (*4-sulfate*)
Emura, C. *et al., J.O.C.*, 2005, **70**, 3031-3038 (*Amphimelibioside A_2*)

3-Aminoheptanedioic acid, 9CI A-308

3-Aminopimelic acid
[71288-40-9]
$HOOC(CH_2)_3CH(NH_2)CH_2COOH$
$C_7H_{13}NO_4$ 175.184

(±)-*form*

Plates (H_2O). Mp 183-185° dec.

Hydrochloride:
Needles (conc. HCl). Mp 148.5-149°.

Mono-Me ester:
$C_8H_{15}NO_4$ 189.211
Cryst. (MeOH) (as hydrochloride). Mp 159.5-160° (hydrochloride).

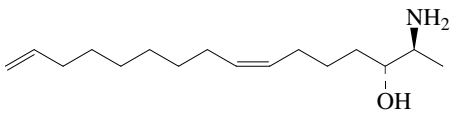
N-*(3,5-Dinitrobenzoyl):*
Pale-yellow rosettes (H_2O). Mp 153.5-154°.

(ξ)-*form*

Bis(L-phenylalaninamide):
$C_{25}H_{31}N_3O_6$ 469.536
Prod. by a *Pseudomonas-Alteromonas* bacterium associated with a Black Sea sponge. Amorph. yellow powder.
Mp *ca.*190° dec. $[\alpha]_D$ -27.5 (c, 0.18 in H_2O).

Nauta, W.T. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1953, **72**, 721 (*synth*)
Romeo, A. *et al., CA*, 1954, **48**, 10592 (*synth*)
De Rosa, S. *et al., J. Nat. Prod.*, 2000, **63**, 1454-1455 (*bisphenylalaninamide*)

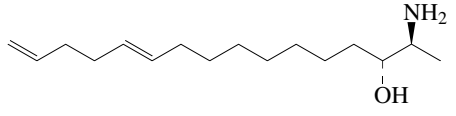
2-Amino-7,15-hexadecadien-3-ol A-309



$C_{16}H_{31}NO$ 253.427

(2*S*,3*R*,7*Z*)-*form*
Obscuraminol B
[350485-82-4]
Isol. from the tunicate *Pseudodistoma obscurum*.
Oil (as di-Ac). $[\alpha]_D^{24}$ -21.1 (c, 0.65 in MeOH) (di-Ac).
Garrido, L. *et al., Tetrahedron*, 2001, **57**, 4579-4588 (*isol, pmr, cmr, abs config*)

2-Amino-11,15-hexadecadien-3-ol A-310



$C_{16}H_{31}NO$ 253.427

(2*S*,3*R*,11*E*)-*form*
Obscuraminol C
[350484-95-6]
Isol. from the tunicate *Pseudodistoma obscurum*.
Amorph. solid (as di-Ac). $[\alpha]_D^{24}$ -24.5 (c, 0.83 in MeOH) (di-Ac).
11,12-Dihydro: 2-Amino-15-hexadecen-3-ol. ***Obscuraminol F***
[350485-01-7]
$C_{16}H_{33}NO$ 255.443
Isol. from *Pseudodistoma obscurum*. Amorph. solid (as di-Ac).
$[\alpha]_D^{24}$ -19.2 (c, 0.71 in MeOH) (di-Ac).
15,16-Dihydro: 2-Amino-11-hexadecen-3-ol. ***Obscuraminol E***
[350485-00-6]
$C_{16}H_{33}NO$ 255.443
Isol. from *Pseudodistoma obscurum*. Oil (as di-Ac).
Garrido, L. *et al., Tetrahedron*, 2001, **57**, 4579-4588 (*Obscuraminols C,E,F, isol, pmr, cmr, abs config*)

2-Amino-1,3-hexadecanediol A-311

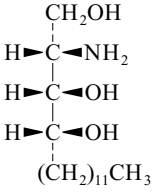
$H_3C(CH_2)_{12}CH(OH)CH(NH_2)CH_2OH$

$C_{16}H_{35}NO_2$ 273.458

(2ξ,3ξ)-*form*
N-*(2,4-Dihydroxytricosanoyl):* [877210-60-1]
$C_{39}H_{79}NO_5$ 642.057
Isol. from an unidentified sponge.
N-*(2,4-Dihydroxytetracosanoyl):* [877210-61-2]
Isol. from an unidentified sponge.
N-*(2,4-Dihydroxypentacosanoyl):* [877210-63-4]
$C_{41}H_{83}NO_5$ 670.11
Isol. from an unidentified sponge.
Guo, W.-C. *et al., CA*, 2006, **144**, 250597z (*isol*)

2-Amino-1,3,4-hexadecanetriol A-312

C_{16}-Phytosphingosine



(2*S*,3*S*,4*R*)–*form*

$C_{16}H_{35}NO_3$ 289.457

(2*S*,3*S*,4*R*)-*form*
D-ribo-*form*
[114379-45-2]
Common phytosphingosine, occurring for example in Acanthacerebroside A, A-38.
N,O,O,O-*Tetra-Ac:*
$C_{24}H_{43}NO_7$ 457.606
Viscous liq. $[\alpha]_D^{25}$ +27.9 (c, 1.5 in $CHCl_3$).
N-*(2*R*-Hydroxydocosanoyl), 1*-O-*β*-D-*glucopyranoside:* ***Acanthacerebroside B***
[122823-43-2]
[110744-72-4]
$C_{44}H_{87}NO_{10}$ 790.172
Isol. from the starfishes *Acanthaster planci* and *Asterina pectinifera*. Needles (MeOH aq.).
Mp 214-215°. $[\alpha]_D$ +9.9 (c, 1.9 in 1-propanol).
N-*(2*R*-Hydroxydocosanoyl), 1*-O-*β*-D-*galactopyranoside:* **Stellaster *Cerebroside S-2b-2***
[166733-14-8]
$C_{44}H_{87}NO_{10}$ 790.172
Isol. from *Agelas clathrodes* and *Stellaster equestris*. Amorph. powder.
Mp 142-143°. $[\alpha]_D$ +3.8 (c, 0.5 in Py). Incorr. sugar struct. given in CA.
N-*(2*R*-Hydroxydocosanoyl), 1*-O-*[β*-D-*galactopyranosyl-(1→4)-β*-D-*glucopyranoside]:* ***Luidialactoside D***
[503856-79-9]
$C_{50}H_{97}NO_{15}$ 952.314
Isol. from the starfish *Luidia maculata*. Amorph. powder.
Mp 223-225°. $[\alpha]_D^{27}$ +7.4 (c, 0.17 in $CHCl_3$/MeOH).
N-*(2*R*-Hydroxy-21-methyldocosanoyl):* [326597-25-5]
$C_{39}H_{79}NO_5$ 642.057
Constit. of the sex pheromone of the crab *Erimacrus isenbeckii*.
N-*(2*R*-Hydroxytricosanoyl):* [202601-30-7]
$C_{39}H_{79}NO_5$ 642.057
Isol. from the starfish *Acanthaster planci*. Constit. of the sex pheromone of the crab *Erimacrus isenbeckii*. Amorph. powder.
Mp 143-145°. $[\alpha]_D$ +10 (c, 0.4 in Py).
N-*(2*R*-Hydroxy-22-methyltricosanoyl):* [326597-28-8]
$C_{40}H_{81}NO_5$ 656.084
Constit. of the pheromone of the crab *Erimacrus isenbeckii*.
N-*Tetracosanoyl, 1*-O-*β*-D-*glucopyranoside:* ***JCer-4***
$C_{46}H_{91}NO_9$ 802.226
Constit. of *Comanthus japonica*. Amorph. powder.
Mp 105-108°. $[\alpha]_D$ +1.2 (c, 0.12 in 1-propanol).
N-*(2*R*-Hydroxytetracosanoyl):* [128802-67-5]
$C_{40}H_{81}NO_5$ 656.084
Isol. from the starfish *Acanthaster planci*. Constit. of the sex pheromone of the crab *Erimacrus isenbeckii*. Amorph. powder.
Mp 142-143°. $[\alpha]_D$ +11.5 (c, 1 in Py).
N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*α*-D-*galactopyranoside:* ***Agelasphin 7a***
[148347-44-8]
$C_{46}H_{91}NO_{10}$ 818.226
Isol. from *Agelas mauritianus*.
Mp 193.5-195°. $[\alpha]_D^{24}$ +52.3 (c, 1 in Py).
N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*[β*-D-*galactofuranosyl-(1→3)-α*-D-*galactopyranoside]:* ***Longiside***
[160436-11-3]
$C_{52}H_{101}NO_{15}$ 980.368
Constit. of the sponge *Agelas longissima*. Oil (as deca-Ac).
$[\alpha]_D^{25}$ +57 (c, 0.03 in $CHCl_3$) (deca-Ac).
N-*(2*R*-Hydroxy-23-methyltetracosanoyl):* [326597-30-2]
$C_{41}H_{83}NO_5$ 670.11
Constit. of the sex pheromone of the crab *Erimacrus isenbeckii*.
N-*(2*R*-Hydroxypentacosanoyl):* [326597-29-9]
[326597-32-4]
$C_{41}H_{83}NO_5$ 670.11
Constit. of the sex pheromone of the crab *Erimacrus isenbeckii*.
Isol. from the sponge *Fasciospongia cavernosa*.
$[\alpha]_D$ +12.3 (c, 0.45 in $CHCl_3$).

N-*(2*R*-Hydroxy-24-methylpentacosanoyl):* [326597-31-3]
$C_{42}H_{85}NO_5$ 684.137
Constit. of the sex pheromone of the crab *Erimacrus isenbeckii*.

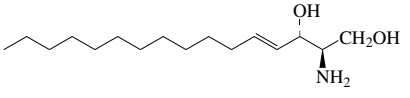
(2*S*,3*R*,4*R*)-*form*
D-xylo-*form*
[128898-88-4]
N,O,O,O-*Tetra-Ac:* $[\alpha]_D^{27}$ +6.13 (c, 0.56 in $CHCl_3$).

(2*S*,3*R*,4*S*)-*form*
D-arabino-*form*
[127061-67-0]
N,O,O,O-*Tetra-Ac:* $[\alpha]_D^{28}$ -23.3 (c, 1.0 in $CHCl_3$).

(2*S*,3*S*,4*S*)-*form*
D-lyxo-*form*
[127062-47-9]
N,O,O,O-*Tetra-Ac:*
$C_{24}H_{43}NO_7$ 457.606
$[\alpha]_D^{28}$ -3.3 (c, 0.46 in $CHCl_3$).
Kawano, Y. *et al., Annalen*, 1988, 19-24 (*Acanthacerebroside B*)
Sugiyama, S. *et al., Annalen*, 1988, 619-625; 1990, 1069-1078 (*synth, pmr, cmr, abs config, bibl*)
Higuchi, R. *et al., Annalen*, 1990, 51-55 (*Acanthacerebroside B*)
Cafieri, F. *et al., Annalen*, 1994, 1187-1189 (*Longiside*)
Natori, T. *et al., Tetrahedron*, 1994, **50**, 2771-2784 (*Agelasphin 7a*)
Higuchi, R. *et al., Annalen*, 1996, 593-599 (*Stellaster Cerebroside S-2b-2*)
Inagaki, M. *et al., Eur. J. Org. Chem.*, 1998, 129-131 (*isol*)
Asai, N. *et al., Tetrahedron*, 2000, **56**, 9895-9899 (*Erimacrus pheromones*)
Ramesh, P. *et al., J. Chem. Res., Synop.*, 2001, 232-234 (*N-2-hydroxypentacosanoyl*)
Asai, N. *et al., J. Nat. Prod.*, 2001, **64**, 1210-1215 (*Erimacrus pheromones, synth*)
Inagaki, M. *et al., Eur. J. Org. Chem.*, 2003, 325-331 (*Luidialactoside D*)
Inagaki, M. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1307-1311 (*JCer-4*)

2-Amino-4-hexadecene-1,3-diol A-313

C_{16}-Sphingosine. Hexadeca-4-sphingenine
[29707-26-4]



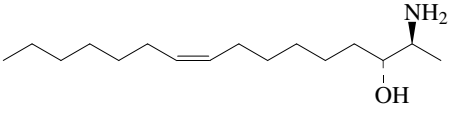
(2*R*,3*S*,4*E*)-*form*

$C_{16}H_{33}NO_2$ 271.442

(2*R*,3*S*,4*E*)-*form* [6982-09-8]
Base constit. of the sphingolipids in various animal spp. incl. *Musca domestica*.

(2*S*,3*R*,4*E*)-*form*
N-*Docosanoyl: JC-3*
$C_{38}H_{75}NO_3$ 594.015
Constit. of *Comanthus japonica*. Amorph. powder.
Mp 77-79°. $[\alpha]_D$ -2.4 (c, 0.25 in $CHCl_3$).
N-*(2*R*-Hydroxy-13*Z*-docosenoyl), 1*-O-*β*-D-glucopyranoside: JCer-2*
$C_{44}H_{83}NO_9$ 770.141
Constit. of *Comanthus japonica*. Amorph. powder.
Mp 128-130°. $[\alpha]_D$ +9.7 (c, 0.17 in 1-propanol).
N-*Tricosanoyl: JC-4*
$C_{39}H_{77}NO_3$ 608.042
Constit. of *Comanthus japonica*. Amorph. powder.
Mp 76-78°. $[\alpha]_D$ -4.6 (c, 0.15 in $CHCl_3$).
N-*(21-Methyldocosanoyl):* ***Oceanapin A***
[155661-01-1]
$C_{39}H_{77}NO_3$ 608.042
Isol. from the sponge *Oceanapia* cf. *tenuis*. Powder (hexane).
Mp 65-75°.
N-*Tetracosanoyl: JC-5*
$C_{40}H_{79}NO_3$ 622.069
Constit. of *Comanthus japonica*. Amorph. powder.
Mp 85-87°. $[\alpha]_D$ -4.3 (c, 0.58 in $CHCl_3$).
N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*β*-D-glucopyranoside: JCer-3*
$C_{46}H_{89}NO_9$ 800.21
Constit. of *Comanthus japonica*. Amorph. powder.
Mp 125-128°. $[\alpha]_D$ +5.6 (c, 0.17 in 1-propanol).
N-*Hexadecanoyl, 1*-O-*β*-D-galactopyranoside:* ***Turbostatin 3***
$C_{38}H_{73}NO_8$ 671.997
Isol. from the mollusc *Turbo stenogyrus*. Amorph. solid.
Mp 213-214°. $[\alpha]_D^{23}$ -6.3 (c, 0.1 in Py).
N-*Hexadecanoyl, 1*-O-*β*-D-glucopyranoside:* ***Turbostatin 1***
$C_{38}H_{73}NO_8$ 671.997
Isol. from *Turbo stenogyrus*. Amorph. solid.
Mp 207-209°. $[\alpha]_D^{23}$ +10.2 (c, 0.1 in Py).
N-*Octadecanoyl, 1*-O-*β*-D-galactopyranoside:* ***Turbostatin 4***
$C_{40}H_{77}NO_8$ 700.05
Isol. from *Turbo stenogyrus*. Amorph. solid.
Mp 214-215°. $[\alpha]_D^{23}$ -6.5 (c, 0.1 in Py).
N-*Octadecanoyl, 1*-O-*β*-D-glucopyranoside:* ***Turbostatin 2***
$C_{40}H_{77}NO_8$ 700.05
Isol. from *Turbo stenogyrus*. Amorph. solid.
Mp 209-210°. $[\alpha]_D^{23}$ +10.7 (c, 0.1 in Py).
N-*Triacontanoyl:* ***Cymiforamide***
[406499-32-9]
$C_{46}H_{91}NO_3$ 706.23
Isol. from the sponge *Sigmadocia cymiformis*.
[123536-50-5]
Polito, A.J. *et al., Biochemistry*, 1968, **7**, 2609 (*isol, ms*)
Sugawara, T. *et al., Carbohydr. Res.*, 1989, **194**, 125 (*synth*)
Mancini, I. *et al., Helv. Chim. Acta*, 1994, **77**, 51-58 (*Oceanapin A*)
Wang, M.-Y. *et al., CA*, 2002, **136**, 276279g (*Cymiforamide*)
Inagaki, M. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1307-1311 (*JC-3,4,5, JCer-2,3*)
Pettit, G.R. *et al., J. Nat. Prod.*, 2005, **68**, 974-978 (*Turbostatins 1-4*)

2-Amino-9-hexadecen-3-ol A-314

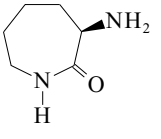


$C_{16}H_{33}NO$ 255.443

(2*S*,3*R*,9*Z*)-*form*
Obscuraminol D
[350484-99-0]
Isol. from the tunicate *Pseudodistoma obscurum*.
Oil (as di-Ac). $[\alpha]_D^{24}$ -21.6 (c, 0.44 in MeOH) (di-Ac).
Garrido, L. *et al., Tetrahedron*, 2001, **57**, 4579-4588 (*isol, ir, pmr, cmr, abs config*)

3-Aminohexahydro-2*H*-azepin-2-one, 9CI A-315

3-Amino-ε-caprolactam
[671-42-1]



(*R*)–*form*

$C_6H_{12}N_2O$ 128.174

(*R*)-*form* [28957-33-7]
Hydrochloride: [26081-03-8]
Solid (MeOH). $[\alpha]_D^{26}$ +26.4 (c, 4 in 1*M* HCl) (>99% ee).
Hydrobromide: [16473-63-5]
$[\alpha]_D^{20}$ +20.7 (c, 5 in H_2O).

(*S*)-*form* [21568-87-6]
Mp 71-72°. $[\alpha]_D^{25}$ -34 (c, 4 in 1*M* HCl) (100% ee).
Hydrochloride: [26081-07-2]
Mp 270°. $[\alpha]_D^{25}$ -27 (c, 2.98 in 1*M* HCl).

Hydrobromide: [16473-62-4]
Mp 285-288° dec. $[\alpha]_D^{20}$ -20.7 (c, 5 in H_2O).

N^3*-(6-Methyloctanoyl):* ***Caprolactin B***
[151379-42-9]
$C_{15}H_{28}N_2O_2$ 268.398
Isol. from a marine bacterium. Cytotoxic agent. $[\alpha]_D^{22}$ +5.4 (c, 1.03 in CH_2Cl_2). Isol. as a mixt. with Caprolactin A. Data given is for the mixt. λ_{max} 219; 274 (sh) (MeOH).

N^3*-(7-Methyloctanoyl):* ***Caprolactin A***
[151379-41-8]
$C_{15}H_{28}N_2O_2$ 268.398
Isol. from a marine bacterium. Cytotoxic agent. Isol. as a mixt. with Caprolactin B. λ_{max} 219; 274 (MeOH) (Berdy).

(±)-*form* [17929-90-7]
Cryst. (EtOAc). Mp 68-71° Mp 147-149°. $Bp_{0.1}$ 105°.

Hydrochloride: [29426-64-0]
Mp 294-296°.

Picrate:
Needles (H_2O). Mp 233° dec.

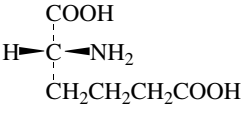
N-*Ac:*
$C_8H_{14}N_2O_2$ 170.211
Cryst. (EtOAc). Mp 160-162°.

N-*Benzoyl:*
$C_{13}H_{16}N_2O_2$ 232.282
Cryst. (EtOH). Mp 203-211°.

Pellegata, R. *et al., Synthesis*, 1978, 614 (*synth, S-form*)
Boyle, W.J. *et al., J.O.C.*, 1979, **44**, 4841 (*synth*)
Davidson, B.S. *et al., Tetrahedron*, 1993, **49**, 6569-6574 (*Caprolactins*)
Uchikawa, J. *et al., J. Het. Chem.*, 1994, **31**, 877 (*N-Ac, N-benzoyl*)
Sakai, K. *et al., Tetrahedron: Asymmetry*, 2003, **14**, 3713-3718 (***resoln***)

2-Aminohexanedioic acid, 9CI A-316

2-Aminoadipic acid. Homoglutamic acid
[542-32-5]



(*R*)-*form*

$C_6H_{11}NO_4$ 161.157
pK_{a3} 9.73 (20°, 0.1*M* KNO_3).

▶ MO1852000

(*R*)-*form* [7620-28-2]
Obt. from hydrol. of Penicillin N.
Cryst. (H_2O). Mp 205-207°. $[\alpha]_D^{20}$ -25 (5*M* HCl).

(*S*)-*form* [1118-90-7]
Found in leaves, roots and seeds of green plants e.g. *Linaria annua*. Prod. by the green alga *Ulva rigida*. Also from fungi and microorganisms. Cryst. (EtOH aq.). Mp 204-206° dec. $[\alpha]_D^{20}$ +25 (5*M* HCl).

6-Amide: 6-Oxolysine, 9CI. 5-Carbamoylnorvaline, 8CI. 2-Amino-5-carbamoylpentanoic acid. 2-Aminoadipamic acid. Homoglutamine
[7433-32-1]
$C_6H_{12}N_2O_3$ 160.172
Cryst. (EtOH aq.). Mp 185-187°. $[\alpha]_D^{20}$ +21.1 (c, 1 in 1*M* HCl). $[\alpha]_D^{25}$ +1.5 (c, 0.6 in H_2O).

(±)-*form* [626-71-1]
Platelets (H_2O, >20°), cryst. + $1H_2O$ (H_2O, Spar. sol. H_2O, EtOH, Et_2O. Mp 206° (anhyd.) dec.

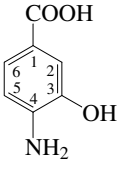
6-Amide: [34218-76-3]
Cryst. (EtOH aq.). Mp 191°.

[5632-90-6, 14258-23-2]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 498B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 591B (*ir*)
Waalkes, T.P. *et al., J.A.C.S.*, 1950, **72**, 5760 (*synth*)
Greenstein, J.P. *et al., J.A.C.S.*, 1953, **75**, 1994-1995 (*resoln, props*)
Abraham, E.P. *et al., Nature (London)*, 1953, **172**, 395 (*R-form, isol*)
Berg, A.M. *et al., Acta Chem. Scand.*, 1954, **8**, 358 (*occur*)
Trown, P.W. *et al., Biochem. J.*, 1963, **86**, 280-284 (*biosynth*)
Blaha, K. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 304-315 (*ord*)
Kimura, R. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1301-1307 (*(±)-Homoglutamine*)
Ghislandi, V. *et al., Farmaco, Ed. Sci.*, 1971, **26**, 474 (*abs config*)
Lerch, E. *et al., Helv. Chim. Acta*, 1974, **57**, 1584-1597 (*synth*)
Kondo, M. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 1171-1173 (*synth*)
Yoshifuji, S. *et al., Chem. Pharm. Bull.*, 1987, **35**, 2994-3001 (*Homoglutamine*)
Low, J.N. *et al., Acta Cryst. C*, 1988, **44**, 1762-1764 (*cryst struct*)
Pellicciari, R. *et al., Synth. Commun.*, 1988, **18**, 1707-1713 (*synth*)
Pham, T. *et al., J.O.C.*, 1994, **59**, 3676-3680 (*synth, pmr, cmr*)
Takano, S. *et al., Synthesis*, 1994, 601-604 (*S-form, synth, pmr*)

4-Amino-3-hydroxybenzoic acid A-317

[2374-03-0]



$C_7H_7NO_3$ 153.137
Microbial degradation product of Chloramphenicol, C-292.
Plates (EtOH aq.).
Mp 216°. pK_a 4.59.

Me ester: [63435-16-5]
$C_8H_9NO_3$ 167.164
Local anaesthetic (no longer in widespread use). Plates (C_6H_6 or H_2O). Mp 120-121°. Log P 1.28 (calc).

Et ester: [87081-52-5]
$C_9H_{11}NO_3$ 181.191
Plates ($CHCl_3$/petrol). Mp 98°.

5-Dodecenyl ester: 5-Dodecenyl 4-amino-3-hydroxybenzoate. ***Antibiotic B 5354A****. B 5354A*
[207570-66-9]
$C_{19}H_{29}NO_3$ 319.443
Prod. by marine bacterium SANK 71896. Sphingosine kinase inhibitor. λ_{max} 229 (ϵ 10200); 281 (ϵ 9200); 295 (ϵ 16100); 309 (ϵ 12700) (MeOH).

7-Z-Tetradecenyl ester: 7-Tetradecenyl 4-amino-3-hydroxybenzoate. ***Antibiotic B 5354C****. B 5354C*
[207570-68-1]
$C_{21}H_{33}NO_3$ 347.497
Prod. by marine bacterium SANK 71896. Sphingosine kinase inhibitor. Powder. λ_{max} 203 (ϵ 16300); 229 (ϵ 9700); 281 (ϵ 8500); 309 (ϵ 11800) (MeOH).

2,7-Tetradecadienyl ester (2E,7ξ): 2,7-Tetradecadienyl 4-amino-3-hydroxybenzoate. ***Antibiotic B 5354B****. B 5354B*
[207570-67-0]
$C_{21}H_{31}NO_3$ 345.481
Prod. by marine bacterium SANK 71896. Sphingosine kinase inhibitor. λ_{max} 203 (ϵ 16600); 229 (ϵ 16600); 283 (ϵ 8800); 309 (ϵ 12200) (MeOH).

N-*Ac:* [10098-40-5]
$C_9H_9NO_4$ 195.174
Solid. Mp 249-250°.

Me ether: 4-Amino-3-methoxybenzoic acid
[2486-69-3]
$C_8H_9NO_3$ 167.164
Mp 186-188°.

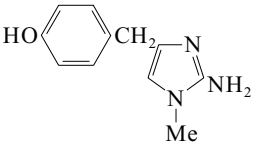
Me ether; Me ester: [41608-64-4]
$C_9H_{11}NO_3$ 181.191
Prisms (MeOH). Mp 126-127°.

Hexyl ether: 4-Amino-3-hexyloxybenzoic acid
[61566-68-5]
$C_{13}H_{19}NO_3$ 237.298
Cryst. (CCl_4). Mp 114-116°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1123A; 1124B (*nmr*)
Einhorn, A. *et al., Annalen*, 1900, **311**, 26-77 (*synth, Me ester, Et ester*)
Lingens, F. *et al., Biochim. Biophys. Acta*, 1966, **130**, 345-354 (*N-Ac, synth*)
Seydel, J.K. *et al., J. Med. Chem.*, 1977, **20**, 439 (*hexyl ether, synth*)
Buess, M.L. *et al., Org. Mass Spectrom.*, 1984, **22**, 233 (*N-14 nqr*)
Rizzacasa, M.A. *et al., Aust. J. Chem.*, 1988, **41**, 1087 (*Me ether, Me ester*)
Singh, S. *et al., J. Med. Chem.*, 1995, **38**, 3217 (*N-Ac*)
Japan. Pat., 1998, 98 101 630; *CA*, **129**, 3906t (*Antibiotic B 5354*)
Kono, K. *et al., J. Antibiot.*, 2000, **53**, 753-758; 759-764 (*Antibiotic B 5354*)
Sellarajah, S. *et al., J. Med. Chem.*, 2004, **47**, 5515-5534 (*Me ether*)
Anderluh, P.S. *et al., J. Med. Chem.*, 2005, **48**, 3110-3113 (*Et ester, synth, pmr, ms*)

2-Amino-4-(4-hydroxybenzyl)-1-methyl-1*H*-imidazole A-318

*4-[(2-Amino-1-methyl-1*H*-imidazol-4-yl)methyl]phenol.* ***Dorimidazole A***
[138935-50-9]

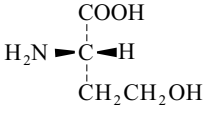


$C_{11}H_{13}N_3O$ 203.243
Alkaloid from the nudibranch *Notodoris gardineri* and *Notodoris citrina*. Anthelminthic, antiparasitic. Yellow powder; cryst. (MeCN) (as hydrobromide).
Mp 175-176° (hydrobromide). λ_{max} 228 (ϵ); 269 (ϵ); 297 (ϵ); 300 (ϵ) (MeOH) (Derep). λ_{max} 228; 269; 297; 360 (MeOH) (Berdy).

Alvi, K.A. *et al., J. Nat. Prod.*, 1991, **54**, 1509-1515 (*isol, uv, pmr, cmr, ms, struct, synth*)
Molina, P. *et al., J.O.C.*, 1999, **64**, 2540-2544 (*synth, pmr, cmr*)

2-Amino-4-hydroxybutanoic acid A-319

Homoserine, 9CI
[498-19-1]



(*S*)–*form*

$C_4H_9NO_3$ 119.12

(*S*)-*form*
L-form
[672-15-1]
Present in germinating peas, Jack bean seeds (*Canavalia ensiformis*) and the seedlings of many leguminous plants. Intermediate in the conversion of Aspartic acid, A-697 into 2-Amino-4-mercaptobutanoic acid and α-ketobutyrate in microbia and fungi.
Mp 203° dec. $[\alpha]_D^{26}$ -8.8 (c, 5 in H_2O).

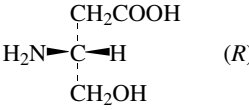
N,N,N-*Tri-Me, betaine:*
$C_7H_{15}NO_3$ 161.2
Occurs as diacylglycerol esters in *Xerocomus langbianensis*. Also in green alga *Monostroma nitidum*.

[53949-21-6, 55596-53-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 580C; 580D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 880B; 880C; 881A (*nmr*)
Guenther, D. *et al., Chem. Ber.*, 1964, **97**, 159 (*synth*)
Kollonitsch, A. *et al., J.A.C.S.*, 1964, **86**, 1857 (*synth*)
Miyoshi, M. *et al., Chem. Lett.*, 1973, 5 (*abs config*)
Lawrence, J.M. *et al., Phytochemistry*, 1973, **12**, 2207 (*isol*)
Curran, W.V. *et al., Prep. Biochem.*, 1981, **11**, 269 (*resoln*)
Baldwin, J.E. *et al., Tetrahedron*, 1988, **44**, 637 (*synth*)
Seebach, D. *et al., Annalen*, 1989, 1215 (*synth*)
Shiraiwa, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2322-2325 (*R-form, S-form, synth*)
Kiet, T.T. *et al., J. Basic Microbiol.*, 2002, **42**, 133-136 (*Xerocomus glycerides*)

3-Amino-4-hydroxybutanoic acid, 9CI A-320

γ-Hydroxy-β-aminobutyric acid. GOBAB
[589-44-6]



(*R*)-*form*

$C_4H_9NO_3$ 119.12
Antiinflammatory, antifungal and antiseptic agent.

(*R*)-*form* [16504-56-6]
Hydrochloride: [196950-52-4]
Mp 177-178°.

*Lactone: 4-Aminodihydro-2(3*H*)-furanone. β-Amino-γ-butyrolactone*
$C_4H_7NO_2$ 101.105
Mp 175-177° (as hydrochloride). $[\alpha]_D^{20}$ +56.7 (c, 1 in H_2O).

N-*Benzyl, lactone:* [152783-42-1]
$C_{11}H_{13}NO_2$ 191.229
Oil. $[\alpha]_D^{25}$ +16.5 (c, 1.0 in $CHCl_3$).

(*S*)-*form* [16504-57-7]
Pharmacol. active isomer.
Lactone: Mp 198-201° (as hydrobromide). $[\alpha]_D^{20}$ -42.6 (c, 1.08 in H_2O).

N-*Benzoyl, lactone:*
$C_{11}H_{11}NO_3$ 205.213
Mp 123.5-126°. $[\alpha]_D^{20}$ -97 (c, 1.41 in $CHCl_3$).

N-tert-*Butyloxycarbonyl, lactone:*
$C_9H_{15}NO_4$ 201.222
Solid. Mp 113-114° (106-108°). $[\alpha]_D^{25}$ -54.3 (c, 1.15 in $CHCl_3$).

N-*Benzyloxycarbonyl, lactone:*
$C_{12}H_{13}NO_4$ 235.239
Cryst. Mp 103-105°. $[\alpha]_D^{20}$ -54.9 (c, 2.27 in $CHCl_3$).

N-*Trifluoroacetyl, benzyl ester:* [673470-50-3]
$C_{13}H_{14}F_3NO_4$ 305.253
Cryst. solid. Mp 70-71°. $[\alpha]_D^{22.5}$ +9.1 (c, 0.99 in $CHCl_3$).

(±)-*form* [16504-55-5]
Needles. Mp 184°.
Lactone: [16504-58-8]
Mp 185-186° (as hydrochloride).
Lactone, N-*benzyl:* [157037-11-1]
$C_{11}H_{13}NO_2$ 191.229
Oil.

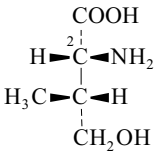
(ξ)-*form*
O-*(4-Hydroxybenzoyl),* N,N,N-*tri-Me, betaine: 1-Carboxy-3-[(4-hydroxybenzoyl)oxy]*-N,N,N-*trimethyl-2-propanaminium, inner salt, 9CI.* ***Zooxanthellabetaine A***
[208256-89-7]
$C_{14}H_{19}NO_5$ 281.308
Isol. from the cultures of a symbiotic dinoflagellate *Symbiodinium* sp. Oil. $[\alpha]_D^{20}$ -13 (c, 0.0035 in MeOH). Zooxanthellabetaine B also isol. but struct. not fully determined.

Jolles, P. *et al., Bull. Soc. Chim. Fr.*, 1951, 862-863 (*synth*)
Chibnall, A.C. *et al., Biochem. J.*, 1958, **68**, 122-128 (*synth*)
Nagai, K. *et al., Arzneim.-Forsch.*, 1967, **17**, 1575-1577 (*synth, isomers, pharmacol*)
Kim, Y.B. *et al., Arch. Pharmacal Res.*, 1985, **8**, 1-6; *CA*, **103**, 98858d (*cryst struct*)
McGarvey, G.J. *et al., J.A.C.S.*, 1986, **108**, 4943-4952 (*lactone N-benzyloxycarbonyl, synth, ir, pmr*)
Hvidt, T. *et al., Can. J. Chem.*, 1988, **66**, 779-782 (*synth, pmr, cmr*)
Hanessian, S. *et al., Can. J. Chem.*, 1993, **71**, 1407-1411 (*lactone, N-tert-butyloxycarbonyl, synth, ir, pmr*)
Maude, A.B. *et al., J.C.S. Perkin 1*, 1997, 2513-2526 (*synth, ir, pmr*)
Calvisi, G. *et al., Synlett*, 1997, 71-74 (*lactone, synth, pmr*)
Nakamura, H. *et al., Bull. Chem. Soc. Jpn.*, 1998, **71**, 781-787 (*Zooanthellabetaine A*)

El Hadri, A. *et al., J. Med. Chem.*, 2002, **45**, 2824-2831 (*N-benzyl lactone, synth*)
Jackson, R.F.W. *et al., Org. Biomol. Chem.*, 2004, **2**, 110-113 (*N-trifluoroacetyl benzyl ester, synth, pmr, cmr*)

2-Amino-4-hydroxy-3-methylbutanoic acid A-321

4-Hydroxyvaline, 9CI



(2R,3R)–form

$C_5H_{11}NO_3$ 133.147

Assignment of props. of stereoisomers uncertain (error in the most recent paper).

(2*R*,3*R*)-*form*
D-iso-*form*
[74431-59-7]
Mp 274°. $[\alpha]_D^{20}$ -8.1 (c, 1 in H_2O). $[\alpha]_{365}^{25}$ -22.7 (c, 1 in H_2O).

(2*R*,3*S*)-*form*
D-allo-*form*
[74431-62-2]
Mp 248°. $[\alpha]_D^{20}$ -10.1 (c, 1 in H_2O). $[\alpha]_{365}^{25}$ -26.9 (c, 1 in H_2O).

(2*S*,3*R*)-*form*
L-allo-*form*
[74431-61-1]
Mp 274°. $[\alpha]_D^{20}$ +8.6 (c, 1 in H_2O). $[\alpha]_{365}^{25}$ +26.4 (c, 1 in H_2O).

(2*S*,3*S*)-*form*
L-iso-*form*
[74431-60-0]
Isol. from crowngall tumours of *Kalanchoe daigremontiana*.
Mp 248°. $[\alpha]_D^{20}$ +10.6 (c, 1 in H_2O). $[\alpha]_{365}^{25}$ +23.3 (c, 1 in H_2O).

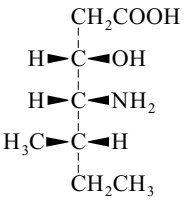
(2*S*)-*form*
L-form
Mp 215° Mp 228° (dimorph.). $[\alpha]_D^{20}$ +10 (H_2O).

(2*RS*,3*RS*)-*form*
(±)-iso-*form*
[127181-57-1]
Mp 230°.

(2*RS*,3*SR*)-*form*
(±)-allo-*form*
[127181-56-0]
Mp 225° (206°).

(2*R*,3*S*)-*form*
Lactone, N-*Ac:* **N-*Acetyl-4-hydroxyvaline lactone***. *3-(Acetylamino)dihydro-4-methyl-2(3*H*)-furanone*
[271796-14-6]
$C_7H_{11}NO_3$ 157.169
Prod. by a marine *Streptomyces* sp. Glassy solid. $[\alpha]_D$ +20.1 (c, 0.01 in MeOH).
Pollard, J.K. *et al., Nature (London)*, 1958, **182**, 1356-1357 (*isol, synth*)
Galantay, E. *et al., J.O.C.*, 1963, **28**, 98-102 (*synth*)
Usher, J.J. *et al., J. Chem. Res., Synop.*, 1980, 30; *J. Chem. Res., Miniprint*, 1980, 361-377 (*synth*)
Englisch-Peters, S. *et al., Tetrahedron*, 1989, **45**, 6127-6134 (*synth, pmr*)
Easton, C.J. *et al., Tetrahedron*, 1997, **53**, 1151-1156 (*2S,3S-form, synth, pmr, cmr, isol*)
Hernandez, I.L.C. *et al., J. Nat. Prod.*, 2000, **63**, 664-665 (*lactone N-Ac*)

4-Amino-3-hydroxy-5-methylheptanoic acid, 9CI A-322



$C_8H_{17}NO_3$ 175.227

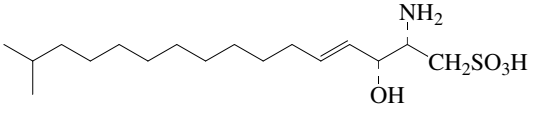
(3*S*,4*R*,5*S*)-*form*
Isostatine
[116261-18-8]
Component of Didemnin A, D-396.
N-tert-*Butyloxycarbonyl:*
Semisolid. $[\alpha]_D$ -8.7 (c, 2.4 in $CHCl_3$).
N-tert-*Butyloxycarbonyl, Me ester:*
Oil. $[\alpha]_D$ -1.5 (c, 1.17 in $CHCl_3$).

(3*R*,4*S*,5*S*)-*form* [114607-51-1]
Component of a depsipeptide isol. from *Tridemnum cyanophorum*.

[116261-18-8, 118812-59-2, 118942-93-1, 119009-32-4, 119009-33-5, 133645-50-8, 135383-55-0]

Guyot, M. *et al., C. R. Hebd. Seances Acad. Sci. Ser. 2*, 1987, **305**, 681-686 (*isol, pmr, ms*)
Rinehart, K.L. *et al., J. Nat. Prod.*, 1988, **51**, 1-21 (*synth*)
Schmidt, U. *et al., Tet. Lett.*, 1988, **29**, 3057-3060 (*synth*)
Hamada, Y. *et al., Tet. Lett.*, 1991, **32**, 931-934 (*synth, deriv*)
Tomioka, K. *et al., Tet. Lett.*, 1991, **32**, 2395-2398 (*synth*)
Lloyd-Williams, P. *et al., J.C.S. Perkin 1*, 1994, 1969-1974 (*synth, bibl*)
Kazmaier, U. *et al., Tet. Lett.*, 1999, **40**, 479-482 (*synth*)

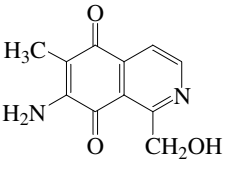
2-Amino-3-hydroxy-15-methyl-4-hexadecene-1-sulfonic acid A-323



$C_{17}H_{35}NO_4S$ 349.534

(2*S*,3*R*,4*E*)-*form*
N-*(2*R*-Hydroxy-13-methyltetradecanoyl):* [205322-93-6]
$C_{32}H_{63}NO_6S$ 589.919
Isol. from the marine bacterium *Cyclobacterium marinus*.
Batrakov, S.G. *et al., Biochim. Biophys. Acta*, 1998, **1391**, 79-91 (*isol*)

7-Amino-1-hydroxymethyl-6-methyl-5,8-isoquinolinedione, 9CI A-324



$C_{11}H_{10}N_2O_3$ 218.212

O-*Angeloyl:* ***Cribrostatin 3***
[276682-84-9]
$C_{16}H_{16}N_2O_4$ 300.313
Alkaloid from *Cribrochalina* sp. Cytotoxic agent. Orange-red needles (CH_2Cl_2/MeOH). Mp 190-192°.

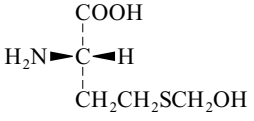
N^7-*Me,* O-*angeloyl:* ***Cribrostatin 5***
[276682-90-7]
$C_{17}H_{18}N_2O_4$ 314.34
Alkaloid from *Cribrochalina* sp. Cytotoxic agent. Red-brown plates ($MeOH/CH_2Cl_2$).

N^7-*(2-Sulfoethyl),* O-*angeloyl:* ***Cribrostatin 7***
[683276-94-0]
$C_{18}H_{20}N_2O_7S$ 408.431
Alkaloid from a *Petrosia* sp. Cytotoxic agent. Dark red film. λ_{max} 210 (ϵ 14500); 282 (ϵ 6500); 338 (ϵ 2000); 474 (ϵ 1700) (MeOH).

Pettit, G.R. *et al., J. Nat. Prod.*, 2000, **63**, 793-798 (*Cribrostatin 3, Cribrostatin 5*)
Sandoval, I.T. *et al., Nat. Prod. Res.*, 2004, **18**, 89-93 (*Cribrostatin 7*)

2-Amino-4-(hydroxymethylthio)butanoic acid A-325

S-*Hydroxymethylhomocysteine*
[23460-00-6]

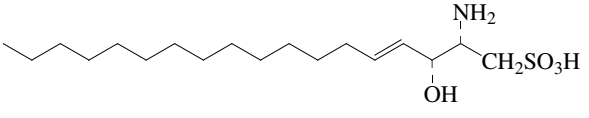


$C_5H_{11}NO_3S$ 165.213

(*S*)-*form*
L-*form*
[6414-80-8]
Isol. from the seaweed *Chondrus ocellatus.*
238-239. $[\alpha]_D$ -73 (c, 1 in H_2O).

Green, M. *et al., J. Biol. Chem.*, 1957, **225**, 387
Takagi, M. *et al., CA*, 1966, **64**, 5326 (*isol*)
Fujiwara, T. *et al., CA*, 1971, **75**, 87282 (*isol*)
Nakagawa, S. *et al., Phytother. Res.*, 1989, **3**, 50 (*props*)

2-Amino-3-hydroxy-4-octadecene-1-sulfonic acid A-326



$C_{18}H_{37}NO_4S$ 363.561

(2*S*,3*R*)-*form*
erythro-*form*

N-*Tetradecanoyl: 1-Deoxydihydroceramide-1-sulfonic acid*
$C_{32}H_{63}NO_5S$ 573.919
Isol. from lipids of the marine diatom *Nitzschia alba*. The name 1-deoxydihydroceramide-1-sulfonic acid actually refers to the mixt. of alkyl homologues (see also below).

N-*Tetradecenoyl:*
$C_{32}H_{61}NO_5S$ 571.904
Component of 1-deoxydihydroceramide-1-sulfonic acid from *Nitzschia alba*. Posn. of double bond not specified.

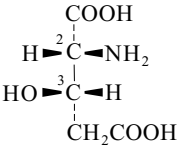
N-*Hexadecanoyl:*
$C_{34}H_{67}NO_5S$ 601.973
Component of 1-deoxydihydroceramide-1-sulfonic acid from *Nitzschia alba*.

N-*3-Hexadecenoyl:*
$C_{34}H_{65}NO_5S$ 599.957
Component of 1-deoxydihydroceramide-1-sulfonic acid from *Nitzschia alba*.

Ohashi, K. *et al., Tetrahedron*, 1989, **45**, 2557

2-Amino-3-hydroxypentanedioic acid A-327

3-Hydroxyglutamic acid, 9CI
[533-62-0]



(2*R*,3*S*)–*form*

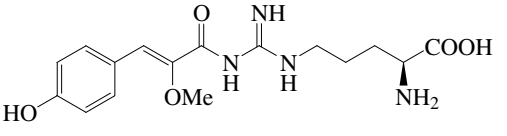
$C_5H_9NO_5$ 163.13

(2*S*,3*S*)-*form*
(+)-erythro-*form*
[6209-00-3]
Found in the ganglions of various molluscs. Neurotransmitter.

[2897-27-0, 5985-23-9, 13593-84-5, 13593-85-6, 17268-00-7, 17598-55-9, 18304-61-5, 23150-61-0, 25541-20-2, 26367-39-5, 32221-84-4, 34266-86-9, 67685-10-3, 115246-61-2, 131320-40-6, 134733-90-7]

Futagawa, S. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 3308 (*nmr*)
Watanabe, K. *et al., Symp. Biol. Hung.*, 1988, **36**, 77 (*rev, props*)
Shiomkawa, S. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1398 (*2S,3S-form*)

2-Amino-5-[[[[3-(4-hydroxyphenyl)-2-methoxy-2-propenoyl]amino](imino)methyl]amino]pentanoic acid A-328

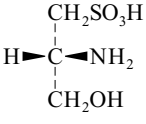


$C_{16}H_{22}N_4O_5$ 350.374
Isol. from the ascidian *Atriolum robustum*. Amorph. solid. $[\alpha]_D^{25}$ -3.2 (c, 0.15 in H_2O). λ_{max} 295 (ϵ 34000) (H_2O).

Kehraus, S. *et al., J. Med. Chem.*, 2004, **47**, 2243-2255 (*isol*)

2-Amino-3-hydroxy-1-propanesulfonic acid A-329

Cysteinolic acid
[3687-17-0]



(*R*)–*form*

$C_3H_9NO_4S$ 155.174
Stereochem. and registry nos. are confused. Wickberg states that the L-form was isol., but his exptl. work shows clearly that it was D (i.e. *S* as it is related to D-Cysteine). CAS uses the same registry no. for L- (in 8CI) and (*S*-)(in 10CI).

(*R*)-*form*
L-*form*
Isol. from red alga *Polysiphonia fastigiata.*
Mp 279-281° dec. $[\alpha]_D$ -6 (c, 2.0 in H_2O).

(*S*)-*form*
D-*form*
Isol. from brown (e.g. *Hijikia fusiforme*) and green (*Ulva pertusa*, *Enteromorpha linza*) algae. Also from diatoms, e.g. *Navicula pelliculosa* and from the starfish *Asterina pectinifera*.
Mp 279-282° dec. $[\alpha]_D$ +7 (H_2O).

[15509-62-3, 16421-58-2, 56942-41-7]

Wickberg, B. *et al., Acta Chem. Scand.*, 1957, **11**, 506 (*isol*)
Yoneda, T. *et al., CA*, 1967, **66**, 113388p (*isol*)
Higashiura, K. *et al., J.O.C.*, 1992, **57**, 764 (*synth*)

3-Amino-2-hydroxy-1-propanesulfonic acid, 9CI A-330

[7013-33-4]

$H_2NCH_2CH(OH)CH_2SO_3H$

$C_3H_9NO_4S$ 155.174

Exists as zwitterion in solid state.

(+)-*form* [27740-29-0]

Constit. of marine red alga *Grateloupia livida*.

(±)-*form* [56892-11-6]

Cryst. (50% EtOH). Mp 299.5-300° (280° dec.).

O-*Ac:* [124930-47-8]

$C_5H_{11}NO_5S$ 197.212

Mp 199-202°.

N-*Benzoyl:* [34155-51-6]

[120088-65-5 (Na salt)]

$C_{10}H_{13}NO_5S$ 259.282

Cryst. (EtOH aq.). Mp 263-264°.

N,N-*Di-Me:* [7013-35-6]

[51732-31-1 (Na salt)]

$C_5H_{13}NO_4S$ 183.228

Prisms or needles (H_2O). Mp 223°.

N,N,N-*Tri-Me, betaine: 2-Hydroxy*-N,N,N-*trimethyl-3-sulfo-1-propanaminium hydroxide inner salt, 9CI*

[7013-36-7]

[62594-39-2, 72372-72-6 (H^+), 125484-45-9 (HCl salt)]

$C_6H_{15}NO_4S$ 197.255

Needles or plates (H_2O). Mp 286-287° dec.

N,N,N-*Tri-Me betaine,* O-*(4-methylbenzenesulfonyl):* [706810-31-3]

$C_{13}H_{21}NO_6S_2$ 351.444

Cryst. (MeOH). Mp 245° dec.

Tsunoo, S. *et al., Ber.*, 1935, **68**, 1334-1341 (*synth, N,N-di-Me, N,N,N-tri-Me betaine*)

Bhattacharyya, P.K. *et al., Arch. Biochem. Biophys.*, 1955, **54**, 424-431 (*synth, N-benzoyl, N,N,N-tri-Me betaine*)

Miyazawa, K. *et al., Nippon Suisan Gakkaishi*, 1970, **36**, 109-114; *CA*, **72**, 129412b (*occur*)

Kim, Y.B. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 2010-2012 (*cryst struct*)

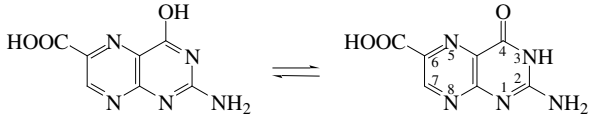
Eur. Pat., 1989, 309 421; *CA*, **112**, 48811y (*O-Ac*)

Condom, M. *et al., Org. Prep. Proced. Int.*, 2003, **35**, 620-622 (*N,N,N-tri-Me betaine O-4-methylbenzenesulfonyl*)

2-Amino-4-hydroxy-6-pteridinecarboxylic acid A-331

*2-Amino-1,4-dihydro-4-oxo-6-pteridinecarboxylic acid. 2-Amino-4(3*H*)-pteridinone-6-carboxylic acid. Pterin-6-carboxylic acid. Ranachrome 5*

[948-60-7]



$C_7H_5N_5O_3$ 207.148

Isol. from various biol. sources incl. human blood, sheep pineals, various amphibians, fish and soybeans. Also from the Chinese drug Jin Yu. Metab. of Pteroylglutamic acid. Cream cryst. Mp 360°.

Me ester: [31010-61-4]

$C_8H_7N_5O_3$ 221.175

Cryst. (DMF). Mp 285° dec.

2-N-*Ac:* [31010-65-8]

$C_9H_7N_5O_4$ 249.185

Cryst. (MeOH). Mp 210°.

2-N-*Ac, Me ester:* [31010-67-0]

$C_{10}H_9N_5O_4$ 263.212

Mp 283°.

7,8-Dihydro: ***7,8-Dihydropterin-6-carboxylic acid***

$C_7H_8N_5O_3$ 210.172

Light emitter of the millipede *Luminodesmus sequoiae.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 896C (*ir*)

Baugh, C.M. *et al., J.O.C.*, 1964, **29**, 3610 (*synth*)

Pfleiderer, W. *et al., Annalen*, 1970, **741**, 64 (*synth, derivs*)

Iwanami, Y. *et al., Tet. Lett.*, 1972, 3219 (*ms*)

Nair, M.G. *et al., J.O.C.*, 1973, **38**, 2185 (*synth*)

Mengel, R. *et al., Chem. Ber.*, 1978, **111**, 3790 (*synth*)

Kohashi, M. *et al., J. Biochem. (Tokyo)*, 1980, **87**, 1581 (*isol*)

Zeitler, M. *et al., Methods Enzymol.*, 1986, **122**, 273 (*isol*)

Sato, N. *et al., J. Het. Chem.*, 1988, **25**, 1737 (*synth, derivs*)

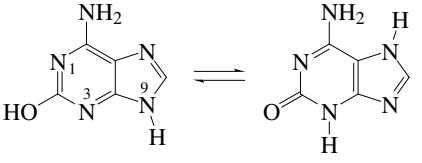
Suga, T. *et al., J. Nat. Prod.*, 1988, **51**, 713 (*isol*)

Kuse, M. *et al., Bioorg. Med. Chem. Lett.*, 2001, **11**, 1037-1040 (*7,8-dihydro*)

6-Amino-2-hydroxypurine A-332

*6-Amino-1,3-dihydro-2*H*-purin-2-one, 9CI. Isoguanine. Guanopterin*

[3373-53-3]



$C_5H_5N_5O$ 151.127

Several tautomers possible. Aglycone from *Croton tiglium*. Isol. from the wings of the butterfly *Prioneris thestylis.* Amorph. powder.

Mp 360°. pK_{a1} 4.47; pK_{a2} 9.03 (20°).

9-(β-D-Arabinofuranosyl): [38819-11-3]

$C_{10}H_{13}N_5O_5$ 283.243

Light yellow powder. Mp 269-272° dec. $[\alpha]_D^{24}$ +29.5 (c, 0.5 in H_2O).

9-β-D-Ribofuranosyl: See Isoguanosine, I-184

*1-Me: 6-Amino-1,3-dihydro-1-methyl-2*H*-purine-2-one, 9CI*

[73691-67-5]

$C_6H_7N_5O$ 165.154

Powder. Mp 300°.

1-Me, 9-β-D-arabinofuranosyl: Ara-doridosine

[77856-33-8]

$C_{11}H_{15}N_5O_5$ 297.27

Shows antiviral props. Plates (H_2O). Mp 223-225° dec. $[\alpha]_D^{24}$ +25.5 (c, 0.5 in H_2O).

1-Me, 6-N-*Ac:* [98933-71-2]

$C_8H_9N_5O_2$ 207.191

Cryst. (MeOH). Mp 222-223° Mp 274° dec.

1-Me, 6,9-di-Ac: [98933-69-8]

$C_{10}H_{11}N_5O_3$ 249.229

Cryst. Mp 222-223° dec. Exists as 6-imino tautomer.

6-N-*Me: 6-(Methylamino)-1,3-dihydro-2*H*-purin-2-one, 9CI.* ***2-Hydroxy-6-methylamino-9H-purine***

[24391-35-3]

$C_6H_7N_5O$ 165.154

Isol. from the blue coral NIO-156 and from the bacterium *Pseudomonas syringae.* Cytokinin. Sol. H_2O. λ_{max} 265; 282 (MeOH) (Berdy).

1,3-Di-Me: ***1,3-Dimethylisoguanine****. 1,3-Dimethylisoguaninium*

[191614-40-1]

$C_7H_9N_5O$ 179.181

Isol. from the sponges *Amphimedon viridis* and *Amphimedon paraviridis.* Also from *Cnemidocarpa bicornuta*. Powder; cryst. (as salt). Isol. by different groups both as the free base and as salts protonated on the imino N. λ_{max} 207 (log ϵ 4.5); 295 (log ϵ 3.9) (MeOH).

3,7-Di-Me: ***3,7-Dimethylisoguanine***

[18904-09-1]

$C_7H_9N_5O$ 179.181

Isol. from the Caribbean sponge *Agelas longissima* and *Zyzzya fuliginosa*. Sol. MeOH, butanol. λ_{max} 245 (ϵ 8500); 285 (ϵ 9900) (MeOH) (Berdy).

N^3,O-*Di-Me:* ***Mucronatine***†

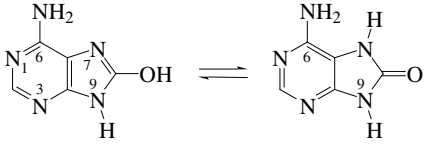
$C_7H_9N_5O$ 179.181

Isol. from the sponge *Stryphnus mucronatus.* Solid. Mp 200-202°. Tautomeric.

Spies, J.R. *et al., J.A.C.S.*, 1939, **61**, 350-351 (*Isoguanine, isol*)
Purrmann, R. *et al., Annalen*, 1940, **544**, 182-190 (*Isoguanine, isol*)
Taylor, E.C. *et al., J.A.C.S.*, 1959, **81**, 2442-2448 (*Isoguanine, synth, uv*)
Veillard, A. *et al., J. Chim. Phys.*, 1962, **59**, 1056-1066 (*pmr*)
Pal, B.C. *et al., J.C.S.*, 1964, 400-405 (*ir*)
Pettit, G.R. *et al., J. Nat. Prod.*, 1976, **39**, 363-367 (*Isoguanine, isol*)
Yamazaki, A. *et al., Nucleic Acids Res.*, 1976, **3**, 251-259 (*Isoguanine, synth*)
Nachman, R.J. *et al., J.C.S. Perkin 1*, 1985, 1315-1321 (*1-Me, 1-Me-6,9-di-Ac, synth, cmr, pmr, ms, uv, ir, cryst struct*)
Farooqi, A.H.A. *et al., Phytochemistry*, 1990, **29**, 2061-2063 (*6-N-Me, isol*)
Cafieri, F. *et al., Tet. Lett.*, 1995, **36**, 7893-7896 (*3,7-Dimethylisoguanine*)
Mitchell, S.S. *et al., J. Nat. Prod.*, 1997, **60**, 727-728 (*1,3-Dimethylisoguanine*)
Chehade, C.C. *et al., J. Nat. Prod.*, 1997, **60**, 729-731 (*1,3-Dimethylisoguanine*)
Do Prado, G.M.T *et al., Acta Cryst. C*, 1999, **55**, 1585-1587 (*1,3-di-Me, cryst struct*)
Bourguet-Kondracki, M.-L. *et al., Tet. Lett.*, 2001, **42**, 7257-7259 (*Mucronatine*)
Jeong, S-J. *et al., Chem. Pharm. Bull.*, 2003, **51**, 731-733 (*1,3-Dimethylisoguaninium*)
Blas, J.R. *et al., J.A.C.S.*, 2004, **126**, 154-164 (*tautom*)
Bats, J.W. *et al., Acta Cryst. E*, 2006, **62**, 2040-2042 (*cryst struct*)

6-Amino-8-hydroxypurine A-333

*6-Amino-1,7-dihydro-8*H*-purin-8-one, 9CI. 6-Amino-8-purinol, 8CI. 7,8-Dihydro-8-oxoadenine. 8-Hydroxyadenine. 8-Oxoadenine*
[21149-26-8]



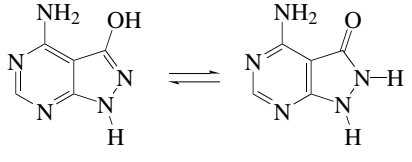
$C_5H_5N_5O$ 151.127

8-Oxo-form predominates. Other tautomers are possible. Results *in vivo* from hydroxylation of DNA by OH radicals. Found in the urine of humans suffering from leukaemia. Isol. from the ascidian *Symplegma rubra*. Potential cause of DNA mismatch in mutagenesis. Needles + $^1/_2H_2SO_4$.
Mp 300° (H_2SO_4). Unlike 2-Amino-6,8-dihydroxypurine, A-272, is not particularly mutagenic.

Lindsay, B.S. *et al., J. Nat. Prod.*, 1999, **62**, 1573-1575 (*Symplegma rubra constit*)

4-Amino-3-hydroxy-1*H*-pyrazolo[3,4-*d*]pyrimidine A-334

*4-Amino-1,2-dihydro-3*H*-pyrazolo[3,4-*d*]pyrimidin-3-one, 9CI.*
Akalone
[128850-54-4]

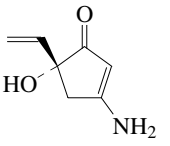


$C_5H_5N_5O$ 151.127
Prod. by the marine bacterium *Agrobacterium aurantiacum* and *Flavobacterium* sp. N-81106. Xanthine oxidase inhibitor. Powder or light green needles. Sol. bases, DMSO; poorly sol. MeOH, hexane, $CHCl_3$.
Mp>350°. λ_{max} 269 (ϵ 1690) (H_2O).

Anderson, J.D. *et al., J. Het. Chem.*, 1990, **27**, 439-453 (*synth*)
Japan. Pat., 1993, 93 317 070; *CA*, **120**, 189879d (*isol*)
Izumida, H. *et al., J. Mar. Biotechnol.*, 1995, **2**, 115-118 (*isol, ir, cmr, pmr*)

3-Amino-5-hydroxy-5-vinyl-2-cyclopenten-1-one A-335

3-Amino-5-ethenyl-5-hydroxy-2-cyclopenten-1-one, 9CI



$C_7H_9NO_2$ 139.154
Incorrect struct. given in CAS.

(R)-form
Myrothenone B
[878633-73-9]
[858126-05-3]
Prod. by *Streptomyces* sp. GT-20026114 obt. from the mangrove plant *Aegiceras comiculatum* and from a marine-derived fungus *Myrothecium* sp.
Yellowish oil. $[\alpha]_D^{20}$ +127.1 (c, 1.54 in MeOH). $[\alpha]_D^{20}$ +35 (c, 0.6 in MeOH). λ_{max} 270 (MeOH). λ_{max} 203 (log ϵ 3.7); 268 (log ϵ 4) (MeOH).

N-*Formyl:* ***Myrothenone A***
$C_8H_9NO_3$ 167.164
Prod. by *Myrothecium* sp. Tyrosinase inhibitor. Oil. $[\alpha]_D^{20}$ +61 (c, 0.6 in MeOH). λ_{max} 203 (log ϵ 3.7); 272 (log ϵ 4.2) (MeOH).

N-*Methoxycarbonyl:* [878633-74-0]
$C_9H_{11}NO_4$ 197.19
Prod. by *Streptomyces* sp. GT-20026114. Yellowish oil. $[\alpha]_D^{20}$ +67.6 (c, 1.16 in MeOH). λ_{max} 261 (MeOH).

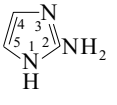
N,N-*Di-Me:* ***3-(Dimethylamino)-5-hydroxy-5-vinyl-2-cyclopenten-1-one****. 3-(Dimethylamino)-5-ethenyl-5-hydroxy-2-cyclopenten-1-one*
[179422-20-9]
Isol. from *Trichoderma koningii*.
Amorph. powder. Sol. H_2O, MeOH, $CHCl_3$, DMSO; fairly sol. Me_2CO, MeCN, EtOAc; poorly sol. hexane.
Mp 137-139°. $[\alpha]_D^{20}$ +69.3 (c, 0.2 in H_2O). Biol. inactive. λ_{max} 280 (ϵ 30000) (MeOH).

N-*[2-(4-Hydroxyphenyl)ethyl]:* [878633-75-1]
$C_{15}H_{17}NO_3$ 259.304
Prod. by *Streptomyces* sp. GT-20026114. Yellowish oil. $[\alpha]_D^{20}$ +59.3 (c, 1.73 in MeOH). λ_{max} 232 (MeOH).

Mukhopadhyay, T. *et al., J. Antibiot.*, 1996, **49**, 210-211 (*N,N-di-Me*)
Li, X. *et al., Chem. Pharm. Bull.*, 2005, **53**, 453-455 (*Myrothenones A,B, isol, pmr, cmr, ms*)
Lin, W. *et al., J. Antibiot.*, 2005, **58**, 594-598 (*isol, cd, pmr, cmr, ms*)

2-Aminoimidazole, 8CI A-336

*1*H*-Imidazol-2-amine, 9CI. 2-Aminoglyoxaline*
[7720-39-0]



$C_3H_5N_3$ 83.093
Isol. from the sponges *Halichondria* sp. and *Reniera cratera*. Also occurs in the seeds of the legume *Mundulea sericea*, and has been shown to be a precursor of the antibiotic 2-Nitroimidazole in *Streptomyces eurocidicus*.

Hydrochloride: [57575-96-9]
Mp 152°. Hygroscopic.

Nitrate: Mp 135-136°.

Sulfate (2:1): [1450-93-7]
[42383-61-9] Mp 270° dec.

Picrate: Mp 236°.

2-N-*Ac: 2-Acetamidoimidazole*
[52737-49-2]

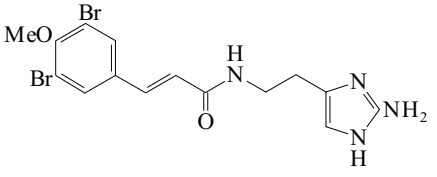
$C_5H_7N_3O$ 125.13
Mp 285° (270-275°) dec.

1-Me: [6646-51-1]
$C_4H_7N_3$ 97.119
Prismatic needles (EtOH/EtOAc) (as hydrochloride). Mp 84° (hydrochloride).

[1450-94-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 614D (*ir*)
Lawson, A. *et al., J.C.S.*, 1956, 307 (*synth*)
Seki, Y. *et al., J. Biochem. (Tokyo)*, 1970, **67**, 389 (*isol, ir, pmr*)
Cimino, G. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1974, **47**, 895 (*isol, uv, pmr, ms*)
Fellows, L.E. *et al., Phytochemistry*, 1977, **16**, 1399 (*isol, pmr, ms*)
Kirk, K.L. *et al., J.O.C.*, 1978, **43**, 4381-4383 (*synth, pmr*)
Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1984, 124-125; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 126-127 (*isol, Halichondria*)
Weinmann, H. *et al., Tet. Lett.*, 2002, **43**, 593-595 (*synth, ir, pmr*)
Yano, S. *et al., Chem. Pharm. Bull.*, 2004, **12**, 3443-3450 (*1-Me, synth, pmr*)

N-[2-(2-Amino-1*H*-imidazol-4-yl)ethyl]-3-(3,5-dibromo-4-methoxyphenyl)-2-propenamide, 9CI A-337



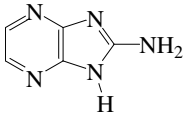
$C_{15}H_{16}Br_2N_4O_2$ 444.125

(*E*)-*form* [160491-72-5]
Metab. from the Caribbean sponge *Verongula* sp.
Amorph. solid (as trifluoroacetate). CAS no. refers to trifluoroacetate.

Ciminiello, P. *et al., J. Nat. Prod.*, 1994, **57**, 1564 (*isol, uv, ir, pmr, cmr, struct*)

2-Amino-1*H*-imidazo[4,5-*b*]pyrazine A-338

*1*H-*Imidazo[4,5-*b*]pyrazin-2-amine. **Zarzissine***



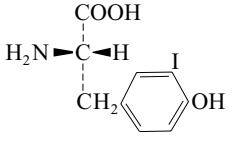
$C_5H_5N_5$ 135.128

Struct. of Zarzissine revised in 2001. Alkaloid from the Mediterranean sponge *Anchinoe paupertas*. Cytotoxic. Active against *Candida*, bacteria and some tumour lines. Cryst. (H_2O or MeOH).
Mp >300° dec. λ_{max} 217 (sh); 244 (log ε 3.3); 318 (log ε 4.03) (MeOH). λ_{max} 206 (log ε 4.31); 230 (sh); 282 (sh); 326 (log ε 5.39) (MeOH/NaOH).

Bouaicha, N. *et al., J. Nat. Prod.*, 1994, **57**, 1455 (*isol*)
Wan, Z.K. *et al., Tetrahedron*, 2001, **57**, 5497-5507 (*synth, uv, pmr, cmr*)

2-Amino-3-(3-iodo-4-hydroxyphenyl)propanoic acid A-339

3-Iodotyrosine, 9CI. Monoiodotyrosine. Iotyrosine



(*S*)–*form*

$C_9H_{10}INO_3$ 307.087
^{131}I labelled compd. is used as a radioactive agent. Log P -1.15 (uncertain value) (calc).

(*S*)-*form*
L-form
[70-78-0]
Occurs in thyroid tissue and human blood serum. Prod. by sponges, *Dendrodoa grossularia*, *Heterochordaria abietina*, *Polysiphonia urceolata*, *Undaria pinnatifida* and *Sargassum thunbergii*.
Cryst. (H_2O). Sol. hot H_2O.
Mp 202-204°. $[\alpha]_D^{20}$ -4.4 (c, 5 in 1*M* HCl).

Me ester: [70277-02-0]
$C_{10}H_{12}INO_3$ 321.114
Mp 211-212° (hydrochloride). $[\alpha]_D$ -6 (c, 0.5 in CH_2Cl_2).

N-*Benzoyl, Me ester:* [188594-27-6]
$C_{17}H_{16}INO_4$ 425.222
Cryst. (CH_2Cl_2/hexane). Mp 123-124°. $[\alpha]_D$ +11 (c, 0.5 in CH_2Cl_2).

N-tert-*Butyloxycarbonyl, Me ester:* [79677-59-1]
$C_{15}H_{20}INO_5$ 421.231
Solid (CH_2Cl_2/hexane). Mp 111-112°. $[\alpha]_D^{25}$ +46 (c, 1 in $CHCl_3$). $[\alpha]_D^{25}$ +14 (c, 1.0 in MeOH).

N-*Benzyloxycarbonyl, Me ester:* [79677-60-4]
$C_{18}H_{18}INO_5$ 455.248
Solid (CH_2Cl_2/hexane). Mp 101-102°. $[\alpha]_D^{25}$ +49 (c, 1 in $CHCl_3$). $[\alpha]_D^{25}$ +2 (c, 1 in MeOH).

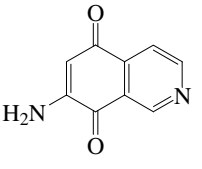
(±)-*form*
Cryst. + $1H_2O$ (H_2O). Mp 200-201° dec.

[16624-40-1, 19254-01-4, 20520-42-7, 60345-92-8, 70277-02-0, 78758-99-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 256C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1189B (*nmr*)
Harington, C.R. *et al., Biochem. J.*, 1944, **38**, 320 (*synth*)
Pitt-Rivers, R. *et al., Chem. Ind. (London)*, 1956, 21 (*synth*)
Hillman, G. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1956, **305**, 177-181 (*synth*)
Wynn, J. *et al., Arch. Biochem. Biophys.*, 1960, **88**, 98-104 (*radioactive exps.*)
Amaral, A.D. *et al., CA*, 1972, **77**, 111749 (*occur*)
Ito, K. *et al., CA*, 1977, **86**, 3897 (*occur*)
Bednar, J. *et al., Radiochem. Radioanal. Lett.*, 1980, **45**, 377-386 (*use*)
Baron, M.H. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1983, **80**, 729-737 (*Raman*)
Okabe, N. *et al., Acta Cryst. C*, 1995, **51**, 1700-1701 (*cryst struct*)
Morera, E. *et al., Synth. Commun.*, 2001, **31**, 2215-2222 (*S-form, Boc Me ester, benzyloxycarbonyl Me ester*)
Khatyr, A. *et al., Synthesis*, 2001, 1665-1670 (*Me ester, N-benzoyl Me ester*)

7-Amino-5,8-isoquinolinedione A-340

7-Amino-5,8-isoquinolinequinone



$C_9H_6N_2O_2$ 174.159

N^7-*Me: 7-(Methylamino)-5,8-isoquinolinedione, 9CI. **Caulibugulone A***
[662167-15-9]
$C_{10}H_8N_2O_2$ 188.185
Alkaloid from the marine bryozoan *Caulibugula intermis*.
Cytotoxic. Dark red solid. λ_{max} 237 (log ε 4.24); 268 (log ε 4.1); 451 (log ε 3.61) (MeOH).

N^7-*(2-Hydroxyethyl): 7-[(2-Hydroxyethyl)amino]-5,8-isoquinolinedione. **Caulibugulone D***
[662167-18-2]
$C_{11}H_{10}N_2O_3$ 218.212
Alkaloid from *Caulibugula intermis*. Cytotoxic. Dark orange solid.
λ_{max} 273 (log ε 3.95); 450 (log ε 3.35) (MeOH).

N^7-*Me, 5-imine: **Caulibugulone E***
[662167-19-3]
$C_{10}H_9N_3O$ 187.201

Alkaloid from *Caulibugula intermis*. Cytotoxic. Dark orange solid (as TFA salt). λ_{max} 213 (log ϵ 3.71); 245 (log ϵ 3.75); 441 (log ϵ 3.09) (MeOH) (TFA salt).

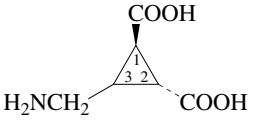
N^7-*Me, 5-(2-hydroxyethyl)imide:* ***Caulibugulone F***
[662167-20-6]
$C_{12}H_{13}N_3O_2$ 231.254
Alkaloid from *Caulibugula intermis*. Cytotoxic. Dark orange solid (as TFA salt). λ_{max} 215 (log ϵ 3.79); 245 (log ϵ 3.75); 440 (log ϵ 3.16) (MeOH) (TFA salt).

6-Chloro, N^7*-Me: 6-Chloro-7-(methylamino)-5,8-isoquinolinedione.* ***Caulibugulone B***
[662167-17-1]
$C_{10}H_7ClN_2O_2$ 222.63
Alkaloid from *Caulibugula intermis*. Cytotoxic. Dark red solid. λ_{max} 251 (log ϵ 4.03); 274 (log ϵ 3.97); 475 (log ϵ 3.36) (MeOH).

6-Bromo, N^7*-Me: 6-Bromo-7-(methylamino)-5,8-isoquinolinedione.* ***Caulibugulone C***
[662167-16-0]
$C_{10}H_7BrN_2O_2$ 267.082
Alkaloid from *Caulibugula intermis*. Cytotoxic. Dark red solid. λ_{max} 254 (log ϵ 4); 272 (log ϵ 3.97); 474 (log ϵ 3.49) (MeOH).

Milanowski, D.J. *et al., J. Nat. Prod.*, 2004, **67**, 70-73 (*Caulibugulones, isol, pmr, cmr*)
Wipf, P. *et al., Org. Biomol. Chem.*, 2004, **2**, 2173-2174 (*synth, activity*)
Alagille, D. *et al., Tet. Lett.*, 2004, **45**, 6179-6181 (*synth*)

3-(Aminomethyl)-1,2-cyclopropanedicarboxylic acid A-341



(1α,2β)-*form*

$C_6H_9NO_4$ 159.141

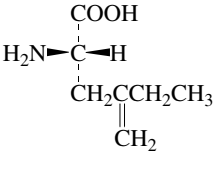
(1α,2β)-*form*
N,N,N-*Tri-Me, betaine:* ***Dysibetaine CPa***
[673499-58-6]
$C_9H_{15}NO_4$ 201.222
Isol. from the marine sponge *Dysidea herbacea*. Amorph. solid. $[\alpha]_D^{18}$ -8.1 (c, 0.12 in H_2O).

(1α,2α,3β)-*form*
N,N,N-*Tri-Me, betaine, monoamide:* ***Dysibetaine CPb***
[673499-60-0]
$C_9H_{16}N_2O_3$ 200.237
Isol. from *Dysidea herbacea*. Amorph. solid. $[\alpha]_D^{18}$ +8.5 (c, 0.13 in H_2O).

Sakai, R. *et al., J.O.C.*, 2004, **69**, 1180-1185 (*isol, cd, pmr, cmr*)

2-Amino-4-methylenehexanoic acid A-342

4-Methylenenorleucine, 9CI

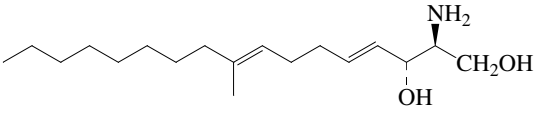


$C_7H_{13}NO_2$ 143.185

(S)-form [252663-79-9]
Isol. from the sponge *Plakortis simplex*. Cytotoxic agent. Solid. $[\alpha]_D^{25}$ -2 (c, 0.005 in MeOH).

Cafieri, F. *et al., Tetrahedron*, 1999, **55**, 13831-13840

2-Amino-9-methyl-4,8-heptadecadiene-1,3-diol A-343



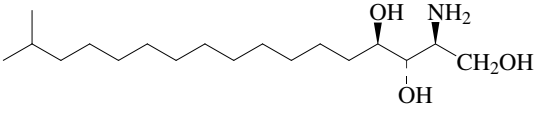
$C_{18}H_{35}NO_2$ 297.48

(2*S*,3*R*,4*E*,8*E*)-*form*
N-*Hexadecanoyl, 1-*O-α-D-*glucopyranoside:* ***Thraustochytroside C***
[251565-82-9]
$C_{40}H_{75}NO_8$ 698.034
Isol. from *Thraustochytrium globosum*.

N-*(2*R*-Hydroxytetradecanoyl), 1-*O-β-D-*glucopyranoside:*
$C_{38}H_{71}NO_9$ 685.98
Isol. from *Cortinarius umidicola*. Amorph. powder (MeOH). $[\alpha]_D^{20}$ +3.5 (c, 0.15 in $CHCl_3$).

Jenkins, K.M. *et al., Tet. Lett.*, 1999, **40**, 7637-7640 (*Thraustochytroside C*)
Liu, J.-K. *et al., Lipids*, 2003, **38**, 669-675 (*Cortinarius glycolipid*)

2-Amino-16-methyl-1,3,4-heptadecanetriol A-344



$C_{18}H_{39}NO_3$ 317.511

(2*S*,3*S*,4*R*)-*form*
N-*Docosanoyl, 1-*O-*(2-acetamido-2-deoxy-β-D-glucopyranoside):* ***Halicylindroside A$_1$***
[161842-86-0]
$C_{48}H_{94}N_2O_9$ 843.279
Isol. from the sponge *Halichondria cylindrata*. Solid. $[\alpha]_D^{23}$ -20.2 (c, 0.2 in Py).

N-*(2*R*-Hydroxyhexadecanoyl), 1-*O-β-D-*glucopyranoside:* ***Linckiacerebroside A****. LLC 2-1*
$C_{40}H_{79}NO_{10}$ 734.065
Isol. from the starfish *Linckia laevigata*. Amorph. powder. Mp 214°. $[\alpha]_D$ +18.9 (c, 0.18 in 1-propanol).

N-*(2*R*-Hydroxydocosanoyl), 1-*O-*(2-acetamido-2-deoxy-β-D-glucopyranoside):* ***Halicylindroside B$_4$***
[161842-93-9]
$C_{48}H_{94}N_2O_{10}$ 859.278
Isol. from the sponge *Halichondria cylindrata*. Solid. $[\alpha]_D^{23}$ -8.5 (c, 0.15 in Py).

N-*(2*R*-Hydroxydocosanoyl), 1-*O-*[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)-[6-deoxy-α-D-galactopyranosyl-(1→3)]-2-acetamido-2-deoxy-β-D-glucopyranoside]:*
$C_{62}H_{117}N_3O_{19}$ 1208.615
Constit. of *Aplysinella rhax*.
$[\alpha]_D^{25}$ +2.6 (c, 0.07 in MeOH).

N-*(2*R*-Hydroxytetracosanoyl), 1-*O-α-D-*galactopyranoside:* ***Agelasphin 9b***
[148766-51-2]
$C_{48}H_{95}NO_{10}$ 846.279
Isol. from the sponge *Agelas mauritianus*. Immunostimulant. Mp 211-212°. $[\alpha]_D^{24}$ +55 (c, 1 in Py).

N-*(2*R*-Hydroxytetracosanoyl), 1-*O-β-D-*galactopyranoside:* **Stellaster *Cerebroside S-2b-16***
[160398-20-9]
$C_{48}H_{95}NO_{10}$ 846.279
Isol. from the starfish *Stellaster equestris*. Amorph. powder. Mp 129-131°. $[\alpha]_D$ +3.8 (c, 1 in Py).

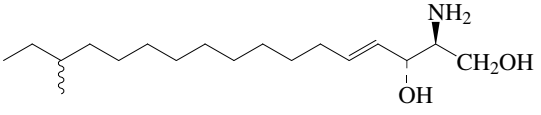
N-*(2*R*-Hydroxytetracosanoyl), 1-*O-β-D-*glucopyranoside:* **Stellaster *Cerebroside S-2a-11***
[122823-48-7]
$C_{48}H_{95}NO_{10}$ 846.279

Isol. from the starfishes *Asterina pectinifera* and *Stellaster equestris*. Amorph. powder.
Mp 146-148°. $[\alpha]_D$ +10.7 (c, 0.1 in 1-propanol).

N-*(2*R*-Hydroxyhexacosanoyl), 1*-O-*[2-acetamido-2-deoxy-β-*D*-galactopyranosyl-(1→4)-[6-deoxy-α-*D*-galactopyranosyl-(1→3)]-2-acetamido-2-deoxy-β-*D*-glucopyranoside]:*
$C_{66}H_{125}N_3O_{19}$ 1264.722
Isol. from *Aplysinella rhax*.
$[\alpha]_D^{25}$ +1.8 (c, 0.05 in MeOH).

Higuchi, R. *et al., Annalen*, 1990, 51-55; 1996, 593-599 (*Stellaster cerebrosides*)
Natori, T. *et al., Tetrahedron*, 1994, **50**, 2771-2784 (*Agelasphin 9b*)
Li, H.-Y. *et al., Tetrahedron*, 1995, **51**, 2273-2280 (*Halicylindrosides*)
Borbone, N. *et al., Eur. J. Org. Chem.*, 2001, 4651-4656 (*Aplysinella rhax cerebrosides*)
Maruta, T. *et al., Chem. Pharm. Bull.*, 2005, **53**, 1255-1258 (*Linckiacerebroside A*)

2-Amino-15-methyl-4-heptadecene-1,3-diol A-345



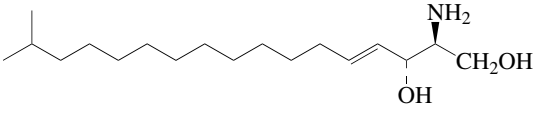
$C_{18}H_{37}NO_2$ 299.496

(2*S*,3*R*,4*E*,15ξ)-*form*

N-*(15*Z*-Tetracosenoyl), 1*-O-*β-D-glucopyranoside: CE 1-3*
[204199-66-6]
$C_{48}H_{91}NO_8$ 810.249
Isol. from the sea cucumber *Cucumaria echinata*.

Yamada, K. *et al., Eur. J. Org. Chem.*, 1998, 371-378 (*CE 1-3*)

2-Amino-16-methyl-4-heptadecene-1,3-diol A-346



$C_{18}H_{37}NO_2$ 299.496

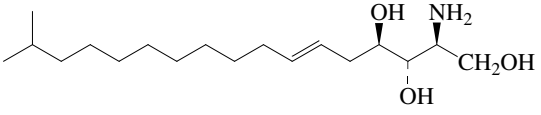
(2*S*,3*R*,4*E*)-*form*

N-*Docosanoyl:* C_{22}*-Ceramide*
[206992-48-5]
$C_{40}H_{79}NO_3$ 622.069
Isol. from the sponge *Haliclona koremella*. Powder. $[\alpha]_D^{25}$ -6 (c, 0.01 in MeOH). λ_{max} 206 (ε 1990) (MeOH).

N-*(21-Methyldocosanoyl):* ***Oceanapin D***
[155661-04-4]
$C_{41}H_{81}NO_3$ 636.096
Isol. from the sponge *Oceanapia* cf. *tenuis*. Powder (hexane).
Mp 70-72°.

Mancini, I. *et al., Helv. Chim. Acta*, 1994, **77**, 51-58 (*Oceanapin D*)
Hattori, T. *et al., J. Nat. Prod.*, 1998, **61**, 823-826 (*C22-Ceramide*)

2-Amino-16-methyl-6-heptadecene-1,3,4-triol A-347



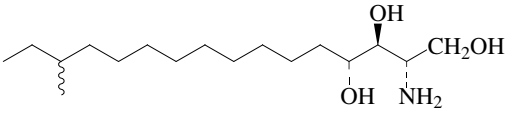
$C_{18}H_{37}NO_3$ 315.495

(2*S*,3*S*,4*R*,6*E*)-*form*

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*[α-D-galactopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Amphimelibioside B***
$C_{52}H_{99}NO_{15}$ 978.352
Isol. from an *Amphimedon* sp. Powder.

Emura, C. *et al., J.O.C.*, 2005, **70**, 3031-3038 (*Amphimelibioside B*)

2-Amino-14-methyl-1,3,4-hexadecanetriol A-348



$C_{17}H_{37}NO_3$ 303.484

(2*S*,3*S*,4*R*,14ξ)-*form*

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*β-D-glucopyranoside: CE 3-2*
[204199-70-2]
$C_{45}H_{89}NO_{10}$ 804.199
Isol. from the sea cucumber *Cucumaria echinata*. Amorph. powder.
Mp 147-149°. $[\alpha]_D$ +10.2 (c, 0.63 in 1-propanol).

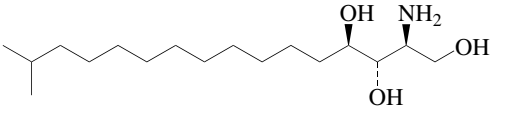
N-*(2*R*-Hydroxydocosanoyl), 1*-O-*[β-D-galactopyranosyl-(1→4)-β-D-glucopyranoside]:* ***Luidialactoside B***
[503856-70-0]
$C_{51}H_{99}NO_{15}$ 966.341
Isol. from the starfish *Luidia maculata*. Amorph. powder.
Mp 235-237°. $[\alpha]_D^{27}$ +7.6 (c, 0.56 in $CHCl_3$/MeOH).

N-*(2*R*-Hydroxy-15*Z*-tetracosenoyl), 1*-O-*β-D-glucopyranoside: CE 3-1*
[204199-68-8]
$C_{47}H_{91}NO_{10}$ 830.237
Isol. from the sea cucumber *Cucumaria echinata*. Amorph. powder.
Mp 138-140°. $[\alpha]_D$ +5.8 (c, 0.13 in 1-propanol).

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*[α-L-fucopyranosyl-(1→4)-*N*-acetyl-α-D-neuraminopyranosyl-(2→2′)-*N*-glycolyl-α-D-neuraminopyranosyl-(2→4)-*N*-acetyl-α-D-neuraminopyranosyl-(2→6)-β-D-glucopyranoside]:* ***HPG 7***
Major component isol. from sea cucumber *Holothuria pervicax*. Amorph. powder.
Mp 185-190°.

Yamada, K. *et al., Eur. J. Org. Chem.*, 1998, 371-378 (*CE 3-1, CE 3-2*)
Yamada, K. *et al., Chem. Pharm. Bull.*, 2000, **48**, 157-159 (*HPG 7*)
Inagaki, M. *et al., Eur. J. Org. Chem.*, 2003, 325-331 (*Luidialactoside B*)

2-Amino-15-methyl-1,3,4-hexadecanetriol A-349



$C_{17}H_{37}NO_3$ 303.484

(2*S*,3*S*,4*R*)-*form*

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*β-D-galactopyranoside:* **Stellaster *Cerebroside S-2b-7***
[178153-50-9]
$C_{45}H_{89}NO_{10}$ 804.199
Isol. from the starfish *Stellaster equestris*. Amorph. powder.
Mp 132-134°. $[\alpha]_D$ +3.9 (c, 0.7 in Py).

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*β-D-glucopyranoside:* **Stellaster *Cerebroside S-2a-3*.** *LLC 2-8*
[122823-44-3]
$C_{45}H_{89}NO_{10}$ 804.199
Isol. from the starfishes *Asterina pectinifera*, *Linckia laevigata* and *Stellaster equestris*. Amorph. powder.
Mp 144-147°. $[\alpha]_D$ +11 (c, 0.1 in 1-propanol).

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*(2-acetamido-2-deoxy-β-D-glucopyranoside):* ***Halicylindroside B₃***

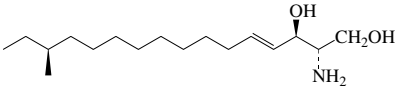
[161842-92-8]
$C_{47}H_{92}N_2O_{10}$ 845.251
Isol. from the sponge *Halichondria cylindrata*. Solid. $[\alpha]_D^{23}$ -9.7 (c, 0.15 in Py).

N-*(2*R*-Hydroxytricosanoyl), 1*-O-*(2-acetamido-2-deoxy-β-*D*-glucopyranoside):* ***Halicylindroside B5***
[161842-94-0]
$C_{48}H_{94}N_2O_{10}$ 859.278
Isol. from the sponge *Halichondria cylindrata*. Solid. $[\alpha]_D^{23}$ -8.6 (c, 0.15 in Py).

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*[α-L-arabinofuranosyl-(1→3)-α-D-galactopyranosyl-(1→4)-*N*-acetyl-α-D-neuraminosyl-(2→6)-β-D-galactofuranosyl-(1→3)-[α-L-arabinofuranosyl-(1→4)]-α-D-galactopyranosyl-(1→4)-*N*-acetyl-α-D-neuraminosyl-(2→3)-β-D-galactopyranosyl-(1→4)-β-D-glucopyranoside]:* ***Ganglioside GP3****. GP3*
$C_{101}H_{179}N_3O_{54}$ 2299.513
Major ganglioside from *Asterina pectinifera*. Amorph. powder.

Higuchi, R. *et al., Annalen*, 1990, 50-51; 1996, 593-599 (*Stellaster cerebrosides*)
Li, H.-Y, *et al., Tetrahedron*, 1995, **51**, 2273-2280 (*Halicylindrosides*)
Maruta, T. *et al., Chem. Pharm. Bull.*, 2005, **53**, 1255-1258 (*LLC 2-8*)
Higuchi, R. *et al., Chem. Pharm. Bull.*, 2006, **54**, 287-291 (*GP3*)

2-Amino-14-methyl-4-hexadecene-1,3-diol A-350



(2*S*,3*R*,4*E*,14*S*)-*form*

$C_{17}H_{35}NO_2$ 285.469

(2*S*,3*R*,4*E*,14*S*)-*form*

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*β-D-glucopyranoside:* [153821-87-5]
$C_{45}H_{87}NO_9$ 786.184
Constit. of *Holothuria leucospilota* and *Cucumaria echinata*. Amorph. powder.
Mp 165-170° (160°). $[\alpha]_D$ +5.6 (c, 0.82 in 1-propanol). The earlier isolates of undetermined C-14 config., to which opt. rotn. refers, appear to be identical.

(2*S*,3*R*,4*E*,14ξ)-*form*

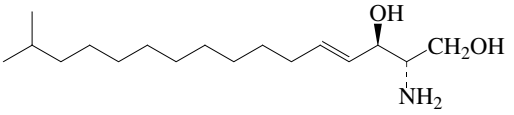
N-*Docosanoyl, 1*-O-*β-D-glucopyranoside:* [157382-83-7]
$C_{45}H_{87}NO_8$ 770.184
Isol. from the sea cucumbers *Cucumaria echinata* and *Pentacta australis*. Amorph. powder.
Mp 138-140°. $[\alpha]_D$ -7.6 (c, 0.89 in 1-propanol).

N-*(2*R*-Hydroxytricosanoyl), 1*-O-*β-D-glucopyranoside:* [153821-88-6]
$C_{46}H_{89}NO_9$ 800.21
Isol. from *Cucumaria echinata* and *Pentacta australis*. Amorph. powder.
Mp 200-205° (185-190°). $[\alpha]_D$ +5.3 (c, 0.96 in 1-propanol).

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*β-D-glucopyranoside:* [153821-89-7]
$C_{47}H_{91}NO_9$ 814.237
Isol. from *Cucumaria echinata* and *Holothuria leucospilota*. Amorph. powder.
Mp 208-212°. $[\alpha]_D$ +5.5 (c, 0.76 in 1-propanol).

Higuchi, R. *et al., Annalen*, 1994, 79-81; 653-658 (*Cucumaria echinata cerebrosides*)
Yamada, K. *et al., Eur. J. Org. Chem.*, 1998, 371-378 (*Pentacta australis cerebrosides*)
Yamada, K. *et al., Chem. Pharm. Bull.*, 2005, **53**, 788-791; 1333-1334 (*Holothuria leucospilota cerebrosides*)

2-Amino-15-methyl-4-hexadecene-1,3-diol A-351



$C_{17}H_{35}NO_2$ 285.469

(2*S*,3*R*,4*E*)-*form*

N-*(21-Methyldocosanoyl):* ***Oceanapin B***
[155661-02-2]
$C_{40}H_{79}NO_3$ 622.069
Isol. from the sponge *Oceanapia* cf *.tenuis*. Powder (hexane).
Mp 63-68°.

N-*Tricosanoyl:* ***Oceanapin C***
[155661-03-3]
$C_{40}H_{79}NO_3$ 622.069
Isol. from the sponge *Oceanapia* cf. *tenuis*. Powder (hexane).
Mp 65-70°.

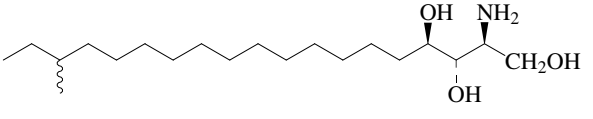
N-*(2*R*-Hydroxyoctadecanoyl), 1*-O-*[*N*-acetyl-8-O-sulfo-α-D-neuraminopyranosyl-(2→6)-β-D-glucopyranoside]:* ***SCG-2***
[76688-82-9]
$C_{52}H_{96}N_2O_{20}S$ 1101.398
Major component of the ganglioside complex from the sea cucumber *Stichopus chloronotus*.

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*[*N*-(α-L-fucopyranosyloxy)acetyl-α-D-neuraminopyranosyl-(2→6)-β-D-glucopyranoside]:* ***SCG-3***
[552322-45-9]
$C_{62}H_{114}N_2O_{22}$ 1239.583
Major component of the ganglioside complex from the sea cucumber *Stichopus chloronotus*.

N-*(2*R*-Hydroxy-15Z-tetracosenoyl), 1*-O-*[*N*-hydroxyacetyl-α-D-neuraminopyranosyl-(2→6)-β-D-glucopyranoside]:* ***SCG-1***
[77322-99-7]
$C_{58}H_{106}N_2O_{18}$ 1119.478
Major component of the ganglioside complex from the sea cucumber *Stichopus chloronotus*.

Mancini, I. *et al., Helv. Chim. Acta*, 1994, **77**, 51-58 (*Oceanapins*)
Yamada, K. *et al., Chem. Pharm. Bull.*, 2003, **51**, 46-52 (*SCG gangliosides*)

2-Amino-17-methyl-1,3,4-nonadecanetriol A-352



$C_{20}H_{43}NO_3$ 345.565

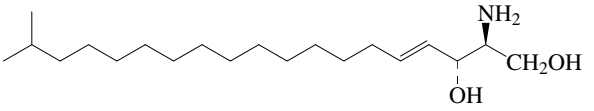
(2*S*,3*S*,4*R*,17ξ)-*form*

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*β-D-glucopyranoside:* [157382-84-8]
$C_{48}H_{95}NO_{10}$ 846.279
Isol. from *Pentacta australis*. Amorph. powder.
Mp 217-220°. $[\alpha]_D$ +6.2 (c, 0.79 in 1-propanol).

N-*(2*R*-Hydroxytricosanoyl), 1*-O-*β-D-glucopyranoside:* [157382-85-9]
$C_{49}H_{97}NO_{10}$ 860.306
Isol. from *Pentacta australis*. Amorph. powder.
Mp 215-220°. $[\alpha]_D$ +9.4 (c, 0.3 in 1-propanol).

Higuchi, R. *et al., Annalen*, 1994, 653-658 (*isol, pmr, cmr*)

2-Amino-18-methyl-4-nonadecene-1,3-diol A-353



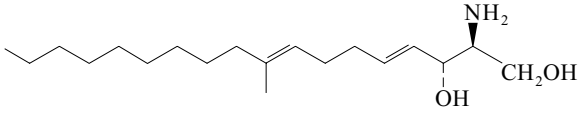
$C_{20}H_{41}NO_2$ 327.549

(2S,3R,4E)-form

N-*(2*R*-Hydroxy-11ξ-methyltridecanoyl), 1*-O-*sulfate:* ***Calyceramide B***
[346425-30-7]
$C_{34}H_{67}NO_7S$ 633.972
Isol. from the sponge *Discodermia calyx*. Neuraminidase inhibitor. Solid (as Na salt). $[\alpha]_D^{20}$ +14.5 (c, 0.1 in MeOH) (Na salt).
Nakao, Y. *et al., Tetrahedron*, 2001, **57**, 3013-3017 (*isol, ir, pmr, cmr*)

2-Amino-9-methyl-4,8-octadecadiene-1,3-diol A-354

9-Methyl-4,8-sphingadienine



$C_{19}H_{37}NO_2$ 311.507

(2S,3R,4E,8E)-form

N-*Hexadecanoyl:* [105243-35-4]
$C_{35}H_{67}NO_3$ 549.919
Isol. from the mushroom *Panellus serotinus*. Amorph. powder. $[\alpha]_D^{21}$ -11.6 (c, 0.09 in $CHCl_3$).

N-*Hexadecanoyl, 1*-O-α-D-*glucopyranoside:* ***Thraustochytroside B***
[251565-81-8]
$C_{41}H_{77}NO_8$ 712.061
Isol. from *Thraustochytrium globosum*. Amorph. solid.

N-*(9Z,12Z-Octadecadienoyl):* [448933-55-9]
$C_{37}H_{67}NO_3$ 573.941
Isol. from the mushrooms *Lyophyllum connatum* and *Panellus serotinus*. Amorph. powder. $[\alpha]_D^{30}$ -13.3 (c, 0.08 in $CHCl_3$).

N-*(2*R*-Hydroxytetradecanoyl):* [448933-57-1]
$C_{33}H_{63}NO_4$ 537.865
Isol. from the mushroom *Amanita pantherina*. Amorph. powder. $[\alpha]_D^{20}$ +6.3 (c, 0.2 in $CHCl_3$).

N-*(2*R*-Hydroxypentadecanoyl):* [448933-56-0]
$C_{34}H_{65}NO_4$ 551.892
Isol. from the mushrooms *Amanita pantherina* and *Sarcodon aspratus*. Amorph. powder. $[\alpha]_D^{21}$ +7 (c, 0.1 in $CHCl_3$).

N-*(2*R*-Hydroxyhexadecanoyl):* [95673-08-8]
$C_{35}H_{67}NO_4$ 565.919
Isol. from the mushrooms *Amanita pantherina*, *Lepista nuda* (wood blewit) and *Sarcodon aspratus*. Amorph. powder. $[\alpha]_D^{19}$ +7.5 (c, 0.1 in $CHCl_3$).

N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-β-D-*glucopyranoside:* ***Cerebroside B***
[88642-46-0]
$C_{41}H_{77}NO_9$ 728.061
From *Pachybasium* sp., *Clitocybe* spp. and *Schizophyllum commune*. Shows elicitor activity. Cell differentiation inducer; fruiting body formation enhancer. Antifungal agent.
Mp 180-190°. $[\alpha]_D^{20}$ +5.2 (c, 1 in MeOH). $[\alpha]_D^{19}$ -7.4 (c, 0.3 in $CHCl_3$).

N-*(2*R*-Hydroxy-3-hexadecenoyl), 1*-O-β-D-*glucopyranoside:* ***Cerebroside A***
[115681-40-8]
$C_{41}H_{75}NO_9$ 726.045
Isol. from a *Pachybasium* sp. Shows elicitor activity. Cell differentiation inducer; fruiting body formation enhancer. Antifungal agent. Cryst. Sol. MeOH.
Mp 170-178°. $[\alpha]_D^{20}$ -6.7 (c, 1 in MeOH).

N-*(2*R*-Hydroxyheptadecanoyl), 1*-O-β-D-*glucopyranoside:*
[120029-71-2]
$C_{42}H_{79}NO_9$ 742.087
Isol. from *Polyporus ellisii*. Amorph. powder.
Mp 154-156°. $[\alpha]_D^{26}$ +4.9 (c, 0.4 in MeOH).

N-*(2*R*-Hydroxyoctadecanoyl):* ***Lactariamide B***
[372178-04-6]
$C_{37}H_{71}NO_4$ 593.972
Isol. from the fungus *Lactarius volemus* (tawny milkcap mushroom). Amorph. powder. $[\alpha]_D^{20}$ +8.4 (c, 0.39 in MeOH). Stereochem. not confirmed.

N-*(2*R*-Hydroxyoctadecanoyl), 1*-O-β-D-*glucopyranoside:* ***Cerebroside D***
[113773-89-0]
$C_{43}H_{81}NO_9$ 756.114
From a *Pachybasium* sp. Shows elicitor activity. Cell differentiation inducer; fruiting body formation enhancer. Cryst. Sol. MeOH.
Mp 178-189°. $[\alpha]_D^{20}$ +4.9 (c, 1 in MeOH).

N-*(2*R*-Hydroxy-3-octadecenoyl), 1*-O-β-D-*glucopyranoside:* ***Cerebroside C***
[98677-33-9]
$C_{43}H_{79}NO_9$ 754.098
Isol. from a *Pachybasium* sp. and *Penicillium funiculosum*. Also isol. (without full stereochem. assignment) from marine fungus *Microsphaeropsis olivacea*. Shows elicitor activity. Cell differentiation inducer; fruiting body formation enhancer. Antifungal agent. Cryst.
Mp 159-169°. $[\alpha]_D^{20}$ -6.2 (c, 1 in MeOH).

N-*(2*R*-Hydroxynonadecanoyl), 1*-O-β-D-*glucopyranoside:*
[852627-54-4]
$C_{44}H_{83}NO_9$ 770.141
Constit. of the soft coral *Lobophytum* sp. Solid.
Mp 218-220°. $[\alpha]_D^{28}$ -13.2 (c, 0.05 in MeOH).

N-*(2*R*-Hydroxyeicosanoyl), 1*-O-β-D-*glucopyranoside:* ***Ircicerebroside***
[854008-50-7]
$C_{45}H_{85}NO_9$ 784.168
Isol. from *Cladiella* sp., *Lobophytum* sp. and *Sinularia* sp. Also from the sponge *Ircinia fasciculata*. Amorph. powder. $[\alpha]_D^{20}$ +9.1 (c, 0.02 in MeOH).

N-*(2*R*-Hydroxyheneicosanoyl), 1*-O-β-D-*glucopyranoside:*
$C_{46}H_{87}NO_9$ 798.195
Isol. from *Cladiella* sp. and *Sinularia* sp.

N-*(2*R*-Hydroxydocosanoyl), 1*-O-β-D-*glucopyranoside:*
$C_{47}H_{89}NO_9$ 812.221
Isol. from *Cladiella* sp. and *Sinularia* sp.

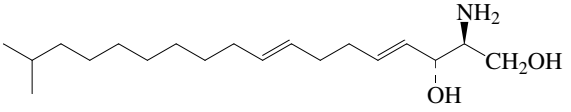
N-*(2*R*-Hydroxy-17Z-tetracosenoyl), 1*-O-β-D-*glucopyranoside:* ***Catacerebroside A***
$C_{49}H_{91}NO_9$ 838.259
Isol. from the fungus *Catathelasma ventricosa*. Amorph. solid. $[\alpha]_D^{20}$ -5 (c, 1.1 in MeOH).

N-*(2*E*-Octadecenoyl), 1*-O-β-D-*glucopyranoside:* [849544-01-0]
$C_{43}H_{79}NO_8$ 738.099
Prod. by a mangrove fungus.

Kawai, G. *et al., Biochim. Biophys. Acta*, 1982, **719**, 612; 1983, **754**, 243 (*isol*)
Kawai, G. *et al., Agric. Biol. Chem.*, 1985, **49**, 2137 (*isol, pmr*)
Kawai, G. *et al., J. Lipid Res.*, 1985, **26**, 338 (*struct*)
Mori, K. *et al., Tetrahedron*, 1985, **41**, 2369; 2379 (*synth*)
Kawai, G. *et al., J. Biol. Chem.*, 1986, **261**, 779-784 (*isol*)
Fogeldal, M. *et al., CA*, 1987, **160**, 29746 (*isol*)
Sitrin, R.D. *et al., J. Antibiot.*, 1988, **41**, 469 (*isol, pmr, cmr, ms, struct*)
Keusgen, M. *et al., Biochem. Syst. Ecol.*, 1996, **24**, 465-468 (*Cerebroside C, isol, marine fungus*)
Striegler, S. *et al., Monatsh. Chem.*, 1996, **127**, 755-761 (*activity*)
Koga, Y. *et al., J. Biol. Chem.*, 1998, **273**, 31985-31991 (*activity, pmr, cmr*)
Jenkins, K.M. *et al., Tet. Lett.*, 1999, **40**, 7637-7640 (*Thraustochytroside B*)
Wang, X.-Z. *et al., J.O.C.*, 2000, **65**, 8146-8151 (*synth*)
Yue, J.-M. *et al., J. Nat. Prod.*, 2001, **64**, 1246-1248 (*Lactariamide B*)
Gao, J.M. *et al., Lipids*, 2001, **36**, 521-527 (*Polyporus ceramide*)

Dmitrenok, A.S. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2001, **50**, 1474-1477 (*Cladiella/Sinularia cerebrosides*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 2002, **50**, 681-684 (*hexadecanoyl, 2-hydroxyacyl, octadecadienoyl*)
Zhan, Z.-J. *et al., J. Nat. Prod.*, 2003, **66**, 1013-1016 (*Catacerebroside A*)
Zhu, F. *et al., CA*, 2005, **142**, 370451c (*N-2-octadecenoyl glucoside*)
Muralidhar, P. *et al., Chem. Pharm. Bull.*, 2005, **53**, 168-171 (*N-2-hydroxynonadecanoyl 1-glucoside*)
Zhang, G.-W. *et al., Helv. Chim. Acta*, 2005, **88**, 885-890 (*Ircicerebroside*)

2-Amino-17-methyl-4,8-octadecadiene-1,3-diol A-355



$C_{19}H_{37}NO_2$ 311.507

(2S,3R,4E,8E)-form

N-*Hexadecanoyl:* [166762-67-0]
$C_{35}H_{67}NO_3$ 549.919
Isol. from the gorgonian *Acabaria undulata*. Solid.
Mp 76-77°. $[\alpha]_D^{25}$ -6 (c, 0.5 in $CHCl_3$).
Shin, J. *et al., J. Nat. Prod.*, 1995, **58**, 948-953 (*N-hexadecanoyl*)

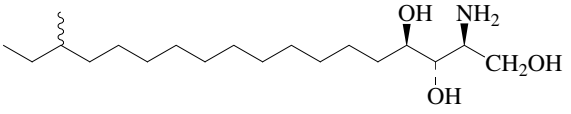
2-Amino-16-methyl-1,3-octadecanediol A-356

$H_3CCH_2CH(CH_3)(CH_2)_{12}CH(OH)CH(NH_2)CH_2OH$
$C_{19}H_{41}NO_2$ 315.538

(2ξ,3ξ,16ξ)-form

N-*(2ξ-Hydroxy-14ξ-methylhexadecanoyl), 1*-O-*β-D-galactofuranoside:* ***Ectyoceramide***
[571194-37-1]
$C_{42}H_{83}NO_9$ 746.119
Constit. of the sponge *Ectyoplasia ferox*. Amorph. solid. $[\alpha]_D^{25}$ -25 (c, 0.11 in MeOH).
Costantino, V. *et al., Eur. J. Org. Chem.*, 2003, 1433-1437 (*Ectyoceramide*)

2-Amino-16-methyl-1,3,4-octadecanetriol A-357



$C_{19}H_{41}NO_3$ 331.538

(2S,3S,4R,16ξ)-form

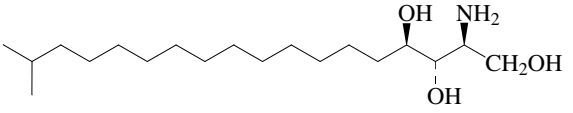
N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-*β-D-glucopyranoside:* ***Luidiacerebroside A***
$C_{41}H_{81}NO_{10}$ 748.092
Isol. from the starfish *Luidia maculata*. Amorph. powder.
Mp 180-181°. $[\alpha]_D^{29}$ +7.7 (c, 0.22 in 1-propanol).

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*β-D-glucopyranoside:* ***Luidiacerebroside B***
$C_{49}H_{97}NO_{10}$ 860.306
Isol. from the starfish *Luidia maculata*. Amorph. powder.
Mp 216-218°. $[\alpha]_D^{29}$ +4.3 (c, 0.22 in 1-propanol).

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*α-D-galactopyranoside:* ***Agelasphin 11***
[152139-44-1]
$C_{49}H_{97}NO_{10}$ 860.306
Isol. from the sponge *Agelas mauritianus*. Immunostimulant.
Mp 189.5-190.5°. $[\alpha]_D^{24}$ +51.9 (c, 1 in Py).

N-*(2*R*-Hydroxypentacosanoyl), 1*-O-*α-D-galactopyranoside:* ***Agelasphin 13***
[155419-38-8]
$C_{50}H_{99}NO_{10}$ 874.333
Isol. from the sponge *Agelas mauritianus*. Immunostimulant.
Mp 215.5-218°. $[\alpha]_D^{24}$ +48.8 (c, 0.5 in Py).
Natori, T. *et al., Tetrahedron*, 1994, **50**, 2771-2784 (*Agelasphins*)
Kawatake, S. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1091-1096 (*Luidiacerebrosides*)

2-Amino-17-methyl-1,3,4-octadecanetriol A-358



$C_{19}H_{41}NO_3$ 331.538

(2S,3S,4R)-form

N-*Docosanoyl, 1*-O-*(2-acetamido-2-deoxy-β-D-glucopyranoside):* ***Halicylindroside A2***
[161842-87-1]
$C_{49}H_{96}N_2O_9$ 857.305
Isol. from the sponge *Halichondria cylindrata*. Solid. $[\alpha]_D^{23}$ -21.1 (c, 0.21 in Py).

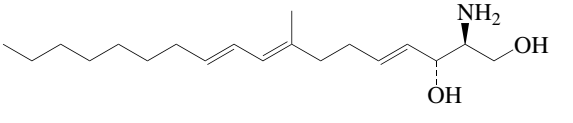
N-*Tricosanoyl, 1*-O-*(2-acetamido-2-deoxy-β-D-glucopyranoside):* ***Halicylindroside A3***
[161842-88-2]
$C_{50}H_{98}N_2O_9$ 871.332
Isol. from the sponge *Halichondria cylindrata*. Solid. $[\alpha]_D^{23}$ -19.5 (c, 0.2 in Py).

N-*Tetracosanoyl, 1*-O-*(2-acetamido-2-deoxy-β-D-glucopyranoside):* ***Halicylindroside A4***
[161842-89-3]
$C_{51}H_{100}N_2O_9$ 885.359
Isol. from the sponge *Halichondria cylindrata*. Solid. $[\alpha]_D^{23}$ -22.3 (c, 0.22 in Py).

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*(2-acetamido-2-deoxy-β-D-glucopyranoside):* ***Halicylindroside B6***
[161842-95-1]
$C_{49}H_{96}N_2O_{10}$ 873.305
Isol. from the sponge *Halichondria cylindrata*. Solid. $[\alpha]_D^{23}$ -8.3 (c, 0.14 in Py).

N-*(2*R*-Hydroxytricosanoyl), 1*-O-*[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)-[6-deoxy-α-D-galactopyranosyl-(1→3)]-2-acetamido-2-deoxy-β-D-glucopyranoside]:*
$C_{64}H_{121}N_3O_{19}$ 1236.669
Isol. from *Aplysinella rhax*.
$[\alpha]_D^{25}$ +2.8 (c, 0.09 in MeOH).
Li, H.-Y. *et al., Tetrahedron*, 1995, **51**, 2273-2280 (*isol, Halicylindrosides*)
Borbone, N. *et al., Eur. J. Org. Chem.*, 2001, 4651-4656 (*Aplysinella rhax cerebroside*)

2-Amino-8-methyl-4,8,10-octadecatriene-1,3-diol A-359



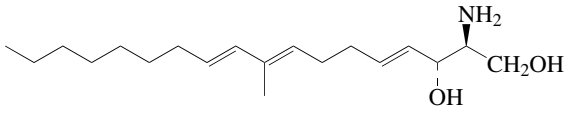
$C_{19}H_{35}NO_2$ 309.491

(2S,3R,4E,8E,10E)-form

N-*(2*R*-Hydroxyhexacosanoyl), 1*-O-*β-D-glucopyranoside:* ***Haliclonacerebroside***
[849618-98-0]
$C_{51}H_{95}NO_9$ 866.313
Constit. of a *Haliclona* sp.
Ayyad, S.-E.N. *et al., CA*, 2005, **142**, 370888a (*Haliclonacerebroside*)

2-Amino-9-methyl-4,8,10-octadecatriene-1,3-diol A-360

9-Methyl-4,8,10-sphingatrienine



$C_{19}H_{35}NO_2$ 309.491

(2*S*,3*R*,4*E*,8*E*,10*E*)-*form*

N-*Hexadecanoyl, 1*-O-α-D-*glucopyranoside:* ***Thraustochytroside A***
[251565-80-7]
$C_{41}H_{75}NO_8$ 710.045
Isol. from *Thraustochytrium globosum.*

N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-β-D-*glucopyranoside:* ***Phallusside 1***
[219308-41-5]
$C_{41}H_{75}NO_9$ 726.045
Constit. of the ascidian *Phallusia fumigata*. Amorph. solid. $[\alpha]_D^{25}$ +7 (c, 0.1 in 1-propanol). Phalluside 4 also isol. Struct. not fully elucidated. λ_{max} 232 (log ϵ 4.43) (MeOH).

N-*(2*R*-Hydroxyheptadecanoyl), 1*-O-β-D-*glucopyranoside:* ***Phalluside 3***
[213622-89-0]
$C_{42}H_{77}NO_9$ 740.072
Isol. from *Phallusia fumigata* and from the starfish *Cosmasterias lurida*. Amorph. solid. $[\alpha]_D^{25}$ +9.4 (c, 0.2 in 1-propanol). Phalluside 4 which is an isomer of Phalluside 3 was also isol. but exact struct. not determined. λ_{max} 233 (log ϵ 4.29) (MeOH).

N-*(2*R*-Hydroxyoctadecanoyl), 1*-O-*sulfate:* [192384-62-6]
$C_{37}H_{69}NO_7S$ 672.021
Isol. from the bryozoan *Watersipora cucullata*. Topoisomerase inhibitor. $[\alpha]_D^{25}$ +16 (c, 0.05 in MeOH). λ_{max} 235 (MeOH) (Berdy).

N-*(2*R*-Hydroxyoctadecanoyl), 1*-O-β-D-*glucopyranoside:* ***Phalluside 2***
[213622-90-3]
$C_{43}H_{79}NO_9$ 754.098
Isol. from *Phallusia fumigata* and from the starfish *Cosmasterias lurida*. Amorph. solid. $[\alpha]_D^{25}$ +10 (c, 0.1 in 1-propanol). λ_{max} 231 (log ϵ 4.52) (MeOH).

N-*(2*R*-Hydroxyeicosanoyl), 1*-O-β-D-*glucopyranoside:* ***Ophidiacerebroside A***
[152247-26-2]
$C_{45}H_{83}NO_9$ 782.152
Isol. from *Ophidiaster ophidiamus.* λ_{max} 225 (MeOH).

N-*(2*R*-Hydroxyheneicosanoyl), 1*-O-β-D-*glucopyranoside:* ***Ophidiacerebroside B***
[152247-27-3]
$C_{46}H_{85}NO_9$ 796.179
Isol. from *Ophidiaster ophidiamus.* λ_{max} 225 (MeOH).

N-*(2*R*-Hydroxydocosanoyl), 1*-O-β-D-*glucopyranoside:* ***Ophidiacerebroside C***. Stellaster *Cerebroside S-1-3*
[152247-25-1]
$C_{47}H_{87}NO_9$ 810.206
Isol. from *Ophidiaster ophidiamus* and *Stellaster equestris.*
Amorph. powder.
Mp 103-105°. $[\alpha]_D$ +9.5 (c, 0.2 in 1-propanol). λ_{max} 230 (log ϵ 4.48) (MeOH).

N-*(2*R*-Hydroxytricosanoyl), 1*-O-β-D-*glucopyranoside:* ***Ophidiacerebroside D***. Stellaster *Cerebroside S-1-4*
[152247-28-4]
$C_{48}H_{89}NO_9$ 824.232
Isol. from *Ophidiaster ophidiamus* and *Stellaster equestris.*
Amorph. powder.
Mp 109-111°. $[\alpha]_D$ +9.9 (c, 0.2 in 1-propanol). λ_{max} 229 (log ϵ 4.55) (MeOH).

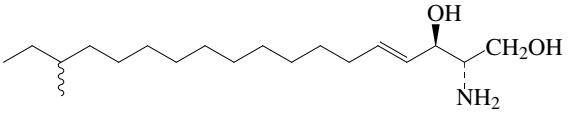
N-*(2*R*-Hydroxytetracosanoyl), 1*-O-β-D-*glucopyranoside:* ***Ophidiacerebroside E***. *Agelasphin 10*. Stellaster *Cerebroside S-1-5*
[152323-72-3]
$C_{49}H_{91}NO_9$ 838.259
Isol. from *Agelas mauritianus, Ophidiaster ophidiamus* and *Stellaster equestris.* Amorph. powder.
Mp 141-142° (98-100°). $[\alpha]_D$ +9.6 (c, 0.2 in propanol). $[\alpha]_D$ -1.6 (c, 1 in propanol). λ_{max} 229 (log ϵ 4.48) (MeOH). λ_{max} 236 (ϵ 5800) (MeOH).

N-*(2*R*-Hydroxypentacosanoyl), 1*-O-β-D-*glucopyranoside:* ***Agelasphin 12***
[155419-37-7]
$C_{50}H_{93}NO_9$ 852.286
Isol. from *Agelas mauritianus.*
Mp 158.5-159.5°. $[\alpha]_D^{24}$ +2.2 (Py). $[\alpha]_D$ -2 (propanol). λ_{max} 236 (ϵ 5500) (MeOH).

N-*(2*R*-Hydroxy-15*Z*-tetracosenoyl), 1*-O-β-D-*glucopyranoside:*
[457645-50-0]
$C_{49}H_{89}NO_9$ 836.243
Isol. from *Allostichaster inaequalis*, *Anasterias minuta* and *Cosmasterias lurida.*

Jin, W. *et al., J.O.C.*, 1994, **59**, 144-147 (*Ophidiacerebrosides*)
Natori, T. *et al., Tetrahedron*, 1994, **50**, 2771-2784 (*Agelasphins*)
Higuchi, R. *et al., Annalen*, 1996, 593-599 (*Stellaster cerebrosides*)
Ojika, M. *et al., Tet. Lett.*, 1997, **38**, 4235-4238 (*Watersipora cucullata constit*)
Maier, M.S. *et al., Lipids*, 1998, **33**, 825-827 (*Cosmasterias lurida derivs*)
Duran, R. *et al., Tetrahedron*, 1998, **54**, 14597-14602 (*Phallusides*)
Jenkins, K.M. *et al., Tet. Lett.*, 1999, **40**, 7637-7640 (*Thraustochytroside A*)
Chludil, H.D. *et al., Z. Naturforsch., C*, 2003, **58**, 433-440 (*Anasterias minuta cerebroside*)

2-Amino-16-methyl-4-octadecene-1,3-diol A-361



$C_{19}H_{39}NO_2$ 313.523

(2*S*,3*R*,4*E*,16ξ)-*form*

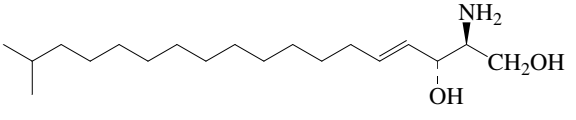
N-*Docosanoyl:* ***Oceanapin E***
[155661-05-5]
$C_{41}H_{81}NO_3$ 636.096
Isol. from the sponge *Oceanapia* cf. *tenuis.* Powder (hexane).
Mp 65-68°.

N-*(21-Methyldocosanoyl):* ***Oceanapin F***
[155661-06-6]
$C_{42}H_{83}NO_3$ 650.123
Isol. from the sponge *Oceanapia* cf. *tenuis.* Powder (hexane).
Mp 70-75°. $[\alpha]_D^{20}$ -2.1 (c, 0.35 in $CHCl_3$).

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*[β-D-galactopyranosyl-(1→4)-β-D-glucopyranoside]:* ***Luidialactoside A***
[503856-65-3]
$C_{55}H_{105}NO_{14}$ 1004.433
Isol. from the starfish *Luidia maculata*. Amorph. powder.
Mp 234-236°. $[\alpha]_D^{27}$ +8.2 (c, 0.17 in $CHCl_3$/MeOH).

Mancini, I. *et al., Helv. Chim. Acta*, 1994, **77**, 51-58 (*Oceanapins E,F*)
Inagaki, M. *et al., Eur. J. Org. Chem.*, 2003, 325-331 (*Luidialactoside A*)

2-Amino-17-methyl-4-octadecene-1,3-diol A-362



$C_{19}H_{39}NO_2$ 313.523

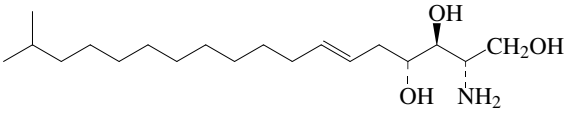
(2*S*,3*R*,4*E*)-*form*

N-*(2*R*-Hydroxy-13-methyltetradecanoyl), 1*-O-*sulfate:* ***Calyceramide A***
[346425-29-4]
$C_{34}H_{67}NO_7S$ 633.972

Isol. from the sponge *Discodermia calyx*. Neuraminidase inhibitor. Solid (as Na salt). $[\alpha]_D^{20}$ +24.8 (c, 0.1 in MeOH) (Na salt).

Nakao, Y. *et al., Tetrahedron*, 2001, **57**, 3013-3017 (*isol, ir, pmr, cmr*)

2-Amino-17-methyl-6-octadecene-1,3,4-triol A-363



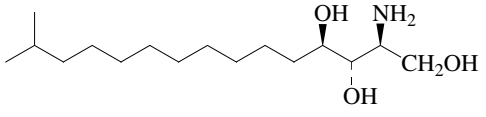
$C_{19}H_{39}NO_3$ 329.522

(2S,3S,4R,6E)-form

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*β-*D*-galactopyranoside:*
[126960-09-6]
$C_{49}H_{95}NO_{10}$ 858.29
Isol. from the sponge *Chondropsis* sp. Cryst.
Mp 218-220°. $[\alpha]_D^{27}$ +18 (c, 0.34 in $CHCl_3$/MeOH).

Endo, M. *et al., Pure Appl. Chem.*, 1986, **58**, 387-394 (*isol*)
Honda, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1385-1391 (*synth, pmr, cmr*)

2-Amino-14-methyl-1,3,4-pentadecanetriol A-364



$C_{16}H_{35}NO_3$ 289.457

(2S,3S,4R)-form

N-*(2*R*-Hydroxydocosanoyl):*
$C_{38}H_{77}NO_5$ 628.03
Isol. from the tunicate *Cystodytes* cf. *dellechiajei*. Amorph. powder. $[\alpha]_D$ +9.6 (c, 0.05 in MeOH).

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*(2-acetamido-2-deoxy-β-*D*-glucopyranoside):* ***Halicylindroside B₁***
[161842-90-6]
$C_{46}H_{90}N_2O_{10}$ 831.224
Isol. from the sponge *Halichondria cylindrata*. Solid. $[\alpha]_D^{23}$ -9.2 (c, 0.15 in Py).

N-*(2*R*-Hydroxytricosanoyl), 1*-O-*(2-acetamido-2-deoxy-β-*D*-glucopyranoside):* ***Halicylindroside B₂***
[161842-91-7]
$C_{47}H_{92}N_2O_{10}$ 845.251
Isol. from the sponge *Halichondria cylindrata*. Solid. $[\alpha]_D^{23}$ -9 (c, 0.15 in Py).

Li, H.-Y. *et al., Tetrahedron*, 1995, **51**, 2273-2280 (*Halicylindrosides*)
Loukaci, A. *et al., J. Nat. Prod.*, 2000, **63**, 799-802 (*isol*)

2-(Aminomethyl)-2-propenoic acid, 9CI A-365

3-Amino-2-methylenepropanoic acid. α-Methylene-β-alanine
[4452-16-8]
$H_2C{=}C(COOH)CH_2NH_2$
$C_4H_7NO_2$ 101.105
Toxic amino acid from the sponge *Fasciospongia cavernosa* and other sponges. Also prod. by a *Streptomyces* sp. Shows herbicidal props. Sol. H_2O.

Hydrochloride: [75509-28-3]
Cryst. (MeOH/Me_2CO). Mp 153-154°.

Me ester: [87375-90-4]
$C_5H_9NO_2$ 115.132
From *Fasciospongia cavernosa*.
Mp 107-108° (as hydrochloride).

N-*Tetradecanoyl:* [70290-27-6]
$C_{18}H_{33}NO_3$ 311.464
Isol. from *Spongia* cf. *zimocca*.

N-*Pentadecanoyl:* [70290-28-7]
$C_{19}H_{35}NO_3$ 325.49
Isol. from *Spongia* cf. *zimocca*.

N-*Hexadecanoyl:* [70290-29-8]
$C_{20}H_{37}NO_3$ 339.517
Isol. from *Spongia* cf. *zimocca*.

N-*Tetradecanoyl, Me ester:* [70290-25-4]
$C_{19}H_{35}NO_3$ 325.49
Isol. from *Fasciospongia cavernosa* and *Spongia* cf. *zimocca*.

N-*Pentadecanoyl, Me ester:* [70290-26-5]
$C_{20}H_{37}NO_3$ 339.517
Isol. from *Fasciospongia cavernosa* and *Spongia* cf. *zimocca*.

N-*Hexadecanoyl, Me ester:* [52634-29-4]
$C_{21}H_{39}NO_3$ 353.544
Isol. from *Fasciospongia cavernosa*, a *Hippospongia* sp. and *Spongia* cf. *zimocca*.

N-*(14-Methylpentadecanoyl), Me ester:* ***Hurghamide A***
$C_{21}H_{39}NO_3$ 353.544
Isol. from a *Hippospongia* sp. Wax.

N-*(15-Methylhexadecanoyl), Me ester:* ***Hurghamide B***
$C_{22}H_{41}NO_3$ 367.571
Isol. from a *Hippospongia* sp. Wax.

N-*(Methylhexadecanoyl), Me ester:* ***Hurghamide C***
$C_{22}H_{41}NO_3$ 367.571
Isol. from a *Hippospongia* sp. Wax. Posn. of methyl on *N*-acyl group not determined.

N-*Heptadecanoyl, Me ester:* [52634-30-7]
$C_{22}H_{41}NO_3$ 367.571
Isol. from *Fasciospongia cavernosa* and a *Hippospongia* sp.

N-*(13-Octadecenoyl), Me ester:* ***Hurghamide D***
$C_{23}H_{41}NO_3$ 379.582
Isol. from a *Hippospongia* sp.

N-*Octadecanoyl, Me ester:* [52634-31-8]
$C_{23}H_{43}NO_3$ 381.598
Isol. from *Fasciospongia cavernosa*.

N-*Nonadecanoyl, Me ester:* [52634-32-9]
$C_{24}H_{45}NO_3$ 395.624
Isol. from *Fasciospongia cavernosa*.

N-*Eicosanoyl, Me ester:* [52634-33-0]
$C_{25}H_{47}NO_3$ 409.651
Isol. from *Fasciospongia cavernosa*.

N-*(2-Oxotetradecanoyl), Me ester:* [70290-19-6]
$C_{19}H_{33}NO_4$ 339.474
Isol. from *Spongia* cf. *zimocca* and *Sinularia dissecta*.

N-*(2-Oxopentadecanoyl), Me ester:* [70290-20-9]
$C_{20}H_{35}NO_4$ 353.501
Isol. from *Spongia* cf. *zimocca* and *Sinularia dissecta*.

N-*(2-Oxohexadecanoyl), Me ester:* [70290-21-0]
$C_{21}H_{37}NO_4$ 367.528
Isol. from *Spongia* cf. *zimocca*.

N-*(2-Hydroxytetradecanoyl), Me ester:* [70290-22-1]
$C_{19}H_{35}NO_4$ 341.49
Isol. from *Spongia* cf. *zimocca*.

N-*(2-Hydroxypentadecanoyl), Me ester:* [70290-23-2]
$C_{20}H_{37}NO_4$ 355.517
Isol. from *Spongia* cf. *zimocca*.

N-*(2-Hydroxyhexadecanoyl), Me ester:* [70290-24-3]
$C_{21}H_{39}NO_4$ 369.543
Isol. from *Spongia* cf. *zimocca*.

N-*(2-Acetoxy-2-tetradecenoyl), Me ester:*
$C_{21}H_{35}NO_5$ 381.511
Isol. from *Fasciospongia cavernosa*.

N-*(2-Acetoxy-2-pentadecenoyl), Me ester:*
$C_{22}H_{37}NO_5$ 395.538
Isol. from *Fasciospongia cavernosa*.

N-*(15-Methyl-8-hexadecenoyl), Me ester:* ***Hurghamide E***
[330203-64-0]
$C_{22}H_{39}NO_3$ 365.555
Isol. from a *Hippospongia* sp. Wax. λ_{max} 205 (ε 14700) (MeOH).

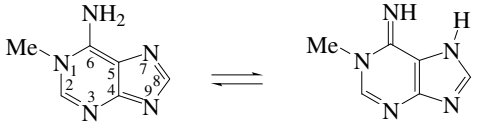
N-*(2-Alkylcyclopropyl)alkanoyl, Me ester (1):* ***Hurghamide F***
[330203-65-1]
$C_{22}H_{39}NO_3$ 365.555
Isol. from a *Hippospongia* sp. Wax. Posn. of cyclopropyl ring in side-chain not yet determined.

N-*(2-Alkylcyclopropylalkanoyl), Me ester (2):* ***Hurghamide G***
[330203-66-2]
$C_{24}H_{43}NO_3$ 393.609
Isol. from a *Hippospongia* sp. Wax. Posn. of cyclopropyl not determined.

Kashman, Y. *et al., Tetrahedron*, 1973, **29**, 3655 (*isol*)
Yunker, M.B. *et al., Tet. Lett.*, 1978, 4651 (*isol*)
Holm, A. *et al., Tet. Lett.*, 1980, 1125 (*synth*)
Neeman, J. *et al., Arch. Toxicol.*, Suppl., 1983, **6**, 258 (*isol*)
Jackson, W.R. *et al., Tet. Lett.*, 1988, **29**, 1983 (*synth*)
Isaac, B.G. *et al., J. Antibiot.*, 1991, **44**, 795 (*isol*)
Guo, Y. *et al., Nat. Prod. Lett.*, 1997, **9**, 281-288 (*Hurghamides A-D*)
Venkateswarlu, Y. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 832-834 (*N-2-acetoxy-2-alkenoyl derivs*)
Ramesh, P. *et al., Biochem. Syst. Ecol.*, 1999, **27**, 661-662 (*2-oxoalkyl derivs, isol, Sinularia*)
Guo, Y.-W. *et al., J. Asian Nat. Prod. Res.*, 2000, **2**, 251-256 (*Hurghamides E-G*)

6-Amino-1-methylpurine A-366

*1-Methyl-1*H*-purin-6-amine, 9CI. 1-Methyladenine. 1-Methyl-6-iminopurine.* ***Spongopurine***
[5142-22-3]



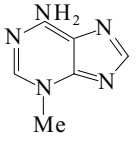
$C_6H_7N_5$ 149.155
Exists in the imino form in nonpolar solvs. and the amino form in H_2O. Isol. from starfishes *Asterias amurensis*, *Asterias rubens* and *Marthasterias glacialis*, and sponges *Geodia gigas* and *Hymeniacidon sanguinea*. Spawning-inducing factor in *Asterias*. Cryst. (H_2O).
Mp 296-299° dec. pK_{a1} 7.2; pK_{a2} 11.

Picrate: Mp 255-257°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 714A (*ir*)
Ackermann, D. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1958, **312**, 210-213; 1961, **323**, 192-193 (*isol, ir, struct*)
Brookes, P. *et al., J.C.S.*, 1960, 539-545 (*synth*)
Karatani, H. *et al., Nature (London)*, 1969, **221**, 273-274 (*isol*)
Lichtenberg, D. *et al., J. Magn. Reson.*, 1972, **6**, 600-604 (*nmr*)
Garrett, E.R. *et al., J.A.C.S.*, 1972, **94**, 8532-8541 (*synth, uv*)
Doree, M. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1976, **73**, 1669-1673 (*biochem, bibl*)
Dreyfus, M. *et al., J.A.C.S.*, 1977, **99**, 7027-7037 (*tautom, bibl*)
Cimino, G. *et al., J. Nat. Prod.*, 1985, **48**, 523-528 (*isol, pmr*)

6-Amino-3-methylpurine A-367

*3-Methyl-3*H*-purin-6-amine, 9CI. 3-Methyladenine, 8CI*
[5142-23-4]



$C_6H_7N_5$ 149.155
Isol. from the marine sponges *Plakortis* aff. *simplex* and *Topsentia genitrix*. Cryst. (H_2O).
Mp 300° (291-292° dec.). pK_a 6.1. λ_{max} 273 (ε 14000) (MeOH) (Derep). λ_{max} 273 (ε 14010) (MeOH) (Berdy).

▶ AU6520000

9-β-D-Ribofuranosyl: 3-Methyladenosine
[72055-63-1]
$C_{11}H_{15}N_5O_4$ 281.271
Plates (MeOH) (as tosylate salt). Mp 150° dec. (tosylate salt). $[\alpha]_D^{20}$ -28.2 (c, 1.00 in H_2O) (tosylate salt). Imino at C-6.

9-(2-Deoxy-β-D-ribofuranosyl): 2′-Deoxy-3-methyladenosine
[76227-26-4]
$C_{11}H_{15}N_5O_3$ 265.271
Powder (as tosylate salt). Mp 120° dec. (tosylate salt). Imino at C-6.

7-Oxide:
$C_6H_7N_5O$ 165.154
Sl. dark prisms. Mp 250-260° (dec.).

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 217A (*nmr*)
Brookes, P. *et al., J.C.S.*, 1960, 539 (*synth*)
Denayer, R. *et al., Bull. Soc. Chim. Fr.*, 1962, 1358 (*synth, uv*)
Jones, J.W. *et al., J.A.C.S.*, 1962, **84**, 1914 (*synth, uv*)
Elion, G.B. *et al., J.O.C.*, 1962, **27**, 2478 (*synth, uv*)
Pal, B.C. *et al., J.C.S.*, 1964, 400 (*ir, cryst struct*)
Lichtenberg, D. *et al., J. Magn. Reson.*, 1972, **6**, 600 (*nmr*)
Yamauchi, K. *et al., J.O.C.*, 1975, **40**, 385 (*synth*)
Stoller, C. *et al., J. Nat. Prod.*, 1988, **51**, 383 (*isol, uv, pmr, cmr, ms*)
Fujii, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2601 (*nucleosides*)
Itaya, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2025 (*7-oxide*)
Rudi, A. *et al., J. Nat. Prod.*, 2003, **66**, 682-685 (*isol, pmr, cmr*)

2-Amino-17-methyl-4,17-triacontadien-1,3-diol A-368

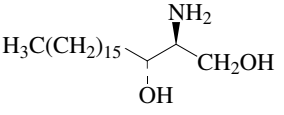
$H_3C(CH_2)_{11}CH{=}C(CH_3)(CH_2)_{11}CH{=}CHCH(OH)CH(NH_2)\text{-}CH_2OH$
$C_{31}H_{61}NO_2$ 479.828

(2ξ,3ξ,4E,17E)-form

N-*(2ξ-Hydroxy-4*E*-heptadecenoyl), 1-*O*-β-D-glucopyranoside:* ***Asperiamide A***
$C_{54}H_{101}NO_9$ 908.393
Prod. by a marine-derived *Aspergillus* sp. (culture MF34). Amorph. powder. $[\alpha]_D^{21}$ -16 (c, 0.46 in MeOH).

Ouyang, M.-A. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 761-765 (*isol, pmr, cmr, ms*)

2-Amino-1,3-nonadecanediol A-369



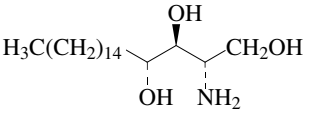
$C_{19}H_{41}NO_2$ 315.538

(2S,3R)-form

N-*Docosanoyl:* [750596-26-0]
$C_{41}H_{83}NO_3$ 638.112
Isol. from *Pseudopterogorgia australiensis*. Cryst. ($CHCl_3$).
Mp 131-133°. $[\alpha]_D^{25}$ +28.5 (c, 0.1 in $CHCl_3$).

Krishna, N. *et al., J. Nat. Prod.*, 2004, **67**, 1423-1425 (*isol, pmr, cmr*)

2-Amino-1,3,4-nonadecanetriol A-370



$C_{19}H_{41}NO_3$ 331.538

(2S,3S,4R)-form

N-*Docosanoyl:* [636589-64-5]
$C_{41}H_{83}NO_4$ 654.111
Constit. of the sponge *Iotrochota baculifera*.

N-*(2*R*-Hydroxynonadecanoyl):*
$C_{38}H_{77}NO_5$ 628.03
Isol. from the gorgonian *Pseudopterogorgia australiensis*. Cryst. (MeOH).
Mp 101-103°. $[\alpha]_D^{25}$ +8.5 (c, 0.1 in Py).

N-*(2*R*,3*S*-Dihydroxyoctacosanoyl), 1*-O-*β-D-glucopyranoside:*
$C_{53}H_{105}NO_{11}$ 932.413
Constit. of *Microcosmus sulcatus.*

N-*(2*R*,3*S*-Dihydroxyoctacosanoyl), 1*-O-*[β-D-galactopyranosyl-(1→4)-β-D-glucopyranoside]:*
$C_{59}H_{115}NO_{16}$ 1094.555
Constit. of *Microcosmus sulcatus.*

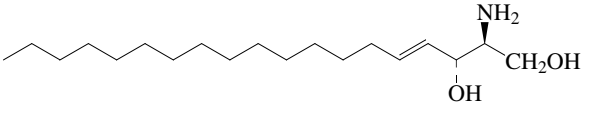
N-*(2*R*,3*S*-Dihydroxyoctacosanoyl), 1*-O-*[α-D-fucopyranosyl-(1→3)-[α-D-galactopyranosyl-(1→4)]-β-D-glucopyranoside]:*
$C_{65}H_{125}NO_{20}$ 1240.697
Main constit. of *Microcosmus sulcatus.*

Muralidhar, P. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1193-1195 (*N-docosanoyl*)

Aiello, A. *et al., Eur. J. Org. Chem.*, 2003, 734-739 (*Microcosmus sulcatus constits*)

Krishna, N. *et al., J. Nat. Prod.*, 2004, **67**, 1423-1425 (*N-2-hydroxynonadecanoyl*)

2-Amino-4-nonadecene-1,3-diol A-371



$C_{19}H_{39}NO_2$ 313.523

(2S,3R,4E)-form

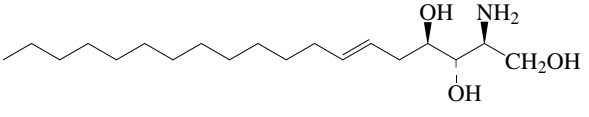
N-*Hexadecanoyl:* [352518-70-8]
$C_{35}H_{69}NO_3$ 551.935
Isol. from a *Pseudopterogorgia* sp. Antibacterial agent. Amorph. powder (hexane/EtOAc).
Mp 104-105°. $[\alpha]_D$ -6 (c, 1.3 in $CHCl_3$).

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*[*N*-acetyl-8*-O*-methyl-α-D-neuraminosyl-(2→3)-β-D-galactopyranosyl-(1→4)-β-D-glucopyranoside]:* ***LMG 3***
Isol. from *Luidia maculata*.
Amorph. powder.
Mp 154-160°.

Vanisree, M. *et al., J. Asian Nat. Prod. Res.*, 2001, **3**, 23-29 (*N-hexadecanoyl*)

Kawatake, S. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1386-1389 (*LMG 3*)

2-Amino-6-nonadecene-1,3,4-triol A-372



$C_{19}H_{39}NO_3$ 329.522

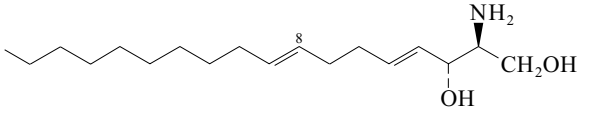
(2S,3S,4R,6E)-form

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*[α-D-galactopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Amphimelibioside D***
$C_{53}H_{101}NO_{15}$ 992.379
Isol. from an *Amphimedon* sp. Powder.

Emura, C. *et al., J.O.C.*, 2005, **70**, 3031-3038 (*Amphimelibioside D*)

2-Amino-4,8-octadecadiene-1,3-diol A-373

4,8-Sphingadiene. 4,8-Octadecasphingadiene. 4,8-Sphingadienine



(2S,3R,4E,8E)–form

$C_{18}H_{35}NO_2$ 297.48

(2S,3R,4E,8E)-form

N-*(2*R*-Hydroxytetradecanoyl), 1*-O-*β-D-glucopyranoside: AS 1-1*
[212777-97-4]
$C_{38}H_{71}NO_9$ 685.98
Constit. of *Allium sativum*. Amorph. powder.
Mp 197-200°. $[\alpha]_D^{28}$ +5.2 (c, 0.25 in propanol).

N-*(2*R*-Hydroxypentadecanoyl), 1*-O-*β-D-glucopyranoside: AS 1-2*
[212777-98-5]
$C_{39}H_{73}NO_9$ 700.007
Constit. of *Allium sativum*. Amorph. powder.
Mp 195-200°. $[\alpha]_D^{28}$ +8.8 (c, 0.13 in 1-propanol).

N-*Hexadecanoyl:* [141980-53-2]
$C_{34}H_{65}NO_3$ 535.892
Isol. from *Acabaria undulata*, *Paracondylactis indicus* and *Vigna angularis* (azuki bean). Also from the marine green alga *Ulva fasciata*. Solid.
Mp 82-83°. $[\alpha]_D^{25}$ -8 (c, 0.5 in $CHCl_3$).

N-*(2ξ-Hydroxyhexadecanoyl):* ***Confertamide A***
$C_{34}H_{65}NO_4$ 551.892
Constit. of *Sinularia conferta*. Powder.
Mp 103-104°. $[\alpha]_D^{20}$ +10.1 (c, 0.19 in $CHCl_3$).

N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-*sulfate:* [192384-61-5]
$C_{34}H_{65}NO_7S$ 631.956
Isol. from the bryozoan *Watersipora cucullata*. DNA topoisomerase I inhibitor. $[\alpha]_D$ +17 (c, 0.06 in MeOH).

N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-*β-D-glucopyranoside:* ***Soyacerebroside I***. *AS 1-4*
[114297-20-0]
$C_{40}H_{75}NO_9$ 714.034
Cerebroside isol. from *Tetragonia tetragonoides* (New Zealand spinach), *Glycine max* (soybean) and *Allium sativum*. Antiulcerogenic principle. Hygroscopic granules or amorph. solid.
Mp 184-186° Mp 193-197°. $[\alpha]_D^{24}$ +10.5 (c, 0.30 in MeOH/$CHCl_3$, 3:2).

N-*(2*R*-Hydroxyheptadecanoyl):*
$C_{35}H_{67}NO_4$ 565.919
Constit. of the coral *Lobophytum* sp. Solid.
Mp 111-112°. $[\alpha]_D^{28}$ -11 (c, 0.5 in $CHCl_3$).

N-*Octadecanoyl: JC-2*
$C_{36}H_{69}NO_3$ 563.946
Constit. of *Comanthus japonica*. Amorph. powder.
Mp 82-85°.

N-*Octadecanoyl, 1*-O-*β-D-glucopyranoside: PA-O-1*
[157478-07-4]
$C_{42}H_{79}NO_8$ 726.088
Isol. from *Pentacta australis*. Amorph. powder.
Mp 150-155°. $[\alpha]_D$ +3.7 (c, 0.21 in 1-propanol).

N-*(2*R*-Hydroxyoctadecanoyl), 1*-O-*β-D-glucopyranoside:* ***JCer-1***
[174176-93-3]
$C_{42}H_{79}NO_9$ 742.087
Constit. of *Monochoria vaginalis* and *Comanthus japonica*. Powder.
Mp 83-85° Mp 182-184°. $[\alpha]_D^{22}$ +4.7 (c, 0.5 in MeOH). $[\alpha]_D$ +7.8 (c, 0.43 in 1-propanol).

N-*(14-Methylheptadecanoyl): JC-1*
$C_{36}H_{69}NO_3$ 563.946
Constit. of *Comanthus japonica*. Amorph. powder.
Mp 68-70°.

N-*(2*R*-Hydroxyeicosanoyl), 1*-O-*β-D-glucopyranoside:* [174176-92-2]
$C_{44}H_{83}NO_9$ 770.141
Constit. of *Monochoria vaginalis*. Powder.
Mp 187-189°. $[\alpha]_D^{22}$ +6.2 (c, 0.6 in MeOH).

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*β-D-glucopyranoside:* ***Typhoniside A***
[444587-23-9]
$C_{46}H_{87}NO_9$ 798.195
Constit. of the dried tubers of *Typhonium giganteum*. Amorph. powder.
Mp 172-174°.

N-*Me,* N-*hexadecanoyl:* [197581-29-6]
$C_{35}H_{67}NO_3$ 549.919
Isol. from *Ulva fasciata* and a *Zoanthus* sp. Amorph. powder.
Mp 86°. $[\alpha]_D^{27}$ +20.1 (c, 0.01 in $CHCl_3$).

N-*Me,* N-*octadecanoyl, 1*-O-*sulfate:* ***Hariamide***
[197703-64-3]
$C_{37}H_{71}NO_6S$ 658.037
Isol. from a *Zoanthus* sp. Cryst.
Mp 165°. $[\alpha]_D^{27}$ +11.3 (c, 0.01 in MeOH).

N-*(2-Hydroxyethyl),* N-*tetradecanoyl:* [684213-91-0]
$C_{34}H_{65}NO_4$ 551.892
Constit. of *Anthopleura pacifica*.

N-*(2-Hydroxyethyl),* N-*hexadecanoyl:* [684213-93-2]
$C_{36}H_{69}NO_4$ 579.945
Constit. of *Anthopleura pacifica*.

N-*(2-Hydroxyethyl),* N-*(9Z-hexadecenoyl):* [684213-92-1]
$C_{36}H_{67}NO_4$ 577.93
Constit. of *Anthopleura pacifica*.

N-*(2-Hydroxyethyl),* N-*(13Z-docosenoyl):* [684213-94-3]
$C_{42}H_{79}NO_4$ 662.09
Constit. of *Anthopleura pacifica*.

(2S,3R,4E,8Z)-form

N-*Hexadecanoyl, 1*-O-*β-D-glucopyranoside:* [127842-89-1]
$C_{40}H_{75}NO_8$ 698.034
Constit. of *Lycium chinense* (Chinese boxthorn). Antihepatotoxic agent. Amorph. powder. $[\alpha]_D^{25}$ +1.2 (c, 0.1 in MeOH).

N-*(2*R-*Hydroxyhexadecanoyl), 1*-O-*β-D-glucopyranoside:* ***Soyacerebroside II****. AS 1-3*
[115074-93-6]
$C_{40}H_{75}NO_9$ 714.034
Isol. from *Tetragonia tetragonoides* (New Zealand spinach), *Glycine max* (soybean) and *Allium sativum*. Antiulcerogenic principle. Hygroscopic granules or amorph. solid.
Mp 192-194° (183°). $[\alpha]_D^{24}$ +13.4 (c, 0.43 in MeOH/$CHCl_3$ 3:2) (+4.6).

N-*(2*R-*Hydroxytetracosanoyl), 1*-O-*β-D-glucopyranoside:* ***Stenochlaena cerebroside****. Longancerebroside II*
[220873-86-9]
$C_{48}H_{91}NO_9$ 826.248
Constit. of *Euphoria longan* and *Stenochlaena palustris.*
$[\alpha]_D^{25}$ +7.9 (c, 0.09 in MeOH).

N-*(15*E-*Tetracosenoyl), 1*-O-*β-D-glucopyranoside: CE 1-2*
[204126-76-1]
$C_{48}H_{89}NO_8$ 808.233
Isol. from the sea cucumber *Cucumaria echinata*. Amorph. powder.
Mp 136-137°. $[\alpha]_D$ -1.9 (c, 0.33 in 1-propanol).

(2ξ,3ξ,4E,8E)-form

N-*(13-Methyltetradecanoyl), 1*-O-*β-D-galactopyranoside:*
$C_{39}H_{73}NO_8$ 684.008
Isol. from sponge *Halichondria panicea*.
$[\alpha]_D$ -11.7 (c, 1.56 in $CHCl_3$) (as penta-Ac).

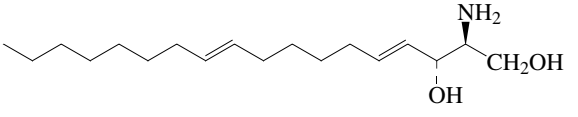
N-*Hexadecanoyl:* ***Sinumeramide***
[124787-56-0]
$C_{34}H_{65}NO_3$ 535.892
Constit. of the soft coral *Sinularia* sp. Cryst. ($CHCl_3$/MeOH).
Mp 98-100°. $[\alpha]_D^{25}$ +2.8 (c, 0.5 in $CHCl_3$).

N-*Nonadecanoyl:* ***Humesamide***
[300715-39-3]
$C_{37}H_{71}NO_3$ 577.973
Isol. from the soft coral *Cladiella humesi*. Amorph. solid.
Mp 79-80°.

[127912-01-0]

Mori, K. *et al., Annalen*, 1988, 807-814 (*abs config, ir, pmr, cmr, synth, bibl, Soyacerebroside*)
Singh, N.P. *et al., J. Carbohydr. Chem.*, 1989, **8**, 199-216 (*synth*)
Kodato, S. *et al., Tetrahedron*, 1989, **45**, 7263-7280 (*Sinumeramide*)
Su, J. *et al., CA*, 1990, **112**, 52558 (*Sinumeramide, isol*)
Shibuya, H. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2933-2938 (*Soyacerebrosides*)
Nagle, D.G. *et al., J. Nat. Prod.*, 1992, **55**, 1013-1017 (*N-13-methyltetradecanoyl galactoside*)
Shibuya, H. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1534-1544 (*synth*)
Higuchi, R. *et al., Annalen*, 1994, 653-658 (*PA-O-1*)
Shin, J. *et al., J. Nat. Prod.*, 1995, **58**, 948-953 (*N-hexadecanoyl*)
Sharma, M. *et al., Bot. Mar.*, 1996, **39**, 213-215 (*N-hexadecanoyl, isol, green alga*)
Kim, S.Y. *et al., J. Nat. Prod.*, 1997, **60**, 274-276 (*Lycium chinense constit*)
Babu, U.V. *et al., J. Nat. Prod.*, 1997, **60**, 1307-1309 (*Hariamide*)
Ojika, M. *et al., Tet. Lett.*, 1997, **38**, 4235-4238 (*N-hydroxyhexadecanoyl 1-sulfate*)
Inagaki, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1153-1156 (*AS compounds*)
Yamada, K. *et al., Eur. J. Org. Chem.*, 1998, 371-378 (*CE 1-2*)
Liu, H. *et al., Phytochemistry*, 1998, **49**, 2403-2408 (*Stenochlaena cerebroside*)
Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 457-460 (*N-hexadecanoyl*)
Wang, M.Y. *et al., Chin. Chem. Lett.*, 2000, **11**, 783-784 (*Humesamide*)
Wang, X.-Z. *et al., J.O.C.*, 2000, **65**, 8146-8151 (*synth*)
Murakami, T. *et al., Tetrahedron*, 2000, **56**, 533-545 (*synth*)
Chen, X. *et al., Tet. Lett.*, 2002, **43**, 3529-3532 (*Typhoniside A*)
Row, L.-C. *et al., J. Chin. Chem. Soc. (Taipei)*, 2003, **50**, 1103-1107 (*Monochoria vaginalis cerebrosides*)
Zhang, S.-Y. *et al., Yaoxue Xuebao*, 2003, **38**, 350-353 (*Anthapleura pacifica ceramides*)
Inagaki, M. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1307-1311 (*JC-1, JC-2, JCer-1*)
Muralidhar, P. *et al., Chem. Pharm. Bull.*2005, **53**, 168-171 (*N-2-hydroxyheptadecanoyl*)
Su, J.-Y. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 107-113 (*Confertamide A*)

2-Amino-4,10-octadecadiene-1,3-diol A-374



$C_{18}H_{35}NO_2$ 297.48

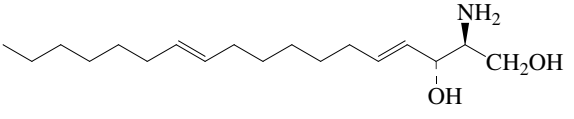
(2S,3R,4E,10E)-form

N-*Hexadecanoyl:* [479411-42-2]
$C_{34}H_{65}NO_3$ 535.892
Constit. of a *Sinularia* sp. Cryst. ($CHCl_3$/MeOH).
Mp 130-132°. $[\alpha]_D^{25}$ +2.5 (c, 0.5 in $CHCl_3$). λ_{max} 210 (MeOH).

Parvataneni, R. *et al., J. Indian Chem. Soc.*, 2002, **79**, 732-738 (*isol, pmr, cmr, ms*)

2-Amino-4,11-octadecadiene-1,3-diol A-375

4,11-Sphingadienine



(2*S*,3*R*,4*E*,11*E*)-*form*

$C_{18}H_{35}NO_2$ 297.48

(2S,3R,4E,11E)-form

N-*(2*R-*Hydroxyhexadecanoyl), 1*-O-*β-D-glucopyranoside:* ***Pinelloside***
$C_{40}H_{75}NO_9$ 714.034
Constit. of the tubers of *Pinellia ternata*. Antimicrobial agent. Amorph. powder.
Mp 136-138°. $[\alpha]_D^{25}$ -6 (c, 0.5 in MeOH).

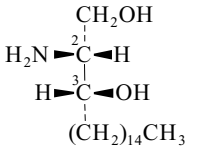
(2S,3R,4E,11Z)-form

N-*Hexadecanoyl:* N-*[2-Hydroxy-1-(hydroxymethyl)-3,10-heptadecadienyl]hexadecanamide, 9CI.* N-*Hexadecanoyl-4,11-sphingadienine.* ***Lobophytamide L8***
[126770-39-6]
$C_{34}H_{65}NO_3$ 535.892
Isol. from the soft coral *Lobophytum chevalieri*.

Li, R. *et al., CA*, 1990, **112**, 195463q (*Lobophytamide L8*)
Chen, J.H. *et al., Phytochemistry*, 2003, **64**, 903-906 (*Pinelloside*)

2-Amino-1,3-octadecanediol, 8CI A-376

Octadecasphinganine. Cerebrin base. Dihydrosphingosine. Sphinganine
[13552-09-5]



(2*R*,3*R*)–*form*

$C_{18}H_{39}NO_2$ 301.512

(2*R*,3*R*)-*form*
D-threo-*form*
[6036-86-8]
Mp 108°. $[\alpha]_{Hg}^{28}$ +13 (10:1 $CHCl_3$/MeOH).

(2*R*,3*S*)-*form*
L-erythro-*form*
Mp 79°. $[\alpha]_{Hg}^{28}$ -6.5 (10:1 $CHCl_3$/MeOH).

(2*S*,3*R*)-*form*
D-erythro-*form*
[764-22-7]
Mp 85-88° (79°) Mp 108-109°. $[\alpha]_{Hg}^{18}$ +6.5 (10:1 $CHCl_3$/MeOH). $[\alpha]_D^{28}$ +13.5 (c, 0.75 in $CHCl_3$).

N,*3-Di-Ac: 2-Acetamido-3-acetoxy-1-octadecanol*
[67492-14-2]
$C_{22}H_{43}NO_4$ 385.586
Constit. of the red alga *Laurencia nidifica*. Cryst. (MeCN aq.).
Mp 91.5-92.5°. $[\alpha]_D$ +10.8 (c, 1.25 in CH_2Cl_2).

N-*(2*R*-Hydroxy-3*E*-hexadecenoyl):* ***Symbioramide C-16***
$C_{34}H_{67}NO_4$ 553.908
Isol. from a *Symbiodinium* sp. Amorph. solid.
Mp 106-108°. $[\alpha]_D^{24}$ +6.8 (c, 0.07 in $CHCl_3$).

N-*(2*R*-Hydroxy-3*E*-octadecenoyl):* ***Symbioramide***. N-*(2-Hydroxy-3-octadecenoyl)dihydrosphingosine*
[118106-53-9]
$C_{36}H_{71}NO_4$ 581.961
Isol. from the dinoflagellate *Symbiodinium* sp. Calcium ATPase activator. Ion channel activator. Cryst.
Mp 105-107°. $[\alpha]_D^{22}$ +5.8 (c, 1 in $CHCl_3$).

(2*S*,3*S*)-*form*
L-threo-*form*. ***Safingol, INN***. *SPC 100270*
[15639-50-6]
Widespread as a component of cerebrosides, in admixture with smaller amts. of homologues. Antipsoriatic agent. Inhibitor of protein kinase C. Increases antitumour effects of chemotherapeutic agents.
Mp 108°. $[\alpha]_D^{28}$ -14.1 ($CHCl_3$).

N-*(9-Octadecenoyl):* N-*(9-Octadecenoylamino)-1,3-octadecanediol*. N-*9-Octadecenoylsphinganine*. N-*Oleoylsphinganine*
$C_{36}H_{71}NO_3$ 565.962
Mp 86-87°.

N-*(9Z,12Z)-Octadecadienoyl: 2-(9,12-Octadecadienoylamino)-1,3-octadecanediol*. N-*9,12-Octadecadienoylsphinganine*. *Linoleoylsphinganine*
[34227-66-2]
$C_{36}H_{69}NO_3$ 563.946

(2ξ,3ξ)-*form*
N-*Nonanoyl: 2-(Nonanoylamino)-1,3-octadecanediol*. N-*Nonanoylsphinganine*
$C_{27}H_{55}NO_3$ 441.736
Constit. of a *Nephthea* sp.

N-*(2ξ,3ξ-Dihydroxyhexacosanoyl):* [849704-44-5]
$C_{44}H_{89}NO_5$ 712.191
Constit. of a mangrove fungus.

Grob, C.A. *et al., Helv. Chim. Acta*, 1957, **40**, 1145 (*synth*)
Shapiro, D. *et al., J.A.C.S.*, 1958, **80**, 1194 (*synth*)
Carter, H.E. *et al., Biochemistry*, 1963, **2**, 389 (*struct, abs config*)
Gigg, J. *et al., J.C.S.(C)*, 1966, 1872 (*synth*)
Reist, E.J. *et al., J.O.C.*, 1970, **35**, 4127 (*synth*)
Stoffel, W. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1972, **353**, 1962; 1973, **354**, 169 (*synth, cmr, metab*)
Alpes, H. *et al., Chem. Phys. Lipids*, 1974, **13**, 109 (*synth, derivs*)
Cardellina, J.H. *et al., Phytochemistry*, 1978, **17**, 554 (*N,3-di-Ac*)
Bongini, A. *et al., J.C.S. Perkin 1*, 1986, 1339 (*synth*)
Kobayashi, J. *et al., Experientia*, 1988, **44**, 800 (*Symbioramide*)
Yoshida, J. *et al., J.C.S. Perkin 1*, 1992, 343-350 (*Symbioramide, synth*)
Mori, K. *et al., Annalen*, 1994, 41 (*2S,3R-form, synth, bibl, tri-Ac, pmr, cmr, ir*)
Wild, R. *et al., Annalen*, 1995, 755 (*2S,3R-form*)
Nakamura, H. *et al., Bull. Chem. Soc. Jpn.*, 1998, **71**, 781-787 (*Symbioramide C-16*)
Hoffman, R.V. *et al., Tet. Lett.*, 1998, **39**, 3953-3956 (*synth*)
Masui, M. *et al., Tet. Lett.*, 1998, **39**, 5199-5200 (*synth*)
Cook, G.R. *et al., Tet. Lett.*, 2002, **43**, 9027-9029 (*synth*)
Rao, C.B. *et al., Asian J. Chem.*, 2003, **15**, 1161-1163 (*N-nonanoyl*)
Azuma, H. *et al., J.O.C.*, 2003, **68**, 2790-2797 (*Symbioramide, synth, pmr*)
Howell, A.R. *et al., Tetrahedron*, 2004, **60**, 11327-11347 (*rev, synth*)
Zhu, F. *et al., CA*, 2005, **142**, 370451c (*2,3-dihydroxyhexacosanoyl*)
Takanami, T. *et al., Tet. Lett.*, 2005, **46**, 3291-3295 (*Symbioramide, synth*)

2-Amino-1,3,4,5-octadecanetetrol A-377

4,5-Dihydro-4,5-dihydroxysphingosine
$H_3C(CH_2)_{12}CH(OH)CH(OH)CH(OH)CH(NH_2)CH_2OH$
$C_{18}H_{39}NO_4$ 333.51

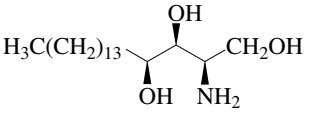
(all-ξ)-*form*
N-*Hexadecanoyl: UF 131*
[141364-80-9]
$C_{34}H_{69}NO_5$ 571.923
Isol. from green alga *Ulva fasciata*. Shows antiviral activity.
Mp 143-144°. $[\alpha]_D$ +8.2 (c, 0.5 in MeOH).

N-*Pentacosanoyl:* [155230-16-3]
$C_{43}H_{87}NO_5$ 698.164
Isol. from red alga *Halymenia durvillae*.
Mp 148-149°.

Garg, H.S. *et al., Tet. Lett.*, 1992, **33**, 1641-1644 (N-*hexadecanoyl*)
Rao, C.B. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 97-98 (N-*pentacosanoyl*)

2-Amino-1,3,4-octadecanetriol, 8CI A-378

C_{18}-*Phytosphingosine. 4-Hydroxysphinganine*



(2*R*,3*S*,4*S*)-*form*

$C_{18}H_{39}NO_3$ 317.511

(2*S*,3*S*,4*R*)-*form*
D-ribo-*form*
[554-62-1]
Present in cerebrosides and gangliosides. Isol. from the basidiomycete *Russula cyanoxantha*.
Amorph. powder.
Mp 103° (95-97°). $[\alpha]_D^{20}$ +10.3 (Py) (+9.4).

N-*Hexadecanoyl, 4-sulfate:* ***Ircisulfamide***
$C_{34}H_{69}NO_7S$ 635.988
Isol. from *Ircinia fasciculata*. Amorph. powder. $[\alpha]_D^{20}$ +16.7 (c, 0.24 in $CHCl_3$).

N-*Octadecanoyl:* ***Confertamide B***
[34354-88-6]
$C_{36}H_{73}NO_4$ 583.977
Constit. of *Sinularia conferta*. Cryst.
Mp 121-123° (99-100°). $[\alpha]_D^{20}$ +13.5 (c, 0.33 in MeOH).

N-*Nonadecanoyl:*
$C_{37}H_{75}NO_4$ 598.004
Constit. of the coral *Lobophytum* sp. Solid.
Mp 122-124°. $[\alpha]_D^{28}$ +19.2 (c, 0.5 in $CHCl_3$).

N-*Tetracosanoyl:* [34437-74-6]
$C_{42}H_{85}NO_4$ 668.138
Constit. of various marine sources and *Physalis philadelphica*. Amorph. powder.
Mp 114-116°. $[\alpha]_D^{20}$ +19.5 (c, 0.2 in Py).

N-*(2*R*-Hydroxyoctadecanoyl):* [65913-97-5]
$C_{36}H_{73}NO_5$ 599.976
Constit. of the coral *Sinularia leptoclados*. Powder (as tetra-Ac).
Mp 54-57° (tetra-Ac). $[\alpha]_D^{28}$ +8 (c, 0.1 in $CHCl_3$) (tetra-Ac).

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*β*-D-*glucopyranoside:* ***Regulosside A***
[193412-76-9]
$C_{46}H_{91}NO_{10}$ 818.226
Isol. from the starfish *Pentaceraster regulus*. Amorph. powder.
Mp 218-219°. $[\alpha]_D^{27}$ +10 (c, 0.05 in Py).

N-*(2*R*-Hydroxytricosanoyl), 1*-O-*β*-D-*glucopyranoside:* ***Regulosside B***
[193412-77-0]
$C_{47}H_{93}NO_{10}$ 832.252
Isol. from the starfish *Pentaceraster regulus*.

N-*(2*R*-Hydroxytetracosanoyl):* ***Russulaceramide***
[154801-30-6]
$C_{42}H_{85}NO_5$ 684.137
Constit. of various marine sources and *Physalis philadelphica*. Also from the basidiomycete *Russula cyanoxantha*. Amorph. powder.
Mp 123-125°. $[\alpha]_D$ +12.6 (c, 0.45 in Py). $[\alpha]_D$ +9.4 (c, 0.21 in Py).

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*β*-D-*glucopyranoside:* ***Regulosside C***
[193412-78-1]
$C_{48}H_{95}NO_{10}$ 846.279
Isol. from the starfish *Pentaceraster regulus*.

N-*(2*R*-Hydroxypentacosanoyl):* [305363-10-4]
$C_{43}H_{87}NO_5$ 698.164
Isol. from the mushrooms *Grifola frondosa* (maitake) and *Phellinus ribis*. Also found in the marine sponge *Iotrochota baculifera*. Amorph. powder.
Mp 145°. $[\alpha]_D^{21}$ +13.8 (c, 0.1 in Py).

N-*(2*R*-Hydroxy-4*E*-tetracosenoyl), 1*-O-*β*-D-*glucopyranoside:* ***Iotroridoside B***
[639088-52-1]
$C_{48}H_{93}NO_{10}$ 844.263
Isol. from the sponge *Iotrochota baculifera*.
Mp 205°. $[\alpha]_D^{28}$ +12 (c, 0.15 in Py).

N-*(2*R*-Hydroxy-4*E*-tetracosenoyl):* [875920-42-6]
$C_{42}H_{83}NO_5$ 682.121
Constit. of *Iotrochota baculifera*.
$[\alpha]_D^{28}$ +8.9 (c, 0.1 in Py).

N-*(2*R*-Hydroxy-4*Z*-tetracosenoyl), 1*-O-*β*-D-*glucopyranoside:* ***Iotroridoside A***
[277756-38-4]
$C_{48}H_{93}NO_{10}$ 844.263
Isol. from the sponge *Iotrochota ridley*. Cytotoxic. Amorph. solid.
$[\alpha]_D^{25}$ -7.2 (c, 0.003 in Py).

Hammarström, S. *et al., J. Lipid Res.*, 1971, **12**, 760-765 (*N-acyl derivs, synth*)
Dahlen, B. *et al., Acta Cryst. B*, 1972, **28**, 2396-2404 (*N-tetracosanoyl, cryst struct*)
Venkannababu, U. *et al., Liebigs Ann./Recl.*, 1997, 1245-1247 (*Regulosides*)
Bala, S.R.G. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1214-1220 (*N-2-hydroxyoctadecanoyl*)
Gao, J.M. *et al., Lipids*, 2001, **36**, 175-180 (*Russulaceramide, 2S,3S,4R-form, isol*)
Su, B.-N. *et al., Tetrahedron*, 2002, **58**, 3453-3466 (*N-tetracosanoyl, N-2-hydroxytetracosanoyl*)
Muralidhar, P. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1193-1195 (*Iotrochota baculifera ceramides*)
Muralidhar, P. *et al., Chem. Pharm. Bull.*, 2005, **53**, 168-171 (*N-nonadecanoyl*)
Zhang, G.-W. *et al., Helv. Chim. Acta*, 2005, **88**, 885-890 (*Ircisulfamide*)
Su, J.-Y. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 107-113 (*Confertamide B*)

2-Amino-1,3,12-octadecanetriol A-379

$H_3C(CH_2)_5CH(OH)(CH_2)_8CH(OH)CH(NH_2)CH_2OH$
$C_{18}H_{39}NO_3$ 317.511

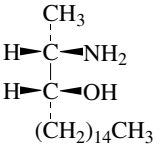
(2ξ,3ξ,12ξ)-*form*

N-*Octadecanoyl:* ***Nephtixamide B***
$C_{36}H_{73}NO_4$ 583.977
Isol. from the soft coral *Nephthea tixierae verseveldt*. Needles (EtOAc).
Mp 125.5-126.5°.

Wang, G.Y.S. *et al., Chin. Chem. Lett.*, 1993, **4**, 499-500 (*Nephtixamide B*)

2-Amino-3-octadecanol A-380

Spisulosine. ES 285
[247067501 2S-,3-S, 378754860 2R-,3-S]



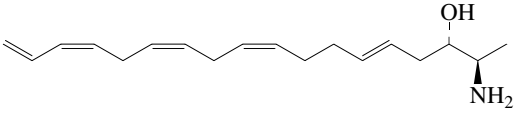
$C_{18}H_{39}NO$ 285.512

(2*S*,3*R*)-*form* [196497-48-0]
Isol. from the clam *Spisula polynyma*. Inhibitor of cell proliferation. Antitumour agent.
Mp 66-67°. $[\alpha]_D^{26}$ +24.9 (c, 1 in $CHCl_3$).

[378753-73-2]

Pat. Coop. Treaty (WIPO), 1999, 99 52 521; *CA*, **131**, 295576q (*isol, synth*)
Cuadros, R. *et al., Cancer Lett. (Shannon, Irel.)*, 2000, **152**, 23-29 (*isol, activity*)
Stokvis, E. *et al., J. Mass Spectrom.*, 2003, **38**, 548-554 (*anal*)
Yun, J.M. *et al., J.O.C.*, 2003, **68**, 7675-7680 (*synth*)

2-Amino-5,9,12,15,17-octadecapentaen-3-ol, 9CI A-381



$C_{18}H_{29}NO$ 275.433

(2*R*,3*S*,5*E*,9*Z*,12*Z*,15*Z*)-*form*
Crucigasterin 275
[150151-84-1]
Isol. from *Pseudodistoma crucigaster*.
Light yellow oil. λ_{max} 204 (ϵ 6200); 227 (ϵ 8700) (MeOH).

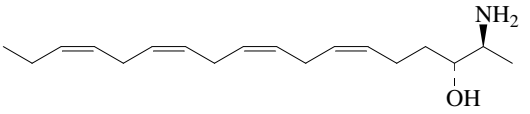
N,O-*Di-Ac:* [149849-81-0]
Oil. $[\alpha]_D^{29}$ +36 (c, 0.26 in MeOH).

17,18-Dihydro: 2-Amino-5,9,12,15-octadecatetraen-3-ol, 9CI. ***Crucigasterin 277***
[150151-83-0]
$C_{18}H_{31}NO$ 277.449
Isol. from *Pseudodistoma crucigaster*. Oil. λ_{max} 204 (ϵ 7900) (MeOH).

17,18-Dihydro, N,O-*di-Ac:* [149849-80-9]
Oil. $[\alpha]_D^{23}$ +36 (c, 0.53 in MeOH).

Jares-Erijman, E.A. *et al., J.O.C.*, 1993, **58**, 5732-5737 (*isol*)
Garrido, L. *et al., Tetrahedron*, 2001, **57**, 4579-4588 (*abs config*)

2-Amino-6,9,12,15-octadecatetraen-3-ol A-382

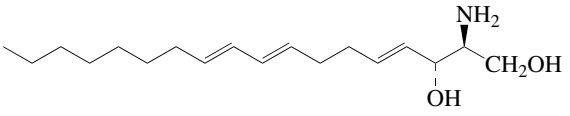


$C_{18}H_{31}NO$ 277.449

(2*S*,3*R*,6*Z*,9*Z*,12*Z*,15*Z*)-*form*
Obscuraminol A. *Halaminol D*
[350484-80-9]
Isol. from the tunicate *Pseudodistoma obscurum*.
Oil. $[\alpha]_D^{20}$ +5 (c, 0.14 in MeOH). $[\alpha]_D$ -23 (c, 0.78 in MeOH) (as di-Ac).
Clark, R.J. *et al., J. Nat. Prod.*, 2001, **64**, 1568-1571 (*Halaminol D*)
Garrido, L. *et al., Tetrahedron*, 2001, **57**, 4579-4588 (*Obscuraminol A*)

2-Amino-4,8,10-octadecatriene-1,3-diol A-383

4,8,10-Sphingatriene

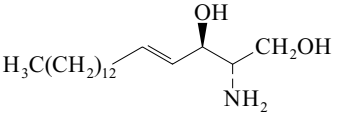


$C_{18}H_{33}NO_2$ 295.464

(2*S*,3*R*,4*E*,8*E*,10*E*)-*form*
N-*Hexadecanoyl:* [166762-66-9]
$C_{34}H_{63}NO_3$ 533.877
Isol. from the gorgonian *Acabaria undulata*. Solid.
Mp 85-86°. $[\alpha]_D^{25}$ -4.1 (c, 0.5 in $CHCl_3$). λ_{max} 223 (ε 9500) (MeCN).
N-*(2*R*-Hydroxy-15*R*-methyl-3*E*-octadecenoyl):* [205582-76-9]
$C_{37}H_{67}NO_4$ 589.941
Isol. from the dinoflagellate *Coolia monotis*.
N-*(2*R*-Hydroxy-14*Z*-tricosenoyl), 1-*O*-β-D-glucopyranoside:* ***Anasterocerebroside A***
[585573-97-3]
$C_{47}H_{85}NO_9$ 808.19
Isol. from the starfish *Anasterias minuta*. Solid. $[\alpha]_D$ -6.7 (c, 0.62 in $CHCl_3$).
N-*(2*R*-Hydroxy-15*Z*-tetracosenoyl), 1-*O*-β-D-glucopyranoside:*
[457645-48-6]
$C_{48}H_{87}NO_9$ 822.217
Isol. from starfish *Allostichaster inaequalis* and *Anasterias minuta*. Amorph. solid.
Mp 182°. $[\alpha]_D$ -12.5 (c, 0.3 in 1-propanol).
Shin, J. *et al., J. Nat. Prod.*, 1995, **58**, 948-953 (*N-hexadecanoyl*)
Tanaka, I. *et al., J. Nat. Prod.*, 1998, **61**, 685-688 (*Coolia monotis cerebroside*)
Akasaka, K. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1842-1846 (*abs config*)
Diaz de Vivar, M.E. *et al., Lipids*, 2002, **37**, 597-603 (*Allostichaster glycolipid*)
Chludil, H.D. *et al., Z. Naturforsch., C*, 2003, **58**, 433-440 (*Anasterias minuta cerebrosides*)

2-Amino-4-octadecene-1,3-diol, 9CI A-384

4-Sphingenine. *C_{18}-Sphingosine*



(2*S*,3*R*,4*E*)–*form*

$C_{18}H_{37}NO_2$ 299.496
See also Gangliosides, G-24. Many syntheses reported of various stereoisomers.

(2*S*,3*R*,4*E*)-*form*
D-erythro-trans-*form*
[123-78-4]
Cryst. (Et_2O). Mp 80-84° (79-81°).
1-Phosphate: Sphingosine-1-phosphate
[26993-30-6]
$C_{18}H_{38}NO_5P$ 379.476
Intermed. in catabolic degradation of sphingosine. Affects cell growth. Amorph. powder.
1-O-β-D-*Glucopyranoside:* ***Glucopsychosine***
[52050-17-6]
$C_{24}H_{47}NO_7$ 461.638
Metab. prod. present in Gaucher's disease.
1-O-β-D-*Galactopyranoside: Psychosine*
[2238-90-6]
[38621-58-8]
$C_{24}H_{47}NO_7$ 461.638
Alkaline hydrol. prod. of the cerebrosides. Cryst. (EtOH or MeOH/MeCN). Mp 195-200° dec. $[\alpha]_D^{20}$ -12.5 (Py).
N-*Ac:* [3102-57-6]
[532-45-6]
$C_{20}H_{39}NO_3$ 341.533
Powder. Mp 85-87°. $[\alpha]_D^{26}$ -10 (c, 13.7 in MeOH).
Tri-Ac: [2482-37-3]
Mp 103.5-104°. $[\alpha]_D^{19}$ -24.1. $[\alpha]_D$ -13 (c, 0.5 in $CHCl_3$).
N-*Hexanoyl:* [124753-97-5]
$C_{24}H_{47}NO_3$ 397.64
Cryst. (MeOH aq.).
N-*Tetradecanoyl:* N-*[2-Hydroxy-1-(hydroxymethyl)-3-heptadecenyl]tetradecanamide, 8CI*. *2-Tetradecanoylamino-4-octadecene-1,3-diol*. N-*Tetradecanoyl-4-sphingenine*
[34227-72-0]
$C_{32}H_{63}NO_3$ 509.855
Present in blood plasma lipids.
N-*Tetradecanoyl, 1*-O-β-D-*galactopyranoside:* N-*Tetradecanoylgalactocerebroside*
[315710-03-3]
$C_{38}H_{73}NO_8$ 671.997
Found in brain tissue.
N-*Pentadecanoyl:* [67492-15-3]
$C_{33}H_{65}NO_3$ 523.881
Constit. of the sponge *Gellius cymiformis*.
N-*(2*R*-Hydroxy-14ξ-methylpentadecanoyl), 1-sulfate:* ***Calyceramide C***
[346425-31-8]
$C_{34}H_{67}NO_7S$ 633.972
Isol. from the sponge *Discodermia calyx*. Neuraminidase inhibitor. Solid (as Na salt). $[\alpha]_D^{20}$ +16.9 (c, 0.1 in MeOH) (Na salt).
N-*Hexadecanoyl:* N-*[2-Hydroxy-1-(hydroxymethyl)-3-heptadecenyl]hexadecanamide, 8CI*. *2-Hexadecanoylamino-4-octadecene-1,3-diol*. N-*Hexadecanoyl-4-sphingenine*
[24696-26-2]
$C_{34}H_{67}NO_3$ 537.908
Present in blood and brain lipids.
N-*Hexadecanoyl, 1*-O-*[*N-*acetyl-α-neuraminosyl-(2→3)-β-D-galactopyranosyl-(1→4)-β-D-glucopyranoside]:* ***Ganglioside GM3***. N-*Acetylganglioside GM3*
[89678-50-2]
$C_{57}H_{104}N_2O_{21}$ 1153.449
Ubiquitous metabolite. Involved in cell differentiation, immunosuppression and other cellular functions. Amorph. solid.
Mp 180-190° (softens). $[\alpha]_D^{22}$ +0.8 (c, 1.2 in $CHCl_3$/MeOH 1:1).
N-*(2-Hydroxyhexadecanoyl): 2-Hydroxy*-N-*[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]hexadecanamide, 9CI*. N-*2-Hydroxyhexadecanoyl-4-sphingenine*
[228579-71-3]
$C_{34}H_{67}NO_4$ 553.908
Found in brain tissue.
Mp 100-101°.
N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-β-D-*glucopyranoside: AS 1-5*
[154967-87-0]
$C_{40}H_{77}NO_9$ 716.05
Constit. of *Allium sativum* (garlic) bulbs. Amorph. powder.
Mp 205-210°. $[\alpha]_D^{28}$ +8.3 (c, 0.15 in propanol).
N-*Heptadecanoyl:*
$C_{35}H_{69}NO_3$ 551.935
Isol. from the red alga *Amansia glomerata* and the gorgonian *Pseudopterogorgia australiensis*. Cryst.
N-*Octadecanoyl: 2-Octadecanoylamino-4-octadecene-1,3-diol*. N-*Octadecanoyl-4-sphingenine*

[2304-81-6]
$C_{36}H_{71}NO_3$ 565.962
Isol. from *Styela canopus*. Present in blood and brain lipids.
Mp 97-98° (91-93°). $[\alpha]_D^{25}$ -3.1 (c, 1.1 in $CHCl_3$).

N-*Octadecanoyl, 1*-O-*β-D-galactopyranoside:* N-*Octadecanoylgalactocerebroside*
[36271-49-5]
$C_{42}H_{81}NO_8$ 728.104
Found in brain tissue.

N-*Octadecanoyl, 1*-O-*[6-deoxy-α-L-galactopyranosyl-(1→3)-[β-D-mannopyranosyl-(1→4)]-β-D-glucopyranoside]:* [319922-63-9]
$C_{54}H_{101}NO_{17}$ 1036.388
Isol. from the millipede *Parafontaria laminata armigera*.

N-*(9-Octadecenoyl):* N-*[2-Hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-9-octadecenamide, 9CI*. *2-Octadec-9-enoylamino-4-octadecene-1,3-diol*. N-*Octadec-9-enoylsphingenine*. N-*Oleoyl-4-sphingenine*
[5966-28-9]
$C_{36}H_{69}NO_3$ 563.946
Present in blood and brain lipids.

N-*(9Z,12Z-Octadecadienoyl):* N-*9,12-Octadecadienoyl-4-sphingenine*. N-*Linoleoyl-4-sphingenine*
[34249-39-3]
$C_{36}H_{67}NO_3$ 561.93
Found in brain lipids.

N-*Nonadecanoyl:*
$C_{37}H_{73}NO_3$ 579.989
Isol. from the gorgonian *Junceella juncea*. Cryst. $[\alpha]_D^{25}$ -11.5 (c, 0.1 in $CHCl_3$).

N-*Eicosanoyl:* N-*[2-Hydroxy-1-(hydroxymethyl)-3-heptadecenyl]eicosanamide, 9CI*. *2-Eicosanoylamino-4-octadecene-1,3-diol*. N-*Eicosanoyl-4-sphingenine*. N-*Icosanoyl-4-sphingenine*
[7344-02-7]
$C_{38}H_{75}NO_3$ 594.015
Present in blood and brain lipids.

N-*Docosanoyl:* N-*[2-Hydroxy-1-(hydroxymethyl)-3-heptadecenyl]docosanamide, 9CI*. *2-Docosanoylamino-4-octadecene-1,3-diol*. N-*Docosanoyl-4-sphingenine*
[27888-44-4]
$C_{40}H_{79}NO_3$ 622.069
Present in brain and blood lipids. Isol. from sponge *Callyspongia spinosissima*. Microcryst. solid (MeOH).
Mp 120°. $[\alpha]_D^{27}$ -7 (c, 0.5 in $CHCl_3$/MeOH 1:1).

N-*(13Z-Docosenoyl):* N-*[2-Hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-13-docosenamide, 9CI*. N-*13-Docosenoyl-4-octadecene-1,3-diol*. N-*13-Docosenoyl-4-sphingenine*. N-*Erucoyl-4-sphingenine*
[54135-66-9]
$C_{40}H_{77}NO_3$ 620.053
Present in blood lipids.

N-*Tetracosanoyl:* N-*[2-Hydroxy-1-(hydroxymethyl)-3-heptadecenyl]tetracosanamide, 9CI*. *2-(Tetracosanoylamino)-4-octadecene-1,3-diol*. N-*Tetracosanoyl-4-sphingenine*. ***Lobophytamide L5***
[34435-05-7]
[34227-72-0]
$C_{42}H_{83}NO_3$ 650.123
Present in blood and brain lipids. Cryst. (MeOH).
Mp 93-95°.

N-*(15Z-Tetracosenoyl), 1*-O-*β-D-galactopyranoside:* N-*15Z-Tetracosenoylgalactocerebroside*. ***Nervone***
[17283-91-9]
$C_{48}H_{91}NO_8$ 810.249
Present in brain cerebrosides.
Mp 154-156°. $[\alpha]_D^{22}$ -3.7 (c, 10 in Py).

N-*(2-Hydroxytetracosanoyl), 1*-O-*galactopyranoside:* See *N*-2-Hydroxytetracosanoylgalactocerebroside in *The Combined Chemical Dictionary.*

N-*(2-Hydroxy-15Z-tetracosenoyl), 1*-O-*β-D-galactopyranoside:* N-*(2-Hydroxy-15-tetracosenoyl)galactocerebroside*. ***Oxynervone***
[17283-90-8]
$C_{48}H_{91}NO_9$ 826.248
Brain cerebroside.
Mp 180-181°. $[\alpha]_D^{22}$ +3.8 (c, 10 in Py).

Tribenzoyl:
Cryst. (EtOH). Mp 121.5-123.5°. $[\alpha]_D^{27}$ -11.2.

N,N-*Di-Me:* [119567-63-4]
$C_{20}H_{41}NO_2$ 327.549
Syrup. $[\alpha]_D$ -3.16 (c, 0.98 in $CHCl_3$).

(2*S*,3*R*,4*Z*)-*form*
D-erythro-cis-*form*
[26308-91-8]
Mp 73-74°. $[\alpha]_D^{21}$ -5 (c, 0.5 in $CHCl_3$).

Tri-Ac: Mp 90-91°.

(2*RS*,3*RS*,4*E*)-*form*
(±)-threo-trans-*form*
[2304-77-0]

N-*Ac:* Mp 69-70°.

N-*Tetradecanoyl:* [16170-10-8]
Mp 88-90°.

(2*RS*,3*RS*,4*Z*)-*form*
(±)-threo-cis-*form*
[17673-73-3]
Mp 80-81°.

N-*Ac:* Mp 97-99°.

Tri-Ac: Mp 40-41°.

N-*Tetradecanoyl:* [17673-78-8]
Mp 96.5-98°.

N-*Hexadecanoyl, 1*-O-*[α-D-galactopyranosyl-(1→4)-β-D-galactopyranosyl-(1→4)-β-D-glucopyranoside]:* ***Globotriaosylceramide***
[137896-85-6]
$C_{52}H_{97}NO_{18}$ 1024.334
Isol. from various tissues, e.g. canine intestine. Cell surface receptor. P^k antigen in the P blood-group system. Associated with various carcinomas.

N-*Hexadecanoyl, 1*-O-*[α-D-galactopyranosyl-(1→3)-β-D-galactopyranosyl-(1→4)-β-D-glucopyranoside]:* ***Isoglobotriaosylceramide***
[137896-95-8]
$C_{52}H_{97}NO_{18}$ 1024.334
Isol. from various tissues. Associated with rat mammary tumours.

N-*Tetracosanoyl:* [17673-74-4]
Mp 100-102°.

(2*RS*,3*SR*,4*E*)-*form*
(±)-erythro-trans-*form*
[2733-29-1]
Mp 71-73° (65-68°).

Tri-Ac: Mp 95-95.5° (91-92°).

N-*Hexadecanoyl:* [52019-77-9]
Cryst. (MeOH aq.). Mp 97-98°.

N-*Octadecanoyl:* Mp 101-102°.

N-*(9-Octadecenoyl):* Mp 68-69°. CAS no. not found 8-14CI.

N-*Tetracosanoyl:* [26549-48-4]
Cryst. (MeOH aq.). Mp 95-96°.

(2*RS*,3*SR*,4*Z*)-*form*
(±)-erythro-cis-*form*
[877761-07-4]
Mp 74-75°.

N-*Ac:* Mp 70-71°.

Tri-Ac: Mp 83-84°.

(2ξ,3ξ,4*E*)-*form*
N-*Tricosanoyl:* ***Sertularamide***
[192938-52-6]
$C_{41}H_{81}NO_3$ 636.096
Isol. from the alga *Caulerpa sertularioides*. Amorph. powder (Me_2CO).
Mp 95-96°.

(2ξ,3ξ,4ξ)-*form* [10140-30-4]
N-*Octadecanoyl:* [335317-17-4]
$C_{36}H_{71}NO_3$ 565.962
Isol. from tunicate *Styela canopus.*
Shapiro, D. *et al., J.A.C.S.*, 1964, **86**, 4472-4476 (*Psychosine, synth*)
Gaver, R.C. *et al., J.A.C.S.*, 1966, **88**, 3643-3647 (*N-Ac, synth*)
Klenk, E. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1967, **348**, 1061-1065 (*Nervone, Oxynervone*)
Auer, E. *et al., Monatsh. Chem.*, 1967, **98**, 802-806 (*synth*)
Samuelsson, B. *et al., J. Lipid Res.*, 1969, **10**, 47-55 (*occur*)
Karlsson, K.A. *et al., J. Lipid Res.*, 1971, **12**, 466-472 (*tlc*)
Stoffel, W. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1972, **353**, 1962-1969 (*cmr*)
Krivit, W. *et al., J. Lipid Res.*, 1972, **13**, 525-530 (*occur*)
Ong, D.E. *et al., J. Lipid Res.*, 1972, **13**, 819-822 (*synth*)
Cardellina, J.H. *et al., Phytochemistry*, 1978, **17**, 554-555 (*N-heptadecanoyl*)
Schmidt, R.R. *et al., Angew. Chem., Int. Ed.*, 1982, **21**, 210-211; 1986, **25**, 725-729 (*synth, bibl*)
Garigipati, R.S. *et al., J.A.C.S.*, 1983, **105**, 4499-4501 (*synth, ir, pmr, cmr*)
Wylida, J. *et al., J.O.C.*, 1984, **49**, 244-249 (*Psychosine, isol*)
Kiso, M. *et al., Carbohydr. Res.*, 1986, **158**, 101-111 (*synth*)
Koike, K. *et al., Carbohydr. Res.*, 1986, **158**, 113-123; 1987, **163**, 189-208 (*synth, Tetracosanoylsphingenine, Globotriaosylceramide, Isoglobotriosylceramide*)
Julina, R. *et al., Helv. Chim. Acta*, 1986, **69**, 368-373 (*synth*)
Radunz, H.E. *et al., Annalen*, 1988, 1103-1105 (*synth*)
Nicolaou, K.C. *et al., Carbohydr. Res.*, 1990, **202**, 177-191 (*synth, Globotriaosylceramide*)
Igarashi, Y. *et al., J. Biol. Chem.*, 1990, **265**, 5385-5389 (*di-Me, synth, pmr*)
Mori, K. *et al., Annalen*, 1991, 253-257 (*synth, glucoside*)
Qiu, D. *et al., Annalen*, 1992, 217-224 (*Globotriaosylceramide, Isoglobotriaosylceramide*)
Ruan, I. *et al., Bioorg. Med. Chem. Lett.*, 1992, **2**, 973-978 (*1-phosphate*)
Metz, K. *et al., Annalen*, 1993, 55-60 (*synth*)
Yadav, J.S. *et al., Tet. Lett.*, 1993, **34**, 1191 (*synth*)
Kratzer, B. *et al., Ann len*, 1995, 957-963 (*1-phosphate*)
Jayadev, S. *et al., J. Biol. Chem.*, 1995, **270**, 2047-2052 (*N-hexanoyl, synth, pmr*)
Li, Y.-L. *et al., Annalen*, 1996, 2079-2082 (*synth, ir, pmr*)
Miyata, O. *et al., Chem. Pharm. Bull.*, 1996, **44**, 636-638 (*synth, bibl*)
Shinozaki, K. *et al., Chem. Pharm. Bull.*, 1996, **44**, 927-932 (*synth*)
Xu, S.H. *et al., Chin. Chem. Lett.*, 1997, **8**, 419-420 (*Sertulamide*)
Agrawal, S. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 343-346 (*N-docosanoyl, isol, sponge*)
Spanu, P. *et al., Tetrahedron: Asymmetry*, 1997, **8**, 3237-3243 (*synth*)
Inagaki, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1153-1156 (*AS 1-5*)
Nugent, T.C. *et al., J.O.C.*, 1998, **63**, 510-520 (*synth*)
Hoffmann, R.V. *et al., J.O.C.*, 1998, **63**, 3979-3985 (*synth*)
Kumar, P. *et al., Synthesis*, 1998, 33-35 (*synth*)
Kobayashi, S. *et al., Tetrahedron*, 1998, **54**, 10275-10294 (*synth*)
Khiar, N. *et al., Tet. Lett.*, 1999, **40**, 5779-5782 (*synth*)
Duclos, R.I. *et al., Carbohydr. Res.*, 2000, **328**, 489-507 (*Ganglioside GM3, synth, bibl*)
Jung, K.-H. *et al., Methods Enzymol.*, 2000, **311**, 441-457 (*synth*)
Koskinen, P.M. *et al., Methods Enzymol.*, 2000, **311**, 458-479 (*rev, synth*)
Bielawska, A. *et al., Methods Enzymol.*, 2000, **311**, 518-535 (*synth*)
Corey, E.J. *et al., Tet. Lett.*, 2000, **41**, 2765-2768 (*synth*)
Hada, N. *et al., Tet. Lett.*, 2000, **41**, 9065-9068 (*Parafontaria glycosphingolipid*)
Wang, C. *et al., CA*, 2001, **134**, 308134 (*Styela canopus constit*)
Nakao, Y. *et al., Tetrahedron*, 2001, **57**, 3013-3017 (*Calyceramide C*)
Nakamura, T. *et al., Tetrahedron*, 2001, **57**, 9087-9092 (*synth*)
Krishna, N. *et al., Nat. Prod. Rep.*, 2004, **18**, 551-555 (*N-nonadecanoyl*)
Disadee, W. *et al., J.O.C.*, 2005, **70**, 9399-9406 (*synth*)
Jacques, S. *et al., Org. Biomol. Chem.*, 2006, **4**, 142-154 (*Ganglioside GM_3, synth*)

2-Amino-9-octadecene-1,3-diol A-385

$H_3C(CH_2)_7CH{=}CH(CH_2)_5CH(OH)CH(NH_2)CH_2OH$
$C_{18}H_{37}NO_2$ 299.496

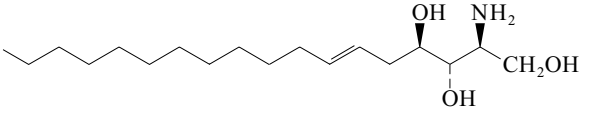
N-*Pentadecanoyl:* ***Isisamide***
[162232-40-8]
$C_{33}H_{65}NO_3$ 523.881
Constit. of the gorgonian *Isis* sp.
Deng, S. *et al., CA*, 1995, **122**, 235560j

2-Amino-5-octadecene-1,3,4-triol A-386

$H_3C(CH_2)_{11}CH{=}CHCH(OH)CH(OH)CH(NH_2)CH_2OH$
$C_{18}H_{37}NO_3$ 315.495

(2ξ,3ξ,4ξ,5*E*)-*form*
N-*(2-Hydroxyhexadecanoyl):* [479411-46-6]
$C_{34}H_{67}NO_5$ 569.907
Constit. of a *Sinularia* sp. Cryst. ($CHCl_3$/MeOH).
Mp 144-145°. $[\alpha]_D^{25}$ +7.2 (c, 0.1 in MeOH).
Parvataneni, R. *et al., J. Indian Chem. Soc.*, 2002, **79**, 732-738 (*isol, pmr, cmr*)

2-Amino-6-octadecene-1,3,4-triol A-387



(2*S*,3*S*,4*R*,6*E*)–*form*

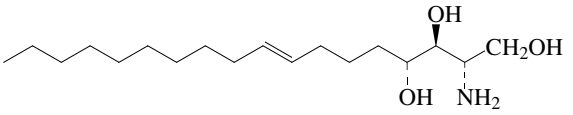
$C_{18}H_{37}NO_3$ 315.495

(2*S*,3*S*,4*R*,6*E*)-*form*
4-O-*Sulfate:*
$C_{18}H_{37}NO_6S$ 395.559
Isol. from the sponge *Spirastrella abata.* Amorph. solid.
N-*(2*R-*Hydroxyheneicosanoyl), 1*-O-*[α-D-galactopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Amphimelibioside A_1***
$C_{51}H_{97}NO_{15}$ 964.325
Isol. from an *Amphimedon* sp. Powder. Isol. as a mixt. with Amphimelibioside A_2.
N-*(2*R-*Hydroxydocosanoyl), 1*-O-*[α-D-galactopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Amphimelibioside C***
$C_{52}H_{99}NO_{15}$ 978.352
Isol. from an *Amphimedon* sp. Powder.
N-*(2*R-*Hydroxytricosanoyl), 1*-O-*[α-D-galactopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Amphimelibioside E***
$C_{53}H_{101}NO_{15}$ 992.379
Isol. from an *Amphimedon* sp. Powder.
N-*(2*R-*Hydroxytetracosanoyl):* [163132-94-3]
$C_{42}H_{83}NO_5$ 682.121
Isol. from *Spirastrella inconstans.* Cryst. (MeOH).
Mp 121-123°. $[\alpha]_D^{27}$ +9.2 (c, 0.05 in MeOH).
N-*(2*R-*Hydroxytetracosanoyl), 1*-O-*[α-D-galactopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Amphimelibioside F***
$C_{54}H_{103}NO_{15}$ 1006.405
Isol. from an *Amphimedon* sp. Powder.
N-*(2*R-*Hydroxy-15Z-tetracosenoyl), 1*-O-*β-D-galactopyranoside:* ***Coralipid***
[146396-36-3]
$C_{48}H_{91}NO_{10}$ 842.248
Isol. from the red alga *Corallina pilulifera*. Cryst.
Mp 61-62°. $[\alpha]_D^{25}$ +12.6 (c, 1.3 in Py).

(2ξ,3ξ,4ξ,6ξ)-*form*
N-*(2-Hydroxydocosanoyl), 1*-O-*β-D-glucopyranoside:* ***Halicerebroside A***
[122794-87-0]
$C_{46}H_{89}NO_{10}$ 816.21
Isol. from the sponge *Haliclona* sp. Viscous oil.
Hirsch, S. *et al., Tetrahedron*, 1989, **45**, 3897 (*Halicerebroside A, isol, struct*)
Ishida, R. *et al., Chem. Lett.*, 1993, 9-12 (*Coralipid, isol*)
Garg, H.S. *et al., J. Nat. Prod.*, 1995, **58**, 442-445 (*Spirastrella inconstans sphingosine*)
Alam, N. *et al., J. Nat. Prod.*, 2002, **65**, 944-945 (*4-sulfate*)
Emura, C. *et al., J.O.C.*, 2005, **70**, 3031-3038 (*Amphimelibiosides*)

2-Amino-8-octadecene-1,3,4-triol, 9CI A-388

[81520-97-0]



(2*S*,3*S*,4*R*,8*E*)-*form*

$C_{18}H_{37}NO_3$ 315.495

(2*S*,3*S*,4*R*,8*E*)-*form*

D-ribo-trans-*form*. *Dehydrophytosphingosine*
[3687-54-5]
Isol. from soybean and flax phosphatides.
Cryst. (Et_2O).
Mp 92-94°. $[\alpha]_D^{25}$ +8.5 (c, 1.2 in EtOH).

N-*(2*R*-Hydroxyoctadecanoyl):*
$C_{36}H_{71}NO_5$ 597.961
Constit. of *Sinularia grandilobata*. Cryst. ($CHCl_3$/MeOH).
Mp 128-130°.

[25277-37-6, 51153-53-8]

Dmitrenok, A.S. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2003, **52**, 1868-1872 (*Sinularia grandilobata constit*)

2-Amino-1,3-pentadecanediol A-389

$H_3C(CH_2)_{11}CH(OH)CH(NH_2)CH_2OH$

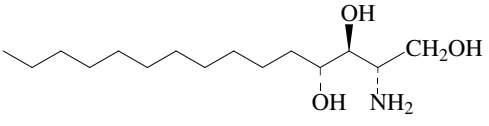
$C_{15}H_{33}NO_2$ 259.431

(2ξ,3ξ)-*form*

N-*(2,4-Dihydroxytricosanoyl):* [877210-62-3]
$C_{38}H_{77}NO_5$ 628.03
Isol. from an unidentified sponge.

Guo, W.-C. *et al., CA*, 2006, **144**, 250597z (*isol*)

2-Amino-1,3,4-pentadecanetriol A-390



$C_{15}H_{33}NO_3$ 275.431

(2*S*,3*S*,4*R*)-*form*

N-*(2*R*-Hydroxytetracosanoyl):* [326597-23-3]
$C_{39}H_{79}NO_5$ 642.057
Constit. of the sex pheromone of the crab *Erimacrus isenbeckii*.

N-*(2*R*-Hydroxy-21-methyldocosanoyl):* [326597-22-2]
$C_{38}H_{77}NO_5$ 628.03
Constit. of the sex pheromone of the crab *Erimacrus isenbeckii*.
Mp 129-133° (synthetic). $[\alpha]_D^{22}$ +14 (c, 0.7 in $CHCl_3$/MeOH) (synthetic).

N-*(2*R*-Hydroxy-22-methyltricosanoyl):* [326597-24-4]
$C_{39}H_{79}NO_5$ 642.057
Constit. of the sex pheromone of the crab *Erimacrus isenbeckii*.

N-*(2*R*-Hydroxypentacosanoyl):* [326597-26-6]
$C_{40}H_{81}NO_5$ 656.084
Constit. of the sex pheromone of the crab *Erimacrus isenbeckii*.

N-*(2*R*-Hydroxy-23-methyltetracosanoyl):* [326597-27-7]
$C_{40}H_{81}NO_5$ 656.084
Constit. of the sex pheromone of the crab *Erimacrus isenbeckii*.

Asai, N. *et al., Tetrahedron*, 2000, **56**, 9895-9899 (*isol*)
Asai, N. *et al., J. Nat. Prod.*, 2001, **64**, 1210-1215 (*synth*)
Masuda, Y. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 1531-1537 (*synth*)

3-Aminopentanedioic acid, 9CI A-391

3-Aminoglutaric acid. β-Glutamic acid
[1948-48-7]
$HOOCCH_2CH(NH_2)CH_2COOH$
$C_5H_9NO_4$ 147.13
Isol. from *Chondria armata*. Cryst. (H_2O).
Mp 295° (280-282°).

Di-Me ester:
$C_7H_{13}NO_4$ 175.184
Oil. $Bp_{0.05}$ 67-70°.

Di-Et ester: [51865-85-1]
$C_9H_{17}NO_4$ 203.238
Mp 83.5-84.5° (as hydrochloride).

Monoamide: 3,5-Diamino-5-oxopentanoic acid, 9CI. 3-Aminoglutaramic acid, 8CI. β-Glutamine
[6706-21-4]
$C_5H_{10}N_2O_3$ 146.146
Cryst. (Me_2CO aq.). Mp 245° dec.

N-*Me: 3-(Methylamino)glutaric acid*
[79755-76-3]
$C_6H_{11}NO_4$ 161.157
Amino acid from the prokaryotic algal symbiont *Prochloron didemnii*. Prisms (EtOH aq.).
Mp 177-179°.

[60793-95-5]

Nauta, W.T. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1953, **72**, 721 (*synth*)
Romeo, A. *et al., CA*, 1954, **48**, 10592 (*synth*)
Feuer, H. *et al., J.A.C.S.*, 1955, **77**, 5427 (*synth*)
Takemoto, T. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1960, **293**, 627 (*isol*)
Josey, A.D. *et al., J.O.C.*, 1962, **27**, 2466 (*synth, ir*)
Khedouri, E. *et al., Biochemistry*, 1964, **3**, 824 (*monoamide*)
Summons, R.E. *et al., Phytochemistry*, 1981, **20**, 1125 (*deriv*)
Crossley, M.J. *et al., J.C.S. Perkin 1*, 1990, 2363 (*synth, pmr*)

5-Aminopentanoic acid, 9CI A-392

[660-88-8]
$H_2NCH_2(CH_2)_3COOH$
$C_5H_{11}NO_2$ 117.147
Leaflets. Mp 157-158° dec. pK_{a1} 4.26; pK_{a2} 10.71 (25°, 0.5*M* NaCl). On melting, forms lactam, 2-Piperidinone, P-433.

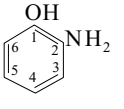
N,N,N-*Tri-Me, betaine: 5-Aminopentanoic acid betaine. δ-Aminovaleric acid betaine*
[6778-33-2]
$C_8H_{17}NO_2$ 159.228
Constit. of an alga of the Florideophyceae.

N,N,N-*Tri-Me, Me ester: 5-Methoxy*-N,N,N-*trimethyl-5-oxo-1-pentanaminium, 9CI. (4-Methoxycarbonylbutyl)trimethylammonium*
[85806-09-3]
$C_9H_{20}NO_2^{\oplus}$ 174.263
Isol. from *Austrovenus stutchburyi*. Neurotoxin. Cryst. (as chloride). Sol. H_2O. λ_{max} 225 (ε 15850) (H_2O).
► LD_{50} (mus, ipr) .30 mg/kg.

Blunden, G. *et al., Biochem. Syst. Ecol.*, 1992, **20**, 373 (*isol, betaine*)
Ishida, H. *et al., Toxicon*, 1994, **32**, 1672-1674 (*N-tri-Me Me ester*)

2-Aminophenol, 9CI A-393

o-*Hydroxyaniline. 1-Amino-2-hydroxybenzene.* ***Questiomycin B***
[95-55-6]
[27598-85-2]



C_6H_7NO 109.127
Manuf. by redn. of 2-nitrophenol. Isol. from *Streptomyces* sp. and *Penicillium notatum*. Also isol. from a purple bacterium from a sponge of *Adocia* sp. Electrochem. polym. gives electroactive

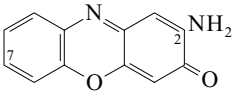
polymer films. Dye intermediate. Tuberculostatic. Possesses antibacterial props. Cryst. (H_2O). Sol. MeOH, H_2O, Et_2O, EtOAc; fairly sol. CCl_4; poorly sol. hexane.
Mp 174°. pK_{a1} 4.78; pK_{a2} 9.97 (20°). Free base readily oxidised. λ_{max} 235 (ϵ 28400); 467 (ϵ 1700) (0.25*N* HCl) (Derep). λ_{max} 335 (ϵ 1230) (0.1*N* KOH) (Derep). λ_{max} 240 (ϵ 26300); 435 (ϵ 2330) (pH 7.4) (Derep). λ_{max} 229; 283 (H_2O) (Berdy). λ_{max} 268 (HCl) (Berdy). λ_{max} 300 (NaOH) (Berdy).

▶ Eye and respiratory tract irritant. LD_{50} (rat, orl) 1300 mg/kg. LD_{50} (mus, ipr) 350 mg/kg. Exp. reprod. and teratogenic effect. SJ4950000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1195D; **2**, 356C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 463C; 1362A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1115D (*ir*)
Aldrich Library of IR Spectra, **2**, 633F (*ir*)
Aldrich Library of NMR Spectra, **5**, 45C (*pmr*)
Forbes, W.F. *et al., Can. J. Chem.*, 1958, **36**, 1371; 1959, **37**, 1294 (*uv*)
Anzai, K. *et al., J. Antibiot., Ser. A*, 1960, **13**, 125 (*isol*)
Neilson, T. *et al., J.C.S.*, 1962, 371 (*synth*)
Portnaya, B.S. *et al., Zh. Org. Khim.*, 1965, 2202 (*synth*)
De Courville, A. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1966, **262**, 1196
Pfeifer, S. *et al., Pharmazie*, 1972, **27**, 536-542 (*isol*)
Vogel, A.I. *et al., Practical Organic Chemistry*, 4th Ed., Longmans, 1978, 662 (*synth*)
Korp, J.D. *et al., J. Cryst. Mol. Struct.*, 1981, **11**, 117 (*cryst struct*)
Fujita, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1151 (*cmr*)
Ide, S. *et al., Anal. Chim. Acta*, 1983, **149**, 235 (*synth, use*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **2**, 580 (*rev*)
Oclarit, J.M. *et al., Fish. Sci.*, 1994, **60**, 559 (*isol*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 53
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ALT000; HIL000

2-Amino-3*H*-phenoxazin-3-one, 9CI, 8CI A-394

Questiomycin A. *AV toxin C*
[1916-59-2]



$C_{12}H_8N_2O_2$ 212.207
Isol. from *Acrospermum viticola, Brevibacterium iodinum, Calocybe gambosa* (St George's mushroom), *Microbispora aerata, Streptomyces thioluteus, Pycnoporus* sp., *Waksmania* sp., and mushroom *Lepiota americana*. Used as a 1m*M* soln. in EtOH as redox indicator for titanometric detn. of Fe(*III*), Au(*III*), $Cr_2O_7^{2\ominus}$, $VO_4^{3\ominus}$ and some organic compds.; redox indicator for stannometry. Aromatase and sulfatase inhibitor. Active against gram-positive bacteria, mycobacteria, *Candida albicans* and shows antitumour activity. Phytotoxin. Dark brown or red cryst. (EtOH). Sol. EtOH. Subl. 255-257. Sometimes occurs in amorph. form with Mp 296-297°. E° + 0.372V (pH 0.92, 23°). λ_{max} 235 (ϵ 28400); 467 (ϵ 1700) (0.25*N* HCl) (Derep). λ_{max} 335 (ϵ 1230) (0.1*N* KOH) (Derep). λ_{max} 240 (ϵ 26300); 435 (ϵ 2330) (pH 7.4) (Derep).

▶ LD_{50} (mus, ipr) 200 mg/kg. SP7695000

N-*β*-D-*Glucopyranosyl:* **N-*β*-D-*Glucopyranosylquestiomycin A***
$C_{18}H_{18}N_2O_7$ 374.349
Prod. by *Microbispora* sp. TP-A0184. Antibacterial and cytotoxic agent. Red powder. Sol. DMSO, Py; fairly sol. MeOH; poorly sol. $CHCl_3$, EtOAc.
Mp >195° dec. $[\alpha]_D^{28}$ +16.5 (c, 0.1 in Py). λ_{max} 240 (log ϵ 4.33); 423 (log ϵ 4.23) (MeOH).

N-*Ac:* N-*(3-Oxo-3*H*-phenoxazin-2-yl)acetamide, 9CI. 2-Acetamido-3*H*-phenoxazin-3-one.* **N-*Acetylquestiomycin A***
[1916-55-8]
$C_{14}H_{10}N_2O_3$ 254.245
From *Brevibacterium iodinum*, *Microbispora aerata*, *Streptomyces thioluteus* and *Waksmania aerata*. Used as a 1m*M* soln. in EtOH as redox indicator for titanometric detn. of Fe(*III*), Au(*III*), Ce(*IV*), $Cr_2O_7^{2\ominus}$, $VO_4^{3\ominus}$ and some organic compounds. Active against *Sarcina lutea* and *Trichophyton* sp. Orange cryst. Sol. EtOH, Et_2O, C_6H_6, MeOH; poorly sol. H_2O. Subl. 165°. E° + 0.375V (pH 0.84, 23°). λ_{max} 240 (E1%/1cm 1400); 405 (E1%/1cm 1100) (EtOH) (Berdy).

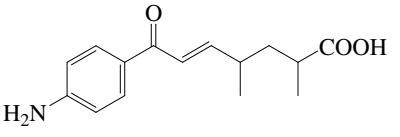
N-*Hydroxyacetyl:* N-*Hydroxyacetylquestiomycin A*. ***Chandrananimycin B***
$C_{14}H_{10}N_2O_4$ 270.244
Prod. by a marine *Actinomadura* sp. M045. Orange solid. λ_{max} 238 (log ϵ 3.85); 399 (log ϵ 3.66) (MeOH).

*6-Hydroxy: 2-Amino-6-hydroxy-3*H*-phenoxazin-3-one.* ***6-Hydroxyquestiomycin A***
$C_{12}H_8N_2O_3$ 228.207
Prod. by the marine *Halomonas* sp. GWS-BW-H8hM. Red solid. λ_{max} 236 (log ϵ 3.93); 277 (log ϵ 3.75); 430 (log ϵ 3.72) (MeOH). λ_{max} 230 (log ϵ 3.91); 284 (log ϵ 3.61); 464 (log ϵ 3.5) (MeOH/HCl).

9-Hydroxy, N-*Ac:* N-*Acetyl-9-hydroxyquestiomycin A*. ***Chandranamimycin A***
$C_{14}H_{10}N_2O_4$ 270.244
Prod. by a marine *Actinomadura* sp. M048. Orange solid. λ_{max} 226 (log ϵ 4.52); 270 (log ϵ 4.38); 423 (log ϵ 4.45) (MeOH).

Fischer, O. *et al., Ber.*, 1961, **27**, 2784 (*synth*)
Gerber, N.N. *et al., Biochemistry*, 1964, **3**, 598; 1966, **5**, 3824 (*isol, uv, ir*)
Gerber, N.N. *et al., J.O.C.*, 1967, **32**, 4055 (*isol, uv, ir, bibl*)
Ruzička, E. *et al., Mikrochim. Acta*, 1967, 277 (*use*)
Ruzička, E. *et al., CA*, 1968, **69**, 40930j (*stannometry*)
Ikekawa, T. *et al., Chem. Pharm. Bull.*, 1968, **16**, 1705 (*synth, ir*)
Sullivan, G. *et al., J. Pharm. Sci.*, 1971, **60**, 1097 (*isol*)
Baer, H. *et al., Pharmazie*, 1971, **26**, 108; 314 (*isol*)
Hishida, T. *et al., Chem. Lett.*, 1974, 293 (*synth*)
Schlunegger, U.V. *et al., Helv. Chim. Acta*, 1976, **59**, 1383 (*isol*)
Motohashi, N. *et al., Yakugaku Zasshi*, 1983, **103**, 364 (*synth, props*)
Bolognese, A. *et al., J. Het. Chem.*, 1986, **23**, 1003 (*synth, pmr, uv, deriv*)
Kinjo, J. *et al., Tet. Lett.*, 1987, **28**, 3697 (*isol*)
Simandi, L.I. *et al., Tet. Lett.*, 1993, **34**, 717 (*synth*)
Igarashi, Y. *et al., J. Antibiot.*, 1998, **51**, 915-920 (*Glucosylquestiomycin A*)
Kim, D.S. *et al., Planta Med.*, 2000, **66**, 78 (*Questiomycin A, isol, activity*)
Bolognese, A. *et al., J. Med. Chem.*, 2002, **45**, 5205-5216 (*synth, N-Ac, uv, pmr*)
Maskey, R.P. *et al., J. Antibiot.*, 2003, **56**, 622-629 (*Chandrananimycins*)
Bitzer, J. *et al., J. Antibiot.*, 2006, **59**, 86-92 (*6-Hydroxyquestiomycin A*)
Giurg, M. *et al., Pol. J. Chem. (Rocz. Chem.)*, 2006, **80**, 297-306 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, QCJ275

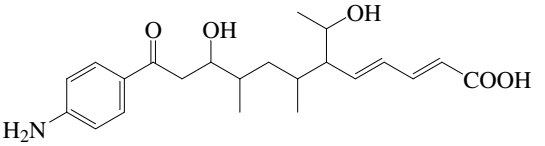
7-(4-Aminophenyl)-2,4-dimethyl-7-oxo-5-heptenoic acid A-395



$C_{15}H_{19}NO_3$ 261.32
Prod. by a *Streptomyces griseus* ssp. from a mangrove plant. Gum. $[\alpha]_D^{25}$ -72.7 (c, 0.22 in MeOH). λ_{max} 202 (ϵ 14680); 237 (ϵ 6970); 330 (ϵ 10640) (MeOH).

Guan, S.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1198-1200 (*isol, pmr, cmr, ms*)

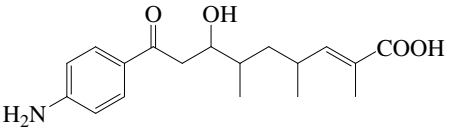
12-(4-Aminophenyl)-10-hydroxy-6-(1-hydroxyethyl)-7,9-dimethyl-12-oxo-2,4-dodecadienoic acid A-396



$C_{22}H_{31}NO_5$ 389.491
Prod. by *Streptomyces griseus* ssp. from a mangrove plant. Gum. $[\alpha]_D^{25}$ -64.1 (c, 1 in MeOH). λ_{max} 202 (ϵ 24010); 259 (ϵ 19230); 317 (ϵ 16273) (MeOH).

Guan, S.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1198-1200 (*isol, pmr, cmr*)

9-(4-Aminophenyl)-7-hydroxy-2,4,6-trimethyl-9-oxo-2-nonenoic acid A-397

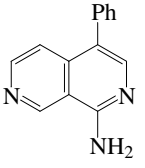


$C_{18}H_{25}NO_4$ 319.4
Prod. by *Streptomyces griseus* ssp. from a mangrove plant. Gum. $[\alpha]_D^{25}$ -320 (c, 0.05 in MeOH). λ_{max} 202 (ϵ 3970); 237 (ϵ 1880); 330 (ϵ 2880) (MeOH).

Guan, S.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1198-1200 (*isol, pmr, cmr*)

1-Amino-4-phenyl-2,7-naphthyridine A-398

*4-Phenyl-2,7-naphthyridin-1-amine, 9CI. **Lophocladine B***

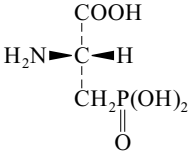


$C_{14}H_{11}N_3$ 221.261
Alkaloid from *Lophocladia* sp. Cytotoxic. Yellowish gum. λ_{max} 220 (log ϵ 4.01); 254 (log ϵ 4.02); 336 (log ϵ 3.89) (MeOH).

Gross, H. *et al., J. Nat. Prod.*, 2006, **69**, 640-644 (*isol, pmr, cmr, ms*)

2-Amino-3-phosphonopropanoic acid A-399

3-Phosphonoalanine, 9CI. AP 3. APPA
[5652-28-8]



$C_3H_8NO_5P$ 169.074
Constit. of *Zoanthus sociatus* and the ciliate, *Tetrahymena pyriformis*.

(*R*)-*form*
Cryst. Mp 224-227°. $[\alpha]_D^{24}$ -8.06 (c, 2 in H_2O).

(*S*)-*form* [23052-80-4]
Cryst. (EtOH aq.). Mp 224-226°. $[\alpha]_D^{24}$ +13.8 (c, 2.0 in 1*M* NaOH). $[\alpha]_D^{24}$ +8.33 (H_2O).

(±)-*form* [20263-06-3]
Solid (EtOH aq.). Mp 226° dec.

N-*Benzoyl:*
$C_{10}H_{12}NO_6P$ 273.182
Cryst. (H_2O or dioxan). Mp 197°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1479A (*nmr*)
Kittredge, J.S. *et al., Biochemistry*, 1964, **3**, 991 (*isol*)
Chambers, J.R. *et al., J.O.C.*, 1964, **29**, 832 (*synth*)
Quin, L.D. *et al., Top. Phosphorus Chem.*, 1967, **4**, 23 (*rev*)
Soroka, M. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1976, **50**, 661 (*synth, ir, pmr*)
Varlet, J.-M. *et al., Can. J. Chem.*, 1979, **57**, 3216 (*synth, pmr*)
Varlet, J.-M. *et al., Tetrahedron*, 1981, **37**, 1377 (*synth, pmr*)
Sawka-Dubrowalska, W. *et al., Acta Cryst. C*, 1985, **41**, 453 (*cryst struct*)
Mikityuk, A.D. *et al., Zh. Obshch. Khim.*, 1987, **57**, 305 (*synth, esters, ir, pmr*)
Smith, E.C.R. *et al., J.O.C.*, 1990, **55**, 4472 (*synth, pmr, cmr*)
Hutchinson, J.P.E. *et al., Tet. Lett.*, 1992, **33**, 7065 (*synth, ester*)
Fields, S.C. *et al., Tetrahedron*, 1999, **55**, 12237-12273 (*rev, synth*)

3-Amino-1-propanesulfonic acid, 9CI A-400

*Homotaurine†. Cerebril. **Tramiprosate, INN***
[3687-18-1]
$H_2NCH_2CH_2CH_2SO_2OH$
$C_3H_9NO_3S$ 139.175
Constit. of marine red algae e.g. *Grateloupia livida* and from the green alga *Cladophora densa*. Inhibits amyloid. A fibril formn. and deposition. Needles (EtOH aq.).
Mp 290-292° dec. (270-271°). pK_a 10.05 (H_2O).

Amide:
$C_3H_{10}N_2O_2S$ 138.19
Cryst. Mp 159-160°.

N-*Ac: 3-Acetylamino-1-propanesulfonic acid, 9CI. **Acamprosate, BAN, INN**. Aotal. Campral*
[77337-76-9]
$C_5H_{11}NO_4S$ 181.212
GABA receptor agonist. Psychotropic agent. Used in treatment of alcoholism. Solid (AcOH). Mp 187-189°. Approved by FDA (2004)

N-*Ac, Ca salt (2:1): Calcium* N-*acetylhomotaurine. **Acamprosate calcium, BAN**. Ca-AOTA*
[77337-73-6]
Mp 270°. Na, K, Li, Mg and Zn salts also reported.

N-*Benzoyl:*
$C_{10}H_{13}NO_4S$ 243.283
Cryst. (EtOH aq.) (as Ag salt).

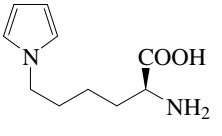
N-*Me:*
$C_4H_{11}NO_3S$ 153.202
Cryst. (EtOH). Mp 210-212°.

[14650-46-5, 81028-90-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 891A (*ir*)
Pinkus, G. *et al., Ber.*, 1893, **26**, 1077 (*synth*)
Rumpf, P. *et al., Bull. Soc. Chim. Fr.*, 1938, **5**, 871 (*synth*)
Miller, E. *et al., J.A.C.S.*, 1940, **62**, 2099 (*amide*)
Ger. Pat., 1957, 1 006 853; *CA*, **53**, 18869h (*N-Ac*)
Miyazawa, K. *et al., CA*, 1970, **72**, 129412b (*occur*)
Ueoka, S. *et al., Bull. Soc. Chim. Fr.*, 1972, **45**, 3634 (*cryst struct*)
Fujii, A. *et al., J. Med. Chem.*, 1975, **18**, 502 (*ir, synth*)
Ito, K. *et al., CA*, 1978, **88**, 2833q (*occur*)
Ger. Pat., 1980, (*Lab Meram*)3 019 350; *CA*, **94**, 174333s (*synth, pharmacol*)
Fujiwara, H. *et al., Chem. Anal. (N.Y.)*, 1987, **91**, 128 (*ms*)
Toffoli, P. *et al., Acta Cryst. C*, 1988, **44**, 1493 (*cryst struct, Acamprosate*)
Durlach, J. *et al., Actual. Chim. Ther.*, 1988, **15**, 169 (*rev*)
Grant, K.A. *et al., Pharmacol., Biochem. Behav.*, 1989, **32**, 607 (*pharmacol*)
Lhuintre, J.P. *et al., Alcohol Alcohol.*, 1990, **25**, 613 (*clin trial*)
Potgieter, A.S. *et al., Lancet*, 1992, **2**, 856 (*tox*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 564
Wilde, M.I. *et al., Drugs*, 1997, **53**, 1038-1053 (*rev*)

α-Amino-1*H*-pyrrole-1-hexanoic acid, 9CI A-401

N$^{\epsilon}$-*Pyrrolylnorleucine. Pyrrole-1-norleucine. 1-(5′-Amino-5′-carboxypentyl)pyrrole*



$C_{10}H_{16}N_2O_2$

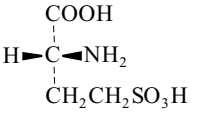
(*S*)-*form*
L-form
[156539-32-1]
Secondary lipid peroxidation prod. derived from L-lysine and 4,5-epoxy-2-alkenols. Widely distributed in fresh foodstuffs, e.g. meats, fish, vegetables and nuts.
Characterised spectroscopically.

Chiang, G.H. *et al., J. Agric. Food Chem.*, 1988, **36**, 506-509 (*hplc, occur*)
Zamora, R. *et al., Lipids*, 1994, **29**, 243-249; 1995, **30**, 477-483 (*synth, detn, pmr, cmr*)
Zamora, R. *et al., Biochim. Biophys. Acta*, 1995, **1258**, 319-327 (*formn*)

Hidalgo, F.J. *et al., J. Agric. Food Chem.*, 1995, **43**, 1023-1028 (*occur, formn*)
Zamora, R. *et al., J. Agric. Food Chem.*, 1999, **47**, 1942-1947 (*occur*)

2-Amino-4-sulfobutanoic acid, 9CI A-402

Homocysteic acid
[1001-13-4]



(*R*)–*form*

$C_4H_9NO_5S$ 183.185

▶ Neurotoxin.

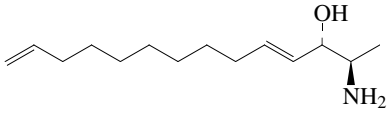
(*R*)-*form* [56892-03-6]
Isol. from the red alga *Palmaria palmata*.
Cryst. (H_2O/EtOH/Et_2O).
Mp 270° dec Mp 267°. $[\alpha]_D^{25}$ -10 (c, 5 in 1*M* HCl). $[\alpha]_D^{21}$ -18 (c, 1.305 in H_2O). Isol. partially racemised.

(*S*)-*form* [14857-77-3]
Cryst. (H_2O/EtOH/Et_2O). Mp 261°. $[\alpha]_D^{19}$ +17 (c, 0.57 in H_2O).

N-*Benzyloxycarbonyl,* S-*amide:* [112898-30-3]
$C_{12}H_{16}N_2O_6S$ 316.334
Mp 78-82°. $[\alpha]_D^{21}$ -10 (c, 1 in H_2O). Comly. available; props. given are from catalogue data.

(±)-*form* [504-33-6]
Cryst. (H_2O).
Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 792D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 891D (*ir*)
Watkins, J.C. *et al., J. Med. Chem.*, 1962, **5**, 1187-1199 (*synth*)
U.S. Pat., 1976, 3 948 922; *CA*, **85**, 160524g (*synth, purifn*)
Clarke, G.R. *et al., J. Cryst. Mol. Struct.*, 1977, **7**, 41 (*cryst struct*)
Lipton, S.H. *et al., J. Agric. Food Chem.*, 1978, **26**, 1406 (*synth*)
Laycock, M.V. *et al., Phytochemistry*, 1979, **18**, 1220 (*isol, pmr, cmr*)

2-Amino-4,13-tetradecadien-3-ol, 9CI A-403



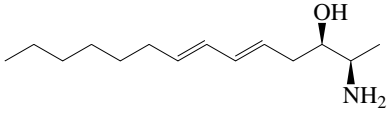
$C_{14}H_{27}NO$ 225.373

(2*R*,3*S*,4*E*)-*form*
Crucigasterin 225
[150151-85-2]
Isol. from *Pseudodistoma crucigaster*.
Light yellow oil. λ_{max} 202 (ε 1200) (MeOH).

N,O-*Di-Ac:* [149849-82-1]
Oil. $[\alpha]_D^{29}$ +45 (c, 0.84 in MeOH).

Jares-Erijman, E.A. *et al., J.O.C.*, 1993, **58**, 5732-5737 (*isol*)
Garrido, L. *et al., Tetrahedron*, 2001, **57**, 4579-4588 (*abs config*)

2-Amino-5,7-tetradecadien-3-ol A-404



(2*R*,3*R*,5*E*,7*E*)-*form*

$C_{14}H_{27}NO$ 225.373

Abs. configs. revised in 2001.

(2*R*,3*R*,5*E*,7*E*)-*form* [117828-55-4]
Isol. from *Xestospongia* sp. Shows antifungal props. λ_{max} 229 (ε 30200) (MeOH) (Derep). λ_{max} 227 (ε 30800) (EtOH) (Berdy).

N-*Ac:* [117828-56-5]
Oil. $[\alpha]_D^{24}$ +43.9 (c, 0.41 in $CHCl_3$). λ_{max} 227 (ε 30900) (MeOH).

N,3-*Di-Ac:* [117828-57-6]
Oil. $[\alpha]_D^{21}$ +16.7 (c, 0.28 in MeOH).

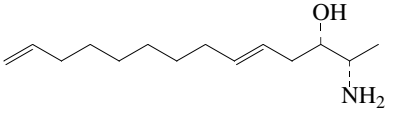
(2*R*,3*S*,5*E*,7*E*)-*form* [117828-59-8]
Isol. from the sponge *Xestospongia* sp. Shows antifungal props. λ_{max} 229 (ε 30200) (MeOH) (Derep). λ_{max} 230 (ε 29500) (EtOH) (Berdy).

N-*Ac:* [117860-01-2]
$C_{16}H_{29}NO_2$ 267.411
Needles. Mp 95-96°. $[\alpha]_D^{23}$ +42.5 (c, 1.1 in $CHCl_3$). λ_{max} 231 (ε 29500) (MeOH).

N,3-*Di-Ac:* [117860-02-3]
$C_{18}H_{31}NO_3$ 309.448
Oil. $[\alpha]_D^{21}$ +50.8 (c, 0.2 in MeOH).

Gulavita, N.K. *et al., J.O.C.*, 1989, **54**, 366-369 (*isol, uv, pmr, cmr*)
Langlois, N. *et al., Tet. Lett.*, 2001, **42**, 5709-5711 (*abs config*)
Garrido, L. *et al., Tetrahedron*, 2001, **57**, 4579-4588 (*abs config*)

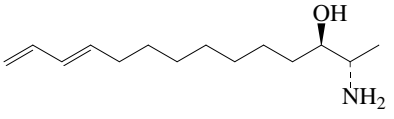
2-Amino-5,13-tetradecadien-3-ol, 9CI A-405



$C_{14}H_{27}NO$ 225.373

(2*S*,3*S*,5*E*)-*form* [181523-17-1]
N,O-*Di-Ac:* [181523-09-1]
$C_{18}H_{31}NO_3$ 309.448
Isol. from a marine ascidian (*Pseudodistoma* sp.).
Hooper, G.J. *et al., Nat. Prod. Lett.*, 1995, **6**, 31-35 (*isol*)
Garrido, L. *et al., Tetrahedron*, 2001, **57**, 4579-4588 (*abs config*)

2-Amino-11,13-tetradecadien-3-ol A-406



$C_{14}H_{27}NO$ 225.373

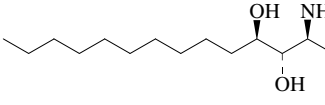
(2*S*,3*R*,11*E*)-*form*
Xestoaminol B
[129825-27-0]
Isol. from the marine sponge *Xestospongia* sp. Reverse transcriptase inhibitor. Oil. $[\alpha]_D$ +6 (c, 0.06 in MeOH). λ_{max} 222 (ε 31600) (MeOH) (Derep). λ_{max} 222 (ε 110000) (MeOH) (Berdy).

13,14-Dihydro: 2-Amino-11-tetradecen-3-ol. ***Xestoaminol A***
[129825-26-9]
$C_{14}H_{29}NO$ 227.389
Isol. from *Xestospongia* sp. Reverse transcriptase inhibitor. Oil. $[\alpha]_D$ +7.7 (c, 0.26 in MeOH).

Tetrahydro: See 2-Amino-3-tetradecanol, A-408

Jimenez, C. *et al., J. Nat. Prod.*, 1990, **53**, 978-982 (*isol*)
Garrido, L. *et al., Tetrahedron*, 2001, **57**, 4579-4588 (*abs config*)

2-Amino-1,3,4-tetradecanetriol A-407



(2*S*,3*S*,4*R*)-*form*

$C_{14}H_{31}NO_3$ 261.404

(2*S*,3*S*,4*R*)-*form*

N-*(2*R*-Hydroxyhexacosanoyl):* ***Alomacrorrhiza A***

$C_{40}H_{81}NO_5$ 656.084

Constit. of the roots of *Alocasia macrorrhiza*. Amorph. powder. Mp 112-114°. $[\alpha]_D^{25}$ +13.1 (c, 1 in Py).

(2ξ,3ξ,4ξ)-*form*

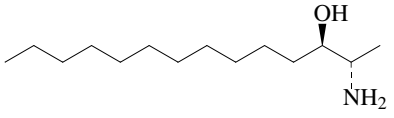
N-*Heneicosanoyl:* [243666-24-2]

$C_{35}H_{71}NO_4$ 569.95

Constit. of *Sinularia crassa*. Cryst. ($CHCl_3$/MeOH). Mp 127-130°. $[\alpha]_D^{25}$ +8.5 (c, 0.5 in MeOH).

Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 457-460 (*Sinularia crassa constit*)
Tien, N.Q. *et al., Arch. Pharmacal Res.*, 2004, **27**, 1020-1022 (*Alomacrorrhiza A*)

2-Amino-3-tetradecanol A-408



(2*S*,3*R*)-*form*

$C_{14}H_{31}NO$ 229.405

(2*S*,3*R*)-*form*

Xestoaminol C

[129825-28-1]

Isol. from *Pseudodistoma obscurum* and *Xestospongia* sp. Oil. $[\alpha]_D$ +7 (c, 0.14 in MeOH). $[\alpha]_D^{24}$ -21.8 (c, 0.4 in MeOH) (as di-Ac).

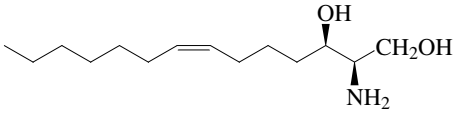
(2ξ,3ξ)-(±)-*form* [72530-18-8]

Cryst. (MeOH). Mp 99-101°.

Turel, R.J. *et al., Indian J. Chem., Sect. B*, 1979, **18**, 219-221 (*synth*)
Jimenez, C. *et al., J. Nat. Prod.*, 1990, **53**, 978-982 (*isol*)
Garrido, L. *et al., Tetrahedron*, 2001, **57**, 4579-4588 (*isol, pmr, cmr, abs config*)
Ichihashi, M. *et al., Biosci., Biotechnol., Biochem.*, 2003, **67**, 329-333 (*synth, abs config*)

2-Amino-7-tetradecene-1,3-diol A-409

Tetradeca-7-sphingenine



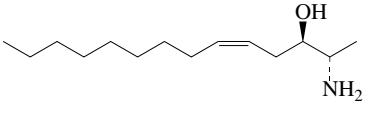
$C_{14}H_{29}NO_2$ 243.389

(2*R*,3*R*,7*Z*)-*form* [288322-52-1]

Isol. from the sponge *Haliclona vansoesti*. $[\alpha]_D^{20}$ +19.7 (c, 0.46 in $CHCl_3$).

Devijver, C. *et al., J. Nat. Prod.*, 2000, **63**, 978-980 (*isol, pmr, cmr*)

2-Amino-5-tetradecen-3-ol A-410



(2*S*,3*R*,5*Z*)-*form*

$C_{14}H_{29}NO$ 227.389

(2*S*,3*R*,5*Z*)-*form*

Halaminol C

[389125-68-2]

Isol. from a marine sponge *Haliclona* n. sp. Oil. $[\alpha]_D$ +1.9 (c, 0.025 in CH_2Cl_2).

(2*S*,3*S*,5*E*)-*form* [181523-19-3]

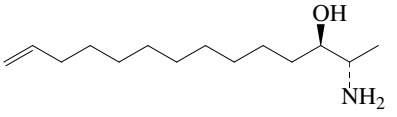
N,O-*Di-Ac:* [181523-11-5]

$C_{18}H_{33}NO_3$ 311.464

Isol. from a marine ascidian (*Pseudodistoma* sp.).

Hooper, G.J. *et al., Nat. Prod. Lett.*, 1995, **6**, 31-35 (*isol*)
Clark, R.J. *et al., J. Nat. Prod.*, 2001, **64**, 1568-1571 (*isol, pmr, cmr*)
Garrido, L. *et al., Tetrahedron*, 2001, **57**, 4579-4588 (*abs config*)

2-Amino-13-tetradecen-3-ol A-411



$C_{14}H_{29}NO$ 227.389

(2*S*,3*R*)-*form*

Halaminol A

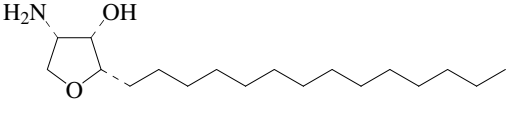
[389125-56-8]

Isol. from the marine sponge *Haliclona* n. sp. Oil. $[\alpha]_D$ +1.7 (c, 0.04 in CH_2Cl_2). $[\alpha]_D$ -30 (c, 0.003 in MeOH) (as *N,O*-di-Ac).

Clark, R.J. *et al., J. Nat. Prod.*, 2001, **64**, 1568-1571 (*Halaminol A, isol, pmr, cmr*)

4-Aminotetrahydro-2-tetradecyl-3-furanol A-412

4-Aminotetrahydro-3-hydroxy-2-tetradecylfuran



$C_{18}H_{37}NO_2$ 299.496

(2*S*,3*S*,4*S*)-*form*

Pachastrissamine*. Jaspine B*

[356043-02-2]

Isol. from the sponges *Pachastrissa* sp. and *Jaspis* sp. Cytotoxic agent. Powder. $[\alpha]_D$ +18 (c, 0.1 in EtOH). $[\alpha]_D$ +7 (c, 0.1 in $CHCl_3$).

(2ξ,3ξ,4ξ)-*form*

N-*(2-Hydroxytetracosanoyl):* ***Ergocerebrin***

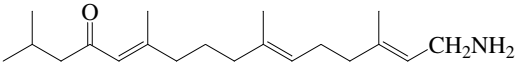
[2433-88-7]

$C_{42}H_{83}NO_4$ 666.122

Isol. from cultures of *Claviceps purpurea*. Needles. Mp 106-107°. $[\alpha]_D^{20}$ +16.3 (c, 0.17 in tetrachloroethane). Accompanied by its lower homologues with dodecyl and tridecyl sidechains.

Simon, J.W.A. *et al., J.C.S.*, 1965, 4164-4168 (*Ergocerebrin*)
Kuroda, I. *et al., J. Nat. Prod.*, 2002, **65**, 1505-1506 (*Pachastrissamine*)
Ledroit, V. *et al., Tet. Lett.*, 2003, **44**, 225-228 (*Jaspine B*)
Bhaket, P. *et al., Org. Lett.*, 2005, **7**, 875-876 (*synth*)
Sudhakar, N. *et al., Tet. Lett.*, 2005, **46**, 325-327 (*synth*)
van den Berg, R.J. *et al., J.O.C.*, 2006, **71**, 836-839 (*synth*)
Du, Y. *et al., J.O.C.*, 2006, **71**, 1251-1253 (*synth*)
Ribes, C. *et al., Tetrahedron*, 2006, **62**, 5421-5425 (*synth*)

16-Amino-2,6,10,14-tetramethyl-5,10,14-hexadecatrien-4-one A-413



$C_{20}H_{35}NO$ 305.503

N-*Formyl:* ***Malonganenone C***

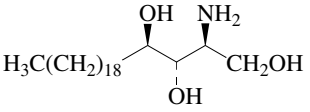
[882403-71-6]

$C_{21}H_{35}NO_2$ 333.513

Isol. from *Leptogorgia gilchristi*. Yellow solid. λ_{max} 230 (ϵ 8800); 276 (ϵ 1400) (MeOH).

Keyzers, R.A. *et al., Tetrahedron*, 2006, **62**, 2200-2206 (*isol, pmr, cmr*)

2-Amino-1,3,4-tricosanetriol A-414



$C_{23}H_{49}NO_3$ 387.645

(2*S*,3*S*,4*R*)-*form*

N-*(2*R*-Hydroxytetradecanoyl):*
$C_{37}H_{75}NO_5$ 614.003
Constit. of the soft coral *Sinularia leptoclados*. Amorph. powder.
Mp 105-107°. $[\alpha]_D^{28}$ +7 (c, 0.1 in $CHCl_3$).

Bala, S.R.G. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1214-1220

2-Amino-4,8-tridecadiene-1,3-diol A-415

$H_3C(CH_2)_3CH{=}CHCH_2CH_2CH{=}CHCH(OH)CH(NH_2)$-$CH_2OH$

$C_{13}H_{25}NO_2$ 227.346

(2ξ,3ξ,4*E*,8*E*)-*form*

N-*Tricosanoyl:* [139649-85-7]
$C_{36}H_{69}NO_3$ 563.946
Isol. from the soft coral *Nephthea albida*.
Mp 85-87°.

Fu, J. *et al., CA*, 1991, **116**, 148521

1-Amino-4,12-tridecadien-2-ol, 9CI A-416

$H_2C{=}CH(CH_2)_6CH{=}CHCH_2CH(OH)CH_2NH_2$

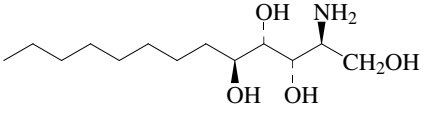
$C_{13}H_{25}NO$ 211.347

(±)-(*E*)-*form* [181523-21-7]

N,O-*Di-Ac:* [181523-13-7]
$C_{17}H_{29}NO_3$ 295.421
Isol. from a marine ascidian (*Pseudodistoma* sp.).

Hooper, G.J. *et al., Nat. Prod. Lett.*, 1995, **6**, 31-35 (*isol*)

2-Amino-1,3,4,5-tridecanetetrol A-417



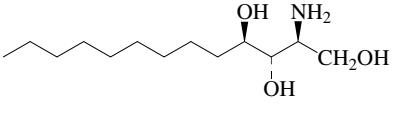
$C_{13}H_{29}NO_4$ 263.376

(2*S*,3*S*,4*S*,5*S*)-*form*

N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-α-D-*glucopyranoside:* ***Phacelliacerebroside A***. *Phakelliacerebroside A*
[405518-90-3]
$C_{35}H_{69}NO_{11}$ 679.93
Constit. of the sponge *Phakellia fusca*. Stereochem. in CA abstract does not coincide with CA name.

Xu, X.-H. *et al., CA*, 2002, **136**, 276280a (*Phacelliacerebroside A*)

2-Amino-1,3,4-tridecanetriol A-418



(2*S*,3*S*,4*R*)-*form*

$C_{13}H_{29}NO_3$ 247.377

(2*S*,3*S*,4*R*)-*form*

N-*(2*R*-Hydroxytricosanoyl):*
$C_{36}H_{73}NO_5$ 599.976
Isol. from a *Lobophytum* sp. Amorph. powder.
Mp 127-129°. $[\alpha]_D^{25}$ +8.2 (c, 0.5 in MeOH).

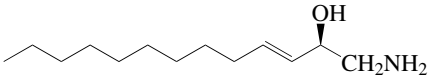
(2ξ,3ξ,4ξ)-*form*

N-*Tricosanoyl:*
$C_{36}H_{73}NO_4$ 583.977
Isol. from the coral *Sinularia* sp.
Mp 127-130°. $[\alpha]_D^{25}$ +8.2 (c, 0.5 in MeOH). CAS no. not found to 14CI.

Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 621-624 (*N-tricosanoyl*)

Radhika, P. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1345-1348 (*N-2-hydroxytricosanoyl*)

1-Amino-3-tridecen-2-ol A-419



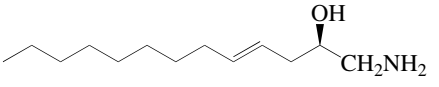
$C_{13}H_{27}NO$ 213.362

(2*R*,3*E*)-*form* [150922-61-5]

Isol. from the ascidian *Didemnum* sp.

Searle, P.A. *et al., J.O.C.*, 1993, **58**, 7578-7580 (*isol*)

1-Amino-4-tridecen-2-ol, 9CI A-420



(2*R*,4*E*)-form

$C_{13}H_{27}NO$ 213.362

(2*R*,4*E*)-*form* [150922-62-6]

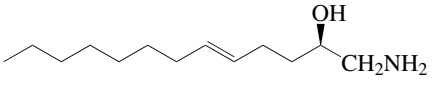
Isol. from the ascidian *Didemnum* sp.

(2*RS*,4*E*)-*form* [181783-05-1]

N,O-*Di-Ac:* [181523-15-9]
$C_{17}H_{31}NO_3$ 297.437
Isol. from a marine ascidian *Pseudodistoma* sp.

Searle, P.A. *et al., J.O.C.*, 1993, **58**, 7578-7580 (*isol*)
Hooper, G.J. *et al., Nat. Prod. Lett.*, 1995, **6**, 31-35 (*isol, di-Ac*)

1-Amino-5-tridecen-2-ol A-421



$C_{13}H_{27}NO$ 213.362

(2*R*,5*E*)-*form* [150922-60-4]

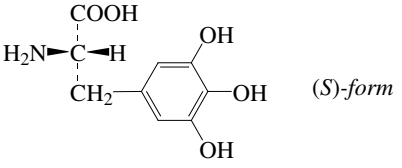
Isol. from the ascidian *Didemnum* sp. Antifungal agent. $[\alpha]_D$ +1.9 (c, 0.4 in MeOH) (as trifluoroacetate salt).

Searle, P.A. *et al., J.O.C.*, 1993, **58**, 7578-7580 (*isol, ir, pmr, abs config*)

2-Amino-3-(3,4,5-trihydroxyphenyl)propanoic acid **A-422**

3,5-Dihydroxytyrosine, 9CI. 3,4,5-Trihydroxyphenylalanine. 5-Hydroxydopa. TOPA

[16032-83-0]



(*S*)-*form*

$C_9H_{11}NO_5$ 213.19

Found in peptide residues isol. from the ascidian *Ascidia ceratodes*. Also isol. from various sea anemones.

(*S*)-*form* [18674-59-4]

Hypotensive agent. Mp 295-300° (dec.).

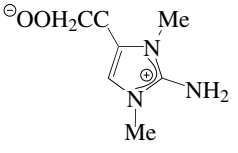
[20225-66-5]

South African Pat., 1968, 68 04 388; *CA*, **71**, 84540c (*synth, props*)
Rapp, P. *et al., Biochem. Biophys. Res. Commun.*, 1975, **64**, 241 (*synth*)
Carlberg, M. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1982, **73**, 23 (*isol*)
Taylor, S.W. *et al., Arch. Biochem. Biophys.*, 1995, **324**, 228 (*occur*)

Aminozooanemonin **A-423**

*2,3-Dihydro-2-imino-1,3-dimethyl-1*H*-imidazole-4-acetic acid, 9CI*

[213749-79-2]



$C_7H_{11}N_3O_2$ 169.183

Alkaloid from the sponge *Agelas dispar*. Amorph. solid. λ_{max} 226 (ϵ 3500); 262 (ϵ 1500) (MeOH).

Cafieri, F. *et al., J. Nat. Prod.*, 1998, **61**, 1171-1173 (*isol, uv, ir, pmr, cmr*)

Ammonium magnesium phosphate (1:1:1), 9CI, 8CI **A-424**

Phosphoric acid ammonium magnesium salt (1:1:1), 8CI

[7785-21-9]

$Mg(NH_4)PO_4$

H_4MgNO_4P 137.315

The anhydrous salt does not appear to have been obtained. Occurs as hexahydrate. Synth. from $Mg(OH)_2$-H_3PO_4-NH_4OH and Na_3PO_4-$MgSO_4$-NH_4OH. Also $MgHPO_4 + NH_3$. Occurs in human urinary calculi, and also guano. Precipitated during course of gravimetric estimation of Mg. Ignited to $Mg_2P_2O_7$. Agricultural fertiliser. Amorph. powder. A trihydrate has been reported.

Monohydrate: [16674-60-5] Obt. from hexahydrate at 80-100°. May be cryst. from aq. solns. containing $MgCl_2$ and $[NH_4]H_2PO_4$. Sol. acids; prac. insol. H_2O (0.023 g per 100 cm^3 at 0°), (0.02 g per 100 cm at 80°); insol. EtOH. Stable below 130-150°.

Hexahydrate: [13478-16-5]
White powder or elongated platelets. Orthorhombic with regular $PO_4^{3\ominus}$ tetrahedra and distorted $Mg(H_2O)_6^{2\oplus}$ octahedra. A slurry in H_2O at 95° → the monohydrate. When heated dry, loses H_2O and NH_3 in three overlapping processes.

Mineral-*form*

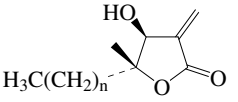
Struvite. *Guanite*
[15490-91-2] Found in peat beds and phosphate caves. Associated with Newberyite and Brushite. Found in human urinary sediments; diatomites, and bird and bat guano deposits in Chile and Australia.
Colourless to pale yellowish-brown, transparent to translucent, brittle, bipyramidal cryst. Essentially the hexahydrate.

[19004-55-8]

Dana's System of Mineralogy, 7th Ed., Wiley, N.Y., 1951, 715 (*mineral*)
Corbridge, C.E. *et al., J.C.S.*, 1954, 493 (*ir*)
Swanson, H.E. *et al., NBS Monogr. (U.S.)*, 1964, **3**, 41 (*cryst struct, hexahydrate*)
Ando, J. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 1716 (*synth, props*)
Fraissard, J. *et al., Bull. Soc. Chim. Fr.*, 1968, 1756 (*ir, struct*)
Étienne, J.J. *et al., Bull. Soc. Chim. Fr.*, 1968, 1805 (*props*)
Sutar, D.J. *et al., J.C.S.(A)*, 1968, 1143 (*props*)
Bridger, G.L. *et al., New Fert. Mater.*, 1968, 256 (*uses*)
Berényi, M. *et al., Talanta*, 1969, **16**, 101 (*props*)
Burriel-Marti, F. *et al., Inf. Quim. Anal.*, 1970, **24**, 84; *CA*, 1971, **74**, 9130 (*synth, ir, dta*)
Rothbaum, H.P. *et al., N.Z. J. Sci.*, 1973, **16**, 539 (*synth, props*)
Nabiev, M.N. *et al., Zh. Prikl. Khim. (Leningrad)*, 1973, **46**, 2377; *J. Appl. Chem. USSR (Engl. Transl.)*, 1973, **46**, 2532 (*synth, props*)
Banks, E. *et al., Inorg. Chem.*, 1975, **14**, 1634 (*synth, ir, cryst struct*)
Paulik, F. *et al., J. Therm. Anal.*, 1975, **8**, 557; 567 (*thermal dec, hexahydrate*)
Saibova, M.T. *et al., Zh. Neorg. Khim.*, 1975, **20**, 1134 (*dta*)
Abbona, F. *et al., J. Cryst. Growth*, 1979, **46**, 339; 1986, **74**, 581 (*synth, cryst struct, morphology*)
Abbona, F. *et al., Acta Cryst. B*, 1984, **40**, 223 (*cryst struct*)
Abbona, F. *et al., Cryst. Res. Technol.*, 1985, **20**, 133 (*synth, morphology*)
Ferraris, G. *et al., Acta Chem. Scand., Ser. B*, 1986, **42**, 253 (*cryst struct, nd, hexahydrate*)
Abdelrazig, B.E.I. *et al., Thermochim. Acta*, 1988, **129**, 197 (*props*)

Amphiasterin A_3 **A-425**

*Dihydro-4-hydroxy-5-methyl-3-methylene-5-tritetracontyl-2(3*H*)-furanone*



Relative Configuration

n = 42

$C_{49}H_{94}O_3$ 731.28

Isol. from *Plakortis quasiamphiaster*. Oil.

*32′,33′-Didehydro(*E-*): Dihydro-4-hydroxy-5-methyl-3-methylene-5-(32-tritetracontenyl)-2(3*H*)-furanone.* ***Amphiasterin A_1***

$C_{49}H_{92}O_3$ 729.264

Isol. from *Plakortis quasiamphiaster*. Oil. λ_{max} 230 (log ϵ 2.99) (MeOH).

Zampella, A. *et al., Tetrahedron*, 2001, **57**, 257-263

Amphiasterin A_4 **A-426**

*5-Heptatetracontyldihydro-4-hydroxy-5-methyl-3-methylene-2(3*H*)-furanone*

As Amphiasterin A_3, A-425 with

n = 46

$C_{53}H_{102}O_3$ 787.387

Isol. from *Plakortis quasiamphiaster*. Oil.

*36′,37′-Didehydro(*E-*): 5-(36-Heptatetracontenyl)dihydro-4-hydroxy-5-methyl-3-methylene-2(3*H*)-furanone. Amphiasterin A_2*

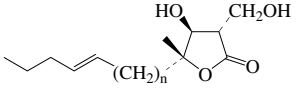
$C_{53}H_{100}O_3$ 785.371

Isol. from *Plakortis quasiamphiaster*. Oil.

Zampella, A. *et al., Tetrahedron*, 2001, **57**, 257-263

Amphiasterin B_1 **A-427**

*Dihydro-4-hydroxy-3-hydroxymethyl-5-methyl-5-(11-pentadecenyl)-2(5*H*)-furanone*



Relative Configuration

n = 10

$C_{21}H_{38}O_4$ 354.529

Isol. from *Plakortis quasiamphiaster*. Oil. $[\alpha]_D^{20}$ -3.3 (c, 0.15 in $CHCl_3$).

*11′,12′-Dihydro: Dihydro-4-hydroxy-3-hydroxymethyl-5-methyl-5-pentadecyl-2(5*H*)-furanone.* ***Amphiasterin B_4***
$C_{21}H_{40}O_4$ 356.545
Isol. from *Plakortis quasiamphiaster.* Oil. $[\alpha]_D^{20}$ -3.3 (c, 0.3 in $CHCl_3$).

Zampella, A. *et al., Tetrahedron*, 2001, **57**, 257-263

Amphiasterin B_2 A-428

*5-(13-Heptadecenyl)dihydro-4-hydroxy-3-hydroxymethyl-5-methyl-2(5*H*)-furanone*
As Amphiasterin B_1, A-427 with
n = 12
$C_{23}H_{42}O_4$ 382.582
Isol. from *Plakortis quasiamphiaster.* Oil. $[\alpha]_D^{20}$ -0.6 (c, 1 in $CHCl_3$).

*13′,14′-Dihydro: 5-Heptadecyldihydro-4-hydroxy-3-hydroxymethyl-5-methyl-2(5*H*)-furanone.* ***Amphiasterin B_5***
$C_{23}H_{44}O_4$ 384.598
Isol. from *Plakortis quasiamphiaster.* Oil. $[\alpha]_D^{20}$ -30 (c, 0.2 in $CHCl_3$).

Zampella, A. *et al., Tetrahedron*, 2001, **57**, 257-263

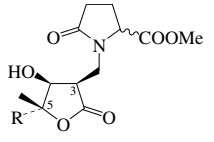
Amphiasterin B_3 A-429

*5-(17-Heneicosenyl)dihydro-4-hydroxy-3-hydroxymethyl-5-methyl-2(5*H*)-furanone*
As Amphiasterin B_1, A-427 with
n = 16
$C_{27}H_{50}O_4$ 438.69
Isol. from *Plakortis quasiamphiaster.* Oil. $[\alpha]_D^{20}$ +3.1 (c, 0.13 in $CHCl_3$).

Zampella, A. *et al., Tetrahedron*, 2001, **57**, 257-263

Amphiasterin C_1 A-430

[330680-37-0]



Relative Configuration

R = -$(CH_2)_3$$\overset{4''}{C}$H=$\overset{5''}{C}H(CH_2)_9CH_3$(*E*-)

$C_{27}H_{45}NO_6$ 479.656
Isol. from *Plakortis quasiamphiaster.* Oil. $[\alpha]_D^{20}$ -19.3 (c, 0.14 in $CHCl_3$).

4′′,5′′-Dihydro: ***Amphiasterin C_3***
[330680-39-2]
$C_{27}H_{47}NO_6$ 481.671
Isol. from *Plakortis quasiamphiaster.* Oil. $[\alpha]_D^{20}$ -8 (c, 0.4 in $CHCl_3$).

3-Epimer: ***Amphiasterin D_1***
[330680-41-6]
$C_{27}H_{45}NO_6$ 479.656
Isol. from *Plakortis quasiamphiaster.* Oil. $[\alpha]_D^{20}$ -16 (c, 0.06 in $CHCl_3$).

3,4,5-Triepimer: ***Amphiasterin E_1***
[330680-44-9]
$C_{27}H_{45}NO_6$ 479.656
Isol. from *Plakortis quasiamphiaster.* Oil. $[\alpha]_D^{20}$ -3.8 (c, 0.11 in $CHCl_3$).

Zampella, A. *et al., Tetrahedron*, 2001, **57**, 257-263 (*Amphiasterins C_1,C_3,D_1,E_1*)

Amphiasterin C_2 A-431

[330680-38-1]
As Amphiasterin C_1, A-430 with
R = -$(CH_2)_5CH$═$CH(CH_2)_9CH_3$(*E*-)
$C_{29}H_{49}NO_6$ 507.709
Isol. from *Plakortis quasiamphiaster.* Oil. $[\alpha]_D^{20}$ -12.3 (c, 0.65 in $CHCl_3$).

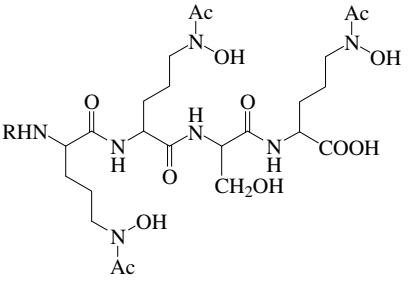
6′′,7′′-Dihydro: ***Amphiasterin C_4***
[330680-40-5]
$C_{29}H_{51}NO_6$ 509.725
Isol. from *Plakortis quasiamphiaster.* Oil. $[\alpha]_D^{20}$ -11.5 (c, 0.13 in $CHCl_3$).

3-Epimer: ***Amphiasterin D_2***
[330680-42-7]
$C_{29}H_{49}NO_6$ 507.709
Isol. from *Plakortis quasiamphiaster.* Oil. $[\alpha]_D^{20}$ -2.9 (c, 0.24 in $CHCl_3$).

3-Epimer, 6′′,7′′-dihydro: ***Amphiasterin D_3***
[330680-43-8]
$C_{29}H_{51}NO_6$ 509.725
Isol. from *Plakortis quasiamphiaster.* Oil. $[\alpha]_D^{20}$ -1.5 (c, 0.1 in $CHCl_3$).

Zampella, A. *et al., Tetrahedron*, 2001, **57**, 257-263 (*Amphiasterins C_2,C_4,D_2,D_3*)

Amphibactins A-432



Amphibactin B R = —$COCH_2CH(OH)(CH_2)_{10}CH_3$
C R = —$COCH_2CH(OH)(CH_2)_5CH\overset{z}{=}CH(CH_2)_5CH_3$
D R = —$CO(CH_2)_{12}CH_3$
E R = —$CO(CH_2)_7CH\overset{z}{=}CH(CH_2)_5CH_3$
F R = —$COCH_2CH(OH)(CH_2)_{12}CH_3$
G R = —$COCH_2CH(OH)(CH_2)_5CH\overset{z}{=}CH(CH_2)_7CH_3$
H R = —$CO(CH_2)_{14}CH_3$
I R = —$CO(CH_2)_7CH\overset{z}{=}CH(CH_2)_7CH_3$

Isol. from the marine bacterium *Vibrio* sp. R-10. Amphiphilic siderophores.

Amphibactin B
$C_{38}H_{69}N_7O_{14}$ 848.002

Amphibactin C
$C_{40}H_{71}N_7O_{14}$ 874.039

Amphibactin D
$C_{38}H_{69}N_7O_{13}$ 832.002

Amphibactin E
$C_{40}H_{71}N_7O_{13}$ 858.04

Amphibactin F
$C_{40}H_{73}N_7O_{14}$ 876.055

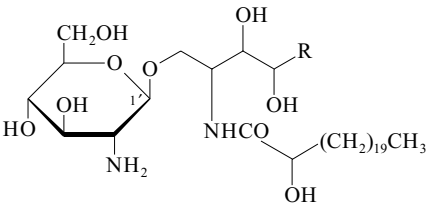
Amphibactin G
$C_{42}H_{75}N_7O_{14}$ 902.093

Amphibactin H
$C_{40}H_{73}N_7O_{13}$ 860.056

Amphibactin I

Martinez, J.S. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2003, **100**, 3754-3759 (*isol, struct*)

Amphicerebrosides A-433



Amphicerebroside B R = $CH_2CH{=}CH(CH_2)_{10}CH(CH_3)_2$
Amphicerebroside C R = $CH{=}CH(CH_2)_{11}CH(CH_3)_2$
Amphicerebroside D R = $(CH_2)_{12}CH(CH_3)_2$

Glycosphingolipid complex. Isol. from the sponge *Amphimedon viridis*.

Amphicerebroside B [122794-88-1]
$C_{48}H_{94}N_2O_9$ 843.279
From *Amphimedon viridis*.

1′-Epimer: ***Amphicerebroside E***
[122872-58-6]
$C_{48}H_{94}N_2O_9$ 843.279
From *Amphimedon viridis*.

Amphicerebroside C [122759-53-9]
$C_{48}H_{94}N_2O_9$ 843.279
From *Amphimedon viridis*.

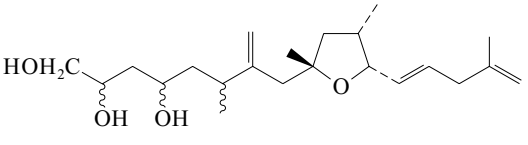
1′-Epimer: ***Amphicerebroside F***
[122799-43-3]
$C_{48}H_{94}N_2O_9$ 843.279
From *Amphimedon viridis*.

Amphicerebroside D [122759-54-0]
$C_{47}H_{94}N_2O_9$ 831.268
From *Amphimedon viridis*.

Hirsch, S. *et al., Tetrahedron*, 1989, **45**, 3897 (*isol, pmr, cmr*)

Amphidinin A A-434

6-Methyl-7-[[tetrahydro-2,4-dimethyl-5-(4-methyl-1,4-pentadienyl)-2-furanyl]methyl]-7-octene-1,2,4-diol, 9CI
[158761-10-5]

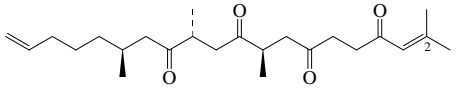


$C_{22}H_{38}O_4$ 366.54
Isol. from *Amphidinium* sp. Cytotoxic. Oil. $[\alpha]_D^{18}$ -300 (c, 0.03 in MeOH). λ_{max} 222 (MeOH).

Kobayashi, J. *et al., Tet. Lett.*, 1994, **35**, 7049-7050 (*isol, pmr, cmr*)

Amphidinoketide I A-435

2,9,12,15-Tetramethyl-2,19-eicosadiene-4,7,10,13-tetrone, 9CI
[162413-57-2]



Absolute Configuration

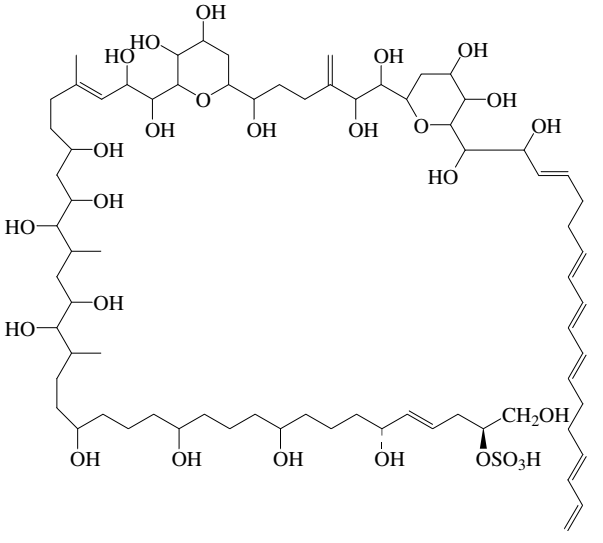
$C_{24}H_{38}O_4$ 390.562
Isol. from the dinoflagellate *Amphidinium* sp. Cytotoxic agent. Oil. $[\alpha]_D^{25}$ +25.3 (CH_2Cl_2). λ_{max} 235 (ϵ 11000) (MeOH).

Δ^1-Isomer: 2,9,12,15-Tetramethyl-1,19-eicosadiene-4,7,10,13-tetrone. ***Amphidinoketide II***
[162413-58-3]
$C_{24}H_{38}O_4$ 390.562
Isol. from *Amphidinium* sp. Cytotoxic agent. Oil. $[\alpha]_D^{25}$ +33.9 (CH_2Cl_2).

Bauer, I. *et al., Tet. Lett.*, 1995, **36**, 991-994 (*isol, pmr, cmr*)
Walsh, L.M. *et al., Chem. Comm.*, 2003, 2616-2617 (*synth, abs config*)

Amphidinol A-436

Amphidinol 1
[132930-70-2]

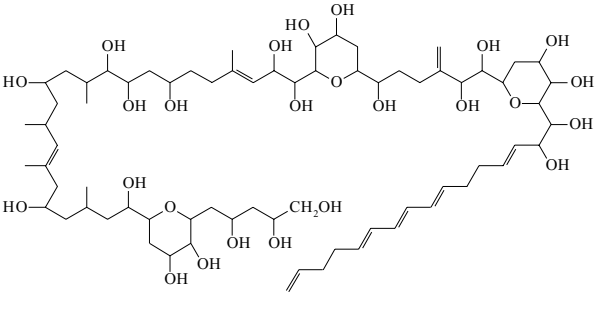


$C_{73}H_{126}O_{27}S$ 1467.848
Constit. of the dinoflagellate *Amphidinium klebsii*. Antifungal agent. Pale yellow solid (as Na salt). $[\alpha]_D^{23}$ -25 (c, 0.18 in MeOH). λ_{max} 259 (ϵ 37500); 270 (ϵ 41900); 282 (ϵ 37500) (MeOH) (Derep).

Satake, M. *et al., J.A.C.S.*, 1991, **113**, 9859-9861 (*isol, struct*)

Amphidinol 2 A-437

[168788-68-9]



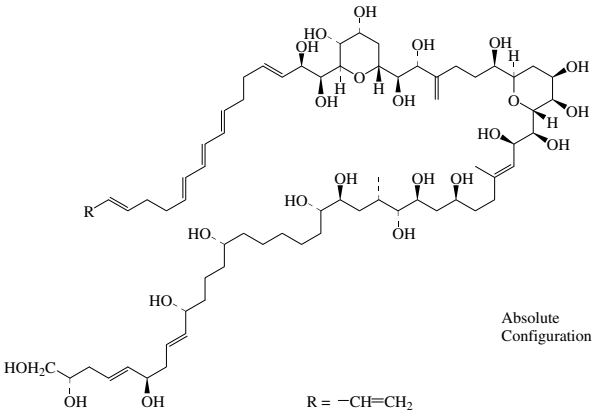
$C_{71}H_{122}O_{25}$ 1375.73
Constit. of the dinoflagellate *Amphidinium klebsii*. Haemolytic and antifungal agent. Algicide. Pale yellow solid. $[\alpha]_D^{25}$ +2.1 (c, 0.1 in MeOH). λ_{max} 248 (ϵ 10300); 270 (ϵ 11200); 280 (ϵ 11700) (MeOH) (Berdy).

1-O-Sulfate: ***Amphidinol 11***
[863453-63-8]
$C_{71}H_{122}O_{28}S$ 1455.794
Constit. of *Amphidinium carterae*.
$[\alpha]_D^{20}$ -18 (c, 0.008 in MeOH).

Paul, G.K. *et al., Tet. Lett.*, 1995, **36**, 6279-6282 (*isol, uv, ir, pmr, cmr, ms*)
Houdai, T. *et al., Tetrahedron*, 2001, **57**, 5551-5557 (*biosynth*)
Echigoya, R. *et al., Harmful Algae*, 2005, **4**, 383-389 (*Amphidinol 11*)

Amphidinol 3 A-438

[190781-74-9]



$C_{70}H_{118}O_{23}$ 1327.688
Constit. of *Amphidinium klebsii*.

Murata, M. *et al., J.A.C.S.*, 1999, **121**, 870-871
Houdai, T. *et al., Tetrahedron*, 2001, **57**, 5551-5555 (*biosynth*)

Amphidinol 4 A-439

[190857-12-6]
As Amphidinol 3, A-438 with
R = H

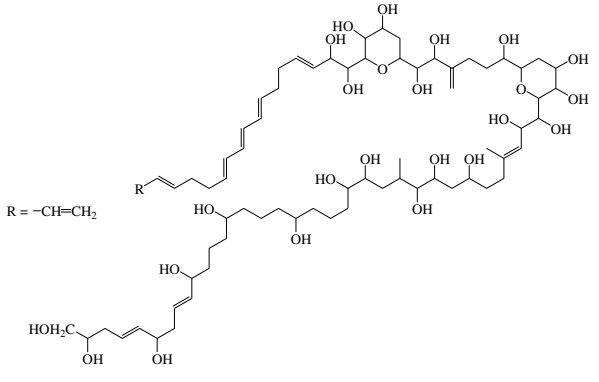
$C_{68}H_{116}O_{23}$ 1301.651
Constit. of *Amphidinium carterae.*

1-O-*Sulfate:* ***Amphidinol 12***
[863453-64-9]
$C_{68}H_{116}O_{26}S$ 1381.715
Constit. of *Amphidinium carterae.*

Houdai, T. *et al., Tetrahedron*, 2001, **57**, 5551-5555 (*biosynth*)
Echigoya, R. *et al., Harmful Algae*, 2005, **4**, 383-389 (*Amphidinol 12*)

Amphidinol 5 A-440

[190781-72-7]



$C_{72}H_{122}O_{24}$ 1371.741
Isol. from *Amphidinium klebsii*.

Paul, G.K. *et al., J. Mar. Biotechnol.*, 1997, **5**, 124-128 (*isol, struct*)
Houdai, T. *et al., Tetrahedron*, 2001, **57**, 5551-5555 (*biosynth*)

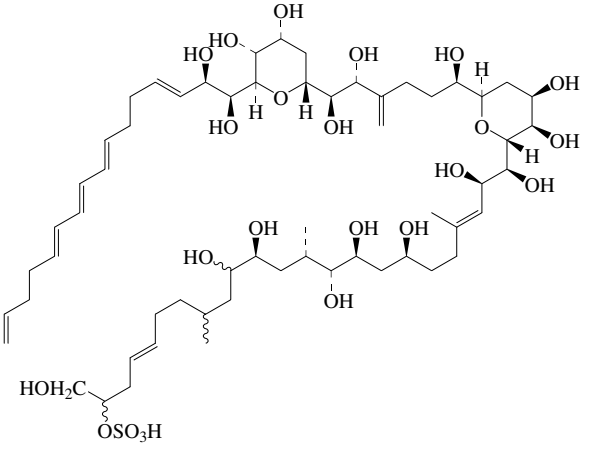
Amphidinol 6 A-441

[190781-73-8]
As Amphidinol 5, A-440 with
R = H

$C_{70}H_{120}O_{24}$ 1345.704
Isol. from *Amphidinium klebsii*.

Paul, G.K. *et al., J. Mar. Biotechnol.*, 1997, **5**, 124-128 (*isol, struct*)
Houdai, T. *et al., Tetrahedron*, 2001, **57**, 5551-5555 (*biosynth*)

Amphidinol 7 A-442

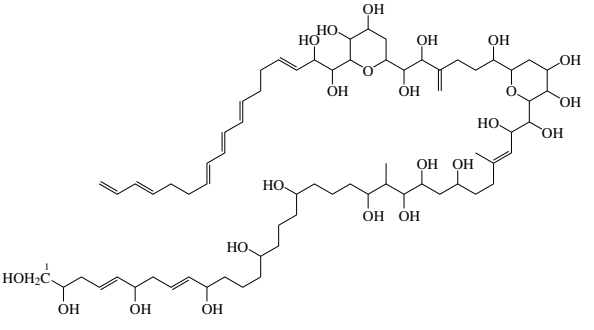


$C_{59}H_{100}O_{23}S$ 1209.491
Constit. of *Amphidinium klebsii*. Pale yellow powder. $[\alpha]_D^{20}$ -14.1 (c, 0.15 in MeOH). λ_{max} 258 (ϵ 19900); 269 (ϵ 25200); 279 (ϵ 19900) (MeOH).

Morsy, N. *et al., Tetrahedron*, 2005, **61**, 8606-8610 (*isol, pmr, cmr, ms*)

Amphidinol 9 A-443

[863453-65-0]



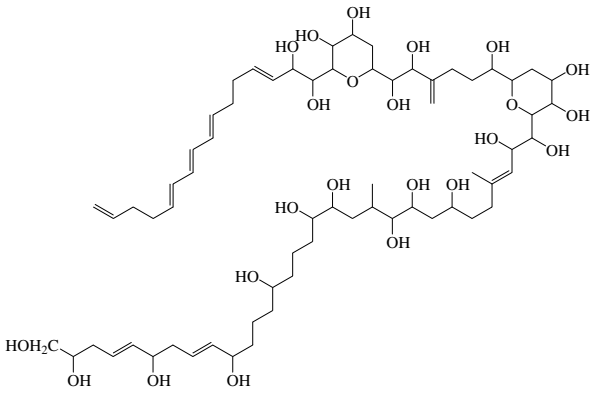
$C_{70}H_{118}O_{23}$ 1327.688
Constit. of *Amphidinium carterae.* Pale yellow solid. $[\alpha]_D^{20}$ -57 (c, 0.03 in MeOH). λ_{max} 230 (ϵ 5600); 279 (ϵ 12400) (no solvent reported).

1-O-*Sulfate:* ***Amphidinol 13***
[863453-66-1]
$C_{70}H_{118}O_{26}S$ 1407.753
Constit. of *Amphidinium carterae.*
$[\alpha]_D^{20}$ -79 (c, 0.02 in MeOH).

Echigoya, R. *et al., Harmful Algae*, 2005, **4**, 383-389 (*isol, pmr, cmr*)

Amphidinol 10 A-444

[863453-67-2]

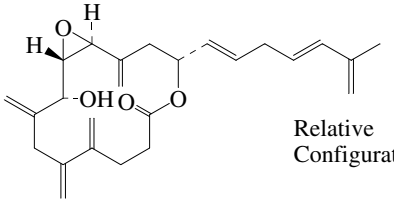


$C_{66}H_{112}O_{23}$ 1273.597
Constit. of *Amphidinium carterae*. Pale yellow oil. $[\alpha]_D^{20}$ -61 (c, 0.02 in MeOH). λ_{max} 269 (ϵ 9940) (no solvent reported).

Echigoya, R. *et al., Harmful Algae*, 2005, **4**, 383-389 (*isol, pmr, cmr*)

Amphidinolide V A-445

[262853-42-9]

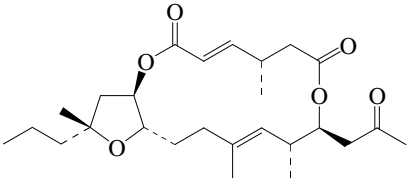


Relative Configuration

$C_{25}H_{32}O_4$ 396.525
Isol. from *Amphidinium* sp. Cytotoxic agent. Oil. λ_{max} 230 (ϵ 11000) (no solvent reported).

Kubota, T. *et al., Tet. Lett.*, 2000, **41**, 713-716

Amphidinolide X A-446



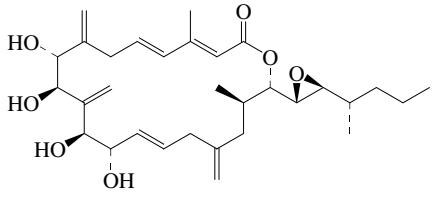
Absolute Configuration

$C_{26}H_{40}O_6$Isol. from *Amphidinium* sp. strain Y-42.
Oil. $[\alpha]_D^{17}$ -12 (c, 1 in $CHCl_3$). λ_{max} 209 (ϵ 6800) (EtOH).

Tsuda, M. *et al., J.O.C.*, 2003, **68**, 5339-5345 (*isol, pmr, cmr, biosynth*)
Fürstner, A. *et al., J.A.C.S.*, 2006, **128**, 9194-9204 (*synth*)

Amphidinolide A A-447

[106463-75-6]



Absolute Configuration

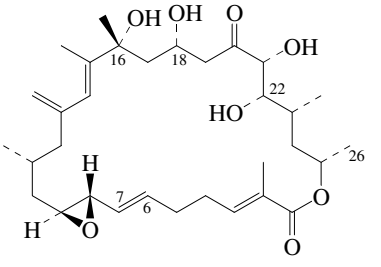
$C_{31}H_{46}O_7$ 530.7

Macrolide antibiotic. Prod. by *Amphidinium* sp. Y5 and *Amphiscolops* sp. Antineoplastic agent. Needles.
Mp 130-133°. $[\alpha]_D^{24}$ +46 (c, 1 in $CHCl_3$). λ_{max} 265 (ϵ 18000) (MeOH) (Derep).

Kobayashi, J. *et al., Tet. Lett.*, 1986, **27**, 5755-5758 (*isol*)
Kobayashi, J. *et al., J. Nat. Prod.*, 1991, **54**, 1435-1439 (*isol, pmr, cmr*)
Trost, B.M. *et al., J.A.C.S.*, 2005, **127**, 13589-13597; 13598-13610 (*synth, abs config*)
Ishiyama, H. *et al., Tetrahedron*, 2006, **62**, 166-170 (*synth, abs config*)

Amphidinolide B A-448

Amphidinolide B_1
[110786-78-2]



Absolute Configuration

$C_{32}H_{50}O_8$ 562.742
Macrolide antibiotic. Isol. from *Amphidinium* sp. Shows antitumour props. Needles (hexane/CH_2Cl_2).
Mp 82-84°. $[\alpha]_D^{25}$ -62.5 (c, 0.4 in $CHCl_3$). $[\alpha]_D^{25}$ -45 (c, 1 in $CHCl_3$). λ_{max} 222 (ϵ 12000) (MeOH).

16-Deoxy: ***Amphidinolide B_4***
$C_{32}H_{50}O_7$ 546.743
Isol. from *Amphidinium* sp. Cytotoxic. Oil. $[\alpha]_D^{23}$ -13 (c, 0.2 in $CHCl_3$). λ_{max} 209 (ϵ 6800) (EtOH).

16-Deoxy, 26-hydroxy: ***Amphidinolide H***. *Amphidinolide H_1*
[134781-24-1]
$C_{32}H_{50}O_8$ 562.742
Isol. from *Amphidinium* sp. and *Amphiscolops* sp. Antitumour agent. Needles (C_6H_6/hexane).
Mp 131-132°. $[\alpha]_D^{18}$ -32.3 (c, 0.2 in $CHCl_3$). λ_{max} 222 (ϵ 12000) (MeOH).

16-Deoxy, 26-hydroxy, 6,7-dihydro: ***Amphidinolide H_4***
$C_{32}H_{52}O_8$ 564.758
Isol. from an *Amphidinium* sp. Oil. $[\alpha]_D^{26}$ -30 (c, 0.1 in $CHCl_3$). λ_{max} 221 (ϵ 9300) (MeOH).

18-Epimer: ***Amphidinolide B_2***
[155683-56-0]
$C_{32}H_{50}O_8$ 562.742
From *Amphidinium* sp. Cytotoxic agent. Amorph. solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -43.9 (c, 0.4 in $CHCl_3$). There is evidence that Amphidinolides B_2 and D are identical. Further research is taking place (1994). λ_{max} 220 (ϵ 16000) (MeOH).

22-Epimer: ***Amphidinolide B_3***
[155683-57-1]
$C_{32}H_{50}O_8$ 562.742
From *Amphidinium* sp. Cytotoxic agent. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -69.4 (c, 0.2 in $CHCl_3$). λ_{max} 220 (ϵ 16000) (MeOH).

22-Epimer, 16-deoxy, 26-hydroxy: ***Amphidinolide H_3***
$C_{32}H_{50}O_8$ 562.742
Isol. from an *Amphidinium* sp. Oil. $[\alpha]_D^{24}$ -61 (c, 0.05 in $CHCl_3$). λ_{max} 222 (ϵ 14900) (MeOH).

16,18-Diepimer: ***Amphidinolide D***
[121350-99-0]
$C_{32}H_{50}O_8$ 562.742
Isol. from an *Amphidinium* sp. and *Amphiscolops* sp. Shows antitumour props. Amorph. solid. $[\alpha]_D^{30}$ -30 (c, 0.5 in $CHCl_3$). λ_{max} 222 (ϵ 12000) (MeOH).

16,18-Diepimer, 16-deoxy: ***Amphidinolide B_5***
$C_{32}H_{50}O_7$ 546.743

Isol. from *Amphidinium* sp. Cytotoxic. Oil. $[\alpha]_D$ -25 (c, 0.2 in $CHCl_3$). λ_{max} 209 (ϵ 6800) (EtOH).

16,18-Diepimer, 16-deoxy, 26-hydroxy: ***Amphidinolide H₂***
$C_{32}H_{50}O_8$ 562.742
Isol. from an *Amphidinium* sp. Oil. $[\alpha]_D^{25}$ -90 (c, 0.1 in $CHCl_3$). λ_{max} 222 (ϵ 20400) (MeOH).

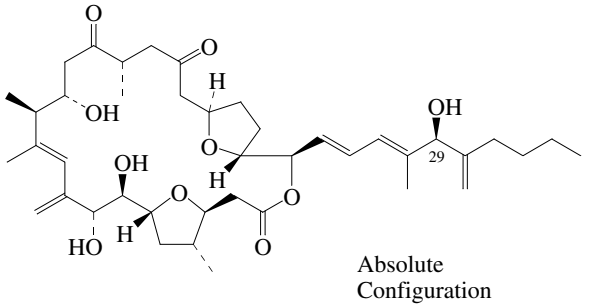
16,18-Diepimer, 16-deoxy, 26-hydroxy, 6,7-dihydro: ***Amphidinolide H₅***
$C_{32}H_{52}O_8$ 564.758
Isol. from an *Amphidinium* sp. Oil. $[\alpha]_D^{26}$ -54 (c, 0.14 in $CHCl_3$). λ_{max} 221 (ϵ 9000) (MeOH).

[155683-55-9]

Ishibashi, M. *et al., Chem. Comm.*, 1987, 1127-1129 (*isol, struct*)
Kobayashi, J. *et al., J. Nat. Prod.*, 1989, **52**, 1036-1041 (*isol, pmr, cmr*)
Kobayashi, J. *et al., J.O.C.*, 1991, **56**, 5221-5224 (*Amphidinolide H*)
Bauer, I. *et al., J.A.C.S.*, 1994, **116**, 2657-2658
Ishibashi, M. *et al., Tet. Lett.*, 1994, **35**, 8241-8242 (*abs config*)
Kobayashi, J. *et al., Org. Lett.*, 2000, **2**, 2805-2807 (*Amphidinolide H, abs config*)
Tsuda, M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1366-1367 (*biosynth*)
Kobayashi, J. *et al., J.O.C.*, 2002, **67**, 6585-6592 (*Amphidinolides H2-H5*)
Kobayashi, J. *et al., Pure Appl. Chem.*, 2003, **75**, 337-342 (*isol, abs config*)
Shimbo, K. *et al., Bioorg. Med. Chem.*, 2005, **13**, 5066-5071 (*Amphidinolide H, conformn*)
Tsuda, M. *et al., Mar. Drugs*, 2005, **3**, 1-8 (*Amphidinolides B4, B5*)

Amphidinolide C A-449

3,26,27-Trioxatricyclo[21.2.1.1^{6,9}]heptacos-13-ene....., 9CI
[112945-21-8]



Absolute Configuration

$C_{41}H_{62}O_{10}$ 714.935

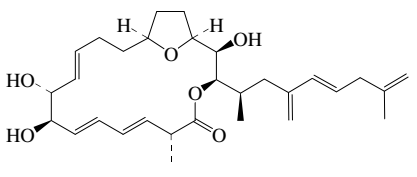
Macrolide antibiotic. Isol. from *Amphidinium* sp. Antineoplastic, ATP-ase activator. Amorph. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{26}$ -106 (c, 1 in $CHCl_3$). λ_{max} 240 (ϵ 26000) (MeOH) (Derep).

29-Ac: ***Amphidinolide C₂***
$C_{43}H_{64}O_{11}$ 756.972
Isol. from *Amphidinium* sp. Cytotoxic. Oil. λ_{max} 230 (ϵ 20000) (MeOH).

Kobayashi, J. *et al., J.A.C.S.*, 1988, **110**, 490 (*isol, pmr, cmr, struct*)
Kubota, T. *et al., Org. Lett.*, 2001, **3**, 1363-1366 (*abs config*)
Kubota, T. *et al., Tetrahedron*, 2001, **57**, 5975-5977 (*biosynth*)
Kubota, T. *et al., Mar. Drugs*, 2004, **2**, 83-87 (*Amphidinolide C₂*)

Amphidinolide E A-450

[126693-94-5]



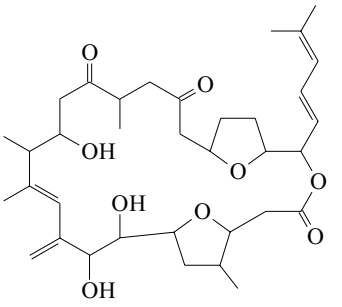
Absolute Configuration

$C_{30}H_{44}O_6$ 500.674
Constit. of an *Amphidinium* sp. symbiotic with an *Amphiscolops* sp. Amorph. solid. λ_{max} 230 (ϵ 26000) (MeOH) (Derep).

Kobayashi, J. *et al., J.O.C.*, 1990, **55**, 3421-3423 (*isol, pmr, cmr*)
Kubota, T. *et al., J.O.C.*, 2002, **67**, 1651-1656 (*abs config*)

Amphidinolide F A-451

[139594-87-9]



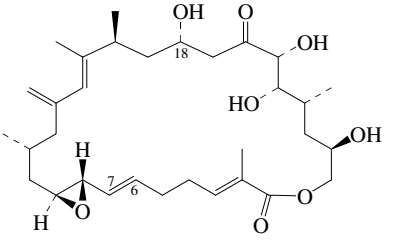
$C_{35}H_{52}O_9$ 616.79

Macrolide antibiotic. Isol. from the marine dinoflagellate *Amphidinium* sp.; also from *Amphiscolops magniviridis.* Cytotoxic agent. Amorph. solid. $[\alpha]_D^{30}$ -57 (c, 0.1 in $CHCl_3$). λ_{max} 237 (ϵ 22000) (MeOH) (Derep).

Kobayashi, J. *et al., J. Antibiot.*, 1991, **44**, 1259-1261 (*isol, struct*)

Amphidinolide G A-452

Amphidinolide G₁
[134781-23-0]



Absolute Configuration

$C_{32}H_{50}O_8$ 562.742
Isol. from the dinoflagellate *Amphidinium* sp. Cytotoxic agent. Amorph. powder. $[\alpha]_D^{25}$ -60.1 (c, 0.15 in $CHCl_3$). λ_{max} 222 (ϵ 11000) (MeOH).

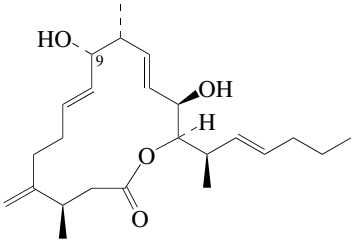
6,7-Dihydro: ***Amphidinolide G₃***
$C_{32}H_{52}O_8$ 564.758
Isol. from an *Amphidinium* sp. Oil. $[\alpha]_D^{24}$ -89 (c, 0.1 in $CHCl_3$). λ_{max} 224 (ϵ 19800) (MeOH).

16,18-Diepimer: ***Amphidinolide G₂***
$C_{32}H_{50}O_8$ 562.742
Isol. from an *Amphidinium* sp. Oil. $[\alpha]_D^{25}$ -47 (c, 0.1 in $CHCl_3$). λ_{max} 222 (ϵ 9600) (MeOH).

Kobayashi, J. *et al., J.O.C.*, 1991, **56**, 5221-5224 (*isol, struct*)
Kobayashi, J. *et al., Org. Lett.*, 2000, **2**, 2805-2807 (*abs config*)
Kobayashi, J. *et al., J.O.C.*, 2002, **67**, 6585-6592 (*Amphidinolides G2,G3*)

Amphidinolide J A-453

[147714-56-5]



$C_{24}H_{38}O_4$ 390.562
Constit. of *Amphidinium* sp. Cytotoxic agent. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{26}$ +1.2 (c, 0.7 in MeOH).

9-Ketone: ***Amphidinolide S***

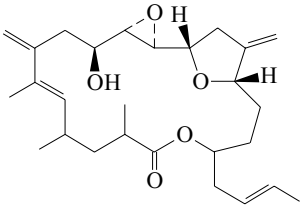
$C_{24}H_{36}O_4$ 388.546

Constit. of *Amphidinium* sp. Oil. $[\alpha]_D^{20}$ +5 (c, 0.17 in MeOH). λ_{max} 224 (ϵ 6300) (MeOH). λ_{max} 284 (ϵ 6300) (MeOH) (Berdy).

Kobayashi, J. *et al., J.O.C.*, 1993, **58**, 2645 (*isol, pmr, cmr, struct*)
Ishibashi, M. *et al., Tetrahedron*, 1997, **53**, 7827 (*Amphidinolide S*)
Williams, D.R. *et al., J.A.C.S.*, 1998, **120**, 11198-11199 (*synth*)

Amphidinolide K A-454

[151656-56-3]



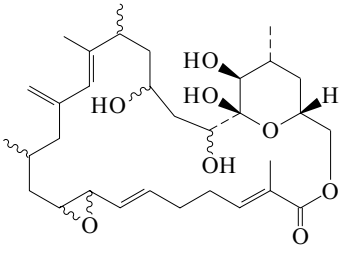
$C_{27}H_{40}O_5$ 444.61

Constit. of an *Amphidinium* sp. Oil. $[\alpha]_D^{21}$ -71 (c, 0.05 in MeOH). λ_{max} 229 (ϵ 11000) (MeOH) (Derep).

Ishibashi, M. *et al., J.O.C.*, 1993, **58**, 6928 (*isol, pmr, cmr, struct*)
Williams, D.R. *et al., J.A.C.S.*, 2001, **123**, 765-766 (*synth*)

Amphidinolide L A-455

[156192-11-9]



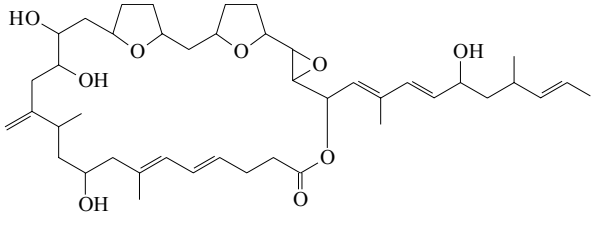
$C_{32}H_{50}O_8$ 562.742

Macrolide antibiotic. Constit. of *Amphidinium* sp. Cytotoxic agent. Amorph. solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{27}$ -50 (c, 0.1 in C_6H_6). λ_{max} 220 (ϵ 16000) (MeOH) (Berdy).

Tsuda, M. *et al., J.O.C.*, 1994, **59**, 3734 (*isol, pmr, cmr*)

Amphidinolide M A-456

[157676-93-2]



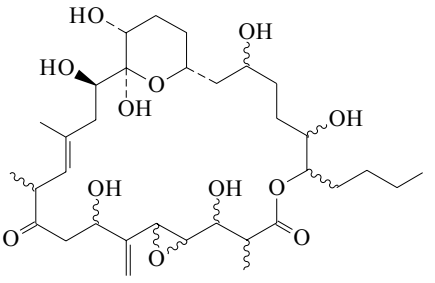
$C_{43}H_{66}O_9$ 726.989

Macrolide antibiotic. Constit. of *Amphidinium* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{26}$ +4.5 (c, 1 in $CHCl_3$).

Kobayaski, J. *et al., J.O.C.*, 1994, **59**, 4698

Amphidinolide N A-457

[157207-92-6]



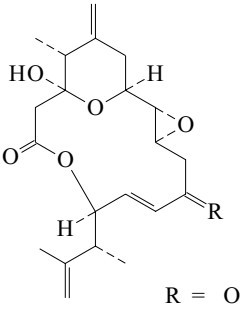
$C_{33}H_{54}O_{12}$ 642.782

Macrolide antibiotic. Isol. from the marine dinoflagellate *Amphidinium* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{20}$ +20 (c, 0.5 in MeOH).

Ishibashi, M. *et al., Chem. Comm.*, 1994, 1455 (*isol, pmr, cmr, ms*)

Amphidinolide O A-458

[167568-91-4]



$C_{21}H_{28}O_6$ 376.449

Macrolide antibiotic. Isol. from the marine dinoflagellate *Amphidinium* sp. Cytotoxic agent. Needles. $[\alpha]_D^{20}$ +65 (c, 0.1 in MeOH). λ_{max} 231 (ϵ 6400) (MeOH).

Ishibashi, M. *et al., J.O.C.*, 1995, **60**, 6062 (*isol, uv, ir, pmr, cmr, ms*)

Amphidinolide P A-459

[167568-92-5]

As Amphidinolide O, A-458 with

R = CH_2

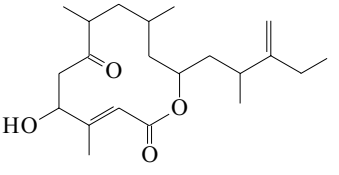
$C_{22}H_{30}O_5$ 374.476

Macrolide antibiotic. Isol. from the marine dinoflagellate *Amphidinium* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{20}$ +31 (c, 0.1 in MeOH). λ_{max} 225 (ϵ 7300) (MeOH).

Ishibashi, M. *et al., J.O.C.*, 1995, **60**, 6062 (*isol, uv, ir, pmr, cmr, ms*)
Williams, D.R. *et al., Org. Lett.*, 2000, **2**, 945-948 (*synth*)
Chakraborty, T.K. *et al., Tet. Lett.*, 2001, **42**, 3387-3390 (*synth*)
Trost, B.M. *et al., J.A.C.S.*, 2004, **126**, 13618-13619 (*synth*)

Amphidinolide Q A-460

[174545-77-8]



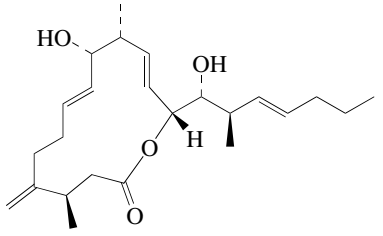
$C_{21}H_{34}O_4$ 350.497

Macrolide antibiotic. Isol. from the dinoflagellate *Amphidinium* sp. Cytotoxic agent. Oil. $[\alpha]_D^{20}$ +47 (c, 0.04 in MeOH). λ_{max} 222 (ϵ 10300) (MeOH).

Kobayashi, J. *et al., Tet. Lett.*, 1996, **37**, 1449 (*isol, ir, pmr, cmr, uv*)

Amphidinolide R A-461

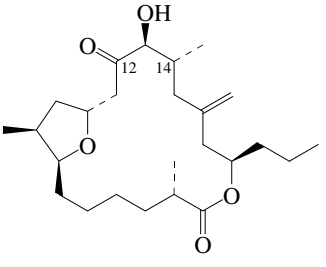
[193221-38-4]



$C_{24}H_{38}O_4$ 390.562
Constit. of *Amphidinium* sp. Oil. $[\alpha]_D^{20}$ +23 (c, 0.5 in MeOH).

Ishibashi, M. *et al., Tetrahedron*, 1997, **53**, 7827-7832 (*isol, pmr, cmr*)

Amphidinolide T_1 A-462



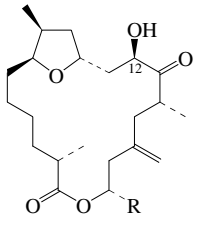
Absolute Configuration

$C_{25}H_{42}O_5$ 422.604
Isol. from *Amphidinium* sp. and *Amphiscolops* sp. Cytotoxic agent. Needles (MeOH aq.).
Mp 63-66°. $[\alpha]_D^{24}$ +18 (c, 0.3 in $CHCl_3$).

*14-Epimer, 13-ketone, 12*S*-alcohol:* ***Amphidinolide T_5***
$C_{25}H_{42}O_5$ 422.604
Isol. from *Amphidinium* sp. and *Amphiscolops* sp. Oil.

Tsuda, M. *et al., J.O.C.*, 2000, **65**, 1349-1352 (*isol, pmr, cmr*)
Kobayashi, J *et al., J.O.C.*, 2001, **66**, 134-142 (*biosynth*)
Kubota, T. *et al., Tetrahedron*, 2001, **57**, 6175-6179 (*isol, cryst struct, abs config*)
Ghosh, A.K. *et al., J.A.C.S.*, 2003, **125**, 2374-2375 (*synth*)
Colby, E.A. *et al., J.A.C.S.*, 2005, **127**, 4297-4307 (*synth*)

Amphidinolide T_2 A-463



R = $-CH_2CH_2CH(OH)CH_3$(*S*-)

$C_{26}H_{44}O_6$ 452.63
Isol. from *Amphidinium* sp. Oil.

Kobayashi, J. *et al., J.O.C.*, 2001, **66**, 134-142

Amphidinolide T_3 A-464

As Amphidinolide T_2, A-463 with
R = $-CH_2CH_2CH_3$

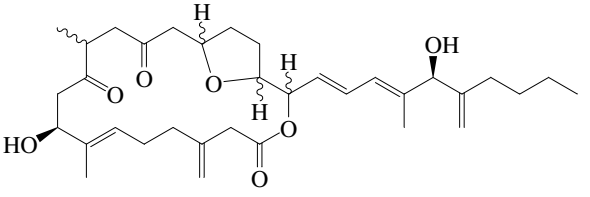
$C_{25}H_{42}O_5$ 422.604
Isol. from *Amphidinium* sp. Oil.

12-Epimer: ***Amphidinolide T_4***
$C_{25}H_{42}O_5$ 422.604
Isol. from *Amphidinium* sp. Oil.

Kobayashi, J. *et al., J.O.C.*, 2001, **66**, 134-142 (*isol, pmr, cmr*)
Fuerstner, A. *et al., Angew. Chem., Int. Ed.*, 2002, **41**, 4763-4766 (*T_4, synth*)
Colby, E.A. *et al., J.A.C.S.*, 2005, **127**, 4297-4307 (*T_4, synth*)
Deng, L.-S. *et al., J.O.C.*, 2006, **71**, 4625-4635 (*synth*)

Amphidinolide U A-465

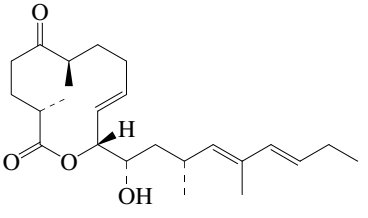
[256493-99-9]



$C_{34}H_{50}O_7$ 570.765
Isol. from *Amphidinium* sp. λ_{max} 230 (ϵ 20000) (MeOH).

Tsuda, M. *et al., Tetrahedron*, 1999, **55**, 14565-14570

Amphidinolide W A-466



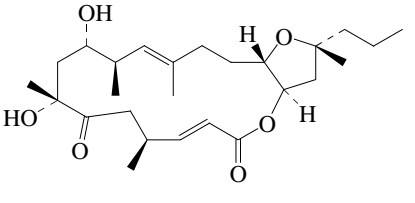
Absolute Configuration

$C_{24}H_{38}O_4$ 390.562
Stereochem. revised in 2004. Isol. from *Amphidinium* sp. strain Y-42; also from *Amphiscolops* sp. Cytotoxic. Oil. λ_{max} 235 (ϵ 14000) (EtOH).

Tsuda, M. *et al., Chem. Pharm. Bull.*, 2002, **50**, 976-977 (*biosynth*)
Shimbo, K. *et al., J.O.C.*, 2002, **67**, 1020-1023 (*isol, pmr, cmr*)
Ghosh, A.K. *et al., J.O.C.*, 2006, **71**, 1085-1093 (*synth, config*)

Amphidinolide Y A-467

[635728-51-7]

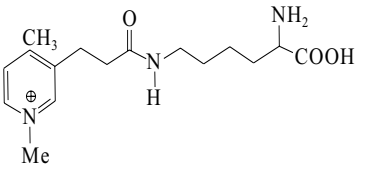


$C_{26}H_{42}O_6$ 450.614
Isol. from an *Amphidinium* sp. Cytotoxic. Oil. $[\alpha]_D^{17}$ -33 (c, 1 in $CHCl_3$). λ_{max} 208 (ϵ 12400) (EtOH).

Tsuda, M. *et al., J.O.C.*, 2003, **68**, 9109-9112 (*isol, pmr, cmr*)
Fürstner, A. *et al., J.A.C.S.*, 2006, **128**, 9194-9204 (*synth*)

Amphikuemin A-468

[105870-54-0]



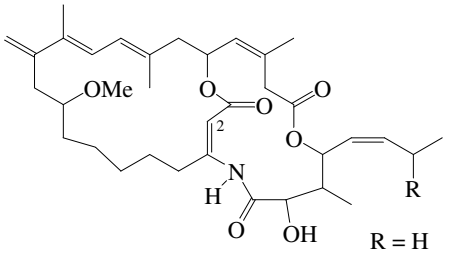
$C_{16}H_{26}N_3O_3^{\oplus}$ 308.4

Isol. from the sea anenome *Radianthus kuekenthali*. Induces symbiosis between sea anenome and anenome fish.

Murata, M. *et al., Science (Washington, D.C.)*, 1986, **234**, 585-587 (*isol, uv, pmr, struct*)
Konno, K. *et al., Heterocycles*, 1990, **30**, 247-251 (*synth*)

Amphilactam A A-469

[221465-59-4]



$C_{35}H_{51}NO_7$ 597.79

Isol. from sponges of the genus *Amphimedon* spp. Nematocide. Yellow oil. $[\alpha]_D$ +11.8 (c, 0.35 in $CHCl_3$). λ_{max} 270 (ϵ 44800) ($CHCl_3$).

*(2*E*)-Isomer:* ***Amphilactam C***
[221465-61-8]
$C_{35}H_{51}NO_7$ 597.79
Isol. from *Amphimedon* spp. Yellow oil. $[\alpha]_D$ +17.3 (c, 0.48 in $CHCl_3$). λ_{max} 280 (ϵ 14000) ($CHCl_3$).
Ovenden, S.P.B. *et al., J.O.C.*, 1999, **64**, 1140-1144 (*isol, uv, ir, pmr, cmr*)

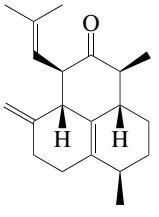
Amphilactam B A-470

[221465-60-7]
As Amphilactam A, A-469 with
R = CH_3
$C_{36}H_{53}NO_7$ 611.817
Isol. from sponges of the genus *Amphimedon* spp. Yellow oil. $[\alpha]_D$ +8.5 (c, 0.38 in $CHCl_3$). λ_{max} 280 (ϵ 18800) ($CHCl_3$).

*(2*E*)-Isomer:* ***Amphilactam D***
[221465-62-9]
$C_{36}H_{53}NO_7$ 611.817
Isol. from *Amphimedon* spp. Yellow oil. $[\alpha]_D$ +2.5 (c, 0.03 in $CHCl_3$). λ_{max} 270 (ϵ 3050) ($CHCl_3$).
Ovenden, S.P.B. *et al., J.O.C.*, 1999, **64**, 1140-1144 (*isol, uv, ir, pmr, cmr*)

8(13),11(20),14-Amphilectatrien-2-one A-471

Sinulobatin B
[189455-96-7]



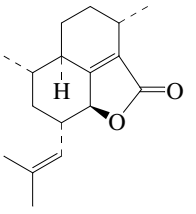
$C_{20}H_{28}O$ 284.441

Constit. of *Sinularia nanolobata*. Amorph. $[\alpha]_D^{25}$ +105.2 (c, 0.1 in $CHCl_3$).

Yamada, K. *et al., Tetrahedron*, 1997, **53**, 4569-4578 (*isol, pmr, cmr*)

Amphilectolide A-472

[290353-50-3]



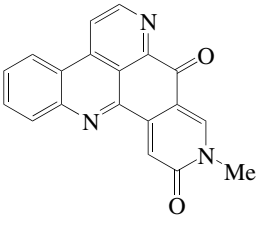
$C_{17}H_{24}O_2$ 260.375

Constit. of *Pseudopterogorgia elisabethae*. Yellow oil. $[\alpha]_D^{25}$ +24.7 (c, 1.7 in $CHCl_3$).

Rodríguez, A.D. *et al., Tet. Lett.*, 2000, **41**, 5177-5180 (*isol, pmr, cmr*)

Amphimedine A-473

*10-Methyl-8*H*-benzo[*b*]pyrido[4,3,2-*de*][1,8]phenanthroline-8,11(10*H*)-dione, 9CI*
[86047-14-5]



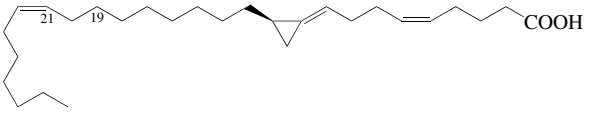
$C_{19}H_{11}N_3O_2$ 313.315

Alkaloid from an *Amphimedon* sp. of Pacific sponge and *Xestospongia carbonaria*. Cytotoxic; topoisomerase II inhibitor. Yellow solid. Fairly sol. MeOH; poorly sol. butanol, hexane. Mp 360°. λ_{max} 210 (ϵ 19700); 233 (ϵ 39400); 281 (ϵ 9100); 341 (ϵ 6060) (EtOH) (Derep). λ_{max} 245 (ϵ 38000); 281 (ϵ 10000); 340 (ϵ 7000) (MeOH) (Berdy). λ_{max} 235 (ϵ 38000); 281 (ϵ 10000); 340 (ϵ 7000) (EtOH) (Berdy).

Schmitz, F.J. *et al., J.A.C.S.*, 1983, **105**, 4835 (*isol, uv, ir, pmr, cmr, ms, struct*)
Kubo, A. *et al., Heterocycles*, 1988, **27**, 2095 (*synth, uv, ir, pmr, ms*)
Echavarren, A.M. *et al., J.A.C.S.*, 1988, **110**, 4051 (*synth*)
Prager, R.H. *et al., Aust. J. Chem.*, 1991, **44**, 277 (*synth, uv, ir*)
Guillier, F. *et al., J.O.C.*, 1995, **60**, 292 (*synth*)
Bracher, F. *et al., Annalen*, 1996, 115 (*synth*)
Nakahara, S. *et al., Heterocycles*, 1996, **43**, 2113 (*synth*)

Amphimic acid B A-474

9-(9-Hexadecenylcyclopropylidene)-5-nonenoic acid, 9CI
[195305-10-3]



$C_{28}H_{48}O_2$ 416.686

Isol. from the sponge *Amphimedon* sp. DNA topoisomerase inhibitor. Oil. $[\alpha]_D^{27}$ +6.2 (c, 1 in MeOH). Props. refer to a mixture with Δ^{19}-isomer. λ_{max} 199 (ϵ 9940) (MeOH).

21,22-Dihydro: ***Amphimic acid A***
[195305-03-4]
[200722-44-7, 200722-45-8]
$C_{28}H_{50}O_2$ 418.702
Isol. from *Amphimedon* sp. DNA topoisomerase I inhibitor.

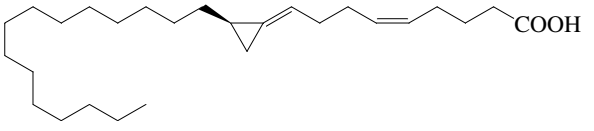
Needles (MeCN/Et_2O).
Mp 39-39.5°. $[\alpha]_D^{22}$ +7.7 (c, 0.5 in MeOH). λ_{max} 196 (ϵ 9210) (MeOH).

21,22-Dihydro, 19,20-didehydro:
$C_{28}H_{48}O_2$ 416.686
Isol. from *Amphimedon* sp.

Nemoto, T. *et al., Tetrahedron*, 1997, **53**, 16699-16710 (*isol, uv, ir, pmr, cmr*)

Amphimic acid C A-475

9-(Pentadecylcyclopropylidene)-5-nonenoic acid, 9CI
[200809-79-6]

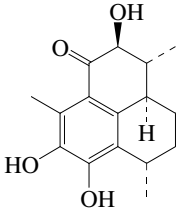


$C_{27}H_{48}O_2$ 404.675
Isol. from the sponge *Amphimedon* sp. Oil. $[\alpha]_D^{27}$ +6.3 (c, 0.1 in MeOH). λ_{max} 199 (ϵ 8210) (MeOH).

Nemoto, T. *et al., Tetrahedron*, 1997, **53**, 16699-16710 (*isol, uv, ir, pmr, cmr*)

Amphiphenalone A-476

[325691-50-7]

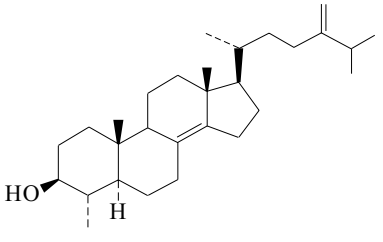


$C_{16}H_{20}O_4$ 276.332
Constit. of *Pseudopterogorgia elisabethae*. Plates.
Mp 218-220°. $[\alpha]_D^{25}$ +86.7 (c, 0.3 in Me_2CO). λ_{max} 216 (ϵ 12000); 288 (ϵ 6000) (MeOH).

Rodríguez, A.D. *et al., Tetrahedron*, 2000, **56**, 9015-9023 (*isol, pmr, cmr*)

Amphisterol A-477

4-Methylergosta-8(14),24(28)-dien-3-ol. 4-Methyl-24-methylene-cholest-8(14)-en-3-ol
[72165-10-7]

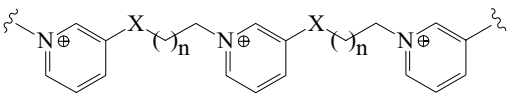


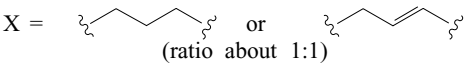
$C_{29}H_{48}O$ 412.698
Constit. of *Amphidinium carterae*. Cryst. (MeOH).
Mp 138-141°. $[\alpha]_D$ +10 (c, 0.07 in $CHCl_3$). Incorrect name in CA.

Withers, N.W. *et al., Phytochemistry*, 1979, **18**, 899-901 (*isol, pmr, ms*)
Kokke, W.C.M.C. *et al., Phytochemistry*, 1981, **20**, 127-134 (*isol, pmr, ms*)

Amphitoxin A-478

[165724-12-9]





n = 5 (mean value)

Polymeric alkaloid from the Caribbean sponge *Amphimedon compressa*. Exhibits antifeedant activity. λ_{max} 266 (H_2O).

Albrizio, S. *et al., J. Nat. Prod.*, 1995, **58**, 647 (*isol, uv, ir, pmr, cmr*)

Amylostreptin A-479

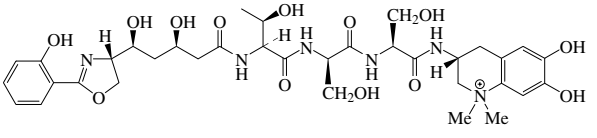
[146479-36-9]

Struct. unknown. Isol. from *Streptomyces corchorusii* ssp. *rhodomarinus* from marine sediment. α-Amylase inhibitor.

Imada, C. *et al., Nippon Suisan Gakkaishi*, 1992, **58**, 2169-2174 (*isol*)

Anachelin 1 A-480

[326490-91-9]



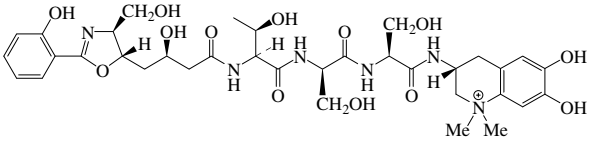
Absolute Configuration

$C_{35}H_{49}N_6O_{13}^{\oplus}$ 761.805
Isol. from *Anabaena cylindrica* NIES-19. Siderophore. Amorph. powder. $[\alpha]_D$ -34.8 (c, 0.05 in H_2O). λ_{max} 286 (ϵ 1900) (H_2O).

Itou, Y. *et al., Tetrahedron*, 2001, **57**, 9093-9099 (*isol, pmr, cmr*)
Gademann, K. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 3327-3329 (*synth*)
Ito, Y. *et al., Tetrahedron*, 2004, **60**, 9075-9080 (*abs config*)

Anachelin 2 A-481

[387816-76-4]



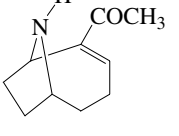
Absolute Configuration

$C_{35}H_{49}N_6O_{13}^{\oplus}$ 761.805
Isol. from *Anabaena cylindrica* NIES-19. Siderophore. Amorph. powder. $[\alpha]_D$ -65.7 (c, 0.06 in H_2O). λ_{max} 286 (ϵ 1800) (H_2O).

Itou, Y. *et al., Tetrahedron*, 2001, **57**, 9093-9099 (*isol, pmr, cmr*)
Ito, Y. *et al., Tetrahedron*, 2004, **60**, 9075-9080 (*abs config*)

Anatoxin a A-482

1-(9-Azabicyclo[4.2.1]non-2-en-2-yl)ethanone, 9CI. 2-Acetyl-9-azabicyclo[4.2.1]non-2-ene



(*R*)-*form*

$C_{10}H_{15}NO$ 165.235

(*R*)-*form*

Very fast death factor. VFDF. AnTx

[64285-06-9]

Alkaloid from *Anabaena flos-aquae* NRC-44h (Euphorbiaceae). Also isol. from *Oscillatoria* spp. *Aphanizomenon flos-aquae* and *Cylindrospermum* sp. Depolarising agent. Potent agonist for the nicotinic acetylcholine receptor. Oil. Sol. H_2O, MeOH. λ_{max} 226 (ϵ 8300) (MeOH) (Berdy). λ_{max} 227 (ϵ 10000) (EtOH) (Berdy).

▶ Exp. reprod. effects. Very toxic by intraperitoneal route; LD_{50} (mus, ipr) .3 mg/kg , LD_{50} (mus, ipr) .2 mg/kg. KM5527000

Hydrochloride: [64314-16-5]

$[\alpha]_D^{24}$ +43.2 (c, 0.676 in EtOH).

▶ KM5528500

N-*Ac:* Mp 117-118°. $[\alpha]_D$ -127 (c, 4.8 in EtOH).

(*S*)-*form* [92142-32-0]

Hydrochloride:

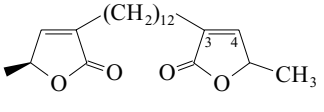
Synthetic. $[\alpha]_D^{23}$ -45 (c, 0.3 in EtOH).

Devlin, J.P. *et al., Can. J. Chem.*, 1977, **55**, 1367-1371 (*isol, pmr, cmr, ms*)
Campbell, H.F. *et al., Can. J. Chem.*, 1977, **55**, 1372 (*synth*)
Bates, H.A. *et al., J.A.C.S.*, 1979, **101**, 1259-1265 (*synth*)
Spivak, C.E. *et al., Mol. Pharmacol.*, 1980, **18**, 384-394; 1983, **23**, 337-343; 1986, **29**, 250-257 (*pharmacol*)
Petersen, J.S. *et al., J.A.C.S.*, 1984, **106**, 4539-4547 (*synth*)
Koskinen, A.M.P. *et al., J. Med. Chem.*, 1985, **28**, 1301-1309 (*synth, cryst struct*)
Danheiser, R.L. *et al., J.A.C.S.*, 1985, **107**, 8066 (*synth*)
Tufariello, J.J. *et al., Tetrahedron*, 1985, **41**, 3447 (*synth*)
Wiseman, J.R. *et al., J.O.C.*, 1986, **51**, 2485 (*synth, bibl*)
Vernon, P. *et al., Chem. Comm.*, 1987, 245 (*synth, bibl*)
Stjernloef, P. *et al., Acta Chem. Scand.*, 1989, **43**, 917 (*synth*)
Matsunaga, S. *et al., J.A.C.S.*, 1989, **111**, 8021 (*isol*)
Sardina, F.J. *et al., J.O.C.*, 1989, **54**, 4654; 1990, **55**, 5025 (*synth, bibl*)
Gallon, J.R. *et al., Phytochemistry*, 1990, **29**, 1107; 1994, **35**, 1195 (*biosynth*)
Somfai, P. *et al., Tet. Lett.*, 1992, **33**, 3791 (*synth*)
Skrinjar, M. *et al., Tetrahedron: Asymmetry*, 1992, **3**, 1263 (*synth*)
Harada, K. *et al., Tetrahedron*, 1993, **49**, 9251 (*isol*)
Newcombe, N.J. *et al., Chem. Comm.*, 1995, 831 (*synth*)
Hemscheidt, T. *et al., Chem. Comm.*, 1995, 1361-1362 (*biosynth*)
Molloy, L. *et al., Eur. J. Pharmacol.*, 1995, **289**, 447-453 (*pharmacol*)
Mansell, H.L. *et al., Tetrahedron*, 1996, **52**, 6025 (*rev, synth*)
Parsons, P.J. *et al., Tetrahedron*, 1996, **52**, 11637 (*synth*)
Oh, C.-Y. *et al., Tet. Lett.*, 1998, **39**, 2133-2136 (*synth*)
Food Sci. Technol., Seafood and Freshwater Toxins, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*revs*)
Parsons, P.J. *et al., Tetrahedron*, 2000, **56**, 309-315 (*synth*)
Brenneman, J.B. *et al., Org. Lett.*, 2004, **6**, 1329-1331 (
Mori, M. *et al., Tet. Lett.*, 2004, **45**, 4397-4399 (*synth*)
Brenneman, J.B. *et al., Tetrahedron*, 2004, **60**, 7301-7314 (*synth*)
Ho, T.-L. *et al., Helv. Chim. Acta*, 2006, **89**, 134-137 (*synth*)
Wonnacott, S. *et al., Mar. Drugs*, 2006, **4**, 228-254 (*rev, activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, AOO120

Ancepsenolide A-483

3,3′-Dodecamethylenebis[5-methyl-2(5H)-furanone], 8CI. 3,3′-(1,12-Dodecanediyl)bis[5-methyl-2(5H)-furanone]

[28028-69-5]



$C_{22}H_{34}O_4$ 362.508

λ_{max} 208 (ϵ 28800) (95% EtOH) (Derep).

(*S*)-*form*

Constit. of the marine gorgon *Pterogorgia (Xiphigorgia) anceps*.

Cryst. (MeOH).

Mp 92.8-94.3°. $[\alpha]_D^{24}$ +7.7 (+13.2). Samples exhibiting variable small opt. rotations, both positive and negative, have been encountered. All samples appeared to be homogeneous.

3,4-Dihydro, 4-acetoxy: ***Ancepsenolide acetate***

$C_{24}H_{38}O_6$ 422.561

Constit. of *Pterogorgia citrina*. Amorph. powder.

Mp 53.9-54.9°. $[\alpha]_D^{25}$ -11.2 (c, 1 in $CHCl_3$). Trivial name is misleading.

3,4-Dihydro, 4-acetoxy, stereoisomer: ***Hydroxyancepsenolide acetate***

$C_{24}H_{38}O_6$ 422.561

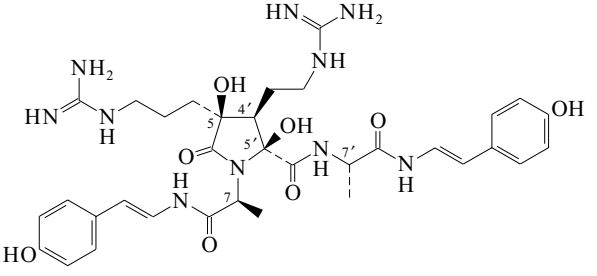
Constit. of *Pterogorgia citrina*. Semisolid.

Mp 68.3-70.3° (semisynthetic). $[\alpha]_D^{25}$ +3.7 (c, 2 in $CHCl_3$) (semisynth). Epimeric with Ancepsenolide acetate at C-3 and C-4. Trivial name is misleading.

Schmitz, F.J. *et al., Tet. Lett.*, 1966, 97 (*struct, pmr*)
Schmitz, F.J. *et al., J.O.C.*, 1969, **34**, 1989; 1971, **36**, 719 (*isol, uv, synth*)
Larson, G.L. *et al., J.O.C.*, 1985, **50**, 5257 (*synth*)
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1994, **57**, 339 (*isol, cmr, derivs*)
Trost, B.M. *et al., J.A.C.S.*, 1994, **116**, 4985 (*synth, abs config*)
Yao, Z.-J. *et al., Synth. Commun.*, 1996, **26**, 3613 (*synth, pmr*)
Takai, K. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 1903-1906 (*synth*)

Anchinopeptolide A A-484

[152369-61-4]



$C_{34}H_{46}N_{10}O_8$ 722.8

Stereochem. at C-5, C-4′ and C-5′ is relative. Isol. from the marine sponge *Anchinoe tenacior*.

$[\alpha]_D$ -103.6 (c, 4 in MeOH). λ_{max} 217 (ϵ 13600); 285 (ϵ 20000) (MeOH) (Derep).

7′-Demethyl: ***Anchinopeptolide B***

[160072-37-7]

$C_{33}H_{44}N_{10}O_8$ 708.773

From *Anchinoe tenacior*.

$[\alpha]_D$ -12.4 (c, 0.7 in MeOH). λ_{max} 284 (ϵ 12070); 318 (MeOH) (Berdy).

7-Demethyl: ***Anchinopeptolide C***

[160041-36-1]

$C_{33}H_{44}N_{10}O_8$ 708.773

From *Anchinoe tenacior*.

$[\alpha]_D$ -6.3 (c, 1 in MeOH). λ_{max} 284 (ϵ 14490); 320 (MeOH) (Berdy).

7,7′-Bisdemethyl: ***Anchinopeptolide D***

[160072-38-8]

$C_{32}H_{42}N_{10}O_8$ 694.746

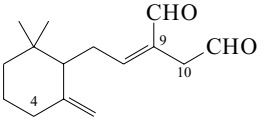
From *Anchinoe tenacior*.

$[\alpha]_D$ +11.4 (c, 1 in MeOH). λ_{max} 284 (ϵ 16940); 318 (MeOH) (Berdy).

Casapullo, A. *et al., Tet. Lett.*, 1993, **34**, 6297 (*isol, uv, ir, pmr, cmr, struct*)
Casapullo, A. *et al., J. Nat. Prod.*, 1994, **57**, 1227 (*Anchinopeptolides B, C and D*)
Snider, B.B. *et al., J.O.C.*, 2000, **65**, 793-800 (*Anchinopeptolide D, synth*)

Ancistrodial A-485

[68398-28-7]



$C_{15}H_{22}O_2$ 234.338

Constit. of *Ancistrotermes cavithorax*.

Δ^9-Isomer: ***2-[2-(2,2-Dimethyl-6-methylenecyclohexyl)ethyl]-2-butenedial***

[85654-10-0]

$C_{15}H_{22}O_2$ 234.338

Constit. of marine alga *Caulerpa bikinensis*. Cytotoxin, ichthyotoxin and antifeedant. Oil. $[\alpha]_D$ +8.5 (c, 0.8 in $CHCl_3$). λ_{max} 227 (ϵ 3010) (solvent not reported) (Derep).

Δ^4-Isomer: ***3-Formyl-5-(2,6,6-trimethyl-2-cyclohexenyl)-3-pentenal***

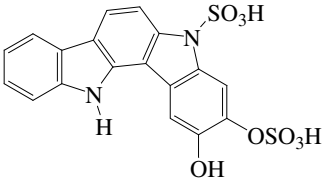
[109326-06-9]

$C_{15}H_{22}O_2$ 234.338

Constit. of *Caulerpa ashmeadii*. Oil. $[\alpha]_D^{21}$ -141 (c, 1.04 in $CHCl_3$).

Baker, R. *et al., Chem. Comm.*, 1978, 410
Paul, V.J. *et al., Tet. Lett.*, 1982, **23**, 5017
Paul, V.J. *et al., J. Chem. Ecol.*, 1987, **13**, 1171-1185 (*isol*)
Mori, K. *et al., Acta Chem. Scand.*, 1992, **46**, 625 (*synth*)
Vidari, G. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 3009 (*synth*)
Horiuchi, S. *et al., Eur. J. Org. Chem.*, 1998, 2851-2854 (*synth*)

Ancorinazole A-486



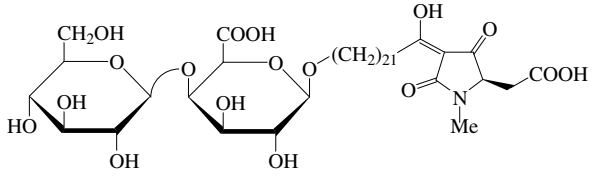
$C_{18}H_{12}N_2O_8S_2$ 448.433

Alkaloid from the sponge *Ancorina* sp. Powder (as di-Na salt). λ_{max} 242 (log ϵ 4.28); 280 (log ϵ 4.23); 296 (sh) (log ϵ 3.97); 308 (log ϵ 4); 340 (log ϵ 3.78); 356 (log ϵ 3.95) (MeOH) (di-Na salt).

Meragelman, K.M. *et al., J.O.C.*, 2002, **67**, 6671-6677 (*isol, pmr, cmr, ms*)

Ancorinoside A A-487

[194426-98-7]



$C_{41}H_{69}NO_{17}$ 847.993

Tetramic acid deriv. Isol. from the sponges *Ancorina* sp. and *Penares sollasi*. Specifically inhibits blastulation of starfish embryos. Inhibits MT1-matrix metalloproteinase. Oil. $[\alpha]_D^{25}$ -5.5 (c, 0.09 in MeOH). λ_{max} 240 (ϵ 5600); 283 (ϵ 7700) (MeOH).

Mg salt:

$C_{41}H_{67}MgNO_{17}$ 870.282

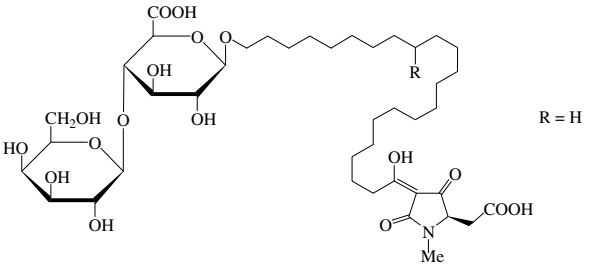
Isol. from *Ancorina* sp. Powder.

Mp 200-208° dec. $[\alpha]_D^{25}$ -7.7 (c, 0.18 in H_2O). λ_{max} 243 (ϵ 8900); 285 (ϵ 9300) (H_2O).

Ohta, S. *et al., J.O.C.*, 1997, **62**, 6452-6453 (*isol, uv, ir, pmr, cmr*)
Fujita, M. *et al., Tetrahedron*, 2001, **57**, 1229-1234 (*isol, activity*)
Ohta, E. *et al., Tetrahedron*, 2001, **57**, 4699-4703 (*Mg salt, isol, cd, pmr, cmr, ms*)

Ancorinoside B A-488

[334519-25-4]



$C_{41}H_{69}NO_{17}$ 847.993

Enolised β-triketone. Isol. from the sponge *Penares sollasi*. Powder. $[\alpha]_D^{24}$ +1.5 (c, 0.1 in MeOH). λ_{max} 282 (ϵ 8540) (MeOH).

Fujita, M. *et al., Tetrahedron*, 2001, **57**, 1229-1234 (*isol, pmr, cmr, uv*)

Ancorinoside C A-489

[334519-26-5]

As Ancorinoside B, A-488 with

R = CH_3

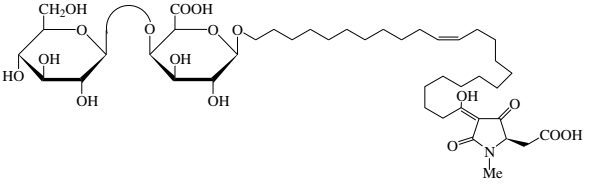
$C_{42}H_{71}NO_{17}$ 862.019

Enolised β-triketone. Isol. from the sponge *Penares sollasi*. Powder. $[\alpha]_D^{24}$ +2.8 (c, 0.1 in MeOH). λ_{max} 282 (ϵ 8430) (MeOH).

Fujita, M. *et al., Tetrahedron*, 2001, **57**, 1229-1234 (*isol, pmr, cmr, uv*)

Ancorinoside D A-490

[334519-27-6]



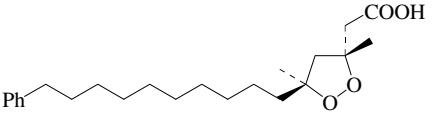
$C_{43}H_{71}NO_{17}$ 874.03

Enolised β-triketone. Isol. from the sponge *Penares sollasi*. Powder. $[\alpha]_D^{24}$ -5.2 (c, 0.1 in MeOH). λ_{max} 282 (ϵ 9630) (MeOH).

Fujita, M. *et al., Tetrahedron*, 2001, **57**, 1229-1234 (*isol, pmr, cmr, uv*)

Andavadoic acid A-491

3,5-Dimethyl-5-(10-phenyldecyl)-1,2-dioxolane-3-acetic acid



Relative Configuration

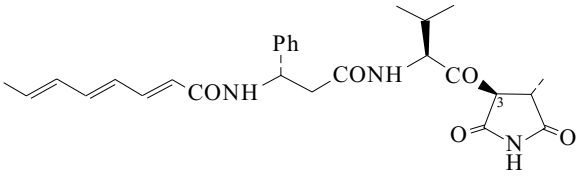
$C_{23}H_{36}O_4$ 376.535

Related to 5-Alkyl-3,5-dimethyl-1,2-dioxolane-3-acetic acids, A-206. Isol. from the sponge *Plakortis* aff. *simplex*. Antitumour agent. Oil. $[\alpha]_D$ +34.7 (c, 0.004 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 2003, **66**, 682-685 (*isol, pmr, cmr, ms*)

Andrimid A-492

[108868-95-7]



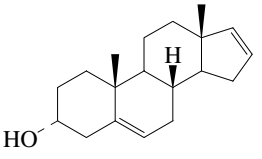
$C_{27}H_{33}N_3O_5$ 479.575

Peptide antibiotic. Prod. by a bacterial symbiont from *Nilaparvata lugens*, a marine *Pseudomonas fluorescens* and an *Enterobacter* sp. Active against *Xanthomonas* sp.
Mp 172-173.5°. λ_{max} 297 (ϵ 38000) (MeOH/AcOH) (Derep). λ_{max} 297 (ϵ 51100) (MeOH/NaOH) (Derep). λ_{max} 297 (ϵ 41200) (MeOH) (Derep).

3-Epimer, 3-hydroxy: ***Moiramide C***
[155233-32-2]
$C_{27}H_{33}N_3O_6$ 495.574
Metab. of a marine *Pseudomonas fluorescens*. Amorph. solid. Sol. MeOH, EtOAc. λ_{max} 289 (ϵ 29711) (MeOH) (Berdy).

Fredenhagen, A. *et al., J.A.C.S.*, 1987, **109**, 4409
Kenny, P.T. *et al., Pestic. Sci.*, 1987, **27**, 117 (*isol*)
McWhorter, W. *et al., Chem. Comm.*, 1989, 299 (*synth*)
Rama Rao, A.V. *et al., Tet. Lett.*, 1991, **32**, 4393 (*synth*)
Needham, J. *et al., J.O.C.*, 1994, **59**, 2058-2063 (*Andrimid, Moiramide C*)
Davies, S.G. *et al., J.C.S. Perkin 1*, 1998, 2635-2643 (*synth*)

Androsta-5,16-dien-3-ol A-493



3α-*form*

$C_{19}H_{28}O$ 272.43

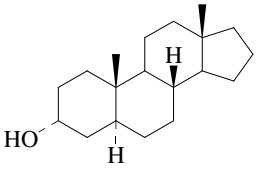
3α-*form* [30505-67-0]
Cryst. (Me_2CO aq.). Mp 138°. $[\alpha]_D$ -77.5 (c, 1.2 in $CHCl_3$).

3β-*form* [1224-94-8]
Sterol identified in sponge *Damiriana hawaiiana*. Metab. of pregnenolone.
Mp 140-141°. $[\alpha]_D$ -71.9 (c, 1.5 in $CHCl_3$).

Ac: [1236-14-2]
$C_{21}H_{30}O_2$ 314.467
Cryst. (MeOH). Mp 94-95°. $[\alpha]_D$ -81 (c, 0.27 in $CHCl_3$).

Sondheimer, F. *et al., J.A.C.S.*, 1955, **77**, 4145 (*synth*)
Barton, D.H.R. *et al., J.C.S.*, 1962, 470 (*synth*)
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476 (*isol*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1983, **66**, 192 (*synth*)
Concepcion, J.I. *et al., J.O.C.*, 1986, **51**, 402 (*deriv*)

Androstan-3-ol A-494



(3α,5α)-*form*

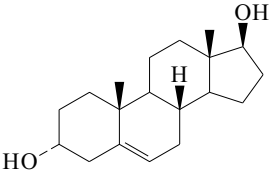
$C_{19}H_{32}O$ 276.461

(3β,5α)-*form* [1224-92-6]
Isol. from Black Sea sponges *Haliclona* spp.
Cryst. (Me_2CO).
Mp 153-155°. $[\alpha]_D^{20}$ +1 ($CHCl_3$).

[1224-93-7, 19308-13-5, 25814-70-4]

Prelog, V. *et al., Helv. Chim. Acta*, 1945, **28**, 618 (*3α,5β, 3β,5β-forms, synth*)
Butenandt, A. *et al., Annalen*, 1951, **575**, 123 (*3α,5α, 3β,5α-forms synth*)
Jones, R.N. *et al., J.A.C.S.*, 1958, **80**, 6121 (*ir*)
Pettit, G.R. *et al., Tetrahedron*, 1962, **18**, 953 (*3β,5α-form, synth*)
Mori, H. *et al., Chem. Pharm. Bull.*, 1963, **11**, 1413 (*3β,5α-form, synth*)
Shapiro, R.H. *et al., J.A.C.S.*, 1964, **86**, 2837 (*3β,5α-form, synth*)
Bridgeman, J.E. *et al., J.C.S.(C)*, 1970, 250 (*3α,5α, 3β,5α-forms, pmr*)
Boul, A.D. *et al., J.C.S.(C)*, 1971, 1130 (*3α,5α, 3β,5α-forms, ir*)
ApSimon, J.W. *et al., Can. J. Chem.*, 1973, **51**, 3874 (*3α,5α, 3β,5α-forms, cmr*)
Kirk, D.N. *et al., J.C.S. Perkin 2*, 1990, 1567 (*pmr*)
Elenkov, I. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1999, **123**, 357-360 (*isol*)

Androst-5-ene-3,17-diol, 9CI A-495



(3α,17β)–*form*

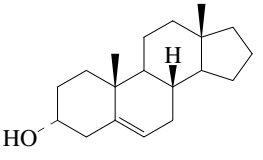
$C_{19}H_{30}O_2$ 290.445

(3β,17β)-*form*
Hermaphrodiol
[521-17-5]
Obt. from the incubation of 3β-hydroxyandrost-5-en-17-one with *Fusidium* sp. Occurs in blood, testes, urine and ovarian follicles. Sterol identified in sponge *Damiriana hawaiiana* and prod. from cholesterol by starfish *Asterias rubens*.
Cryst. (Me_2CO).
Mp 180.5-183°. $[\alpha]_D$ -56 (c, 0.4 in EtOH).
► Exp. reprod. effects. BV8091000

[14504-94-0, 42921-37-9, 64162-67-0, 75767-22-5]

Dodson, R.M. *et al., J.A.C.S.*, 1959, **81**, 6295 (*synth, 3β,17β-form*)
Shoppee, C.W. *et al., J.C.S.*, 1959, 345 (*synth, 3β,17β-form*)
Dannenberg, H. *et al., Chem. Ber.*, 1961, **94**, 3094 (*synth, uv*)
Ohrt, J.M. *et al., Acta Cryst.*, 1965, **19**, 479 (*cryst struct*)
Hampel, B. *et al., Tetrahedron*, 1966, **22**, 1607 (*pmr*)
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476 (*isol, sponge*)
Castonguay, A. *et al., J. Med. Chem.*, 1978, **21**, 391 (*pharmacol*)
Andersson, S.H.G. *et al., J. Chromatogr.*, 1984, **289**, 195 (*gcms*)
Sahlberg, B.L. *et al., J. Steroid Biochem.*, 1986, **25**, 379; 1987, **26**, 609 (*occur*)
Bartsch, W. *et al., J. Steroid Biochem.*, 1987, **28**, 35 (*metab*)

Androst-5-en-3-ol, 9CI A-496



3α-*form*

$C_{19}H_{30}O$ 274.445

3α-*form* [5232-33-7]
Cryst. (MeOH). Mp 138-139°.

Ac:
$C_{21}H_{32}O_2$ 316.483
Cryst. (MeOH). Mp 129-131°.

3β-*form* [1476-64-8]
Sterol identified in sponge *Damiriana hawaiiana*.
Cryst. (Me_2CO).
Mp 136.5-137°. $[\alpha]_D$ -75 (c, 1.03 in dioxan). $[\alpha]_D$ -68 (EtOH).

Ac: [13067-44-2]

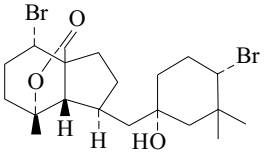
Cryst. ($CHCl_3$). Mp 99°. $[\alpha]_D$ -76.9 (c, 0.528 in $CHCl_3$).

Benzoyl:
$C_{26}H_{34}O_2$ 378.553
Mp 188-189°. $[\alpha]_D$ -34.

Shoppee, C.W. *et al., J.C.S.*, 1961, 3641 (*synth, 3β-form*)
Weinman, J. *et al., Steroids*, 1965, **6**, 683 (*synth, ir*)
Habermehl, G. *et al., Annalen*, 1969, **723**, 181 (*synth, 3β-form*)
Van Lier, J.E. *et al., J.O.C.*, 1970, **35**, 2627 (*synth, ir, 3β-form*)
Van Lier, J.E. *et al., Steroids*, 1973, **21**, 521 (*synth, ms, 3β-form*)
Budzikiewicz, H. *et al., Tetrahedron*, 1976, **32**, 143 (*ms, 3β-form*)
Hudec, J. *et al., Tetrahedron*, 1976, **32**, 2475 (*cd, 3β-form*)
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476 (*isol*)
Deive, N. *et al., J. Med. Chem.*, 2001, **44**, 2612-2618 (*3β-form, synth, pmr, cmr*)

Angasiol A-497

[68081-51-6]



$C_{20}H_{30}Br_2O_3$ 478.263
Constit. of *Aplysia angasi*. Cryst. (Me_2CO/hexane).
Mp 189-191°.

Ac: ***Angasiol acetate***
[123967-75-9]
$C_{22}H_{32}Br_2O_4$ 520.3
Metab. of *Aplysia juliana*. Cryst. (MeOH).
Mp 176°. $[\alpha]_D$ +27 ($CHCl_3$).

Pettit, G.R. *et al., J.O.C.*, 1978, **43**, 4685 (*isol, cryst struct*)
Atta-ur-Rahman, *et al., J. Nat. Prod.*, 1991, **54**, 886 (*isol, pmr, cmr, cryst struct*)

Triakis scyllia Angiotensin I A-498

Dogfish angiotensin I
[152839-32-2]
Asn-Arg-Pro-Tyr-Ile-His-Pro-Phe-Gln-Leu
$C_{61}H_{89}N_{17}O_{14}$ 1284.48
Isol. from plasma and kidney extracts of the dogfish *Triakis scyllia*.

Takei, Y. *et al., J. Endocrinol.*, 1993, **139**, 281-285 (*isol*)

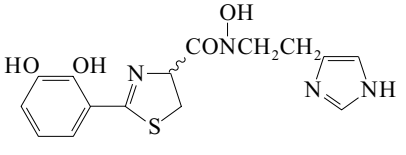
Thunnus albacares Angiotensin-converting enzyme inhibitor A-499

[117620-76-5]
Pro-Thr-His-Ile-Lys-Trp-Gly-Asp
$C_{44}H_{64}N_{12}O_{12}$ 953.063
Isol. from muscle of the yellowfin tuna *Thunnus albacares*.
Inhibitor of angiotensin-converting enzyme.

Kohama, Y. *et al., Biochem. Biophys. Res. Commun.*, 1988, **155**, 332-337 (*isol*)
Kohama, Y. *et al., J. Pharmacobio-Dyn.*, 1989, **12**, 566-571 (*synth, props*)

Anguibactin A-500

2-(2,3-Dihydroxyphenyl)-4,5-dihydro-N-*hydroxy*-N-*[2-(1*H*-imidazol-4-yl)ethyl]-4-thiazolecarboxamide, 9CI*
[117308-63-1]

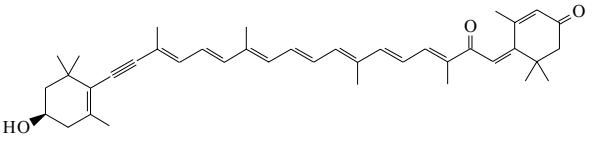


$C_{15}H_{16}N_4O_4S$ 348.382
Isol. from the iron-deficient cultures of a marine *Vibrio anguillarum*. Siderophore. λ_{max} 216; 266; 327 (MeOH) (Berdy). λ_{max} 214; 260 (ε 11000); 315; 410 (pH 7 buffer) (Berdy). λ_{max} 214; 258; 335; 415 (pH 10 buffer) (Berdy).

Actis, L.A. *et al., J. Bacteriol.*, 1986, **167**, 57 (*isol*)
Jalal, M.A.F. *et al., J.A.C.S.*, 1989, **111**, 292-296 (*Anguibactin*)

Anhydroamarouciaxanthin B A-501

6′,7,7′,8-Tetrahydro-6′,8′-dihydro-3-hydroxy-β,ε-carotene-3′,8′-dione
[119286-10-1]

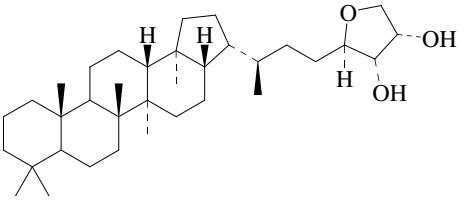


$C_{40}H_{50}O_3$ 578.833
Constit. of *Mytilus edulis* (blue mussel). λ_{max} 458; 485 (hexane).

Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495 (*occur, uv, ms, pmr*)

32,35-Anhydrobacteriohopane-33,34-diol A-502

[346578-23-2]

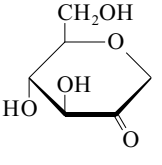


$C_{35}H_{60}O_3$ 528.857
Constit. of *Plakortis simplex*. Powder.
Mp 266-267° dec. $[\alpha]_D$ +17 (c, 2.2 in Py).

Costantino, V. *et al., Tetrahedron*, 2001, **57**, 4045-4048 (*isol, pmr, cmr*)

1,5-Anhydrofructose, 9CI A-503

1,5-Anhydro-arabino-*hex-2-ulose*



$C_6H_{10}O_5$ 162.142
In aq. soln. the oxo form illus. is in equilib. with the 2-enol form (1,5-Anhydro-*arabino*-hex-1-enitol), the 2,3-enediol form and the 3,3-diol covalent hydrate, which is the predominating species. In nonaqueous solvs. exists as a mixt. of two dimers. Acetylation gives spiro-dimers.

D-*form* [75414-43-6]
Prod. by the action of α-1,4-glucan lyase on α-glucans such as starch. Exists in rat liver, fungi and algae. Precursor of 2-Hydroxy-2-(hydroxymethyl)-2*H*-pyran-3(6*H*)-one, H-696 in *Morchella vulgaris* (morel) and of Echinosporin in *Peziza echinospora*. Antioxidant. Amorph. solid.
Mp 107-112°. $[\alpha]_D^{20}$ -32.9 (c, 0.86 in H_2O).

Oxime: [75414-31-2]
$C_6H_{11}NO_5$ 177.157
Mp 178-180°. $[\alpha]_D^{21}$ -43 (c, 0.3 in H_2O).

Tri-Ac: 3,4,6-Tri-O-*acetyl-1,5-anhydro-D*-arabino-*hex-2-ulose*
$C_{12}H_{16}O_8$ 288.254
Mp 93-94° (86-88°). $[\alpha]_D$ -7.2 (c, 1.5 in $CHCl_3$).

Tri-Ac, oxime: [88851-59-6]

[75414-20-9]
$C_{12}H_{17}NO_8$ 303.268
Mp 89-90°. $[\alpha]_D^{21}$ -52.9 (c, 0.3 in $CHCl_3$).

*Tribenzoyl: 1,5-Anhydro-3,4,6-tri-*O*-benzoyl-D-fructose*
[75414-32-3]
$C_{27}H_{22}O_8$ 474.466
Mp 126-127°. $[\alpha]_D^{20}$ -24 (c, 0.8 in $CHCl_3$).

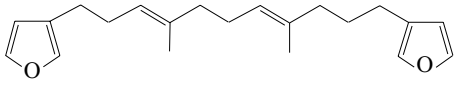
Tribenzoyl, oxime: [82569-81-1]
[75414-21-0]
$C_{27}H_{23}NO_8$ 489.481
Mp 176-177°. $[\alpha]_D^{21}$ -39 (c, 0.4 in $CHCl_3$).

*4,6-Benzylidene, 3-(*tert*-butyldimethylsilyl): 1,5-Anhydro-4,6-*O*-benzylidene-3-*O*-(*tert*-butyldimethylsilyl)-D-fructose*
[89872-98-0]
$C_{19}H_{28}O_5Si$ 364.513
Syrup + $1H_2O$. $[\alpha]_D^{20}$ -49.9 (c, 2.7 in $CHCl_3$).

Lichtenthaler, F.W. *et al., Tet. Lett.*, 1980, **21**, 1429-1432 (*synth, tri-Ac, tribenzoyl*)
Tulshian, D.B. *et al., J.O.C.*, 1984, **49**, 2347-2355 (*benzylidene butyldimethylsilyl*)
Deffieux, G. *et al., Phytochemistry*, 1987, **26**, 1391-1393 (*biosynth, isol, oxime, cryst struct*)
Baute, M.A. *et al., Phytochemistry*, 1991, **30**, 1419-1423 (*biosynth*)
Yu, S. *et al., Carbohydr. Res.*, 1998, **305**, 73-82 (*anal, bibl*)
Kopper, S. *et al., Chem. Eur. J.*, 1998, **4**, 2442-2455 (*synth*)
Andersen, S.M. *et al., J. Carbohydr. Chem.*, 1998, **17**, 1027-1035 (*acetyl dimers, cryst struct*)
Andersen, S.M. *et al., J. Carbohydr. Chem.*, 2000, **19**, 717-723; 2002, **21**, 569-578 (*synth, struct, tri-Ac, props*)
Andersen, S.M. *et al., Carbohydr. Res.*, 2002, **337**, 873-890 (***rev***)
Yamaji, K. *et al., Planta Med.*, 2002, **68**, 16-19 (*activity*)
Lichtenthaler, F.W. *et al., Eur. J. Org. Chem.*, 2003, 3094-3104 (*tribenzoyl*)
Yu, S. *et al., Food Chem. Toxicol.*, 2004, **42**, 1677-1686 (*anal, metab, toxicol*)

Anhydrofurospongin 1 A-504

[35671-06-8]

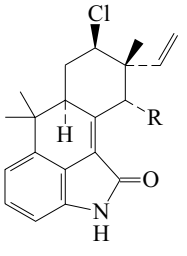


$C_{21}H_{28}O_2$ 312.451
Constit. of *Spongia officinalis* and *Hippospongia communis*. Oil.

Cimino, G. *et al., Tetrahedron*, 1972, **28**, 267

Anhydrohapaloxindole A A-505

[109217-16-5]



R = NC

$C_{21}H_{21}ClN_2O$ 352.862
Minor alkaloid from the blue-green alga *Hapalosiphon fontinalis*. Mp 123° dec. $[\alpha]_D$ +150 (c, 0.4 in EtOH). Appears to be a $^1O_2$ oxidn. prod. of Hapalindole A, H-80, the major alkaloid in this cyanophyte.

Moore, R.E. *et al., J.O.C.*, 1987, **52**, 3773 (*isol, uv, pmr, cmr, struct*)

Anhydrohapaloxindole B A-506

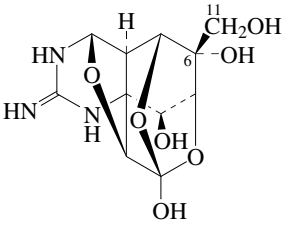
[123519-73-3]
As Anhydrohapaloxindole A, A-505 with
R = NCS
$C_{21}H_{21}ClN_2OS$ 384.928
Minor alkaloid from the blue-green alga *Hapalosiphon fontinalis*.

Dechloro: ***Anhydrohapaloxindole M***
[123498-03-3]
$C_{21}H_{22}N_2OS$ 350.484
Minor alkaloid from *Hapalosiphon fontinalis*.

Moore, R.E. *et al., Phytochemistry*, 1989, **28**, 1565 (*isol, pmr, struct*)

4,9-Anhydrotetrodotoxin A-507

[13072-89-4]



$C_{11}H_{15}N_3O_7$ 301.255
Isol. from puffer fish, newts, other marine animals incl. *Cynops ensicauda*, *Fugu* spp. and *Octopus maculosus*. Bacteria has been suggested as the source within these organisms. Toxic sodium channel blocker; phycotoxin. Amorph.
▶ Paralytic poison.

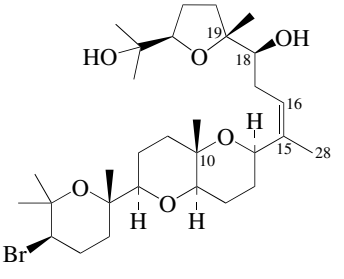
6-Epimer: ***4,9-Anhydro-6-epitetrodotoxin***
[113565-40-5]
$C_{11}H_{15}N_3O_7$ 301.255
Isol. from the newt *Cynops ensicauda*. Amorph. $[\alpha]_D^{25}$ +10 (c, 0.08 in AcOH aq.).

11-Deoxy: ***4,9-Anhydro-11-deoxytetrodotoxin***
[113507-22-5]
$C_{11}H_{15}N_3O_6$ 285.256
Isol. from the newt *Cynops ensicauda*. Amorph.

Tsuda, K. *et al., Chem. Pharm. Bull.*, 1964, **12**, 634-642; 642-645; 1357-1374
Tamura, C. *et al., Acta Cryst. C*, 1966, **21**, 226-236 (*cryst struct*)
Nakamura, M. *et al., Toxicon*, 1985, **23**, 271-276 (*isol*)
Yasumoto, T. *et al., Agric. Biol. Chem.*, 1986, **50**, 793-795 (*isol*)
Yasumoto, T. *et al., J.A.C.S.*, 1988, **110**, 2344-2345 (*isol, pmr, cmr*)
Dyankonov, A.L. *et al., Khim. Prir. Soedin.*, 1997, **33**, 297-351; *Chem. Nat. Compd. (Engl. Transl.)*, 1997, **33**, 221-267 (*rev*)

15-Anhydrothyrsiferol A-508

15,16-Dehydrothyrsiferol



$C_{30}H_{51}BrO_6$ 587.633

Di-Ac: 15-Anhydrothyrsiferyl diacetate
[107040-99-3]
$C_{34}H_{55}BrO_8$ 671.708
Constit. of red alga *Laurencia obtusa*. Cytotoxic agent. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 163-164°. $[\alpha]_D$ +12.9 (c, 1.00 in $CHCl_3$).

$\Delta^{15(28)}$-Isomer: ***Dehydrothyrsiferol***
[93413-35-5]
$C_{30}H_{51}BrO_6$ 587.633

Isol. from *Laurencia pinnatifida*. Needles (Me_2CO).
Mp 103-104°. $[\alpha]_D$ -203 (c, 0.64 in $CHCl_3$).

$\Delta^{15(28)}$-Isomer, di-Ac: 15(28)-Anhydrothyrsiferyl diacetate
[107065-86-1]
$C_{34}H_{55}BrO_8$ 671.708
Constit. of *Laurencia obtusa*. Cytotoxic agent. Cryst.
Mp 94-95°. $[\alpha]_D$ +8.8 (c, 1.00 in $CHCl_3$).

$\Delta^{15(28)}$-Isomer, 16α-hydroxy: ***16-Hydroxydehydrothyrsiferol***
$C_{30}H_{51}BrO_7$ 603.633
Constit. of *Laurencia viridis*. Amorph. solid. $[\alpha]_D^{25}$ -2.2 (c, 0.23 in $CHCl_3$).

$\Delta^{15(28)}$-Isomer, 16β-hydroxy: ***16-Epihydroxydehydrothyrsiferol***
[346583-60-6]
$C_{30}H_{51}BrO_7$ 603.633
Constit. of *Laurencia viridis*. Amorph. solid. $[\alpha]_D^{25}$ +12 (c, 0.07 in $CHCl_3$).

3-Epimer, $\Delta^{15(28)}$-isomer: ***3-Epidehydrothyrsiferol***
[477853-62-6]
$C_{30}H_{51}BrO_6$ 587.633
Constit. of *Laurencia viridis*. Amorph. solid. $[\alpha]_D^{25}$ +3.9 (c, 0.18 in $CHCl_3$).

10-Epimer: ***10-Epi-15,16-dehydrothyrsiferol***
$C_{30}H_{51}BrO_6$ 587.633
Constit. of *Laurencia viridis*. Amorph. solid. $[\alpha]_D^{25}$ +8 (c, 0.2 in $CHCl_3$).

10-Epimer, $\Delta^{15(28)}$-isomer: ***10-Epidehydrothyrsiferol***
[176589-47-2]
$C_{30}H_{51}BrO_6$ 587.633
Constit. of *Laurencia viridis*. Oil. $[\alpha]_D^{25}$ +20.7 (c, 0.76 in $CHCl_3$).

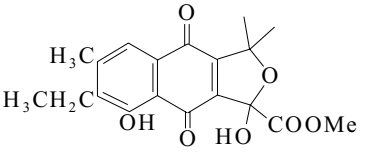
18,19-Diepimer: ***15,16-Dehydrovenustatriol***
$C_{30}H_{51}BrO_6$ 587.633
Constit. of *Laurencia viridis*. Amorph. solid. $[\alpha]_D^{25}$ -5.4 (c, 0.26 in $CHCl_3$).

18,19-Diepimer, $\Delta^{15(28)}$-isomer: ***Dehydrovenustatriol***
$C_{30}H_{51}BrO_6$ 587.633
Constit. of *Laurencia viridis*. Amorph. solid. $[\alpha]_D^{25}$ +4.6 (c, 0.26 in $CHCl_3$).

Gonzalez, A.G. *et al., Tetrahedron*, 1984, **40**, 2751
Suzuki, T. *et al., Chem. Lett.*, 1987, 361
Norte, M. *et al., Tet. Lett.*, 1996, **37**, 2671 (*10-Epidehydrothyrsiferol*)
Norte, M. *et al., Tetrahedron*, 1997, **53**, 4649 (*derivs*)
Manriquez, C.P. *et al., Tetrahedron*, 2001, **57**, 3117-3123 (*16-Epihydroxydehydrothyrsiferol*)
Souto, M.L. *et al., Tetrahedron*, 2002, **58**, 8119-8125 (*3-Epidehydrothyrsiferol*)

Annulin A A-509

[105335-73-7]

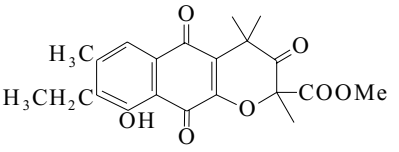


$C_{19}H_{20}O_7$ 360.363
Constit. of *Garveia annulata*. Shows antibacterial activity. Orange cryst. (EtOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 174-176°. λ_{max} 286 (ϵ); 559 (ϵ) (MeOH/NaOH) (Derep). λ_{max} 217 (ϵ); 247 (ϵ); 439 (ϵ) (MeOH) (Derep).

Fahy, E. *et al., J.O.C.*, 1986, **51**, 5145 (*isol, cryst struct*)

Annulin B A-510

[105335-74-8]



$C_{21}H_{22}O_7$ 386.401
Constit. of *Garveia annulata*. Orange oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +8 (c, 0.2 in $CHCl_3$). λ_{max} 235 (ϵ); 270 (sh) (ϵ); 307 (sh) (ϵ); 530 (ϵ) (MeOH/NaOH) (Derep). λ_{max} 208 (ϵ); 255 (ϵ); 293 (ϵ); 425 (ϵ) (MeOH) (Derep).

Fahy, E. *et al., J.O.C.*, 1986, **51**, 5145

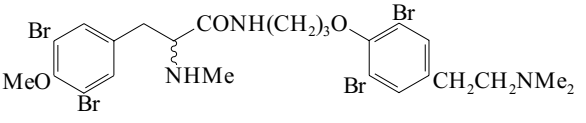
Anodontatachykin A-511

[157171-96-5]
H-5-OxoPro-Tyr-Gly-Phe-His-Ala-Val-Arg-NH_2
$C_{45}H_{62}N_{14}O_{10}$ 959.073
Isol. from the ganglia of the mollusc *Anodonta cygnea*.

Fujisawa, Y. *et al., Pept. Chem.*, 1993, **31**, 161-164 (*isol*)

Anomoian A A-512

[129602-20-6]

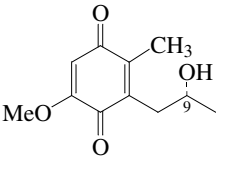


$C_{24}H_{31}Br_4N_3O_3$ 729.143
Metab. of the verongid sponge *Anomoianthella popeae*. Powder (as hydrochloride).
Mp 200° dec. (hydrochloride). $[\alpha]_D$ +5.1 (c, 0.013 in MeOH). λ_{max} 245 (ϵ 12300); 276 (ϵ 9400); 283 (ϵ 7800) (MeOH).

Kernan, M.R. *et al., J. Nat. Prod.*, 1990, **53**, 720-723 (*isol, uv, ir, pmr, cmr, ms*)

Anserinone B A-513

3-(2-Hydroxypropyl)-5-methoxy-2-methyl-1,4-benzoquinone
[190895-96-6]



$C_{11}H_{14}O_4$ 210.229
Abs. config. revised in 2004.

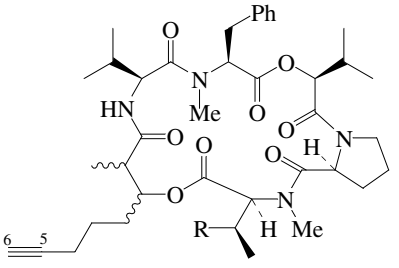
(R)-form
Prod. by *Podospora anserina* and strains of the marine *Penicillium corylophilum*. Exhibits antibacterial, antifungal and cytotoxic props. Yellow oil. $[\alpha]_D$ +43 (c, 1 in MeOH). λ_{max} 233 (ϵ 4500); 275 (ϵ 10000); 369 (ϵ 500) (CH_2Cl_2).

O-*Formyl:* ***Formylanserinone B***
$C_{12}H_{14}O_5$ 238.24
Isol. from a mixture of strains of the marine *Penicillium corylophilum*. Amber cryst. $[\alpha]_D^{27}$ +11.6 (c, 0.2 in MeOH). λ_{max} 279 (log ϵ 3.93); 360 (log ϵ 2.67) (CH_2Cl_2).

Ketone: 5-Methoxy-2-methyl-3-(2-oxopropyl)-1,4-benzoquinone. ***Anserinone A***
[190895-95-5]
$C_{11}H_{12}O_4$ 208.213

Prod. by *Podospora anserina* and *Penicillium corylophilum*. Exhibits antibacterial, antifungal and cytotoxic props. Yellow needles.
Mp 122-124°. λ_{max} 265 (ϵ 7100); 359 (360) (CH_2Cl_2).
Wang, H.-J. *et al., J. Nat. Prod.*, 1997, **60**, 629-631; 2004, **67**, 1637 (*Anserinones*)
Gautschi, J.T. *et al., J. Nat. Prod.*, 2004, **67**, 362-367 (*Formylanserinone B*)

Antanapeptin A **A-514**



R = CH_2CH_3

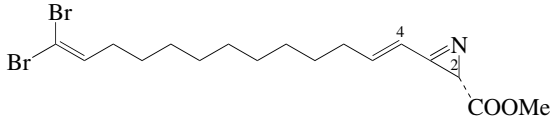
$C_{41}H_{60}N_4O_8$ 736.947
Depsipeptide antibiotic. Isol. from *Lyngbya majuscula*. Pale yellow oil. $[\alpha]_D^{21}$ -50 (c, 0.13 in MeOH). λ_{max} 212 (log ϵ 4.5) (MeOH).

5,6-Dihydro: ***Antanapeptin B***
$C_{41}H_{62}N_4O_8$ 738.963
Isol. from *Lyngbya majuscula*. Pale yellow oil. $[\alpha]_D^{21}$ -42 (c, 0.09 in MeOH). λ_{max} 212 (log ϵ 4.6) (MeOH).

5,5,6,6-Tetrahydro: ***Antanapeptin C***
$C_{41}H_{64}N_4O_8$ 740.979
Isol. from *Lyngbya majuscula*. Pale yellow oil. $[\alpha]_D^{21}$ -42 (c, 0.09 in MeOH). λ_{max} 212 (log ϵ 4.6) (MeOH).
Nogle, L.M. *et al., J. Nat. Prod.*, 2002, **65**, 21-24

Antanapeptin D **A-515**
As Antanapeptin A, A-514 with
R = CH_3
$C_{40}H_{58}N_4O_8$ 722.92
Isol. from *Lyngbya majuscula*. Pale yellow oil. $[\alpha]_D^{21}$ -30 (c, 0.05 in MeOH).
Nogle, L.M. *et al., J. Nat. Prod.*, 2002, **65**, 21-24

Antazirine **A-516**



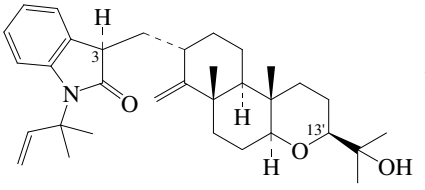
(2*S*,4*E*)-*form*

$C_{17}H_{25}Br_2NO_2$ 435.198

(2*S*,4*E*)-*form* [170385-24-7]
Isol. from the sponge *Dysidea fragilis*.
Oil. $[\alpha]_D$ +10.3 (c, 0.39 in $CHCl_3$). λ_{max} 213; 220 (sh) (MeOH).

(4*Z*)-*form* [170554-75-3]
Very minor constit. of *Dysidea fragilis*.
Oil. C-2 config. not clear. λ_{max} 215; 220 (sh) (MeOH).
Salomon, C.E. *et al., J. Nat. Prod.*, 1995, **58**, 1463-1466 (*isol, uv, ir, pmr, cmr, ms, struct*)

Anthcolorin A **A-517**
[358334-50-6]



Absolute Configuration

$C_{33}H_{47}NO_3$ 505.739
Prod. by *Aspergillus versicolor* OUPS-N136 isol. from the sea urchin *Anthocidaris crassispina*.

3-Hydroxy: ***Anthcolorin G***
[358334-56-2]
$C_{33}H_{47}NO_4$ 521.739
Prod. by *Aspergillus versicolor* OUPS-N136.

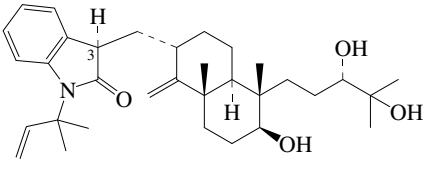
3-Epimer: ***Anthcolorin B***
[358334-51-7]
$C_{33}H_{47}NO_3$ 505.739
Prod. by *Aspergillus versicolor* OUPS-N136.

3-Epimer, 3-hydroxy: ***Anthcolorin H***
[358334-57-3]
$C_{33}H_{47}NO_4$ 521.739
Prod. by *Aspergillus versicolor* OUPS-N136.

13′-Epimer: ***Anthcolorin C***
[358334-52-8]
$C_{33}H_{47}NO_3$ 505.739
Prod. by *Aspergillus versicolor* OUPS-N136.

3,13′-Diepimer: ***Anthcolorin D***
[358334-53-9]
$C_{33}H_{47}NO_3$ 505.739
Prod. by *Aspergillus versicolor* OUPS-N136.
Yamada, K. *et al., CA*, 2001, **135**, 204898 (*isol*)

Anthcolorin E **A-518**
[358334-54-0]

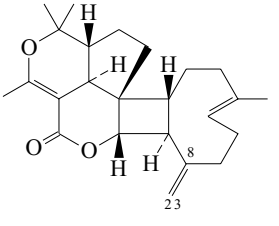


Absolute Configuration

$C_{33}H_{49}NO_4$ 523.754
Prod. by *Aspergillus versicolor* OUPS-N136 isol. from the sea urchin *Anthocidaris crassispina*.

3-Epimer: ***Anthcolorin F***
[358334-55-1]
$C_{33}H_{49}NO_4$ 523.754
Prod. by *Aspergillus versicolor* OUPS-N136.
Yamada, K. *et al., CA*, 2001, **135**, 204898 (*isol*)

Antheliolide A **A-519**
[114915-36-5]



$C_{24}H_{32}O_3$ 368.515

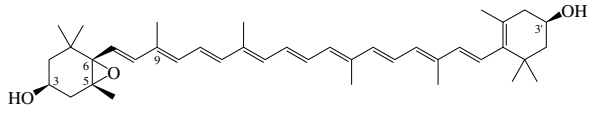
Novel acetoacetylated diterpenoid skeleton. Constit. of soft coral *Anthelia glauca*.
Mp 180°. Exists as mixt. of two conformers. λ_{max} 245 (ϵ 10000) (MeOH) (Derep).

8ξ,23-Epoxide: ***Antheliolide B***
[114933-19-6]
$C_{24}H_{32}O_4$ 384.514
Constit. of *Anthelia glauca*. Oil. λ_{max} 245 (ϵ 10000) (MeOH) (Derep).

Green, D. *et al., Tet. Lett.*, 1988, **29**, 1605 (*isol*)
Smith, A.B. *et al., Tet. Lett.*, 1989, **30**, 3363 (*cryst struct*)

Antheraxanthin A-520

5,6-Epoxy-5,6-dihydro-β,β-carotene-3,3′-diol, 9CI. Zeaxanthin epoxide. 5,6-Epoxyzeaxanthin



(3*S*,3'*R*,5*S*,6*R*,9*E*)-*form*

$C_{40}H_{56}O_3$ 584.881

(3*S*,3′*R*,5*S*,6*R*,9*E*)-*form*
Antheraxanthin A
[25494-44-4]
Constit. of *Lilium* spp., *Euonymus europaeus*, *Capsicum annuum* and other sources. Minor xanthophyll of Chrysophyceae algae. Potential nutriceutical. Cryst. (MeOH).
Mp 197°.

(3*S*,3′*R*,5*S*,6*R*,9*Z*)-*form*
cis-*Antheraxanthin*
[68831-78-7]
Constit. of *Lilium* spp.
Cryst. (MeOH).
Mp 108°.

(3*S*,3′*R*,5*R*,6*S*)-*form*
Antheraxanthin B
[640-03-9]
Constit. of the common freshwater goby *Rhinogobius brunneus*.
λ_{max} 420; 445; 475 (Et_2O).

Tappi, G. *et al., Helv. Chim. Acta*, 1949, **32**, 50 (*isol*)
Bartlett, L. *et al., J.C.S.(C)*, 1969, 2527 (*synth, pmr, ms, uv, ord*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 1841 (*occur*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1982, **65**, 2198 (*abs config*)
Molnar, P. *et al., Acta Chim. Hung.*, 1983, **112**, 477 (*cmr*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 231 (*bibl*)
Tsushima, M. *et al., J. Nat. Prod.*, 2000, **63**, 960-964 (*Antheraxanthin B*)

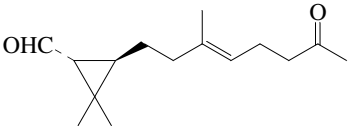
Antho-KA amide A-521

[137350-94-8]
$PhCH_2CH(OH)CO$-Phe-Lys-Ala-NH_2
$C_{27}H_{37}N_5O_5$ 511.62
Isol. from the sea anemone *Anthopleura elegantissima*. Neuropeptide. Sol. H_2O, MeOH.

Nothacker, H.P. *et al., Biochem. Biophys. Res. Commun.*, 1991, **179**, 1205-1211 (*isol, struct*)

Anthoplalone A-522

2,2-Dimethyl-3-(3-methyl-7-oxo-3-octenyl)cyclopropanecarboxaldehyde
[129145-58-0]



$C_{15}H_{24}O_2$ 236.353
CAS name incorrect, based on incorrect struct. in first 1990 paper. Metab. of *Anthopleura pacifica*. Cytotoxic. Pale yellow oil. $[\alpha]_D$ -4.4 (c, 0.09 in $CHCl_3$).

Deformyl: ***Noranthoplone***
[129145-59-1]
$C_{14}H_{24}O$ 208.343
Metab. of *Anthopleura pacifica*. Cytotoxic. $[\alpha]_D$ -10.5 (c, 0.56 in $CHCl_3$).

[100693-05-8, 100762-47-8 ((±)-form)]

McMurry, J.E. *et al., J.O.C.*, 1987, **52**, 4885-4893 (*synth*)
Zheng, G.-C. *et al., Tet. Lett.*, 1990, **31**, 2617-2618; 4522 (*Anthoplalone, Noranthoplone*)
Ihara, M. *et al., J.O.C.*, 1994, **59**, 8092-8100 (*synth*)
Hanessian, S. *et al., J.O.C.*, 1999, **64**, 4893-4900 (*synth*)

Anthopleurins A-523

Heart stimulant.

Anthopleurin A, 9CI
Neurotoxin AX1
[60880-63-9]
Isol. from the sea anemone *Anthopleura xanthogrammica*. A single chain peptide of 49 amino acid residues with 3 intramol. disulfide bridges.

Anthopleurin B
Isol. from the sea anemone *Anthopleura xanthogrammica*. A single chain peptide containing 49 amino acids.

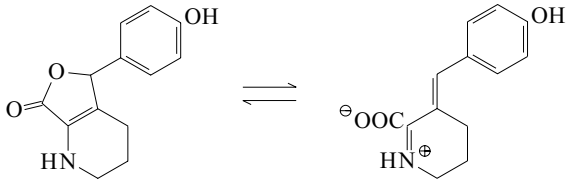
Anthopleurin C
Isol. from the sea anemone *Anthopleura elegantissima*. A single chain peptide containing 47 amino acids.

[62079-80-5, 72067-68-6, 78207-22-4]

Norton, T.R. *et al., J. Pharm. Sci.*, 1976, **65**, 1368 (*isol*)
Tanaka, M. *et al., Biochemistry*, 1977, **16**, 204-208 (*struct*)
Norton, R.S. *et al., J. Biol. Chem.*, 1979, **254**, 10220-10226 (*struct, cmr*)
Shibata, S. *et al., Jpn. J. Pharmacol.*, 1980, **30**, 7 (*rev*)
Smith, C.D. *et al., J. Biol. Chem.*, 1984, **259**, 8010-8011 (*cryst struct*)
Gooley, P.R. *et al., Eur. J. Biochem.*, 1985, **153**, 529-539 (*pmr*)
Reimer, N.S. *et al., J. Biol. Chem.*, 1985, **260**, 8690 (*Anthopleurin B*)

Anthosamine A A-524

3,4,5,6-Tetrahydro-3-[(4-hydroxyphenyl)methylene]-2-pyridinecarboxylic acid, 9CI
[165074-97-5]



$C_{13}H_{13}NO_3$ 231.251

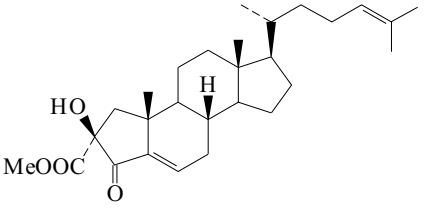
Shows reversible equilib. between lactone and zwitterion form; the latter predominates in protic solv. the former in aprotic solvs. Metab. from the marine sponge *Anthosigmella* aff. *raromicrosclera*. Induces larval metamorphosis in ascidians. Yellow solid. λ_{max} 229 (ϵ 7300); 249 (ϵ 6400); 283 (ϵ 4200); 368 (ϵ 14500) (MeOH) (Berdy). λ_{max} 287 (ϵ 7000) (DMSO) (Berdy).

N-*Me:* ***Anthosamine B****. 1,3,4,5-Tetrahydro-5-(4-hydroxyphenyl)-1-methylfuro[3,4-*b*]pyridin-7(2*H*)-one, 9CI*
[165074-96-4]
$C_{14}H_{15}NO_3$ 245.277
Metab. of *Anthosigmella* aff. *raromicrosclera*. Induces larval metamorphosis in ascidians. Yellow solid. $[\alpha]_D^{24}$ 0 (c, 0.15 in MeOH). λ_{max} 249 (ϵ 7100); 369 (ϵ 18400); 453 (ϵ 1900) (MeOH) (Berdy). λ_{max} 285 (ϵ 6000); 357 (ϵ 2400); 486 (ϵ 3600) (DMSO) (Berdy).

Tsukamoto, S. *et al., Tetrahedron*, 1995, **51**, 6687 (*isol, uv, ir, pmr, cmr, struct*)

Anthosterone A A-525

Methyl 2-hydroxy-3-oxo-4-norcholesta-5,24-diene-2-carboxylate
[116374-18-6]



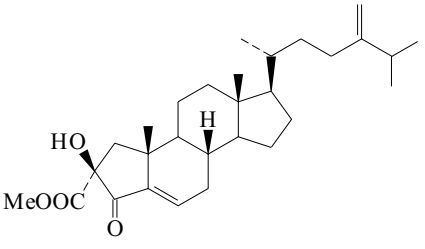
$C_{28}H_{42}O_4$ 442.637
Constit. of sponge *Anthoarcuata graceae*. Needles (MeCN). Mp 142-143°.

24,25-Dihydro: ***Phorbasterone B***
[682808-88-4]
$C_{28}H_{44}O_4$ 444.653
Constit. of *Phorbas amaranthus*. Solid. $[\alpha]_D$ -54.6 (c, 0.28 in $CHCl_3$). λ_{max} 250 (ϵ 9300) (MeCN).

Tischler, M. *et al., Can. J. Chem.*, 1988, **66**, 1173 (*isol, pmr, cmr, cryst struct*)
Masuno, M.N. *et al., J. Nat. Prod.*, 2004, **67**, 731-733 (*Phorbasterone B*)

Anthosterone B A-526

Methyl 2-hydroxy-3-oxo-4-norergosta-5,24(28)-diene-2-carboxylate
[116368-92-4]



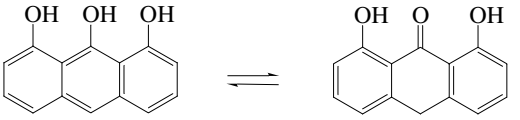
$C_{29}H_{44}O_4$ 456.664
Constit. of sponge *Anthoarcuata graceae*. Needles (MeCN). Mp 155-157°.

*22,23-Didehydro(*E-*), 24,28-dihydro:* ***Phorbasterone A***
[682808-87-3]
$C_{29}H_{44}O_4$ 456.664
Constit. of *Phorbas amaranthus*. Solid. $[\alpha]_D$ -45.4 (c, 0.19 in $CHCl_3$). λ_{max} 250 (ϵ 9600) (MeCN).

Tischler, M. *et al., Can. J. Chem.*, 1988, **66**, 1173-1178 (*Anthosterone B*)
Masuno, M.N. *et al., J. Nat. Prod.*, 2004, **67**, 731-733 (*Phorbasterone A*)

1,8,9-Anthracenetriol A-527

*1,8,9-Trihydroxyanthracene. 1,8,9-Anthratriol. 1,8-Dihydroxyanthrone. 1,8-Dihydroxy-9(10*H*)-anthracenone.* ***Dithranol, BAN, INN****. Anthralin, USAN. Chrysanthranol. Cignolin. Many other names*



$C_{14}H_{10}O_3$ 226.231
Tautomeric, anthrone form predominates. Isol. from the coral *Tubastrea micrantha*. Has been used in treatment of dermatitis, psoriasis and other skin complaints. Use limited by skin irritancy and staining. Shows antiproliferative effects on keratinocytes and antiinflammatory activity. Yellow plates or needles (petrol).
Mp 178-180°.
▶ Skin, eye and mucous membrane irritant. Exp. neoplastic agent. LD_{50} (rat, orl) 3216 mg/kg. CB8927000

Diol-*form* [1143-38-0]

Mono-Ac: [2891-34-1]
$C_{16}H_{12}O_4$ 268.268
Mp 159°.

Di-Ac: [38165-75-2]
$C_{18}H_{14}O_5$ 310.306
Mp 210-212°.

Mono-Me ether: 1-Hydroxy-8-methoxyanthrone
[138591-01-2]
$C_{15}H_{12}O_3$ 240.258
Yellow platelets or needles. Mp 154° Mp 183-185°.

Di-Me ether: 1,8-Dimethoxyanthrone
[104970-46-9]
[176505-06-9]
$C_{16}H_{14}O_3$ 254.285
Yellow needles (AcOH). Mp 196-197°.

Triol-*form* [480-22-8]
▶ CB1225000

Tri-Ac: Triacetoxyanthracene. Exolan. Psoralex
[16203-97-7]
$C_{20}H_{16}O_6$ 352.343
Used in treatment of psoriasis. Yellow needles. Mp 209-210°.
Log P 2.71 (calc).
▶ Severe eye irritant. CB1410000

[72045-47-7, 72045-51-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1114A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 313C (*nmr*)
Schrobsdorff, H. *et al., Ber.*, 1902, **35**, 2930 (*synth, tri-Ac*)
Hirosé, Y. *et al., Ber.*, 1912, **45**, 2474
Attree, G.F. *et al., J.C.S.*, 1931, 144-173 (*mono-Me ether, di-Me ether*)
Zahn, K. *et al., Ber.*, 1938, **71**, 172 (*synth*)
Barnes, R.A. *et al., Chem. Ind. (London)*, 1956, 873 (*uv*)
Sammul, O.R. *et al., J. Assoc. Off. Agric. Chem.*, 1964, **47**, 918 (*ir*)
Hofer, P. *et al., Pharm. Acta Helv.*, 1974, **49**, 35 (*mono-Ac, di-Ac, tri-Ac*)
IARC Monog., 1977, **13**, 75; *Suppl.* 7, 63 (*rev, tox*)
Ahmed, F.R. *et al., Acta Cryst. B*, 1980, **36**, 3184 (*cryst struct*)
Avdovich, H.M. *et al., Can. J. Spectrosc.*, 1980, **25**, 110 (*struct*)
Ippen, H. *et al., Br. J. Dermatol.*, 1981, **105**, 28; 72 (*revs*)
Schaefer, H. *et al., Psoriasis, Proc. Int. Symp., 3rd, 1981 (1982)*, 1981, 111 (*rev*)
Farber, E.M. *et al., Acta Derm. Venereol.*, Suppl., 1984, **112**, 11 (*rev*)
Mueller, K. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1984, **317**, 120 (*synth, C-14*)
Sanduja, R. *et al., J. Chem. Res., Synop.*, 1986, 450 (*isol*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 2996 (*synonyms*)
Cheah, I.C.L. *et al., J. Chromatogr.*, 1989, **467**, 414 (*hplc*)
Müller, K. *et al., Biochem. Pharmacol.*, 1993, **46**, 1695; 1995, **49**, 1607 (*pharmacol*)
Hayden, P.T. *et al., Chem. Res. Toxicol.*, 1993, **6**, 231 (*epr*)
Wiegrebe, W. *et al., Skin Pharmacol.*, 1995, **8**, 1 (*rev, pharmacol*)
Prinz, H. *et al., J.O.C.*, 1996, **61**, 2853; 2857 (*Me ether, synth*)

Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1085
Mrowietz, U. *et al., Br. J. De matol.*, 1997, **136**, 542 (*pharmacol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, APH250; APH500

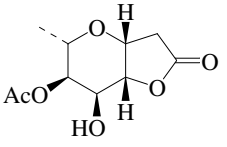
Laminaria angustata Antibiotic **A-528**

Polysaccharide antibiotic of unknown struct. Constit. of *Laminaria angustata* var. *longissima*. Antitumour agent. Powder.

Suzuki, Y. *et al., Chemotherapy (Tokyo)*, 1980, **28**, 165-170; *CA*, **93**, 143013

Antibiotic 386A **A-529**

3,7-Anhydro-2,8-dideoxy-D-glycero-*D*-gluco-*octonic acid γ-lactone 6-acetate, 9CI. 6-Acetoxy-3,3*a*,5,6,7,7*a*-hexahydro-7-hydroxy-5-methylfuro[3,2-*b*]pyran-2-one. 386A*
[264200-55-7]



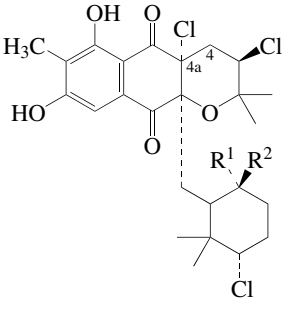
Relative Configuration

$C_{10}H_{14}O_6$ 230.217
Prod. by a marine *Penicillium* sp. No. 386.

Shao, Z. *et al., CA*, 2000, **132**, 290797y (*isol*)

Antibiotic A 80915A **A-530**

A 80915A
[127875-60-9]



$R^1, R^2 = =CH_2$

$C_{26}H_{31}Cl_3O_5$ 529.886
Naphthoquinone antibiotic. Prod. by *Streptomyces aculeolatus* A80915 and marine actinomycete strain CNQ-525. Antibacterial agent. Cytotoxic. Pale yellow powder. Sol. MeOH, EtOAc, DMSO; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -89.7 (c, 1 in MeOH). λ_{max} 266 (ϵ 22600); 331 (ϵ 8860); 356 (sh) (ϵ 8270) (EtOH/HCl) (Derep). λ_{max} 246 (ϵ 15500); 302 (ϵ 21100); 400 (ϵ 15200) (EtOH/NaOH) (Derep). λ_{max} 267 (ϵ 19500); 314 (ϵ 9430); 356 (ϵ 7890) (EtOH) (Derep).
▶ LD_{50} (mus, ipr) 212 mg/kg.

*4*a*-Dechloro, 4,4*a*-didehydro:*
$C_{26}H_{30}Cl_2O_5$ 493.425
Prod. by marine actinomycete strain CNQ-525. Cytotoxic. Pale yellow cryst.
Mp 179-181°. $[\alpha]_D^{25}$ -7.7 (c, 0.4 in MeOH).

Fukuda, D.S. *et al., J. Antibiot.*, 1990, **43**, 623-633 (*isol*)
Soria-Mercado, I.E. *et al., J. Nat. Prod.*, 2005, **68**, 904-910 (*isol, pmr, cmr*)

Antibiotic A 80915C **A-531**

A 80915C
[127875-62-1]
As Antibiotic A 80915A, A-530 with
$R^1 = CH_3$, $R^2 = OH$
$C_{26}H_{33}Cl_3O_6$ 547.901
Naphthoquinone antibiotic. Prod. by *Streptomyces aculeolatus* A80915 and marine actinomycete strain CNQ-525. Antibacterial agent. Cytotoxic. Yellow prisms. Sol. MeOH, EtOAc, DMSO; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -190 (c, 0.03 in $CHCl_3$). $[\alpha]_D^{25}$ -115.4 (c, 0.56 in MeOH). λ_{max} 266 (ϵ 22600); 331 (ϵ 8860); 356 (sh) (ϵ 8270) (EtOH/HCl) (Derep). λ_{max} 246 (ϵ 15500); 302 (ϵ 21100); 400 (ϵ 15200) (EtOH/NaOH) (Derep). λ_{max} 267 (ϵ 19500); 314 (ϵ 9430); 356 (ϵ 7890) (EtOH) (Derep).

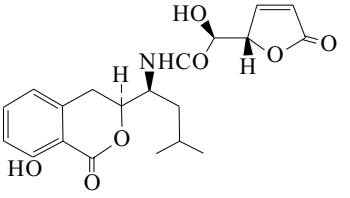
*4*a*-Dechloro:*
$C_{26}H_{34}Cl_2O_6$ 513.456
Prod. by a marine actinomycete strain CNQ-525. Cytotoxic. Pale yellow cryst.
Mp 197-198°. $[\alpha]_D^{25}$ -24.3 (c, 0.14 in MeOH).

*4*a*-Dechloro, 4,4*a*-didehydro:*
$C_{26}H_{32}Cl_2O_6$ 511.441
Prod. by a marine actinomycete strain CNQ-525. Pale yellow oil. $[\alpha]_D^{25}$ -6.3 (c, 0.13 in MeOH).

Fukuda, D.S. *et al., J. Antibiot.*, 1990, **43**, 623-633 (*isol*)
Soria-Mercado, I.E. *et al., Acta Cryst. E*, 2004, **60**, 1627-1629 (*cryst struct*)
Soria-Mercado, I.E. *et al., J. Nat. Prod.*, 2005, **68**, 904-910 (*isol, pmr, cmr*)

Antibiotic AI 77F **A-532**

AI 77F
[77675-02-6]

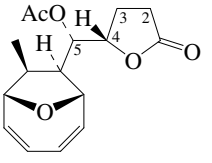


$C_{20}H_{23}NO_7$ 389.404
Prod. by *Bacillus pumilus*, incl. strains associated with marine sponges *Dendrilla* sp. Also prod. by the marine-derived *Alternaria tenuis* Sg17-1. Shows weak antibacterial and antiulcer props. Needles (EtOH aq.).
Mp 182-183°. Related to the Amicoumacins. λ_{max} 248 (sh); 347 (0.1*M* NaOH) (Derep). λ_{max} 208 (ϵ 27300); 248 (ϵ 6000); 314 (ϵ 4000) (H_2O) (Derep). λ_{max} 245; 312 (MeOH).

Netherlands Pat., 1980, 3 985; *CA*, **95**, 78461 (*isol*)
Shimojima, Y. *et al., Agric. Biol. Chem.*, 1982, **46**, 1823
Shimojima, Y. *et al., Tet. Lett.*, 1982, **23**, 5435
Shimojima, Y. *et al., J. Med. Chem.*, 1983, **26**, 1370
Shimojima, Y. *et al., Tetrahedron*, 1984, **40**, 2519 (*struct*)
Afiyatullov, S.S. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1991, **27**, 765-766 (*isol, sponge*)
Huang, Y.-F. *et al., J. Antibiot.*, 2006, **59**, 355-357 (*Alternaria, marine isol*)

Antibiotic 1893B **A-533**

1893B



Absolute Configuration

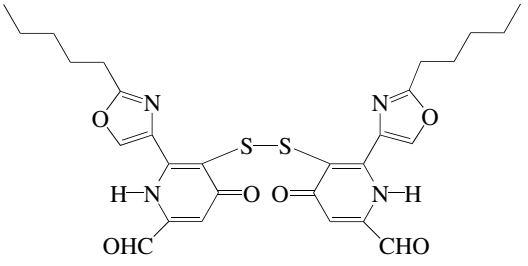
$C_{16}H_{20}O_5$
Stereochem. revised in 2006. Related to Mycoepoxydiene, M-666.
Metab. of a marine endophytic fungus no. 1893. Cryst.
Mp 140-142°. $[\alpha]_D^{20}$ +10.8 (c, 0.02 in Me_2CO). λ_{max} 274 (log ϵ 4.3) (MeOH).

*Deacetoxy, 2,3,4*E*,5-tetradehydro:* ***Antibiotic 1893A****. 1893A*
$C_{14}H_{14}O_3$ 230.263
Metab. of a marine endophytic fungus no. 1893. Cytotoxic and insecticide. Needles.
Mp 95-96°. $[\alpha]_D^{20}$ +4 (c, 0.07 in Me_2CO). λ_{max} 278 (log ϵ 4.7) (MeOH).

Chen, G. *et al., Tetrahedron*, 2003, **59**, 4907-4909 (*isol, pmr, cmr, cryst struct*)
Takao, K. *et al., J.O.C.*, 2004, **69**, 8789-8795 (*1893A, synth*)
Yasui, H. *et al., Heterocycles*, 2006, **67**, 123-128 (*synth, abs config*)
Yasui, H. *et al., J. Antibiot.*, 2006, **59**, 456-463 (*synth, pmr, cmr*)

Antibiotic B 90063 A-534

5,5′-Dithiobis[1,4-dihydro-4-oxo-6-(2-pentyl-4-oxazolyl)-2-pyridinecarboxaldehyde], 9CI. B 90063. 5,5′-Dithiobis[4-hydroxy-6-(2-pentyl-4-oxazolyl)-2-pyridinecarboxaldehyde]
[215377-24-5]
[181634-31-1]

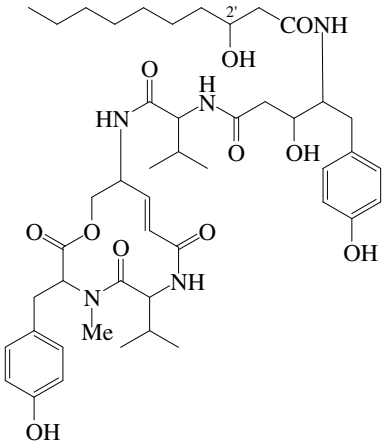


$C_{28}H_{30}N_4O_6S_2$ 582.7
Prod. by the marine bacterium *Blastobacter* sp. SANK 71894. Endothelin-converting enzyme inhibitor. Yellow cryst.
Mp 73-74° Mp 116-118° (+ 2MeOH). The alternative CAS no. refers to the bis(4-hydroxypyridine) tautomeric struct. under which it was originally descr. λ_{max} 214 (ϵ 47400); 261 (ϵ 37200); 340 (sh) (ϵ 8100); 360 (sh) (ϵ 4100) (MeCN).

Japan. Pat., 1996, 96 208 646; *CA*, **125**, 219743c
Takaishi, S. *et al., J. Antibiot.*, 1998, **51**, 805-815 (*isol, uv, ir, pmr, cmr, ms*)

Antibiotic B 1371A A-535

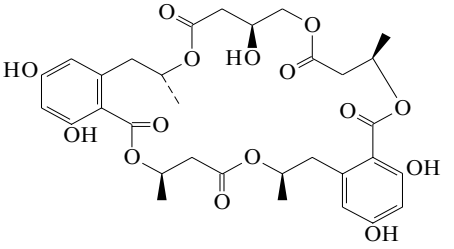
B 1371A



$C_{46}H_{67}N_5O_{11}$ 866.062
Peptide antibiotic. Prod. by the marine bacteria *Oceanospirillium* sp. SANK 70992.
$[\alpha]_D$ -26.4 (MeOH). λ_{max} 224 (ϵ 19100); 227 (ϵ 3450) (MeOH).
2′-Deoxy, 2′,3′-didehydro: ***Antibiotic B 1371F****. B 1371F*
[176952-11-7]
$C_{46}H_{65}N_5O_{10}$ 848.047
Prod. by *Oceanospirillium* sp. SANK 70992.
Pat. Coop. Treaty (WIPO), 1994, 94 19 481; *CA*, **121**, 279063h (*B 1371F*)
Japan. Pat., 1996, 96 81 431; *CA*, **125**, 8687z (*B 1371A*)

Antibiotic BK 223B A-536

BK 223B. NG 011. Antibiotic NG 011. Antibiotic 15G256α-1
[151271-58-8]

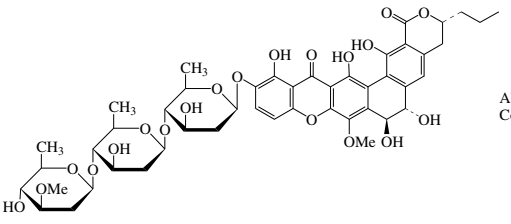


$C_{32}H_{38}O_{15}$ 662.643
Struct. of NG 011 revised in 2002. Prod. by *Penicillium verruculosum* and the marine fungus *Hypoxylon oceanicum*. Antifungal agent. Sol. MeOH; poorly sol. H_2O. $[\alpha]_D^{22}$ -5 (c, 0.8 in MeOH). λ_{max} 216 (ϵ 40800); 264 (ϵ 22460); 302 (ϵ 9760) (MeOH).

Ito, M. *et al., J. Antibiot.*, 1992, **45**, 1559-1565; 1566-1572 (*NG 011*)
Breinholt, J. *et al., J. Antibiot.*, 1993, **46**, 1101-1108 (*isol, pmr, cmr, struct*)
Schlingmann, G. *et al., Tetrahedron*, 2002, **58**, 6825-6835 (*isol, cd, pmr, cmr, ms*)

Antibiotic FD 594 A-537

FD 594



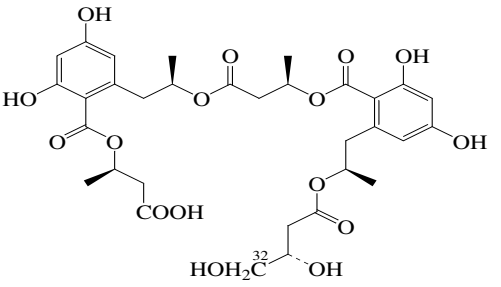
Absolute Configuration

$C_{47}H_{56}O_{20}$ 940.947
Similar to Antibiotic MSO 901809. Prod. by *Streptomyces* sp. TA-0256 and marine *Streptomyces* sp. B7936. Antitumour and antibacterial agent. Yellow powder. Sol. DMSO, Py; fairly sol. MeOH; poorly sol. Me_2CO, hexane.
Mp 199-202°. $[\alpha]_D^{26}$ -215 (c, 0.6 in $CHCl_3$). λ_{max} 214 (ϵ 24800); 233 (ϵ 23200); 276 (ϵ 27500); 363 (ϵ 12600); 420 (ϵ 3200) (MeOH). λ_{max} 206 (ϵ 40700); 215 (ϵ 40600); 235 (ϵ 36700); 276 (ϵ 49000); 365 (ϵ 23300); 420 (ϵ 6100) (MeOH/HCl). λ_{max} 232 (ϵ 26300); 277 (ϵ 21400); 379 (ϵ 11700); 440 (ϵ 5200) (MeOH/NaOH).

Qiao, Y-F. *et al., J. Antibiot.*, 1998, **51**, 282-287; 288-295 (*isol, uv, ir, pmr, cmr, ms, biosynth, activity*)
Eguchi, T. *et al., J.O.C.*, 1999, **64**, 5371-5376 (*uv, cd, conformn, abs config*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)

Antibiotic 15G256α-2 A-538

15G256α-2
[482374-47-0]



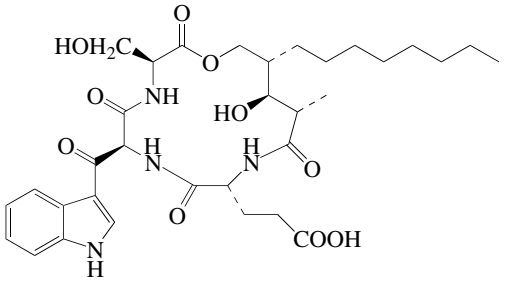
$C_{32}H_{40}O_{16}$ 680.658

Prod. by the marine fungus *Hypoxylon oceanicum* LL-15G256. λ_{max} 216 (ϵ 40800); 264 (ϵ 22460); 302 (ϵ 9760) (MeOH).

32-Deoxy: ***Antibiotic 15G256β-2****. 15G256β-2*
[482374-48-1]
$C_{32}H_{40}O_{15}$ 664.659
Prod. by the marine fungus *Hypoxylon oceanicum* LL-15G256. λ_{max} 216 (ϵ 40800); 264 (ϵ 22460); 302 (ϵ 9760) (MeOH).
Schlingmann, G. *et al., Tetrahedron*, 2002, **58**, 6825-6835 (*isol, pmr, cmr, ms*)

Antibiotic 15G256δ A-539

15G256δ
[185378-41-0]



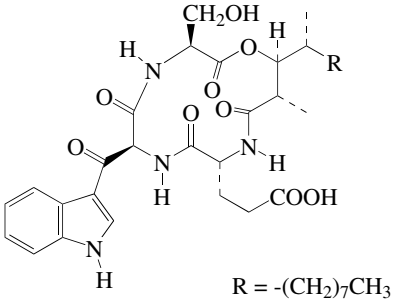
$C_{33}H_{46}N_4O_{10}$ 658.747
Lipodepsipeptide antibiotic. Prod. by the marine fungus *Hypoxylon oceanicum*. λ_{max} 208 (ϵ 33720); 246 (ϵ 13600); 262 (ϵ 9920); 310 (ϵ 13100) (MeOH).
Abbanat, D. *et al., J. Antibiot.*, 1998, **51**, 296-302 (*isol*)
Schlingmann, G. *et al., J. Antibiot.*, 1998, **51**, 303-316 (*isol, uv, ir, pmr, cmr, ms*)

Antibiotic 15G256ϵ A-540

15G256ϵ
[185378-42-1]
As Antibiotic 15G256γ, A-541 with
R = $-(CH_2)_5CH_3$
$C_{31}H_{42}N_4O_9$ 614.694
Prod. by the marine fungus *Hypoxylon oceanicum*. λ_{max} 208 (ϵ 41000); 246 (ϵ 16200); 264 (ϵ 11800); 311 (ϵ 15400) (MeOH).
Abbanat, D. *et al., J. Antibiot.*, 1998, **51**, 296-302 (*isol*)
Schlingmann, G. *et al., J. Antibiot.*, 1998, **51**, 303-316 (*isol, uv, ir, pmr, cmr, ms*)

Antibiotic 15G256γ A-541

Arthrichitin. 15G256γ
[180462-26-4]

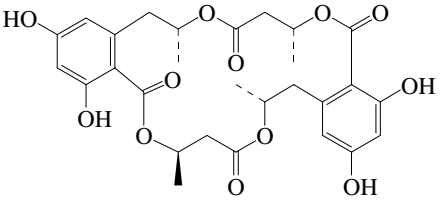


R = $-(CH_2)_7CH_3$

$C_{33}H_{46}N_4O_9$ 642.748
Depsipeptide. Stereochem. of Arthrichitin was not determined. Cell wall active metab. from *Arthrinium phaeospermum* and the marine fungus *Hypoxylon oceanicum*. Solid.
Mp 245°. $[\alpha]_D$ +24.1 (c, 0.5 in MeOH). λ_{max} 247; 266; 310 (MeOH).
Vijayakumar, E.K.S. *et al., J.O.C.*, 1996, **61**, 6591-6593 (*isol, uv, ir, pmr, cmr*)
Abbanat, D. *et al., J. Antibiot.*, 1998, **51**, 296-302 (*isol*)
Schlingman, G. *et al., J. Antibiot.*, 1998, **51**, 303-316 (*isol, uv, ir, pmr, cmr, ms*)
Albaugh, D. *et al., J. Antibiot.*, 1998, **51**, 317-322 (*activity*)

Antibiotic 15G256ι A-542

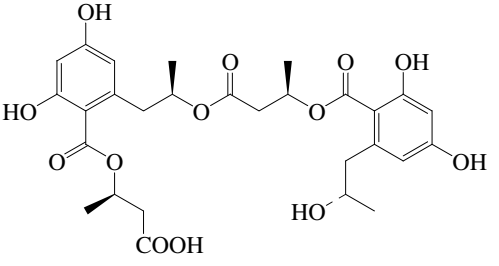
15G256ι
[482374-44-7]



$C_{28}H_{32}O_{12}$ 560.554
Prod. by the marine fungus *Hypoxylon oceanicum* LL-15G256. Antifungal agent. Cryst.
Mp 156°. λ_{max} 216 (ϵ 46420); 264 (ϵ 23420); 302 (ϵ 10240) (MeOH).
Schlingmann, G. *et al., Tetrahedron*, 2002, **58**, 6825-6835 (*isol, cd, pmr, cmr, ms*)

Antibiotic 15G256π A-543

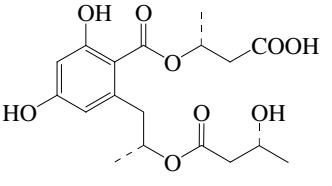
15G256π
[482374-50-5]



$C_{28}H_{34}O_{13}$ 578.569
Prod. by the marine fungus *Hypoxylon oceanicum* LL-15G256. λ_{max} 216 (ϵ 46420); 264 (ϵ 23420); 302 (ϵ 10240) (MeOH).
Schlingmann, G. *et al., Tetrahedron*, 2002, **58**, 6825-6835 (*isol, pmr, cmr, ms*)

Antibiotic 15G256 A-544

15G256
[482374-49-2]

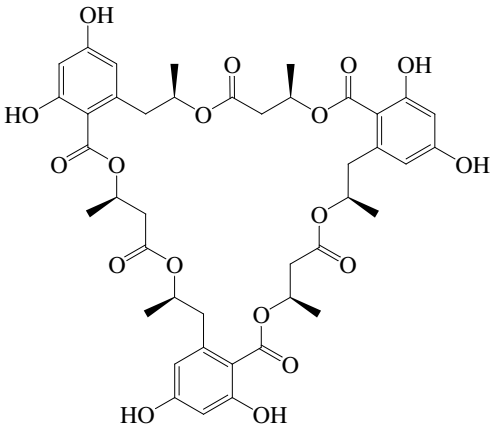


$C_{18}H_{24}O_9$ 384.382
Prod. by the marine fungus *Hypoxylon oceanicum* LL-15G256. λ_{max} 216 (ϵ 22390); 264 (ϵ 11300); 302 (ϵ 4940) (MeOH).
Schlingmann, G. *et al., Tetrahedron*, 2002, **58**, 6825-6835 (*isol, pmr, cmr, ms*)

Antibiotic 15G256ω A-545

15G256ω

[482374-45-8]



$C_{42}H_{48}O_{18}$ 840.83

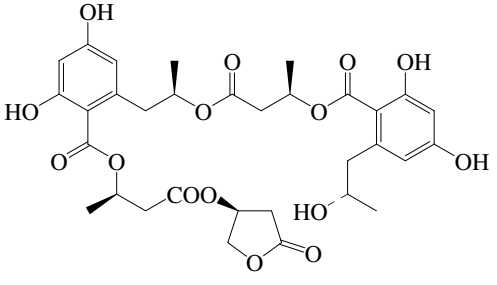
Prod. by the marine fungus *Hypoxylon oceanicum* LL-15G256. Antifungal agent. λ_{max} 216 (ϵ 62000); 264 (ϵ 34100); 302 (ϵ 14820) (MeOH).

Schlingmann, G. *et al., Tetrahedron*, 2002, **58**, 6825-6835 (*isol, cd, pmr, cmr, ms*)

Antibiotic 15G256o A-546

15G256o

[482374-46-9]



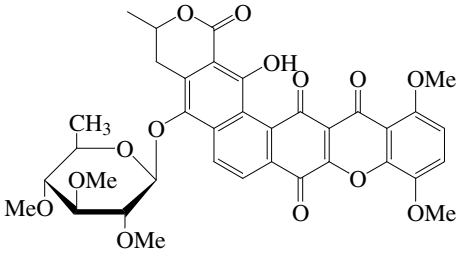
$C_{32}H_{38}O_{15}$ 662.643

Prod. by the marine fungus *Hypoxylon oceanicum* LL-15G256. λ_{max} 216 (ϵ 40800); 264 (ϵ 22460); 302 (ϵ 9760) (MeOH).

Schlingmann, G. *et al., Tetrahedron*, 2002, **58**, 6825-6835 (*isol, pmr, cmr, ms*)

Antibiotic IB 00208 A-547

IB 00208



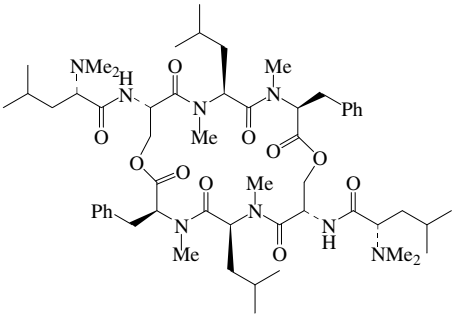
$C_{36}H_{34}O_{14}$ 690.656

Prod. by a marine-derived *Actinomadura* sp. Cytotoxic. Orange powder. $[\alpha]_D^{25}$ -65 (c, 0.15 in $CHCl_3$). λ_{max} 225; 255; 325; 385 (no solvent reported).

Malet-Cascón, L. *et al., J. Antibiot.*, 2003, **56**, 219-225; 318-321 (*isol, pmr, cmr*)

Antibiotic IB 01212 A-548

IB 01212



Absolute Configuration

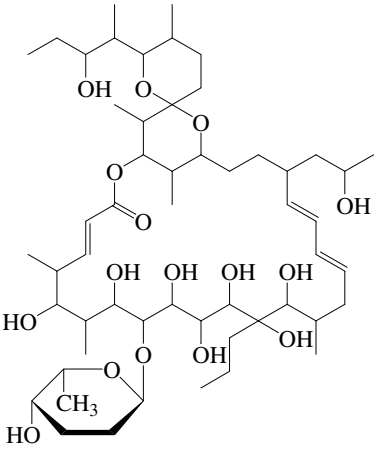
$C_{56}H_{88}N_8O_{10}$ 1033.359

Depsipeptide antibiotic. Prod. by the marine fungus *Clonostachys* sp. ESNA-A009. Cytotoxic. Powder. $[\alpha]_D$ -106 (c, 1 in $CHCl_3$).

Cruz, L.J. *et al., J.O.C.*, 2006, **71**, 3335-3338; 3339-3344 (*isol, synth, pmr, cmr, ms*)

Antibiotic IB 96212 A-549

IB 96212



$C_{54}H_{94}O_{16}$ 999.327

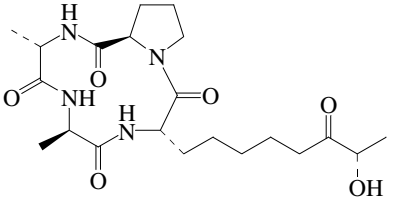
Prod. by the marine-derived *Micromonospora* sp. L-25-ES25-008. Cytotoxic. Cryst.

Mp 165-166°. $[\alpha]_D^{25}$ -42.3 (c, 0.22 in $CHCl_3$). λ_{max} 225 (no solvent reported).

Canedo, L.M. *et al., J. Antibiot.*, 2000, **53**, 474-478; 479-483

Antibiotic JM 47 A-550

Tetrapeptide JM 47. JM 47



Absolute Configuration

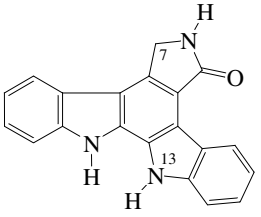
$C_{21}H_{34}N_4O_6$ 438.523

Cyclic peptide. Related to HC Toxin I. Prod. by a marine *Fusarium* sp. isol. from the alga *Codium fragile*. Powder. Mp 114-116°. $[\alpha]_D^{21}$ -71.4 (c, 1.43 in $CHCl_3$).

Jiang, Z. *et al., Phytochemistry*, 2002, **60**, 33-38 (*isol, pmr, cmr, ms*)

Antibiotic K 252c A-551

*6,7,12,13-Tetrahydro-5*H*-indolo[2,3-*a*]pyrrolo[3,4-*c*]carbazol-5-one, 9CI. Staurosporine aglycone. Staurosporinone. K 252c*
[85753-43-1]



$C_{20}H_{13}N_3O$ 311.342

Isol. from *Nocardiopsis* sp. K290e and from the marine ascidian *Eudistoma* sp., also from *Streptomyces longisoroflavus* R19, *Streptomyces mediocidicus* ATCC 13279 and the fruiting bodies of the myxomycete *Lycogala epidendrum*. Protein kinase C inhibitor, calmodulin inhibitor, serotonin release inhibitor and cell adhesion inhibitor. Pale yellow needles. Sol. DMSO; fairly sol. MeOH, $CHCl_3$; poorly sol. H_2O, acids, bases.

Mp >300°. λ_{max} 230 (ϵ 37000); 238 (sh) (ϵ 34000); 246 (sh) (ϵ 28000); 257 (sh) (ϵ 29000); 287 (ϵ 86000); 320 (sh) (ϵ 16000); 331 (ϵ 20000); 341 (ϵ 16000); 358 (ϵ 11000) (MeOH) (Derep).

N^{13}*-(α-L-Rhamnopyranosyl):* ***Antibiotic K 252d***. *K 252d*
[105114-22-5]
$C_{26}H_{23}N_3O_5$ 457.485

Isol. from *Nocardiopsis* sp. K290e. Protein kinase C inhibitor, calmodulin inhibitor and serotonin release inhibitor. Pale yellow needles. Sol. MeOH, $CHCl_3$, DMSO; poorly sol. H_2O, bases, acids.

Mp 240-245° dec. $[\alpha]_D^{20}$ +35 (c, 0.4 in MeOH). λ_{max} 223 (ϵ 40000); 233 (ϵ 39700); 248 (sh) (ϵ 31000); 260 (sh) (ϵ 34000); 268 (sh) (ϵ 38000); 280 (sh) (ϵ 61000); 290 (ϵ 98800); 320 (sh); 322 (ϵ 17000); 335 (ϵ 20300); 347 (ϵ 13200); 364 (ϵ 11500) (MeOH) (Derep).

N^{13}*-(2,6-Dideoxy-α-D-*ribo*-hexopyranosyl):* ***Antibiotic RK 286D***. *RK 286D*
[140429-37-4]
$C_{26}H_{23}N_3O_4$ 441.485

Prod. by *Streptomyces* sp. RK-286/P10634. Inhibitor of protein kinase C, also antiinflammatory, platelet agglutination inhibitor, bleb formation inhibitor and antioncotic promoter. Pale yellow powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 225-230°. $[\alpha]_D^{20}$ -60 (c, 0.13 in MeOH). λ_{max} 223 (ϵ 40000); 233 (ϵ 39700); 248 (sh) (ϵ 31000); 260 (sh) (ϵ 34000); 268 (sh) (ϵ 38000); 280 (sh) (ϵ 61000); 290 (ϵ 98800); 320 (sh); 322 (ϵ 17000); 335 (ϵ 20300); 347 (ϵ 13200); 364 (ϵ 11500) (MeOH) (Derep).

N^{13}*-(3-Amino-2,3,6-trideoxy-α-L-*ribo*-hexopyranosyl):* ***Holyrine A***
[249512-77-4]
$C_{26}H_{24}N_4O_3$ 440.501

Prod. by a marine actinomycete.

N^{13}*-(3-Amino-2,3,6-trideoxy-5-hydroxy-α-L-*erythro*-hexopyranosyl):* ***Holyrine B***
[249512-78-5]
$C_{26}H_{24}N_4O_4$ 456.5

Prod. by a marine actinomycete.

N^6*-(1-Methylethoxy)methyl:* [178276-03-4]
$C_{24}H_{21}N_3O_2$ 383.449

Prod. by *Streptomyces longisporoflavus*. Yellowish solid.
Mp 45-50°.

7-Oxo: See Arcyriaflavin A, A-647

2-Hydroxy: ***2-Hydroxystaurosporinone***
$C_{20}H_{13}N_3O_2$ 327.342
Isol. from *Lycogala epidendrum*. Protein tyrosine kinase inhibitor. Cytotoxic. Light brown solid. λ_{max} 226 (log ϵ 10.2); 294 (log ϵ 10.9); 342 (log ϵ 9.8) (MeOH).

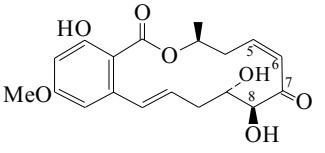
7-Methoxy: [137888-73-4]
$C_{21}H_{15}N_3O_2$ 341.368

Prod. by *Saccharothrix aerocolonigenes* ssp. *copiosa* ATCC 53856. Yellow powder. λ_{max} 206 (ϵ 24000); 234 (ϵ 23000); 296 (ϵ 45600); 332 (ϵ 8000); 344 (ϵ 6500); 361 (ϵ 4700) (MeOH) (Berdy).

Sarstedt, B. *et al., Heterocycles*, 1983, **20**, 469-476 (*synth*)
Nakanishi, S. *et al., J. Antibiot.*, 1986, **39**, 1066-1071 (*isol, props*)
Yasuzawa, T. *et al., J. Antibiot.*, 1986, **39**, 1072-1078 (*isol, uv, ir, pmr, cmr, ms, struct*)
Hughes, I. *et al., J.C.S. Perkin 1*, 1990, 2475-2480 (*synth, uv, pmr*)
Pat. Coop. Treaty (WIPO), 1991, 91 9 034; *CA*, **116**, 39768v (*7-methoxy*)
Osada, H. *et al., J. Antibiot.*, 1992, **45**, 278-279 (*Antibiotic RK286D*)
Moody, C.J. *et al., J.O.C.*, 1992, **57**, 2105-2114 (*synth*)
Horton, P.A. *et al., Experientia*, 1994, **50**, 843-845 (*isol*)
Xie, G. *et al., Tet. Lett.*, 1994, **35**, 5555-5558 (*synth*)
Cai, Y. *et al., J. Antibiot.*, 1996, **49**, 519-526 (*N^6-(1-methylethoxy)methyl, ir, pmr, cmr, cd*)
Mahboobi, S. *et al., J.O.C.*, 1999, **64**, 4697-4704 (*synth*)
Williams, D.E. *et al., Tet. Lett.*, 1999, **40**, 7171-7174 (*Holyrines*)
Hosoya, T. *et al., Bioorg. Med. Chem. Lett.*, 2005, **15**, 2776-2780 (*2-Hydroxystaurosporinone*)

Antibiotic LL-Z1640-2 A-552

LL-Z1640-2. C 292. Antibiotic C 292. Antibiotic L 783278. L 783278
[66018-38-0]



$C_{19}H_{22}O_7$ 362.379

Macrolide-type antibiotic. Isol. from *Deuteromyces* sp. Protein kinase inhibitor, mycotoxin. Cryst. (EtOAc/hexane).
Mp 172-176°. $[\alpha]_D$ -75.9 (c, 0.41 in MeOH). Related to Zearalenone. λ_{max} 234 (ϵ 30900); 271 (ϵ 12000); 314 (ϵ 6100) (MeOH) (Derep).

7-Alcohol: ***Antibiotic LL-Z1640-4***. *LL-Z1640-4. Zeaenol*
[66018-41-5]
$C_{19}H_{24}O_7$ 364.394

Isol. from *Deuteromyces* sp. and *Cochliobolus lunata*. Shows antiviral and antiprotozoal activity. Cryst. (EtOAc/hexane).
Mp 193-195°. $[\alpha]_D$ -102 (c, 0.49 in MeOH). Stereochem. unknown and may not correspond with that of LL-Z1640-2. λ_{max} 234 (ϵ 30900); 271 (ϵ 12000); 314 (ϵ 6100) (MeOH) (Derep).

5,6-Dihydro: ***Antibiotic LL-Z1640-1***. *LL-Z1640-1. Antibiotic L 783279. L 783279*
[66018-37-9]
$C_{19}H_{24}O_7$ 364.394

From *Deuteromyces* sp. Cryst. (C_6H_6/hexane).
Mp 151-153°. $[\alpha]_D$ -80 (c, 0.48 in MeOH). λ_{max} 234 (ϵ 30900); 271 (ϵ 12000); 314 (ϵ 6100) (MeOH) (Derep).

5,6-Dihydro, 7-alcohol: ***Antibiotic LL-Z1540-3***. *LL-Z1640-3*
[66018-40-4]
$C_{19}H_{26}O_7$ 366.41

From *Deuteromyces* sp. Cryst.
Mp 175°. $[\alpha]_D$ -112 (c, 0.28 in MeOH). λ_{max} 234 (ϵ 30900); 271 (ϵ 12000); 314 (ϵ 6100) (MeOH) (Derep).

*11*R*,12*R*-Epoxide:* ***Hypothemycin***
[76958-67-3]
$C_{19}H_{22}O_8$ 378.378

Macrolide antibiotic. Isol. from *Hypomyces trichothecoides*. Also from *Coriolus versicolor* and *Aigialus parvus*. Active against protozoa and plant pathogenic fungi. Cytotoxic. Inhibits MEK kinase. Prisms (MeOH).
Mp 173-174°. $[\alpha]_D^{25}$ -18 (c, 0.5 in $CHCl_3$). Struct. revised in 1993. λ_{max} 220 (ϵ 38000); 267 (ϵ 14000); 307 (ϵ 7000) (MeOH) (Derep).

*11*R*,12*R*-Epoxide, 7*R*-alcohol:* ***Aigialomycin B***
$C_{19}H_{24}O_8$ 380.394
Prod. by *Aigialus parvus* BCC 5311. Cryst.
Mp 82-84°. $[\alpha]_D^{24}$ -10 (c, 0.27 in $CHCl_3$). λ_{max} 220 (log ϵ 4.37); 266 (log ϵ 4.28); 306 (log ϵ 3.74) (MeOH).

*11*R,*12*R-*Epoxide, 5,6-dihydro:* ***Dihydrohypothemycin***
[80325-04-8]
$C_{19}H_{24}O_8$ 380.394
Isol. from *Hypomyces trichothecoides*. Active against protozoa and plant pathogenic fungi. Unstable cryst. Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 178-179°. $[\alpha]_D^{26}$ -16 (c, 0.17 in $CHCl_3$). λ_{max} 220 (ϵ 31000); 265 (ϵ 14900); 305 (ϵ 7000) (MeOH) (Berdy).

*9-Deoxy, 11*R,*12*R-*epoxide, 7*R-*alcohol:* ***Aigialomycin C***
$C_{19}H_{24}O_7$ 364.394
Prod. by *Aigialus parvus* BCC 5311. Amorph. solid. $[\alpha]_D^{27}$ -20 (c, 0.25 in $CHCl_3$). λ_{max} 219 (log ϵ 4.45); 265 (log ϵ 4.14); 306 (log ϵ 3.82) (MeOH).

*5*E-*Isomer, 11*R,*12*R-*epoxide:* ***Aigialomycin A***
$C_{19}H_{22}O_8$ 378.378
Prod. by *Aigialus parvus* BCC 5311. Cryst.
Mp 166-168°. $[\alpha]_D$ +17 (c, 0.5 in $CHCl_3$). λ_{max} 220 (log ϵ 4.5); 266 (log ϵ 4.04); 306 (log ϵ 3.74) (MeOH).

9-Epimer, 11,12-dihydro: ***Antibiotic L 783277****. L 783277*
[219917-92-7]
$C_{19}H_{24}O_7$ 364.394
Prod. by a *Phoma* sp. Selective inhibitor of MEK kinase. Cryst. (MeOH).

*9-Epimer, 5*E-*isomer, 11,12-dihydro:* ***Antibiotic L 783290****. L 783290*
[219917-93-8]
$C_{19}H_{24}O_7$ 364.394
Prod. by a *Phoma* sp. Selective inhibitor of MEK kinase.

[69427-14-1]

Ellestad, G.A. *et al., J.O.C.*, 1978, **43**, 2339-2343 (*isol, uv, ir, struct*)
Nukina, M. *et al., CA*, 1979, **90**, 99737 (*Zeaenol, isol, uv, ir, pmr, cmr*)
Nair, M.S.R. *et al., Tetrahedron*, 1981, **37**, 2445-2449 (*Hypothemycin, isol*)
Sugawara, F. *et al., Phytochemistry*, 1992, **31**, 1987-1990 (*isol, pmr, cmr, struct*)
Agatsuma, T. *et al., Chem. Pharm. Bull.*, 1993, **41**, 373-375 (*Hypothemycin, struct*)
Pat. Coop. Treaty (WIPO), 1996, 13 259; *CA*, **125**, 105084h (*C 292*)
Dombrowski, A.W. *et al., J. Antibiot.*, 1999, **52**, 1077-1085; 1086-1094 (*L-783277, L-783290*)
Zhao, A. *et al., J. Antibiot.*, 1999, **52**, 1086-1094 (*Hypothemycin, activity*)
Tatsuta, K. *et al., Chem. Lett.*, 2001, 172-173 (*synth*)
Isaka, M. *et al., J.O.C.*, 2002, **67**, 1561-1566 (*Aigialomycins*)
Selles, P. *et al., Tet. Lett.*, 2002, **43**, 4621-4625 (*synth*)

Antibiotic MA 39 A-553

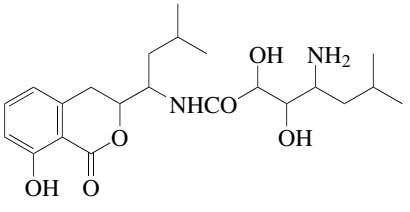
[158827-81-7]
Struct. unknown. Prod. by *Streptomyces* MA-39, isol. from seaweed. Shows antimicrobial activity.
Japan. Pat., 1994, 06 181 753; *CA*, **121**, 279066m (*isol*)

Antibiotic NAT 13 A-554

Prod. by *Streptomyces* sp. NAT-4 isol. from seaweed. Shows antimicrobial activity.
Japan. Pat., 1994, 94 181 753; *CA*, **121**, 279066m (*isol*)

Antibiotic PM 94128 A-555

PM 94128
[182292-49-5]

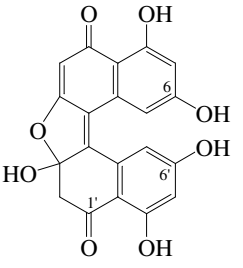


$C_{22}H_{34}N_2O_6$ 422.52
Prod. by a marine *Bacillus* sp. Antitumour agent.
Mp 172-173°. $[\alpha]_D^{25}$ -88.9 (c, 2 in $CHCl_3$). Related to Amicoumacin B, A-245. λ_{max} 208 (ϵ 27000); 246 (ϵ 6400); 314 (ϵ 4380) (no solvent reported).

Canedo, L.M. *et al., J. Antibiot.*, 1997, **50**, 175-176 (*isol, uv, ir, pmr, cmr*)
Patel, S.K. *et al., Org. Lett.*, 2003, **5**, 4081-4084 (*synth*)

Antibiotic RF 3192C A-556

*6,6*a-*Dihydro-2,4,6*a*,10,12-pentahydroxydinaphtho[2,1-*b*:1′,2′-*d*]furan-5,9-dione, 9CI. RF 3192C*
[151545-57-2]



$C_{20}H_{12}O_8$ 380.31
Prod. by *Chaetomella circinoseta*. Aldose reductase inhibitor. Orange-red cryst. (Me_2CO/CH_2Cl_2). Mp. >150° dec. Incorrect CAS name. λ_{max} 220 (sh); 273; 347; 440 (sh) (MeOH). λ_{max} 273 (E1%/1cm 500); 347 (E1%/1cm 487); 440 (E1%/1cm 130) (MeOH) (Berdy). λ_{max} 218 (E1%/1cm 700); 273 (E1%/1cm 460); 347 (E1%/1cm 440); 440 (E1%/1cm 130) (MeOH-HCl) (Berdy). λ_{max} 265 (E1%/1cm 500); 318 (E1%/1cm 460); 358 (E1%/1cm 340) (MeOH-NaOH) (Berdy).

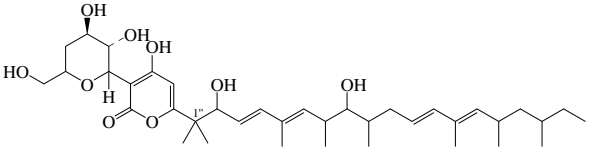
6,6′-Dideoxy: ***Sphaerolone***
$C_{20}H_{12}O_6$ 348.311
Prod. by an imperfect fungus (order Sphaeropsidales) sp. F-24707 and the marine-derived *Alternaria* sp. Stamm 6588. Amorph. red powder.
Mp 210° dec. λ_{max} 254 (log ϵ 3.93); 286 (log ϵ 3.92); 327 (log ϵ 4.07); 423 (log ϵ 3.84) (MeOH).

6,6′-Dideoxy, 1′-alcohol: ***Dihydrosphaerolone***
$C_{20}H_{14}O_6$ 350.327
Prod. by an imperfect fungus (order Sphaeropsidales) sp. F-24707. Amorph. orange solid.
Mp 139° dec. $[\alpha]_D^{20}$ +57 (c, 0.94 in MeOH). λ_{max} 201 (log ϵ 4.49); 264 (log ϵ 3.72); 329 (log ϵ 4.19); 419 (log ϵ 3.92) (MeOH).

Eur. Pat., 1993, 557 939; *CA*, **119**, 269194w (*RF 3192C*)
Bode, H.B. *et al., Phytochemistry*, 2000, **54**, 597-601 (*Sphaerolone*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*Sphaerolone, marine, isol*)

Antibiotic S 39163F1 A-557

S 39163F1
[118117-43-4]



$C_{38}H_{60}O_9$ 660.887
Lactone antibiotic. Related to Dactylfungin A and Fusapyrone. Prod. by *Microsphaeropsis* sp. Antimicrobial agent. Amorph. powder. Sol. MeOH, $CHCl_3$, DMSO, Py; poorly sol. H_2O, Et_2O, hexane.
Mp 105-115° (sinters). $[\alpha]_D^{20}$ -15 (c, 0.5 in MeOH). Dec. from 124°. λ_{max} 205 (ϵ 50); 235 (ϵ 79); 290 (ϵ 15) (MeOH) (Berdy).

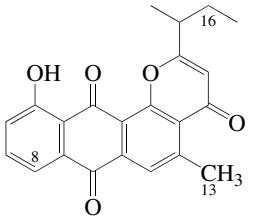
1″-Demethyl: ***Antibiotic YM 202204****. YM 202204*
$C_{37}H_{58}O_9$ 646.86
Prod. by the marine *Phoma* sp. Q60596. Antifungal agent. Yellow syrup. $[\alpha]_D^{25}$ -16 (c, 0.1 in MeOH). λ_{max} 208 (ϵ 17000); 236 (ϵ 32000); 289 (ϵ 5400) (MeOH).

[118117-44-5]

U.S. Pat., 1988, 4 753 959; *CA*, **110**, 22315 (*isol, ir, uv, pmr*)
Nagai, K. *et al., J. Antibiot.*, 2002, **55**, 1036-1041 (*YM 202204*)

Antibiotic SS 43405E A-558

*SS 43405E. 11-Hydroxy-5-methyl-2-(1-methylpropyl)-4*H*-anthra[1,2-*b*]pyran-4,7,12-trione, 9CI*
[106577-65-5]



$C_{22}H_{18}O_5$ 362.381
Quinone antibiotic. Prod. by *Streptomyces* sp. SS 43405. Antigenic agent. Sol. $CHCl_3$, DMSO, bases; poorly sol. H_2O, hexane. Mp 210-212°. $[\alpha]_D^{25}$ -14 (c, 0.5 in MeOH).

13-Hydroxy: ***Espicufolin A***
[182232-96-8]
$C_{22}H_{18}O_6$ 378.381
Prod. by *Streptomyces* sp. cu39 and the marine -derived *Streptomyces* sp. B5543. Neuronal cell protecting agent. Yellow powder. Sol. MeOH, Me_2CO, EtOAc; poorly sol. H_2O. Mp 184-186°. $[\alpha]_D^{21}$ -2.5 (c, 0.02 in $CHCl_3$). The isolate named Espicufolin A possesses *R*-config. λ_{max} 208 (ϵ 15400); 239 (ϵ 28100); 266 (ϵ 13500); 406 (ϵ 4700) (MeOH).

14-Hydroxy: ***γ-Indomycinone****. BE 26554B. Antibiotic BE 26554B*
[164907-62-4]
[160492-53-5]
$C_{22}H_{18}O_6$ 378.381
Isol. from a marine *Streptomyces* sp. and from *Streptomyces* sp. A26554. Cytotoxic agent. Yellow powder. λ_{max} 208; 236; 420 (EtOH).

16-Hydroxy: ***Antibiotic AH 1763IIa****. AH 1763IIa*
[199795-31-8]
$C_{22}H_{18}O_6$ 378.381
Prod. by *Streptomyces cyaneus*. Antiherpetic agent. Yellow needles (MeOH).
Mp 224-226°. $[\alpha]_D^{25}$ +6.6 (c, 0.1 in $CHCl_3$). λ_{max} 239 (ϵ 22600); 267 (ϵ 12000); 287 (sh) (ϵ 7000); 417 (ϵ 6400) (MeOH).

8,13-Dihydroxy: ***Espicufolin B***
$C_{22}H_{18}O_7$ 394.38
Prod. by the marine-derived *Streptomyces* sp. B5543.

Japan. Pat., 1986, 86 189 280; *CA*, **106**, 65844 (*isol*)
Japan. Pat., 1994, 06 228 121; *CA*, **122**, 114902p (*BE 26554B*)
Schumacher, R.W. *et al., J. Nat. Prod.*, 1995, **58**, 613-617 (*γ-Indomycinone*)
Kim, J.S. *et al., J. Antibiot.*, 1996, **49**, 947-948 (*Espicufolin A*)
Uyeda, M. *et al., J. Antibiot.*, 1997, **50**, 828-832 (*AH 1763IIa*)
Uno, H. *et al., J.C.S. Perkin 1*, 2001, 229-238 (*Espicufolin A, synth*)
Abdelfattah, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*Espicufolins A,B*)

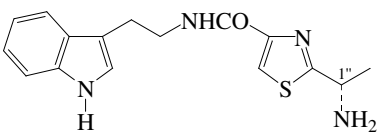
Antibiotic TA 13 A-559

[158827-83-9]
Struct. unknown. Prod. by *Streptomyces* TA 13 isol. from seaweed. Shows antimicrobial activity.

Japan. Pat., 1994, 06 181 753; *CA*, **121**, 279066m (*isol*)

Antibiotic TM 64 A-560

*2-(1-Aminoethyl)-*N*-[2-(1*H*-indol-3-yl)ethyl]-4-thiazolecarboxamide, 9CI. TM 64*



$C_{16}H_{18}N_4OS$ 314.41

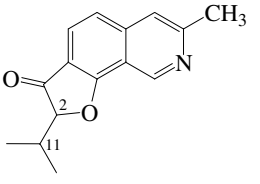
(S)-form [58887-22-2]
Prod. by *Thermoactinomyces* sp. TM-64. Sol. acids, MeOH, $CHCl_3$; fairly sol. C_6H_6; poorly sol. H_2O.
Mp 120° (145-147°). $[\alpha]_D^{20}$ -6 (c, 1 in MeOH). $[\alpha]_D$ -8.3 (c, 1 in EtOH). λ_{max} 223 (ϵ 51750); 275 (ϵ 10500); 282 (ϵ 10500); 291 (ϵ 8350) (MeOH).

*1″-*N*-Ac:* ***Microbiaeratin***
$C_{18}H_{20}N_4O_2S$ 356.448
Isol. from the marine-derived *Microbispora aerata*.

Omura, S. *et al., J. Antibiot.*, 1975, **28**, 609-610 (*isol*)
Konda, Y. *et al., Chem. Pharm. Bull.*, 1976, **24**, 92-96 (*uv, ir, pmr, ms, struct*)
Onda, M. *et al., Chem. Pharm. Bull.*, 1978, **26**, 2167-2169 (*synth*)
Laatsch, H. *et al., Dissertation*, Univ. of Göttingen, 2005, (*Microbiaeratin*)

Antibiotic TMC 120A A-561

*2,3-Dihydro-7-methyl-2-(1-methylethyl)furo[3,2-*h*]isoquinolin-3-one, 9CI. TMC 120A*
[250231-80-2]



$C_{15}H_{15}NO_2$ 241.289
Prod. by *Aspergillus ustus*. Pale yellow solid.
Mp 115-116°. $[\alpha]_D^{23}$ -18 (c, 0.5 in MeOH). λ_{max} 210 (log ϵ 4.5); 250 (log ϵ 4.53); 323 (sh) (log ϵ 3.85); 340 (log ϵ 4.05); 354 (log ϵ 4.11) (MeOH).

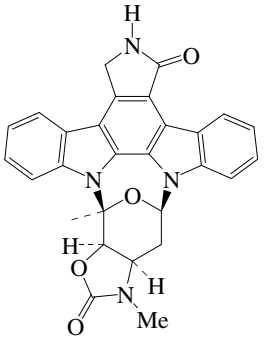
2,11-Didehydro: ***Antibiotic TMC 120B****. TMC 120B*
[250231-81-3]
$C_{15}H_{13}NO_2$ 239.273
Prod. by *Aspergillus ustus* and the marine *Aspergillus pseudodeflectus*. Moderate inhibitor of eosinophil survival. Pale yellow needles.
Mp 176-177°. λ_{max} 212 (log ϵ 4.54); 233 (log ϵ 4.11); 239 (log ϵ 4.11); 271 (log ϵ 4.37); 295 (sh) (log ϵ 4.33); 302 (log ϵ 4.33); 365 (log ϵ 3.89) (MeOH).

2-Hydroxy: ***Antibiotic TMC 120C****. TMC 120C*
[250231-82-4]
$C_{15}H_{15}NO_3$ 257.288
Prod. by *Aspergillus ustus*. Pale yellow needles.
Mp 176-177° dec. Possibly racemic. λ_{max} 211 (log ϵ 4.51); 253 (log ϵ 4.5); 354 (log ϵ 4.01); 413 (sh) (log ϵ 3.05) (MeOH).

Kohno, J. *et al., J. Antibiot.*, 1999, **52**, 913-916 (*isol, activity*)
Kohno, J. *et al., Tetrahedron*, 1999, **55**, 11247-11252 (*uv, ir, pmr, cmr, TMC 120B, TMC 120C, cryst struct*)
Ogawa, A. *et al., Bioorg. Med. Chem. Lett.*, 2004, **14**, 3539-3543 (*TMC 120B, isol, pmr, cmr*)
Kumemura, T. *et al., Chem. Pharm. Bull.*, 2005, **53**, 393-397 (*TMC 120B, synth*)

Antibiotic ZHD 0501 A-562

ZHD 0501



Absolute Configuration

$C_{28}H_{22}N_4O_4$ 478.506

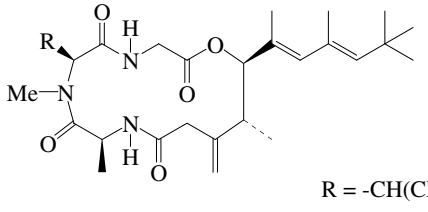
Related to Staurosporine, S-360. Prod. by a marine-derived *Actinomadura* sp. 007. Cytotoxic. Pale yellow cryst. ($CHCl_3$/MeOH).

Mp 283.4-285.5°. $[\alpha]_D^{20}$ +83.2 (c, 0.1 in MeOH). λ_{max} 232 (ϵ 19610); 243 (sh) (ϵ 19020); 275 (sh) (ϵ 19720); 290 (ϵ 33210); 318 (ϵ 9940); 332 (ϵ 9640); 351 (ϵ 6750); 369 (ϵ 6920) (MeOH).

Han, X.-X. *et al., Tet. Lett.*, 2005, **46**, 6137-6140 (*isol, uv, pmr, cmr*)

Antillatoxin A-563

[165967-02-2]



Absolute Configuration

R = -$CH(CH_3)_2$

$C_{28}H_{45}N_3O_5$ 503.681

Lipodepsipeptide antibiotic. Isol. from the blue-green alga *Lyngbya majuscula*. Ichthyotoxin and neurotoxin. Amorph. powder. $[\alpha]_D$ -140 (c, 0.1 in MeOH). λ_{max} 230 (ϵ 12000) (MeOH).

Orjala, J. *et al., J.A.C.S.*, 1995, **117**, 8281-8282 (*isol, pmr, cmr*)
Yokokawa, F. *et al., Tetrahedron*, 2000, **56**, 1759-1775 (*synth, config*)
Li, W.I. *et al., J. Nat. Prod.*, 2004, **67**, 559-568 (*pmr, cmr, activity*)

Antillatoxin B A-564

[357638-90-5]

As Antillatoxin, A-563 with

R = -CH_2CH_2Ph

$C_{33}H_{47}N_3O_5$ 565.751

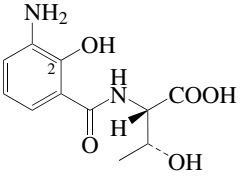
Cyclic lipopeptide antibiotic. Isol. from *Lyngbya majuscula*. Ichthyotoxin and neurotoxin. Oil. $[\alpha]_D^{23}$ -113.8 (c, 0.21 in MeOH). λ_{max} 209 (log ϵ 4.7); 240 (log ϵ 4.06) (MeOH).

Nogle, L.M. *et al., J. Nat. Prod.*, 2001, **64**, 983-985 (*isol, pmr, cmr, uv*)

Antimycic acid A-565

N-*(3-Amino-2-hydroxybenzoyl)threonine, 9CI.* N-*(3-Aminosalicoyl)threonine*

[642-82-0]



Absolute Configuration

$C_{11}H_{14}N_2O_5$ 254.242

Degradn. prod. of Antimycin A, A-566. Intermediate for manuf. of Antimycins. Needles (MeOH). Mp 224-225° (219-220°). $[\alpha]_D^{25}$ +14.9 (c, 1.8 in 3% HCl).

N-*Formyl, Me ester:* [380228-43-3]

$C_{13}H_{16}N_2O_6$ 296.279

Prod. by a marine-derived *Streptomyces* sp. M03033.

2-Me ether, Me ester: [132857-17-1]

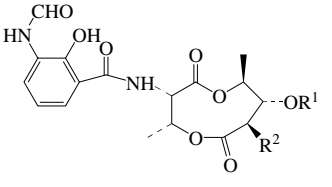
Needles (EtOAc). Mp 155-156°.

Tener, G.M. *et al., J.A.C.S.*, 1953, **75**, 1100; 3623 (*struct*)
Okumura, S. *et al., J.A.C.S.*, 1959, **81**, 5215 (*synth*)
Japan. Pat., 1959, 23 487; *CA*, **57**, 16742b (*synth*)
Seo, Y. *et al., J. Microbiol. Biotechnol.*, 2001, **11**, 663-667; *CA*, **136**, 34428 (*N-formyl Me ester*)

Antimycin A A-566

Antipiriculin. Levoristatin. Virosin†. Antibiotic 720A. ***Vulgarin***

[1397-94-0]



Antimycin A_{1a}	R^1 = -$COCH(CH_3)CH_2CH_3$, R^2 = $(CH_2)_5CH_3$
Antimycin A_{1b}	R^1 = -$COCH_2CH(CH_3)_2$, R^2 = $(CH_2)_5CH_3$
Antimycin A_{2a}	R^1 = -$COCH(CH_3)_2$, R^2 = $(CH_2)_5CH_3$
Antimycin A_{2b}	R^1 = -$COCH_2CH_2CH_3$, R^2 = $(CH_2)_5CH_3$
Antimycin A_{3a}	R^1 = -$COCH(CH_3)CH_2CH_3$(*S*-), R^2 = $(CH_2)_3CH_3$
Antimycin A_{3b}	R^1 = -$COCH_2CH(CH_3)_2$, R^2 = $(CH_2)_3CH_3$
Antimycin A_{4a}	R^1 = -$COCH(CH_3)_2$, R^2 = $(CH_2)_3CH_3$
Antimycin A_{4b}	R^1 = -$COCH_2CH_2CH_3$, R^2 = $(CH_2)_3CH_3$
Antimycin A_5	R^1 = -$COCH_2CH(CH_3)_2$, R^2 = CH_2CH_3
Antimycin A_6	R^1 = -$COCH_2CH_2CH_3$, R^2 = CH_2CH_3
Antimycin A_{7a}	R^1 = -$COCH(CH_3)_2$, R^2 = $(CH_2)_2CH(CH_3)_2$
Antimycin A_{7b}	R^1 = -$COCH_2CH_2CH_3$, R^2 = $(CH_2)_2CH(CH_3)_2$
Antimycin A_{8a}	R^1 = -$COCH(CH_3)CH_2CH_3$, R^2 = $(CH_2)_2CH(CH_3)_2$
Antimycin A_{8b}	R^1 = -$COCH_2CH(CH_3)_2$, R^2 = $(CH_2)_2CH(CH_3)_2$
Antibiotic I 2743C	R^1 = -$COCH_3$, R^2 = $(CH_2)_3CH_3$
Antimycin A_9	R^1 = -COPh, R^2 = $(CH_2)_3CH_3$

Macrolide antibiotic complex. Has been separated into various pure components and subcomplexes of which the most important is Blastmycin. Prod. by *Streptomyces* sp. NRRL 2288. Antifungal agent. Inhibitor of ATP-citrate lyase.

► Toxic to mammals and insects.

Antimycin A_3

Blastmycin

[522-70-3]

$C_{26}H_{36}N_2O_9$ 520.578

From *Streptomyces blastmyceticus*. Antifungal, antiviral and antitumour agent. Inhibitor of ATP-citrate lyase. Needles (C_6H_6/petrol). Mp 174.5-175°. $[\alpha]_D^{26}$ +79.4 (c, 1 in $CHCl_3$). Log P 4.54 (calc). A mixt. of factors 3a and 3b which are v. difficult to separate. λ_{max} 222

(ϵ 40000); 343 (ϵ 8220) (MeOH/NaOH) (Derep). λ_{max} 225 (ϵ 33110); 320 (ϵ 7240) (MeOH).

▶ LD_{50} (mus, scu) 1.6 mg/kg. NY1502900

De(3-methylbutanoyl): ***Deisovalerylblastmycin***
[60504-95-2]
$C_{21}H_{28}N_2O_8$ 436.461
Prod. by *Streptomyces* spp. incl. a marine-derived sp. Antifungal agent. Inhibitor of ATP-citrate lyase.
Mp 186-188°. $[\alpha]_D^{24}$ +36 (c, 1 in MeOH). λ_{max} 225 (ϵ 35300); 345 (ϵ 8500) (MeOH/NaOH) (Derep). λ_{max} 226 (ϵ 30400); 320 (ϵ 6000) (MeOH) (Derep).

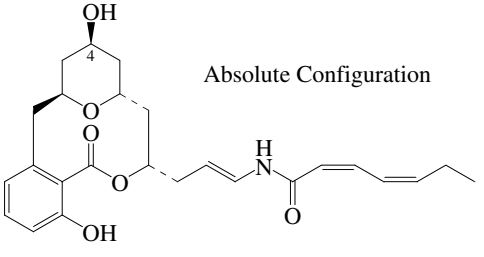
▶ LD_{50} (mus, ipr) 25 mg/kg; LD_{50} (mus, ivn) 15 mg/kg. VN7007000

[27220-56-0]

Ishiyama, T. *et al., J. Antibiot.*, 1976, **29**, 804-808 (*Deisovalerylblastmycin*)
Yao, C.B.F. *et al., Z. Naturforsch., B*, 2006, **61**, 320-325 (*Deisovalerylblastmycin, marine isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, AQM260; DAM000; DUO350; BLX750 (*A_1, A_4, Deisovalerylblastmycin*)

Apicularen A A-567

[220757-04-0]



Absolute Configuration

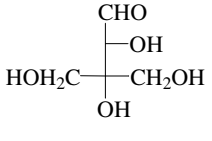
$C_{25}H_{31}NO_6$ 441.523
Prod. by *Chondromyces apiculatus*, *Chondromyces robustus* and other *Chondromyces* spp. Cytotoxic agent. Vacuolar-type ATPase inhibitor. Antineoplastic agent.
Mp 139-141° dec. $[\alpha]_D$ -36.1 (c, 1 in MeCN). λ_{max} 278 (log ϵ 4.43) (MeOH).

4-O-*(2-Acetamido-2-deoxy-β-D-glucopyranoside):* ***Apicularen B***
[220757-06-2]
$C_{33}H_{44}N_2O_{11}$ 644.717
Prod. by *Chondromyces* spp. Cytotoxic agent. $[\alpha]_D$ -5.5 (c, 0.3 in MeOH). λ_{max} 280 (log ϵ 4.49) (MeOH).

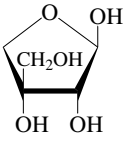
Kunze, B. *et al., J. Antibiot.*, 1998, **51**, 1075-1080 (*isol, ir, activity*)
Jansen, R. *et al., Eur. J. Org. Chem.*, 2000, 913-919 (*pmr, cmr, ms, abs config*)
Bhattacharjee, A. *et al., Tet. Lett.*, 2001, **42**, 1217-1220 (*synth*)
Yet, L. *et al., Chem. Rev.*, 2003, **103**, 4283-4306 (*rev*)
Lewis, A. *et al., Org. Biomol. Chem.*, 2003, **1**, 104-116 (*synth*)
Graetz, B.R. *et al., Org. Lett.*, 2003, **5**, 3357-3360 (*synth*)
Petri, A.F. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 5821-5823 (*synth*)
Nicolaou, K.C. *et al., Chem. Eur. J.*, 2004, **9**, 6177-6191 (*synth*)
Su, Q. *et al., J.A.C.S.*, 2004, **126**, 2425-2430 (*synth*)
Hilli, F. *et al., Org. Lett.*, 2004, **6**, 1289-1292 (*synth*)
Huss, M. *et al., BMC Biochem.*, 2005, **6**, 13 (*pharmacol*)
Hong, J. *et al., J. Pharmacol. Exp. Ther.*, 2005, **312**, 968-977 (*pharmacol*)

Apiose, 9CI, 8CI A-568

2,3,4-Trihydroxy-3-(hydroxymethyl)butanal. 3-C-*(Hydroxymethyl)*-glycero-*tetrose. Tetrahydroxyisovaleraldehyde*



D-*form*



β-D-erythro-Tetrofuranose-*form*

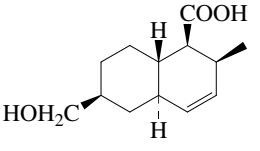
$C_5H_{10}O_5$ 150.131
Care needed with naming and numbering of derivs. C-3 is not a chiral centre in the acyclic sugar. In L-Apio-α-D-furanose for example, L- defines the config. at C-2 (L-apiose), while D- defines the config. at C-3 (D-furanosyl stereoisomeric form of L-apiose).

D-*form*
(R)-form
[639-97-4]
First found in parsley as the glycoside Apiin, also present in celery, *Dalbergia lanceolaria*, *Hevea brasiliensis*, *Taraxacum koksaghyz*, *Zostera marina*, *Lemna* spp., and *Platycodon grandiflorum*.
Isol. from the marine aquatic plant *Posidonia australis.*
Syrup. $[\alpha]_D$ +7.6 (c, 0.7 in H_2O).

[6477-44-7, 30912-14-2, 41546-43-4, 41546-44-5, 41546-46-7, 41546-47-8, 41546-49-0, 94943-41-6]

Watson, R.R. *et al., Adv. Carbohydr. Chem. Biochem.*, 1975, **31**, 135 (***rev***)
Vyas, D.M. *et al., Can. J. Chem.*, 1975, **53**, 2748 (*cmr*)
Ho, P.-T. *et al., Can. J. Chem.*, 1979, **57**, 381 (*D-form, L-form, synth, β-D-isopropylidene*)
Koos, M. *et al., Carbohydr. Res.*, 1986, **146**, 335 (***synth***)

Apiosporic acid A-569



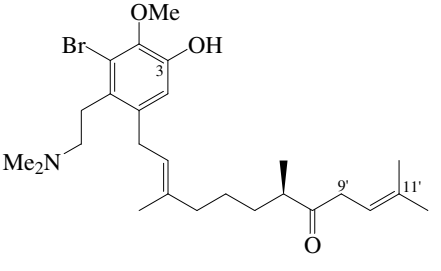
Relative Configuration

$C_{13}H_{20}O_3$ 224.299
Isol. from the marine fungus *Apiospora montagnei*. Oil. $[\alpha]_D^{28}$ -103.6 (c, 0.5 in MeOH). λ_{max} 202 (log ϵ 3.3); 242 (log ϵ 3.03); 248 (log ϵ 3.03) (MeOH).

Klemke, C. *et al., J. Nat. Prod.*, 2004, **67**, 1058-1063 (*isol, pmr, cmr*)

Aplaminone A-570

12-[3-Bromo-2-[2-(dimethylamino)ethyl]-5-hydroxy-4-methoxyphenyl]-2,6,10-trimethyl-2,10-dodecadien-5-one, 9CI
[131815-20-8]



$C_{26}H_{40}BrNO_3$ 494.511

(R)-form
Isol. from the marine mollusc *Aplysia kurodai*. Cytotoxic. Oil. $[\alpha]_D^{23}$ -2.9 (c, 1.18 in MeOH). λ_{max} 225 (ϵ 11000); 285 (ϵ 2900) (MeOH) (Berdy).

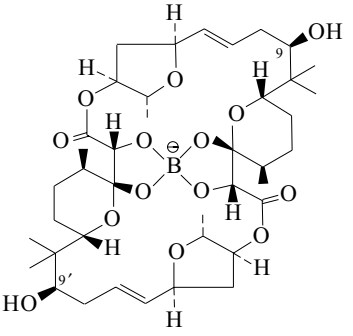
*$\Delta^{9'}$-Isomer(*E-*), 11'-hydroxy:* ***Neoaplaminone***
[131815-21-9]
$C_{26}H_{40}BrNO_4$ 510.51
Alkaloid from the marine mollusc *Aplysia kurodai*. Cytotoxic. Oil. $[\alpha]_D^{23}$ -5.3 (c, 0.65 in MeOH). λ_{max} 226 (ϵ 11000); 284 (ϵ 2500) (MeOH) (Derep).

*$\Delta^{9'}$-Isomer(*E-*), 11'-hydroxy, 3*-O-*sulfate:* ***Neoaplaminone sulfate***
[131815-22-0]
$C_{26}H_{40}BrNO_7S$ 590.574
Isol. from the marine mollusc *Aplysia kurodai*. Cytotoxic. $[\alpha]_D^{27}$ -3 (c, 1.29 in $CHCl_3$). λ_{max} 227 (ϵ 11000); 282 (ϵ 1700) (MeOH) (Derep).

Kigoshi, H. *et al., Tet. Lett.*, 1990, **31**, 4911-4914; 1992, **33**, 4195-4198 (*isol, uv, ir, pmr, cmr, ms, struct, abs config*)

Aplasmomycin **A-571**

Aplasmomycin A
[61230-25-9]



$C_{40}H_{60}BO_{14}^{\ominus}$ 775.717
Isol. from *Streptomyces griseus* and *Plasmodium berghei*. Active against gram-positive bacteria and shows insecticidal and acaricidal props. Ionophore. Needles (MeOH) (as Na salt). Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O.
Mp 283-285° dec. (as Na salt). $[\alpha]_D^{22}$ +225 (c, 1.24 in $CHCl_3$) (Na salt). Belongs to small group of boron-containing antibiotics. Closely related to Boromycin.
▶ LD_{50} (mus, ipr) 125 mg/kg. CD8835000

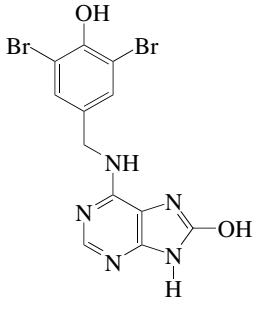
9-Ac: ***Aplasmomycin B***
[68193-20-4]
$C_{42}H_{62}BO_{15}^{\ominus}$ 817.754
Isol. from *Streptomyces griseus* from a Japanese marine sediment. Active against gram-positive bacteria. Ionophore. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D$ +188 (MeOH) (as Na salt).

9,9′-Di-Ac: ***Aplasmomycin C***
[68193-21-5]
$C_{44}H_{64}BO_{16}^{\ominus}$ 859.791
Prod. by *Streptomyces griseus* from a marine sediment. Weakly active against gram-positive bacteria. Ionophore. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D$ +134 (MeOH) (as Na salt).

Okami, Y. *et al., J. Antibiot.*, 1976, **29**, 1019 (*isol, ir, uv, ms, pmr, cmr, struct*)
Nakamura, H. *et al., J. Antibiot.*, 1977, **30**, 714 (*struct*)
Sato, K. *et al., J. Antibiot.*, 1978, **31**, 632 (*deriv*)
Chen, T.S.S. *et al., J. Antibiot.*, 1980, **33**, 1316 (*biosynth, pmr, cmr*)
Floss, H.G. *et al., Antibiotics (N.Y.)*, 1981, **4**, 193 (*biosynth, rev*)
Corey, E.J. *et al., J.A.C.S.*, 1982, **104**, 6816; 6818 (*synth*)
White, J.D. *et al., Tet. Lett.*, 1984, **25**, 3671 (*synth*)
Lee, J.J. *et al., Diss. Abstr. Int., B*, 1985, **45**, 3233 (*biosynth*)
White, J.D. *et al., J.A.C.S.*, 1986, **108**, 8105 (*synth*)
Matsuda, F. *et al., Tetrahedron*, 1990, **46**, 3469 (*synth*)
Stout, T.J. *et al., Tetrahedron*, 1991, **47**, 3511-3520 (*Aplasmomycin C, cryst struct, bibl*)
Norcross, R.D. *et al., Chem. Rev.*, 1995, **95**, 2041 (*rev, synth*)

Aplidiamine **A-572**

[188348-59-6]



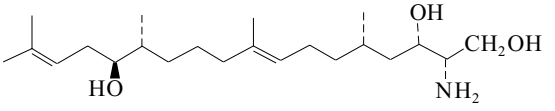
$C_{12}H_9Br_2N_5O_2$ 415.043

Tautomeric with oxo-form. Isol. from the marine ascidian *Aplidiopsis* sp. Sol. H_2O, MeOH.
Mp 241-243°. λ_{max} 221 (ϵ 17300); 273 (ϵ 15800) (MeOH/CH_2Cl_2 1:1). λ_{max} 223 (ϵ 19000); 290 (ϵ 15200) (MeOH/CH_2Cl_2/HCl). λ_{max} 223 (ϵ 52500); 250 (sh); 283 (ϵ 30700); 313 (sh); 377 (sh) (MeOH/CH_2Cl_2/NaOH).

Kang, H. *et al., Tet. Lett.*, 1997, **38**, 941-944 (*isol, uv, ir, pmr, cmr, struct*)
Itaya, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1297-1300 (*synth, struct*)

Aplidiasphingosine **A-573**

[68862-28-2]



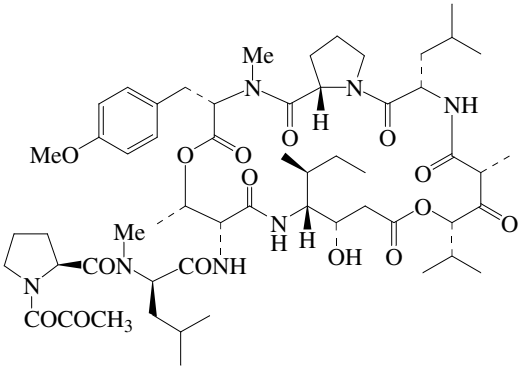
Absolute configuration

$C_{22}H_{43}NO_3$ 369.587
Constit. of *Aplidium* spp. Oil.

Carter, G.T. *et al., J.A.C.S.*, 1978, **100**, 7441-7442
Mori, K. *et al., Tet. Lett.*, 1981, **22**, 4429-4432; 4433-4436 (*stereochem*)
Mori, K. *et al., Tet. Lett.*, 1982, **23**, 3391-3394 (*synth*)
Umemora, T. *et al., Agric. Biol. Chem.*, 1987, **51**, 1973-1982 (*synth*)

Aplidine **A-574**

N-*[1-(1,2-Dioxopropyl)-L-prolyl]didemnin A, 9CI. Dehydrodidemnin B. [Pyruvyl*^{9}*]didemnin B.* ***Plitidepsin, INN. DDB***
[137219-37-5]

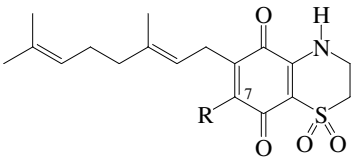


$C_{57}H_{87}N_7O_{15}$ 1110.352
Depsipeptide antibiotic. Isol. from the Mediterranean tunicate *Aplidium albicans*. Inhibits vascular endothelial growth factor (VEGF) secretion. Antineoplastic agent. Phase II clin. trial (2002). Granted orphan drug status by FDA (2004) for the treatment of acute lymphoblastic leukaemia and multiple myeloma. Solid.
Mp 152-160°. $[\alpha]_D$ -95.9 (c, 1.8 in $CHCl_3$).

Schmitz, F.J. *et al., J. Nat. Prod.*, 1991, **54**, 1469-1490 (*isol*)
Sakai, R. *et al., J. Med. Chem.*, 1996, **39**, 2819-2834 (*pharmacol*)
Jou, G. *et al., J.O.C.*, 1997, **62**, 354-366 (*synth, pmr, cmr*)
Cárdenas, F. *et al., J.O.C.*, 2001, **66**, 4580-4584; 2003, **68**, 9554-9562 (*pmr, conformn*)
Yao, L. *et al., IDrugs*, 2003, **6**, 246-250 (*rev*)
Cuadrado, A. *et al., J. Biol. Chem.*, 2003, **278**, 241-250 (*bibl, pharmacol*)

Aplidinone A A-575

[875057-52-6]



R = -OMe

$C_{19}H_{25}NO_5S$ 379.476
Alkaloid from the ascidian *Aplidium conicum*. Orange amorph. solid. λ_{max} 310 (ϵ 5700) (MeOH).

Aiello, A. *et al., Eur. J. Org. Chem.*, 2005, 5024-5030 (*isol, pmr, cmr*)

Aplidinone B A-576

[875081-15-5]
As Aplidinone A, A-575 with
R = -NH_2

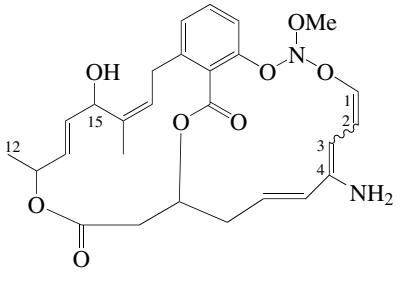
$C_{18}H_{24}N_2O_4S$ 364.465
Alkaloid from the ascidian *Aplidium conicum*. Violet amorph. solid. λ_{max} 3300 (ϵ 2600) (MeOH).

N^7*-(2-Sulfoethyl):* ***Aplidinone C***
[875082-39-6]
$C_{20}H_{28}N_2O_7S_2$ 472.582
Alkaloid from *Aplidium conicum*. Red-violet amorph. solid. λ_{max} 340 (ϵ 2900) (MeOH).

Aiello, A. *et al., Eur. J. Org. Chem.*, 2005, 5024-5030 (*isol, pmr, cmr*)

Aplidite A A-577

[165689-34-9]



$C_{27}H_{32}N_2O_8$ 512.558
Unique orthonitrite functionality. Alkaloid from the Australian marine tunicate *Aplidium* sp. Solid.
Mp 126-128°. $[\alpha]_D$ -15.8 (c, 0.58 in MeOH). λ_{max} 213 (ϵ 14300); 284 (ϵ 3785) (MeOH) (Berdy).

N,O-*Di-Ac:*
Synthetic. Yellow solid. Mp 84-86.5°.

12-Hydroxy: ***Aplidite C***
[165689-35-0]
$C_{27}H_{32}N_2O_9$ 528.558
From *Aplydium* sp. Solid.
Mp 103.5-105.5°. λ_{max} 208 (ϵ 11733); 280 (ϵ 6746) (MeOH) (Berdy).

12-Hydroxy, 15-Ac: ***Aplidite E***
[165689-36-1]
$C_{29}H_{34}N_2O_{10}$ 570.595
From *Aplidium* sp. Solid.
Mp 104-105°. $[\alpha]_D$ -50 (c, 0.71 in MeOH). λ_{max} 208 (ϵ 12892); 280 (ϵ 8686) (MeOH) (Berdy).

Geom. isomer: ***Aplidite B***
[165883-78-3]
$C_{27}H_{32}N_2O_8$ 512.558
From *Aplidium* sp. Solid.
Mp 124.5-126°. $[\alpha]_D$ -32.9 (c, 0.665 in MeOH). Possibly has opposite config. at the Δ^1 double bond. λ_{max} 213 (ϵ 14300); 284 (ϵ 3785) (MeOH) (Berdy).

Geom. isomer, 12-hydroxy: ***Aplidite D***
[165883-79-4]
$C_{27}H_{32}N_2O_9$ 528.558
From *Aplidium* sp. Solid.
Mp 107.5-109°. $[\alpha]_D$ -17.8 (c, 0.105 in MeOH). λ_{max} 206 (ϵ 15000); 282 (ϵ 8800) (MeOH) (Berdy).

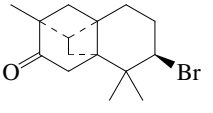
Geom. isomer, 12-hydroxy, 15-Ac: ***Aplidite F***
[165883-80-7]
$C_{29}H_{34}N_2O_{10}$ 570.595
From *Aplidium* sp. Solid.
Mp 105-109°. $[\alpha]_D$ -8.6 (c, 0.245 in MeOH). λ_{max} 208 (ϵ 5286); 285 (ϵ 2830) (MeOH) (Berdy).

Geom. isomer, 12-acetoxy: ***Aplidite G***
[165689-37-2]
$C_{29}H_{34}N_2O_{10}$ 570.595
From *Aplidium* sp. Solid.
Mp 106-108°. $[\alpha]_D$ -26.9 (c, 0.60 in MeOH). λ_{max} 201 (ϵ 27400); 286 (ϵ 11000) (MeOH) (Berdy).

Murray, L. *et al., Aust. J. Chem.*, 1995, **48**, 1253-1266 (*isol, uv, ir, pmr, cmr, ms, struct*)

Aplydactone A-578

[325689-20-1]

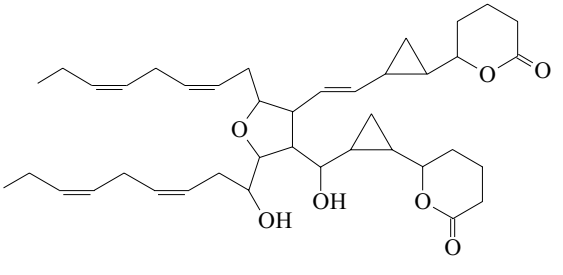


$C_{15}H_{21}BrO$
Constit. of *Aplysia dactylomela*.
Cryst. Mp 195-196°. $[\alpha]_D^{20}$ +33 (c, 0.2 in EtOH).

Fedorov, S.N. *et al., J.A.C.S.*, 2001, **123**, 504-505 (*isol, pmr, cmr, cryst struct*)

Aplydilactone A-579

[125295-94-5]

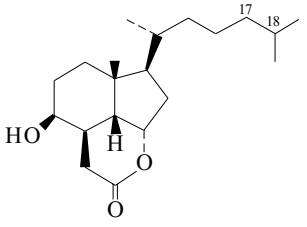


$C_{40}H_{58}O_7$ 650.894
Metab. of *Aplysia kurodai*. Shows phospholipase A2 activating activity. Oil. $[\alpha]_D^{27}$ -1.63 (c, 1.00 in $CHCl_3$). λ_{max} 204 (ϵ 20000) (MeCN) (Derep).

Ojika, M. *et al., Tet. Lett.*, 1990, **31**, 4907 (*isol, struct*)

Aplykurodin A A-580

[101691-10-5]



$C_{20}H_{34}O_3$ 322.487

Possibly a degraded steroid. Constit. of mollusc *Aplysia kurodai*. Needles. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 138°. $[\alpha]_D$ -44 (c, 0.96 in $CHCl_3$).

17,18-Didehydro: ***Aplykurodin B***
[101691-09-2]
$C_{20}H_{32}O_3$ 320.471
Constit. of *Aplysia kurodai*. Plates.
Mp 130-131°. $[\alpha]_D$ -36 (c, 0.90 in $CHCl_3$).

17,18-Didehydro, 4-Ac: ***4-Acetylaplykurodin B***
[142780-49-2]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Aplysia fasciata*. Ichthyotoxic, antifeedant. $[\alpha]_D^{20}$ -26.1 (c, 0.74 in $CHCl_3$).

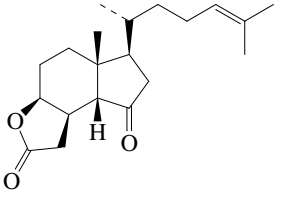
17,18-Didehydro, 4-ketone: ***Aplykurodinone B***
[142780-50-5]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Aplysia fasciata*. Solid (hexane).
Mp 60°. $[\alpha]_D^{20}$ -198 (c, 0.73 in $CHCl_3$).

17,18-Didehydro, 4-ketone, 3-epimer: ***3-Epiaplykurodinone B***
[189818-73-3]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Aplysia fasciata*. Amorph. powder. $[\alpha]_D^{25}$ -98 (c, 0.2 in $CHCl_3$).

Miyamoto, T. *et al., Tet. Lett.*, 1986, **27**, 1153 (*cryst struct*)
Spinella, A. *et al., J. Nat. Prod.*, 1992, **55**, 989-993 (*derivs*)
Ortega, M.J. *et al., J. Nat. Prod.*, 1997, **60**, 488-489 (*3-Epiaplykurodinone B*)

Aplykurodinone 1 A-581

[837424-47-2]



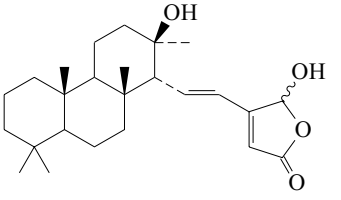
$C_{20}H_{30}O_3$ 318.455
Constit. of *Syphonota geographica*. Amorph. solid. $[\alpha]_D^{25}$ +51.2 (c, 0.3 in $CHCl_3$).

Parent hydroxyacid, Me ester: ***Aplykurodinone 2***
[837424-48-3]
$C_{21}H_{34}O_4$ 350.497
Constit. of *Syphonota geographica*. Amorph. solid. $[\alpha]_D^{25}$ +9.1 (c, 0.24 in $CHCl_3$).

Gavagnin, M. *et al., Tetrahedron*, 2005, **61**, 617-621 (*isol, pmr, cmr*)

Aplyolide A† A-582

[135288-73-2]

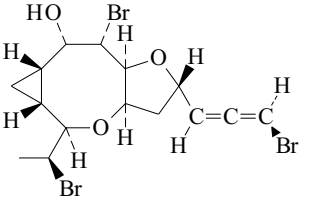


$C_{25}H_{38}O_4$ 402.573
Constit. of an *Aplysinopsis* sponge. Antiinflammatory agent. Oil. $[\alpha]_D$ -20 (c, 0.3 in MeOH). λ_{max} 269 (ϵ 51067) (MeOH) (Berdy).

Crews, P. *et al., Tetrahedron*, 1991, **47**, 3585-3600 (*isol, pmr, cmr*)

Aplyparvunin A-583

[167425-79-8]



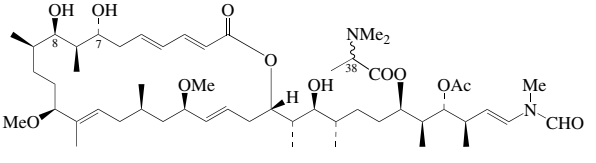
$C_{15}H_{19}Br_3O_3$ 487.025

Acetogenin. Isol. from the sea hare *Aplysia parvula*. Ichthyotoxic agent. Rods ($CHCl_3$).
Mp 138-139°. $[\alpha]_D^{22}$ -131.4 (c, 1.5 in $CHCl_3$).

Miyamoto, T. *et al., Tet. Lett.*, 1995, **36**, 6073-6074 (*isol, ir, pmr, cmr, ms*)

Aplyronine C A-584

[151923-86-3]



Absolute Configuration

$C_{53}H_{90}N_2O_{12}$ 947.3

Macrolide antibiotic. Obt. as a mixt. of C-38 epimers. Isol. from the sea hare *Aplysia kurodai*. Cytotoxic agent. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{27}$ +18 (c, 0.017 in MeOH). λ_{max} 259 (MeOH) (Berdy). λ_{max} 259 (ϵ 33000) (MeCN) (Berdy).

O^7*-(2-Dimethylamino-3-methoxypropanoyl):* ***Aplyronine A***
[151923-84-1]
$C_{59}H_{101}N_3O_{14}$ 1076.459
Isol. from *Aplysia kurodai*. Cytotoxic agent. Sol. MeOH, DMSO, THF, $CHCl_3$. $[\alpha]_D^{28}$ +32 (c, 0.26 in MeOH). λ_{max} 256 (ϵ 43500) (MeOH) (Berdy). λ_{max} 256 (ϵ 31000) (MeCN) (Berdy).

O^8*-(2-Dimethylamino-3-methoxypropanoyl):* ***Aplyronine B***
[151923-85-2]
$C_{59}H_{101}N_3O_{14}$ 1076.459
Isol. from *Aplysia kurodai*. Cytotoxic agent. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{27}$ +3.7 (c, 0.19 in MeOH). λ_{max} 258 (MeOH) (Berdy). λ_{max} 258 (ϵ 30200) (MeCN) (Berdy).

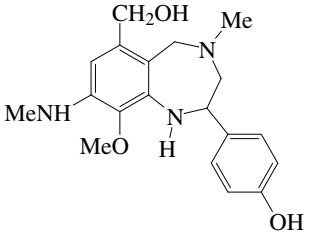
[125751-80-6]

Yamada, K. *et al., J.A.C.S.*, 1993, **115**, 11020-11021 (*isol, pmr, cmr*)

Ojika, M. *et al., J.A.C.S.*, 1994, **116**, 7441-7442 (*Aplyronine A, abs config*)
Kigoshi, H. *et al., J.O.C.*, 1996, **61**, 5326-5351 (*synth, abs config*)
Suenaga, K. *et al., Bioorg. Med. Chem. Lett.*, 1997, **7**, 269-274 (*Aplyronine A, activity*)

Aplysepine A-585

[151756-71-7]

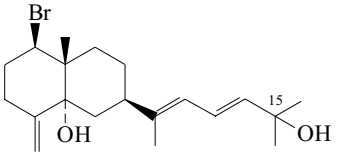


$C_{19}H_{25}N_3O_3$ 343.425
Alkaloid from the sea hare *Aplysia kurodai*.
$[\alpha]_D^{12}$ -3 (c, 0.47 in MeOH). λ_{max} 231 (ϵ 33600); 256 (sh) (ϵ 9400); 298 (sh) (ϵ 1600) (MeOH) (Derep).

Ojika, M. *et al., Tet. Lett.*, 1993, **34**, 5307-5308 (*isol, ir, pmr, cmr, struct*)

Aplysiadiol A-586

[132436-04-5]



$C_{20}H_{31}BrO_2$ 383.368
Constit. of *Aplysia kurodai* and *Laurencia japonensis*. Oil. $[\alpha]_D^{20}$ -50.8 (c, 0.44 in $CHCl_3$). λ_{max} 239 (ϵ 25600) (cyclohexane) (Berdy).

15-Me ether: [132328-04-2]
$C_{21}H_{33}BrO_2$ 397.394
Constit. of *Aplysia kurodai*. Plates (hexane).
Mp 102-103°. $[\alpha]_D^{11}$ -62.5 (c, 0.848 in $CHCl_3$).

15-Deoxy, 15,16-didehydro: ***Anhydroaplysiadiol***
[212331-29-8]
$C_{20}H_{29}BrO$ 365.353
Constit. of *Laurencia japonensis*. Oil. $[\alpha]_D^{27}$ -116.2 (c, 0.1 in $CHCl_3$).

Ojika, M. *et al., J. Nat. Prod.*, 1990, **53**, 1619 (*isol, pmr, cmr*)
Niwa, H. *et al., Tet. Lett.*, 1990, **31**, 7157 (*synth*)
Takahashi, Y. *et al., Phytochemistry*, 1998, **48**, 987-990 (*Anhydroaplysiadial*)

Aplysianin A-587

[101550-77-0]

Aplysianin A [105521-56-0]
Glycoprotein consisting of 4 subunits. Isol. from the albumen gland of the sea hare *Aplysia kurodai*. Shows antitumour and antimicrobial activities.

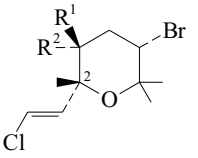
Aplysianin E [112130-75-3]
Glycoprotein consisting of 3 subunits. Isol. from eggs of *Aplysia kurodai*. Shows antitumour activity.

Aplysianin P [102510-57-6]
Single polypeptide. Isol. from purple fluid of *Aplysia kurodai*. Cytolytic. Sol. H_2O.

Kamiya, H. *et al., Experientia*, 1986, **42**, 1065-1067 (*Aplysianin A*)
Kisugi, J. *et al., Cancer Res.*, 1987, **47**, 5649-5653 (*Aplysianin E*)
Yamazaki, H. *et al., Cancer Res.*, 1989, **49**, 3834-3838 (*Aplysianin P*)
Kisugi, J. *et al., Chem. Pharm. Bull.*, 1989, **37**, 3050-3053 (*Aplysianin E, activity*)
Takamatsu, N. *et al., FEBS Lett.*, 1995, **377**, 373-376 (*Aplysianin A, struct*)

Aplysiapyranoid A A-588

[109927-30-2]



R^1 = Br, R^2 = H

$C_{10}H_{15}Br_2ClO$ 346.489
Constit. of *Aplysia kurodai*. Cytotoxic against various cell lines. Oil. Sol. MeOH, $CHCl_3$, C_6H_6; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D$ +4.4 (c, 1 in $CHCl_3$).

2-Epimer: ***Aplysiapyranoid B***
[108212-12-0]
$C_{10}H_{15}Br_2ClO$ 346.489
Constit. of *Aplysia kurodai*. Cytotoxic against various cell lines. Cryst. (EtOH). Sol. MeOH, C_6H_6, $CHCl_3$; fairly sol. hexane; poorly sol. H_2O.
Mp 46-49°. $[\alpha]_D$ -27 (c, 0.91 in $CHCl_3$).
Kusumi, T. *et al., J.O.C.*, 1987, **52**, 4597

Aplysiapyranoid C A-589

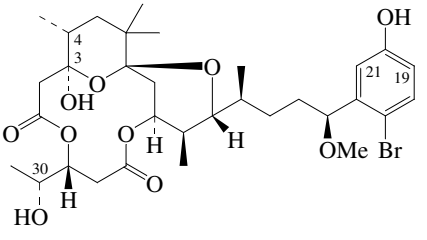
[109927-31-3]
As Aplysiapyranoid A, A-588 with
R^1 = H, R^2 = Cl
$C_{10}H_{15}BrCl_2O$ 302.037
Constit. of *Aplysia kurodai*. Cytotoxic to various cell lines. Oil. Sol. MeOH, $CHCl_3$, C_6H_6; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D$ +52 (c, 1 in $CHCl_3$).

2-Epimer: ***Aplysiapyranoid D***
[109927-32-4]
$C_{10}H_{15}BrCl_2O$ 302.037
From *Aplysia kurodai*. Cytotoxic to various cell lines. Oil. $[\alpha]_D$ +3.4 (c, 1.1 in $CHCl_3$).

Kusumi, T. *et al., J.O.C.*, 1987, **52**, 4597-4600 (*isol, Aplysia*)
Jung, M.E. *et al., J.O.C.*, 1991, **56**, 1347; 1998, **63**, 2982-2987 (*synth*)

Aplysiatoxin A-590

[52659-57-1]



$C_{32}H_{47}BrO_{10}$ 671.621
Related to Oscillatoxin A, O-133. Isol. from *Stylocheilus longicauda*, also from *Oscillatoria nigroviridis*, *Schizothrix calcicola*, *Lyngbya gracilis*, *Lyngbya majuscula* and *Gracillaria coronopifolia*. Oil. Sol. MeOH, C_6H_6, Et_2O; poorly sol. H_2O. λ_{max} 290 (ϵ 3000) (MeOH/NaOH) (Derep). λ_{max} 283 (ϵ 1950) (MeOH) (Derep).
▶ Carcinogenic, skin irritant. LD_{100} (mus, ipr) 0.3 mg/kg.
CD8870000

3-Deoxy, 3,4-didehydro: ***Anhydroaplysiatoxin***
[90359-03-8]
$C_{32}H_{45}BrO_9$ 653.606
Constit. of *Lyngbya majuscula*.

19-Bromo: ***19-Bromoaplysiatoxin***
$C_{32}H_{46}Br_2O_{10}$ 750.517

Minor component of *Schizothrix calcicola* and *Oscillatoria nitroviridis*. λ_{max} 283 (ϵ 1950) (MeOH) (Derep).

19-Bromo, 3-deoxy, 3,4-didehydro: ***Anhydro-19-bromoaplysiatoxin***
[90414-34-9]
$C_{32}H_{44}Br_2O_9$ 732.502
Constit. of *Lyngbya majuscula*.

19,21-Dibromo, 3-deoxy, 3,4-didehydro: ***Anhydro-19,21-dibromoaplysiatoxin***
[90414-35-0]
$C_{32}H_{43}Br_3O_9$ 811.398
Constit. of *Lyngbya majuscula*.

Debromo: ***Debromoaplysiatoxin***
[52423-28-6]
$C_{32}H_{48}O_{10}$ 592.725
Isol. from sea hare *Stylocheilus longicauda*, also from *Lyngbya gracilis*, *Schizothrix calcicola*, *Oscillatoria nigroviridis* and *Gracilaria coronopifolia*. Sol. MeOH, C_6H_6; poorly sol. H_2O. λ_{max} 290 (ϵ 3000) (MeOH/NaOH) (Derep). λ_{max} 283 (ϵ 1950) (MeOH) (Derep).
▶ Tumour promotor, toxin, LD_{50} (mus, ipr) 0.5 mg/kg. CD8880000

Debromo, 30-Ac: ***Manauealide C***
$C_{34}H_{50}O_{11}$ 634.762
Isol. from the red alga *Gracilaria coronopifolia*.
$[\alpha]_D$ +33.1 (c, 1 in MeOH). Config. not confirmed. λ_{max} 231 (ϵ 554); 276 (ϵ 582) (MeOH).

Debromo, 19-bromo: ***Manauealide B***
$C_{32}H_{47}BrO_{10}$ 671.621
Isol. from the red alga *Gracilaria coronopifolia*.
$[\alpha]_D$ +21.3 (c, 0.3 in MeOH). λ_{max} 232 (ϵ 740); 278 (ϵ 740); 704; 740 (MeOH).

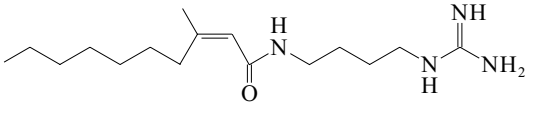
Debromo, 3-deoxy, 3,4-didehydro: ***Anhydrodebromoaplysiatoxin***
[63543-22-6]
$C_{32}H_{46}O_9$ 574.71
Isol. from *Gracilaria coronopifolia*, *Schizothrix calcicola*, *Oscillatoria nigroviridis* and *Lyngbya majuscula*. Phycotoxin. Diarrhetic agent. Cryst. (Et_2O/pentane).
Mp 116-117.5°. $[\alpha]_D$ +25.6 (c, 0.02 in MeOH). Originally obt. as an artifact. λ_{max} 208 (ϵ 6800); 274 (ϵ 1790) (MeOH).

Debromo, 19-chloro: ***Manauealide A***
$C_{32}H_{47}ClO_{10}$ 627.17
Isol. from the red alga *Gracilaria coronopifolia*.
$[\alpha]_D$ +13.8 (c, 0.5 in MeOH). Config. not confirmed. λ_{max} 233 (ϵ 776); 279 (ϵ 738) (MeOH).

Watson, M. *et al., Toxicon*, 1973, **11**, 259 (*isol*)
Kato, Y. *et al., J.A.C.S.*, 1974, **96**, 2245-2246 (*isol, struct*)
Scheuer, P. *et al., J. Nat. Prod.*, 1975, **38**, 1 (*rev*)
Kato, Y. *et al., Pure Appl. Chem.*, 1975, **41**, 1-14 (*isol, struct*)
Scheuer, P.J. *et al., Acc. Chem. Res.*, 1977, **10**, 39 (*rev*)
Mynderse, J.S. *et al., J.O.C.*, 1978, **43**, 2021 (*19-Bromoaplysiatoxin*)
Moore, R.E. *et al., J.O.C.*, 1984, **49**, 2484-2489 (*isol, abs config*)
Park, P. *et al., J.A.C.S.*, 1987, **109**, 6205 (*Debromoaplysiatoxin, synth*)
Okamura, H. *et al., Tetrahedron*, 1993, **49**, 10531 (*synth*)
Nagai, H. *et al., Toxicon*, 1996, **34**, 753-761 (*isol*)
Nagai, H. *et al., J. Nat. Prod.*, 1997, **60**, 925-928 (*Manauealides*)
Nagai, H. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 1011-1013 (*Manauealide C, Anhydrodebromoaplysiatoxin*)
Ito, E. *et al., Toxicon*, 2000, **38**, 123-132 (*isol*)

Aplysillamide A A-591

N-[4-[(Aminoiminomethyl)amino]butyl]-3-methyl-2-decenamide, 9CI. 3-Methyl-2-decenoic acid (4-guanidinobutyl)amide
[164301-82-0]



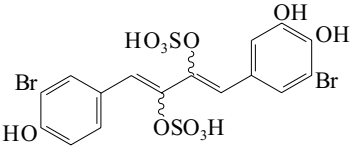
$C_{16}H_{32}N_4O$ 296.455
Alkaloid from the Okinawan marine sponge *Psammaplysilla purea*. Exhibits modest antimicrobial activity against some fungi and bacteria. Cytotoxic against murine lymphoma L1210 and human epidermoid carcinoma KB cells. Oil. Sol. MeOH. λ_{max} 225 (ϵ 10000) (MeOH) (Berdy).

*2,3*S*-Dihydro:* ***Aplysillamide B***
[164301-83-1]
$C_{16}H_{34}N_4O$ 298.471
Alkaloid from *Psammaplysilla purea*. Exhibits modest antimicrobial activity against some fungi and bacteria. Not cytotoxic. Oil. Sol. MeOH. $[\alpha]_D^{21}$ -2.4 (c, 0.1 in MeOH) (natural). $[\alpha]_D^{22}$ -5.1 (c, 1.6 in MeOH) (synthetic).

Honma, K. *et al., Tetrahedron*, 1995, **51**, 3745 (*isol, uv, ir, pmr, cmr, ms, synth, struct*)

Aplysillin A A-592

3-Bromo-5-[4-(3-bromo-4-hydroxyphenyl)-2,3-bis(sulfoxy)-1,3-butadienyl]-1,2-benzenediol, 9CI
[166833-91-6]

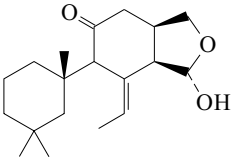


$C_{16}H_{12}Br_2O_{11}S_2$ 604.204
Isol. from the sponge *Aplysina fistularis fulva*. Thrombin receptor antagonist. Isol. as di-Na salt to which CAS no. refers.

Gulavita, N.K. *et al., J. Nat. Prod.*, 1995, **58**, 954-957 (*isol, pmr, cmr*)

Aplysillolide A A-593

[130221-22-6]

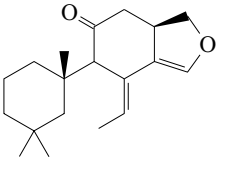


$C_{19}H_{30}O_3$ 306.444
Constit. of *Aplysilla glacialis*. Glass. $[\alpha]_D$ +30 (c, 2.4 in $CHCl_3$).

Tischler, M. *et al., J.O.C.*, 1991, **56**, 42 (*isol, pmr, cmr*)

Aplysillolide B A-594

[130221-23-7]

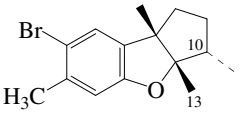


$C_{19}H_{28}O_2$ 288.429
Constit. of *Aplysilla glacialis*. Oil.

Tischler, M. *et al., J.O.C.*, 1991, **56**, 42 (*isol, pmr*)

Aplysin A-595

[6790-63-2]



$C_{15}H_{19}BrO$ 295.218
Constit. of *Aplysia kurodai* and *Aplysia californica*. Cryst. (MeOH).

Mp 85-86°. $[\alpha]_D^{27}$ -85.4 ($CHCl_3$). λ_{max} 234 (ϵ 8910); 294 (ϵ 4570) (EtOH) (Derep).

13-Oxo: ***Aplysinal***
[64052-99-9]
$C_{15}H_{17}BrO_2$ 309.202
Constit. of *Marginisporum aberrans.*

10-Hydroxy: ***10-Hydroxyaplysin***
[885328-74-5]
$C_{15}H_{19}BrO_2$ 311.218
Constit. of *Laurencia tristicha*. Cryst. (MeOH).
Mp 48-50°. $[\alpha]_D^{20}$ -50.1 (c, 0.81 in MeOH).

13-Hydroxy: ***Aplysinol***
[6790-64-3]
[73088-67-2]
$C_{15}H_{19}BrO_2$ 311.218
Constit. of *Aplysia kurodai*. Cryst. (CCl_4).
Mp 158-160°. $[\alpha]_D^{19}$ -55.6 ($CHCl_3$). λ_{max} 234 (ϵ 8910); 294 (ϵ 4570) (EtOH) (Derep).

13-Hydroperoxy: ***Laureperoxide****. Aplysinol peroxide*
[862288-23-1]
$C_{15}H_{19}BrO_3$ 327.217
Constit. of *Laurencia okamurai*. Oil. $[\alpha]_D^{20}$ -48 (c, 0.25 in $CHCl_3$). λ_{max} 207 (log ϵ 4.51); 232 (log ϵ 3.55); 299 (log ϵ 3.51) (MeOH).

13-Bromo: ***10-Bromoisoaplysin***
[862288-24-2]
$C_{15}H_{18}Br_2O$ 374.115
Constit. of *Laurencia okamurai*. Oil. $[\alpha]_D^{20}$ -20.9 (c, 0.42 in $CHCl_3$). λ_{max} 209 (log ϵ 4.35); 232 (log ϵ 3.53); 299 (log ϵ 3.48) (MeOH).

Debromo: ***Debromoaplysin***
[23444-68-0]
$C_{15}H_{20}O$ 216.322
Constit. of *Aplysia kurodai*. Oil. λ_{max} 236 (ϵ 8130); 290 (ϵ 3890) (EtOH) (Derep).

Debromo, 13-hydroxy: ***Debromoaplysinol***
[72782-84-4]
[126252-17-3]
$C_{15}H_{20}O_2$ 232.322
Constit. of *Laurencia okamurai*. Cryst. (hexane).
Mp 85-87°. $[\alpha]_D^{21}$ -32 (c, 0.44 in $CHCl_3$).

Debromo, 13-bromo: ***Isoaplysin***
[68773-08-0]
[126252-18-4]
$C_{15}H_{19}BrO$ 295.218
Constit. of *Laurencia nipponica* and *Aplysia* sp. Oil. $[\alpha]_D$ -33 (c, 0.69 in $CHCl_3$). λ_{max} 240 (ϵ 30000) (EtOH) (Derep). λ_{max} 234 (ϵ 8910); 294 (ϵ 4570) (EtOH) (Derep).

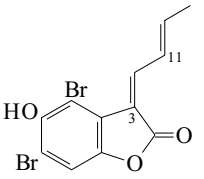
10-Epimer, 10-hydroxy: ***10-Hydroxyepiaplysin***
[885328-73-4]
$C_{15}H_{19}BrO_2$ 311.218
Constit. of *Laurencia tristicha*. Oil. $[\alpha]_D^{20}$ -8.1 (c, 0.06 in MeOH).

10-Epimer, debromo, 10-hydroxy: ***10-Hydroxydebromoaplysin***
[154800-88-1]
$C_{15}H_{20}O_2$ 232.322
Constit. of *Laurencia tristicha*. Oil. $[\alpha]_D^{20}$ -19.7 (c, 0.1 in MeOH).

Yamamura, S. *et al., Tetrahedron*, 1963, **19**, 1485 (*isol*)
Irie, T. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 843-844 (*Aplysin, Debromoaplysin, Aplysinol*)
Cameron, A.F. *et al., J.C.S.(B)*, 1969, 692 (*struct*)
Yamada, K. *et al., Tetrahedron*, 1969, **25**, 3509 (*synth*)
McMillan, J.A. *et al., Tet. Lett.*, 1976, 4219 (*struct, Aplysinol*)
Ronald, R.C. *et al., Tet. Lett.*, 1976, 4413 (*synth, deriv, bibl*)
Ohta, K. *et al., Phytochemistry*, 1977, **16**, 1062 (*Aplysinal*)
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 3352-3354 (*Debromoaplysinol*)
Ronald, R.C. *et al., J.O.C.*, 1980, **45**, 2224 (*synth*)
Goldsmith, D.J. *et al., J.O.C.*, 1980, **45**, 3989 (*synth*)
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 3981 (*Isoaplysin*)
Ghosh, A. *et al., Chem. Comm.*, 1988, 1421 (*synth*)
Biswas, S. *et al., J.O.C.*, 1990, **55**, 3498 (*synth*)
Laronze, J.Y. *et al., Tetrahedron*, 1991, **47**, 10003 (*synth*)
Nath, A. *et al., J.O.C.*, 1992, **57**, 1467 (*synth*)
Takano, S. *et al., Tet. Lett.*, 1992, **33**, 329 (*synth*)
Nemoto, H. *et al., J.O.C.*, 1994, **59**, 74 (*synth*)
Srikrishna, A. *et al., Tet. Lett.*, 2001, **42**, 4913-4914 (*synth*)
Harrowven, D.C. *et al., Tetrahedron*, 2001, **57**, 791-804 (*synth*)
Sun, J. *et al., Chin. Chem. Lett.*, 2005, **16**, 1611-1614 (*Laurencia tristicha constits*)
Mao, S.-C. *et al., Helv. Chim. Acta*, 2005, **88**, 1034-1039 (*Laureperoxide, 10-Bromoisoaplysin*)

Aplysinadiene A-596

*4,6-Dibromo-3-(2-butenylidene)-5-hydroxy-2(3*H*)-benzofuranone, 9CI*



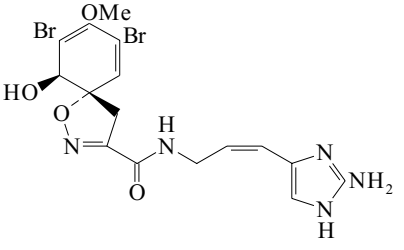
$C_{12}H_8Br_2O_3$ 360.001

(3Z,11E)-form [108940-55-2]
Constit. of *Aplysina aerophoba*.
Yellow amorph. powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 218-220°. λ_{max} 209 (ϵ 64000); 335 (ϵ 47222) (EtOH) (Berdy).
[108940-97-2]

Norte, M. *et al., Tetrahedron*, 1988, **44**, 4973 (*isol, pmr, cmr, synth*)

Aplysinamisine I A-597

[150417-67-7]

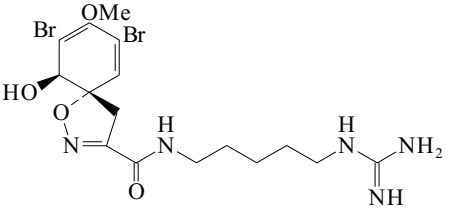


$C_{16}H_{17}Br_2N_5O_4$ 503.149
Alkaloid from the Caribbean sponge *Aplysina cauliformis.* Oil. $[\alpha]_D^{26}$ +121.9 (c, 5.7 in MeOH). λ_{max} 226 (ϵ 13700); 266 (ϵ 13100) (MeOH) (Berdy).

Rodríguez, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 907 (*isol, uv, ir, pmr, cmr, ms, struct*)

Aplysinamisine II A-598

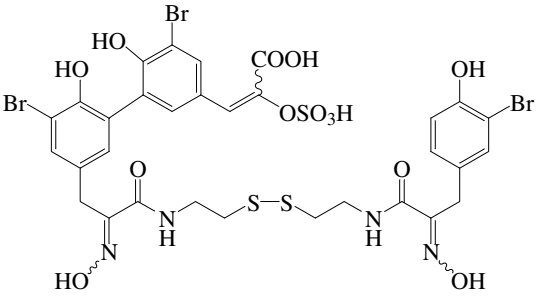
[150417-68-8]



$C_{16}H_{23}Br_2N_5O_4$ 509.197
Alkaloid from the Caribbean sponge *Aplysina cauliformis.*
Semisolid. $[\alpha]_D^{26}$ +47 (c, 7.9 in MeOH). λ_{max} 218 (ϵ 4600); 284 (ϵ 2500) (MeOH) (Berdy).

Rodríguez, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 907 (*isol, uv, ir, pmr, cmr, ms, struct*)

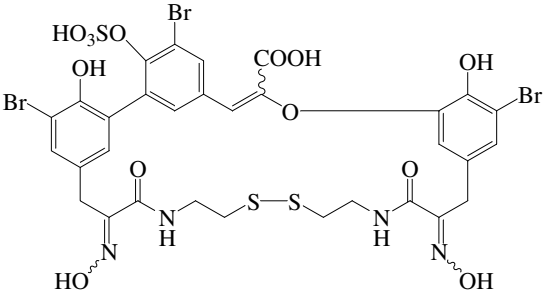
Aplysinellin A A-599



$C_{31}H_{29}Br_3N_4O_{13}S_3$ 1001.499
Isol. from the sponge *Aplysinella rhax*. Amorph. yellow solid (as di-Na salt).
Mp 191-194° dec. (di-Na salt). λ_{max} 204 (log ϵ 4.83); 291 (log ϵ 4.11) (MeOH) (di-Na salt).

Shin, J. *et al., Tetrahedron*, 2000, **56**, 9071-9077

Aplysinellin B A-600

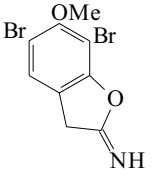


$C_{31}H_{27}Br_3N_4O_{13}S_3$ 999.483
Isol. from the sponge *Aplysinella rhax*. Amorph. yellow solid (as mono-Na salt).
Mp 236-239° dec. (Na salt). λ_{max} 205 (log ϵ 4.88); 280 (log ϵ 3.93) (MeOH) (Na salt).

Shin, J. *et al., Tetrahedron*, 2000, **56**, 9071-9077

Aplysinimine A-601

[129138-55-2]

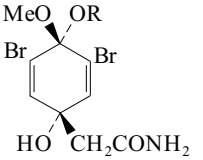


$C_9H_7Br_2NO_2$ 320.968
Constit. of *Aplysina thiona*. Amorph. solid.
Mp 146°.

Cruz, F. *et al., J. Nat. Prod.*, 1990, **53**, 543 (*isol, pmr*)

Aplysinketal A A-602

[129138-56-3]



R = $(CH_2)_3CH_3$

$C_{13}H_{19}Br_2NO_4$ 413.105
Related to 3,5-Dibromo-1-hydroxy-4,4-dimethoxy-2,5-cyclohexadiene-1-acetamide, D-259. Metab. of *Aplysina thiona*. Cryst. Mp 194-195°.

Cruz, F. *et al., J. Nat. Prod.*, 1990, **53**, 543-548 (*isol, pmr, ms*)
Toscano, R.A. *et al., Acta Cryst. C*, 1992, **48**, 2235-2237 (*cryst struct*)

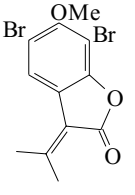
Aplysinketal B A-603

[129138-57-4]
As Aplysinketal A, A-602 with
R = $(CH_2)_4CH_3$
$C_{14}H_{21}Br_2NO_4$ 427.132
Metab. of *Aplysina thiona*. Cryst.
Mp 194-195°.

Cruz, F. *et al., J. Nat. Prod.*, 1990, **53**, 543-548 (*isol, pmr, ms*)

Aplysinolide A-604

[129138-54-1]

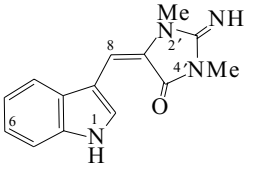


$C_{12}H_{10}Br_2O_3$ 362.017
Metab. of *Aplysina thiona*. Yellow cryst.
Mp 142-144°.

Cruz, F. *et al., J. Nat. Prod.*, 1990, **53**, 543 (*isol, pmr*)

Aplysinopsin A-605

*2-Imino-5-(1*H*-indol-3-ylmethylene)-1,3-dimethyl-4-imidazolidinone, 9CI*
[63153-56-0]
[138127-90-9]



$C_{14}H_{14}N_4O$ 254.291
Metab. of the marine sponges *Verongia spengelii* and *Thorecta* sp. and from the anthozoan *Astroides calycularis*. Antibiotic with antitumour props. Fine yellow needles + $1H_2O$ (MeOH aq. + Et_2NH).
Mp 235-237° dec. (232-233°). λ_{max} 217 (ϵ 27500); 280 (ϵ 10300); 406 (ϵ 24800) (EtOH aq./HCl) (Derep). λ_{max} 260 (ϵ 10000); 376 (ϵ 21200) (EtOH aq./NaOH) (Derep). λ_{max} 225 (ϵ 23000); 268 (ϵ 8800br); 383 (ϵ 21500) (50% EtOH) (Derep).

Di-Ac:
Fine yellow needles (EtOH). Mp 221-222° dec. (217-220°).

N^1-*Propanoyl:* **N^1-*Propionylaplysinopsin***
[100667-70-7]
$C_{17}H_{18}N_4O_2$ 310.355
Metab. from the anthozoan *Astroides calycularis*. Cryst. (MeOH). Mp 300°.

3′-N-*Me:* **N-*3′-Methylaplysinopsin***
[66492-97-5]
[66492-99-7]
$C_{15}H_{16}N_4O$ 268.318
Prod. by *Aplysinopsis reticulata*. Monoamine oxidase inhibitor, serotonergic neurotransmission potentiator. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

3′-N-*Et:* **N-*3′-Ethylaplysinopsin***
$C_{16}H_{18}N_4O$ 282.344
Isol. from the Jamaican sponge *Smenospongia aurea*. Yellowish gum. No CAS no. found to CA 136-139. λ_{max} 219 (log ϵ 4.13); 276 (log ϵ 3.74) (MeOH).

$N^{2'}$-*De-Me:* ***2′*-N-*Demethylaplysinopsin***
[72479-07-3]
$C_{13}H_{12}N_4O$ 240.264
Metab. of the marine sponge *Dercitus* sp., also isol. from the nudibranch *Phestilla melanobranchia* and the corals *Tubastrea coccinea* and *Dendrophyllia* sp.
Mp 235° (with charring from 180°). λ_{max} 217 (ϵ 27500); 280 (ϵ 10300); 406 (ϵ 24800) (EtOH aq./HCl) (Derep). λ_{max} 260 (ϵ 10000); 376 (ϵ 21200) (EtOH aq./NaOH) (Derep). λ_{max} 225 (ϵ 23000); 268 (ϵ 8800br); 383 (ϵ 21500) (50% EtOH) (Derep). λ_{max} 385 (ϵ 25000) (MeOH) (Berdy).

$N^{2'}$-*De-Me, 3′*-N-*Me:* ***2′*-N-*Demethyl*-N-*3′-methylaplysinopsin***
[126149-80-2]
$C_{14}H_{14}N_4O$ 254.291
Isol. from *Dendrophyllia* sp. Yellow solid.
Mp >250° dec. Obt. as an *E*/*Z*-mixt., Z-form predominates.

$N^{4'}$-*De-Me, 3′*-N-*Me:* ***Isoplysin A***
[158761-04-7]
$C_{14}H_{14}N_4O$ 254.291
Metab. from the Okinawan marine sponge *Aplysina* sp. Weakly cytotoxic. Yellow needles.
Mp 310° dec. λ_{max} 220 (ϵ 14000); 278 (ϵ 5400); 405 (ϵ 13000) (MeOH) (Berdy).

1′,8-Dihydro: ***1′,8-Dihydroaplysinopsin***
[85079-46-5]
$C_{14}H_{16}N_4O$ 256.307
Isol. from the coral *Tubastrea coccinea*.

3′-Deimino, 3′-oxo: [63153-57-1]
[117603-69-7, 117604-23-6]
$C_{14}H_{13}N_3O_2$ 255.276
Alkaloid from the coral *Tubastrea* sp. Obt. as an *E*/*Z*-mixt.

3′-Deimino, 3′-oxo, $N^{2'}$,$N^{4'}$*-di-de-Me:*
[117490-33-2, 117490-34-3]
$C_{12}H_9N_3O_2$ 227.222
Alkaloid from the coral *Leptopsammia pruvoti*. Obt. as an *E*/*Z*-mixt.

6-Bromo: ***6-Bromoaplysinopsin***
[85079-45-4]
$C_{14}H_{13}BrN_4O$ 333.187
Isol. from the marine sponge *Smenospongia aurea*, the anthozoan *Astroides calycularis* and the coral *Tubastrea coccinea*. Cryst. (MeOH). Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 283-285°. λ_{max} 230 (ϵ 35000); 284 (ϵ 15000); 364 (ϵ 26000); 385 (ϵ 24000) (MeOH) (Berdy).

6-Bromo, N^1*-propanoyl:* ***6-Bromo*-N^1*-propionylaplysinopsin***
[100667-71-8]
$C_{17}H_{17}BrN_4O_2$ 389.251
Metab. from the anthozoan *Astroides calycularis*. Cryst. (MeOH). Mp 300°.

6-Bromo, $N^{2'}$*-de-Me:* ***6-Bromo-2′*-N-*demethylaplysinopsin***
[72479-08-4]
$C_{13}H_{11}BrN_4O$ 319.16
Metab. of the marine sponge *Dercitus* sp. Also isol. from the nudibranch *Phestilla melanobranchia* and the coral *Tubastrea coccinea*.
Mp 186-188° (with charring from 175°). λ_{max} 390 (ϵ 23000) (MeOH) (Derep).

6-Bromo, $N^{2'}$*-de-Me, 3′*-N-*Me:* ***6-Bromo-2′*-N-*demethyl*-N-*3′-methylaplysinopsin***
[126149-81-3 (*Z*-form), 126149-84-6 (*E*-form)]
$C_{14}H_{13}BrN_4O$ 333.187
Isol. from *Dendrophyllia* sp. Yellow solid.
Mp >280° dec. Obt. as an *E*/*Z*-mixt., *Z*-form predominates.
λ_{max} 238 (ϵ 8500); 286 (ϵ 5200); 385 (ϵ 10700) (MeOH).

6-Bromo, $N^{4'}$*-de-Me:* ***6-Bromo-4′*-N-*demethylaplysinopsin***
[97480-15-4]
$C_{13}H_{11}BrN_4O$ 319.16
Metab. of the marine sponge *Smenospongia aurea*. Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 290° (as Ac). Characterised as the Ac deriv. λ_{max} 390 (ϵ 23000) (MeOH) (Derep). λ_{max} 230 (ϵ 35000); 284 (ϵ 15000); 364 (ϵ 26000) (MeOH) (Berdy).

6-Bromo, 1′,8-dihydro: ***6-Bromo-1′,8-dihydroaplysinopsin***
[85079-47-6]
$C_{14}H_{15}BrN_4O$ 335.203
Isol. from the coral *Tubastrea coccinea*.

6-Bromo, 1′,8-dihydro, 1′ξ-hydroxy: ***6-Bromo-1′,8-dihydro-1′-hydroxyaplysinopsin***
[868830-18-6]
$C_{14}H_{15}BrN_4O_2$ 351.202
Isol. from a *Thorectandra* sp. Red solid. $[\alpha]_D^{25}$ +1 (c, 0.5 in MeOH).

6-Bromo, 1′,8-dihydro, 1′ξ-methoxy: ***6-Bromo-1′,8-dihydro-1′-methoxyaplysinopsin***
[868830-19-7]
$C_{15}H_{17}BrN_4O_2$ 365.229
Isol. from a *Thorectandra* sp. Red solid. $[\alpha]_D^{25}$ +3 (c, 1.4 in MeOH).

6-Bromo, 1′,8-dihydro, 1′ξ-ethoxy: ***6-Bromo-1′-ethoxy-1′,8-dihydroaplysinopsin***
[868830-20-0]
$C_{16}H_{19}BrN_4O_2$ 379.256
Isol. from a *Smenospongia* sp. Red solid. $[\alpha]_D^{25}$ +19.3 (c, 0.05 in MeOH).

6-Bromo, 3′-deimino, 3′-oxo: ***6-Bromo-3′-deimino-3′-oxoaplysinopsin***
[117490-31-0, 117490-32-1]
$C_{14}H_{12}BrN_3O_2$ 334.172
Alkaloid from the coral *Tubastrea* sp. Obt. as an *E*-/*Z*-mixt.

6-Bromo, 3′-deimino, 3′-oxo, $N^{2'}$,$N^{4'}$*-di-de-Me:* ***6-Bromo-3′-deimino-2′,4′-bis(demethyl)-3′-oxoaplysinopsin***
[117490-29-6, 117490-30-9]
$C_{12}H_8BrN_3O_2$ 306.118
Alkaloid from the coral *Leptopsammia pruvoti*. Obt. as an *E*-/*Z*-mixt.

5,6-Dibromo, $N^{2'}$*-de-Me: 5,6-Dibromo-2′*-N-*demethylaplysinopsin*
[376598-41-3]
$C_{13}H_{10}Br_2N_4O$ 398.056
Isol. from the sponge *Hyrtios erecta*. Yellow powder. λ_{max} 246 (ϵ 8500); 293 (ϵ 2700); 385 (ϵ 8600) (MeOH).

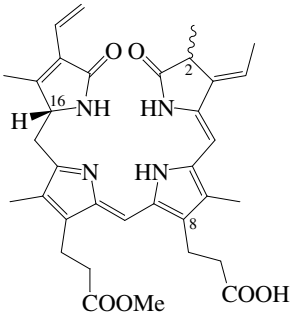
Z-Isomer, 5,6-dibromo, $N^{2'}$*-de-Me:* [376598-39-9]
$C_{13}H_{10}Br_2N_4O$ 398.056
Isol. from *Hyrtios erecta*. Yellow powder. λ_{max} 247 (ϵ 17300); 294 (ϵ 4400); 383 (ϵ 20700) (MeOH).

Hollenbeak, K.H. *et al., J. Nat. Prod.*, 1977, **40**, 479-481 (*isol, uv, ir, pmr, ms, struct*)
Kazlauskas, R. *et al., Tet. Lett.*, 1977, 61-64 (*uv, ir, pmr, ms, struct*)
Djura, P. *et al., J.O.C.*, 1980, **45**, 735-737 (*2′-N-Demethylaplysinopsin, 6-Bromo-2′-N-demethylaplysinopsin*)
Okuda, R.K. *et al., Pure Appl. Chem.*, 1982, **54**, 1907-1914 (*1′,8-Dihydroaplysinopsin, 6-Bromo-1′,8-dihydroaplysinopsin*)
Fattorusso, E. *et al., J. Nat. Prod.*, 1985, **48**, 924-927 (N^1-*Propionylaplysinopsin, 6-Bromo-*N^1*-propionylaplysinopsin*)
Tymiak, A.A. *et al., Tetrahedron*, 1985, **41**, 1039-1047 (*6-Bromoaplysinopsin, 6-Bromo-4′-N-demethylaplysinopsin*)
Guella, G. *et al., Helv. Chim. Acta*, 1988, **71**, 773-781; 1989, **72**, 1444-1450 (*Dendrophyllia constits, Tubastrea constits*)

Dalkafouki, A. *et al., Tet. Lett.*, 1991, **32**, 5325-5328 (*synth*)
Gulati, D. *et al., Indian J. Chem.*, 1994, **33**, 4-9; 10-16 (*synth*)
Kondo, K. *et al., J. Nat. Prod.*, 1994, **57**, 1008-1011 (*Isoplysin A*)
Molina, P. *et al., Tetrahedron*, 1994, **50**, 2241-2254 (*synth, derivs*)
Aoki, S. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1372-1374 (*5,6-Dibromo-N-demethylaplysinopsin*)
Hu, J.-F. *et al., J. Nat. Prod.*, 2002, **65**, 476-480 (*N-3′-Ethylaplysinopsin, N-3′-Methylaplysinopsin*)
Segraves, N.L. *et al., J. Nat. Prod.*, 2005, **68**, 1484-1488 (*6-Bromo-1′,8-dihydro-1′-hydroxyaplysinopsin*)

Aplysioviolin A-606

Phycobiliviolin monomethyl ester. Phycoerythrobilin monomethyl ester. Aplysiaviolin
[15265-71-1]

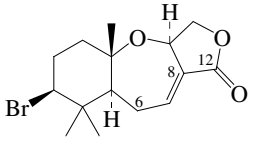


$C_{34}H_{40}N_4O_6$ 600.713
Me ester posn. revised in 2002. Major violet pigment from the defensive secretion of the sea hares *Aplysina parvula*, *Aplysina limacina* and *Aplysia dactylomela*. Defensive secretion. Mauve cryst. ($CHCl_3$). Sol. $CHCl_3$.
Mp 315° dec. $[\alpha]_D^{20}$ +730 (c, 0.1 in MeOH). Isol. as a mixt. of (2*R*,16*R*)- and (2*S*,16*R*)- stereoisomers. λ_{max} 203 (4.29); 329 (4.18); 595 (4.46) (MeOH).

Rüdiger, W. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1967, **348**, 129; 1554; 1969, **350**, 1291 (*isol, uv, struct*)
Lightner, D.A. *et al., The Porphyrins*, (Dolphin, D., Ed.), Academic Press, N.Y., Vol. VI, 1979, 521
Appleton, D.R. *et al., Tetrahedron*, 2001, **57**, 10181-10189 (*isol, uv, ir, pmr, cmr*)
Jongaramruong, J. *et al., Aust. J. Chem.*, 2002, **55**, 275-280 (*isol, pmr, cmr, ms*)

Aplysistatin A-607

[62003-89-8]



Absolute Configuration

$C_{15}H_{21}BrO_3$ 329.233
Constit. of *Aplysia angasi*. Shows weak antimycobacterial and cytotoxic activities. Cryst.
Mp 173-175°. $[\alpha]_D^{25}$ -375 (MeOH). λ_{max} 215 (ϵ 9000) (MeOH) (Derep).

12-Deoxo: 12-Deoxyaplysistatin. ***Palisadin A***
[77249-86-6]
$C_{15}H_{23}BrO_2$ 315.249
Constit. of *Laurencia* cf. *palisada*. Oil. $[\alpha]_D$ +19.5 (c, 1.5 in $CHCl_3$). Slowly oxid. to Aplysistatin in air.

6β-Hydroxy: ***6β-Hydroxyaplysistatin***
[79493-95-1]
$C_{15}H_{21}BrO_4$ 345.232
Constit. of *Laurencia filiformis*. Shows weak antimycobacterial and cytotoxic activities. Cryst. (MeOH).
Mp 153.5-155.5°. $[\alpha]_D^{25}$ +130 (c, 0.4 in MeOH). λ_{max} 237 (ϵ 2500) (EtOH) (Berdy).

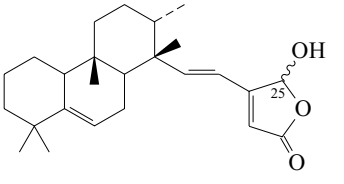
12-Deoxo, 7ξ,8ξ-epoxide: ***3,4-Epoxypalisadin A***
[150998-89-3]
$C_{15}H_{23}BrO_3$ 331.249
Constit. of *Laurencia flexilis*. Cryst.
Mp 119-122°. $[\alpha]_D^{25}$ +10 (c, 0.1 in $CHCl_3$).

12-Deoxo, 6β-acetoxy: ***5β-Acetoxypalisadin A***
[150712-71-3]
$C_{17}H_{25}BrO_4$ 373.286
Constit. of *Laurencia flexilis*. Oil. $[\alpha]_D^{25}$ -45 (c, 0.1 in $CHCl_3$).

Pettit, G.R. *et al., J.A.C.S.*, 1977, **99**, 262-263 (*isol, cryst struct*)
Paul, V.J. *et al., Tet. Lett.*, 1980, **21**, 2787-2790 (*Palisadin A*)
Capon, R. *et al., Tetrahedron*, 1981, **37**, 1613-1621 (*6β-Hydroxyaplysistatin, cryst struct, abs config*)
White, J.D. *et al., J.A.C.S.*, 1982, **104**, 3923 (*synth*)
Hoye, T.R. *et al., J.A.C.S.*, 1982, **104**, 6704 (*synth*)
Shieh, H.-M. *et al., Tet. Lett.*, 1982, **23**, 4643 (*synth*)
Kraus, G.A. *et al., J.O.C.*, 1983, **48**, 5356 (*synth*)
Gosselin, P. *et al., Tet. Lett.*, 1983, **24**, 5515 (*synth*)
Tanaka, A. *et al., Agric. Biol. Chem.*, 1984, **48**, 2535; 1986, **50**, 1069 (*synth*)
De Nys, R. *et al., J. Nat. Prod.*, 1993, **56**, 877-883 (*isol, derivs, pmr, cmr*)
Koenig, G.M. *et al., J. Nat. Prod.*, 1994, **57**, 151-154 (*3,4-Epoxypalisadin A, cryst struct*)
Koenig, G.M. *et al., Planta Med.*, 2000, **66**, 337-342 (*Aplysistarin, 6β-hydroxy, activity*)
Couladouros, E.A. *et al., Chem. Eur. J.*, 2004, **10**, 3822-3835 (*synth*)

Aplysolide A A-608

[135261-91-5]

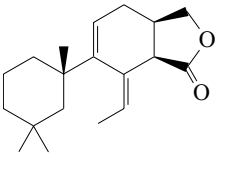


$C_{25}H_{36}O_3$ 384.558
Constit. of an *Aplysinopsis* sponge. Oil (as acetate). $[\alpha]_D$ -20 (c, 0.7 in $CHCl_3$) (acetate).

25-Epimer: ***Aplysolide B***
[135356-90-0]
$C_{25}H_{36}O_3$ 384.558
Constit. of an *Aplysinopsis* sponge. Oil (as acetate). $[\alpha]_D$ -9 (c, 0.4 in $CHCl_3$) (acetate).

Crews, P. *et al., Tetrahedron*, 1991, **47**, 3585 (*isol, pmr, cmr*)

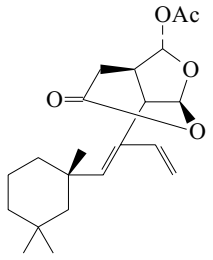
Aplytandiene 1 A-609



$C_{19}H_{28}O_2$ 288.429
Constit. of *Aplysilla tango*. Needles (Et_2O).
Mp 91-94°. $[\alpha]_D$ -134 (c, 1 in $CHCl_3$).

Poiner, A. *et al., Aust. J. Chem.*, 1990, **43**, 1713 (*isol, pmr, cmr*)

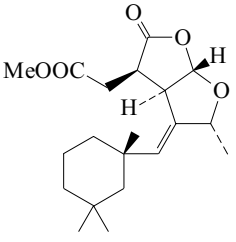
Aplytangene 1 A-610



$C_{21}H_{30}O_5$ 362.465
Constit. of *Aplysilla tango*. Gum. $[\alpha]_D$ +13.3 (c, 1 in $CHCl_3$).

Poiner, A. *et al., Aust. J. Chem.*, 1990, **43**, 1713 (*isol, pmr, cmr*)

Aplytangene 2 A-611

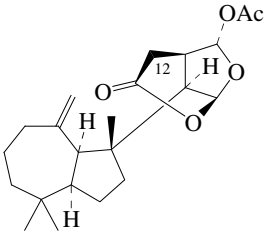


$C_{20}H_{30}O_5$ 350.454
Constit. of *Aplysilla tango*. Oil. $[\alpha]_D$ +32.3 (c, 1 in $CHCl_3$).

Poiner, A. *et al., Aust. J. Chem.*, 1990, **43**, 1713 (*isol, pmr, cmr*)

Aplyviolene A-612

[104371-86-0]



$C_{22}H_{32}O_5$ 376.492

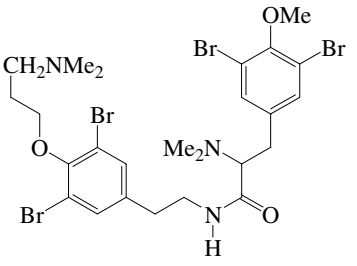
This struct. was originally assigned to Dendrillolide A (see Dendrillolide A, D-68). Constit. of *Chelonaplysilla violacea* and *Aplysilla polyrhaphis*. Cryst. (EtOAc/petrol).
Mp 163-164°. $[\alpha]_D$ -29.5 (c, 1 in $CHCl_3$).

12β-Acetoxy: ***Aplyviolacene****. Macfarlandin E*
[104311-71-9]
$C_{24}H_{34}O_7$ 434.528
Constit. of *Chelonaplysilla violacea*, *Chromodoris macfarlandi* and *Dysidea* sp. Glass. Sol. MeOH, $CHCl_3$, Me_2CO; poorly sol. H_2O.
$[\alpha]_D$ -34 (c, 0.05 in $CHCl_3$).

Buckleton, J.S. *et al., Acta Cryst. C*, 1986, **42**, 1846 (*cryst struct*)
Molinski, T.F. *et al., J.O.C.*, 1986, **51**, 4564-4567 (*Macfarlandin E*)
Carmely, S. *et al., J.O.C.*, 1988, **53**, 4801-4807 (*isol, pmr, cmr*)
Bobzin, S.C. *et al., J.O.C.*, 1989, **54**, 3902-3907 (*Aplysilla polyrhaphis constits*)
Hambley, T.W. *et al., Aust. J. Chem.*, 1990, **43**, 1861-1870 (*isol, pmr, cmr, cryst struct*)

Aplyzanzine A A-613

[327165-67-3]

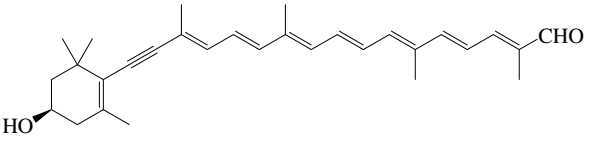


$C_{25}H_{33}Br_4N_3O_3$ 743.17
Isol. from an *Aplysina* sp. Pale orange oil.

Evan, T. *et al., J. Nat. Prod.*, 2001, **64**, 226-227

Apoalloxanthinal A-614

7,8-Didehydro-3-hydroxy-8′-apo-β-caroten-8′-al
[190849-79-7]

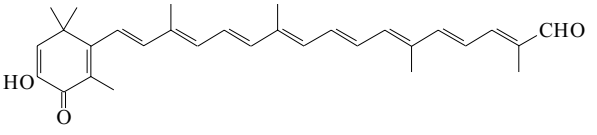


$C_{30}H_{38}O_2$ 430.629
Isol. from the mussel *Mytilus coruscus* and the oyster *Crassostrea gigas*.

Maoka, T. *et al., J. Nat. Prod.*, 1997, **60**, 616-617 (*isol, cd, pmr, ms*)

Apoastacenal A-615

2,3-Didehydro-3-hydroxy-4-oxo-8′-apo-β,ψ-carotenal, 9CI
[59076-74-3]

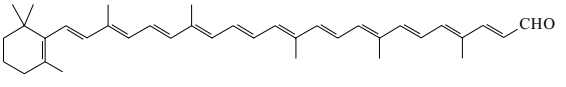


$C_{30}H_{36}O_3$ 444.613
Isol. from the egg masses of *Hexabranchus* sp. Cryst. ($CHCl_3$/hexane).
Mp 196-197° (synthetic).

Coman, R.E. *et al., J.C.S. Perkin 1*, 1975, 2529 (*synth*)
Tanaka, Y. *et al., CA*, 1993, **118**, 36149v (*isol*)

β-Apo-2′-carotenal A-616

3′,4′-Didehydro-2′-apo-β-caroten-2′-al

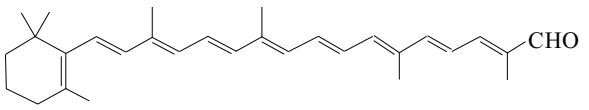


$C_{37}H_{48}O$ 508.786
Identified in *Aplysia* sp. Glistening metallic violet cryst. (petrol).
Mp 160-161°. λ_{max} 498 (petrol).

Rüegg, R. *et al., Helv. Chim. Acta*, 1959, **42**, 854 (*synth*)
Schwieter, U. *et al., Helv. Chim. Acta*, 1966, **49**, 369 (*synth*)
Czeczuga, B. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1984, **78**, 259 (*occur*)

8′-Apo-β-caroten-8′-al A-617

β-Carotinal. *β-Apo-2-carotinal*. *C.I. Food Orange 6*
[1107-26-2]



$C_{30}H_{40}O$ 416.645
Constit. of orange peel, spinach, marigolds and egg yolks. Obt. by oxidn. of β-Carotene, C-129. Colour additive. Violet cryst. (MeOH).
Mp 139°.

8′-Alcohol: ***8′-Apo-β-caroten-8′-ol***
[6541-41-9]
$C_{30}H_{42}O$ 418.661
Constit. of *Aplysia kurodai*. Orange needles.
Mp 148-149°.

8′-Carboxylic acid: ***8′-Apo-β-caroten-8′-oic acid***. *β-Apo-8′-carotenoic acid*
[1962-15-8]
$C_{30}H_{40}O_2$ 432.645
Isol. from *Staphylococcus aureus*. Cryst. (C_6H_6).
Mp 189-190°. λ_{max} 448 (petrol).

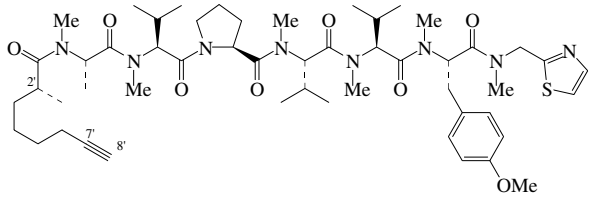
8′-Carboxylic acid, Me ester: [4273-73-8]
$C_{31}H_{42}O_2$ 446.672
Isol. from *Staphylococcus aureus*. Red cryst. (petrol or Et_2O/petrol).
Mp 136-137°. λ_{max} 445; 471 (petrol).

8′-Carboxylic acid, Et ester: all-trans *Carophyll yellow. C.I. Food Orange 7*
[1109-11-1]
$C_{32}H_{44}O_2$ 460.698
Colour additive for foods, e.g. egg yolks. Dark red cryst. (CH_2Cl_2/EtOH). Mp 137-138°. λ_{max} 445; 470 (petrol).

Rüegg, R. *et al., Helv. Chim. Acta*, 1959, **42**, 854-864 (*synth*)
Isler, O. *et al., Helv. Chim. Acta*, 1959, **42**, 864-871 (*synth, acid*)
Winterstein, A. *et al., Chem. Ber.*, 1960, **93**, 2951-2965 (*isol*)
Isler, O. *et al., Chimia*, 1961, **15**, 208-226 (*synth*)
Schwieter, H. *et al., Helv. Chim. Acta*, 1966, **49**, 369-390 (*carboxylic acid, Et ester, uv*)
Fischli, A. *et al., Helv. Chim. Acta*, 1975, **58**, 1492-1497 (*Et ester, synth, ir, uv, pmr*)
Englert, G. *et al., Helv. Chim. Acta*, 1975, **58**, 2367-2390 (*cmr*)
Sharma, R.V. *et al., Biochim. Biophys. Acta*, 1977, **486**, 183-194 (*biochem*)
Taylor, R.F. *et al., Can. J. Biochem.*, 1983, **61**, 892-905 (*isol, carboxylic acid*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 482 (*bibl*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AQO300
Yamashita, E. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1990, **96**, 465-470 (*Aplysia, isol*)
Bernhard, K. *et al., Pure Appl. Chem.*, 1991, **63**, 35-44 (*rev, total synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 192-193 (*use*)
Sliwka, H.-R. *et al., Chem. Eur. J.*, 1998, **4**, 113-117 (*acid, synth, uv, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AQO300

Apramide A A-618

[290298-29-2]



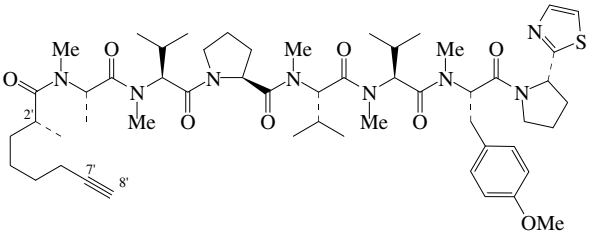
$C_{52}H_{80}N_8O_8S$ 977.319
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{22}$ -206 (c, 2.7 in $CHCl_3$). λ_{max} 201 (log ϵ 4.74); 230 (sh) (log ϵ 4.29) (MeOH).

7′,8′-Dihydro: ***Apramide C***
[290298-31-6]
$C_{52}H_{82}N_8O_8S$ 979.335
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{22}$ -206 (c, 0.56 in $CHCl_3$). λ_{max} 201 (log ϵ 4.74); 230 (sh) (log ϵ 4.3) (MeOH).

2′-Demethyl: ***Apramide B***
[290298-30-5]
$C_{51}H_{78}N_8O_8S$ 963.292
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D$ -189 (c, 0.2 in $CHCl_3$). λ_{max} 201 (log ϵ 4.74); 230 (sh) (log ϵ 4.27) (MeOH).

Luesch, H. *et al., J. Nat. Prod.*, 2000, **63**, 1106-1112 (*Apramides A-C, isol, ir, uv, pmr, cmr, ms*)

Apramide D A-619



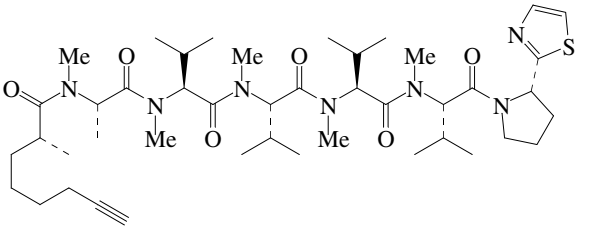
$C_{54}H_{82}N_8O_8S$ 1003.357
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{22}$ -234 (c, 0.55 in $CHCl_3$). λ_{max} 201 (log ϵ 4.75); 230 (sh) (log ϵ 4.3) (MeOH).

7′,8′-Dihydro: ***Apramide F***
$C_{54}H_{84}N_8O_8S$ 1005.372
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{22}$ -160 (c, 0.15 in $CHCl_3$). λ_{max} 201 (log ϵ 4.44); 240 (sh) (log ϵ 3.77) (MeOH).

2′-Demethyl: ***Apramide E***
$C_{53}H_{80}N_8O_8S$ 989.33
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{22}$ -213 (c, 0.23 in $CHCl_3$). λ_{max} 201 (log ϵ 4.75); 230 (sh) (log ϵ 4.29) (MeOH).

Luesch, H. *et al., J. Nat. Prod.*, 2000, **63**, 1106-1112

Apramide G A-620

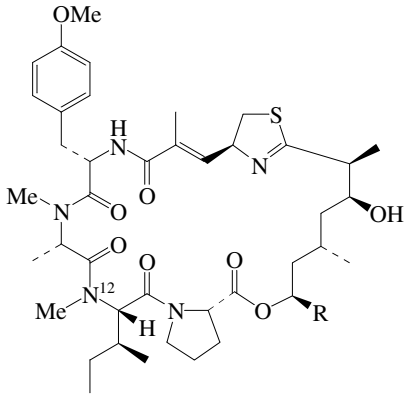


$C_{44}H_{73}N_7O_6S$ 828.17
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{22}$ -160 (c, 0.15 in $CHCl_3$). λ_{max} 201 (log ϵ 4.44); 240 (sh) (log ϵ 3.77) (MeOH).

Luesch, H. *et al., J. Nat. Prod.*, 2000, **63**, 1106-1112

Apratoxin A A-621

[350791-64-9]



Absolute Configuration

R = -C(CH$_3$)$_3$

$C_{45}H_{69}N_5O_8S$ 840.135
Isol. from *Lyngbya majuscula*. Potent cytotoxin. Amorph. solid. $[\alpha]_D^{25}$ -161 (c, 1.3 in MeOH).

N^{12}*-De-Me:* ***Apratoxin B***
[444885-29-4]
$C_{44}H_{67}N_5O_8S$ 826.108
Isol. from *Lyngbya* sp. Amorph. solid. $[\alpha]_D^{25}$ -73 (c, 0.2 in MeOH). λ_{max} 200 (log ϵ 4.64); 230 (log ϵ 4.36) (MeOH).

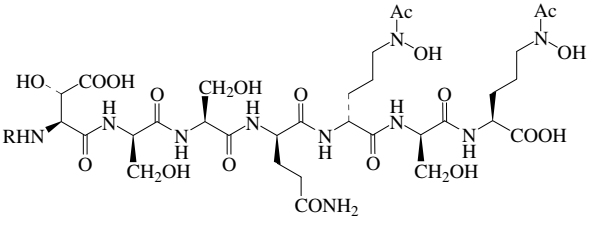
Luesch, H. *et al., J.A.C.S.*, 2001, **123**, 5418-5423 (*isol, pmr, cmr*)
Luesch, H. *et al., Bioorg. Med. Chem.*, 2002, **10**, 1973-1978 (*Apratoxin B*)
Chen, J. *et al., J.A.C.S.*, 2003, **125**, 8734-8735 (*synth*)
Doi, T. *et al., Org. Lett.*, 2006, **8**, 531-534 (*synth*)

Apratoxin C A-622

[444885-30-7]
As Apratoxin A, A-621 with
R = -CH(CH$_3$)$_2$
$C_{44}H_{67}N_5O_8S$ 826.108
Isol. from *Lyngbya* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{25}$ -171 (c, 0.22 in MeOH). λ_{max} 201 (log ϵ 4.64); 230 (log ϵ 4.31) (MeOH).

Luesch, H. *et al., Bioorg. Med. Chem.*, 2002, **10**, 1973-1978

Aquachelins A-623



Aquachelin A R = $-CO(CH_2)_3CH\overset{Z}{=}CH(CH_2)_5CH_3$
B R = $-CO(CH_2)_{10}CH_3$
C R = $-CO(CH_2)_5CH\overset{Z}{=}CH(CH_2)_5CH_3$
D R = $-CO(CH_2)_{12}CH_3$

Isol. from the marine bacterium *Halomonas aquamarina* DS40M3. Amphiphilic siderophores.

Aquachelin A [265319-78-6]
$C_{44}H_{74}N_{10}O_{20}$ 1063.124

Aquachelin B [265319-79-7]
$C_{44}H_{76}N_{10}O_{20}$ 1065.139

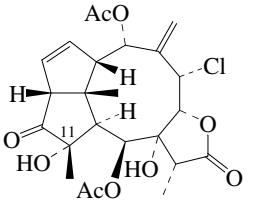
Aquachelin C [265319-80-0]
$C_{46}H_{78}N_{10}O_{20}$ 1091.177

Aquachelin D [265319-81-1]
$C_{46}H_{80}N_{10}O_{20}$ 1093.193

Martinez, J.S. *et al., Science (Washington, D.C.)*, 2000, **287**, 1245-1247 (*isol, struct*)

Aquariolide A A-624

[477243-87-1]



$C_{24}H_{29}ClO_9$ 496.94
Constit. of *Erythropodium caribaeorum*. Glass.

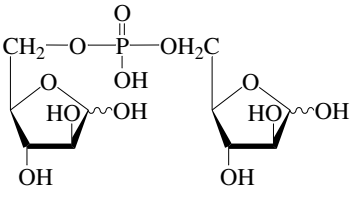
11-Ac: ***Aquariolide C***
[627878-07-3]
$C_{26}H_{31}ClO_{10}$ 538.978
Constit. of *Erythropodium caribaeum*. Glass. $[\alpha]_D^{25}$ -167.2. λ_{max} 213 (ϵ 3500) (MeOH).

11-Me ether: ***Aquariolide B***
[627878-06-2]
$C_{25}H_{31}ClO_9$ 510.967
Constit. of *Erythropodium caribaeorum*. Glass. $[\alpha]_D^{25}$ -62.5. λ_{max} 213 (ϵ 3800) (MeOH).

Taglialatela-Scafati, O. *et al., Org. Lett.*, 2002, **4**, 4085-4088 (*Aquariolide A*)
Taglialatela-Scafati, O. *et al., Eur. J. Org. Chem.*, 2003, 3515-3523 (*Aquariolides B and C*)

D-Arabinofuranose 5,5′-(hydrogen phosphate), 9CI A-625

[121808-61-5]

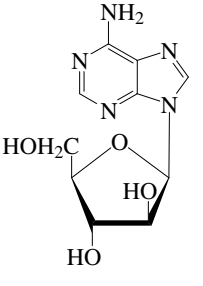


$C_{10}H_{19}O_{12}P$ 362.227
Constit. of an extracellular glycoprotein found in the alga *Volvox carteri* f. *nagariensis*.

Holst, O. *et al., Eur. J. Biochem.*, 1989, **181**, 345-350 (*isol, cmr, ms*)

9-Arabinofuranosyladenine, 8CI A-626

*9-Arabinofuranosyl-9*H*-purin-6-amine, 9CI*
[2006-02-2]



β-D-*form*

$C_{10}H_{13}N_5O_4$ 267.244

β-D-*form*

Vidarabine, BAN, INN, JAN, USAN. *Spongoadenosine. Adena-A. Ara-A. Arasena-A. Panavirin. Plosarabine forte. Vira-A. CI 673. NSC 404241. Araadenosine*

[5536-17-4]

Isol. from the marine gorgonian *Eunicella cavolini* and *Streptomyces* spp. Antiviral agent; shows significant activity against Herpes simplex and vaccinia viruses in cell cultures and in experimental animals. Nucleoside transporter substrate. Needles + ½ H_2O (H_2O).

Mp 257-257.5°. $[\alpha]_D^{40}$ +12 (c, 0.25 in H_2O). $[\alpha]_D^{27}$ -5 (c, 0.25 in H_2O).

Log P -2.88 (calc). λ_{max} 260 (ϵ 12000) (H_2O) (Derep).

▶ Human systemic effects when used therapeutically. Adverse ocular effects following topical administration. Exp. reprod. and teratogenic effects (large doses). LD_{50} (mus, orl) 7.8 mg/kg. Eye irritant. AU6200000

3′-Ac: [65286-65-9]

$C_{12}H_{15}N_5O_5$ 309.281

Isol. from *Eunicella cavolini*. Antiviral agent. Cryst. (MeOH). Sol. MeOH, butanol, H_2O; poorly sol. $CHCl_3$, hexane.

Mp 214-215°. λ_{max} 258 (ϵ 14000) (MeOH) (Berdy).

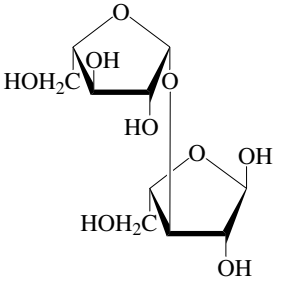
[24356-66-9, 71002-10-3]

Cimino, G. *et al., Experientia*, 1984, **40**, 339 (*β-D-Ac, isol*)

3-*O*-β-L-Arabinofuranosyl-L-arabinose, 9CI A-627

Arabinofuranobiose

[52287-00-0]



β-Furanose-*form*

$C_{10}H_{18}O_9$ 282.247

Formed on partial acid hydrolysis of sugar beet araban and certain plant gums, e.g. *Acacia pycnantha* gum and *Rhizophora mangle* gum.

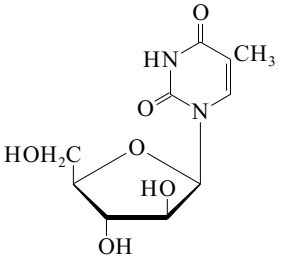
$[\alpha]_D$ +94 (H_2O).

Phenylosazone: Mp 200°.

Andrews, P. *et al., Chem. Ind. (London)*, 1956, 658 (*isol*)
Aspinall, G.O. *et al., J.C.S.*, 1959, 1697 (*isol*)
Sarkar, M. *et al., Indian J. Chem.*, 1974, **11**, 1129
Sarkar, M. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 369 (*isol, pmr*)

1-Arabinofuranosylthymine A-628

*1-Arabinofuranosyl-5-methyl-2,4(1*H*,3*H*)-pyrimidinedione, 9CI. 1-(Arabinofuranosyl)-5-methyluracil*



$C_{10}H_{14}N_2O_6$ 258.23

Log P -2.33 (calc).

β-D-*form*

Spongothymidine. *Ara-T*

[605-23-2]

Isol. from Caribbean sponge, *Cryptotethia crypta*. Antiviral agent. HIV reverse transcriptase (HIV-rt) inhibitor.

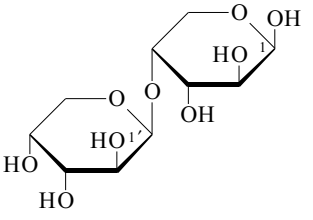
Mp 194-195° Mp 242°. $[\alpha]_D^{28}$ +90 (c, 0.8 in Py). Low acute toxicity. λ_{max} 267 (pH 12) (Derep). λ_{max} 267 (ϵ 9600) (pH 7.2) (Derep). λ_{max} 269 (ϵ 9250) (H_2O) (Berdy).

▶ XP2100200

[2946-29-4]

Bergmann, W. *et al., J.O.C.*, 1955, **20**, 1501-1507 (*isol, struct*)
Fr. Pat., 1965, (*Upjohn*)1 396 003; *CA*, **63**, 13392d (*synth*)
Tougard, P. *et al., Acta Cryst. B*, 1973, **29**, 2227-2232 (*cryst struct*)
Mueller, W.E.G. *et al., FEBS-Symp.*, 1979, **57**, 327-341 (*rev*)
Ooka, T. *et al., Virology*, 1980, **104**, 219-223 (*activity*)
Soike, K.F. *et al., Antiviral Res.*, 1984, **4**, 245-257 (*pharmacol, activity*)
Gosselin, G. *et al., Nucleosides Nucleotides*, 1984, **3**, 265-275 (*synth*)
Machida, H. *et al., Microbiol. Immunol.*, 1991, **35**, 963-973 (*pharmacol*)
Hirota, K. *et al., Synthesis*, 1993, 213-215 (*synth, bibl, pmr, ms*)

4-*O*-β-D-Arabinopyranosyl-D-arabinose A-629



$C_{10}H_{18}O_9$ 282.247

2,2′,3-Tri-Ac, 1-O-*(3,7,11-trimethyl-2,6,10-dodecatrienyl):*

[143838-79-3]

$C_{31}H_{48}O_{12}$ 612.713

Isol. from the coral *Sinularia* sp. Enhances glucose transport in rat adipocytes. Oil. $[\alpha]_D$ -196 (c, 0.7 in $CHCl_3$).

Shindo, T. *et al., Experientia*, 1992, **48**, 688 (*isol, pmr, cmr, ms*)

Arachidonate lipoxygenases A-630

Fe-dependent oxidoreductase enzymes.

Arachidonate 5-lipoxygenase

E.C. 1.13.11.34. Arachidonate:oxygen 5-oxidoreductase. 5-Lipoxygenase. Leukotriene A_4 synthase

[80619-02-9]

Present in a number of mammalian cells and in plants. Catalyses the reaction of arachidonate with O_2 to give (5*S*,6*E*,8*Z*,11*Z*,14*Z*)-5-hydroperoxy-6,8,11,14-eicosatetraenoate.

Arachidonate 8-lipoxygenase

E.C. 1.13.11.40. Arachidonate:oxygen 8-oxidoreductase. 8-Lipoxygenase

[100900-72-9]

Isol. from the coral *Pseudoplexaura porosa*. Catalyses the reaction of arachidonate with O_2 to give (5*Z*,8*R*,9*E*,11*Z*,14*Z*)-8-hydroperoxy-5,9,11,14-eicosatetraenoate.

Arachidonate 12-lipoxygenase

E.C. 1.13.11.31. Arachidonate:oxygen 12-oxidoreductase. 12-Lipoxygenase

[82391-43-3]

Present in mammalian platelets, leucocytes and epidermis. Catalyses the reaction of arachidonate with O_2 to give (5*Z*,8*Z*,10*Z*,12*S*,14*Z*)-12-hydroperoxy-5,8,10,14-eicosatetraenoate (see 12-Hydroperoxy-5,8,10,14-eicosatetraenoic acid, H-430) which is rapidly reduced to the 12-hydroxy compd.

Arachidonate 15-lipoxygenase

E.C. 1.13.11.33. Arachidonate:oxygen 15-oxidoreductase. 15-Lipoxygenase. ω-6 Lipoxygenase

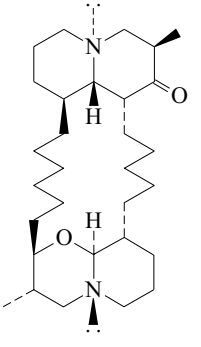
[82249-77-2]

Present in animal reticulocytes and leucocytes; also occurs in some plants. Catalyses the reaction of arachidonate with O_2 to give (5*Z*,8*Z*,11*Z*,13*E*,15*S*)-15-hydroperoxy-5,8,11,13-eicosatetraenoate which is rapidly reduced to the 15-hydroxy compd.

Nugteren, D.H. *et al., Biochim. Biophys. Acta*, 1975, **380**, 299-307 (*E.C. 1.13.11.31, blood platelets*)
Wallach, D.P. *et al., Biochim. Biophys. Acta*, 1981, **663**, 361-372 (*E.C. 1.13.11.31, human blood platelets*)
Nugteren, D.H. *et al., Methods Enzymol.*, 1982, **86**, 49-54 (*E.C. 1.13.11.31, bovine platelets*)
Bundy, G.L. *et al., J. Biol. Chem.*, 1986, **261**, 747-751 (*E.C. 1.13.11.40, Pseudoplexaura porosa*)
Shibata, D. *et al., J. Biol. Chem.*, 1987, **262**, 10080-10085 (*E.C. 1.13.11.33, soybean*)
Ohishi, N. *et al., J. Biol. Chem.*, 1987, **262**, 10200-10205 (*E.C. 1.13.11.34, human lung*)
Sigal, E. *et al., J. Biol. Chem.*, 1988, **263**, 5328-5332 (*E.C. 1.13.11.33, human leucocytes*)
Soberman, R.J. *et al., Methods Enzymol.*, 1988, **163**, 344-349 (*E.C. 1.13.11.33, E.C. 1.13.11.34, human leukocytes*)
Sloane, D.L. *et al., Biochem. Biophys. Res. Commun.*, 1990, **173**, 507-513 (*E.C. 1.13.11.33, rabbit reticulocytes*)
Reddanna, P. *et al., Methods Enzymol.*, 1990, **187**, 268-277 (*E.C. 1.13.11.34, potato tubers*)
Rouzer, C.A. *et al., Methods Enzymol.*, 1990, **187**, 312-319 (*E.C. 1.13.11.34, human leukocytes*)
Ford-Hutchinson, A.W. *et al., Eicosanoids*, 1991, **4**, 59-74 (*E.C. 1.13.11.33, rev*)
Ford-Hutchinson, A.W. *et al., Annu. Rev. Biochem.*, 1994, **63**, 383-417 (*E.C. 1.13.11.34, rev*)
Kuhn, H. *et al., J. Lipid Mediators Cell Signalling*, 1995, **12**, 157-170 (*E.C. 1.13.11.33, rev*)
Radmark, O. *et al., J. Lipid Mediators Cell Signalling*, 1995, **12**, 171-184 (*E.C. 1.13.11.34, rev*)
Yoshimoto, T. *et al., J. Lipid Mediators Cell Signalling*, 1995, **12**, 195-212 (*E.C. 1.13.11.31, rev*)
Yamamoto, S. *et al., Prog. Lipid Res.*, 1997, **36**, 23-41 (*E.C. 1.13.11.31, rev*)
Dailey, L.A. *et al., Curr. Med. Chem.*, 1999, **6**, 389-398 (*E.C. 1.13.11.31, rev*)
Radmark, O. *et al., Prostaglandins Other Lipid Mediat.*, 2002, **68-69**, 211-234 (*E.C. 1.13.11.34, rev*)
Furstenburger, C. *et al., Prostaglandins Other Lipid Mediat.*, 2002, **68-69**, 235-243 (*E.C. 1.13.11.40, rev*)
Yoshimoto, H. *et al., Prostaglandins Other Lipid Mediat.*, 2002, **68-69**, P245-262 (*E.C. 1.13.11.31, rev*)
Kuhn, H. *et al., Prostaglandins Other Lipid Mediat.*, 2002, **68-69**, 263-290 (*E.C. 1.13.11.33, rev*)
Peters-Golden, M. *et al., Prostaglandins, Leukotrienes, Essent. Fatty Acids*, 2003, **69**, 89-97 (*E.C. 1.13.11.34, rev*)

Aragupetrosine A A-631

[125236-58-0]

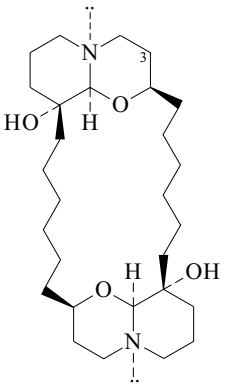


$C_{30}H_{52}N_2O_2$ 472.753
Alkaloid from an Okinawan marine sponge *Xestospongia* sp. Exhibits vasodilatory activity. $[\alpha]_D$ -18.8 ($CHCl_3$).

Kobayashi, M. *et al., Tet. Lett.*, 1989, **30**, 4149 (*isol, ir, pmr, cmr, struct, abs config*)

Araguspongine C A-632

[122908-10-5]



Relative configuration

$C_{28}H_{50}N_2O_4$ 478.714
Alkaloid from an Okinawan marine sponge, *Xestospongia* sp. and from the sponge *Haliclona exigua*. Exhibits vasodilative activity. $[\alpha]_D$ +11.1 ($CHCl_3$).

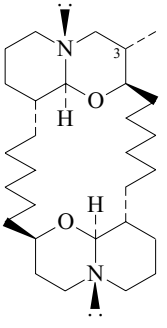
N-*Oxide:* ***Araguspongine L***
$C_{28}H_{50}N_2O_5$ 494.713
Alkaloid from *Xestospongia exigua*. Needles. $[\alpha]_D^{25}$ +1.7 (c, 0.36 in $CHCl_3$).

3α-Methyl: ***3α-Methylaraguspongine C***
[159392-28-6]
$C_{29}H_{52}N_2O_4$ 492.741
Alkaloid from the sponge *Haliclona exigua*. Amorph. solid. $[\alpha]_D$ +1.2 (c, 0.15 in $CHCl_3$).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1676 (*isol, pmr, cmr, struct*)
Venkateswarlu, Y. *et al., J. Nat. Prod.*, 1994, **57**, 1283 (*3α-Methylaraguspongine C*)
Orabi, K.Y. *et al., J. Nat. Prod.*, 2002, **65**, 1782-1785 (*Araguspongines C,L*)

Araguspongine F A-633

[122908-11-6]



Absolute configuration

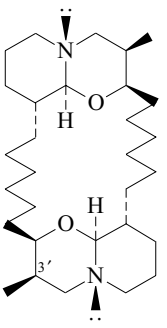
$C_{29}H_{52}N_2O_2$ 460.742
Alkaloid from an Okinawan marine sponge, *Xestospongia* sp. Exhibits vasodilatory activity. $[\alpha]_D$ +8.6 ($CHCl_3$). Work in 1998 suggested that the stereochemistries may require revision.

3-Epimer: ***Araguspongine G***
[123000-04-4]
$C_{29}H_{52}N_2O_2$ 460.742
Alkaloid from *Xestospongia* sp. Shows vasodilatory activity. $[\alpha]_D$ -16 ($CHCl_3$).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1676 (*isol, pmr, cmr, struct, abs config*)
Baldwin, J.E. *et al., J.A.C.S.*, 1998, **120**, 8559-8560 (*configs*)

Araguspongine J A-634

[123000-05-5]



$C_{30}H_{54}N_2O_2$ 474.769
Alkaloid from an Okinawan marine sponge, *Xestospongia* sp. Exhibits vasodilatory activity. $[\alpha]_D$ -23.4 ($CHCl_3$). Work in 1998 suggested that the stereochem. may need revision.

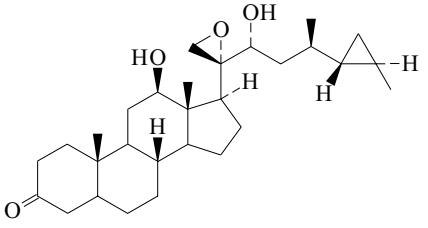
3′-Epimer: ***Araguspongine H***
[122908-12-7]
$C_{30}H_{54}N_2O_2$ 474.769
Alkaloid from *Xestospongia* sp. Shows vasodilatory activity. $[\alpha]_D$ -9 ($CHCl_3$).

3,3′,5,9-Tetraepimer: ***3R,3′R-Dimethylxestospongin C***
[203576-22-1]
$C_{30}H_{54}N_2O_2$ 474.769
Isol. from a *Xestospongia* sp.

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1676 (*isol, ir, pmr, cmr, struct, abs config*)
Reddy, M.V.R. *et al., Nat. Prod. Lett.*, 1997, **11**, 53-59 (*3,3′-Dimethylxestospongin C*)
Baldwin, J.E. *et al., J.A.C.S.*, 1998, **120**, 8559-8560 (*configs*)

Aragusterol A A-635

Aragusterol
[152887-09-7]



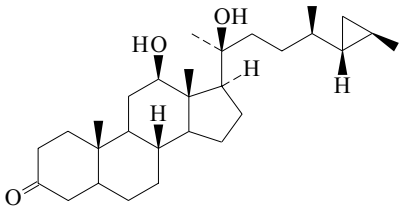
$C_{29}H_{46}O_4$ 458.68
Constit. of a *Xestospongia* sp. Needles.
Mp 157-158°. $[\alpha]_D$ +37.6 (c, 1.06 in $CHCl_3$).

Di-Me ketal: ***Aragusteroketal A***
$C_{31}H_{52}O_5$ 504.749
Constit. of a *Xestospongia* sp. Amorph. solid. $[\alpha]_D^{25}$ +25.3 (c, 0.12 in $CHCl_3$).

Iguchi, K. *et al., Tet. Lett.*, 1993, **34**, 6277 (*isol, pmr, cmr*)
Mitome, H. *et al., Tet. Lett.*, 1995, **36**, 8231 (*synth*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1840 (*Aragusteroketal A*)
Honda, T. *et al., J.C.S. Perkin 1*, 1996, 2291 (*synth*)
Mitome, H. *et al., Bioorg. Med. Chem. Lett.*, 1997, **7**, 691 (*synth*)

Aragusterol B A-636

[156918-74-0]

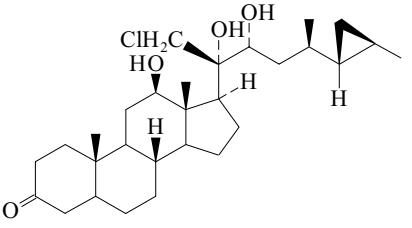


$C_{29}H_{48}O_3$ 444.696
Constit. of a *Xestospongia* sp. Cryst. (EtOAc/hexane).
Mp 194-195°. $[\alpha]_D$ +4 (c, 1.56 in $CHCl_3$).

Iguchi, K. *et al., J.O.C.*, 1994, **59**, 7499 (*isol, pmr, cmr, cryst struct*)
Mitome, H. *et al., Tet. Lett.*, 1995, **36**, 8231 (*synth*)
Honda, T. *et al., J.C.S. Perkin 1*, 1996, 2291 (*synth*)

Aragusterol C A-637

[156009-76-6]



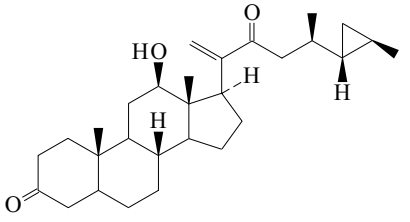
$C_{29}H_{47}ClO_4$ 495.141
Constit. of a *Xestospongia* sp. Cryst.
Mp 204-205°. $[\alpha]_D$ +20.1 (c, 0.35 in $CHCl_3$).

3-Di-Me ketal: ***Aragusteroketal C***
[182889-75-4]
$C_{31}H_{53}ClO_5$ 541.209
Constit. of a *Xestospongia* sp. Amorph. solid. $[\alpha]_D^{25}$ +8 (c, 1.5 in $CHCl_3$).

Shimura, H. *et al., Experientia*, 1994, **50**, 134 (*isol, pmr, cmr, cryst struct*)
Mitome, H. *et al., Tet. Lett.*, 1995, **36**, 8231 (*synth*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1840 (*Aragusteroketal C*)
Honda, T. *et al., J.C.S. Perkin 1*, 1996, 2291 (*synth*)

Aragusterol D A-638

Xestokerol C
[158931-58-9]
[151515-26-3]

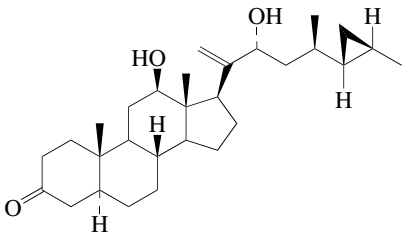


$C_{29}H_{44}O_3$ 440.665
Constit. of a *Xestospongia* sp. Cryst. (MeOH).
Mp 152.5-153.5° (137-140°). $[\alpha]_D$ -61.3 (c, 0.3 in $CHCl_3$). λ_{max} 225 (ϵ 5700) (MeOH) (Berdy).

Kobayashi, J. *et al., J. Nat. Prod.*, 1993, **56**, 1350-1355 (*isol, pmr,cmr*)
Iguchi, K. *et al., J.O.C.*, 1994, **59**, 7499-7502 (*isol, pmr, cmr*)
Mitome, H. *et al., Tet. Lett.*, 1995, **36**, 8231-8234 (*synth*)
Honda, T. *et al., J.C.S. Perkin 1*, 1996, 2291-2296 (*synth*)

Aragusterol E A-639

[171419-86-6]

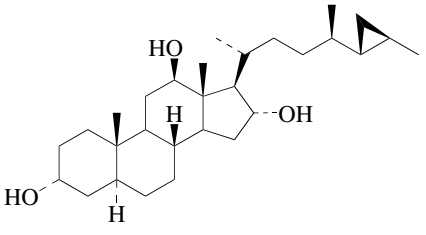


$C_{29}H_{46}O_3$ 442.681
Constit. of *Xestospongia* sp. Glassy solid. $[\alpha]_D$ +12.1 (c, 0.24 in $CHCl_3$).

Miyaoka, H. *et al., Tetrahedron*, 1997, **53**, 5403-5412 (*isol, pmr, cmr*)

Aragusterol G A-640

[189573-86-2]



$C_{29}H_{50}O_3$ 446.712
Constit. of *Xestospongia* sp. Glassy solid. $[\alpha]_D$ +1.6 (c, 0.5 in $CHCl_3$).

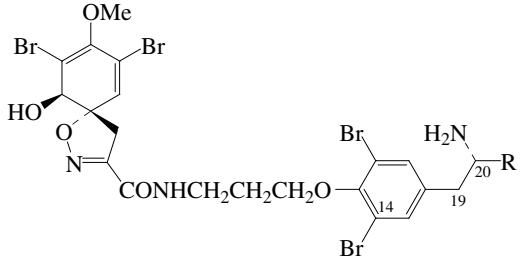
3-Epimer: ***Aragusterol H***
[189573-90-8]
$C_{29}H_{50}O_3$ 446.712
Constit. of a *Xestospongia* sp. Rods.
Mp 189-190°. $[\alpha]_D$ -1.5 (c, 0.13 in $CHCl_3$).

3-Ketone: ***Aragusterol F***
[189573-85-1]
$C_{29}H_{48}O_3$ 444.696
Constit. of a *Xestospongia* sp. Plates.
Mp 168-170°. $[\alpha]_D$ +20.3 (c, 0.79 in $CHCl_3$).

Miyaoka, H. *et al., Tetrahedron*, 1997, **53**, 5403-5412 (*isol, pmr, cmr*)

Araplysillin I A-641

N-*[3-[4-(2-Aminoethyl)-2,6-dibromophenoxy]propyl]-7,9-dibromo-10-hydroxy-8-methoxy-1-oxa-2-azaspiro[4.5]deca-2,6,8-triene-3-carboxamide, 9CI. Hexadellin A*
[129313-98-0]



R = H

$C_{21}H_{23}Br_4N_3O_5$ 717.046

Relatative configs. only known in this series. The compds. covered by this entry have not been correlated. Identity of Araplysillin I and Hexadellin A not confirmed. Isol. from the sponge *Psammaplysilla arabica*. ATPase inhibitor. Shows antimicrobial props. Amorph.
Mp 140-142°. $[\alpha]_D$ -70 (c, 0.7 in MeOH).

N^{20}-*(13-Methyltetradecanoyl):* ***Araplysillin II***
[129277-05-0]
$C_{36}H_{51}Br_4N_3O_6$ 941.431
From the sponge *Psammaplysilla arabica*. ATPase inhibitor. Shows antimicrobial props. Amorph.
Mp 40-42°. $[\alpha]_D$ -38 (c, 0.73 in $CHCl_3$). λ_{max} 270 (ϵ 11650) (MeOH) (Berdy).

N^{20},N^{20}-*Di-Me:* ***Purealidin P***
[167394-81-2]
$C_{23}H_{27}Br_4N_3O_5$ 745.099
Alkaloid from the Okinawan sponge *Psammaplysilla purea*. Cytotoxic against murine lymphoma and human KB carcinoma cells. Oil (as trifluoroacetate). Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D$ +6.6 (c, 0.75 in MeOH). λ_{max} 277 (ϵ 1700); 284 (ϵ 1400) (MeOH) (Berdy).

N^{20},N^{20},N^{20}-*Tri-Me:* ***Purealidin B***
[138590-55-3]
$C_{24}H_{30}Br_4N_3O_5^{\oplus}$ 760.134
Quaternary alkaloid from *Psammaplysilla purea* and *Pseudoceratina verrucosa*. Antibacterial and cytotoxic. Amorph. solid (prob. as trifluoroacetate). $[\alpha]_D^{18}$ -4.5 (c, 1.3 in MeOH). λ_{max} 220 (ϵ 10000); 284 (ϵ 1000) (MeOH) (Berdy).

14-Debromo: ***14-Debromoaraplysillin I***
[136685-29-5]
$C_{21}H_{24}Br_3N_3O_5$ 638.15
From the sponge *Psammaplysilla purpurea*. Glass. $[\alpha]_D$ +21 (c, 0.47 in MeOH/$CHCl_3$). λ_{max} 240 (ϵ 23000); 287 (ϵ 16700) (MeOH) (Berdy).

19-Hydroxy, N^{20}*-Ac:* ***Aplysinamisine III***
[150417-69-9]
$C_{23}H_{25}Br_4N_3O_7$ 775.082
Isol. from the Caribbean sponge *Aplysina cauliformis*. Semisolid. $[\alpha]_D^{26}$ +69 (c, 6.4 in MeOH). λ_{max} 218 (ϵ 14500); 282 (ϵ 5200) (MeOH) (Berdy).

[121135-00-0]

Morris, S.A. *et al., Can. J. Chem.*, 1989, **67**, 677 (*Hexadellin A, isol, ir, pmr, cmr, ms*)
Longeon, A. *et al., Experientia*, 1990, **46**, 548 (*Araplysillin I*)
James, D.M. *et al., J. Nat. Prod.*, 1991, **54**, 1137 (*14-Debromoaraplysillin I*)
Kobayashi, J. *et al., Tetrahedron*, 1991, **47**, 6617 (*Purealdin B, isol, pmr, cmr, uv, ir, ms, cd*)
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 907 (*Aplysinamisine III*)
Kobayashi, J. *et al., Chem. Pharm. Bull.*, 1995, **43**, 403 (*Purealidin P*)

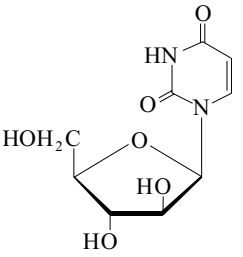
Araplysillin III A-642

[245436-90-2]
As Araplysillin I, A-641 with
R = COOH
$C_{22}H_{23}Br_4N_3O_7$ 761.056
Isol. from the sponge *Aiolochroia crassa*. Amorph. solid. $[\alpha]_D$ +96.3 (c, 0.19 in MeOH). λ_{max} 208 (ϵ 8100); 284 (ϵ 1200) (EtOH).

Gao, H. *et al., Tetrahedron*, 1999, **55**, 9717-9726

Arauridine A-643

1-β-D-Arabinofuranosyl-2,4(1H,3H)-pyrimidinedione, 9CI. 1-β-D-Arabinofuranosyluracil. ***Spongouridine****. Ara-U*
[3083-77-0]



$C_9H_{12}N_2O_6$ 244.204
Isol. from the Caribbean sponge *Cryptotethia crypta* and the gorgonian *Eunicella cavolini*. Drug intermed. Cryst. (MeOH). Sol. H_2O.
Mp 220-221° (226-228°). $[\alpha]_D$ +131.1 (c, 0.63 in H_2O).

▶ Exp. reprod. effects. YQ8818000

2′,3′-Di-Ac: [21016-88-6]
$C_{13}H_{16}N_2O_8$ 328.278
Mp 168-169°.

3′,5′-Di-Ac: [25383-79-3]
$C_{13}H_{16}N_2O_8$ 328.278
Cryst. (C_6H_6/hexane). Mp 78-79°. λ_{max} 258 (ϵ 10000) (MeOH).

2′,3′,5′-Tri-Ac: [14057-18-2]
$C_{15}H_{18}N_2O_9$ 370.315
Cryst. (EtOH). Mp 131-132°. $[\alpha]_D^{20}$ +83.9 (c, 0.5 in MeOH). λ_{max} 259 (EtOH).

5′-Phosphate:
$C_9H_{13}N_2O_9P$ 324.183
$[\alpha]_D^{20}$ +48.15 (H_2O, as Ba salt).

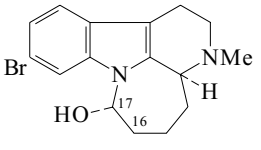
5′-Trityl:
$C_{28}H_{26}N_2O_6$ 486.523
Mp 113-114°.

5′-Trityl, 2′,3′-di-Ac:
$C_{32}H_{30}N_2O_8$ 570.598
Mp 153-154°.

Bergmann, W. *et al., J.O.C.*, 1955, **20**, 1501 (*isol, struct*)
Brown, D.M. *et al., J.C.S.*, 1956, 2388 (*synth*)
Privat de Garilhe, M. *et al., Bull. Soc. Chim. Fr.*, 1968, 1485 (*2′,3′-di-Ac, phosphate, trityl, trityl di-Ac*)
Verheyden, J.P.H. *et al., J.O.C.*, 1970, **35**, 2868 (*3′,5′-di-Ac, 2′-methylphosphonate salt*)
Sherfinski, J. *et al., Acta Cryst. B*, 1974, 873 (*cryst struct*)
Zemlicka, J. *et al., J.A.C.S.*, 1975, **97**, 4089 (*pmr*)
Hruska, F.E. *et al., Can. J. Chem.*, 1982, **60**, 3026 (*pmr, cmr*)
Divakar, K.J. *et al., J.C.S. Perkin 1*, 1982, 1171 (*tri-Ac, synth*)
Cech, D. *et al., J. Prakt. Chem.*, 1983, 325 (*synth*)
Cimino, G. *et al., Experientia*, 1984, **40**, 339-340 (*isol*)
Alder, L. *et al., Z. Chem.*, 1986, **26**, 136 (*ms*)

Arborescidine C A-644

[147395-94-6]



$C_{16}H_{19}BrN_2O$ 335.243
Alkaloid from the marine tunicate *Pseudodistoma arborescens*. Cryst. (MeOH).
Mp 172-173°. $[\alpha]_D$ +3 (c, 1 in $CHCl_3$).

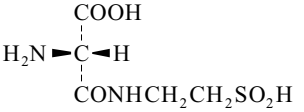
17-Epimer: ***Arborescidine D***
[147512-45-6]
$C_{16}H_{19}BrN_2O$ 335.243
Alkaloid from the marine tunicate *Pseudodistoma arborescens*. Exhibits moderate cytotoxicity *in vitro* against KB human buccal carcinoma. Amorph. solid. λ_{max} 231 (ϵ 29800); 285 (ϵ 8000) (MeOH) (Berdy).

17-Deoxy, 16,17-didehydro: ***Arborescidine B***
[147395-93-5]
$C_{16}H_{17}BrN_2$ 317.228
Alkaloid from *Pseudodistoma arborescens*. Oil. $[\alpha]_D$ +70 (c, 0.6 in $CHCl_2$).

Chbani, M. *et al., J. Nat. Prod.*, 1993, **56**, 99-104 (*isol, cd, uv, ir, pmr, cmr, ms*)
Burm, B.E.A. *et al., Tetrahedron*, 1998, **54**, 6135-6146 (*synth, pmr, cmr*)
Santos, L.S. *et al., J.O.C.*, 2004, **69**, 1283-1289 (*synth*)

Arcamine A-645

3-Oxo-3-[(2-sulfinoethyl)amino]alanine, 9CI

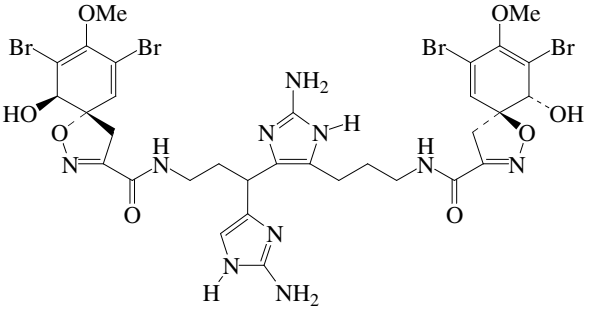


$C_5H_{10}N_2O_5S$ 210.21

(S)-form [56857-48-8]
Isol. from *Arca zebra*. Fish attractant. Syrup.

Sangster, A.W. *et al., Tetrahedron*, 1975, **31**, 1135

Archerine A-646

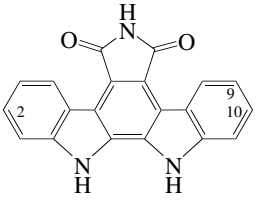


$C_{32}H_{36}Br_4N_{10}O_8$ 1008.315
Isol. from *Aplysina archeri*. Amorph. brown solid. $[\alpha]_D^{25}$ +111.4 (c, 0.07 in MeOH). λ_{max} 221 (ϵ 17600); 279 (ϵ 9500) (MeOH).

Ciminiello, P. *et al., Eur. J. Org. Chem.*, 2001, 55-60

Arcyriaflavin A A-647

12,13-Dihydro-5H-indolo[2,3-a]pyrrolo[3,4-c]carbazole-5,7(6H)-dione, 9CI
[118458-54-1]



$C_{20}H_{11}N_3O_2$ 325.326
Minor pigment from the fruiting bodies of the slime mould *Arcyria denudata*. Also isol. from the tunicate *Eudistoma* sp. and from *Nocardiopsis* sp. Orange solid.
Mp 360°. λ_{max} 235 (log ϵ 4.8); 257 (log ϵ 4.42); 272 (log ϵ 4.45); 281 (log ϵ 4.55); 300 (sh) (log ϵ 4.64); 314 (log ϵ 4.86); 402 (log ϵ 3.81) (MeOH).

N^{12}-*β*-D-*Glucopyranosyl:* ***Antibiotic BMY 41219***. *BMY 41219*. *Didechloro-4′*-O-*demethylrebeccamycin*
[158204-55-8]
$C_{26}H_{21}N_3O_7$ 487.468
Prod. by *Saccharothrix aerocolonigenes*. Orange-yellow powder. Sol. MeOH, DMSO, THF; poorly sol. H_2O. λ_{max} 236 (ϵ 29970); 284 (ϵ 17750); 316 (ϵ 37420); 404 (ϵ 3020) (MeOH).

Deoxo: See Antibiotic K 252c, A-551

2-Hydroxy: ***Arcyriaflavin B***
[73697-64-0]
$C_{20}H_{11}N_3O_3$ 341.325
Isol. from *Arcyria denudata* and *Metatrichia vesparium*. Pale yellow.
Mp 350°. λ_{max} 229 (log ϵ 4.07); 271 (log ϵ 3.7); 280 (log ϵ 3.75); 323 (log ϵ 4.11); 414 (log ϵ 3.19) (MeOH).

1,11-Dihydroxy: ***Antibiotic BE 13793C***. *BE 13793C*. *Antibiotic J 104303*. *J 104303*
[133805-03-5]
$C_{20}H_{11}N_3O_4$ 357.325
Prod. by *Streptomyces mobaraensis* sp. BA-13793. Antitumour agent. Topoisomerase inhibitor. Yellow-orange powder. Sol. THF, DMSO; fairly sol. MeOH; poorly sol. H_2O.
Mp 295°. λ_{max} 245 (ϵ 63500); 298 (ϵ 38100); 307 (ϵ 37400); 325 (sh) (ϵ 21900); 430 (ϵ 5600) (MeOH) (Derep).

▶ NM3457000

2,3-Dihydroxy: ***2,3-Dihydroxyarcyriaflavin A***
$C_{20}H_{11}N_3O_4$ 357.325
Isol. from *Lycogala epidendrum*. Cytotoxic. Amorph. yellow solid. λ_{max} 230 (log ϵ 10.5); 284 (log ϵ 9.8); 330 (log ϵ 10.5) (MeOH).

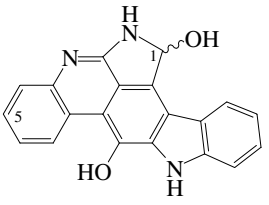
2,9-Dihydroxy: ***Arcyriaflavin D***
[179077-55-5]
$C_{20}H_{11}N_3O_4$ 357.325
Pigment from *Dictydiaethalium plumbeum*. Yellow cryst. powder. Mp >300°.

2,10-Dihydroxy: ***Arcyriaflavin C***
[73697-65-1]
$C_{20}H_{11}N_3O_4$ 357.325
Isol. from *Arcyria denudata*, *Metatrichia vesparium* and *Streptosporangium vulgare* K254. Enzyme inhibitor, calmodulin antagonist, shows insecticidal props. Pale yellow.
Mp 350°. λ_{max} 229 (ϵ 13800); 255 (sh) (ϵ 5890); 270 (ϵ 4570); 280 (ϵ 5010); 318 (sh) (ϵ 12300); 331 (ϵ 19500); 422 (ϵ 2190) (MeOH) (Derep).

Steglich, W. *et al., Angew. Chem., Int. Ed.*, 1980, **19**, 459-460 (*Arcyriaflavins, isol, uv, ir, pmr, struct*)
Bergman, J. *et al., J.O.C.*, 1989, **54**, 824-828 (*synth, ir, pmr*)
Steglich, W. *et al., Pure Appl. Chem.*, 1989, **61**, 281-288 (*Arcyriaflavin D*)
U.S. Pat., 1990, 5 326 754; *CA*, **121**, 221985u (*BMY 41219*)
Kojiri, K. *et al., J. Antibiot.*, 1991, **44**, 723-728 (*BE 13793C*)
Horton, P.A. *et al., Experientia*, 1994, **50**, 843-845 (*isol*)
Ohkubo, M. *et al., Tetrahedron*, 1996, **52**, 8099-8112 (*synth*)
Marques, M.M.B. *et al., Tet. Lett.*, 1999, **40**, 3795-3796 (*synth*)
Ohuchi, T. *et al., J. Antibiot.*, 2000, **53**, 393-403 (*BE13793C, biosynth*)
Bergman, J. *et al., J.C.S. Perkin 1*, 2000, 2609-2614 (*synth*)
Marques, M.M.B. *et al., Tet. Lett.*, 2000, **41**, 9835-9838 (*synth*)
Hosoya, T. *et al., Bioorg. Med. Chem. Lett.*, 2005, **15**, 2776-2780 (*2,3-Dihydroxyarcyriaflavin A*)
Alonso, D. *et al., Tet. Lett.*, 2005, **46**, 4839-4841 (*synth*)

Arcyrin A A-648

*2,9-Dihydro-1*H-*indolo[3,2-*j*]pyrrolo[2,3,4-*gh*]phenanthridine-1,8-diol*



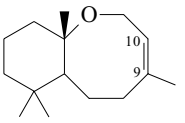
$C_{20}H_{13}N_3O_2$ 327.342
Systematic numbering shown. Isol. from *Arcyria* sp. No phys. props. reported. Not indexed by CAS.

1-Deoxy, 5-hydroxy: ***Arcyrin B***
$C_{20}H_{13}N_3O_2$ 327.342
Isol. from *Arcyria* sp. No phys. props. reported. Not indexed by CAS.

Steglich, W. *et al., Pure Appl. Chem.*, 1989, **61**, 281-288 (*occur*)

Arenaran A A-649

[162559-00-4]



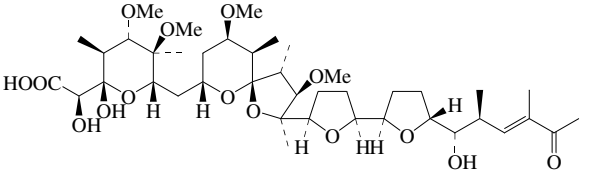
$C_{15}H_{26}O$ 222.37
Constit. of *Dysidea arenaria*. Amorph. solid. $[\alpha]_D$ +154 (c, 0.01 in $CHCl_3$).

9β,10β-Epoxide: ***Arenaran B***
[162559-01-5]
$C_{15}H_{26}O_2$ 238.369
Constit. of *Dysidea arenaria*. Amorph. solid. $[\alpha]_D$ -24.4 (c, 0.23 in $CHCl_3$).

Horton, P.A. *et al., J. Nat. Prod.*, 1995, **58**, 44 (*isol, pmr, cmr*)

Arenaric acid A-650

Antibiotic 27C6
[196202-51-4]
[223392-57-2]

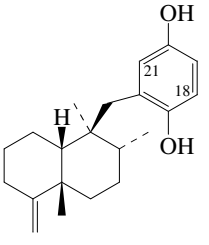


$C_{41}H_{68}O_{15}$ 800.979
Polyether antibiotic. Related to Antibiotic K 41. Prod. by a marine *Streptomyces* sp. (isolate CNH-248). Cryst. (as Na salt). Mp 185-187° Mp 106-108° (Na salt). $[\alpha]_D^{25}$ -17.6 (c, 1.2 in MeOH) (Na salt). λ_{max} 230 (log ϵ 4.54) (MeOH) (Na salt).

Hoshi, M. *et al., J. Antibiot.*, 1997, **50**, 631-634 (*synth*)
Cheng, X.C. *et al., J. Nat. Prod.*, 1999, **62**, 605-607 (*isol, uv, ir, pmr, cmr*)

Arenarol A-651

[87764-13-4]



$C_{21}H_{30}O_2$ 314.467
Constit. of *Dysidea arenaria*. Cryst. (MeOH aq.). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 128-130°. $[\alpha]_D$ +19 (c, 0.1 in $CHCl_3$). λ_{max} 298 (ϵ 3900) (solvent not reported) (Derep). λ_{max} 220 (ϵ 4085); 293 (ϵ 2713); 312 (ϵ 510) (MeOH) (Berdy).

Quinone: ***Arenarone***
[87764-16-7]
$C_{21}H_{28}O_2$ 312.451

Isol. from *Dysidea arenaria*. Yellow oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +8.3 (c, 0.18 in $CDCl_3$). λ_{max} 246 (ϵ 12300); 315 (ϵ 750); 440 (ϵ 30) (solvent not reported) (Derep). λ_{max} 245 (ϵ 4753); 330 (ϵ 245) (MeOH) (Berdy).

Quinone, 19-methoxy, 21-hydroxy: ***21-Hydroxy-19-methoxyarenarone***
[267650-85-1]
$C_{22}H_{30}O_4$ 358.477
Constit. of *Hyrtios tubulatus*. Amorph. solid. λ_{max} 293 (ϵ 6520); 424 (ϵ 240) (MeOH).

Δ^3-Isomer: ***Isoarenarol***
[637774-35-7]
$C_{21}H_{30}O_2$ 314.467
Constit. of *Dysidea arenaria*.

Schmitz, F.J. *et al., J.O.C.*, 1984, **49**, 241-244 (*isol, pmr, cmr*)
Watson, A.T. *et al., J.O.C.*, 1995, **60**, 5102 (*synth*)
Kawano, H. *et al., Tet. Lett.*, 1997, **38**, 7769-7772 (*synth*)
Anderson, J.C. *et al., J.C.S. Perkin 1*, 1998, 2023-2030 (*synth*)
Salmoun, M. *et al., J. Nat. Prod.*, 2000, **63**, 452-456 (*21-Hydroxy-19-methoxyarenarone*)
Yoo, H.-D. *et al., Pharm. Biol.*, 2003, **41**, 223-225 (*Isoarenarol*)

Arenicins A-652

Isol. from coelomocytes of the lugworm *Arenicola marina*. Show antimicrobial and antibacterial activity.

Arenicin 1

$C_{127}H_{193}N_{41}O_{25}S_2$ 2758.313

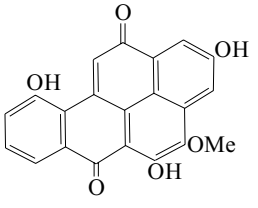
Arenicin 2

$C_{128}H_{195}N_{41}O_{25}S_2$ 2772.34

Ovchinnikova, T.V. *et al., FEBS Lett.*, 2004, **577**, 209-214 (*isol, struct*)

Arenicochromene A-653

*2,5,10-Trihydroxy-4-methoxybenzo[*a*]pyrene-6,12-dione, 9CI*
[27575-46-8]

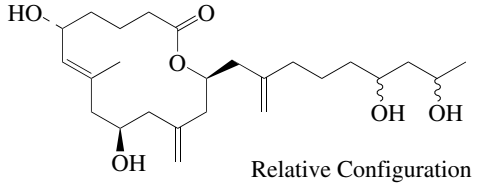


$C_{21}H_{12}O_6$ 360.322
Pigment from *Arenicola marina*.

Tri-Ac: Mp 210-211°.

v. Duijn, P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1952, **71**, 585; 595 (*isol, struct*)
Morimoto, I. *et al., Chem. Comm.*, 1970, 550 (*struct*)

Arenolide A-654

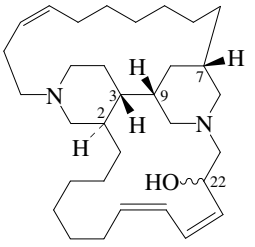


Relative Configuration

$C_{25}H_{42}O_6$ 438.603
Macrolide antibiotic. Isol. from a *Dysidea* sp. from Palau. Shows modest cytotoxic activity. Viscous oil. $[\alpha]_D$ +13 (c, 0.64 in $CHCl_3$). Unstable.

Lu, Q. *et al., J. Nat. Prod.*, 1998, **61**, 1096-1100 (*isol, ir, pmr, cmr, ms*)

Arenosclerin A A-655



$C_{32}H_{54}N_2O$ 482.791
Alkaloid from the sponge *Arenosclera brasiliensis*. Glassy solid. $[\alpha]_D^{25}$ -3 (c, 0.01 in MeOH). λ_{max} 235 (ϵ 15100) (MeOH).

Deoxy: ***Haliclonacyclamine E***
$C_{32}H_{54}N_2$ 466.792
Alkaloid from *Arenosclera brasiliensis*. Glassy solid. $[\alpha]_D^{25}$ +14 (c, 0.02 in MeOH). λ_{max} 236 (ϵ 14900) (MeOH).

Deoxy, 23,24-dihydro: ***Halichondramine***
$C_{32}H_{56}N_2$ 468.808
Alkaloid from *Halichondria* sp. Yellow oil. $[\alpha]_D^{25}$ +3.3 (c, 0.5 in MeOH).

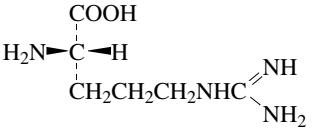
2,3-Diepimer: ***Arenosclerin C***
$C_{32}H_{54}N_2O$ 482.791
Alkaloid from *Arenosclera brasiliensis*. Glassy solid. $[\alpha]_D^{25}$ -17 (c, 0.02 in MeOH). λ_{max} 235 (ϵ 15150) (MeOH).

2,3,7-Triepimer: ***Arenosclerin B***
$C_{32}H_{54}N_2O$ 482.791
Alkaloid from *Arenosclera brasiliensis*. Glassy solid. $[\alpha]_D^{25}$ +8.6 (c, 0.008 in MeOH). λ_{max} 235 (ϵ 15000) (MeOH).

Torres, Y.R. *et al., J. Nat. Prod.*, 2000, **63**, 1098-1105 (*isol*)
Chill, L. *et al., J. Nat. Prod.*, 2002, **65**, 1738-1741 (*Halichondramine*)
Torres, Y.R. *et al., Toxicon*, 2002, **40**, 885-891 (*props*)

Arginine, INN, USAN A-656

2-Amino-5-[(aminoiminomethyl)amino]pentanoic acid. 2-Amino-5-guanidinovaleric acid. Arg
[7004-12-8]



(*S*)-*form*

$C_6H_{14}N_4O_2$ 174.202
Basic genetically coded amino acid. Essential amino acid for human development. Precursor of nitric oxide and is synth. by the body from 2,5-Diaminopentanoic acid, D-122. Diuretic agent. Growth hormone releaser. Immune stimulating agent and wound healing agent. Acidifying agent. Dietary supplement. Ammonia detoxicant (hepatic failure). Diagnostic aid for pituitary function. Log P -4.79 (calc).

(S)-form
L-form. L-Arginine. FEMA 3819
[74-79-3]
Found in seeds/shoots of pine, fir, acacia, arachis etc. and in many proteins. Reagent for the fluorimetric anal. of reducing sugars by hplc. Diagnostic aid (pituitary function determination); ammonia detoxicant; dietary supplement, nutrient. Plates or prisms + $2H_2O$ (H_2O), plates (EtOH). Sol. H_2O (15.0g/100g at 21°).
Mp 207° Mp 244° dec. (anhyd. 105°). $[\alpha]_D$ +21.8 (H_2O). $[\alpha]_D^{25}$ +48.1 (c, 1 in 5*M* HCl). pK_{a1} 2.17; pK_{a2} 9.04; pK_{a3} 12.48 (guanido). Isoelectric point 10.76. Bitter taste. *N*-Protected derivs. useful in peptide synth. have been listed alphabetically elsewhere.

▶ CF1934200

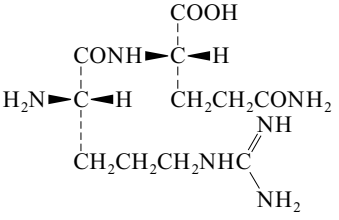
N^2*-(4-Hydroxybenzoyl):* ***N^2-(4-Hydroxybenzoyl)arginine***
[178495-39-1]
$C_{13}H_{18}N_4O_4$ 294.31

Isol. from the ascidian *Leptoclinides dubius*. Sol. MeOH, butanol. $[\alpha]_D^{20}$ +19.5 (c, 2 in MeOH). λ_{max} 210 (log ϵ 3.46); 256 (log ϵ 3.49) (MeOH). λ_{max} 216; 294 (MeOH/NaOH) (Berdy).

[14975-30-5, 32042-43-6, 50912-92-0, 63238-98-2, 78851-84-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 785A; 785D; 786A; 786B; **2**, 259C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1281A (*nmr*)
Org. Synth., 1932, **12**, 4 (*synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 1841 (*rev*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Bak, B. *et al., J. Mol. Spectrosc.*, 1968, **26**, 78 (*pmr*)
Voelter, W. *et al., Z. Naturforsch., B*, 1971, **26**, 213 (*cmr*)
Lehmann, M.S. *et al., J.C.S. Perkin 2*, 1973, 133 (*cryst struct*)
Torgerson, D.F. *et al., Biochem. Biophys. Res. Commun.*, 1974, **60**, 616 (*ms*)
Garcia, A. *et al., J. Nat. Prod.*, 1996, **59**, 782-785 (*4-hydroxybenzoyl*)
Shervington, A. *et al., Anal. Profiles Drug Subst.*, 2001, **27**, 1-32 (*rev*)

N^2-Arginylglutamine A-657



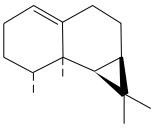
$C_{11}H_{22}N_6O_4$ 302.333

L-L-*form* [2483-17-2]
Isol. from *Euglena gracilis* and from the green algae *Cladophora* spp., *Enteromorpha linza* and *Ulva pertusa*.
Cryst. (EtOH aq.).
Mp 205°.

Ac:
$C_{13}H_{24}N_6O_5$ 344.37
Cryst. (Me_2CO/MeOH). Mp 160°. $[\alpha]_D^{25}$ +19.2 (c, 3.87 in H_2O).

Makisumi, S. *et al., J. Biochem. (Tokyo)*, 1959, **46**, 63 (*isol*)
Berse, C. *et al., Can. J. Chem.*, 1960, **38**, 1946 (*synth*)
Kempner, E.S. *et al., J. Protozool.*, 1974, **21**, 363 (*isol*)
Miyazawa, K. *et al., CA*, 1977, **86**, 167528 (*occur*)

1(10)-Aristolene A-658



(+)–*form*

$C_{15}H_{24}$ 204.355

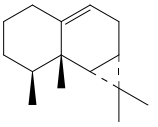
(+)-*form*
ent-form. ***β-Gurjunene***. *Calarene*
[17334-55-3]
Constit. of the essential oils of many plants including gurjun balsam.
Oil. Bp_{13} 120-123°. $[\alpha]_D^{20}$ +81.8.

(-)-*form* [20501-51-3]
Isol. from the grey form of the soft coral *Paraerythropodium fulvum fulvum*, *Pseudopterogorgia americana*, *Eunicea mammosa* and the liverwort *Jungermannia infusa*.
$[\alpha]_D$ -41 (c, 0.3 in CH_2Cl_2). $[\alpha]_D^{25}$ -78.5 (neat).

[73464-47-8]

Narayanan, C.S. *et al., Tetrahedron*, 1964, **20**, 963 (*isol*)
Coates, R.M. *et al., Chem. Comm.*, 1968, 515 (*synth, bibl*)
Weinheimer, A.J. *et al., Chem. Comm.*, 1968, 1070 (*isol, pmr*)
Khoo, S.F. *et al., Tetrahedron*, 1973, **24**, 3379 (*isol*)
Green, D. *et al., J. Nat. Prod.*, 1992, **55**, 1186 (*isol, pmr, cmr*)
Nagashima, K. *et al., Phytochemistry*, 1997, **46**, 1203-1208 (*isol, pmr, cmr*)

9-Aristolene A-659



(+)-*form*

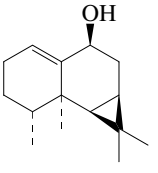
$C_{15}H_{24}$ 204.355

(+)-*form*
ent-*9-Aristolene*. ***α-Ferulene***
[27862-07-3]
Constit. of *Ferula communis*, also isol. from *Acanthella cavernosa* and *Pseudopterogorgia americana*.
Oil. Bp_8 110°. $[\alpha]_D$ +68 (neat). $[\alpha]_D$ +40 (c, 0.1 in $CHCl_3$).

(-)-*form*
Aristolene
[6831-16-9]
Constit. of calarene from sweet flag oil and essence of nard (*Nardostachys jatamansi*).
Oil. $[\alpha]_D$ -98.7 (neat).

Pesnelle, P. *et al., Bull. Soc. Chim. Fr.*, 1963, 912 (*isol*)
Carboni, S. *et al., Tet. Lett.*, 1965, 3017 (*isol*)
Weinheimer, A.J. *et al., Chem. Comm.*, 1968, 1070 (*isol*)
Hirota, H. *et al., Tetrahedron*, 1996, **52**, 2359 (*isol, pmr, cmr*)

1(10)-Aristolen-9-ol A-660



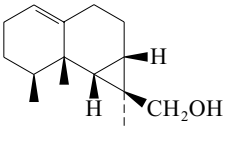
$C_{15}H_{24}O$ 220.354

(ent-9α)-form [150577-91-6]
Constit. of marine algae.

Mayer, A.M.S. *et al., Hydrobiologia*, 1993, **260**, 521-529; *CA*, **119**, 199280v (*isol, pmr*)

1(10)-Aristolen-12-ol A-661

[602278-94-4]



$C_{15}H_{24}O$ 220.354
Constit. of *Bazzania japonica*. Oil. Not clear from ref. if this is 12- or 13-ol.

Ac: [148371-05-5]
$C_{17}H_{26}O_2$ 262.391
Constit. of *Lemnalia africana*. Oil. $[\alpha]_D$ -62 (c, 1 in $CHCl_3$).

12-Aldehyde: ***1(10)-Aristolen-12-al***
[602278-95-5]
$C_{15}H_{22}O$ 218.338
Constit. of *Bazzania japonica*. Oil. Not clear from the ref. if this is 12- or 13-al. It may be identical with 1(10)-Aristolen-13-al.

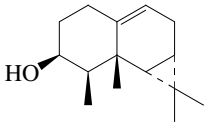
Jurek, J. *et al., J. Nat. Prod.*, 1993, **56**, 508 (*Ac*)
Lu, R. *et al., Phytochemistry*, 2003, **63**, 581 (*Bazzania japonica constits*)

9-Aristolen-1-ol A-662

$C_{15}H_{24}O$ 220.354

(*ent*-1β)-*form* [26128-14-3]
Constit. of *Nardostachys chinensis* and marine algae.
Cryst.
Mp 85°. $[\alpha]_D^{24}$ +35.9 (c, 5.3 in $CHCl_3$).
Teisseire, P. *et al., Recherches*, 1969, **17**, 121 (*synth*)
Rücker, G. *et al., Annalen*, 1971, **748**, 214 (*isol*)
Mayer, A.M.S. *et al., Hydrobiologia*, 1993, **260**, 521-529; *CA*, **119**, 199280v (*isol*)

9-Aristolen-3-ol A-663

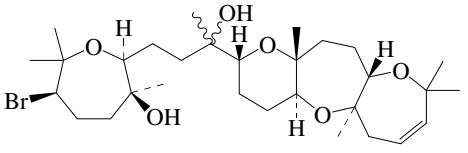


$C_{15}H_{24}O$ 220.354

3β-*form* [74075-09-5]
Constit. of *Lemnalia humesi*.
Cryst.
Mp 83-85°. $[\alpha]_D$ +90.6 (c, 0.2 in $CHCl_3$).
3-Ketone: ***9-Aristolen-3-one***
[74075-08-4]
$C_{15}H_{22}O$ 218.338
Constit. of *Lemnalia humesi*. Solid.
Mp 29-30°. $[\alpha]_D$ +14.3 (c, 0.2 in $CHCl_3$).
Bowden, B.F. *et al., Aust. J. Chem.*, 1980, **33**, 681-684 (*isol, pmr, cmr*)

Armatol A A-664

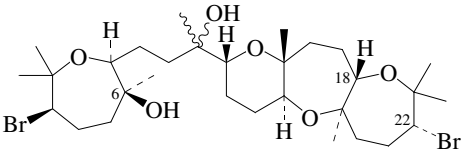
[330938-99-3]



$C_{30}H_{51}BrO_6$ 587.63
Constit. of *Chondria armata*. Oil. $[\alpha]_D$ +43.4 (c, 2 in $CHCl_3$).
Ciavatta, M.L. *et al., Tetrahedron*, 2001, **57**, 617-623 (*isol, pmr, cmr*)

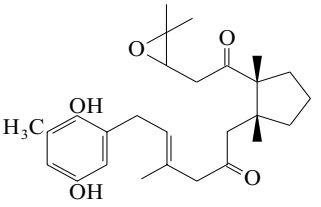
Armatol B A-665

[330939-00-9]



$C_{30}H_{52}Br_2O_6$ 668.545
Constit. of *Chondria armata*. Oil. $[\alpha]_D$ +25.4 (c, 0.4 in $CHCl_3$).
6-Epimer: ***Armatol C***
[330939-01-0]
$C_{30}H_{52}Br_2O_6$ 668.545
Constit. of *Chondria armata*. Oil. $[\alpha]_D$ +20.4 (c, 0.15 in $CHCl_3$).
18-Epimer: ***Armatol F***
[330939-04-3]
$C_{30}H_{52}Br_2O_6$ 668.545
Constit. of *Chondria armata*. Oil. $[\alpha]_D$ +17.9 (c, 1.5 in $CHCl_3$).
22-Epimer: ***Armatol D***
[330939-02-1]
$C_{30}H_{52}Br_2O_6$ 668.545
Constit. of *Chondria armata*. Oil. $[\alpha]_D$ +25.1 (c, 2 in $CHCl_3$).
6,22-Diepimer: ***Armatol E***
[330939-03-2]
$C_{30}H_{52}Br_2O_6$ 668.545
Constit. of *Chondria armata*. Oil. $[\alpha]_D$ +13.6 (c, 0.18 in $CHCl_3$).
Ciavatta, M.L. *et al., Tetrahedron*, 2001, **57**, 617-623 (*isol, pmr, cmr*)

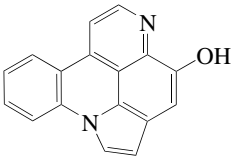
Armentaepoxide A-666



$C_{27}H_{38}O_5$ 442.594
Constit. of *Cystoseira stricta*. Oil. $[\alpha]_D^{20}$ +14.6 (c, 1.25 in EtOH).
Amico, V. *et al., Phytochemistry*, 1987, **26**, 1715 (*isol, pmr*)

Arnoamine A A-667

Pyrido[4,3,2-mn*]pyrrolo[3,2,1*-de*]acridin-4-ol, 9CI. 4-Hydroxypyrido[4,3,2*-mn*]pyrrolo[3,2,1*-de*]acridine, 9CI*
[202652-44-6]

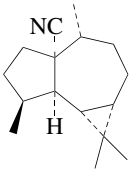


$C_{17}H_{10}N_2O$ 258.279
Alkaloid from the ascidian *Cystodytes* sp. Yellow glass. λ_{max} 278 (log ϵ 4.11); 401 (log ϵ 3.09); 486 (log ϵ 3.17) (trifluoroacetic acid/MeOH). λ_{max} 258 (ϵ 14125); 328 (ϵ 7762); 431 (ϵ 1023) (MeOH) (Berdy).

Me ether: 4-Methoxypyrido[4,3,2-mn*]pyrrolo[3,2,1*-de*]acridine.*
Arnoamine B
[202652-47-9]
$C_{18}H_{12}N_2O$ 272.306
Alkaloid from *Cystodytes* sp. Yellow glass. λ_{max} 280 (log ϵ 4.15); 398 (log ϵ 3.15); 467 (log ϵ 3.22) (trifluoroacetic acid/MeOH). λ_{max} 254 (ϵ 13800); 309 (ϵ 7582); 400 (ϵ 1483) (MeOH) (Berdy).
Plubrukarn, A. *et al., J.O.C.*, 1998, **63**, 1657-1659 (*isol, uv, ir, pmr, cmr, ms*)
Delfourne, E. *et al., J.O.C.*, 2000, **65**, 5476-5479 (*synth*)

Aromadendrane 1-isonitrile A-668

1-Isocyanoaromadendrane



(1α,4β,5α,6β,7β,10α)-*form*

$C_{16}H_{25}N$ 231.38

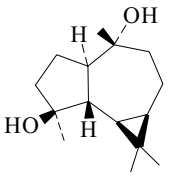
(1α,4β,5α,6β,7β,10α)-*form*
Isothiocyanate:
$C_{16}H_{25}NS$ 263.446
Constit. of *Axinyssa aplysinoides*. Oil. $[\alpha]_D$ +128 (c, 0.24 in $CHCl_3$).

(1β,4β,5α,6β,7β,10β)-*form* [112757-34-3]
Metab. of marine sponge *Acanthella acuta*. Ichthyotoxin, spongicide. Cryst. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 65-66°. $[\alpha]_D$ -13.7 (c, 1.4 in $CHCl_3$).

Isothiocyanate: ***Aromadendrane 1-isothiocyanate****. 1-Isothiocyanatoaromadendrane*
[112767-01-8]
$C_{16}H_{25}NS$ 263.446
Metab. of *Acanthella acuta*. Oil. $[\alpha]_D$ -32.8 (c, 0.7 in $CHCl_3$). Has -NCS replacing -NC.
Mayol, L. *et al., Tetrahedron*, 1987, **43**, 5381-5388 (*Acanthella acuta constits*)
He, H.-Y. *et al., J.O.C.*, 1992, **57**, 3191-3194 (*Axinyssa aplysinoides constit*)

4,10-Aromadendranediol A-669

4,10-Dihydroxyaromadendrane



(1α,4β,5β,6α,7α,10α)–*form*

$C_{15}H_{26}O_2$ 238.369

(1α,4β,5β,6α,7α,10α)-*form* [70051-38-6]
Constit. of *Artemisia adamsii*, *Brasilia sickii* and *Sinularia mayi*.
Cryst.
Mp 132°. $[\alpha]_D^{24}$ -17 (c, 0.1 in $CHCl_3$).

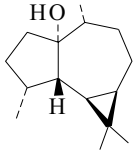
(1α,4β,5β,6α,7α,10β)-*form* [70051-37-5]
Constit. of *Baccharis dracunculifolia* and *Aristolochia heterophylla*.
Cryst.
Mp 136-137°. $[\alpha]_D$ -20.2 (c, 0.24 in $CHCl_3$).

(1β,4α,5α,6α,7α,10β)-*form*
10-Me ether. 10-Methoxy-4-aromadendranol
[279680-98-7]
$C_{16}H_{28}O_2$ 252.396
Constit. of *Lepicolea ochroleuca*. Oil. $[\alpha]_D$ +9.2 (c, 0.085 in CH_2Cl_2).

(1β,4α,5α,6β,7β,10β)-*form* [70000-15-6]
Constit. of *Plagiochila ovalifolia* and *Sinularia mayi*.
Oil.
Mp 134.8-135.5°. $[\alpha]_D$ +22.4 (c, 1.4 in $CHCl_3$).

(1β,4α,5β,6α,7α,10β)-*form*
Alloaromadendrane-4α,10β-diol
[109360-94-3]
Constit. of *Ambrosia peruviana*.
Cryst. Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 112-113°. $[\alpha]_D^{25}$ +7 (c, 0.45 in $CHCl_3$).
Beechan, C.M. *et al., Tetrahedron*, 1978, **34**, 2503 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1983, **22**, 1213 (*isol, struct*)
Goldsby, G. *et al., Phytochemistry*, 1987, **26**, 1059 (*isol, struct*)
Jenniskens, L.H.D. *et al., J.O.C.*, 1991, **56**, 6585 (*synth*)
Nagashima, F. *et al., Phytochemistry*, 1994, **36**, 1425 (*isol, pmr, cmr*)
Wu, T.-S. *et al., Chem. Pharm. Bull.*, 2000, **48**, 357-361 (*isol, pmr, cmr, cryst struct*)
Liu, H.-J. *et al., Phytochemistry*, 2000, **53**, 845-849 (*10-Me ether*)

1-Aromadendranol A-670



(1α,4α,5β,6α,7α,10α)–*form*

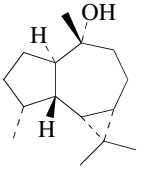
$C_{15}H_{26}O$ 222.37

(1α,4α,5β,6α,7α,10α)-*form*
Palustrol
[5986-49-2]
Constit. of *Baccharis genistelloides* and *Ledum palustre*.
Oil. Bp_2 118°. $[\alpha]_D^{20}$ -17.8.

(1β,4β,5α,6β,7β,10β)-*form*
Constit. of *Cespitularia* aff. *subviridis*.
Oil.
Dolejš, L. *et al., Coll. Czech. Chem. Comm.*, 1961, **26**, 811 (*isol*)
Braekman, J.C. *et al., Bull. Soc. Chim. Belg.*, 1989, **98**, 869 (*isol, cryst struct*)

10-Aromadendranol A-671

*Decahydro-1,1,4,7-tetramethyl-1*H*-cycloprop[e]azulen-4-ol, 9CI*
[19078-39-8]



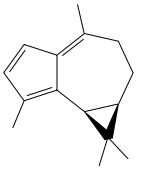
(1α,4α,5β,6α,7α,10α)-*form*

$C_{15}H_{26}O$ 222.37

(1α,4β,5α,6β,7β,10α)-*form*
ent-*Viridiflorol*. *(-)-Viridiflorol*
[64665-36-7]
Constit. of the soft coral *Cespitularia* aff. *subviridis* and the liverworts *Porella canariensis*, *Calypogeia muelleriana* and *Bazzania trilobata*.
$[\alpha]_D^{20}$ -10 (EtOH).

(1β,4α,5β,6β,7β,10α)-*form*
Ledol. *Ledum camphor. Porschcamphor*
[577-27-5]
Constit. of *Ledum palustre* and of *Valeriana officinalis* (valerian), *Baccharis genistelloides*, *Piper* spp., *Aristolochia indica* and others.
Isol. from soft coral *Cespitularia* aff. *subviridis*.
Cryst. (petrol). Mp 105°. Bp 282-283°. $[\alpha]_D$ +8 (EtOH). Stereochem. revised in 2000.
Birch, A.J. *et al., Aust. J. Chem.*, 1955, **8**, 550 (*isol*)
Büchi, G. *et al., Tet. Lett.*, 1959, **No. 6**, 14 (*struct, synth*)
Graham, B.A. *et al., Aust. J. Chem.*, 1960, **13**, 372 (*struct*)
Büchi, G. *et al., J.A.C.S.*, 1969, **91**, 6473 (*synth, abs config*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 1908 (*occur*)
Marshall, J.A. *et al., J.O.C.*, 1974, **39**, 1971 (*synth*)
Braeckman, J.C. *et al., Experientia*, 1977, **33**, 993 (*(-)-Viridiflorol, Ledol, isol, coral*)
El-Seedi, H. *et al., Phytochemistry*, 1994, **35**, 1495 (*Ledol, cmr*)
Wassmuth-Wagner, I. *et al., Planta Med.*, 1995, **61**, 196 (*pmr, cmr*)
Nagashima, F. *et al., Phytochemistry*, 1996, **42**, 1361-1366 (*(-)-Viridiflorol*)
Topçu, G. *et al., Phytochemistry*, 1997, **44**, 1393 (*Ledol, pmr, cmr*)
Warmers, U. *et al., Phytochemistry*, 1998, **49**, 1723-1731; 1999, **52**, 99-104 (*(-)-Viridiflorol*)
Cao, S.-G. *et al., Nat. Prod. Lett.*, 2000, **14**, 447-452 (*Ledol, synth*)
Kaplan, M.A.C. *et al., Phytochemistry*, 2000, **55**, 749-753 (*Ledol, struct, bibl*)

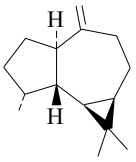
1(10),2,4-Aromadendratriene A-672



$C_{15}H_{20}$ 200.323

(6α,7α)-*form*
Fulfulvene
[144027-73-6]
Constit. of *Parerythropodium fulvum fulvum*.
Yellow-orange oil. $[\alpha]_D$ -437 (c, 0.2 in CCl_4).
Green, D. *et al., J. Nat. Prod.*, 1992, **55**, 1186-1196 (*isol, pmr, cmr*)

10(14)-Aromadendrene A-673



(1α,4α,5β,6α,7α)–*form*

$C_{15}H_{24}$ 204.355

(1α,4α,5β,6α,7α)-*form*
(-)-Aromadendrene. *β-Diploalbicene*
[14682-34-9]
[72747-25-2]
Constit. of *Bixa orellana* (annatto) and *Eucalyptus sideroxylon*.
Oil. $[\alpha]_D$ -11 (EtOH).

10β,14-Epoxide: 10,14-Epoxyaromadendrane. ***Aromadendrene epoxide***
[85710-39-0]
$C_{15}H_{24}O$ 220.354
Constit. of *Thymus borgiae* and hops.

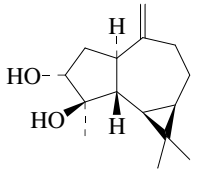
(1β,4α,5β,6β,7β)-*form*
Alloaromadendrene. *α-Aromadendrene*
[25246-27-9]
[72747-25-2]
Constit. of many essential oils incl. *Ledum palustre*, *Croton* spp. *Eucalyptus globulus*, *Metrosideros scandens*, *Perovskia scrophulariaefolia*, *Glycyrrhiza triphylla*. Trace constit. of soft coral *Cespitularia* aff. *subviridis* and gorgonian *Pseudoplexaura flagellosa*.
Oil. Bp_2 96°. $[\alpha]_D^{20}$ -21.6. n_D^{18} 1.5010.

10β,14-Epoxide: ***Alloaromadendrene epoxide***
[85760-81-2]
$C_{15}H_{24}O$ 220.354
Constit. of *Thymus borgiae*.

(1β,4β,5α,6β,7β)-*form*
(+)-Aromadendrene
[489-39-4]
[72747-25-2]
Constit. of *Agathis australis, Artemisia vestita* and *Eucalyptus* oils.
Oil. Bp 260-265°. $[\alpha]_D$ +24.5.

Dolejš, L. *et al., Coll. Czech. Chem. Comm.*, 1960, **25**, 1483 (*isol*)
Büchi, G. *et al., J.A.C.S.*, 1969, **91**, 6473 (*synth, abs config, bibl*)
Braeckman, J.C. *et al., Experientia*, 1977, **33**, 993 (*Alloaromadendrene, isol, coral*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1983, **31**, 892 (*Aromadendrene epoxide*)
Bohlmann, F. *et al., Planta Med.*, 1984, **50**, 1950 (*Alloaromadendrene epoxide*)
Zafra-Polo, M.C. *et al., J. Chromatogr.*, 1990, **518**, 230 (*Aromadendrene epoxide*)
Williams, H.J. *et al., Phytochemistry*, 1995, **40**, 1633 (*pmr, cmr, ms*)
Tanaka, T. *et al., Tetrahedron*, 1996, **52**, 4257 (*synth*)

10(14)-Aromadendrene-3,4-diol A-674



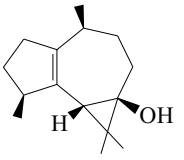
(1α,3α,4β,5β,6β,7β)-*form*

$C_{15}H_{24}O_2$ 236.353

(1α,3α,4β,5β,6β,7β)-*form*
3-Ac: ***3-Acetoxyspathulenol***
[334872-12-7]
$C_{17}H_{26}O_3$ 278.391
Constit. of *Parerythropodium fulvum*. Oil. $[\alpha]_D$ -0.9 (c, 0.29 in $CHCl_3$).

(1β,3α,4α,5α,6α,7α)-*form* [279680-99-8]
Constit. of *Lepicolea ochroleuca*.
Oil. $[\alpha]_D$ -9.9 (c, 0.08 in CH_2Cl_2).
Liu, H.-J. *et al., Phytochemistry*, 2000, **53**, 845-849 (*isol, pmr, cmr*)
Wessels, M. *et al., J. Nat. Prod.*, 2001, **64**, 370-372 (*3-Acetoxyspathulenol*)

1(5)-Aromadendren-7-ol A-675

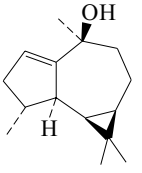


$C_{15}H_{24}O$ 220.354

(4β,6β,7β,10β)-*form*
Constit. of the soft coral *Xenia novae-britanniae.*
Cryst. (EtOAc).
Mp 121-124°. $[\alpha]_D$ +66 (c, 0.1 in $CHCl_3$).
Bowden, B.F. *et al., Aust. J. Chem.*, 1987, **40**, 1483

1-Aromadendren-10-ol A-676

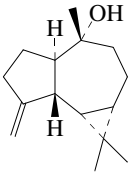
10-Hydroxy-1-aromadendrene



$C_{15}H_{24}O$ 220.354

(4α,5α,6α,7α,10β)-*form* [63181-42-0]
Metab. of *Laurencia subopposita*.
Oil. $[\alpha]_D^{20}$ -46 (c, 1 in $CHCl_3$).
Wratten, S.J. *et al., J.O.C.*, 1977, **42**, 3343

4(15)-Aromadendren-10-ol A-677



(1α,5β,6α,7α,10α)-*form*

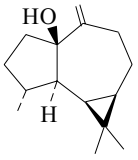
$C_{15}H_{24}O$ 220.354

(1α,5β,6α,7α,10α)-*form*
4(15)-Dehydroglobulol
[133443-03-5]
Isol. from the liverwort *Mylia taylorii*.

(1β,5α,6β,7β,10α)-*form* [680210-17-7]
Constit. of *Clavularia koellikeri*.
Oil. $[\alpha]_D^{25}$ +7.1 (c, 0.21 in $CHCl_3$).

(1β,5β,6α,7α,10α)-*form* [133443-02-4]
Isol. from *Mylia taylorii*.
Matsuo, A. *et al., Proc. Phytochem. Soc. Eur.*, 1990, **29**, 59-69; *CA*, **114**, 182059d
Nagashina, F. *et al., Phytochemistry*, 2001, **56**, 347-352 (*isol*)
Iguchi, K. *et al., J. Nat. Prod.*, 2004, **67**, 577-583 (*isol, pmr, cmr*)

10(14)-Aromadendren-1-ol A-678



(1β,4α,5α,6α,7α)–*form*

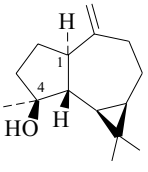
$C_{15}H_{24}O$ 220.354

(1β,4α,5α,6α,7α)-*form*
1β-Hydroxyalloaromadendrene
Metab. of *Laurencia subopposita*.
Oil. $[\alpha]_D^{20}$ +99 (c, 1 in $CHCl_3$).

(1β,4α,5β,6α,7α)-*form* [63181-41-9]
Constit. of *Cassinia subtropica*.
Wratten, S.J. *et al., J.O.C.*, 1977, **42**, 3343
Jakupovic, J. *et al., Phytochemistry*, 1988, **27**, 3831 (*isol, pmr*)

10(14)-Aromadendren-4-ol A-679

[72203-24-8]



(1α,4β,5β,6α,7α)–*form*

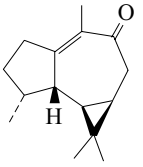
$C_{15}H_{24}O$ 220.354

(1α,4β,5β,6α,7α)-*form*
***Spathulenol*†**
[6750-60-3]
Constit. of the essential oil of *Eucalyptus spathulata* var. *grandiflora* and *Salvia sclarea* (clary sage). Also from *Sinularia kavarattiensis.*
Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane. $[\alpha]_D$ +56.
3,5-Dinitrobenzoyl:
Cryst. Mp 148°.

(1β,4α,5β,6β,7β)-*form*
Espathulenol
Constit. of *Taonia lacheana*.
Cryst.
Mp 102-103°. $[\alpha]_D$ +2 (c, 0.7 in Me_2CO).

(1β,4α,5α,6β,7β)-*form*
ent-*Spathulenol*
[77171-55-2]
Constit. of many liverworts. Possibly an artifact as it is readily produced by autoxidation of bicyclogermacrene.
$[\alpha]_D$ -20 (c, 1 in $CHCl_3$).
Bowyer, R.C. *et al., Chem. Ind. (London)*, 1963, 1245 (*isol, struct*)
Juell, S. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1976, **309**, 458 (*pmr*)
Asakawa, Y. *et al., Phytochemistry*, 1980, **19**, 2141 (*ent-Spathulenol*)
Surburg, H. *et al., Chem. Ber.*, 1981, **114**, 118 (*synth*)
Ulubelen, A. *et al., Phytochemistry*, 1994, **36**, 971 (*isol, pmr, cmr*)
Tringali, C. *et al., Phytochemistry*, 1995, **40**, 827 (*Epispathulenol*)
Toyota, M. *et al., Phytochemistry*, 1996, **41**, 1347 (*ent-Spathulenol*)
Goud, V.T. *et al., Biochem. Syst. Ecol.*, 2002, **30**, 493-495 (*Spathulenol, isol, Sinularia*)

1(10)-Aromadendren-9-one A-680

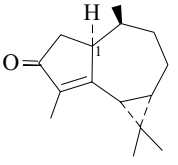


$C_{15}H_{22}O$ 218.338

(4α,5β,6α,7α)-*form*
Squamulosone
[34413-94-0]
Constit. of *Phebalium squamulosum*.
Cryst. (hexane).
Mp 45-46°. $[\alpha]_D$ -234 (c, 1.2 in $CHCl_3$).

(4β,5α,6β,7β)-*form*
Millecrone B
Constit. of *Leminda millecra*.
Oil. $[\alpha]_D$ +151 (c, 0.32 in heptane). λ_{max} 246 (ϵ 5600) (MeOH) (Berdy).
Batey, I.L. *et al., Aust. J. Chem.*, 1971, **24**, 2173

4-Aromadendren-3-one A-681



(1α,6β,7β,10β)–*form*

$C_{15}H_{22}O$ 218.338

(1α,6β,7β,10β)-*form*
(+)-Cyclocolorenone. ent-*Colorenone*
[53584-68-2]
[106190334 (±)-form]
Constit. of *Plagiochila acanthophylla* ssp. *japonica*, *Porella vernicosa*, *Bazzania tridens* and *Nephthea chabrolii*.
Oil. $[\alpha]_D$ +404 (c, 0.9 in $CHCl_3$). λ_{max} 264 (ϵ 12900) (EtOH) (Berdy).

(1β,6α,7α,10α)-*form*
(-)-Cyclocolorenone
[489-45-2]
Constit. of *Pseudowintera colorata* and *Solidago canadensis.*
Phytotoxin. Oil. Bp_5 136-138°. $[\alpha]_D^{20}$ -400 (c, 8.75 in EtOH).
2,4-Dinitrophenylhydrazone:
Red cryst. (EtOAc). Mp 217-218°.

(1α,6α,7α,10α)-*form*
Epicyclocolorenone
[1911-75-7]
Constit. of *Dipterocarpus kerrii.*
Cryst.
Mp 68-68.5°. $[\alpha]_D$ -198 (c, 6.9 in $CHCl_3$).
Corbett, R.E. *et al., J.C.S.*, 1958, 3710-3715 (*Pseudowintera colorata constit*)
Büchi, G. *et al., J.A.C.S.*, 1966, **88**, 3403-3408 (*struct*)
Caine, D. *et al., J.O.C.*, 1972, **37**, 3751-3752 (*synth*)
Matsuo, A. *et al., Experientia*, 1974, **30**, 321-322 (*Plagiochila acanthophylla constit*)
Asakawa, Y. *et al., Phytochemistry*, 1976, **15**, 1929-1931 (*Porella vernicosa constit*)
Saha, M. *et al., Tet. Lett.*, 1986, **27**, 915-918 (*synth*)

Richardson, D.P. *et al., J. Chem. Ecol.*, 1989, **15**, 731-747 (*Dipterocarpus kerrii constit*)
Wu, C.-L. *et al., Phytochemistry*, 1992, **31**, 4213-4217 (*Bazzania tridens constit*)
Banerjee, A.K. *et al., Tetrahedron*, 1993, **49**, 4761-4788 (*synth, rev*)
Stefanello, M.E.A. *et al., Fitoterapia*, 1997, **68**, 475-476 (*cmr*)
Handayani, D. *et al., J. Nat. Prod.*, 1997, **60**, 716-718 (*Nephthea chabrolii constit*)

ARS 2 A-682

Glycoprotein containing 66.9% carbohydrate, mainly D-galactose; MW 63100. Isol. from *Chlorella vulgaris*. Shows antitumour activity. Immunostimulant. Powder. Sol. H_2O.

Noda, K. *et al., Planta Med.*, 1996, **62**, 423-426 (*isol, pmr, cmr*)

Arsenobetaine A-683

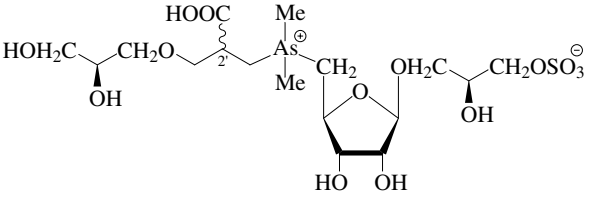
(Carboxymethyl)trimethylarsonium hydroxide inner salt, 9CI
[64436-13-1]
$Me_3As^{\oplus}CH_2COO^{\ominus}$
$C_5H_{11}AsO_2$ 178.062
Constit. of *Panulirus longipes cygnus*. Found in algae, lobsters, sharks and dogfish *Squalus acanthias*, etc. Metab of (2-Hydroxyethyl)trimethylarsonium(1+), H-620. Not produced in mammals. Deliquescent cryst. (Me_2CO/MeOH).
Mp 204-210° dec. Low mammalian toxicity, excreted unchanged e.g. from seafood sources.

▶ LD_{50} (mus, orl) 10000 mg/kg. CH9750000

Hydrobromide: [71642-15-4]
$C_5H_{12}AsBrO_2$ 258.974
Synth. from $AsMe_3$ + $BrCH_2COOH$ in toluene at 5° followed by stirring for 6 h then cooling (-20°; 30 min.). Non-hygroscopic white shiny cryst. (EtOH at 5°).

Edmonds, J.S. *et al., Tet. Lett.*, 1977, 1543-1546 (*synth, pmr, cryst struct*)
Cannon, J.R. *et al., Aust. J. Chem.*, 1981, **34**, 787-798 (*isol, synth*)
Edmonds, J.S. *et al., Chemosphere*, 1981, **10**, 1041-1044 (*isol, ir, pmr*)
Norin, H. *et al., Chemosphere*, 1982, **11**, 287-298 (*isol, ms, pmr, reaction*)
Luten, J.B. *et al., Chemosphere*, 1983, **12**, 131-141 (*isol, ms, reaction*)
Edmonds, J.S. *et al., J.C.S. Perkin 1*, 1983, 2375-2382 (*pmr, cmr*)
Edmonds, J.S. *et al., Appl. Organomet. Chem.*, 1988, **2**, 297-302 (*biosynth, occur, uv*)
Hanaoka, K. *et al., Appl. Organomet. Chem.*, 1988, **2**, 371-376 (*occur, metab*)
Ismail, H. *et al., Pertanika J. Trop. Agric. Sci.*, 1988, **11**, 437-439; *CA*, **112**, 7249 (*synth, cmr*)
Siu, K.W.M. *et al., Rapid Commun. Mass Spectrom.*, 1988, **2**, 69-71 (*ms*)
Beauchemin, D. *et al., J. Anal. At. Spectrom.*, 1989, **4**, 285-289 (*hplc, ms*)
Arsenic Environ., Part II:, (ed. Nriagu, J.O.), J. Wiley, 1994, (*rev, props*)
Minhas, R. *et al., Appl. Organomet. Chem.*, 1998, **12**, 635-641 (*synth, pmr, cmr, ms*)

Sargassum lacerifolium Arsenomethionine A-684



$C_{17}H_{33}AsO_{14}S$ 568.427
Isol. from *Sargassum lacerifolium*. Isol. as a mixt. of C-2′ epimers.

Edmonds, J.S. *et al., Bioorg. Med. Chem. Lett.*, 2000, **10**, 1105-1108 (*isol*)

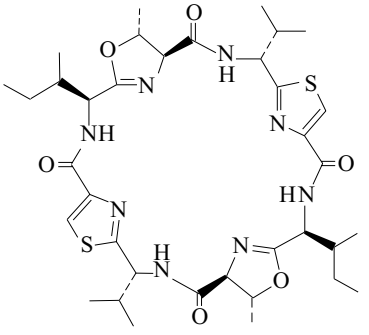
ARYFL amide A-685

[152247-51-3]
Ala-Arg-Tyr-Phe-Leu-NH_2
$C_{33}H_{49}N_9O_6$ 667.807
Isol. from the echiuroid worm *Urechis unicinctus*.

Ikeda, T. *et al., Pept. Chem.*, 1992, **30**, 583-585 (*isol*)

Ascidiacyclamide A-686

[86701-12-4]

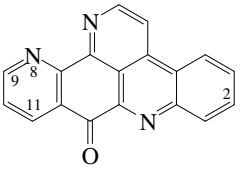


$C_{36}H_{52}N_8O_6S_2$ 756.989
Cyclic peptide antibiotic. Prod. by an unidentified ascidian. Cytotoxic. Active against PV_4 cultured cells transformed with Polyoma virus. Prisms (C_6H_6). Sol. Me_2CO, $CHCl_3$; poorly sol. H_2O.
Mp 245-246° (139-139.5°). $[\alpha]_D^{25}$ +164 (c, 0.466 in $CHCl_3$). λ_{max} 232 (ϵ 21000) (MeOH) (Derep).

Hamamoto, Y. *et al., Chem. Comm.*, 1983, 323-324 (*struct, pmr, cmr*)
Hamada, Y. *et al., Tet. Lett.*, 1985, **26**, 3223 (*synth, config*)
Ishida, T. *et al., J.O.C.*, 1988, **53**, 107 (*struct, conformn*)
In, Y. *et al., Acta Cryst. C*, 1994, **50**, 2015 (*cryst struct*)

Ascididemin A-687

9H-Quino[4,3,2-de][1,10]phenanthrolin-9-one, 9CI. Leptoclinidinone
[114622-04-7]



$C_{18}H_9N_3O$ 283.289
CAS numbering shown. Other systems have been used. Alkaloid from the Okinawan tunicate *Didemnum* sp., *Cystodytes delle chiajei*, *Didemnum rubeum* and the Seychelles tunicate *Eudistoma* sp. Exhibits potent antineoplastic activity. Ca release agent. DNA intercalator and cleavage agent. Yellow solid. Sol. MeOH, EtOAc.
Mp 300°. λ_{max} 220 (ϵ 49500); 248 (ϵ 48000); 273 (sh) (ϵ 27500); 298 (ϵ 17000); 308 (ϵ 15700); 340 (sh) (ϵ 11300); 377 (ϵ 13600) (MeOH) (Derep). λ_{max} 220; 247; 270; 308; 340; 375 (EtOH) (Berdy).

10-Hydroxy: ***11-Hydroxyascididemin***. *Cystodamine*
[129741-41-9]
[158761-11-6]
$C_{18}H_9N_3O_2$ 299.288
Alkaloid from the ascidian *Leptoclinides* sp. and *Cystodytes delle chiajei*. Cytotoxic agent. Yellow amorph. solid.
Mp 250°. Struct. of Cystodamine revised in 2000. λ_{max} 203 (ϵ 25000); 227 (ϵ 38000); 275 (ϵ 18000); 285 (ϵ 17000); 370 (ϵ 11000) (MeOH) (Derep).

10-Hydroxy, 12,13-dihydro: ***8,9-Dihydro-11-hydroxyascididemin***
[151392-04-0]
$C_{18}H_{11}N_3O_2$ 301.304
Alkaloid from the Okinawan marine sponge *Biemna* sp. Cytotoxic agent. Yellow amorph. powder.
Mp 300°. λ_{max} 218 (ϵ 17000); 273 (ϵ 9300); 319 (ϵ 6700); 355 (ϵ 5300) (MeOH) (Berdy).

6-Bromo: ***2-Bromoleptoclinidinone***
[109802-17-7]
$C_{18}H_8BrN_3O$ 362.185

Alkaloid from an ascidian, prob. *Leptoclinides* sp. Toxic to lymphocytic leukaemia cells *in vitro*. Protein phosphatase inhibitor. Yellow powder ($CHCl_3$/MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 300°. Revised struct. λ_{max} 227 (ϵ 152000); 247 (ϵ 27800); 254 (sh) (ϵ 27300); 278 (ϵ 32000); 298 (ϵ 30600); 335 (ϵ 18500); 371 (ϵ 21000) (EtOH) (Derep).

5-Hydroxy: Neocalliactine

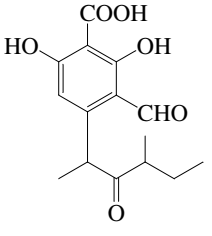
[143370-24-5]

Obt. from Calliactine, C-53 by treatment with dil. acid. Cryst. (CH_2Cl_2/Et_2O)(as Ac). Mp 280-290° (Ac).

Bloor, S.J. *et al., J.A.C.S.*, 1987, **109**, 6134-6136 (*2-Bromoleptoclinidinone*)
Kitahara, Y. *et al., Tetrahedron*, 1987, **53**, 17029-17038 (*Neocalliactine*)
Kobayashi, J. *et al., Tet. Lett.*, 1988, **29**, 1177-1180 (*isol, uv, ir, pmr, cmr, ms, struct*)
Bracher, F. *et al., Heterocycles*, 1989, **29**, 2093-2095 (*synth*)
De Guzman, F.S. *et al., Tet. Lett.*, 1989, **30**, 1069-1070 (*2-Bromoleptoclinidinone, struct*)
Bracher, F. *et al., Annalen*, 1990, 205; 1992, 1205-1207 (*2-Bromoleptoclinidinone, Neocalliactine, synth, ir, pmr, cmr, ms*)
Schmitz, F.J. *et al., J.O.C.*, 1991, **56**, 804-808 (*11-Hydroxyascididemin*)
He, H.-Y. *et al., J.O.C.*, 1991, **56**, 5369-5371 (*isol*)
Moody, C.J. *et al., Tetrahedron*, 1992, **48**, 3589-3602 (*synth*)
Zeng, C.-M. *et al., Tetrahedron*, 1993, **49**, 8337-8342 (*8,9-Dihydro-11-hydroxyascididemin*)
Gellerman, G. *et al., Synthesis*, 1994, 239-241 (*synth*)
Lindsay, B.S. *et al., J. Chem. Crystallogr.*, 1998, **28**, 645-648 (*2-Bromoleptoclinidinone, cryst struct*)
Alvarez, M. *et al., Eur. J. Org. Chem.*, 2000, 849-855 (*synth*)
Delfourne, E. *et al., Tet. Lett.*, 2000, **41**, 3863-3864 (*Cystodamine, struct*)
Alvarez, M. *et al., Tetrahedron*, 2000, **56**, 3703-3708 (*11-Hydroxyascididemin, synth*)
Cuerva, J.M. *et al., J.C.S. Perkin 1*, 2002, 1360-1365 (*synth*)

Ascochital A-688

4-(1,3-Dimethyl-2-oxopentyl)-3-formyl-2,6-dihydroxybenzoic acid



$C_{15}H_{18}O_6$ 294.304

Related to Ascochitin, A-689. Prod. by the marine fungi *Ascochyta salicorniae* and *Kirschsteiniothelia maritima*. Antibacterial agent.

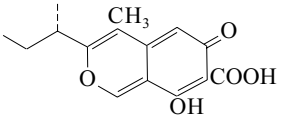
Mp 122-124°. λ_{max} 235; 251; 281; 334 (MeOH).

Kusnick, C. *et al., Pharmazie*, 2002, **57**, 510-512 (*isol, uv, ir, pmr, cmr, ms*)
Siebert, S.F. *et al., Org. Biomol. Chem.*, 2006, **4**, 2233-2240 (*isol*)

Ascochitin A-689

Ascochytin

[3615-05-2]



$C_{15}H_{16}O_5$ 276.288

Tautomerism possible. Metab. of *Ascochyta pisa*, *Ascochyta fabae* and *Ascochyta salicorniae*. Causes brown rot in broad beans. Active against gram-positive and -negative bacteria, and phytopathogen bacteria and fungi. Yellow cryst. Sol. MeOH, Et_2O; poorly sol. H_2O, hexane.

Mp 196-198°. $[\alpha]_D^{25}$ -86 ($CHCl_3$). λ_{max} 220 (ϵ 20617); 286 (ϵ 17550); 415 (ϵ 5700) (EtOH) (Berdy).

▶ Toxic.

Oku, H. *et al., Phytopathology*, 1963, **53**, 1321
Mishima, H. *et al., Sankyo Kenkyusho Nenpo*, 1970, **22**, 67; *CA*, **75**, 48824x (*struct*)
Galbraith, M.N. *et al., J.C.S.(C)*, 1971, 3557 (*synth*)
Colombo, L. *et al., J.C.S. Perkin 1*, 1980, 675; 2549 (*biosynth, cmr, struct*)
Beed, F.D. *et al., Mycol. Res.*, 1994, **98**, 1069 (*manuf*)
Seibert, S.F. *et al., Org. Biomol. Chem.*, 2006, **4**, 2233-2240 (*isol*)

Ascorbate peroxidase A-690

E.C. 1.11.1.11. L-Ascorbate:hydrogen-peroxide oxidoreductase

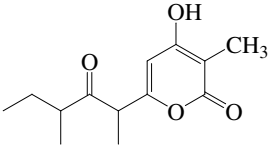
[72906-87-7]

Oxidoreductase enzyme. Isol. from leguminous plants; also from *Euglena gracilis*. Catalyses the reaction of L-ascorbate with H_2O_2 to give L-dehydroascorbate and H_2O.

Shigeoka, S. *et al., Arch. Biochem. Biophys.*, 1980, **201**, 121-127 (*Euglena gracilis*)
Shigeoka, S. *et al., Biochem. J.*, 1980, **186**, 377-380 (*Euglena gracilis*)
Dalton, D.A. *et al., Plant Physiol.*, 1987, **83**, 789-794 (*legumes*)
Marquez, L.A. *et al., FEBS Lett.*, 1996, **389**, 153-156 (*pea*)

Ascosalipyrone A-691

6-(1,3-Dimethyl-2-oxopentyl)-4-hydroxy-3-methyl-2H-pyran-2-one



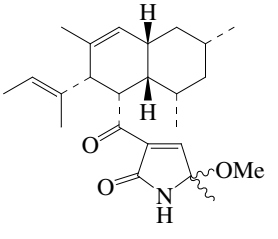
$C_{13}H_{18}O_4$ 238.283

Constit. of *Ascochyta salicorniae* isol. from an *Ulva* sp. Amorph. yellow powder. λ_{max} 210 (log ϵ 3.81); 290 (log ϵ 3.51) (EtOH).

Osterhage, C. *et al., J.O.C.*, 2000, **65**, 6412-6417 (*isol, pmr, cmr*)

Ascosalipyrrolidinone B A-692

[303052-08-6]



$C_{24}H_{35}NO_3$ 385.545

Prod. by the marine fungus *Ascochyta salicorniae*. Powder. Racemic. Related to Oteromycin. λ_{max} 207 (log ϵ 4.38); 225 (log ϵ 4.08); 273 (log ϵ 3.24) (EtOH).

O-*De-Me,* O-*butyl:* ***Ascosalipyrrolidinone A***

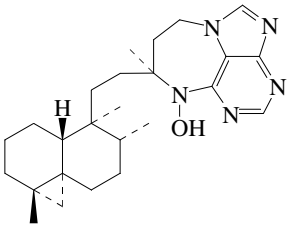
[303052-07-5]

$C_{27}H_{41}NO_3$ 427.626

Prod. by *Ascochyta salicorniae*. Antiplasmodial and antimicrobial agent. Inhibitor of tyrosine kinase. Amorph. powder. $[\alpha]_D^{20}$ -51.3 (c, 0.16 in EtOH). λ_{max} 211 (log ϵ 4.1); 225 (sh) (log ϵ 3.89); 267 (log ϵ 3.08) (EtOH).

Osterhage, C. *et al., J.O.C.*, 2000, **65**, 6412-6417 (*Ascosalipyrrolidinones A,B*)

Asmarine I A-693

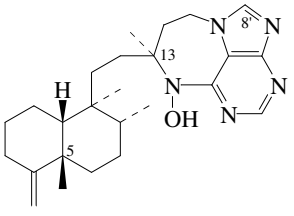


$C_{25}H_{37}N_5O$ 423.6
Alkaloid from the sponge *Raspailia* sp. Oil. $[\alpha]_D^{25}$ +24 (c, 0.6 in MeOH).

Deoxy: ***Asmarine J***
$C_{25}H_{37}N_5$ 407.601
Alkaloid from a *Raspailia* sp. Oil. $[\alpha]_D^{25}$ +20 (c, 0.6 in MeOH).
Rudi, A. *et al., J. Nat. Prod.*, 2004, **67**, 1932-1935 (*isol, pmr, cmr*)

Asmarine B A-694

[208391-67-7]



$C_{25}H_{37}N_5O$ 423.6
Alkaloid from the sponge *Raspailia* sp. Cytotoxic agent. Oil. $[\alpha]_D$ +60 (c, 0.5 in $CHCl_3$). λ_{max} 292 (ϵ 1000) (MeOH) (Berdy).

Deoxy: ***Asmarine K***
$C_{25}H_{37}N_5$ 407.601
Alkaloid from a *Raspailia* sp. Oil. $[\alpha]_D^{25}$ +28 (c, 0.5 in MeOH).

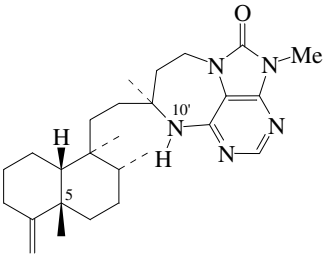
5-Epimer: ***Asmarine A***
[208391-66-6]
$C_{25}H_{37}N_5O$ 423.6
Alkaloid from a *Raspailia* sp. Cytotoxic agent. Cryst. (MeOH). Mp 232°. $[\alpha]_D$ +55 (c, 0.5 in $CHCl_3$). λ_{max} 292 (ϵ 10000) (MeOH) (Berdy).

5-Epimer, Me ether: ***Asmarine G***
[662166-94-1]
$C_{26}H_{39}N_5O$ 437.627
Alkaloid from a *Raspailia* sp. Oil. $[\alpha]_D^{25}$ +40 (c, 1.2 in CH_2Cl_2).

5-Epimer, deoxy: ***Asmarine H***
[662166-95-2]
$C_{25}H_{37}N_5$ 407.601
Alkaloid from a *Raspailia* sp. Oil. $[\alpha]_D^{25}$ +10 (c, 0.37 in CH_2Cl_2).
Yosief, T. *et al., J. Nat. Prod.*, 2000, **63**, 299-304 (*Asmarines A,B, isol, pmr, cmr, cryst struct, activity*)
Rudi, A. *et al., J. Nat. Prod.*, 2004, **67**, 106-109; 1932-1935 (*Asmarines G,H,K*)

Asmarine C A-695

[208391-68-8]



$C_{26}H_{39}N_5O$ 437.627
Alkaloid from the sponge *Raspailia* sp. Oil.

$N^{10'}$*-Methoxy:* ***Asmarine F***
[261630-39-1]
$C_{27}H_{41}N_5O_2$ 467.653
Constit. of a *Raspailia* sp.

5-Epimer: ***Asmarine D***
[261630-37-9]
$C_{26}H_{39}N_5O$ 437.627
Alkaloid from a *Raspailia* sp.

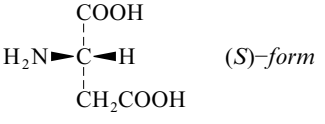
5-Epimer, $N^{10'}$*-methoxy:* ***Asmarine E***
[261630-38-0]
$C_{27}H_{41}N_5O_2$ 467.653
Alkaloid from a *Raspailia* sp.
Yosief, T. *et al., J. Nat. Prod.*, 2000, **63**, 299-304 (*isol, pmr, cmr*)

Asparaginyl-D-tryptophylphenylalaninamide A-696

[201225-56-1]
H-Asn-D-Trp-Phe-NH_2
$C_{24}H_{28}N_6O_4$ 464.523
Isol. from the heart of the sea hare, *Aplysia kurodai*; also isol. from the land snail, *Euhadra congenita* and the freshwater snail, *Lymnaea stagnalis*. Cardioactive neuropeptide.
Morishita, F. *et al., Biochem. Biophys. Res. Commun.*, 1997, **240**, 354-358 (*isol*)
Morishita, F. *et al., Pept. Sci.*, 1998, **35**, 165-168 (*activity*)
Morishita, F. *et al., Peptides (N.Y.)*, 2003, **24**, 1533-1544 (*isol*)

Aspartic acid, INN, USAN A-697

Aminobutanedioic acid, 9CI. Aminosuccinic acid. Asparagic acid. Asparaginic acid. Asp
[6899-03-2]



(S)–form

$C_4H_7NO_4$ 133.104

(R)-form
D-form
[1783-96-6]
Obt. from bacterial hydrolysates and from the red alga *Chondria armata*. Sol. H_2O, HCl; insol. EtOH, Et_2O.
Mp 251°. $[\alpha]_D$ -5.05 (c, 1 in H_2O). $[\alpha]_D$ -25.4 (c, 1 in 5*M* HCl).
▶ CI9097500

N-*Me: (Methylamino)butanedioic acid*. N-*Methyl-D-aspartic acid, 9CI. NMDA*
[6384-92-5]
$C_5H_9NO_4$ 147.13
Isol. from the mollusc *Scapharca broughtonii* and from the green alga *Bryopsis plumosa*. NMDA receptor competitive agonist.
Cryst. + $1H_2O$ (EtOH aq.).
Mp 190°. $[\alpha]_{578}^{25}$ -17.1 (c, 1.49 in H_2O). $[\alpha]_D$ -30 (5*M* HCl).
▶ CI9457000

(S)-form
L-form. FEMA 3656
[56-84-8]
Found in sugar cane and sugar beet molasses and proteins/peptides. Made comly. by biotransformation of ammonium fumarate using *Escherichia alcalescens* immobilised on polymer gel. Glutamate receptor agonist. Dietary supplement, nutrient.
Leaflets (H_2O). Spar. sol. H_2O (0.5g/100g at 25°).
Mp 269-271° dec. $[\alpha]_D^{25}$ +5.05 (c, 1 in H_2O). $[\alpha]_D$ +25.4 (c, 1 in 5*M* HCl). pK_{a1} 2.09 (COOH); pK_{a2} 3.86 (4-COOH); pK_{a3} 9.82 (1-COOH) (25°). Isoelectric point 2.77. Bitter taste.
▶ LD_{50} (mus, ipr) 6000 mg/kg. CI9098500

[1115-63-5, 3792-50-5, 14007-45-5, 17090-93-6, 17833-53-3]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 496C; 496D; 497A (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 588D; 589A; 589B (*ir*)
Vickery, H.B. *et al., Biochem. Prep.*, 1952, **2**, 71-73 (*L-form, synth*)
Takemoto, T. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1960, **293**, 627-633 (*isol, D-form*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 1856-1878; 2759 (*synth, resoln, rev*)
Watkins, J.C. *et al., J. Med. Chem.*, 1962, **5**, 1187-1199 (*N-Me, synth*)
Org. Synth., Coll. Vol., 4, 1963, 55-58 (*synth*)
Fujiwara, S. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 344-349 (*pmr*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679-681 (*cd*)
Young, D.P. *et al., Chem. Ind. (London)*, 1967, 1251 (*synth*)
Zintel, J.A. *et al., Can. J. Chem.*, 1969, **47**, 411-415 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 2369 (*occur*)
Rao, S.T. *et al., Acta Cryst. B*, 1973, **29**, 1718-1720 (*cryst struct*)
Sergeev, G.M. *et al., CA*, 1977, **89**, 208521r (*use*)
Hardin, E.D. *et al., Anal. Chem.*, 1981, **53**, 1492-1497 (*ms*)
Harada, K. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 653-654 (*resoln*)
Sawka-Dobrowolska, W. *et al., Acta Cryst. C*, 1990, **46**, 1679 (*N-Me, cryst struct*)
Euerby, M.R. *et al., J. Chromatogr.*, 1990, **502**, 226-229 (*N-Me, tlc, enantiomers*)
The NMDA Receptor, (Eds. Collingridge, G.L. *et al*), Oxford University Press, 1994, (*book*)
Castro, J.L. *et al., J. Mol. Struct.*, 1995, **349**, 113-116 (*ir, Raman*)
GulzarM.S. *et al., J.C.S. Perkin 1*, 1997, 649-655 (*N-Me, N,N-di-Me, N-Et, N-methoxy, synth, ir, pmr, cmr, ms*)

Aspartocin†, INN, USAN A-698

4-L-Asparagineoxytocin. A 8999

[4117-65-1]

H-Cys-Tyr-Ile-Asn-Asn-Cys-Pro-Leu-Gly-NH_2

$C_{42}H_{64}N_{12}O_{12}S_2$ 993.173

Reduced form shown. Isol. from the spiny dogfish (*Squalus acanthias*) and *Streptomyces griseus*. Antibacterial agent.

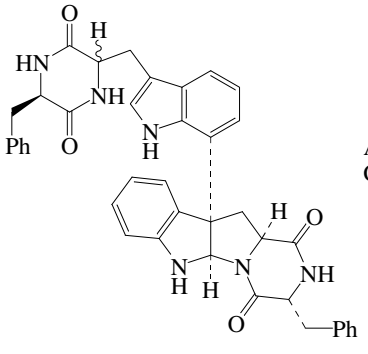
▶ RS7535000

[1402-89-7, 30769-11-0]

Acher, R. *et al., Eur. J. Biochem.*, 1972, **29**, 12 (*isol*)
Hruby, V.J. *et al., J.A.C.S.*, 1979, **101**, 202 (*cmr*)
Gazis, D. *et al., Int. J. Pept. Protein Res.*, 1989, **34**, 353 (*props*)

Asperazine A-699

[198953-76-3]



Absolute Configuration

$C_{40}H_{36}N_6O_4$ 664.762

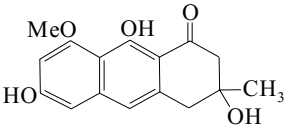
Alkaloid from the sponge-derived culture of *Aspergillus niger*. Amorph. powder. $[\alpha]_D$ +53 (c, 0.2 in MeOH). λ_{max} 225; 285; 300 (MeOH).

Varoglu, M. *et al., J.O.C.*, 1997, **62**, 7078-7079 (*isol, uv, ir, pmr, ms*)
Govek, S.P. *et al., J.A.C.S.*, 2001, **123**, 9468-9469 (*synth*)

Asperflavin A-700

3,4-Dihydro-3,6,9-trihydroxy-8-methoxy-3-methylanthracen-1(2H)-one, 9CI

[38371-01-6]



$C_{16}H_{16}O_5$ 288.299

(+)-form

Constit. of *Aspergillus flavus*, *Aspergillus repens*, *Leucopaxillus tricolor* and *Microascus tardifaciens*. Mycotoxin. Immunosuppressant. Yellow needles (EtOAc). Sol. MeOH, bases; poorly sol. H_2O, hexane.

Mp 180° Mp 225-230°. $[\alpha]_D$ +4 (c, 0.3 in MeOH). $[\alpha]_D$ +89 (c, 0.2 in MeOH). Differences in phys. props. between the isolates suggest partial racemates. λ_{max} 232 (log ϵ 4.23); 270 (log ϵ 4.56); 318 (log ϵ 3.68); 332 (log ϵ 3.57); 389 (log ϵ 4.02) (MeOH). λ_{max} 230 (ϵ 13500); 269 (ϵ 32360); 317 (ϵ 43600); 335 (ϵ 28200); 392 (ϵ 8130) (MeOH) (Berdy).

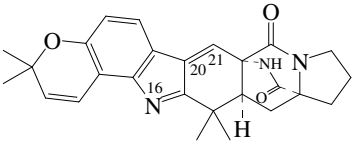
6-O-α-D-Ribofuranoside:

$C_{21}H_{24}O_9$ 420.415

Prod. by the marine-derived *Microsporum* sp. Yellow oil. $[\alpha]_D^{20}$ +23.8 (c, 0.2 in MeOH). λ_{max} 225 (log ϵ 0.91); 269 (log ϵ 1.22); 312 (log ϵ 0.44); 388 (log ϵ 0.62) (MeOH).

Grove, J.F. *et al., J.C.S. Perkin 1*, 1972, 2406-2411 (*isol*)
Fujimoto, H. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1426-1432 (*isol, uv, pmr, cmr, cd*)
Li, Y. *et al., Chem. Pharm. Bull.*, 2006, **54**, 882-883 (*riboside*)

Aspergamide B A-701



Relative Configuration

$C_{26}H_{27}N_3O_3$ 429.518

Prod. by *Aspergillus ochraceus*. No phys. props. reported.

N^{16}-Oxide: ***Avrainvillamide****. CJ 17665. Antibiotic CJ 17665*

[269741-97-1]

$C_{26}H_{27}N_3O_4$ 445.517

Prod. by a marine *Aspergillus* sp. CNC358 and *Aspergillus ochraceus* CL 41582. Cytotoxic and antibacterial agent. Powder or yellow gum. $[\alpha]_D^{25}$ +12 (c, 0.6 in MeOH). λ_{max} 280 (ϵ 6300); 370 (ϵ 2720) (MeOH).

16,21-Dihydro: ***Stephacidin A***

[360765-74-8]

$C_{26}H_{29}N_3O_3$ 431.533

Prod. by *Aspergillus ochraceus* WC 76466. Cytotoxic. Amorph. solid. λ_{max} 211 (log ϵ 3.96); 242 (log ϵ 4.54); 309 (log ϵ 4.54); 335 (sh) (log ϵ 3.64) (MeOH).

20β-Hydroxy, 20,21-dihydro, N^{16}-oxide: ***Aspergamide A***

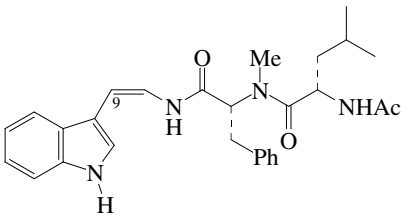
$C_{26}H_{29}N_3O_5$ 463.532

Prod. by *Aspergillus ochraceus*. No phys. props. reported.

U.S. Pat., 2000, 6 066 635; *CA*, **132**, 346709r (*Avrainvillamide*)
Sugie, Y. *et al., J. Antibiot.*, 2001, **54**, 911-916 (*CJ 17665*)
U.S. Pat., 2001, 6 291 461; *CA*, **135**, 2364119 (*Stephacidin A*)
Qian-Cutrone, J. *et al., J.A.C.S.*, 2002, **124**, 14556-14557 (*Stephacidin A*)
Von Nussbaum, F. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 3068-3071 (*rev*)
Baran, P.S. *et al., J.A.C.S.*, 2006, **128**, 8678-8693 (*Stephacidin A, Avrainvillamide, synth*)

Aspergillamide A A-702

[217489-31-1]



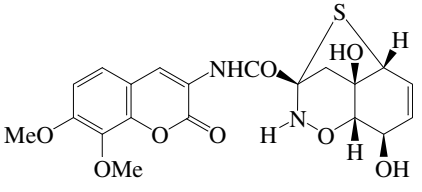
$C_{28}H_{34}N_4O_3$ 474.602

Prod. by a marine *Aspergillus* sp. Cytotoxic agent. Amorph. powder. $[\alpha]_D$ -26.2 (c, 3.05 in MeOH). Exists as a 1:1 mixt. of *cis*- and *trans*-amide rotational conformers. λ_{max} 200 (log ϵ 4.68); 221 (log ϵ 4.59); 286 (log ϵ 4.44) (MeOH).

(E)-Isomer: ***Aspergillamide B***
[217489-32-2]
$C_{28}H_{34}N_4O_3$ 474.602
Prod. by a marine *Aspergillus* sp. Amorph. powder.

Toske, S.G. *et al., Tetrahedron*, 1998, **54**, 13459-13466 (*isol*)
Rivas, L. *et al., Tet. Lett.*, 2002, **43**, 7639-7641 (*Aspergillamide B, synth*)
Su, S. *et al., Tetrahedron*, 2003, **59**, 8931-8946 (*synth, pmr, cmr*)

Aspergillazine A A-703

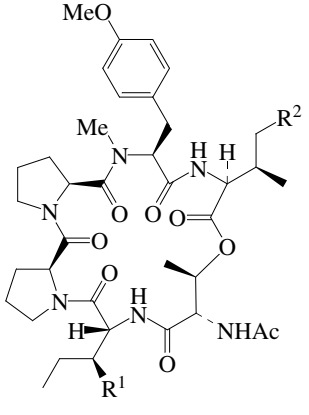


$C_{20}H_{20}N_2O_8S$ 448.453

Related to Trichodermamide A, T-492. Prod. by *Aspergillus unilateralis* (MST-F8675) and the marine-derived *Spicaria elegans*. Cytotoxic. Amorph. yellow solid. $[\alpha]_D$ -103 (c, 0.14 in MeOH). $[\alpha]_D$ -366.4 (c, 0.11 in MeOH). λ_{max} 205 (ϵ 19270); 245 (sh); 337 (ϵ 11100) (MeOH). λ_{max} 270 (log ϵ 3.95); 338 (log ϵ 4.29) (MeOH).

Liu, R. *et al., Arch. Pharmacal Res.*, 2005, **28**, 1042-1046 (*isol, pmr, cmr, ms*)
Capon, R.J. *et al., Org. Biomol. Chem.*, 2005, **3**, 123-129 (*isol, pmr, cmr*)

Aspergillicin A A-704



Absolute Configuration

$R^1 = CH_3$, $R^2 = H$

$C_{38}H_{56}N_6O_9$ 740.895

Prod. by a marine-derived *Aspergillus carneus*. Solid. $[\alpha]_D^{20}$ -51.9 (c, 0.03 in MeOH). λ_{max} 212 (ϵ 9870); 227 (ϵ 7530); 277 (ϵ 990); 283 (ϵ 870) (MeOH).

Demethoxy: ***Aspergillicin C***
$C_{37}H_{54}N_6O_8$ 710.869
Prod. by a marine-derived *Aspergillus carneus*. Isol. as a mixt. with Aspergillicin D.

Demethoxy, N*-de-Me:* ***Aspergillicin D***
$C_{36}H_{52}N_6O_8$ 696.842
Prod. by a marine-derived *Aspergillus carneus*. Isol. as a mixt. with Aspergillicin C.

Capon, R.J. *et al., Org. Biomol. Chem.*, 2003, **1**, 1856-1862 (*isol, pmr, cmr, ms*)

Aspergillicin B A-705

As Aspergillicin A, A-704 with
$R^1 = R^2 = H$

$C_{37}H_{54}N_6O_9$ 726.868
Prod. by a marine-derived *Aspergillus carneus*. Solid. $[\alpha]_D^{20}$ -46.6 (c, 0.02 in MeOH). λ_{max} 210 (ϵ 9800); 225 (ϵ 7500); 277 (ϵ 980); 283 (ϵ 880) (MeOH).

Capon, R.J. *et al., Org. Biomol. Chem.*, 2003, **1**, 1856-1862 (*isol, pmr, ms*)

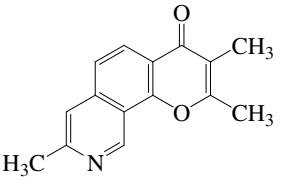
Aspergillicin E A-706

As Aspergillicin A, A-704 with
$R^1 = R^2 = CH_3$

$C_{39}H_{58}N_6O_9$ 754.922
Prod. by a marine-derived *Aspergillus carneus*. Solid.

Capon, R.J. *et al., Org. Biomol. Chem.*, 2003, **1**, 1856-1862 (*isol, pmr*)

Aspergillitine A-707

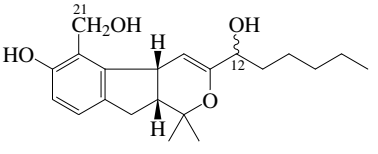


$C_{15}H_{13}NO_2$ 239.273

Prod. by the fungus *Aspergillus versicolor* isol. from the sponge *Xestospongia exigua*. Yellow powder (MeOH). λ_{max} 214; 245; 265; 295; 315; 370 (MeOH aq.).

Lin, W. *et al., J. Nat. Prod.*, 2003, **66**, 57-61 (*isol, pmr, cmr, ms*)

Aspergillodiol A-708



Relative Configuration

$C_{21}H_{30}O_4$ 346.466

Prod. by the marine *Aspergillus versicolor*.

21-Aldehyde: ***Aspergillol***
$C_{21}H_{28}O_4$ 344.45
Prod. by *Aspergillus versicolor*.

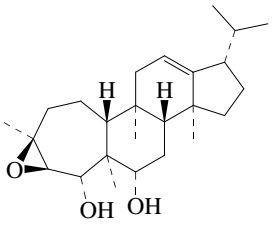
21-Aldehyde, 12-Ac: ***12-O-Acetylaspergillol***
$C_{23}H_{30}O_5$ 386.487
Prod. by *Aspergillus versicolor*.

12-Ketone, 21-aldehyde: ***Aspergillone***
$C_{21}H_{26}O_4$ 342.434
Prod. by *Aspergillus versicolor*. Amorph. solid. λ_{max} 220; 263; 350 (no solvent reported).

Lin, W.H. *et al., Chin. Chem. Lett.*, 2001, **12**, 435-438

Aspergilloxide A-709

[436144-24-0]

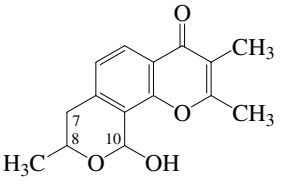


$C_{25}H_{40}O_3$ 388.589
Metab. of a marine derived *Aspergillus* sp. Amorph. powder. $[\alpha]_D$ -29 (c, 0.65 in CH_2Cl_2). λ_{max} 227 (log ϵ 5.4) ($CHCl_3$).

Cueto, M. *et al., Org. Lett.*, 2002, **4**, 1583-1585 (*isol, pmr, cmr*)

Aspergione B A-710

*7,8-Dihydro-10-hydroxy-2,3,8-trimethyl-4*H*-benzo[2,1-*b*:3,4-c′]dipyran-4-one*



$C_{15}H_{16}O_4$ 260.289
Struct. was incorrectly reported in a preliminary communication.
Prod. by *Aspergillus versicolor* isol. from *Xestospongia exigua*. Amorph. solid (MeOH). $[\alpha]_D^{20}$ +1.9 (c, 1.6 in MeOH). λ_{max} 231; 291; 352 (MeOH aq.).

Me ether: ***Aspergione A***
$C_{16}H_{18}O_4$ 274.316
Prod. by *Aspergillus versicolor* isol. from *Xestospongia exigua*. Amorph. solid (MeOH). $[\alpha]_D^{20}$ +8.8 (c, 0.28 in MeOH). λ_{max} 235; 291; 350 (MeOH aq.).

*7,8-Didehydro, Me ether: 10-Methoxy-2,3,8-trimethyl-4*H*,10*H*-benzo[2,1-*b*:3,4-c′]dipyran-4-one.* ***Aspergione C***
$C_{16}H_{16}O_4$ 272.3
Prod. by *Aspergillus versicolor* isol. from *Xestospongia exigua*. Amorph. yellow solid (MeOH). $[\alpha]_D^{20}$ +1.9 (c, 0.58 in MeOH).

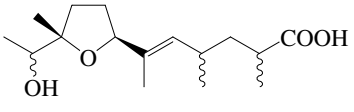
*7,8-Didehydro, ketone: 2,3,8-Trimethyl-4*H*,10*H*-benzo[2,1-*b*:3,4-c′]dipyran-4,10-dione.* ***Aspergione D***
$C_{15}H_{12}O_4$ 256.257
Prod. by *Aspergillus versicolor* isol. from *Xestospongia exigua*. Amorph. solid (MeOH). λ_{max} 211; 270; 325; 335; 390 (MeOH aq.).

10-Deoxy, 8-hydroxy: ***Aspergione F***
$C_{15}H_{16}O_4$ 260.289
Prod. by *Aspergillus versicolor* isol. from *Xestospongia exigua*. Amorph. solid (MeOH). $[\alpha]_D^{20}$ -1.7 (c, 1.5 in MeOH). λ_{max} 235; 291; 350 (MeOH aq.).

10-Deoxy, 8-methoxy: ***Aspergione E***
$C_{16}H_{18}O_4$ 274.316
Prod. by *Aspergillus versicolor* isol. from *Xestospongia exigua*. Amorph. solid (MeOH). $[\alpha]_D^{20}$ +2.5 (c, 0.6 in MeOH). λ_{max} 235; 291; 350 (MeOH aq.).

Lin, W. *et al., J. Nat. Prod.*, 2003, **66**, 57-61 (*isol, pmr, cmr, ms*)

Asperic acid A-711

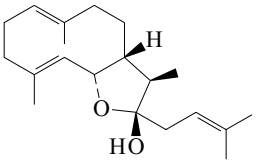


$C_{16}H_{28}O_4$ 284.395
Isol. from *Aspergillus niger* derived from the sponge *Hyrtios proteus*. Yellow wax. $[\alpha]_D$ +35 (c, 0.5 in CH_2Cl_2). λ_{max} 225; 280 (no solvent reported).

Varoglu, M. *et al., J. Nat. Prod.*, 2000, **63**, 41-43 (*isol, pmr, cmr*)

Asperketal A A-712

[114763-50-7]



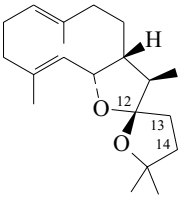
$C_{20}H_{32}O_2$ 304.472
Constit. of *Eunicea asperula*. Cryst.
Mp 75-77°. $[\alpha]_D^{20}$ +75 (c, 0.97 in C_6H_6).

Me ether: ***Asperketal C***
[114763-52-9]
$C_{21}H_{34}O_2$ 318.498
Constit. of *Eunicea asperula*. Cryst.
Mp 72-73°. $[\alpha]_D^{20}$ +190 (c, 1.88 in C_6H_6).

Shin, J. *et al., J.O.C.*, 1988, **53**, 3271 (*isol, pmr, cmr*)

Asperketal D A-713

[114763-53-0]



$C_{20}H_{32}O_2$ 304.472
Constit. of *Eunicea asperula*. Cryst.
Mp 75-76°. $[\alpha]_D^{20}$ +126 (c, 0.6 in C_6H_6).

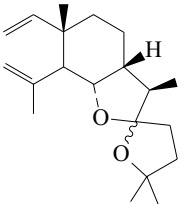
12-Epimer: ***Asperketal E***
[114818-67-6]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Eunicea asperula*. Oil. $[\alpha]_D^{20}$ +54 (c, 0.57 in C_6H_6).

13,14-Didehydro: ***Asperketal B***
[114763-51-8]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Eunicea asperula*. Cryst.
Mp 62-63°. $[\alpha]_D^{20}$ +88 (c, 0.65 in C_6H_6).

Shin, J. *et al., J.O.C.*, 1988, **53**, 3271 (*isol, pmr, cmr*)

Asperketal F A-714

[114763-54-1]

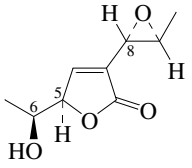


$C_{20}H_{32}O_2$ 304.472
Constit. of *Eunicea asperula*. Cryst.
Mp 54-55°. $[\alpha]_D^{20}$ +71 (c, 0.77 in C_6H_6).

Shin, J. *et al., J.O.C.*, 1988, **53**, 3271 (*isol, pmr, cmr*)

Asperlactone A-715

*5-(1-Hydroxyethyl)-3-(3-methyloxiranyl)-2(5*H*)-furanone, 9CI. 5-(1-Hydroxyethyl)-3-(2,3-epoxypropyl)butenolide*
[76375-62-7]



Absolute Configuration

$C_9H_{12}O_4$ 184.191
Metab. of *Aspergillus melleus* and *Aspergillus ochracens*. Shows bactericidal and fungicidal activity. Yellow oil. $Bp_{0.4}$ 140°. $[\alpha]_D$ +61.8 (c, 0.11 in $CHCl_3$).

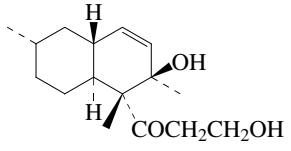
*Deepoxy, 8ξ-chloro, 9ξ-hydroxy: 3-(1-Chloro-2-hydroxypropyl)-5-(1-hydroxyethyl)-2(5*H*)-furanone.* ***8-Chloro-9-hydroxy-8,9-deoxyasperlactone***
$C_9H_{13}ClO_4$ 220.652
Prod. by a marine *Aspergillus ostianus* strain TUF 01F313. Antibacterial agent. $[\alpha]_D^{24}$ +22.5 (c, 0.17 in $CHCl_3$). λ_{max} 230 (ϵ 2500) (MeOH/$CHCl_3$).

*Deepoxy, 9ξ-chloro, 8ξ-hydroxy: 3-(2-Chloro-1-hydroxypropyl)-5-(1-hydroxyethyl)-2(5*H*)-furanone.* ***9-Chloro-8-hydroxy-8,9-deoxyasperlactone***
$C_9H_{13}ClO_4$ 220.652
Prod. by a marine *Aspergillus ostianus* strain TUF 01F313. Antibacterial agent. $[\alpha]_D^{26}$ +76 (c, 0.01 in $CHCl_3$). λ_{max} 230 (ϵ 2300) (MeOH/$CHCl_3$).

5,6-Diepimer: ***Isoasperlactone***
[91840-97-0]
$C_9H_{12}O_4$ 184.191
From *Aspergillus melleus*. Yellow oil. $[\alpha]_D$ -51.6 (c, 0.124 in $CHCl_3$).

Garson, M.J. *et al., J.C.S. Perkin 1*, 1984, 1021 (*isol, struct*)
Brereton, R.G. *et al., J.C.S. Perkin 1*, 1984, 1027 (*biosynth*)
Ahmed, S.A. *et al., Chem. Comm.*, 1985, 1685 (*biosynth*)
Staunton, J. *et al., Chem. Comm.*, 1991, 1106 (*biosynth*)
Torres, M. *et al., Pestic. Sci.*, 1998, **53**, 9-14 (*activity*)
Namikoshi, M. *et al., J. Antibiot.*, 2003, **56**, 755-761 (*Chlorohydroxydeoxyasperlactones*)

Aspermytin A A-716



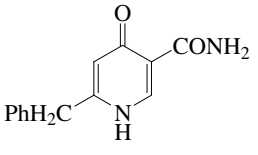
Absolute Configuration

$C_{16}H_{26}O_3$ 266.38
Prod. by a marine-derived *Aspergillus* sp. Neurotrophic agent. $[\alpha]_D^{25}$ +1.2 (c, 0.1 in $CHCl_3$). λ_{max} 201 (log ϵ 3) (MeOH).

Tsukamoto, S. *et al., Bioorg. Med. Chem. Lett.*, 2004, **14**, 417-420 (*isol, pmr, cmr*)

Aspernigrin A A-717

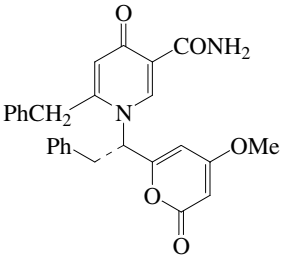
*1,4-Dihydro-4-oxo-6-(phenylmethyl)-3-pyridinecarboxamide. 2-Benzyl-5-carbamoyl-4(1*H*)-pyridinone*



$C_{13}H_{12}N_2O_2$ 228.25
Struct. revised in 2005. Prod. by *Aspergillus niger* isol. from the sponge *Axinella damicornis*. Also prod. by a terrestrial *Cladosporium herbarum* IFB-E002. Prisms ($CHCl_3$/MeOH). Mp 197-199°. λ_{max} 217 (log ϵ 4.25); 257 (log ϵ 4.68) (MeOH).

Hiort, J. *et al., J. Nat. Prod.*, 2004, **67**, 1532-1543; 2005, **68**, 1821 (*isol, pmr, cmr*)
Ye, Y.H. *et al., J. Nat. Prod.*, 2005, **68**, 1106-1108 (*isol, pmr, cmr, ms, cryst struct*)

Aspernigrin B A-718



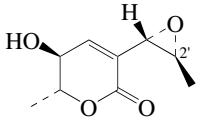
Absolute Configuration

$C_{27}H_{24}N_2O_5$ 456.497
Struct. revised in 2005. Prod. by *Aspergillus niger* isol. from the sponge *Axinella damicornis*. Neuroprotective agent. Oil. $[\alpha]_D^{20}$ +37.8 (c, 0.5 in DMSO).

Hiort, J. *et al., J. Nat. Prod.*, 2004, **67**, 1532-1543; 2005, **68**, 1821 (*isol, cd, pmr, cmr*)

Aspyrone A-719

*5,6-Dihydro-5-hydroxy-6-methyl-3-(3-methyloxiranyl)-2*H*-pyran-2-one, 9CI. 3-(1,2-Epoxypropyl)-5,6-dihydro-5-hydroxy-6-methyl-2*H*-pyran-2-one, 8CI*
[17398-00-4]



Absolute Configuration

$C_9H_{12}O_4$ 184.191
Isol. from *Aspergillus melleus, Aspergillus elegans* and *Aspergillus ochraceus*. Weak broad-spectrum antibiotic. Cryst. (C_6H_6 or Me_2CO/petrol).
Mp 112-112.5°. $[\alpha]_D$ -14 (c, 1 in EtOH). λ_{max} 204 (ϵ 12000) (MeOH) (Derep).

Ac: [17397-86-3]
Needles. Mp 65-67°.

*Deepoxy, 2′S-hydroxy: 5,6-Dihydro-5-hydroxy-3-(2-hydroxypropyl)-6-methyl-2*H*-pyran-2-one.* ***Dihydroaspyrone***
$C_9H_{14}O_4$ 186.207
Prod. by *Aspergillus ochraceus*.
$[\alpha]_D^{20}$ +17.8 (c, 0.7 in MeOH). λ_{max} 204 (log ϵ 3.69) (MeOH).

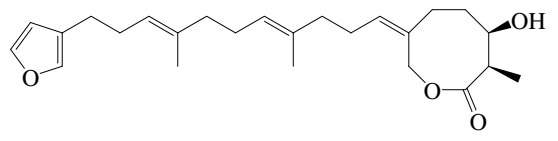
*Deepoxy, 2′ξ-chloro, 1′ξ-hydroxy: 3-(2-Chloro-1-hydroxypropyl)-5,6-dihydro-5-hydroxy-6-methyl-2*H*-pyran-2-one.* ***9-Chloro-8-hydroxy-8,9-deoxyaspyrone***
$C_9H_{13}ClO_4$ 220.652
Prod. by a marine *Aspergillus ostianus* strain TUF 01F313. Antibacterial agent. $[\alpha]_D^{25}$ +17.2 (c, 0.17 in $CHCl_3$). λ_{max} 230 (ϵ 1600) (MeOH/$CHCl_3$).

Mills, S.D. *et al., J.C.S.(C)*, 1967, 2242 (*isol*)
Rosenbrook, W. *et al., Tet. Lett.*, 1970, 1867 (*isol, uv, ir, ms, pmr*)
Moore, J.H. *et al., J. Agric. Food Chem.*, 1974, **22**, 697 (*isol*)
Simpson, T.J. *et al., Tet. Lett.*, 1975, 4693 (*cmr, biosynth*)
Tanabe, M. *et al., Heterocycles*, 1976, **5**, 355 (*isol, cmr, biosynth*)
Lesage, S. *et al., Can. J. Chem.*, 1978, **56**, 3117 (*cmr*)
Holker, J.S.E. *et al., J.C.S. Perkin 1*, 1981, 1397 (*cmr, biosynth*)
Nair, M.S.R. *et al., J. Nat. Prod.*, 1982, **45**, 644 (*biosynth*)
Copeland, R.J. *et al., J.C.S. Perkin 1*, 1984, 1013; 1021 (*isol, cryst struct, biosynth*)
Ahmed, S.A. *et al., Chem. Comm.*, 1985, 1685 (*biosynth*)

Staunton, J. *et al., Chem. Comm.*, 1991, 1106; 1108; 1110; 1113 (*biosynth*)
Sugiyama, T. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1921 (*synth, ir, pmr, bibl*)
Kimura, y. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 1375 (*isol, uv, ir, pmr, cmr*)
Fuchser, J. *et al., Liebigs Ann./Recl.*, 1997, 87 (*isol, uv, pmr, cmr, Dihydroaspyrone*)
Namikoshi, M. *et al., J. Antibiot.*, 2003, **56**, 755-761 (*Chlorohydroxydeoxyaspyrone*)

Astakolactin A-720

[508226-57-1]

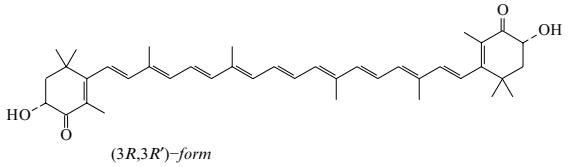


$C_{25}H_{36}O_4$ 400.557
Constit. of *Cacospongia scalaris*. Oil. $[\alpha]_D$ -36 (c, 0.05 in CH_2Cl_2).

Tsoukatou, M. *et al., J. Nat. Prod.*, 2003, **66**, 444-446 (*isol, pmr, cmr*)

Astaxanthin A-721

3,3′-Dihydroxy-β,β-carotene-4,4′-dione. 3,3′-Dihydroxycanthaxanthin. 3,3′-Dihydroxy-4,4′-diketo-β-carotene. Ovoester
[7542-45-2]



(3*R*,3*R*′)–*form*

$C_{40}H_{52}O_4$ 596.848

(3*R*,3′*R*)-*form* [60760-95-4]
Isol. from the yeast *Phaffia rhodozyma*.
Mp 222-223°. CD:$\Delta\epsilon_{385}$ -6.2, $\Delta\epsilon_{324}$ +24.0. λ_{max} 492 ($CHCl_3$).

(3*S*,3′*S*)-*form* [472-61-7]
Prosthetic group of carotenoprotein Alloporin ex *Allopora californica*.
Mp 223-225°. λ_{max} 472 (MeOH) (Berdy). λ_{max} 466 (hexane) (Berdy). λ_{max} 485 ($CHCl_3$) (Berdy). λ_{max} 492 ($CHCl_3$).

3-O-*β*-D-*Glucopyranoside:*
$C_{46}H_{62}O_9$ 758.99
Constit. of *Agrobacterium aurantiacum*. λ_{max} 487 (C_6H_6).

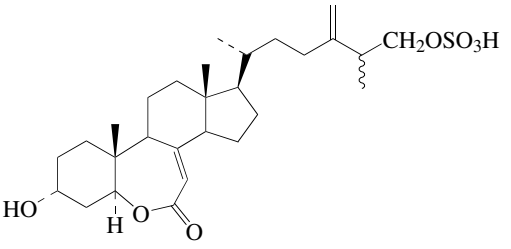
(3′*RS*,3′*SR*)-*form* [71772-51-5]
Isol. from lobster shells and lobster eggs along with both enantiomers. 85% of carotenoid content of alga *Pleurastrum tercinoideum*. Used in fish farming to induce trout flesh colouring.
Mp 216-219°. Meso-isomer.

[74601-68-6]

Andrewes, A.G. *et al., Phytochemistry*, 1976, **15**, 1009 (*isol*)
Muller, R.K. *et al., Helv. Chim. Acta*, 1980, **63**, 1654 (*hplc, isol, isom*)
Zell, R. *et al., Helv. Chim. Acta*, 1981, **64**, 2447 (*synth*)
Renstrom, B. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **71**, 249 (*isol, isomers*)
Berger, H. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **71**, 253 (*isol*)
Yokoyama, A. *et al., J. Nat. Prod.*, 1995, **58**, 1929 (*glucoside*)
Choi, S. *et al., J.O.C.*, 2005, **70**, 3328-3331 (*synth*)
Hussein, G. *et al., J. Nat. Prod.*, 2006, **69**, 443-449 (*rev*)

Asterasterol A A-722

[193008-25-2]

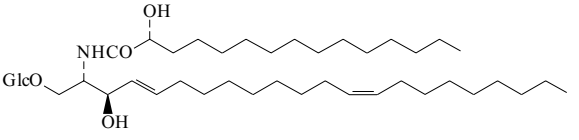


$C_{28}H_{44}O_7S$ 524.717
Constit. of an Antarctic starfish (Asteriidae).
$[\alpha]_D$ +4.5.

De Marino, S. *et al., Tetrahedron*, 1997, **53**, 8625-8628 (*isol, pmr, cmr*)

Asteriacerebroside A A-723

[134178-88-4]

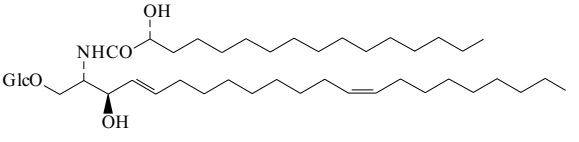


$C_{43}H_{81}NO_9$ 756.114
Glycosphingolipid. Isol. from the starfish *Asterias amurensis versicolor*. Needles + $4H_2O$ (MeOH).
Mp 182-184°. $[\alpha]_D^{25}$ +8.5 (c, 0.27 in 1-propanol).

Higuchi, R. *et al., Annalen*, 1991, 745-752 (*isol, pmr, cmr, struct*)

Asteriacerebroside B A-724

[134178-89-5]

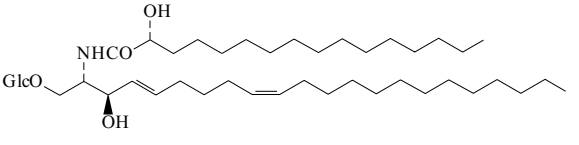


$C_{44}H_{83}NO_9$ 770.141
Glycosphingolipid. Isol. from the starfish *Asterias amurensis versicolor*. Needles + $3H_2O$ (MeOH).
Mp 178-180°. $[\alpha]_D^{25}$ +8.3 (c, 0.28 in 1-propanol).

Higuchi, R. *et al., Annalen*, 1991, 745-752 (*isol, pmr, cmr, struct*)

Asteriacerebroside C A-725

[134178-90-8]

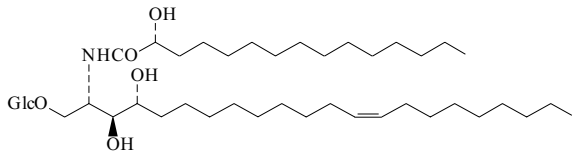


$C_{44}H_{83}NO_9$ 770.141
Glycosphingolipid. Isol. from the starfish *Asterias amurensis versicolor*. Needles + $3H_2O$ (MeOH).
Mp 183-186°. $[\alpha]_D^{25}$ +9.4 (c, 0.28 in 1-propanol).

Higuchi, R. *et al., Annalen*, 1991, 745-752 (*isol, pmr, cmr, struct*)

Asteriacerebroside D **A-726**

[134178-91-9]



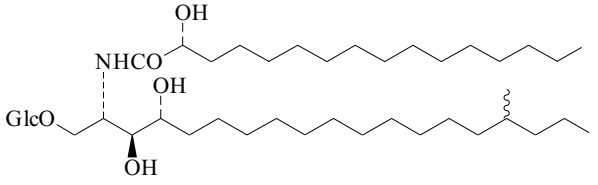
$C_{43}H_{83}NO_{10}$ 774.129

Glycosphingolipid. Isol. from the starfish *Asterias amurensis versicolor*. Needles + $2H_2O$ (MeOH).
Mp 174-176°. $[\alpha]_D^{25}$ +10.5 (c, 0.4 in 1-propanol).

Higuchi, R. *et al., Annalen*, 1991, 745-752 (*isol, pmr, cmr, struct*)

Asteriacerebroside E **A-727**

[134178-92-0]



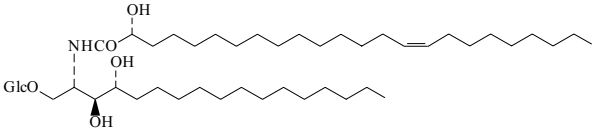
$C_{42}H_{83}NO_{10}$ 762.118

Glycosphingolipid. Isol. from the starfish *Asterias amurensis versicolor*. Needles + $1H_2O$ (MeOH).
Mp 216-218°. $[\alpha]_D^{25}$ +12.2 (c, 0.32 in 1-propanol).

Higuchi, R. *et al., Annalen*, 1991, 745-752 (*isol, pmr, cmr, struct*)

Asteriacerebroside F **A-728**

[134178-93-1]



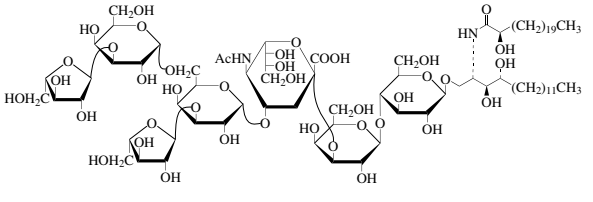
$C_{47}H_{91}NO_{10}$ 830.237

Glycosphingolipid. Isol. from the starfish *Asterias amurensis versicolor*. Needles + $4H_2O$ (MeOH).
Mp 167-169°. $[\alpha]_D^{25}$ +12.6 (c, 0.33 in 1-propanol).

Higuchi, R. *et al., Annalen*, 1991, 745-752 (*isol, pmr, cmr, struct*)

Asterinaganglioside A **A-729**

[131489-38-8]

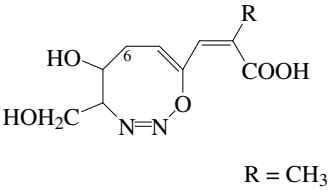


$C_{83}H_{150}N_2O_{41}$ 1832.087

Constit. of the starfish *Asterias pectinifera*. Amorph. powder.
Mp 163-165°. $[\alpha]_D^{24}$ +19.9 (c, 0.1 in H_2O).

Higuchi, R. *et al., Annalen*, 1991, 1 (*isol, ir, struct*)

Asterionellin A **A-730**



$R = CH_3$

$C_{10}H_{14}N_2O_5$ 242.231

Isol. from an *Asterionella* sp. Not indexed by CAS.

Shimizu, Y. *et al., Chem. Rev.*, 1993, **93**, 1685-1698

Asterionellin B **A-731**

As Asterionellin A, A-730 with
R = H

$C_9H_{12}N_2O_5$ 228.204

Isol. from the microalga *Asterionella* sp. Antibiotic.

6-Hydroxy: ***Asterionellin C***
$C_9H_{12}N_2O_6$ 244.204
Isol. from *Asterionella* sp.

Shimizu, Y. *et al., Chem. Rev.*, 1993, **93**, 1685-1698

Asterubin **A-732**

2-[[(Dimethylamino)iminomethyl]amino]ethanesulfonic acid, 9CI
[6249-86-1]

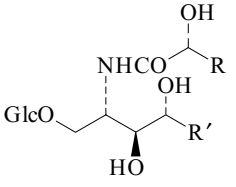
$HN{=}C(NMe_2)NHCH_2CH_2SO_3H$

$C_5H_{13}N_3O_3S$ 195.242

Isol. from starfish. Needles (MeOH aq.).
Mp 272-273° dec.

Ackermann, D. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1935, **232**, 206; **235**, 233 (*isol, synth*)

Astrocerebrosides **A-733**



A, R = $(CH_2)_{12}CH_3$,
R′ = $(CH_2)_4CH{=}CH(CH_2)_{11}CH_3$ (*Z*–)
B, R = $(CH_2)_{13}CH_3$,
R′ = $(CH_2)_4CH{=}CH(CH_2)_{11}CH_3$ (*Z*–)
C, R = $(CH_2)_{21}CH_3$, R′ = $(CH_2)_{10}CH(CH_3)_2$

Isol. from $CHCl_3$/MeOH extract of the starfish *Astropecten latespinosus*.

Astrocerebroside A [126665-07-4]

$C_{43}H_{83}NO_{10}$ 774.129
Needles + $1H_2O$ (MeOH). Mp 188-192°. $[\alpha]_D^{25}$ +10.3 (c, 1 in 1-propanol).

Astrocerebroside B [122823-41-0]

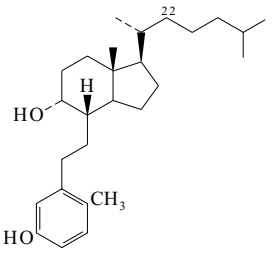
$C_{44}H_{85}NO_{10}$ 788.156
Needles + $3H_2O$ (MeOH). Mp 198-202°. $[\alpha]_D^{25}$ +10.8 (c, 1 in 1-propanol).

Astrocerebroside C [122823-47-6]

$C_{47}H_{93}NO_{10}$ 832.252
Needles + $2H_2O$ (MeOH). Mp 218-219°. $[\alpha]_D^{25}$ +10.7 (c, 1 in 1-propanol).

Higuchi, R. *et al., Annalen*, 1990, 659-663

Astrogorgiadiol A-734



$C_{27}H_{44}O_2$ 400.643
Metab. of gorgonian *Astrogorgia* sp. Inhibits cell division in fertilised starfish eggs. Solid. Sol. MeOH, $CHCl_3$, Et_2O; poorly sol. H_2O. $[\alpha]_D$ -16.4 (c, 0.058 in $CHCl_3$). λ_{max} 218 (ϵ 7080); 281 (ϵ 2291) (MeOH) (Berdy).

9-Ketone: ***Calicoferol E***
$C_{27}H_{42}O_2$ 398.628
Constit. of a gorgonian *Muricella* sp. Cryst. (Me_2CO/hexane). Mp 94-95°. $[\alpha]_D^{25}$ +21.4 (c, 0.6 in $CHCl_3$).

24,25-Didehydro: 9,10-Secocholesta-1,3,5(10),24-tetraene-3,9-diol. ***Calicoferol G***
[214962-74-0]
$C_{27}H_{42}O_2$ 398.628
Constit. of a *Muricella* sp. Oil. $[\alpha]_D^{25}$ -7.5 (c, 0.1 in $CHCl_3$). λ_{max} 218 (log ϵ 3.85); 281 (log ϵ 3.38) (MeOH).

*22,23-Didehydro(22*E*-), 9-ketone:* ***Calicoferol A***
$C_{27}H_{40}O_2$ 396.612
Constit. of *Calicogorgia* sp. Solid. $[\alpha]_D^{15}$ +4.2 (c, 0.24 in $CHCl_3$). λ_{max} 218 (ϵ 4980); 280 (ϵ 1730) (EtOH) (Berdy).

16β-Hydroxy, 9-ketone: 3,16-Dihydroxy-9,10-secocholesta-1,3,5(10)-trien-9-one. ***Calicoferol I***
[214962-76-2]
$C_{27}H_{42}O_3$ 414.627
Constit. of a *Muricella* sp. Oil. $[\alpha]_D^{25}$ +18.4 (c, 0.1 in $CHCl_3$). λ_{max} 218 (log ϵ 3.82); 283 (log ϵ 3.32) (MeOH).

Fusetani, N. *et al., Tet. Lett.*, 1989, **30**, 7079
Ochi, M. *et al., Chem. Lett.*, 1991, 427 (*Calicoferol A*)
Seo, Y. *et al., J. Nat. Prod.*, 1995, **58**, 1291 (*Calicoferols, isol, pmr, cmr*)
Seo, Y. *et al., J. Nat. Prod.*, 1998, **61**, 1441-1443 (*Calicoferols*)
Della Sala, G. *et al., Tet. Lett.*, 1998, **39**, 4741-4744 (*synth*)
Taber, D. F. *et al., J.O.C.*, 2001, **66**, 944-953 (*synth*)
Singh, T.V. *et al., ARKIVOC*, 2002, **vii**, 82-90 (*Calicoferol E, synth*)

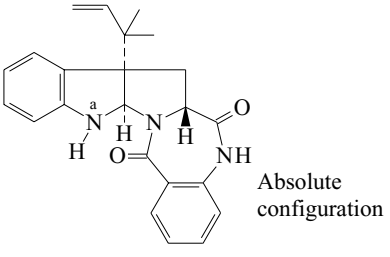
Asvatocin A-735

[144334-52-1]
Cys-Tyr-Ile-Asn-Asn-Cys-Pro-Val-Gly-NH_2
$C_{41}H_{62}N_{12}O_{12}S_2$ 979.146
Peptide of the oxytocin/vasopressin family; struct. of reduced form shown. Isol. from the pituitary of the spotted dogfish *Scyliorhinus caniculus.* Neurohypophysial hormone.

Chauvet, J. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1994, **91**, 11266-11270 (*isol, struct*)

Aszonalenin A-736

[81797-27-5]



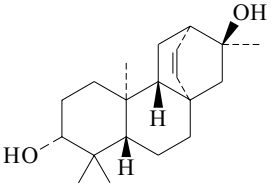
$C_{23}H_{23}N_3O_2$ 373.454
Prod. by *Aspergillus zonatus.* Induces abnormal development of embryos. Mycotoxin. Needles (MeOH/$CHCl_3$). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 244-247°. $[\alpha]_D^{20}$ +53 (c, 1.31 in $CHCl_3$). λ_{max} 210 (ϵ 44700); 233 (sh) (ϵ 25100); 290 (ϵ 5050) (EtOH) (Derep). λ_{max} 210 (ϵ 44700); 290 (ϵ 5050) (EtOH) (Berdy).

N^a*-Ac:* ***Antibiotic LL-S 490β****. LL-S 490β*
[42230-55-7]
$C_{25}H_{25}N_3O_3$ 415.491
Metab. of *Aspergillus zonatus* and marine-derived *Aspergillus carneus.* Cryst. (EtOAc/C_6H_6). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 238-240°. $[\alpha]_D$ +425 (c, 0.20 in MeOH). λ_{max} 210 (ϵ 61000); 245 (ϵ 22000); 284 (sh) (ϵ 3940) (MeOH) (Derep). λ_{max} 210; 290 (MeOH) (Berdy).

N^a,N^b*-Di-Ac:*
Amorph. solid. Mp 218-221°.

Ellestad, G.A. *et al., J.O.C.*, 1973, **38**, 4204 (*isol, uv, ir, pmr, ms, struct, deriv*)
Floss, H.G. *et al., CA*, 1980, **98**, 175942 (*biosynth*)
Kimura, Y. *et al., Tet. Lett.*, 1982, **23**, 225 (*isol, struct, uv, ir, pmr, deriv*)
White, J.D. *et al., J.A.C.S.*, 1983, **105**, 6517 (*synth*)
White, J.D. *et al., Tet. Lett.*, 1984, **25**, 3671 (*synth*)
Lee, J.J. *et al., Diss. Abstr. Int., B*, 1985, **45**, 3233 (*biosynth*)
Bhat, B. *et al., Tetrahedron*, 1993, **49**, 10655 (*abs config*)
Capon, R.J. *et al., Org. Biomol. Chem.*, 2003, **1**, 1856-1862 (*marine isol*)

13-Atisene-3,16-diol A-737



$C_{20}H_{32}O_2$ 304.472

(ent-3β,16α)-form
Constit. of *Viguiera insignis.*
Cryst. (diisopropyl ether/EtOAc).
Mp 192-193°.

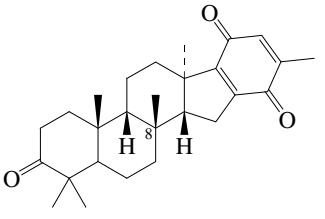
3-Ketone: ent*-16α-Hydroxy-13-atisen-3-one.* ***Yucalexin A16***
[119642-81-8]
$C_{20}H_{30}O_2$ 302.456
Gum. Stress metab. of cassava root (*Manihot esculenta*).

13,14-Dihydro: **ent-*3β,16α-Atisanediol***
[87013-77-2]
$C_{20}H_{34}O_2$ 306.487
Isol. from *Tedania ignis.* Cryst. (C_6H_6).
Mp 205-206°. $[\alpha]_D$ -28 (c, 0.22 in $CHCl_3$).

Schmitz, F.J. *et al., J.O.C.*, 1983, **48**, 3941
Delgado, G. *et al., Phytochemistry*, 1984, **23**, 2285
Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769 (*Yucalexin A16*)
De Heluani, C.S. *et al., Magn. Reson. Chem.*, 1998, **36**, 947-950 (*Yucalexin A16, pmr, cmr*)

Atomarianone A A-738

[872130-67-1]



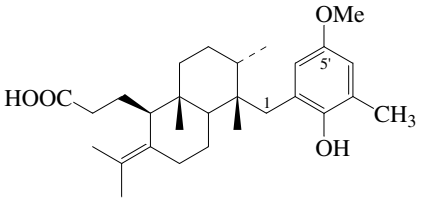
$C_{27}H_{36}O_3$ 408.58

Constit. of *Taonia atomaria*. Oil. $[\alpha]_D^{20}$ +3.3 (c, 1.21 in $CHCl_3$).

8-Epimer: ***Atomarianone B***
[872130-68-2]
$C_{27}H_{36}O_3$ 408.58
Constit. of *Taonia atomaria*. Oil. $[\alpha]_D^{20}$ +32.6 (c, 1.09 in $CHCl_3$).
Abatis, D. *et al., Tet. Lett.*, 2005, **46**, 8525-8529

Atomaric acid A-739

[55907-34-1]



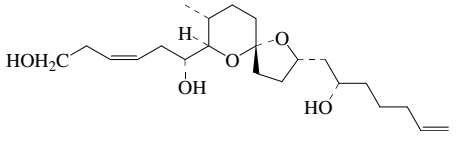
$C_{28}H_{42}O_4$ 442.637
Constit. of *Taonia atomaria* and brown alga *Stypopodium zonale*. Narcotic to fish. Tyrosine kinase inhibitor. Oil. $[\alpha]_D$ +49 (c, 0.42 in $CHCl_3$). λ_{max} 293 (ϵ 3270) (MeOH) (Berdy).

Me ester:
Cryst. Mp 112-115°.
O-*De-Me:* [476478-80-5]
$C_{27}H_{40}O_4$ 428.611
Constit. of *Stypopodium zonale*. Oil (as Me ester). $[\alpha]_D^{25}$ +52.1 (c, 0.05 in $CHCl_3$) (Me ester).
O-*De-Me, 5′-Ac:* [548785-86-0]
$C_{29}H_{42}O_5$ 470.648
Constit. of *Stypopodium zonale*. Cryst.
1-Ketone, O-*de-Me:* [548752-96-1]
$C_{27}H_{38}O_5$ 442.594
Constit. of *Stypopodium zonale*. Yellow oil. $[\alpha]_D^{25}$ +145.9 (c, 0.18 in $CHCl_3$).

González, A.G. *et al., Tet. Lett.*, 1974, 3951-3954 (*Atomaric acid*)
Gerwick, W.H. *et al., Phytochemistry*, 1985, **24**, 1279-1283 (*5′-O-de-Me-5′-Ac*)
Dorta, E. *et al., J. Nat. Prod.*, 2002, **65**, 1727-1730 (*O-de-Me*)
Dorta, E. *et al., Tetrahedron*, 2003, **59**, 2059-2062 (*isol, pmr, cmr, stereochem*)

Attenol A A-740

[250729-79-4]



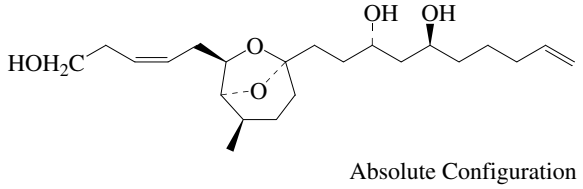
Absolute Configuration

$C_{22}H_{38}O_5$ 382.539
Isol. from the bivalve *Pinna attenuata*. Cytotoxic agent.

Takada, N. *et al., Chem. Lett.*, 1999, 1025-1026 (*isol*)
Araki, K. *et al., Tetrahedron*, 2002, **58**, 1983-1995 (*synth*)

Attenol B A-741

[250729-80-7]



Absolute Configuration

$C_{22}H_{38}O_5$ 382.539
Isol. from the bivalve *Pinna attenuata*. Cytotoxic agent.

Takada, N. *et al., Chem. Lett.*, 1999, 1025-1026 (*isol*)
Araki, K. *et al., Tetrahedron*, 2002, **58**, 1983-1995 (*synth*)

Attractin A-742

[210299-69-7]

Peptide containing 58 amino acid residues and 21 wt % carbohydrate as a result of *N*-linked glycosylation. Released by the marine mollusc *Aplysia* during egg laying. Water-borne pheromone.

Painter, S.D. *et al., Biol. Bull. (Woods Hole, Mass.)*, 1998, **194**, 120-131 (*isol, struct*)
Garimella, R. *et al., Biochemistry*, 2003, **42**, 9970-9979 (*soln struct*)
Cummins, S.F. *et al., Peptides (N.Y.)*, 2005, **26**, 121-129 (*rev*)

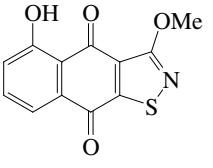
Augertoxins A-743

Three peptides containing 40-41 amino acid residues and 3 intramol. disulfide bridges. Isol. from venom of the toxoglossate gastropod *Terebra subulata*.

Imperial, J.S. *et al., Toxicon*, 2003, **42**, 391-398 (*isol*)

Aulosirazole A-744

*5-Hydroxy-3-methoxynaphth[2,3-*d*]isothiazole-4,9-dione, 9CI*
[159194-92-0]

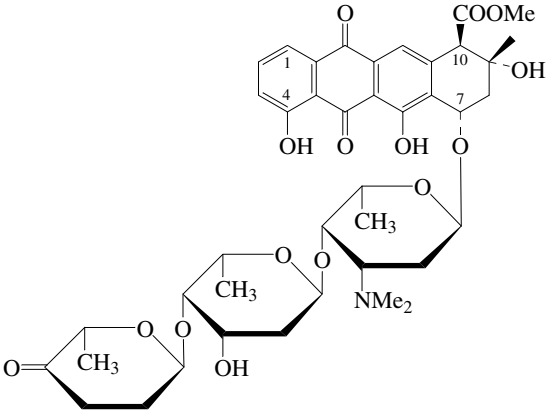


$C_{12}H_7NO_4S$ 261.258
Isol. from the blue-green alga *Aulosira fertilissima*. Cytotoxic agent. Deep yellow cryst. (MeOH aq.). λ_{max} 216 (ϵ 20500); 248 (ϵ 11200); 272 (ϵ 8500); 424 (ϵ 6300) (MeOH). λ_{max} 226; 280; 312; 536 (MeOH/NaOH) (Berdy).

Stratmann, K. *et al., J.O.C.*, 1994, **59**, 6279-6281

Auramycin A A-745

[78173-92-9]



$C_{41}H_{51}NO_{15}$ 797.852
Anthracycline antibiotic. Numbering systems vary. Isol. from *Streptomyces galilaeus* (OBB-111). Active against gram-positive bacteria, mycobacteria and tumours. Yellow powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 141°. $[\alpha]_D^{20}$ -8 (c, 0.1 in $CHCl_3$). λ_{max} 228 (E1%/1cm 620); 258 (E1%/1cm 375); 288 (E1%/1cm 135); 433 (E1%/1cm 200) (MeOH) (Berdy). λ_{max} 239 (E1%/1cm 575); 288 (E1%/1cm 165); 315 (E1%/1cm 90); 525 (E1%/1cm 180) (MeOH/NaOH) (Berdy).

▶ LD_{50} (mus, ipr) 100 mg/kg. QI9290700

Aglycone: Auramycinone
[78173-89-4]
Yellow powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 153.5°. $[\alpha]_D^{20}$ +198 (c, 0.1 in $CHCl_3$).

1-Hydroxy: ***1-Hydroxyauramycin A****. 10-Hydroxyauramycin A*
[79217-17-7]
$C_{41}H_{51}NO_{16}$ 813.851
Prod. by *Streptomyces melanogenes* and *Streptomyces galilaeus*. Active against gram-positive bacteria and tumours. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 108.5°. $[\alpha]_D^{20}$ +93.1 (c, 0.1 in $CHCl_3$). λ_{max} 234 (E1%/1cm 500); 292 (E1%/1cm 103); 493 (E1%/1cm 150); 511 (E1%/1cm 130); 526 (E1%/1cm 140); 570 (E1%/1cm 80) (MeOH) (Berdy). λ_{max} 241 (E1%/1cm 535); 565 (E1%/1cm 210); 602 (E1%/1cm 170) (MeOH/NaOH) (Berdy).

1-Hydroxy, aglycone: 1-Hydroxyauramycinone. 10-Hydroxyauramycinone
[76023-81-9]
Red powder. Mp 180.5°. Shows same gross structure as ϵ_1-Pyrromycinone.

11-Hydroxy, aglycone: ***11-Hydroxyauramycinone***
[88458-06-4]
$C_{21}H_{18}O_9$ 414.368
Prod. by *Streptomyces* sp. (MST-77755). Red solid.
Mp 177°. $[\alpha]_D$ +60 (c, 0.1 in $CHCl_3$). λ_{max} 234 (E1%/1cm 950); 252 (E1%/1cm 605); 295 (E1%/1cm 193); 494 (E1%/1cm 300); 528 (E1%/1cm 276); 576 (E1%/1cm 136) (no solvent reported).

7-Deoxy, aglycone: ***7-Deoxyauramycinone****. 4-Deoxyauramycinone*
[78173-93-0]
$C_{21}H_{18}O_7$ 382.369
Prod. by *Streptomyces galilaeus* (OBB-111).
Mp 200°. $[\alpha]_D^{20}$ +81.2 (c, 0.1 in $CHCl_3$).

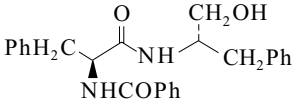
9-Epimer, 1-hydroxy, 4′-deglycosyl: ***1-Hydroxyauramycin T***
$C_{29}H_{33}NO_{11}$ 571.58
Prod. by marine-derived *Streptomyces* sp. (CANU Fox 21-2-6a). Cytotoxic. Deep red solid. λ_{max} 202; 234; 258; 290; 492 (MeOH).

10-Epimer, 7-deoxy, aglycone: ***Resomycin A***
$C_{21}H_{18}O_7$ 382.369
Prod. by *Streptomyces* sp. (GW71/2497). Orange solid. $[\alpha]_D^{20}$ -63 (c, 0.1 in $CHCl_3$). λ_{max} 261 (log ϵ 4.23); 292 (log ϵ 3.83); 435 (log ϵ 3.88) ($CHCl_3$).

Fujiwara, A. *et al., J. Antibiot.*, 1981, **34**, 912-915; 1982, **35**, 164-175 (*isol, ir, pmr, cmr*)
Rao, A.V.R. *et al., Tet. Lett.*, 1982, **23**, 775-778 (*synth, deriv*)
Hoshino, T. *et al., J. Antibiot.*, 1983, **36**, 1463-1467; 1984, **37**, 1469-1472 (*derivs*)
Krohn, K. *et al., Tetrahedron*, 1984, **40**, 3677-3694 (*synth*)
Jones, D.W. *et al., J.C.S. Perkin 1*, 1995, 2747-2755 (*synth, aglycone*)
Maskey, R.P. *et al., J. Antibiot.*, 2003, **56**, 795-800 (*7-Deoxyauramycinone, Resomycin A*)
Phipps, R.K. *et al., ARKIVOC*, 2004, **x**, 94-100 (*1-Hydroxyauramycin T*)
Clark, B. *et al., J. Nat. Prod.*, 2004, **67**, 1729-1731 (*11-Hydroxyauramycinone*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ARS130

Aurantiamide A-746

N-*Benzoylphenylalanylphenylalaninol. Antibiotic TMC 58B. TMC 58B*
[58115-31-4]



Absolute configuration

$C_{25}H_{26}N_2O_3$ 402.492

Alkaloid from *Piper aurantiacum* and *Hybanthus enneasperma*. Prod. by *Aspergillus penicilloides*. Cryst. (C_6H_6).
Mp 194° (184°). $[\alpha]_D^{30}$ -51 ($CHCl_3$).

O-*Ac:* ***Asperglaucide****. Anomalamide. Lyciumamide. Aurantiamide acetate. Antibiotic TMC 58A. TMC 58A. Saropeptate*
[56121-42-7]
$C_{27}H_{28}N_2O_4$ 444.529
Alkaloid from *Aspergillus glaucus*, *Aspergillus penicilloides*, *Euphorbia fischeriana*, *Malachra fasciata* and *Cystoseira corniculata*, *Sargassum carpophylum*, *Euphorbia fischeriana*, *Malachra fasciata*, *Pteris multifida* and *Acanthophora spicifera*. Selective cathepsin inhibitor. Antiallergic agent. Shows specific antimicrobial activity.
Mp 185-186°. $[\alpha]_D^{30}$ -45 ($CHCl_3$).

O-*Benzoyl:* ***Aurantiamide benzoate****.* O-*Benzoylaurantiamide*
[150881-02-0]
[150881-03-1]
$C_{32}H_{30}N_2O_4$ 506.6
Alkaloid from *Piper aurantiacum* and *Zeyheria digitalis*. Needles (C_6H_6/cyclohexane).
Mp 211°. $[\alpha]_D^{30}$ -26.3 ($CHCl_3$).

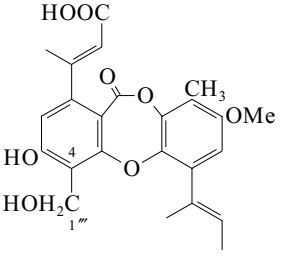
L-D-Diastereomer, Ac: ***Diaaurantiamide acetate***
$C_{27}H_{28}N_2O_4$ 444.529
Isol. from the red alga *Acanthophora spicifera*.
Mp 167°. Genus name misspelt as Acantophora in the paper.

[112924-28-4, 125276-43-9, 150881-04-2]

Maiti, B.C. *et al., Experientia*, 1976, **32**, 1166 (*deriv*)
Cox, R.E. *et al., J.C.S. Perkin 1*, 1976, 578-580 (*deriv*)
McCorkindale, N.J. *et al., Tetrahedron*, 1978, **34**, 2791-2795 (*synth, ms, pmr, ir*)
Banerji, A. *et al., Phytochemistry*, 1981, **20**, 2217-2220 (*isol, synth, pmr, cmr, ms*)
Wahidulla, S. *et al., Phytochemistry*, 1991, **30**, 3323-3325 (*Aurantiamide acetate, Diaaurantiamide acetate, isol, Acanthophora*)
Banerji, A. *et al., Indian J. Chem., Sect. B*, 1993, **32**, 776-778 (*Benzoylaurantiamide*)
Ferreira, D.T. *et al., J. Braz. Chem. Soc.*, 1995, **6**, 323-326 (*Benzoylaurantiamide*)
Ragasa, C.Y. *et al., Philipp. J. Sci.*, 1998, **127**, 267-276; *CA*, **131**, 167716y (*activity*)
Lu, H. *et al., Planta Med.*, 1999, **65**, 586 (*isol, activity, Asperglaucide*)
Hayashi, Y. *et al., J.O.C.*, 2000, **65**, 8402-8405 (*synth*)
Isshiki, K. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 1195-1197 (*isol*)

Auranticin A A-747

[133943-50-7]



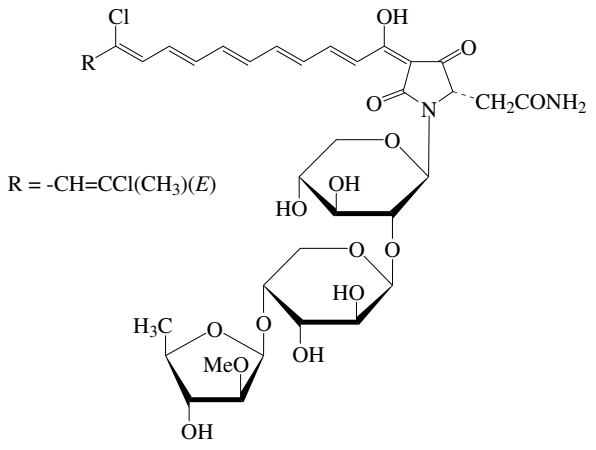
$C_{24}H_{24}O_8$ 440.449
Metab. of *Preussia aurantiaca* ATCC14745 isol. from a mangrove sediment. Cryst.
Mp 264° dec. λ_{max} 284 (ϵ 23823) (MeOH) (Berdy).

1‴-Aldehyde: ***Auranticin B***
[133943-51-8]
$C_{24}H_{22}O_8$ 438.433
Metab. of *Preussia aurantiaca* ATCC14745. Orange oil. λ_{max} 266 (ϵ 18578); 350 (ϵ 5957) (MeOH) (Berdy).

Poch, G.K. *et al., J. Nat. Prod.*, 1991, **54**, 213-217 (*isol, pmr, cmr*)

Aurantoside A A-748

[137895-70-6]



$C_{36}H_{46}Cl_2N_2O_{15}$ 817.669

Tetramic acid glycoside. Geom. isom. of terminal double bond revised in 1999. Isol. from the sponge *Theonella* sp. Cytotoxic agent. Orange solid. $[\alpha]_D^{23}$ -568 (c, 0.1 in MeOH). λ_{max} 242 (ϵ 12100); 414 (ϵ 46700) (H_2O).

O-*De-Me:* ***Aurantoside B***

[137895-71-7]

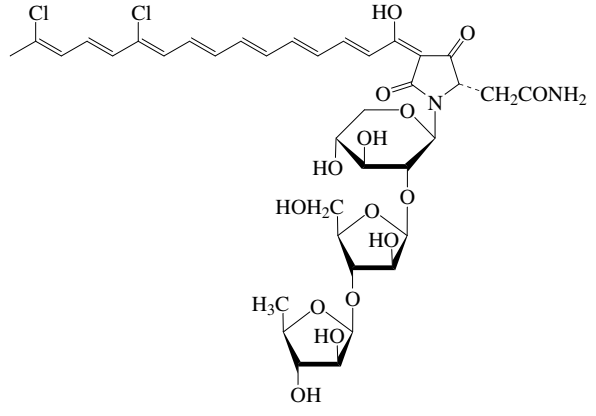
$C_{35}H_{44}Cl_2N_2O_{15}$ 803.642

Isol. from *Theonella* sp. Cytotoxic agent. Orange solid. $[\alpha]_D^{23}$ -492 (c, 0.1 in MeOH). λ_{max} 242 (ϵ 10900); 414 (ϵ 49100) (H_2O).

Matsunaga, S. *et al., J.A.C.S.*, 1991, **113**, 9690-9692 (*isol, uv, ir, pmr, cmr, ms*)
Sata, N.U. *et al., J. Nat. Prod.*, 1999, **62**, 969-971 (*struct*)

Aurantoside C A-749

[219297-37-7]



$C_{37}H_{46}Cl_2N_2O_{15}$ 829.68

Tetramic acid deriv. Isol. from the sponge *Homophymia conferta*. Amorph. red powder. $[\alpha]_D^{20}$ -480 (c, 0.2 in CH_2Cl_2/MeOH). λ_{max} 252 (ϵ 9700); 426 (ϵ 41600) (H_2O).

Wolf, D. *et al., J. Nat. Prod.*, 1999, **62**, 170-172 (*isol, uv, ir, pmr, cmr, ms*)

Aurantoside E A-750

[233608-98-5]

As Aurantoside A, A-748 with

R = -CH=CHCH=CCl(CH_3) (*E,Z*-)

$C_{38}H_{48}Cl_2N_2O_{15}$ 843.707

Tetramic acid glycoside. Isol. from the sponge *Siliquariaspongia japonica*. Antifungal agent. Red solid. $[\alpha]_D^{24}$ -1038 (c, 0.001 in MeOH). λ_{max} 250 (log ϵ 4.12); 423 (log ϵ 4.99) (MeOH).

O-*De-Me:* ***Aurantoside D***

[233608-94-1]

$C_{37}H_{46}Cl_2N_2O_{15}$ 829.68

Isol. from *Siliquariaspongia japonica*. Antifungal agent. Red solid. $[\alpha]_D^{24}$ -536 (c, 0.001 in MeOH). λ_{max} 244 (log ϵ 4.3); 433 (log ϵ 4.83) (MeOH).

Sata, N.U. *et al., J. Nat. Prod.*, 1999, **62**, 969-971 (*isol, uv, pmr, cmr*)

Aurantoside F A-751

[233608-99-6]

As Aurantoside A, A-748 with

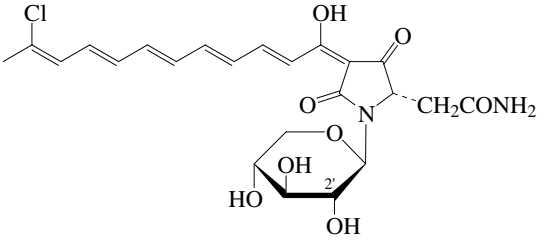
R = -CH=CHCH=CHCH=CClCH$_3$ (*Z*-)

$C_{40}H_{50}Cl_2N_2O_{15}$ 869.745

Tetramic acid glycoside. Isol. from the sponge *Siliquariaspongia japonica*. Antifungal agent. Red solid. $[\alpha]_D^{24}$ -1012 (c, 0.001 in MeOH). λ_{max} 440 (log ϵ 4.79); 465 (log ϵ 4.85) (MeOH).

Sata, N.U. *et al., J. Nat. Prod.*, 1999, **62**, 969-971 (*isol, uv, pmr, cmr*)

Aurantoside G A-752



$C_{23}H_{27}ClN_2O_8$ 494.928

Tetramic acid glycoside. Isol. from the sponge *Theonella swinhoei*. Orange solid. $[\alpha]_D^{24}$ -116 (c, 0.1 in MeOH). λ_{max} 240 (log ϵ 3.72); 280 (log ϵ 3.69); 376 (log ϵ 3.57) (MeOH).

2′-O-*β*-D-*Arabinopyranosyl:* ***Aurantoside H***

$C_{28}H_{35}ClN_2O_{12}$ 627.043

Isol. from *Theonella swinhoei*. Orange solid. $[\alpha]_D^{24}$ -295 (c, 0.1 in MeOH). λ_{max} 240 (log ϵ 3.79); 280 (log ϵ 3.79); 434 (log ϵ 3.95) (MeOH).

2′-O-*[5-Deoxy-2*-O*-methyl-β-*D*-arabinofuranosyl-(1→4)-β-*D*-arabinopyranosyl]:* ***Aurantoside I***

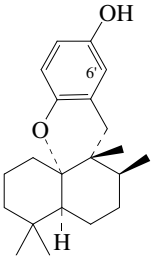
$C_{34}H_{45}ClN_2O_{15}$ 757.187

Isol. from *Theonella swinhoei*. Orange solid. $[\alpha]_D^{24}$ -210 (c, 0.1 in MeOH). λ_{max} 242 (log ϵ 3.68); 282 (log ϵ 3.68); 430 (log ϵ 3.72) (MeOH).

Ratnayake, A.S. *et al., J. Nat. Prod.*, 2005, **68**, 104-107 (*isol, pmr, cmr*)

Aureol† A-753

[72853-81-7]



$C_{21}H_{30}O_2$ 314.467

Constit. of *Smenospongia aurea* and *Aplysina lacunosa*. Cryst. (hexane). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O, hexane.

Mp 144-144.5°. $[\alpha]_D$ +65 (c, 2 in $CHCl_3$). λ_{max} 227 (ϵ 5000); 302 (ϵ 2700) (MeOH/NaOH) (Derep). λ_{max} 216 (ϵ 4600); 299 (ϵ 3100) (MeOH) (Derep). λ_{max} 225 (ϵ 4200); 295 (ϵ 2170) (EtOH) (Berdy).

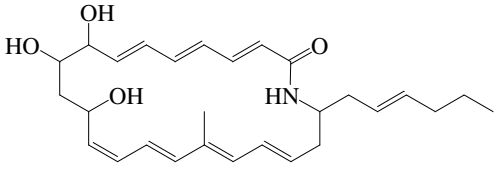
Ac: ***Aureol acetate***
$C_{23}H_{32}O_3$ 356.504
Isol. from sponge *Smenospongia aurea*.

6′-Chloro: ***6′-Chloroaureol***
[147228-70-4]
$C_{21}H_{29}ClO_2$ 348.912
Isol. from sponge *Smenospongia aurea*. Yellow cryst. (MeOH). Mp 143-144°. $[\alpha]_D$ +27.8 (c, 0.02 in $CHCl_3$). λ_{max} 226 (ϵ 8000); 299 (ϵ 4500) (MeOH).

Djura, P. *et al., J.O.C.*, 1980, **45**, 1435-1441 (*isol, pmr, cmr, cryst struct*)
Tymiak, A.A. *et al., Tetrahedron*, 1985, **41**, 1039-1047 (*isol, pmr, cmr*)
Aiello, A. *et al., Z. Naturforsch., B*, 1993, **48**, 209-212 (*pmr, cmr, 6′-Chloroaureol, Aureol acetate*)
Urban, S. *et al., Aust. J. Chem.*, 1994, **47**, 1023-1029 (*synth*)
Nakamura, M. *et al., Tet. Lett.*, 2002, **43**, 6929-6932 (*synth*)

Aureoverticillactam A-754

22-(2-Hexenyl)-9,10,12-trihydroxy-17-methylazacyclodocosa-3,5,7,13,15,17,19-heptaen-2-one, 9CI
[682774-28-3]

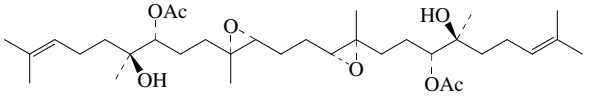


$C_{28}H_{39}NO_4$ 453.62
Closely related to Antibiotic BE 14106. Prod. by the marine *Streptomyces aureoverticillatus* (NPS001583). Shows moderate cytotoxic activity. Amorph. solid. λ_{max} 283 (sh); 290; 310 (sh); 330 (sh) (MeCN aq.).

Mitchell, S.S. *et al., J. Nat. Prod.*, 2004, **67**, 1400-1402 (*isol, pmr, cmr*)

Auriculol A-755

[381217-83-0]

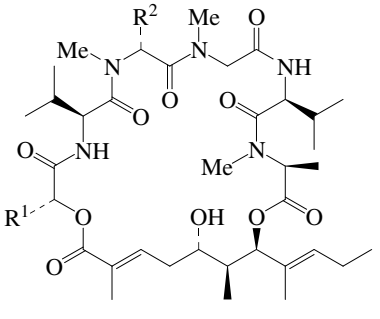


$C_{34}H_{58}O_8$ 594.827
Constit. of *Dolabella auricularia*. Oil. $[\alpha]_D^{25}$ +0.12 (c, 0.1 in $CHCl_3$).

Kigoshi, H. *et al., Tet. Lett.*, 2001, **42**, 7461-7464 (*isol, pmr, cmr, synth*)

Aurilide A-756

[182863-03-2]



R^1 = -CH(CH$_3$)CH$_2$CH$_3$(*S*), R^2 = -CH$_2$CH(CH$_3$)$_2$

$C_{44}H_{75}N_5O_{10}$ 834.104
Depsipeptide antibiotic. Isol. from the sea hare *Dolabella auricularia*. Cytotoxic. Powder. $[\alpha]_D^{25}$ -17 (c, 0.06 in MeOH).

Suenaga, K. *et al., Tetrahedron*, 2004, **60**, 8509-8527 (*isol, synth, ir, pmr, cmr*)

Aurilide B A-757

As Aurilide, A-756 with
R^1 = -CH(CH$_3$)CH$_2$CH$_3$(*S*-), R^2 = -CH(CH$_3$)CH$_2$CH$_3$(*R*-)
$C_{44}H_{75}N_5O_{10}$ 834.104
Isol. from *Lyngbya majuscula*. Cytotoxic. Amorph. solid. $[\alpha]_D^{24}$ -17 (c, 0.34 in MeOH). λ_{max} 222 (log ϵ 4.65) (MeOH).

Han, B. *et al., J. Nat. Prod.*, 2006, **69**, 572-575 (*isol, pmr, cmr*)

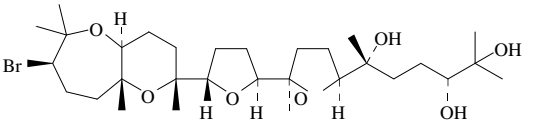
Aurilide C A-758

As Aurilide, A-756 with
R^1 = -CH(CH$_3$)$_2$, R^2 = -CH(CH$_3$)CH$_2$CH$_3$(*R*-)
$C_{43}H_{73}N_5O_{10}$ 820.077
Isol. from *Lyngbya majuscula*. Cytotoxic. Amorph. solid. $[\alpha]_D^{24}$ -19 (c, 0.39 in MeOH). λ_{max} 222 (log ϵ 4.56) (MeOH).

Han, B. *et al., J. Nat. Prod.*, 2006, **69**, 572-575 (*isol, pmr, cmr*)

Aurilol A-759

[205251-96-3]



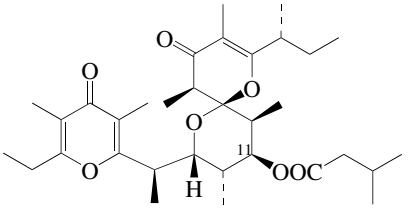
Absolute Configuration

$C_{30}H_{53}BrO_7$ 605.649
Constit. of *Dolabella auricularia*. Cytotoxic. Oil. $[\alpha]_D^{30}$ +4.6 (c, 0.41 in $CHCl_3$).

Suenaga, K. *et al., J. Nat. Prod.*, 1998, **61**, 515-518 (*isol, pmr, cmr*)
Morimoto, Y. *et al., J.A.C.S.*, 2005, **127**, 5806-5807 (*synth, abs config*)

Auripyrone A A-760

[179600-02-3]



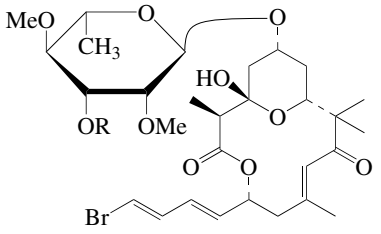
$C_{33}H_{50}O_7$ 558.754
Isol. from the sea hare *Dolabella auricularia*. Cytotoxic agent. Cryst. (pentane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 172-176°. $[\alpha]_D^{26}$ +28 (c, 0.08 in $CHCl_3$). λ_{max} 220 (ϵ 9500); 260 (ϵ 13000) (MeOH).

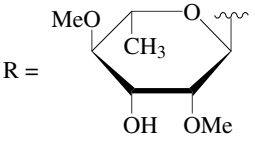
*11-Deacyl, 11-*O*-(2-methylbutanoyl):* ***Auripyrone B***
[179600-03-4]
$C_{33}H_{50}O_7$ 558.754
Isol. from *Dolabella auricularia*. Cytotoxic agent. Cryst. (pentane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 126-128°. $[\alpha]_D^{26}$ +39 (c, 0.1 in $CHCl_3$). λ_{max} 217 (ϵ 6800); 260 (ϵ 14000) (MeOH).

Suenaga, K. *et al., Tet. Lett.*, 1996, **37**, 5151-5154 (*isol, uv, ir, pmr, cmr*)
Lister, T. *et al., Angew. Chem., Int. Ed.*, 2006, **45**, 2560-2564 (*synth*)

Auriside A A-761

[184974-84-3]





$C_{37}H_{57}BrO_{14}$ 805.753
Isol. from *Dolabella auricularia*. Cytotoxic agent. Amorph. solid. Sol. MeOH, EtOAc, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{31}$ -43 (c, 0.05 in MeOH). λ_{max} 245 (ϵ 31000) (MeCN).

Sone, H. *et al., J.O.C.*, 1996, **61**, 8956-8960 (*isol, uv, ir, pmr, cmr*)
Paterson, I. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 1130-1133 (*synth*)

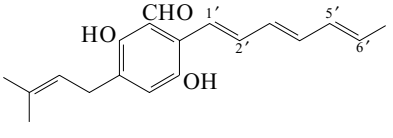
Auriside B A-762

[184974-85-4]
As Auriside A, A-761 with
R = $CONH_2$
$C_{30}H_{44}BrNO_{11}$ 674.582
Isol. from *Dolabella auricularia*. Cytotoxic agent. Amorph. solid. Sol. MeOH, EtOAc, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{33}$ -30 (c, 0.9 in MeOH). λ_{max} 245 (ϵ 35000) (MeCN).

Sone, H. *et al., J.O.C.*, 1996, **61**, 8956-8960 (*isol, uv, ir, pmr, cmr*)
Paterson, I. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 1130-1133 (*synth*)

Auroglaucin A-763

2-(1,3,5-Heptatrienyl)-3,6-dihydroxy-5-(3-methyl-2-butenyl)benzaldehyde, 9CI
[41451-81-4]



$C_{19}H_{22}O_3$ 298.381
Constit. of *Aspergillus* spp. Orange-red.
Mp 153°.

▶CU6340000

Oxime:
Yellowish-green cryst. Mp 117° dec.

1′,2′-Dihydro: 2-(3,5-Heptadienyl)-3,6-dihydroxy-5-(3-methyl-2-butenyl)benzaldehyde, 9CI. ***Isodihydroauroglaucin***
[74886-31-0]
$C_{19}H_{24}O_3$ 300.397
Metab. of *Aspergillus ruberEurotium chevalieri* and a marine-derived *Microsporum* sp. Yellow needles (hexane). Sol. Me_2CO, hexane; poorly sol. H_2O.
Mp 114-115°. λ_{max} 227 (ϵ 38000); 273 (ϵ 10000); 391 (ϵ 4700) (EtOH) (Berdy).

5′,6′-Dihydro: 2-(1,3-Heptadienyl)-3,6-dihydroxy-5-(3-methyl-2-butenyl)benzaldehyde, 9CI. ***Dihydroauroglaucin***
[77102-91-1]
$C_{19}H_{24}O_3$ 300.397
Metab. of *Aspergillus chevalieri* and *Eurotium chevalieri*. Yellow needles (hexane). Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 114-115°. λ_{max} 249 (ϵ 26000); 298 (ϵ 13700); 410 (ϵ 5700) (EtOH) (Berdy).

1′,2′,3′,4′-Tetrahydro: 2-(5-Heptenyl)-3,6-dihydroxy-5-(3-methyl-2-butenyl)benzaldehyde, 9CI. ***Isotetrahydroauroglaucin***
[74886-32-1]
$C_{19}H_{26}O_3$ 302.413
Metab. of *Aspergillus ruber*. Yellow needles (hexane). Sol. Me_2CO, hexane; poorly sol. H_2O.
Mp 85.5-86.5°. λ_{max} 238 (ϵ 10000); 275 (ϵ 10000); 392 (ϵ 4270) (EtOH) (Berdy).

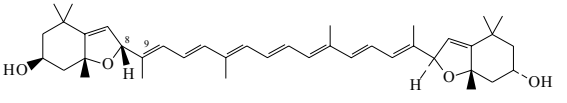
3′,4′,5′,6′-Tetrahydro: 2-(1-Heptenyl)-3,6-dihydroxy-5-(3-methyl-2-butenyl)benzaldehyde, 9CI. ***Aspergin****. Tetrahydroauroglaucin*
[33514-92-0]
$C_{19}H_{26}O_3$ 302.413
Yellow cryst. (hexane) or yellow powder. Mp 60-61° Mp 90.5-91.5°.

[40434-07-9]

Raistrick, H. *et al., J.C.S.*, 1937, 80 (*struct*)
Cruickshank, J.H. *et al., J.C.S.*, 1938, 2056 (*struct*)
Birch, A.J. *et al., J.C.S.*, 1965, 1231 (*biosynth*)
Natori, S. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2727 (*Aspergin*)
Grove, J.F. *et al., J.C.S. Perkin 1*, 1972, 2406 (*Aspergin*)
Hashizume, K. *et al., Yakugaku Zasshi*, 1977, **97**, 569; *CA*, **87**, 201216v
Gatti, G. *et al., J. Chem. Res., Synop.*, 1979, 366 (*cmr*)
Hamasaki, T. *et al., Agric. Biol. Chem.*, 1980, **44**, 1685; 1981, **45**, 313 (*isol, ir, uv, pmr, derivs*)
Nagao, M. *et al., Agric. Biol. Chem.*, 1981, **45**, 313 (*Dihydroauroglaucin*)
Li, Y. *et al., Chem. Pharm. Bull.*, 2006, **54**, 882-883 (*Isodihydroauroglaucin, marine, isol*)

Auroxanthin A-764

5,8:5′,8′-Diepoxy-5,5′,8,8′-tetrahydro-β,β-carotene-3,3′-diol
[27785-15-5]



(8*R*,8′*R*)–*form*

$C_{40}H_{56}O_4$ 600.88
Isol. from *Viola tricolor, Lonicera japonica, Delonix regia* and other plants. Present in red algae. Yellow cryst. (EtOH).
Mp 203°. A *cis*-isomer was reported from *D. regia*.

3,3′-Dideoxy: 5,8:5′,8′-Diepoxy-5,5′,8,8′-tetrahydro-β,β-carotene. ***Aurochrome***
[6821-09-6]
$C_{40}H_{56}O_2$ 568.881
Widespread carotenoid. Present in red algae. Cryst.(C_6H_6/MeOH).
Mp 185°.

3′-Deoxy: 5,8:5′,8′-Diepoxy-5,5′,8,8′-tetrahydro-β,β-caroten-3-ol. ***Cryptochrome***
[73745-06-9]
$C_{40}H_{56}O_3$ 584.881
Isol. from *Prunus persica* (peach) and fruits of *Averrhoa carambola*. Isol. only in trace amounts. λ_{max} 424; 456 (CS_2). λ_{max} 399; 424 (EtOH).

(8R,8′R)-form [95034-12-1]
Isol. from *Rosa foetida* petals. λ_{max} 378; 398; 423 (no solvent reported).

(8R,8′S)-form [51921-06-3]
Isol. from *Rosa foetida* petals. λ_{max} 378; 398; 423 (no solvent reported).

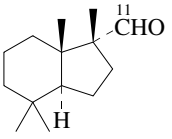
(8S,8′S)-form [51921-05-2]
Isol. from *Rosa foetida* petals. λ_{max} 378; 398; 423 (no solvent reported).

(8R,8′R,9Z)-form [95119-78-1]
Isol. from *Rosa foetida* petals. λ_{max} 378; 398; 423 (no solvent reported).

[22350-65-8]

Karrer, P. *et al., Helv. Chim. Acta*, 1944, **27**, 1684; 1945, **28**, 427 (*struct*)
Goodwin, T.W. *et al., Biochem. J.*, 1956, **62**, 346 (*isol*)
Jungalwala, F.B. *et al., Biochem. J.*, 1962, **85**, 1 (*isol*)
Stobart, A.K. *et al., Phytochemistry*, 1967, **6**, 1467 (*isol*)
Gross, J. *et al., Phytochemistry*, 1983, **22**, 1479 (*Cryptochrome*)
Acemoglu, M. *et al., Helv. Chim. Acta*, 1984, **67**, 471 (*synth, uv, pmr, cmr*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1984, **67**, 2143 (*isol*)

Austrodoral A-765



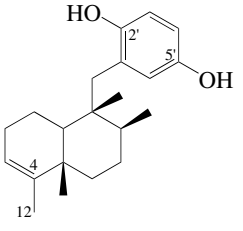
$C_{14}H_{24}O$ 208.343
Constit. of *Austrodoris kerguelenensis*.
$[\alpha]_D$ +5 (c, 0.3 in $CHCl_3$).

11-Carboxylic acid: ***Austrodoric acid***
[511546-05-7]
$C_{14}H_{24}O_2$ 224.342
Constit. of *Austrodoris kerguelenensis*.
$[\alpha]_D$ +16 (c, 0.1 in $CHCl_3$).

Gavagnin, M. *et al., Tet. Lett.*, 2003, **44**, 1495-1498 (*isol, pmr, cmr*)
Kulcitki, V. *et al., Eur. J. Org. Chem.*, 2005, 1816-1822 (*synth*)
Alvarez-Manzaneda, E.J. *et al., Tet. Lett.*, 2005, **46**, 5321-5324 (*synth*)

Avarol A-766

[55303-98-5]



Absolute Configuration

$C_{21}H_{30}O_2$ 314.467
Constit. of *Dysidea avara*. Immunostimulant. Shows antiinflammatory, analgesic, ichthyotoxic, antimutagenic and anti-HIV activity. Cryst. ($CHCl_3$). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 148-150°. $[\alpha]_D$ +6.1. Log P 6.98 (calc). λ_{max} 298 (ϵ 3900) (no solvent reported) (Derep).
▶ LD_{50} (mus, ipr) 269 mg/kg. Antimutagenic activity with inhibiting effect on benzo[*a*]pyrene monooxygenase. CZ9026700

5′-Ac: [122143-92-4]
$C_{23}H_{32}O_3$ 356.504
Constit. of *Dysidea avara*. Cryst. (Et_2O/hexane).
Mp 151-152°. $[\alpha]_D^{25}$ +11 (c, 3.1 in $CHCl_3$). λ_{max} 286 (no solvent reported) (Derep).

Di-Ac: [61187-44-8]
$C_{25}H_{34}O_4$ 398.541
Constit. of *Dysidea avara*. Cryst. (hexane).
Mp 92-94°. $[\alpha]_D$ +12.5 (c, 1.0 in $CHCl_3$).

6′-Hydroxy: ***6′-Hydroxyavarol***
[130203-72-4]
$C_{21}H_{30}O_3$ 330.466
Metab. of *Dysidea cinerea*. HIV reverse transcriptase and DNA polymerase inhibitor. Oil. $[\alpha]_D^{25}$ +60 (c, 0.02 in MeOH). λ_{max} 242 (ϵ 2750); 294 (ϵ 2200); 385 (ϵ 500) (MeOH) (Berdy).

6′-Acetoxy: ***6′-Acetoxyavarol***
[130203-69-9]
$C_{23}H_{32}O_4$ 372.503
Metab. of *Dysidea cinerea*. DNA polymerase inhibitor. Oil. $[\alpha]_D^{25}$ +18.9 (c, 0.44 in $CHCl_3$). λ_{max} 298 (ϵ 4000) (MeOH) (Berdy).

6′-Hydroxy, 5′-Ac: ***5′-O-Acetyl-6′-hydroxyavarol***
[132194-46-8]
$C_{23}H_{32}O_4$ 372.503
Isol. from *Dysidea avara*. Cryst. (Et_2O/hexane).
Mp 113-115°. $[\alpha]_D$ +16 (c, 0.8 in $CHCl_3$).

2′,5′-Quinone: ***Avarone***
[55303-99-6]
$C_{21}H_{28}O_2$ 312.451
From *Dysidea avara*. Immunostimulant. Antiiflammatory, antimutagenic and antileukaemic activity. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 246 (ϵ 12300); 315 (ϵ 750); 440 (ϵ 30) (no solvent reported) (Derep). λ_{max} 247 (ϵ 14700) (EtOH) (Berdy).
▶ LD_{50} (mus, ipr) 181 mg/kg. GU5405000

2′,5′-Quinone, 3′-hydroxy: ***3′-Hydroxyavarone****. Avarone A*
[130203-67-7]
$C_{21}H_{28}O_3$ 328.45
Metab. of *Dysidea cinerea*. Oil. $[\alpha]_D^{25}$ +45 (c, 0.06 in $CHCl_3$). λ_{max} 256 (ϵ 10200); 284 (ϵ 3300) (MeOH) (Berdy).

2′,5′-Quinone, 3′,6′-dihydroxy: ***3′,6′-Dihydroxyavarone****. Avarone B*
[114019-20-4]
$C_{21}H_{28}O_4$ 344.45
Metab. of *Dysidea cinerea*. Oil. $[\alpha]_D^{25}$ +65.6 (c, 0.32 in $CHCl_3$). λ_{max} 256 (ϵ 11400); 282 (ϵ 8140) (MeOH) (Berdy).

2′,5′-Quinone, 6′-acetoxy: ***6′-Acetoxyavarone***
[130203-70-2]
$C_{23}H_{30}O_4$ 370.488
Metab. of *Dysidea cinerea*. Oil. $[\alpha]_D^{25}$ -4.2 (c, 0.018 in $CHCl_3$). λ_{max} 250 (ϵ 10300); 330 (ϵ 550) (MeOH) (Berdy).

2′,5′-Quinone, 6′-hydroxy, 4′-methoxy: ***6′-Hydroxy-4′-methoxyavarone***
[130203-71-3]
$C_{22}H_{30}O_4$ 358.477
Metab. of *Dysidea cinerea*. Oil. $[\alpha]_D^{25}$ +75 (c, 0.040 in $CHCl_3$). λ_{max} 256 (ϵ 12700); 294 (ϵ 5400) (MeOH) (Berdy).

2′,5′-Quinone, 3′-methoxy: ***18-Methoxyavarone***
[117686-16-5]
$C_{22}H_{30}O_3$ 342.477
Constit. of *Dysidea avara*. Yellow solid.
Mp 120-125°. $[\alpha]_D^{20}$ -14.5 (c, 0.02 in CH_2Cl_2). λ_{max} 270 (ϵ 7980) (EtOH) (Derep).

2′,5′-Quinone, 4′-methoxy: ***19-Methoxyavarone****. 4′-Methoxyavarone*
[129357-96-6]
$C_{22}H_{30}O_3$ 342.477
Constit. of *Dysidea avara*. Yellow solid.
Mp 149-151°. $[\alpha]_D$ +16.4 (c, 0.15 in $CHCl_3$). λ_{max} 270 (ϵ 7980) (EtOH) (Derep).

$\Delta^{4(12)}$-Isomer: ***Isoavarol****. Neoavarol*
[129443-87-4]
$C_{21}H_{30}O_2$ 314.467
Isol. from a sponge *Dysidea* sp. Ichthyotoxic agent. Needles.
Mp 151-153°. $[\alpha]_D$ -38.6 (c, 0.1 in $CHCl_3$). λ_{max} 298 (ϵ 3700) (EtOH).

$\Delta^{4(12)}$-Isomer, 5′-Ac: ***20-O-Acetylneoavarol***
[852629-62-0]
$C_{23}H_{32}O_3$ 356.504
Constit. of a *Dysidea* sp. Yellow oil. $[\alpha]_D^{25}$ -31.9 (c, 0.1 in $CHCl_3$).

$\Delta^{4(12)}$-Isomer, 2′,5′-quinone: ***Neoavarone***
[129445-46-1]
$C_{21}H_{28}O_2$ 312.451
Isol. from a sponge *Dysidea* sp. Ichthyotoxic agent. Yellow cryst.
Mp 78-79°. $[\alpha]_D$ -55.2 (c, 0.07 in $CHCl_3$). λ_{max} 247 (ϵ 14900) (EtOH).

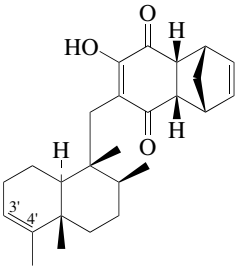
$\Delta^{4(12)}$-Isomer, 2′,5′-quinone, 4′-methoxy: ***4′-Methoxyneoavarone***
$C_{22}H_{30}O_3$ 342.477
Constit. of the sponges *Chelonaplysilla violacea* and *Dysidea* sp.

Yellow cryst.
Mp 161-163°. $[\alpha]_D$ -8.1 (c, 0.22 in $CHCl_3$). λ_{max} 270 (ϵ 7900) (EtOH).

Minale, L. *et al., Tet. Lett.*, 1974, 3401-3404 (*isol*)
De Rosa, S. *et al., J.C.S. Perkin 1*, 1976, 1408-1414 (*struct*)
Sarma, A.S. *et al., J.O.C.*, 1982, **47**, 1727-1731 (*synth*)
Muller, W.E. *et al., Cancer Res.*, 1985, **45**, 4822-4826 (*activity*)
Kurelec, B. *et al., Mutat. Res.*, 1985, **144**, 63-66 (*tox*)
Sarin, P.S. *et al., J. Natl. Cancer Inst.*, 1987, **78**, 663-666 (*anti-HIV activity*)
Crispino, A. *et al., J. Nat. Prod.*, 1989, **52**, 646-648 (*5′-Ac, isol, pmr, cmr*)
Iguchi, K. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1121-1123 (*Avarol, Neoavarol, Neoavarone*)
Shubina, L.K. *et al., Khim. Prir. Soedin.*, 1990, **26**, 358-361; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 296-298 (*Isoavarol*)
De Guilio, A. *et al., Tetrahedron*, 1990, **46**, 7971-7976 (*5′-O-Acetyl-6′-hydroxyavarol, di-Ac*)
Hirsch, S. *et al., J. Nat. Prod.*, 1991, **54**, 92-97 (*isol, pmr, cmr, Dysidea cinerea constits*)
Alvi, K.A. *et al., J.O.C.*, 1992, **57**, 6604-6607 (*Methoxyavarones*)
Sarma, A.S. *et al., Secondary Metabolites from Marine Sponges*, Ullstein Mosby, 1993, 142 (*Avarol, Avarone, pharmacol, activity*)
Puliti, R. *et al., Acta Cryst. C*, 1994, **50**, 830-833; 1995, **51**, 1195-1198; 2163-2166 (*cryst struct*)
Ferrándiz, M.L. *et al., Eur. J. Pharmacol.*, 1994, **253**, 75-82 (*pharmacol*)
Locke, E.P. *et al., Chem. Comm.*, 1996, 2717-2718 (*synth, Avarone*)
An, J. *et al., J.O.C.*, 1996, **61**, 8775-8779 (*synth*)
Stewart, M. *et al., Aust. J. Chem.*, 1997, **50**, 341-347 (*Avarones, pmr, cmr*)
Ilyin, S.G. *et al., Acta Cryst. C*, 1999, **55**, 266-268 (*Isoavarol, cryst struct*)
Ling, T. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 3089-3091 (*synth*)
Ling, T. *et al., J.A.C.S.*, 2002, **124**, 12261-12267 (*synth*)
Pérez-Garcia, E. *et al., J. Nat. Prod.*, 2005, **68**, 6 3-658 (*20-Acetylneoavarol*)

Avarone adduct A A-767

[193157-86-7]



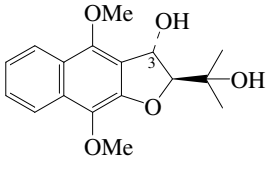
$C_{26}H_{34}O_3$ 394.553
Not named in paper. Constit. of a *Dysidea* sp. Oil. λ_{max} 205; 220; 290 (MeOH).

3′,4′,7′,8′-Tetraepimer: ***Avarone adduct B***
[193157-87-8]
$C_{26}H_{34}O_3$ 394.553
Oil.

3′,4′-Dihydro: ***Avarone adduct C***
[193284-78-5]
$C_{26}H_{36}O_3$ 396.569
Constit. of a *Dysidea* sp. Orange oil. λ_{max} 208; 285 (MeOH).

Stewart, M. *et al., Aust. J. Chem.*, 1997, **50**, 341-347 (*isol, pmr, cmr*)

Avicenol A A-768



Absolute Configuration

$C_{17}H_{20}O_5$ 304.342
Constit. of the stem bark of *Avicennia alba*. Oil. $[\alpha]_D$ +5.1 (c, 0.39 in $CHCl_3$). λ_{max} 210; 239; 290; 300; 321; 335 (MeOH).

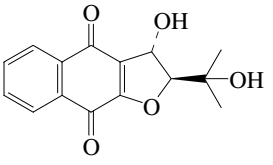
Di-O-*de*-*Me:* ***Dide*-O-*methylavicenol A***
$C_{15}H_{16}O_5$ 276.288
Constit. of *Tabebuia heptaphylla*. Resin.

3-Deoxy: ***Avicenol C***
$C_{17}H_{20}O_4$ 288.343
Constit. of *Avicennia alba* and *Avicennia officinalis*. Oil. $[\alpha]_D$ +22 (c, 1.03 in $CHCl_3$). λ_{max} 210; 239; 286; 297; 326; 338 (MeOH).

Ito, C. *et al., Chem. Pharm. Bull.*, 2000, **48**, 339-343 (*Avicenols*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 2003, **42**, 3117-3119 (*isol*)
Schmeda-Hirschmann, G. *et al., Z. Naturforsch., C*, 2003, **58**, 495-501 (*Dide-O-methylavicenol A*)
Zou, Y. *et al., J.O.C.*, 2005, **70**, 1761-1770 (*synth, abs config*)

Avicequinone A A-769

2,3-Dihydro-3-hydroxy-2-(1-hydroxy-1-methylethyl)naphtho[2,3-b]furan-4,9-dione



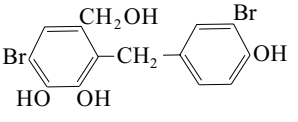
Relative Configuration

$C_{15}H_{14}O_5$ 274.273
Constit. of the stem bark of *Avicennia alba*. Phytoalexin. Yellow oil. $[\alpha]_D$ +35 (c, 0.11 in $CHCl_3$). λ_{max} 206; 245; 251; 286; 334 (MeOH).

Ito, C. *et al., Chem. Pharm. Bull.*, 2000, **48**, 339-343

Avrainvilleol A-770

6-Bromo-3-[(3-bromo-4-hydroxyphenyl)methyl]-4-(hydroxymethyl)-1,2-benzenediol, 9CI
[87402-66-2]



$C_{14}H_{12}Br_2O_4$ 404.054
Feeding deterrent from *Avrainvillea longicaulis*. Ichthyotoxic agent. IMP dehydrogenase inhibitor. Viscous oil. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 288 (ϵ 4400) (MeOH) (Derep).

Sun, H.H. *et al., Phytochemistry*, 1983, **22**, 743

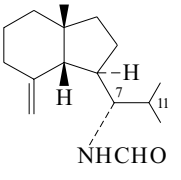
AX II A-771

Peptide containing 51 amino acid residues. Isol. from the sea anemone *Anthopleura xanthogrammica*. Toxin. Na Channel Inhibitor. Ichthyotoxic agent. For Neurotoxin AX I see Anthopleurins, A-523. λ_{max} 280 (H_2O) (Berdy).
▶ LD_{50} (mus, ipr) 0.008 mg/kg.

Schweitz, H. *et al., Biochemistry*, 1981, **20**, 5245-5252 (*isol, struct*)

Axamide 1 A-772

[56012-88-5]



$C_{16}H_{27}NO$ 249.395
Constit. of *Axinella cannabina*. Oil. $[\alpha]_D$ +10 (c, 1.2 in $CHCl_3$).

7,11-Didehydro: ***Axamide 4***
[62078-09-5]

$C_{16}H_{25}NO$ 247.38
Constit. of *Axinella cannabina*. Cryst.
Mp 81-84°. $[\alpha]_D$ +63.3.

Isothiocyanate: ***Axisothiocyanate 1***
[53822-97-2]
$C_{16}H_{25}NS$ 263.446
Isol. from *Axinella cannabina*. Oil. $[\alpha]_D$ +5.9 (c, 2.5 in $CHCl_3$). Has -NCS replacing -NHCHO.

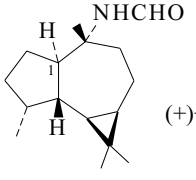
Isocyanide: ***Axisonitrile 1***
[53822-96-1]
$C_{16}H_{25}N$ 231.38
From *Axinella cannabina* and *Phyllidia pulitzeri*. Ichthyotoxic agent. Cryst.
Mp 43-45°. $[\alpha]_D$ +22.6 (c, 1 in $CHCl_3$). Has -NC replacing -NHCHO.

7,11-Didehydro, isocyanide: ***Axisonitrile 4***
[62078-10-8]
$C_{16}H_{23}N$ 229.364
Isol. from *Axinella cannabina*. Cryst.
Mp 56-58°. $[\alpha]_D$ +51.4 (c, 1 in $CHCl_3$).

7,11-Didehydro, isothiocyanate: ***Axisothiocyanate 4***
[62078-11-9]
$C_{16}H_{23}NS$ 261.43
Isol. from *Axinella cannabina*. Oil. $[\alpha]_D$ -35.9 (c, 1.2 in $CHCl_3$).

Cafieri, F. *et al., Tetrahedron*, 1973, **29**, 4259 (*isol*)
Fattorusso, E. *et al., Tetrahedron*, 1975, **31**, 269 (*isol*)
Iengo, A. *et al., Experientia*, 1977, **33**, 11; 1979, **35**, 10 (*isol, struct*)
Adinolfi, M. *et al., Tet. Lett.*, 1977, 2815 (*struct*)
Piers, E. *et al., Can. J. Chem.*, 1986, **64**, 2475 (*synth*)
Piers, E. *et al., Tetrahedron*, 1987, **43**, 5521 (*synth*)
Chenera, B. *et al., J.O.C.*, 1992, **57**, 2018 (*synth*)
Ohkubo, T. *et al., Tet. Lett.*, 1995, **36**, 3365 (*synth*)
Guevel, A.-C. *et al., J.O.C.*, 1996, **61**, 473 (*synth*)

Axamide 2 A-773



(+)–*form*

$C_{16}H_{27}NO$ 249.395

(+)-form [56012-89-6]
Constit. of *Axinella cannabina*.
Oil. $[\alpha]_D$ +37.5 (c, 0.9 in $CHCl_3$).

Isocyanide: ***Axisonitrile 2***
[55907-33-0]
$C_{16}H_{25}N$ 231.38
From *Axinella cannabina*, *Phyllidia pustulosa* and *Cadlina luteomarginata*. Oil. $[\alpha]_D$ +29 (c, 0.5 in $CHCl_3$). Has -NC replacing -NHCHO.

Isothiocyanate: ***Axisothiocyanate 2***
[56012-90-9]
$C_{16}H_{25}NS$ 263.446
Isol. from *Axinella cannabina*. Oil. $[\alpha]_D$ +12.8 (c, 1.5 in $CHCl_3$). Has -NCS replacing -NHCHO.

1-Epimer: ***10α-Formamidoalloaromadendrane***
[108739-41-9]
$C_{16}H_{27}NO$ 249.395
Constit. of *Axinella cannabina*. Oil.

1-Epimer, isocyanide: ***10α-Isocyanoalloaromadendrane***
[108739-39-5]
$C_{16}H_{25}N$ 231.38
Isol. from *Axinella cannabina*. Oil. $[\alpha]_D$ -17.21 (c, 0.7 in $CHCl_3$).

1-Epimer, isothiocyanate: ***10α-Isothiocyanatoalloaromadendrane***
[108739-40-8]
$C_{16}H_{25}NS$ 263.446
From *Axinella cannabina*. Oil. $[\alpha]_D$ -6.95 (c, 0.9 in $CHCl_3$).

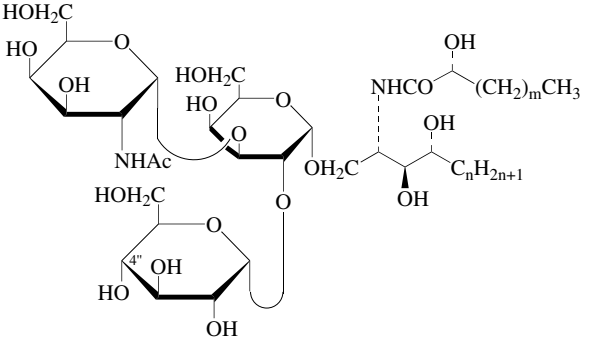
(-)-form

1-Epimer, isothiocyanate:
$C_{16}H_{25}NS$ 263.446
Constit. of *Acanthella cavernosa*. Oil. $[\alpha]_D$ +8 (c, 0.1 in $CHCl_3$). Not indexed by CAS.

Fattorusso, E. *et al., Tetrahedron*, 1974, **30**, 3911-3913; 1975, **31**, 269-270 (*Axisonitrile 2, Axisothiocyanate 2, Axamide 2*)
Ciminiello, P. *et al., Can. J. Chem.*, 1987, **65**, 518-522 (*Axinella cannabina constits*)
Fusetani, N. *et al., Tet. Lett.*, 1991, **32**, 7291-7294 (*Axisonitrile 2*)
Da Silva, C.C. *et al., J.O.C.*, 1994, **59**, 2880-2881 (*synth*)
Hirota, H. *et al., Tetrahedron*, 1996, **52**, 2359 (*isol, pmr, cmr*)

Axiceramide A A-774

[160338-33-0]



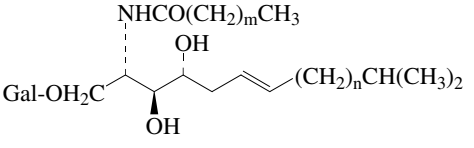
m = 21,22 or 23
n = 12,13,14,15 or 17

Glycosphingolipid complex. Isol. from the sponge *Axinella* sp. Oil (as per-Ac). $[\alpha]_D^{25}$ +88 (c, 0.01 in $CHCl_3$) (per-Ac).

4″-Epimer: ***Axiceramide B***
[160338-32-9]
Isol. from *Axinella* sp.
Oil (as per-Ac). $[\alpha]_D^{25}$ +82 (c, 0.01 in $CHCl_3$) (per-Ac).

Costantino, V. *et al., Annalen*, 1994, 1181-1186 (*isol, pmr, cmr, ms*)

Axidjiferosides A-775



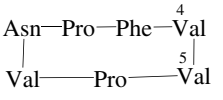
m = 19-23
n = 4-12

Glycosphingolipid complex. Isol. from the mangrove sponge *Axinyssa djiferi*.

Genin, E. *et al., Boll. Mus. Ist. Biol. Univ. Genova*, 2004, **68**, 327-334

Axinastatin 1 A-776

Malaysiatin. Pseudoaxinellin
[145038-60-4]



$C_{38}H_{56}N_8O_8$ 752.909
Cyclic peptide antibiotic. Isol. from the marine sponges *Pseudaxinyssa* sp., *Axinella* sp. and *Pseudaxinella* sp. Cytotoxic agent. Cryst. (CH_2Cl_2).
Mp 283-287° dec. $[\alpha]_D$ -162 (c, 0.1 in MeOH). Similar to Pseudoaxinellin. Struct. of Malaysiatin revised in 1995.

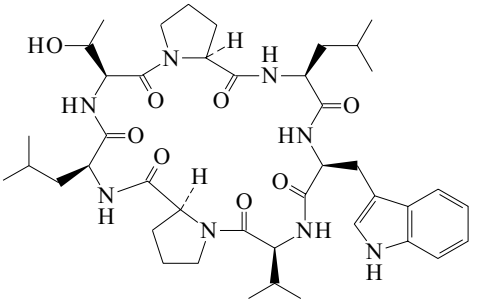
5-L-Leucine analogue: ***Axinastatin 2***
[153723-34-3]
$C_{39}H_{58}N_8O_8$ 766.936
From *Axinella* sp. Cytotoxic agent. Cryst. (MeOH aq.).
Mp 280-282°. $[\alpha]_D$ -153 (c, 0.2 in MeOH).

4-L-Isoleucine, 5-L-leucine analogue: ***Axinastatin 3***
[153723-35-4]
$C_{40}H_{60}N_8O_8$ 780.963
From *Axinella* sp. Cytotoxic agent. Cryst. (MeOH aq.).
Mp 291-294°. $[\alpha]_D$ -185 (c, 0.2 in MeOH).

Pettit, G.R. *et al., J. Med. Chem.*, 1991, **34**, 3339; 1994, **37**, 1165 (*isol*)
Kong, F. *et al., Tet. Lett.*, 1992, **33**, 3269-3272 (*Pseudoaxinellin*)
Fernandez, R. *et al., Tet. Lett.*, 1992, **33**, 6017 (*isol, pmr, cmr, struct*)
Konat, R.K. *et al., Annalen*, 1995, 765 (*synth, pmr, cmr, ms, conformn*)
Pettit, G.R. *et al., J.C.S. Perkin 1*, 1996, 2411 (*synth*)
Mechnich, O. *et al., Helv. Chim. Acta*, 1997, **80**, 1338-1342 (*derivs, pmr, conformn*)

Axinastatin 4 A-777

[150731-25-2]

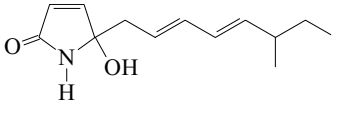


$C_{42}H_{62}N_8O_8$ 807.001
Cyclic heptapeptide antibiotic. Isol. from the sponge *Axinella* cf. *carteri*. Cytotoxic agent. Amorph. solid.
Mp 201-206°. $[\alpha]_D^{25}$ -92.8 (c, 0.5 in MeOH). λ_{max} 219 (ϵ 30000); 281 (ϵ 6000); 288 (ϵ 5000) (EtOH) (Derep).

Pettit, G.R. *et al., Heterocycles*, 1993, **35**, 711 (*isol, pmr, cmr, struct*)
Mechnich, O. *et al., Helv. Chim. Acta*, 1997, **80**, 1338-1342 (*pmr, conformn*)
Bates, R.B. *et al., J. Nat. Prod.*, 1998, **61**, 405 (*synth, config*)

Axinellamide A-778

*1,5-Dihydro-5-hydroxy-5-(6-methyl-2,4-octadienyl)-2*H*-pyrrol-2-one, 9CI. 5-Hydroxy-5-(6-methyl-2,4-octadienyl)-3-pyrrolin-2-one*
[167425-78-7]

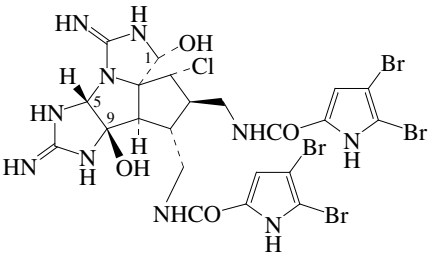


$C_{13}H_{19}NO_2$ 221.299
Alkaloid from the marine sponge *Axinella* sp. Pale yellow gum. $[\alpha]_D$ -26.2 (c, 0.08 in $CHCl_3$). λ_{max} 277 (ϵ 8700) (MeOH) (Berdy).

Miller, S.L. *et al., Tet. Lett.*, 1995, **36**, 5851 (*isol, uv, ir, pmr, cmr, struct*)

Axinellamine A† A-779

[221225-27-0]



$C_{22}H_{23}Br_4ClN_{10}O_4$ 846.557
CAS nos. refer to bis(trifluoroacetates). Alkaloid from the Australian sponge *Axinella* sp. Powder (as bistrifluoroacetate salt). $[\alpha]_D^{20}$ -18 (c, 0.16 in MeOH). λ_{max} 277 (ϵ 11400) (MeOH).

1-Me ether: ***Axinellamine C***
[221226-05-7]
$C_{23}H_{25}Br_4ClN_{10}O_4$ 860.584
Alkaloid from an *Axinella* sp. Pale yellow oil. $[\alpha]_D^{20}$ -9 (c, 1.1 in MeOH). λ_{max} 277 (ϵ 6500) (MeOH).

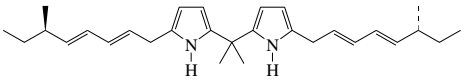
5,9-Diepimer: ***Axinellamine B***†
[221226-09-1]
$C_{22}H_{23}Br_4ClN_{10}O_4$ 846.557
Alkaloid from an *Axinella* sp. Pale yellow oil. $[\alpha]_D^{20}$ -7 (c, 0.21 in MeOH). λ_{max} 277 (ϵ 8000) (MeOH).

5,9-Diepimer, 1-Me ether: ***Axinellamine D***
[221226-07-9]
$C_{23}H_{25}Br_4ClN_{10}O_4$ 860.584
Alkaloid from an *Axinella* sp. Pale yellow oil. $[\alpha]_D^{20}$ -6 (c, 0.5 in MeOH). λ_{max} 276 (ϵ 8000) (MeOH).

Urban, S. *et al., J.O.C.*, 1999, **64**, 731-735 (*isol, uv, ir, pmr, cmr, ms*)
Dransfield, P.J. *et al., Tetrahedron*, 2006, **62**, 5223-5247 (*synth*)

Axinellamine B† A-780

[213269-07-9]



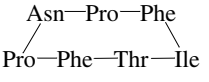
Probable Configuration

$C_{29}H_{42}N_2$ 418.664
Alkaloid from the marine sponge *Axinella* sp. Pale yellow gum. $[\alpha]_D$ -8.9 (c, 0.2 in $CHCl_3$). λ_{max} 228 (ϵ 6500) (MeOH).

Bascombe, K.C. *et al., Heterocycles*, 1998, **48**, 1461-1464 (*isol, uv, ir, pmr, cmr, ms*)
Seki, M. *et al., Eur. J. Org. Chem.*, 2001, 503-506 (*config*)

Axinellin A A-781

[215586-19-9]

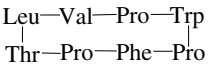


$C_{42}H_{56}N_8O_9$ 816.953
Cyclic peptide antibiotic. Isol. from the marine sponge *Axinella carteri*. Moderate antitumour agent. Amorph. solid. $[\alpha]_D$ -98.2 (c, 0.003 in MeOH).

Randazzo, A. *et al., Eur. J. Org. Chem.*, 1998, 2659-2665 (*isol ir, pmr, cmr, ms*)

Axinellin B A-782

[215586-20-2]

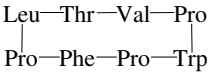


$C_{50}H_{67}N_9O_9$ 938.134

Cyclic peptide antibiotic. Isol. from the marine sponge *Axinella carteri*. Moderate antitumour agent. Amorph. solid. $[\alpha]_D$ +50 (c, 0.001 in MeOH).

Randazzo, A. *et al., Eur. J. Org. Chem.*, 1998, 2659-2665 (*isol, ir, pmr, cmr, ms*)

Axinellin C A-783



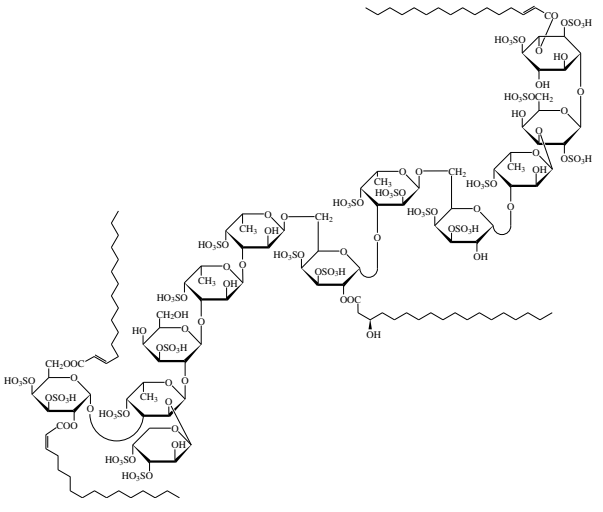
$C_{50}H_{67}N_9O_9$ 938.134

Cyclic peptide antibiotic. Isol. from the marine sponge *Stylotella aurantium*. Oil. $[\alpha]_D^{25}$ -53.1 (c, 0.001 in MeOH). λ_{max} 290 (ϵ 3320) (MeOH).

Tabudravu, J.N. *et al., Tetrahedron*, 2002, **58**, 7863-7868 (*isol, pmr, cmr, ms, cryst struct*)

Axinelloside A A-784

[868081-48-5]



$C_{137}H_{238}O_{117}S_{19}$ 4366.571

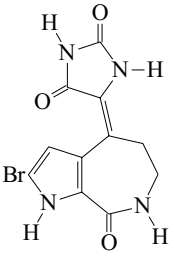
Highly sulfated lipopolysaccharide. Isol. from *Axinella infundibula*. Human telomerase inhibitor. Amorph. solid. $[\alpha]_D^{26}$ -10 (c, 0.1 in MeOH). λ_{max} 210 (MeOH).

Warabi, K. *et al., J.A.C.S.*, 2005, **127**, 13262-13270 (*isol, pmr, cmr, ms*)

Axinohydantoin A-785

5-(2-Bromo-5,6,7,8-tetrahydro-8-oxopyrrolo[2,3-c]azepin-4(1H)-ylidene)-2,4-imidazolidinedione, 9CI

[132160-42-0]



$C_{11}H_9BrN_4O_3$ 325.121

Alkaloid from the sponges *Axinella* sp. and *Monanchora* sp. Yellow prisms (MeOH).

Mp 350°. λ_{max} 264; 345 (ϵ 14400) (MeOH) (Berdy).

Debromo: ***Debromoaxinohydantoin***

$C_{11}H_{10}N_4O_3$ 246.225

Isol. from the Papua New Guinea sponge *Monanchora* sp.

Mp 300° dec. λ_{max} 208 (ϵ 16000); 225 (ϵ 11200); 255 (ϵ 15500); 339 (ϵ 27500) (MeOH) (Berdy).

(Z)-Isomer: ***Spongiacidin D****. (Z)-Axinohydantoin. Fuscin*†

$C_{11}H_9BrN_4O_3$ 325.121

Isol. from the sponges *Phakellia fusca*, *Stylotella aurantium* and *Hymeniacidon* sp. Inhibitor of protein kinase C. Amorph. solid.

Mp 221-227° (dec.). There is confusion in CAS w.r.t. the config. of the *Phakellia* isolate. λ_{max} 272 (ϵ 10000); 310 (ϵ 4000) (MeOH).

Debromo, (Z)-isomer: ***Spongiacidin C****. (Z)-Debromoaxinohydantoin*

$C_{11}H_{10}N_4O_3$ 246.225

Isol. from the sponge *Stylotella aurantia* and *Hymeniacidon* sp. Inhibitor of protein kinase C. Amorph. solid.

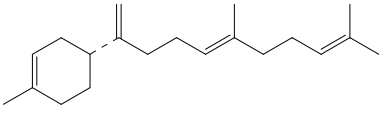
Mp 213-218° (dec.). λ_{max} 273 (ϵ 9700); 312 (ϵ 3800) (MeOH).

[132160-43-1]

Pettit, G.R. *et al., Can. J. Chem.*, 1990, **68**, 1621 (*isol, uv, ir, pmr, cryst struct*)
Fu, X. *et al., Chem. Res. Chin. Univ.*, 1991, **7**, 178; *CA*, **118**, 36148y (*Fuscin*)
Groszek, G. *et al., Annalen*, 1995, 715 (*Debromoaxinohydantoin*)
Patil, A.D. *et al., Nat. Prod. Lett.*, 1997, **9**, 201-207 (*Z-isomers*)
Inaba, K. *et al., J. Nat. Prod.*, 1998, **61**, 693-695 (*Spongiacidins C and D*)
Sosa, A.C.B. *et al., J.O.C.*, 2002, **67**, 4498-4500 (*synth*)

Axinyssene A-786

[497143-31-4]



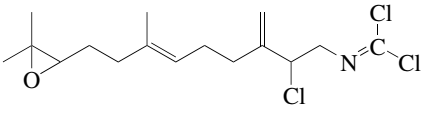
$C_{20}H_{32}$ 272.473

Constit. of an *Axinyssa* sp. and of *Otostegia integrifolia*. Oil. $[\alpha]_D$ -34.2 (c, 0.2 in $CHCl_3$).

Kodama, K. *et al., Org. Lett.*, 2003, **5**, 169-171 (*isol, pmr, cmr, synth*)
Tesso, H. *et al., Phytochemistry*, 2004, **65**, 2057-2062 (*isol, pmr, cmr*)

Axinyssimide A A-787

[184173-50-0]



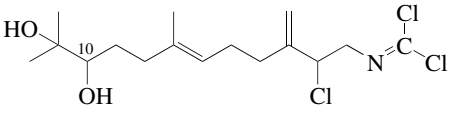
$C_{16}H_{24}Cl_3NO$ 352.73

Constit. of an *Axinyssa* sponge and *Phyllidia pustulosa*. Antifouling agent. $[\alpha]_D$ +1.7 (c, 0.06 in $CHCl_3$).

Hirota, H. *et al., Tetrahedron*, 1998, **54**, 13971-13980 (*isol, pmr, cmr*)

Axinyssimide B A-788

[184173-51-1]



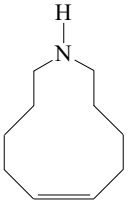
$C_{16}H_{26}Cl_3NO_2$ 370.745

Constit. of an *Axinyssa* sponge. Antifouling agent. $[\alpha]_D$ -22.5 (c, 0.02 in $CHCl_3$).

10-Epimer: ***Axinyssimide C***
[217481-01-1]
$C_{16}H_{26}Cl_3NO_2$ 370.745
Constit. of an *Axinyssa* sponge. Antifouling agent. $[\alpha]_D$ +7.3 (c, 0.015 in $CHCl_3$).

Hirota, H. *et al., Tetrahedron*, 1998, **54**, 13971-13980 (*isol, pmr, cmr*)

Azacyclo-6-undecene, 9CI A-789

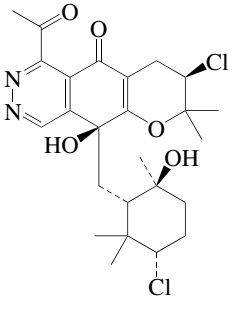


$C_{10}H_{19}N$ 153.267

(Z)-form
Keramaphidin C
[126412-12-2]
Isol. from the Okinawan marine sponge *Amphimedon* sp. Plausible biogenetic precursor of Manzamine C, M-97. Amorph. solid. Mp 106-109°.

Torisawa, Y. *et al., Tetrahedron*, 1991, **47**, 8067 (*synth*)
Tsuda, M. *et al., Tet. Lett.*, 1994, **35**, 4387 (*isol, ir, pmr, cmr*)
Tsuda, M. *et al., Heterocycles*, 1997, **46**, 765-794 (*rev*)

Azamerone A-790

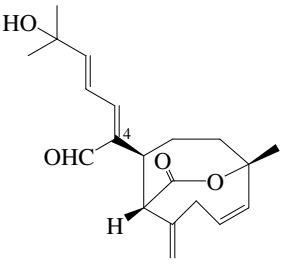


$C_{25}H_{32}Cl_2N_2O_5$ 511.444
Isol. from the marine-derived *Streptomyces* sp. CNQ766. Cryst. Mp 210-212°. $[\alpha]_D$ -8.8 (c, 0.002 in MeOH). λ_{max} 217 (sh) (log ϵ 3.9); 250 (sh) (log ϵ 3.4); 323 (log ϵ 3.3) (MeOH).

Cho, J.Y. *et al., Org. Lett.*, 2006, **8**, 2471-2474 (*isol, pmr, cmr, cryst struct*)

Azamial A A-791

[182806-35-5]



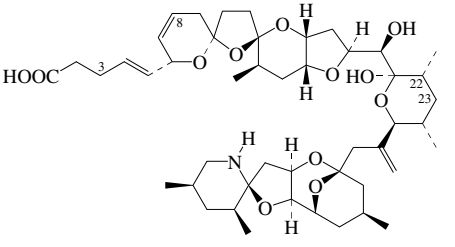
$C_{20}H_{26}O_4$ 330.423
Isol. from a soft coral, *Xenia* sp. Oil. Isol. as a mixture with Azamial B. λ_{max} 281 (ϵ 11300) (no solvent reported).

*4*E-*Isomer:* ***Azamial B***
[182968-28-1]
$C_{20}H_{26}O_4$ 330.423
Isol. from a *Xenia* sp.

Iwagawa, T. *et al., Tetrahedron*, 1996, **52**, 13121-13128

Azaspiracid 1 A-792

Killarytoxin 3
[214899-21-5]



Absolute Configuration

$C_{47}H_{71}NO_{12}$ 842.077

Struct. finally confirmed in 2004. Alkaloid from *Mytilus edulis* (blue mussel). Shellfish toxin. Amorph. solid. $[\alpha]_D^{20}$ -21 (c, 0.1 in MeOH).

*3*R-*Hydroxy:* ***Azaspiracid 7***
[629656-50-4]
$C_{47}H_{71}NO_{13}$ 858.077
Alkaloid from *Mytilus edulis* (blue mussel).

*23*R-*Hydroxy:* ***Azaspiracid 8***
[629656-53-7]
$C_{47}H_{71}NO_{13}$ 858.077
Alkaloid from *Mytilus edulis* (blue mussel).

22-Demethyl: ***Azaspiracid 3***
[265996-93-8]
$C_{46}H_{69}NO_{12}$ 828.051
Alkaloid from *Mytilus edulis* (blue mussel).

*22-Demethyl, 3*R-*hydroxy:* ***Azaspiracid 4***
[344422-49-7]
$C_{46}H_{69}NO_{13}$ 844.05
Alkaloid from *Mytilus edulis* (blue mussel).

*22-Demethyl, 23*S-*hydroxy:* ***Azaspiracid 5***
[344422-51-1]
$C_{46}H_{69}NO_{13}$ 844.05
Alkaloid from *Mytilus edulis* (blue mussel).

8-Methyl: ***Azaspiracid 2***
[265996-92-7]
$C_{48}H_{73}NO_{12}$ 856.104
Alkaloid from *Mytilus edulis* (blue mussel).

*8-Methyl, 3*R*-hydroxy:* ***Azaspiracid 11***
[629656-62-8]
$C_{48}H_{73}NO_{13}$ 872.104
Alkaloid from *Mytilus edulis* (blue mussel).

*8-Methyl, 23*R*-hydroxy: Azaspiracid 12*
[629656-65-1]
$C_{48}H_{73}NO_{13}$ 872.104
Existence as a natural prod. has been predicted but not proven.

8-Methyl, 22-demethyl: ***Azaspiracid 6***
[629656-47-9]
$C_{47}H_{71}NO_{12}$ 842.077
Alkaloid from *Mytilus edulis* (blue mussel).

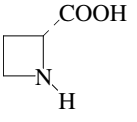
*8-Methyl, 22-demethyl, 3*R*-hydroxy:* ***Azaspiracid 9***
[629656-56-0]
$C_{47}H_{71}NO_{13}$ 858.077
Alkaloid from *Mytilus edulis* (blue mussel).

*8-Methyl, 22-demethyl, 23*R*-hydroxy:* ***Azaspiracid 10***
[629656-59-3]
$C_{47}H_{71}NO_{13}$ 858.077
Alkaloid from *Mytilus edulis* (blue mussel). Cahn-Ingold-Prelog priorities change at C-23.

Satake, M. *et al., J.A.C.S.*, 1998, **120**, 9967-9968 (*Azaspiracid 1*)
Ofuji, K. *et al., Nat. Toxins*, 1999, **7**, 99-102 (*Azaspiracids 2,3*)
Food Sci. Technol., Seafood and Freshwater Toxins, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**,
Ofuji, K. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 740-742 (*Azaspiracids 4,5*)
James, K.J. *et al., Toxicon*, 2003, **41**, 277-283 (*isol, ms*)
Lehane, M. *et al., J. Chromatogr., A*, 2004, **1024**, 63-70 (*hplc-ms*)
Nicolaou, K.C. *et al., Angew. Chem., Int. Ed.*, 2006, **45**, 2609-2615 (*Azaspiracid 2,3, synth*)
Nicolaou, K.C. *et al., J.A.C.S.*, 2006, **128**, 2244-2257; 2258-2267; 2859-2872 (*synth, struct*)

2-Azetidinecarboxylic acid, 9CI A-793

[2517-04-6]



(*R*)-*form*

$C_4H_7NO_2$ 101.105

(*R*)-*form* [7729-30-8]
$[\alpha]_D^{20}$ +102 (c, 3.6 in H_2O).

N-*Benzyl, Me ester:* [205443-23-8]
$C_{12}H_{15}NO_2$ 205.256
$[\alpha]_D^{20}$ +125.2 (c, 1 in CH_2Cl_2) (>99% ee).

(*S*)-*form* [2133-34-8]
Present in roots and leaves of *Convallaria majalis* (lily-of-the-valley) and other liliaceous plants and seeds of *Fritillaria meleagris*. Isol. from marine sponges *Haliclona* and *Chalinopsilla* spp. Seedling growth inhibitor. Proline antagonist. Antidermatophytic agent. Cryst. (MeOH). Sol. H_2O.
Mp >121° dec. $[\alpha]_D^{21}$ -121.7 (c, 0.5 in H_2O). Unstable in mineral acids.
▶ Exp. reprod. and teratogenic effects. LD_{50} (mus, scu) 1000 mg/kg. CM4310500

Me ester: [69684-70-4]
$C_5H_9NO_2$ 115.132
Cryst. (Et_2O/CH_2Cl_2) (as hydrochloride). $[\alpha]_D$ -86.8 (c, 0.5 in H_2O) (hydrochloride).

Amide:
$C_4H_8N_2O$ 100.12
Cryst. (CH_2Cl_2/EtOAc). Mp 114-116°. $[\alpha]_D^{28}$ -182.9 (c, 1.007 in $CHCl_3$).

N-*Benzyloxycarbonyl:* [25654-52-8]
$C_{12}H_{13}NO_4$ 235.239
Oil. $[\alpha]_D^{20}$ -99 (c, 3.9 in $CHCl_3$).

N-*Benzyl,* N-*oxide:*
$C_{11}H_{13}NO_3$ 207.229
Cryst. (CH_2Cl_2).

N-*Benzyl, Me ester:* [127382-20-1]
$C_{12}H_{15}NO_2$ 205.256
$[\alpha]_D$ -115 (c, 1.3 in CH_2Cl_2).

N-*(3-Hydroxypropyl):* ***Medicanine***
[91106-30-8]
$C_7H_{13}NO_3$ 159.185
Amino acid from seeds of *Medicago sativa* (alfalfa). Hygroscopic cryst.
Mp 124-126° (synthetic). $[\alpha]_D$ -92.2 (c, 0.13 in H_2O) (natural). $[\alpha]_D$ -100.5 (c, 0.45 in H_2O) (synthetic).

(±)-*form* [20063-89-2]
Darkens without melting >200°.

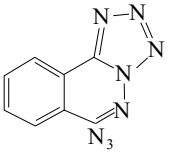
N-*Benzyl, Me ester:* [18085-37-5]
$C_{12}H_{15}NO_2$ 205.256
Bp_1 107-109°.

1-(1-Adamantyl): 1-Tricyclo[3.3.1.1^{3,7}]dec-1-yl-2-azetidinecarboxylic acid, 9CI. 1-(1-Adamantyl)-2-azetidinecarboxylic acid. ***Carmantadine, INN, USAN.*** *Sch 15427*
[38081-67-3]
$C_{14}H_{21}NO_2$ 235.325
Antiparkinsonian drug. Cryst. ($CHCl_3$/hexane). Mp 172-173°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 582D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 885C (*nmr*)
Berman, H.M. *et al., J.A.C.S.*, 1969, **91**, 6177-6182 (*cryst struct*)
Ger. Pat., 1972, 2 156 499; *CA*, **77**, 88330f (*synth, pharmacol*)
Miyoshi, M. *et al., Chem. Lett.*, 1973, 5-6 (*synth, abs config*)
Phillips, B.A. *et al., J. Het. Chem.*, 1973, **10**, 795-799 (*synth, ir, pmr*)
Leete, E. *et al., Phytochemistry*, 1975, **14**, 1983-1984 (*biosynth*)
Bach, B. *et al., Experientia*, 1978, **34**, 688-691 (*isol, sponges*)
Cromwell, N.H. *et al., Chem. Rev.*, 1979, **79**, 331-358 (*rev, bibl*)
Fushiya, S. *et al., Heterocycles*, 1984, **22**, 1039-1040 (*Medicanine*)
Baldwin, J.E. *et al., Tetrahedron*, 1988, **44**, 637-642 (*synth*)
Seebach, D. *et al., Annalen*, 1990, 687-695 (*derivs*)
O'Neill, I.A. *et al., Chem. Comm.*, 1998, 1487-1488 (*N-benzyl N-oxide, cryst struct*)
Fujita, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 787-796 (*amide, synth, ir, pmr*)
Wim, A.J. *et al., Tetrahedron: Asymmetry*, 1998, **9**, 429-435 (*1-benzoyl Me ester, synth, resoln, pmr, cmr*)
Futamura, Y. *et al., Biosci., Biotechnol., Biochem.*, 2005, **69**, 1892-1897 (*synth, pmr*)
Couty, F. *et al., J.O.C.*, 2005, **70**, 9028-9031 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ASC500

6-Azidotetrazolo[5,1-*a*]phthalazine, 9CI A-794

[51627-67-9]

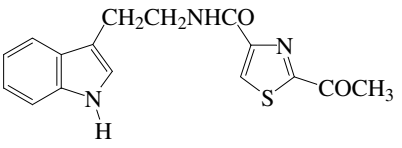


$C_8H_4N_8$ 212.173
Isol. from the toxic flagellate *Gymnodinium breve*. Ichthyotoxin.
Mp 152° (synthetic).
▶ LD_{50} 0.4 μg/ml (fish). Potentially explosive.

Reynolds, G.A. *et al., J.O.C.*, 1959, **24**, 1205 (*synth, struct*)
Waller, A.R. *et al., J. Chromatogr.*, 1979, **179**, 392 (*ir*)
Hossain, M.B. *et al., Acta Cryst. C*, 1985, **41**, 1199 (*cryst struct*)

Bacillamide B-1

[637344-98-0]



$C_{16}H_{15}N_3O_2S$ 313.379

Prod. by the marine *Bacillus* sp. SY-1. Algicide active against *Cochlodinium polykrikoides*. Amorph. powder. λ_{max} 279 (log ϵ 3.72) (no solvent reported).

Jeong, S.-Y. *et al., Tet. Lett.*, 2003, **44**, 8005-8007 (*isol, pmr, cmr*)

Bacillariolide I B-2

*Hexahydro-4-hydroxy-3-(1,4,7,10-tridecatetraenyl)-1*H*-cyclopenta[c]furan-1-one, 9CI*

[126857-23-6]

$C_{20}H_{28}O_3$ 316.439

Cyclopentane eicosanoid. Isol. from the diatom *Nitzschia pungens*. $[\alpha]_D^{24}$ -25.9 (c, 0.21 in MeOH).

3-Epimer: ***Bacillariolide II***

[126923-96-4]

$C_{20}H_{28}O_3$ 316.439

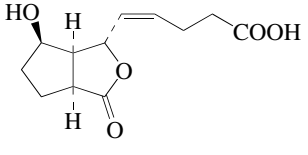
Isol. from *Nitzschia pungens*.

$[\alpha]_D^{23}$ -59.2 (c, 0.33 in MeOH).

Wang, R. *et al., Chem. Comm.*, 1990, 413; 1993, 379 (*isol, pmr, struct, abs config*)
Miyaoka, H. *et al., Tetrahedron*, 2000, **56**, 8083-8094 (*synth*)
Ghosh, S. *et al., Org. Lett.*, 2006, **8**, 3781-3784 (*synth*)

Bacillariolide III B-3

[188827-33-0]



$C_{12}H_{16}O_5$ 240.255

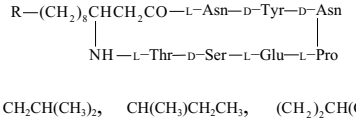
Metab. of the diatom *Pseudonitzschia multiseries*. Amorph. solid. $[\alpha]_D^{24}$ -25.3 (c, 0.3 in MeOH).

Zheng, N. *et al., Chem. Comm.*, 1997, 399 (*isol, ir, pmr, cmr*)
Seo, S.-Y. *et al., Org. Lett.*, 2004, **6**, 429-432 (*synth*)

Bacillomycin D B-4

Raubitschek substance

[76012-17-4]



R = $CH_2CH(CH_3)_2$, $CH(CH_3)CH_2CH_3$, $(CH_2)_2CH(CH_3)$ or $(CH_2)_4CH_3$

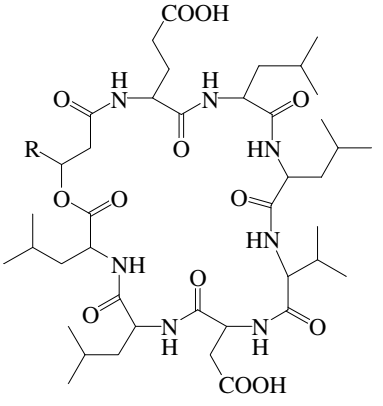
Cyclic lipopeptide antibiotic complex. Essentially $C_{48}H_{74}N_{10}O_{15}$ and $C_{49}H_{76}N_{10}O_{15}$. Isol. from a *Bacillus subtilis* strain. Antifungal agent. Powder.
Mp 287°.

Me ester: Isol. from the marine *Bacillus subtilis* KMM 457. Powder.
Mp 257-260°.

Peypoux, F. *et al., J. Antibiot.*, 1980, **33**, 1146-1149 (*isol, ir*)
Peypoux, F. *et al., Eur. J. Biochem.*, 1981, **118**, 323-327 (*struct*)
Peypoux, F. *et al., J. Antibiot.*, 1984, **37**, 1600-1604 (*struct*)
Besson, F. *et al., FEBS Lett.*, 1992, **308**, 18-21 (*biosynth*)
Moyne, A.L. *et al., J. Appl. Microbiol.*, 2001, **90**, 622-629 (*isol, ms, activity*)
Oleinikova, G.K. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2003, **39**, 609-610; 2005, **41**, 240-242; 461-464 (*isol, pmr, cmr, ms*)

Bacircines B-5

Batsirtsines, 9CI. Bacirtcines. Bacirtsins



Bacircine 1 R = $-(CH_2)_6CH(CH_3)CH_2CH_3$
2 R = $-(CH_2)_8CH(CH_3)_2$
3 R = $-(CH_2)_{10}CH_3$
4 R = $-(CH_2)_8CH(CH_3)CH_2CH_3$
5 R = $-(CH_2)_9CH(CH_3)_2$

Depsipeptide antibiotic complex. Several alternative spellings in the lit., including CAS. Prod. by *Bacillus pumilis* KMM150 isol. from an Australian sponge *Ircinia* sp.

Bacircine 1 [169276-09-9]

$C_{51}H_{89}N_7O_{13}$ 1008.303

Sol. MeOH, EtOAc. $[\alpha]_D$ -36.5 (c, 0.5 in MeOH).

Bacircine 2 [169276-10-2]

$C_{52}H_{91}N_7O_{13}$ 1022.33

Sol. MeOH, EtOAc. $[\alpha]_D$ -31.5 (c, 0.5 in MeOH).

Bacircine 3 [169276-11-3]

$C_{52}H_{91}N_7O_{13}$ 1022.33

Sol. MeOH, EtOAc. $[\alpha]_D$ -32.4 (c, 0.5 in MeOH).

Bacircine 4 [169276-12-4]

$C_{53}H_{93}N_7O_{13}$ 1036.357

Cryst. Sol. MeOH, EtOAc. Mp 143.5-144.5°. $[\alpha]_D$ -28.6 (c, 0.5 in MeOH).

Bacircine 5 [169276-13-5]

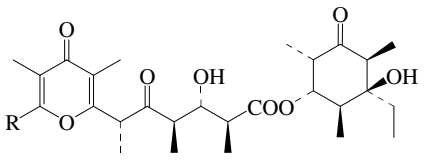
$C_{53}H_{93}N_7O_{13}$ 1036.357

Cryst. Sol. MeOH, EtOAc. Mp 142.5-143.5°. $[\alpha]_D$ -33.6 (c, 0.5 in MeOH).

Kalinovskaya, N.I. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1995, **44**, 951-955 (*Bacirines 1-5, isol, struct*)
Prokof'eva, N.G. *et al., Toxicon*, 1999, **37**, 801-813 (*activity*)

Baconipyrone A B-6

[123003-45-2]



Absolute Configuration

R = CH_2CH_3

$C_{29}H_{44}O_8$ 520.662

Constit. of the pulmonate mollusc *Siphonaria baconi*. Oil. $[\alpha]_D$ -82 (c, 0.47 in $CHCl_3$). λ_{max} 220 (ϵ 10300); 260 (ϵ 12700) (MeOH) (Derep).

Manker, D.C. *et al., J.O.C.*, 1989, **54**, 5371-5374 (*isol, pmr, cmr*)
Turks, M. *et al., Org. Lett.*, 2004, **6**, 3031-3034 (*synth, abs config*)

Baconipyrone B B-7

[123003-46-3]

As Baconipyrone A, B-6 with

R = -CH_3

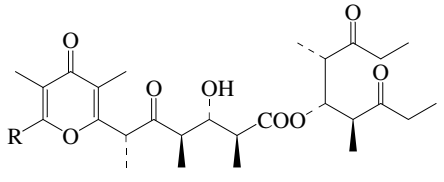
$C_{28}H_{42}O_8$ 506.635

Constit. of the pulmonate mollusc *Siphonaria baconi*. Oil. $[\alpha]_D$ -65.9 (c, 0.66 in $CHCl_3$). λ_{max} (solvent not reported) (Derep). λ_{max} 220 (ϵ 10300); 260 (ϵ 12700) (MeOH) (Derep).

Manker, D.C. *et al., J.O.C.*, 1989, **54**, 5371-5374 (*isol, pmr, cmr*)
Turks, M. *et al., Org. Lett.*, 2004, **6**, 3031-3034 (*abs config*)

Baconipyrone C B-8

[123003-47-4]



Absolute Configuration

R = CH_2CH_3

$C_{29}H_{44}O_8$ 520.662

Constit. of the pulmonate mollusc *Siphonaria baconi*. Oil. $[\alpha]_D$ -19 (c, 0.9 in MeOH). λ_{max} 220 (ϵ 10300); 260 (ϵ 12700) (MeOH) (Derep).

Manker, D.C. *et al., J.O.C.*, 1989, **54**, 5371-5374 (*isol, pmr, cmr, struct*)
Paterson, I. *et al., Tet. Lett.*, 1994, **35**, 6925; 6929 (*abs config, biosynth*)
Paterson, I. *et al., Org. Lett.*, 2000, **2**, 1513-1516 (*synth*)

Baconipyrone D B-9

[123003-48-5]

As Baconipyrone C, B-8 with

R = –CH_3

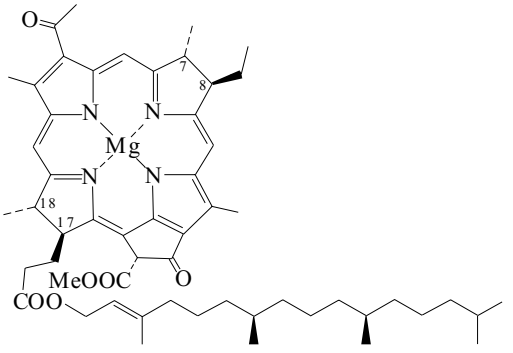
$C_{28}H_{42}O_8$ 506.635

Constit. of the pulmonate mollusc *Siphonaria baconi*. Oil. $[\alpha]_D$ -61.7 (c, 1.17 in MeOH). λ_{max} (solvent not reported) (Derep). λ_{max} 220 (ϵ 10300); 260 (ϵ 12700) (MeOH) (Derep).

Manker, D.C. *et al., J.O.C.*, 1989, **54**, 5371-5374 (*isol, pmr, cmr, struct*)
Paterson, I. *et al., Tet. Lett.*, 1994, **35**, 6925-6928; 6929-6932 (*abs config, biosynth*)

Bacteriochlorophyll a B-10

[17499-98-8]



$C_{55}H_{74}MgN_4O_6$ 911.518

Occurs in *Rhodopseudomonas spheroides*, *Rhodospirillum rubrum*, *Rhodospirillum fulvum*, *Rhodopseudomonas viridis*, *Thiocystis violacea*, *Oscillatoria* sp. and sulfur and chlorobacteria. Dark-purple amorph. solid (petrol).

Mp 94° dec. In *R. rubrum* the esterifying alcohol is 2,6,10,14-Phytatetraen-1-ol, P-393 instead of 2-Phyten-1-ol, P-396. λ_{max} 358; 390; 771 (no solvent reported).

Scheer, H. *et al., Porphyrins and Metalloporphyrins*, (ed. Smith, K.M.), Elsevier (Ed. Smith, K.M.), Elsevier, Amsterdam, 1975, 399
Jackson, A.H. *et al., Chem. Biochem. Plant Pigm.*, (Ed. Goodwin, T.W.), Academic Press, N.Y., Vol. I, 1976, 1
Brockmann, H. *et al., The Porphyrins*, (Ed. Dolphin, D. *et al*), Academic Press, N. Y., Vol. II, 1979, 287
Scholz, B. *et al., Angew. Chem., Int. Ed.*, 1981, **20**, 956-958 (*struct*)
Oelze, J. *et al., Methods Microbiol.*, 1985, **18**, 257-284 (*rev, isol, anal*)
Leeper, F.J. *et al., Nat. Prod. Rep.*, 1985, **2**, 19-47; 561-568; 1987, **4**, 441-469; 1989, **6**, 171-203 (*revs, biosynth*)
Simpson, D.J. *et al., Diss. Abstr. Int., B*, 1987, **47**, 4168 (*synth, struct*)
Berger, G. *et al., J. Liq. Chromatogr.*, 1987, **10**, 1519-1531 (*purifn*)
Grese, R.P. *et al., J. Am. Soc. Mass Spectrom.*, 1990, **1**, 72-84 (*ms*)
Smith, K.M. *et al., New Compr. Biochem.*, 1991, **19**, 237 (*rev, struct, biosynth*)

Bacteriorhodopsin B-11

Protein consisting of 247 aminoacid residues with a prosthetic group of Retinal, R-32. Purple photosynthetic pigment of the membrane of halophilic archaebacteria, e.g. *Halobacterium halobium*. Light-driven proton pump.

Miercke, L.J. *et al., J. Biol. Chem.*, 1989, **264**, 7531-7535 (*isol*)
Lorder, B. *et al., FEBS Lett.*, 1990, **261**, 14-18 (*isol*)
Haupts, U. *et al., Annu. Rev. Biophys. Biomol. Struct.*, 1999, **28**, 367-399 (*rev*)
Lanyi, J.K. *et al., Int. Rev. Cytol.*, 1999, **187**, 161-202 (*rev*)
Lanyi, J.K. *et al., Curr. Opin. Struct. Biol.*, 2000, **11**, 415-419 (*rev*)
Lanyi, J.K. *et al., Annu. Rev. Physiol.*, 2004, **66**, 665-688 (*rev*)

Aplysia californica ϵ-Bag cell peptide B-12

[109024-45-5]

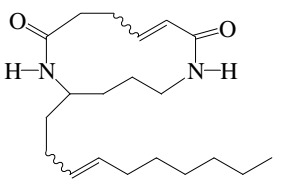
H-Ser-Val-Leu-Thr-Pro-Ser-Leu-Ser-Ser-Leu-Gly-Glu-Ser-Leu-Glu-Ser-Gly-Ile-Ser-OH

Isol. from bag cells of the marine mollusc *Aplysia californica*. Released during egg-laying.

Newcomb, R. *et al., J. Neurosci.*, 1987, **7**, 857 (*isol, struct*)
Nagle, G.T. *et al., Biol. Bull. (Woods Hole, Mass.)*, 1989, **177**, 210 (*isol, struct*)

Bahamamide B-13

2-(3-Decenyl)-1,6-diazacyclododec-8-ene-7,12-dione, 9CI
[190782-45-7]

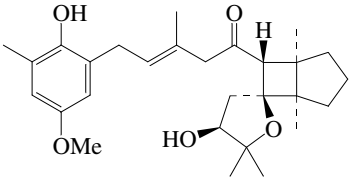


$C_{20}H_{34}N_2O_2$ 334.501
Prod. by an unidentified marine bacterium. Oil. $[\alpha]_D$ +27.8 (c, 0.5 in $CHCl_3$). λ_{max} 227 (ϵ 1700) (THF).

Boehler, M. *et al., Nat. Prod. Lett.*, 1997, **10**, 75-78 (*isol, uv, ir, pmr, cmr*)

Balearone B-14

[92675-09-7]



Absolute configuration

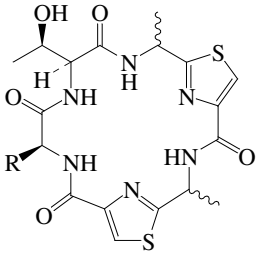
$C_{28}H_{40}O_5$ 456.621
Metabolite of brown alga *Cystoseira balearica*. Cryst. (hexane). Mp 94-96°. $[\alpha]_D^{20}$ +52.

Z-*Isomer:* ***Isobalearone***
[110351-75-2]
$C_{28}H_{40}O_5$ 456.621
Constit. of *Cystoseira stricta*. Oil. $[\alpha]_D^{20}$ +38.3 (c, 1.2 in EtOH).

Amico, V. *et al., Tetrahedron*, 1984, **40**, 1721 (*isol, struct*)
Amico, V. *et al., Phytochemistry*, 1987, **26**, 1719 (*isol*)
Amico, V. *et al., Gazz. Chim. Ital.*, 1991, **121**, 335 (*pmr, cmr*)
Amico, V. *et al., J. Nat. Prod.*, 1997, **60**, 1088-1093 (*abs config*)

Banyascyclamide B B-15

[501904-00-3]



R = $-CH_2CH(CH_3)_2$

$C_{22}H_{30}N_6O_5S_2$ 522.648
Isol. from *Nostoc* sp. TAU strain IL-235.

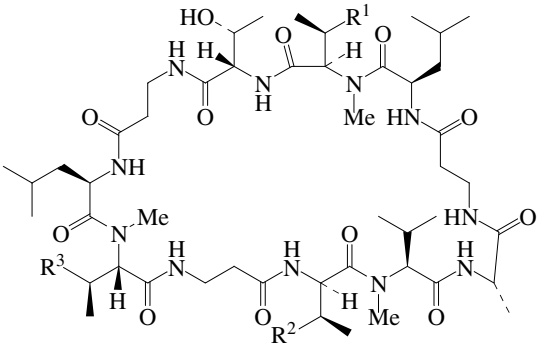
Ploutno, A. *et al., Tetrahedron*, 2002, **58**, 9949-9957 (*isol, pmr, cmr, ms*)

Banyascyclamide C B-16

[501904-01-4]
As Banyascyclamide B, B-15 with
R = $-CH_2Ph$
$C_{25}H_{28}N_6O_5S_2$ 556.665
Isol. from *Nostoc* sp. TAU strain IL-235.
$[\alpha]_D^{25}$ +50.1 (c, 0.1 in MeOH). This is an isomer of Didmolamide B, D-409. λ_{max} 222 (ϵ 15100); 238 (ϵ 16300) (MeOH).

Ploutno, A. *et al., Tetrahedron*, 2002, **58**, 9949-9957 (*isol, pmr, cmr, ms*)

Barangamides B-17



Barangamide A	$R^1 = R^2 = R^3 = -CH_2CH_3$
Barangamide B	$R^1 = R^2 = -CH_2CH_3$, $R^3 = CH_3$
Barangamide C	$R^1 = R^3 = -CH_2CH_3$, $R^2 = CH_3$
Barangamide D	$R^1 = CH_3$, $R^2 = R^3 = -CH_2CH_3$

Cyclic peptide. Isol. from the sponge *Theonella swinhoei*.

Barangamide A

$C_{54}H_{97}N_{11}O_{12}$ 1092.427
Glassy solid. $[\alpha]_D^{25}$ -38.4 (c, 0.3 in MeOH).

Barangamide B

$C_{53}H_{95}N_{11}O_{12}$ 1078.4
Glassy solid. $[\alpha]_D^{29}$ +76.5 (c, 0.04 in $CHCl_3$).

Barangamide C

$C_{53}H_{95}N_{11}O_{12}$ 1078.4
Glassy solid. $[\alpha]_D^{26}$ +57.8 (c, 0.07 in $CHCl_3$).

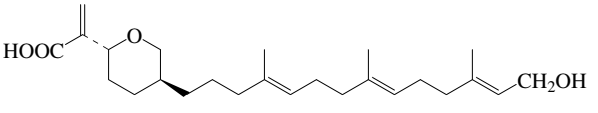
Barangamide D

$C_{53}H_{95}N_{11}O_{12}$ 1078.4
Glassy solid. $[\alpha]_D^{29}$ +84.6 (c, 0.1 in $CHCl_3$).

Roy, M.C. *et al., Tetrahedron*, 2000, **56**, 9079-9092 (*isol, ir, pmr, cmr*)

Barangcadoic acid A B-18

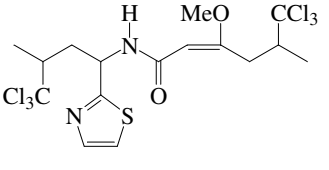
[457938-80-6]



$C_{25}H_{40}O_4$ 404.589
Isol. from the sponge *Hippospongia* sp. RCE-protease inhibitor. $[\alpha]_D^{28}$ +34.9 (c, 3.8 in CH_2Cl_2).

Craig, K.S. *et al., Tet. Lett.*, 2002, **43**, 4801-4804 (*isol, pmr, cmr*)

Barbaleucamide A B-19



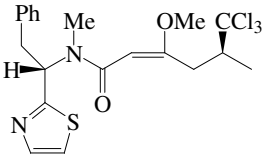
$C_{16}H_{20}Cl_6N_2O_2S$ 517.128
Isol. from a *Dysidea* sp. Pale yellow oil.

N-*Me:* ***Barbaleucamide B***
$C_{17}H_{22}Cl_6N_2O_2S$ 531.155
Isol. from a *Dysidea* sp. Pale yellow oil.

Harrigan, G.G. *et al., J. Nat. Prod.*, 2001, **64**, 1133-1138

Barbamide B-20

[174630-03-6]



Absolute Configuration

$C_{20}H_{23}Cl_3N_2O_2S$ 461.838

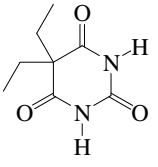
Metab. from the Caribbean cyanobacterium *Lyngbya majuscula*. Possesses molluscicidal activity. Pale yellow oil. Sol. MeOH, $CHCl_3$, EtOAc; poorly sol. hexane, H_2O. $[\alpha]_D^{26}$ -89 (c, 1.9 in MeOH). The first marine nat. prod. for which the biosynthetic gene cluster has been sequenced. λ_{max} 240 (ϵ 16000) (MeOH) (Berdy).

Dechloro: ***Dechlorobarbamide***
[327613-98-9]
$C_{20}H_{24}Cl_2N_2O_2S$ 427.393
Metab. of *Lyngbya majuscula*. Pale yellow oil. $[\alpha]_D^{25}$ -67 (c, 0.05 in MeOH). λ_{max} 238 (ϵ 16000) (MeOH).

Orjala, J. *et al., J. Nat. Prod.*, 1996, **59**, 427-430 (*isol, uv, ir, pmr, cmr, struct*)
Hartung, J. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 1209-1211 (*biosynth*)
Sitachitta, N. *et al., Tetrahedron*, 2000, **56**, 9103-9113 (*isol, biosynth, abs config, Dechlorobarbamide*)
Nguyen, V.-A. *et al., Chem. Comm.*, 2001, 1934-1935 (*synth*)
Flatt, P.M. *et al., J. Nat. Prod.*, 2006, **69**, 938-944 (*biosynth*)

Barbital, INN B-21

*5,5-Diethyl-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione, 9CI. 5,5-Diethylbarbituric acid. Diethylmalonylurea. Barbitone, BAN. Veronal. Many other names*
[57-44-3]



$C_8H_{12}N_2O_3$ 184.194

Exists in several tautomeric forms. Isol. from tissues of the Indian puffer fish *Sphaeroides oblongus*. Powerful hypnotic and sedative of long duration. Faintly bitter cryst. (H_2O); polymorphic forms; trigonal cryst., monoclinic prisms, monoclinic needles, triclinic cryst.
Mp 190° Mp 183° (181°, 176°). pK_{a1} 8.02 (25°). pK_a 7.43. Log P 0.66 (calc). λ_{max} 224 (EtOH) (Berdy). λ_{max} 224; 240 (EtOH-NaOH) (Berdy). λ_{max} 243 (NAOH) (Berdy).

▶ LD_{50} (mus, orl) 600 mg/kg. CQ3500000

Na salt: ***Barbital sodium, INN***
[144-02-5]

▶ Fatal in large doses. LD_{50} (rat, orl) 600 mg/kg. Exp. reprod. and teratogenic effects. CQ3850000

N-*Me:* See Metharbital in *The Combined Chemical Dictionary.*

N-*Isopropyl:* [85432-35-5]
$C_{11}H_{18}N_2O_3$ 226.275
Cryst. (EtOH aq.). Mp 116°.

▶ CQ3550000

N^1,N^3-*Di-Me:* [714-59-0]
$C_{10}H_{16}N_2O_3$ 212.248
Cryst. Mp 37°.

▶ CQ3508600

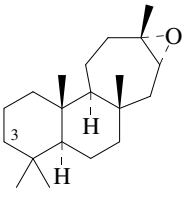
N-*Ph: 5,5-Diethyl-1-phenyl-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione.* ***Phetharbital, INN****. Pyrictal. Fedibaretta*
[357-67-5]
$C_{14}H_{16}N_2O_3$ 260.292
Anticonvulsant, also for the treatment of hyperbilirubinaemia. Plates (EtOH). Mp 178° (197°).

▶ CQ3774000

Sadtler Standard Proton NMR Spectra, 1173 (*pmr*)
Fischer, E. *et al., Annalen*, 1904, **335**, 334 (*synth*)
Köfler, A. *et al., CA*, 1947, **41**, 3584 (*props*)
Craven, B.M. *et al., J. Mol. Struct.*, 1973, **16**, 331 (*cryst struct*)
Japan. Pat., 1975, 7 537 673; *CA*, **85**, 108659 (*synth*)
McMullen, R.K. *et al., Acta Cryst. B*, 1978, **34**, 3719 (*cryst struct*)
Asada, S. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 3379 (*cmr*)
Voronin, V.G. *et al., Khim. Geterotsikl. Soedin.*, 1978, 813; *Chem. Heterocycl. Compd.*, 1978, 667 (*ms*)
Barnes, A.J. *et al., J. Mol. Struct.*, 1979, **56**, 29 (*ir*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1985, **A13**, 542 (*props*)
Koval'chukova, O.V. *et al., Zh. Neorg. Khim.*, 1985, **30**, 1769; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1985, **30**, 1006 (*uv*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 969 (*synonyms*)
Mitra, S.K. *et al., Chem. Comm.*, 1989, 16 (*isol, uv, ir, pmr, cmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 566
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BAG000; BAG250

Barekoxide B-22

[145458-09-9]



$C_{20}H_{34}O$ 290.488

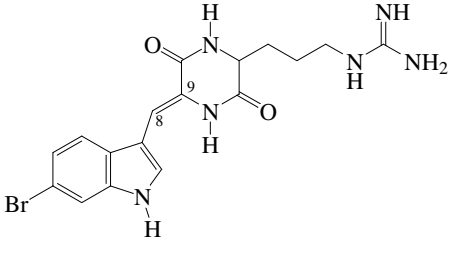
Stereochem. revised in 2001. Constit. of *Chelonaplysilla erecta*. Cryst. (hexane).
Mp 140°. $[\alpha]_D^{24}$ +5.3 (c, 0.26 in $CHCl_3$).

3β-Bromo: ***3-Bromobarekoxide***
[291507-24-9]
$C_{20}H_{33}BrO$ 369.384
Constit. of *Laurencia luzonensis*. Cryst. (CCl_4).
Mp 165°. $[\alpha]_D^{27}$ +6.2 (c, 0.3 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 1992, **55**, 1408 (*isol, pmr, cmr*)
Kuniyoshi, M. *et al., J. Nat. Prod.*, 2001, **64**, 696-700 (*3-Bromobarekoxide, pmr, cmr, cryst struct*)
Justicia, J. *et al., J.A.C.S.*, 2005, **127**, 14911-14921 (*synth*)

Barettin B-23

[104311-70-8]



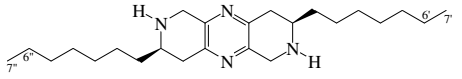
$C_{17}H_{19}BrN_6O_2$ 419.28

Struct. and MF revised in 2002. Isol. from the sponge *Geodia barretti*. Yellow solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 207-210°. $[\alpha]_D$ -25 (c, 3 in MeOH). λ_{max} 235 (ϵ 13000); 294 (sh) (ϵ 5200); 340 (ϵ 9700) (MeOH) (Derep).

8,9-Dihydro: ***8,9-Dihydrobarettin***
$C_{17}H_{21}BrN_6O_2$ 421.296
Isol. from *Geodia barretti*. Brownish solid. $[\alpha]_D^{21}$ -24 (c, 0.096 in MeOH). λ_{max} 225 (log ϵ 1.27); 286 (log ϵ 0.16) (MeOH).

Sölter, S. *et al., Tet. Lett.*, 2002, **43**, 3385-3386 (*isol, pmr, cmr, struct*)
Sjögren, M. *et al., J. Nat. Prod.*, 2004, **67**, 368-372 (*isol, activity*)
Johnson, A.-L. *et al., Tetrahedron*, 2004, **60**, 961-965 (*synth*)

Barrenazine A B-24



Relative Configuration

$C_{24}H_{42}N_4$ 386.623
Isol. from an unidentified tunicate. Mildly cytotoxic. Oil. $[\alpha]_D^{21}$ -55 (4) (c, 0.48 in MeOH). λ_{max} 288 (ϵ 6950); 313 (sh) (MeOH).

6′,6″,7′,7″-Tetradehydro: ***Barrenazine B***
$C_{24}H_{38}N_4$ 382.591
Isol. from an unidentified tunicate. Oil. $[\alpha]_D^{21}$ -21 (c, 0.26 in MeOH). λ_{max} 288 (ϵ 6950); 313 (sh) (MeOH).

Chill, L. *et al., Org. Lett.*, 2003, **5**, 2433-2435 (*isol, pmr, cmr*)
Focken, T. *et al., Org. Lett.*, 2006, **8**, 2985-2988 (*synth*)

Bass hepcidin B-25

Morone *Hepcidin*
[452112-54-8]
Gly-Cys-Arg-Phe-Cys-Cys-Asn-Cys-Cys-Pro-Asn-Met-Ser-Gly-Cys-Gly-Val-Cys-Cys-Arg-Phe

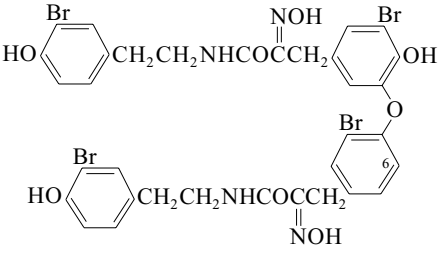
$C_{86}H_{128}N_{29}O_{25}S_9$ 2256.731

Struct. of reduced form shown. Isol. from gills of the hybrid striped bass, (white bass (*Morone chrysops*) × striped bass (*Morone saxatilis*). Shows antimicrobial activity.

Shike, H. *et al., Eur. J. Biochem.*, 2002, **269**, 2232-2237 (*isol*)

Bastadin 1 B-26

[75513-48-3]



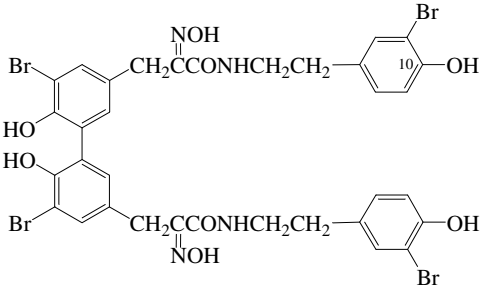
$C_{34}H_{30}Br_4N_4O_8$ 942.249
Isol. from the sponge *Ianthella basta*. Active against gram-positive bacteria. Foam. λ_{max} 220 (ϵ 63100); 283 (ϵ 10700); 288 (sh) (ϵ 8510) (MeOH) (Derep). λ_{max} 220 (ϵ 63000); 282 (ϵ 11400); 288 (ϵ 11000) (MeOH) (Berdy).

6-Bromo: ***Bastadin 2***
[75513-47-2]
$C_{34}H_{29}Br_5N_4O_8$ 1021.145
From *Ianthella basta*. Active against gram-positive bacteria. Foam. λ_{max} 220 (sh) (ϵ 50100); 280 (ϵ 8510); 293 (sh) (ϵ 7410) (MeOH) (Derep).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1981, **34**, 765 (*isol, uv, pmr, cmr, ms, struct*)
Nishiyama, S. *et al., Tet. Lett.*, 1982, **23**, 1281 (*synth, ir*)
Guo, Z. *et al., J.O.C.*, 1998, **63**, 4269-4276 (*Bastadin 2, synth*)

Bastadin 3 B-27

[79067-77-9]



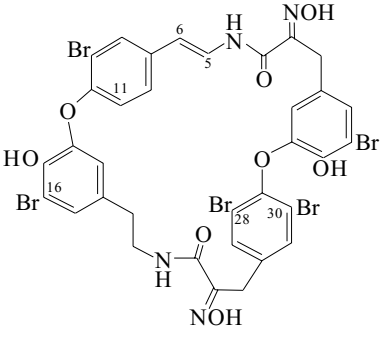
$C_{34}H_{30}Br_4N_4O_8$ 942.249
Isol. from the sponge *Ianthella basta*. Active against gram-positive bacteria. Pale yellow foam. Poorly sol. hexane. λ_{max} 220 (ϵ 63100); 283 (ϵ 10700); 288 (sh) (ϵ 8510) (MeOH) (Derep). λ_{max} 220 (ϵ 57200); 285 (ϵ 8700) (MeOH) (Berdy).

*10-*O*-Sulfate:* ***10-O-Sulfatobastadin 3***
[184478-47-5]
$C_{34}H_{30}Br_4N_4O_{11}S$ 1022.313
Isol. from *Ianthella basta*. Calcium ion release inducer. Calcium ion channel modulator. Powder (as Na salt). λ_{max} 209 (ϵ 84400); 279 (ϵ 5550) (MeOH) (as Na salt).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1981, **34**, 765 (*isol, uv, pmr, cmr, ms, struct*)
Nishimaya, S. *et al., Tet. Lett.*, 1982, **23**, 1281 (*synth, ir*)
Franklin, M.A. *et al., J. Nat. Prod.*, 1996, **59**, 1121-1127 (*10-sulfate*)
Guo, Z. *et al., J.O.C.*, 1998, **63**, 4269-4276 (*synth*)

Bastadin 4 B-28

Cyclobastadin 1
[79067-76-8]



$C_{34}H_{25}Br_5N_4O_8$ 1017.113

Some Bastadins were renumbered in 1993. Isol. from the sponge *Ianthella basta*. Antiinflammatory agent. Active against gram-positive bacteria. Yellow needles (DMF aq.). Poorly sol. hexane. Mp 250° dec. λ_{max} 209 (ϵ 126000); 289 (ϵ 20000); 300 (sh) (ϵ 15800); 310 (ϵ 15800) (MeOH) (Derep). λ_{max} 210 (ϵ 68400); 228 (ϵ 10000); 315 (ϵ 10000) (MeOH) (Berdy).

5,6-Dihydro: ***Bastadin 5***. *Cyclobastadin 2*
[79067-75-7]
$C_{34}H_{27}Br_5N_4O_8$ 1019.129
From *Ianthella basta*. Cryst. (MeCN) (as tetra-Me ether). Poorly sol. hexane.
Mp 262-264° (tetra-Me ether). λ_{max} 208 (ϵ 126000); 280 (ϵ 7940) (MeOH) (Derep).

*5,6-Dihydro, 6*S*-hydroxy:* ***Bastadin 8***
[127709-45-9]
$C_{34}H_{27}Br_5N_4O_9$ 1035.129
From *Ianthella basta*. Film. Fortuitously given the same trivial name by 2 independent groups. λ_{max} 208 (ϵ 126000); 280 (ϵ 7940) (MeOH) (Derep).

11-Bromo, 5,6-dihydro: ***Bastadin 6***. *Cyclobastadin 3*
[79067-74-6]
$C_{34}H_{26}Br_6N_4O_8$ 1098.025
From *Ianthella basta* and *Psammaplysilla purpurea*. Antiangiogenic agent. Powder. Poorly sol. hexane. λ_{max} 220 (sh) (ϵ 50000); 281 (ϵ 5500) (MeOH) (Derep).

16-Debromo: ***Bastadin 11***
[127687-09-6]
$C_{34}H_{26}Br_4N_4O_8$ 938.217
From *Ianthella basta*. Antiinflammatory agent. Film. λ_{max} 208 (ϵ 20000); 285 (ϵ 2510); 331 (ϵ 3160) (MeOH) (Derep).

16-Debromo, 5,6-dihydro: ***Bastadin 9***†
[127687-07-4]
$C_{34}H_{28}Br_4N_4O_8$ 940.233
From *Ianthella basta*. Antiinflammatory agent. Powder (MeOH aq.). λ_{max} 208 (ϵ 126000); 279 (ϵ 10000) (MeOH) (Derep).

*16-Debromo, 5,6-dihydro, 34-*O*-sulfate:* ***34-O-Sulfobastadin 9***
$C_{34}H_{28}Br_4N_4O_{11}S$ 1020.297
Isol. from *Ianthella basta*. Amorph. solid (as Na salt).

28-Debromo: ***Bastadin 7***. *Cyclobastadin 4*
[79067-73-5]
$C_{34}H_{26}Br_4N_4O_8$ 938.217
From *Ianthella basta*. Foam. Poorly sol. hexane. λ_{max} 290 (ϵ 15100); 315 (ϵ 15500) (MeOH) (Derep).

28-Debromo, 15,34-disulfate: ***15,34-Di-O-sulfatobastadin 7***
[184478-46-4]
$C_{34}H_{26}Br_4N_4O_{14}S_2$ 1098.346
From *Ianthella basta*. Calcium ion release inducer. Calcium ion channel modulator. Yellow solid (as di-Na salt). λ_{max} 207 (ϵ 82300); 321 (ϵ 12400) (MeOH) (di-Na salt).

*28-Debromo, 6*S*-hydroxy, 5,6-dihydro:* ***Bastadin 10***
[127687-08-5]
$C_{34}H_{28}Br_4N_4O_9$ 956.233
From *Ianthella basta*. Antiinflammatory agent. Inosine 5′-phosphate dehydrogenase inhibitor. Oil. λ_{max} 208 (ϵ 126000); 279 (ϵ 10000) (MeOH) (Derep). λ_{max} 210 (ϵ 50000); 277 (ϵ 5000) (MeOH) (Berdy).

28-Debromo, 11-bromo: ***Bastadin 14***. *Isobastadin 4*
[146345-73-5]
$C_{34}H_{25}Br_5N_4O_8$ 1017.113
Isol. from sponge *Psammaplysilla purpurea*. Dehydrofolate reductase inhibitor. λ_{max} 284 (ϵ 20000); 292 (ϵ 20000); 314 (ϵ 25000) (MeOH) (Berdy).

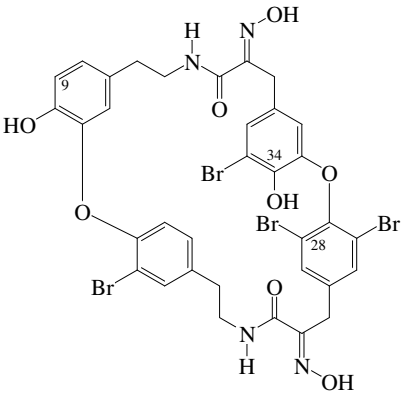
28-Debromo, 11-bromo, 5,6-dihydro: ***Bastadin 15***
[149420-79-1]
$C_{34}H_{27}Br_5N_4O_8$ 1019.129
Metab. of a temperate marine sponge *Ianthella* sp. Small -ve opt. rotn.

*28-Debromo, 11-bromo, 5,6-dihydro, 6*S*-hydroxy:* ***Bastadin 12***. *Bastadin 9 (obsol.)*†
[150204-46-9]
$C_{34}H_{27}Br_5N_4O_9$ 1035.129
From *Ianthella basta*. Amorph. Renumbered in 1993. Name changed from Bastadin 9 to Bastadin 12 as the name Bastadin 9 was duplicated.

Kazlauskas, R. *et al., Aust. J. Chem.*, 1981, **34**, 765 (*isol, uv, ir, pmr, ms, cryst struct, derivs*)
Nishiyama, S. *et al., Tet. Lett.*, 1982, **23**, 3699 (*synth*)
Miao, S. *et al., J. Nat. Prod.*, 1990, **53**, 1441 (*isol, pmr, cmr, struct*)
Pordesimo, E.O. *et al., J.O.C.*, 1990, **55**, 4704 (*isol, pmr, cmr, struct*)
Carney, J.R. *et al., J. Nat. Prod.*, 1993, **56**, 153-157 (*nomencl*)
Dexter, A.F. *et al., J. Nat. Prod.*, 1993, **56**, 782 (*Bastadin 15*)
Pettit, G.R. *et al., J. Nat. Prod.*, 1995, **58**, 680-688 (*abs config*)
Franklin, M.A. *et al., J. Nat. Prod.*, 1996, **59**, 1121-1127 (*15,34-Disulfatobastadin 7*)
Guo, Z. *et al., J.O.C.*, 1998, **63**, 4269-4276 (*Bastadin 6, synth*)
Masuno, M.N. *et al., Mar. Drugs*, 2004, **2**, 176-184 (*34-Sulfobastadin 9*)
Kotoku, N. *et al., Tetrahedron*, 2005, **61**, 7211-7218 (*Bastadin 6, synth*)

Bastadin 13 B-29

Bastadin 12 (obsol.)†
[134981-78-5]



$C_{34}H_{28}Br_4N_4O_8$ 940.233
Originally isol. as Bastadin 12. Renumbered in 1993. Constit. of the sponge *Ianthella basta*. Powder.
Mp 177-179°. λ_{max} 204 (ϵ 141000); 280 (ϵ 11200) (MeOH).

34-Sulfate: ***34-Sulfobastadin 13***
[152213-67-7]
$C_{34}H_{28}Br_4N_4O_{11}S$ 1020.297
Constit. of an *Ianthella* sp. Endothelin A binding inhibitor; inhibitor of ATP citrate lyase. CAS no. refers to the Na salt. λ_{max} 204 (ϵ 74000); 280 (ϵ 4800) (MeOH).

9-Bromo: ***Bastadin 19***
[158982-26-4]
$C_{34}H_{27}Br_5N_4O_8$ 1019.129
Isol. from *Ianthella basta*. Calcium channel modulator.

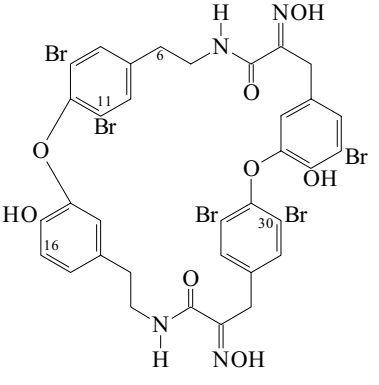
28-Debromo: ***Bastadin 21***
$C_{34}H_{29}Br_3N_4O_8$ 861.337
Isol. from *Ianthella quadrangulata*. Amorph. solid. λ_{max} 195 (log ϵ 4.56); 279 (log ϵ 3.4); 384 (log ϵ 2.99) (MeOH).

28-Debromo, 9-bromo: ***Bastadin 20***
[184679-29-6]
$C_{34}H_{28}Br_4N_4O_8$ 940.233
Isol. from *Ianthella basta*. Calcium channel modulator. Solid. λ_{max} 209 (ϵ 84400); 279 (ϵ 5550) (MeOH).

Butler, M.S. *et al., Aust. J. Chem.*, 1991, **44**, 287-296 (*isol, pmr, cmr*)
Carney, J.R. *et al., J. Nat. Prod.*, 1993, **56**, 153-157 (*nomencl*)
Gulavita, N.K. *et al., J. Nat. Prod.*, 1993, **56**, 1613-1617 (*34-sulfate*)
Franklin, M.A. *et al., J. Nat. Prod.*, 1996, **59**, 1121-1127 (*Bastadin 19, Bastadin 20*)
Coll, J.C. *et al., J. Nat. Prod.*, 2002, **65**, 753-756 (*Bastadin 21*)

Bastadin 16 B-30

[156312-12-8]



$C_{34}H_{27}Br_5N_4O_8$ 1019.129

Constit. of the sponge *Ianthella basta* and *Psammaplysilla purpurea*. λ_{max} 280 (ϵ 3980) (MeOH) (Berdy).

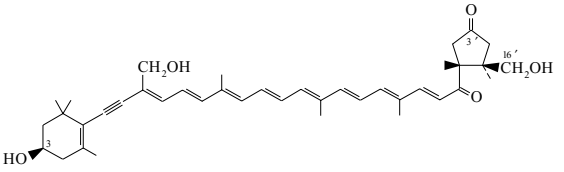
6-Hydroxy, 11-debromo: ***Bastadin 17***
[156312-13-9]
$C_{34}H_{28}Br_4N_4O_9$ 956.233
Constit. of *Ianthella basta*. λ_{max} 278 (ϵ 12600) (MeOH) (Berdy).

11,30-Bisdebromo, 16-bromo: ***Bastadin 18***
[157536-51-1]
$C_{34}H_{28}Br_4N_4O_8$ 940.233
Constit. of *Ianthella basta*. Inosine 5′-phosphate dehydrogenase inhibitor. Amorph. solid.

Park, S.K. *et al., J. Nat. Prod.*, 1994, **57**, 407 (*isol, pmr, cmr, struct*)
Jaspars, M. *et al., Tetrahedron*, 1994, **50**, 7367 (*Bastadin 18*)

Bastaxanthol B-31

Bastaxanthol c



$C_{40}H_{52}O_5$ 612.848

3-O-*Sulfate:* ***Bastaxanthin****. Bastaxanthin c*
[80802-72-8]
$C_{40}H_{52}O_8S$ 692.912
Constit of sponge *Ianthella basta*. Cryst. (Me_2CO/hexane) (as Na salt).
Mp 190° (Na salt). First known carotenoid sulfate.

16′-Aldehyde: 7,8-Didehydro-3,19-dihydroxy-3′,6′-dioxo-β, χ-caroten-16′-al, 9CI. ***Bastaxanthol b***
[88930-50-1]
Minor carotenoid from *Ianthella basta*. λ_{max} 358; 468 (MeOH).

16′-Aldehyde, 3-O-*sulfate:* ***Bastaxanthin b***
[80802-71-7]
$C_{40}H_{50}O_8S$ 690.896
Isol. from *Ianthella basta*. Cryst. (Me_2CO/hexane) (as Na salt). λ_{max} 360; 463 (MeOH).

16′-Carboxylic acid, 3-O-*sulfate:* ***Bastaxanthin e***
[80802-74-0]
$C_{40}H_{50}O_9S$ 706.896
Isol. from *Ianthella basta*. Isol. as Na salt.

3′β-Alcohol, 3-O-*sulfate:* ***Bastaxanthin d***
[80802-73-9]
$C_{40}H_{54}O_8S$ 694.928
Isol. from *Ianthella basta*. Isol. as Na salt.

16′-Deoxy, 3-O-*sulfate:* ***Bastaxanthin b₂***
[88907-74-8]
$C_{40}H_{52}O_7S$ 676.913
Isol. from *Ianthella basta*. Isol. as Na salt, not sepd. from its congeners.

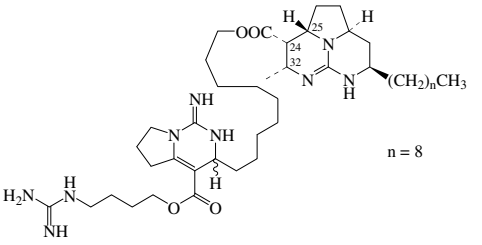
16′-Deoxy, 3′β-alcohol, 3-O-*sulfate:* ***Bastaxanthin c₂***
[88907-75-9]
$C_{40}H_{54}O_7S$ 678.928
Isol. from *Ianthella basta*. Tentative stereochem. Not separated from Bastaxanthin c. Isol. as Na salt.

3′β-Alcohol, 16′-carboxylic acid, 3-O-*sulfate:* ***Bastaxanthin f***
[80802-75-1]
$C_{40}H_{52}O_9S$ 708.911
Isol. from *Ianthella basta*. Isol. as Na salt. λ_{max} 468 (MeOH).

Hertzberg, S. *et al., Biochem. Syst. Ecol.*, 1981, **9**, 211; 1983, **11**, 267
Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1983, **37**, 267

Batzelladine A B-32

[147664-18-4]



$C_{42}H_{73}N_9O_4$ 768.097
Major component of complex where in addn. *n* = 9 and 10. Alkaloids from the Caribbean sponge *Batzella* sp. Inhibits the binding of HIVgp-120 to CD4. Amorph. powder. $[\alpha]_D^{25}$ +8.9 (c, 2.3 in MeOH). λ_{max} 205 (ϵ 20100); 288 (ϵ 6820) (MeOH) (Derep).

[162047-79-2, 162047-80-5]

Patil, A.D. *et al., J.O.C.*, 1995, **60**, 1182 (*isol, uv, ir, pmr, cmr, struct*)
Snider, B.B. *et al., J.O.C.*, 1999, **62**, 1707-1711 (*config*)
Franklin, A.S. *et al., J.O.C.*, 1999, **64**, 1512-1519 (*config*)
Shimokawa, J. *et al., Chem. Eur. J.*, 2005, **11**, 6878-6888 (*synth*)
Arnold, M.A. *et al., J.A.C.S.*, 2006, **128**, 13255-13260 (*synth*)

Batzelladine B B-33

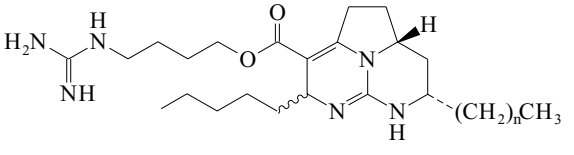
[161503-23-7]
As Batzelladine A, B-32 with
n = 6, $\Delta^{24,32}$, 25-epimer
$C_{40}H_{67}N_9O_4$ 738.027
Major component of complex where in addn. *n* = 7 and 8. Alkaloids from the Caribbean sponge *Batzella* sp. Inhibitor of HIVgp-120-human CD4 binding. Interleukin binding inhibitor. Amorph. powder. Sol. H_2O; fairly sol. MeOH; poorly sol. Me_2CO, hexane. $[\alpha]_D^{25}$ +44.3 (c, 3.7 in MeOH). λ_{max} 206 (ϵ 16600); 289 (ϵ 9300); 340 (ϵ 4380) (MeOH) (Derep).

[162047-81-6, 162047-82-7]

Patil, A.D. *et al., J.O.C.*, 1995, **60**, 1182 (*isol, uv, ir, pmr, cmr, struct*)
Franklin, A.S. *et al., J.O.C.*, 1999, **64**, 1512-1519 (*synth, config*)

Batzelladine C B-34

[161503-24-8]



n = 6

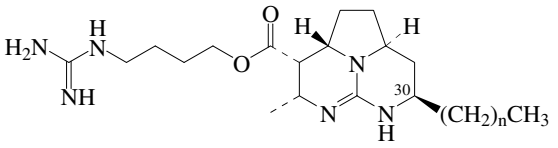
$C_{27}H_{48}N_6O_2$ 488.715
Major component of complex where in addn. *n* = 7 and 8. Alkaloids from the Caribbean sponge *Batzella* sp. Amorph. powder. $[\alpha]_D^{25}$ -3.7 (c, 2.4 in MeOH). λ_{max} 211 (ϵ 8080); 230 (ϵ 7830); 298 (ϵ 6940) (MeOH) (Derep).

[162047-83-8, 162047-84-9]

Patil, A.D. *et al., J.O.C.*, 1995, **60**, 1182 (*isol, uv, ir, pmr, cmr, struct*)

Batzelladine D B-35

[161596-65-2]



n = 8

$C_{25}H_{46}N_6O_2$ 462.677

Major component of complex where in addn. *n* = 9 and 10. Alkaloids from the Caribbean sponge *Batzella* sp. Amorph. powder. $[\alpha]_D^{25}$ -1.2 (c, 0.9 in MeOH). λ_{max} 205 (ϵ 9170); 298 (ϵ 2380) (MeOH) (Derep).

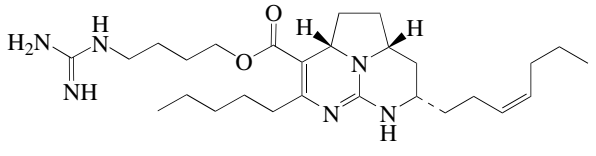
30-Epimer: ***30-Epibatzelladine D***
[147664-20-8]
$C_{25}H_{46}N_6O_2$ 462.677
Alkaloid from a *Batzella* sp. Cytotoxic agent. Powder. Sol. MeOH, H_2O.

[162047-85-0, 162047-86-1]

Pat. Coop. Treaty (WIPO), 1993, 93 1 193; *CA*, **118**, 225662x (*30-epimer*)
Patil, A.D. *et al., J.O.C.*, 1995, **60**, 1182 (*isol, uv, ir, pmr, cmr, struct*)
Franklin, A.S. *et al., J.O.C.*, 1999, **64**, 1512-1519 (*config*)
Cohen, F. *et al., Org. Lett.*, 1999, **1**, 2169-2172 (*synth*)
Ishiwata, T. *et al., Org. Lett.*, 2002, **4**, 2921-2924 (*synth*)
Shimokawa, J. *et al., Chem. Eur. J.*, 2005, **11**, 6878-6888 (*synth*)
Arnold, M.A. *et al., J.A.C.S.*, 2006, **128**, 13255-13260 (*synth*)

Batzelladine E B-36

[161503-25-9]

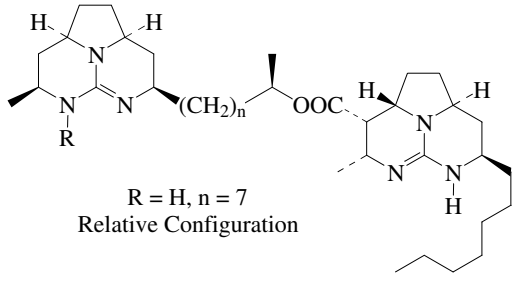


$C_{27}H_{46}N_6O_2$ 486.699
Alkaloid from the Caribbean sponge *Batzella* sp. Protein kinase C and interleukin binding inhibitor. Gum. Sol. H_2O; fairly sol. MeOH; poorly sol. Me_2CO, hexane. $[\alpha]_D^{25}$ +87.1 (c, 1.9 in MeOH). λ_{max} 207 (ϵ 7954); 227 (ϵ 7012); 291 (ϵ 3311); 345 (ϵ 2876) (MeOH) (Berdy).

Patil, A.D. *et al., J.O.C.*, 1995, **60**, 1182 (*isol, uv, ir, pmr, cmr, struct*)
Snider, B.B. *et al., Tet. Lett.*, 1998, **39**, 5697-5700 (*synth, config*)

Batzelladine F B-37

[188112-82-5]



R = H, n = 7
Relative Configuration

$C_{37}H_{64}N_6O_2$ 624.952

Struct. finalised in 2001. Alkaloid from the sponge *Monanchora arbuscula* (formerly *Batzella* sp.). Gum. $[\alpha]_D$ +19.4 (c, 0.87 in MeOH). λ_{max} 236; 254; 296 (MeOH).

Patil, A.D. *et al., J.O.C.*, 1997, **62**, 1814-1819 (*isol, uv, ir, pmr, cmr, struct*)
Snider, B.B. *et al., J. Nat. Prod.*, 1999, **62**, 1707-1711 (*config*)
Black, G.P. *et al., Tetrahedron*, 1999, **55**, 6547-6554 (*synth, pmr, cmr, config*)
Cohen, F. *et al., J.A.C.S.*, 2006, **128**, 2594-2603; 2604-2608 (*synth, struct*)

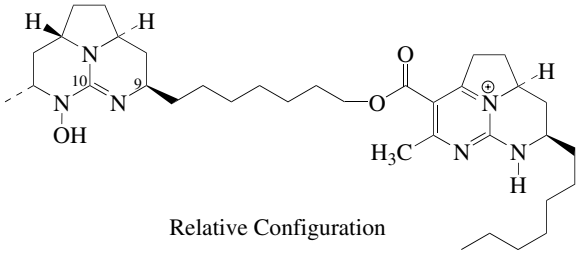
Batzelladine G B-38

[188112-84-7]
As Batzelladine F, B-37 with
R = OH, n = 7
$C_{39}H_{68}N_6O_3$ 669.005
Alkaloid from the sponge *Batzella* sp. Immunosuppressant. Powder. Sol. H_2O; fairly sol. MeOH; poorly sol. Me_2CO, hexane. $[\alpha]_D$ +14.7 (c, 0.79 in MeOH). λ_{max} 233; 258; 295 (MeOH).

Patil, A.D. *et al., J.O.C.*, 1997, **62**, 1814-1819 (*isol, uv, ir, pmr, cmr, struct*)

Batzelladine H B-39

[188112-85-8]



Relative Configuration

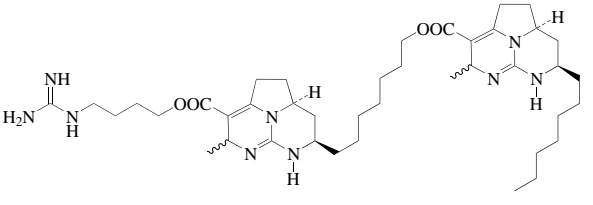
$C_{35}H_{57}N_6O_3^{\oplus}$ 609.874

Isol. as a 43:57 inseparable mixt. with Batzelladine I. Alkaloid from the sponge *Batzella* sp. Oil (as formate). Sol. H_2O; fairly sol. MeOH; poorly sol. Me_2CO, hexane. $[\alpha]_D$ +33.7 (c, 0.56 in MeOH) (formate). λ_{max} 217; 258 (MeOH).

Isomer: ***Batzelladine I***
[188112-86-9]
$C_{35}H_{57}N_6O_3^{\oplus}$ 609.874
From *Batzella* sp. Isomer of Batzelladine H in which the N-hydroxy group is located on the N between C-9 and C-10.

Patil, A.D. *et al., J.O.C.*, 1997, **62**, 1814-1819 (*isol, uv, ir, pmr, cmr, struct*)

Batzelladine J B-40

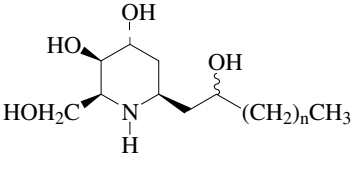


$C_{41}H_{67}N_9O_4$ 750.038
Alkaloid from the sponge *Monanchora unguifera*.
$[\alpha]_D^{25}$ -11.8 (c, 0.13 in MeOH). λ_{max} 228 (ϵ 8800); 295 (ϵ 7200) (MeOH).

Gallimore, W.A. *et al., J. Nat. Prod.*, 2005, **68**, 1420-1423 (*isol, pmr, cmr, ms*)

Batzellaside A B-41

6-(2-Hydroxydodecyl)-2-(hydroxymethyl)-3,4-piperidinediol



Relative Configuration

n = 9

$C_{18}H_{37}NO_4$ 331.495

Alkaloid from the sponge *Batzella* sp. Oil. $[\alpha]_D^{25}$ +8.1 (c, 0.44 in MeOH).

Segraves, N.L. *et al., J. Nat. Prod.*, 2005, **68**, 118-121 (*isol, pmr, cmr*)

Batzellaside B **B-42**

2-(Hydroxymethyl)-6-(2-hydroxyundecyl)-3,4-piperidinediol
As Batzellaside A, B-41 with
n = 8

$C_{17}H_{35}NO_4$ 317.468
Alkaloid from the sponge *Batzella* sp. Oil. $[\alpha]_D^{25}$ +10 (c, 0.5 in MeOH).

Segraves, N.L. *et al., J. Nat. Prod.*, 2005, **68**, 118-121 (*isol, pmr, cmr*)

Batzellaside C **B-43**

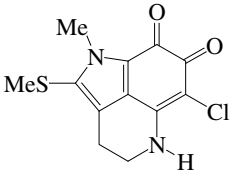
2-(Hydroxymethyl)-6-(2-hydroxytridecyl)-3,4-piperidinediol
As Batzellaside A, B-41 with
n = 10

$C_{19}H_{39}NO_4$ 345.521
Alkaloid from the sponge *Batzella* sp. Oil. $[\alpha]_D^{25}$ +12 (c, 0.4 in MeOH).

Segraves, N.L. *et al., J. Nat. Prod.*, 2005, **68**, 118-121 (*isol, pmr, cmr*)

Batzelline A **B-44**

6-Chloro-1,3,4,5-tetrahydro-1-methyl-2-(methylthio)pyrrolo[4,3,2-de]quinoline-7,8-dione, 9CI
[123064-89-1]



$C_{12}H_{11}ClN_2O_2S$ 282.75
Alkaloid from the deep water Bahamas sponge *Batzella* sp. Black prisms ($CHCl_3$/MeOH).
Mp 205°. λ_{max} 214 (ϵ 8900); 269 (ϵ 22100); 356 (ϵ 7900); 376 (ϵ 8000); 548 (ϵ 600) (MeOH) (Derep).

N-*Me:* Mp 202°.

N-*De-Me:* ***Batzelline B***
[123064-90-4]
$C_{11}H_9ClN_2O_2S$ 268.723
Isol. from *Batzella* sp. Herbicide. Dark brown solid. No definite Mp (dec.). λ_{max} 211 (ϵ 58300); 266 (ϵ 120800); 330 (sh); 387 (ϵ 51800); 550 (ϵ 4000) (MeOH) (Derep).

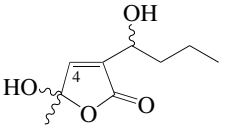
De(methylthio): ***Batzelline C***
[123064-91-5]
$C_{11}H_9ClN_2O_2$ 236.657
Isol. from *Batzella* sp. and *Zyzzya massalis*. Herbicide. Dark brown solid. No definite Mp (dec.). λ_{max} 211 (ϵ 7900); 250 (ϵ 17300); 331 (ϵ 9100); 380 (sh); 540 (ϵ 900) (MeOH) (Derep).

De(methylthio), N-*de-Me:* ***Batzelline D***
[437980-22-8]
$C_{10}H_7ClN_2O_2$ 222.63
Isol. from *Zyzzya fuliginosa* and *Zyzzya massalis*. Purple solid. λ_{max} 248 (log ϵ 4); 328 (log ϵ 3.73) (MeOH).

Sakemi, S. *et al., Tet. Lett.*, 1989, **30**, 2517 (*isol, uv, ir, pmr, cmr, ms, struct*)
Tao, X.L. *et al., Tetrahedron*, 1994, **50**, 2017 (*Batzelline C, synth*)
Yamada, F. *et al., Heterocycles*, 1995, **41**, 1905 (*Batzelline C, synth*)
Roberts, D. *et al., J.O.C.*, 1997, **62**, 568 (*Batzelline C, synth*)
Alvarez, M. *et al., Eur. J. Org. Chem.*, 1999, 1173-1183 (*synth*)
Chang, L.C. *et al., J. Nat. Prod.*, 2002, **65**, 776-778 (*Batzelline D*)
Dijou, M.-G. *et al., Bioorg. Med. Chem.*, 2005, **13**, 6035-6044 (*Batzelline C, D*)

Beckerelide **B-45**

5-Hydroxy-3-(1-hydroxybutyl)-5-methyl-2(5H)-furanone, 9CI



$C_9H_{14}O_4$ 186.207
Parent lactone unknown.

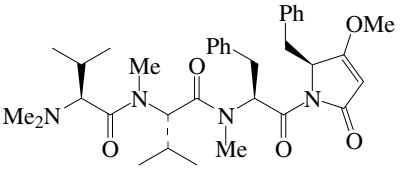
4-Chloro: ***Chlorobeckerelide***
[65428-11-7]
$C_9H_{13}ClO_4$ 220.652
Isol. from the red alga *Beckerella subcostatum*. Obt. as a mixt. of stereoisomers.

4-Bromo: ***Bromobeckerelide***
$C_9H_{13}BrO_4$ 265.103
From *Beckerella subcostatum*. Obt. as a mixt. of stereoisomers.
λ_{max} 227 (ϵ 8900) (MeOH) (Berdy).

[71386-14-6, 71386-15-7, 71386-16-8, 71386-17-9]

Ohta, K. *et al., Agric. Biol. Chem.*, 1977, **41**, 2105 (*isol*)
Jefford, C.W. *et al., Tet. Lett.*, 1989, **30**, 1237 (*synth*)
Katsumura, S. *et al., Chem. Lett.*, 1993, 1525 (*synth*)

Belamide A **B-46**

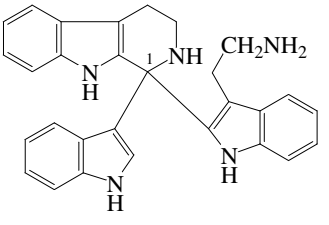


$C_{35}H_{48}N_4O_5$ 604.788
Isol. from a marine *Symploca* sp. Antimitotic. Yellow oil. $[\alpha]_D^{25}$ +16 (c, 0.002 in $CHCl_3$). λ_{max} 240 ($CHCl_3$).

Simmons, T.L. *et al., Tet. Lett.*, 2006, **47**, 3387-3390 (*isol, pmr, cmr*)

Bengacarboline **B-47**

[192947-81-2]

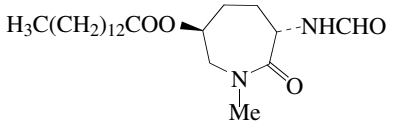


$C_{29}H_{27}N_5$ 445.566
Isol. from the ascidian *Didemnum* sp. Cytotoxic agent. Brown solid. λ_{max} 226 (ϵ 6719); 284 (ϵ 1877) (MeOH).

Foderaro, T.A. *et al., J.O.C.*, 1997, **62**, 6064-6065 (*isol, uv, ir, cd, pmr, cmr*)

Bengamide K **B-48**

[193894-98-3]



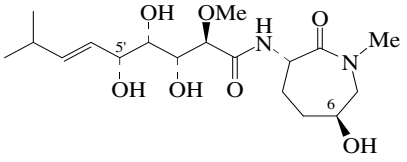
$C_{22}H_{40}N_2O_4$ 396.569
Isol. from the sponge *Jaspis carteri*.

$[\alpha]_D^{25}$ +78.7 (c, 0.08 in MeOH).

D'Auria, M.V. *et al., J. Nat. Prod.*, 1997, **60**, 814-816 (*isol, pmr, cmr, ms*)

Bengamide Z B-49

[118477-10-4]



Absolute Configuration

$C_{18}H_{32}N_2O_7$ 388.46
Isol. from the sponge *Jaspis* cf. *coriacea* and from *Pachastrissa* sp. Cytotoxic agent; anthelmintic; nematocide; shows antiproliferative action. $[\alpha]_D^{20}$ +45 (c, 0.11 in MeOH).

6-O-*(3*R*,4*S*,5*R*-Trihydroxy-2*R*-methoxy-8-methyl-6-nonenoyl):* ***Bengamide D***
[118477-02-4]
$C_{29}H_{50}N_2O_{12}$ 618.72
From a Choristid sponge (Jaspidae). Anthelmintic, nematocide. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ +19.8 (c, 0.086 in MeOH). Unstable in $CDCl_3$ soln.

6-O-*Tridecanoyl:* ***Bengamide H***
[193894-95-0]
$C_{31}H_{56}N_2O_8$ 584.792
Isol. from *Jaspis carteri* and *Jaspis* cf. *coriacea*.
$[\alpha]_D^{25}$ +9.2 (c, 0.1 in MeOH).

6-O-*(12-Methyltridecanoyl):* ***Bengamide O***
$C_{32}H_{58}N_2O_8$ 598.819
Isol. from *Jaspis* cf. *coriacea*. Oil. $[\alpha]_D$ +35.8 (c, 23.9 in MeOH).

6-O-*Tetradecanoyl:* ***Bengamide B****. NSC 646846*
[104947-69-5]
$C_{32}H_{58}N_2O_8$ 598.819
Isol. from *Jaspis* cf. *coriacea* and *Pachastrissa* sp. Anthelminthic and cytotoxic agent. Exhibits antiparasitic and antimicrobial activity. Shows antiproliferative action. Viscous oil. $[\alpha]_D^{20}$ +34.6 (c, 0.075 in MeOH).

6-O-*(13-Methyltetradecanoyl):* ***Bengamide M***
$C_{33}H_{60}N_2O_8$ 612.846
Isol. from *Jaspis* cf. *coriacea*. Oil. $[\alpha]_D$ +2.1 (c, 61.9 in MeOH).

6-O-*Pentadecanoyl:* ***Bengamide J***
[193894-97-2]
$C_{33}H_{60}N_2O_8$ 612.846
Isol. from *Jaspis carteri*.
$[\alpha]_D^{25}$ +33 (c, 0.1 in MeOH).

N-*De-Me:* ***Bengamide Y***
[118477-09-1]
$C_{17}H_{30}N_2O_7$ 374.433
Isol. from *Jaspis* cf. *coriacea*. Cytotoxic agent. Shows antiproliferative action. $[\alpha]_D$ +14 (c, 0.11 in MeOH).

N-*De-Me, 6*S-*(3*R*,4*S*,5*R*-trihydroxy-2*R*-methoxy-8-methyl-6-nonenoyl):* ***Bengamide C***
[104975-72-6]
$C_{28}H_{48}N_2O_{12}$ 604.693
Constit. of a Choristid sponge (Jaspidae). Anthelmintic, nematocide. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Unstable in $CDCl_3$ soln.

N-*De-Me, 6*-O-*tridecanoyl:* ***Bengamide G***
[193894-94-9]
$C_{30}H_{54}N_2O_8$ 570.765
Isol. from *Jaspis carteri* and *Jaspis* cf. *coriacea*. Shows antiproliferative action. $[\alpha]_D^{25}$ +14 (c, 0.1 in MeOH).

N-*De-Me, 6*-O-*(12-methyltridecanoyl):* ***Bengamide N***
$C_{31}H_{56}N_2O_8$ 584.792
Isol. from *Jaspis* cf. *coriacea*. Oil. $[\alpha]_D$ +20.7 (c, 38 in MeOH).

N-*De-Me, 6*-O-*tetradecanoyl:* ***Bengamide A****. NSC 613012*
[104947-68-4]
$C_{31}H_{56}N_2O_8$ 584.792
Isol. from *Jaspis* cf. *coriacea* and *Pachastrissa* sp. Anthelminthic, antiparasitic, antimicrobial and cytotoxic agent. Shows antiproliferative action. Cryst. (MeOH).
Mp 114-115°. $[\alpha]_D^{20}$ +30.3 (c, 0.081 in MeOH).

N-*De-Me, 6*-O-*(13-methyltetradecanoyl):* ***Bengamide L***
[226922-85-6]
$C_{32}H_{58}N_2O_8$ 598.819
Isol. from the sponges *Pachastrissa* sp. and *Jaspis* cf. *coriacea*.
$[\alpha]_D$ +18.5 (c, 1.4 in MeOH).

N-*De-Me, 6*-O-*pentadecanoyl:* ***Bengamide I***
[193894-96-1]
$C_{32}H_{58}N_2O_8$ 598.819
Isol. from *Jaspis carteri* and *Jaspis* cf. *coriacea*.
$[\alpha]_D^{25}$ +32.4 (c, 0.7 in MeOH).

6-Deoxy: ***Bengamide F***
[118477-04-6]
$C_{18}H_{32}N_2O_6$ 372.461
Isol. from *Jaspis* cf. *coriacea*. Cytotoxic agent. Shows antiproliferative action. $[\alpha]_D^{20}$ +27.9 (c, 0.039 in MeOH).

6-Deoxy, 5′-O-*tetradecanoyl:* ***Bengamide Q***
$C_{32}H_{58}N_2O_7$ 582.819
Isol. from *Jaspis* cf. *coriacea*. Oil. $[\alpha]_D$ +14.1 (c, 10.7 in MeOH).

6-Deoxy, N-*de-Me:* ***Bengamide E***
[118477-03-5]
$C_{17}H_{30}N_2O_6$ 358.434
Isol. from *Jaspis* cf. *coriacea* and *Pachastrissa* sp. Cytotoxic agent; shows antiproliferative action; anthelmintic; nematocide. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ +36.9 (c, 0.043 in MeOH).

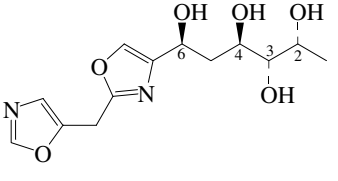
6-Deoxy, N-*de-Me, 5′*-O-*tetradecanoyl:* ***Bengamide P***
$C_{31}H_{56}N_2O_7$ 568.793
Isol. from *Jaspis* cf. *coriacea*. Oil. $[\alpha]_D$ +47.2 (c, 3.6 in MeOH).

6-Deoxy, N-*de-Me, 5′*-O-*hexadecanoyl:* ***Bengamide R***
$C_{33}H_{60}N_2O_7$ 596.846
Isol. from *Jaspis* cf. *coriacea*. Oil (impure).

Quiñoà, E. *et al., J.O.C.*, 1986, **51**, 4494-4497 (*isol, ir, pmr, cmr, ms, struct*)
Adamczeski, M. *et al., J.A.C.S.*, 1989, **111**, 647-654 (*isol, ir, pmr, cmr, ms, struct*)
Adamczeski, M. *et al., J.O.C.*, 1990, **55**, 240-242 (*abs config*)
Chida, N. *et al., Chem. Comm.*, 1992, 1064 (*synth, abs config*)
Marshall, J.A. *et al., J.O.C.*, 1993, **58**, 6229-6234 (*synth, bibl*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1997, **60**, 814-816 (*Bengamides G-J*)
Fernandez, R. *et al., J. Nat. Prod.*, 1999, **62**, 678-680 (*Bengamide L*)
Groweiss, A. *et al., J. Nat. Prod.*, 1999, **62**, 1691-1693 (*Bengamides Y,Z*)
Thale, Z. *et al., J.O.C.*, 2001, **66**, 1733-1741 (*Bengamides M-Q, isol, activity*)
Kinder, F.R. *et al., J.O.C.*, 2001, **66**, 2118-2122 (*Bengamides B,E, synth*)
Banwell, M.G. *et al., J.O.C.*, 2001, **66**, 6768-6774 (*Bengamide E, synth*)
Boeckman Jr., R.K. *et al., Org. Lett.*, 2002, **4**, 2109-2112 (*synth*)
Liu, W. *et al., Tet. Lett.*, 2002, **43**, 1373-1375 (*Bengamide E, synth*)
Sarabia, F. *et al., Tet. Lett.*, 2005, **46**, 1131-1135 (*synth*)

Bengazole Z B-50

[153549-05-4]



Absolute Configuration

$C_{13}H_{18}N_2O_6$ 298.295
Isol. from a *Jaspis* sp. sponge. Oil. $[\alpha]_D$ -7.5 (c, 0.17 in MeOH).

O^2-*Tetradecanoyl:* ***Bengazole C_2***
[153516-65-5]
$C_{27}H_{44}N_2O_7$ 508.654
Alkaloid from the Papua New Guinean marine sponge *Jaspis* cf. *coriacea*. Isol. as an insep. mixt. with 6 bengazoles C_3, C_4, C_6, D_2-D_4.

O^2-*(13-Methyltetradecanoyl):* ***Bengazole D_2***
[153516-66-6]
$C_{28}H_{46}N_2O_7$ 522.681

From *Jaspis* cf. *coriacea*.

O^3-*Tetradecanoyl:* ***Bengazole C$_3$***
[153590-03-5]
$C_{27}H_{44}N_2O_7$ 508.654
From *Jaspis* cf. *coriacea*.

O^3-*(13-Methyltetradecanoyl):* ***Bengazole D$_3$***
[153590-04-6]
$C_{28}H_{46}N_2O_7$ 522.681
From *Jaspis* cf. *coriacea*.

O^4-*Tetradecanoyl:* ***Bengazole C$_4$***
[153590-05-7]
$C_{27}H_{44}N_2O_7$ 508.654
From *Jaspis* cf. *coriacea*.

O^4-*(13-Methyltetradecanoyl):* ***Bengazole D$_4$***
[153590-06-8]
$C_{28}H_{46}N_2O_7$ 522.681
From *Jaspis* cf. *coriacea*.

O^6-*Tetradecanoyl:* ***Bengazole C$_6$***
[153516-67-7]
$C_{27}H_{44}N_2O_7$ 508.654
From *Jaspis* cf. *coriacea*.

O^2-*Pentadecanoyl:* [226922-32-3]
$C_{28}H_{46}N_2O_7$ 522.681
Isol. from *Pachastrissa* sp.
$[\alpha]_D$ -10.5 (c, 0.6 in MeOH). λ_{max} 209 (MeOH).

O^2-*(14-Methylpentadecanoyl):* [226922-28-7]
$C_{29}H_{48}N_2O_7$ 536.707
Isol. from *Pachastrissa* sp.
$[\alpha]_D$ -12.9 (c, 0.2 in MeOH). λ_{max} 209 (MeOH).

O^6-*Pentadecanoyl:* [226922-37-8]
$C_{28}H_{46}N_2O_7$ 522.681
Isol. from *Pachastrissa* sp.
$[\alpha]_D$ -9.3 (c, 1.8 in MeOH). λ_{max} 209 (MeOH).

O^6-*(14-Methylpentadecanoyl):* [226922-30-1]
$C_{29}H_{48}N_2O_7$ 536.707
Isol. from *Pachastrissa* sp.
$[\alpha]_D$ -8.5 (c, 0.9 in MeOH). λ_{max} 209 (MeOH).

O^2-*Hexadecanoyl:* [226922-26-5]
$C_{29}H_{48}N_2O_7$ 536.707
Isol. from *Pachastrissa* sp.
$[\alpha]_D$ -9.5 (c, 0.3 in MeOH). λ_{max} 209 (MeOH).

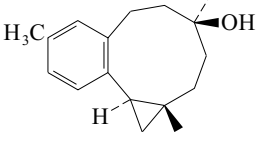
O^6-*Hexadecanoyl:* [226922-27-6]
$C_{29}H_{48}N_2O_7$ 536.707
Isol. from *Pachastrissa* sp.
$[\alpha]_D$ -11.4 (c, 1.1 in MeOH). λ_{max} 209 (MeOH).

O^6-*Heneicosanoyl:* ***Digonazole***
[157536-06-6]
$C_{34}H_{58}N_2O_7$ 606.841
Metab. from the marine sponge *Jaspis digonoxea*. Viscous oil.
$[\alpha]_D^{20}$ -8.9 (c, 2.2 in $CHCl_3$).

Rodríguez, J. *et al., J. Nat. Prod.*, 1993, **56**, 2034-2040 (*isol, pmr, cmr, struct*)
Rudi, A. *et al., J. Nat. Prod.*, 1994, **57**, 829-836 (*Digonazole*)
Fernandez, R. *et al., J. Nat. Prod.*, 1999, **62**, 678-680 (*Pachastrissa Bengazoles*)
Groweiss, A. *et al., J. Nat. Prod.*, 1999, **62**, 1691-1693 (*isol*)

Benkarlaol B-51

[181527-95-7]

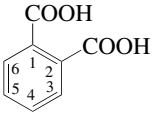


$C_{17}H_{24}O$ 244.376
Constit. of *Laurencia karlae*. Oil. $[\alpha]_D^{20}$ -55 (c, 0.02 in CH_2Cl_2).

Zeng, L.-M. *et al., Chin. J. Chem.*, 1996, **14**, 370-372 (*isol, pmr, cmr*)

1,2-Benzenedicarboxylic acid, 9CI B-52

Phthalic acid, 8CI. Alizarinic acid. Naphthalinic acid†*. Phthalinic acid*
[88-99-3]



$C_8H_6O_4$ 166.133
Obt. industrially by oxidn. of 1,2-Dimethylbenzene and Naphthalene. Found in *Gibberella fujikuroi*. Esters are important plasticisers. Used for gravimetric detn. of Pb. Used as aq. soln. in buffer solns.; alkalimetric standard (as K salt). Plates (H_2O). Sol. hot H_2O, alkalis; mod. sol. H_2O, EtOH; spar. sol. Et_2O.
Mp 210° dec Mp 234°. pK_{a1} 2.95; pK_{a2} 5.41 (25°,H_2O). Forms anhydride at Mp. Frequent reports of the isol. of phthalate esters as nat. prods. are in prob. all cases erroneous because of their ubiquitous presence in solvs., laboratory plastics, etc. as plasticisers.

▶ Fl. p. 168°. Violent reaction on heating with $NaNO_2$. Skin and mucous membrane irritant. Low acute mammalian toxicity. TH9625000

Dioctyl ester: Dioctyl phthalate. Vinicizer 85
[117-84-0]
$C_{24}H_{38}O_4$ 390.562
Reported as a nat. prod. from the brown alga *Sargassum wightii* and various plant spp. Plasticiser. Oil. d_{20}^{20} 0.98.
Mp -25°. Bp_1 185° $Bp_{0.1}$ 165°. n_D^{25} 1.4848. Almost certainly a contaminant.

Bis(2-ethylnonyl) ester: Bis(2-ethylnonyl) phthalate
$C_{30}H_{50}O_4$ 474.723
Reported as a nat. prod. from the red alga *Acanthophora spicifera*. Nat. occurrence doubtful in view of the widespread presence of phthalate esters in the environment.

Benzyl butyl ester: Benzyl butyl phthalate. Santicizer 160. Spatozoate. Unimoll BB. BBP
[85-68-7]
$C_{19}H_{20}O_4$ 312.365
Reported isol. from the alga *Spatoglossum variabile*. Plasticiser. Liq. Insol. H_2O. d^{25} 1.12. Bp 370° Bp_{10} 235-255°. n_D^{25} 1.5380. Struct. of Spatozoate revised in 2003.

[131-15-7, 523-24-0, 3198-29-6, 4409-98-7, 10197-71-4, 15968-01-1, 79723-02-7, 102904-15-4]

Matsuda, S. *et al., CA*, 1958, **52**, 9995c (*esters, synth, props*)
Toxicol. Ind. Health, 1987, **3**, 7; 99; 151; 165 (*esters, tox*)
Alger, M. *et al., Polymer Science Dictionary*, 2nd edn., Chapman & Hall, 1997, 61; 129-132; 132-136; 141; 144-147; 150; 157 (*diesters, use*)
Wahidulla, S. *et al., Phytochemistry*, 1998, **48**, 1203-1206 (*isol, bis-2-ethylnonyl ester*)
Cheng, K.-T. *et al., Indian J. Chem., Sect. B*, 2003, **42**, 1190-1192 (*Spatozoate, synth, struct*)

1,4-Benzenedicarboxylic acid, 9CI B-53

Terephthalic acid, 8CI. p-*Phthalic acid*
[100-21-0]
$C_8H_6O_4$ 166.133
Isol. from pods of *Cassia roxburghii* and *Tephrosia hamiltonii*. Manuf. by oxidn. of *p*-xylene. Acid and derivs. are important feedstocks for polymerisations, used for making polyester resins, e.g. terylene, for fibres and films. Important industrial chemical, 24th in order of volume for USA in 1994 (production 4.32 million tons/year). Cryst. Prac. insol. H_2O, $CHCl_3$, Et_2O, AcOH; mod. sol. hot EtOH; sol. Py, DMSO, DMF. Subl. *ca.* 300. pK_{a1} 3.54; pK_{a2} 4.34 (25°).

▶ Eye irritant. Low acute mammalian tox. WZ0875000

2-Ethylhexyl 2-methylpropyl ester: [887650-33-1]
$C_{20}H_{30}O_4$ 334.455

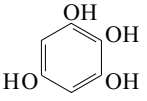
Isol. from *Sarcophyton* sp. Presumably an environmental contaminant.

[3856-02-8, 10028-70-3, 60088-54-2]

Ma, X. *et al., CA*, 2006, **144**, 484835c (*2-ethylhexyl 2-methylpropyl ester*)

1,2,3,5-Benzenetetrol, 9CI, 8CI B-54

1,2,3,5-Tetrahydroxybenzene
[634-94-6]



$C_6H_6O_4$ 142.111
Isol. from brown alga *Carpophyllum maschalocarpum*. Needles (H_2O).
Mp 168-170° (165°).

2-O-*Sulfate:* [67173-67-5]
$C_6H_6O_7S$ 222.175
Constit. of brown algae *Petalonia fascia*, *Scytosiphon lomentaria*, *Dictyota dichotoma*, *Ascophyllum nodosum*, *Fucus vesiculosus* and *Himanthalia elongata*.

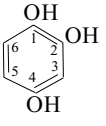
2,5-O-*Disulfate:* [67173-65-3]
$C_6H_6O_{10}S_2$ 302.239
Constit. of the brown algae *Ascophyllum nodosum*, *Petalonia fascia*, *Scytosiphon lomentaria*, *Chorda filum*, *Fucus distichus* ssp. *anceps*, *Fucus vesiculosus*, *Pelvetia canaliculata* and *Dictyota dichotoma*. Biogenetic precursor of the wide range of oligomeric phlorotannins which are a major component of brown algae.

[67173-66-4, 68944-24-1, 87562-77-4, 108543-42-6]

Jensen, A. *et al., Tet. Lett.*, 1978, 847-850 (*sulfates*)
Ragan, M.A. *et al., Phytochemistry*, 1979, **18**, 261-262 (*sulfates, occur*)

1,2,4-Benzenetriol, 9CI, 8CI B-55

1,2,4-Trihydroxybenzene. Hydroxyhydroquinone. Hydroxyquinol
[533-73-3]



$C_6H_6O_3$ 126.112
Constit. of the sponge *Axinella polycapella*. Also isol. from the fruiting bodies of *Gomphidius* spp. Prod. by hydrothermal treatment of biomass carbohydrates. Used as 1% aq. soln. for photometric detn. of Os. Antibacterial agent. Plates (Et_2O). Sol. H_2O.
Mp 140.5° subl. pK_{a1} 9.08; pK_{a2} 11.82 (20°).
▶ LD_{50} (mus, scu) 120 mg/kg. DC4200000

1,2-Di-Me ether: 3,4-Dimethoxyphenol
[2033-89-8]
$C_8H_{10}O_3$ 154.165
Constit. of various plant spp. including *Croton*, *Passiflora* and *Lysimachia* spp. and marine bacterium Ta-6 isol. from *Tapes philippinarum* (short-necked clam). Prod. by a range of marine microorganisms isol. from fish and shellfish. Antioxidant. Cryst. (petrol).
Mp 79-82°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1049A; 1091C; 1104A; **2**, 313A (*ir, di-Me ether*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 199C; 279A; 299B; 1289C (*nmr, di-Me ether*)
Böesenken, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1939, **53**, 528-537 (*di-Me ether*)
Von Ardenne, R. *et al., Z. Naturforsch., C*, 1974, **29**, 446; 1981, **36**, 488-489 (*isol*)
Wratten, S.J. *et al., Experientia*, 1981, **37**, 13-14 (*isol*)
Takao, T. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1780-1783 (*1,2-di-Me ether, isol, occur*)
Zaitsev, V.G. *et al., Tetrahedron*, 1994, **50**, 6377-6386 (*synth*)

1,3,5-Benzenetriol, 9CI B-56

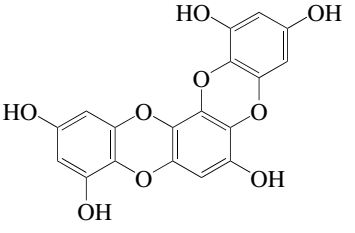
1,3,5-Trihydroxybenzene. ***Phloroglucinol****. Phloroglucin. Dilospan S. Spasfon-Lyoc*
[108-73-6]
$C_6H_6O_3$ 126.112
Isol. from *Eucalyptus kino* and *Acacia arabica*. In the free state, a minor constit. of brown algae, e.g. *Halidrys siliquosa*, *Cystophora retroflexa*, *Eisenia arborea*, *Laminaria ochroleuca*, *Analipus japonicus*, *Cystophora congesta* and *Carpophyllum angustifolium*. Present in brown algae as a range of phlorotannin oligomers. Reagent used for the detn. of aldehydes. Used in diazo-type-copying and textile-dyeing. Spasmolytic agent. Leaflets or plates + $2H_2O$ (H_2O). Mod. sol. H_2O; sol. EtOH, Et_2O, Py, Me_2CO.
Mp 117° (dihydrate) Mp 217-219° (anhyd.) (rapid heat) Mp 200-209° (slow heat). pK_{a1} 7.97; pK_{a2} 9.23 (20°). Log P 0.14 (calc). Forms polymers with aldehydes and with diamines; no coml. importance.
▶ Skin and eye irritant. LD_{50} (rat, orl) 5200 mg/kg. Exp. reprod. effects. SY1050000

[6099-90-7]

Glombitza, K.W. *et al., Phytochemistry*, 1976, **15**, 1082-1083 (*isol, Analipus*)
Sattler, E. *et al., Tetrahedron*, 1977, **33**, 1239-1244 (*isol, Halidrys*)
Glombitza, K.W. *et al., Phytochemistry*, 1985, **24**, 543-551 (*isol, Eisenia*)
Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol, Cystophora*)

Benzo[1,2-*b*:3,4-*b′*]bis[1,4]benzodioxin-1,3,6,9,11-pentol, 9CI B-57

Dioxinodehydroeckol*. Eckstolonol*
[96820-12-1]



$C_{18}H_{10}O_9$ 370.272
Constit. of the brown algae *Eisenia arborea*, *Ecklonia maxima* and *Ecklonia stolonifera*. Powder. Isol. as penta-Ac.

Glombitza, K.-W. *et al., Phytochemistry*, 1985, **24**, 543-551 (*isol*)
Glombitza, K.-W. *et al., Planta Med.*, 1985, **51**, 308-312 (*isol, pmr, cmr*)
Kang, H.S. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1012-1014 (*isol, pmr, cmr*)

Benzoic acid, 9CI, USAN B-58

Benzenecarboxylic acid. E210. FEMA 2131
[65-85-0]
PhCOOH
$C_7H_6O_2$ 122.123
Prod. industrially mainly by oxidn. of toluene. Widespread in plants esp. in essential oils, e.g. *Cucumis sativus*, mostly in esterified form. Obt. in 17th Century by sublimation of *Styrax* spp. resin. Prod. by *Streptomyces lavendulae* (K82), *Sasa albomarginata*, *Aspergillus raperi*, *Fusarium oxysporum*, *Letharia vulpina*, *Rhizoctonia solani*, *Sporobolomyces odorus* and *Lactobacillus plantarum* (Vtte.78076). Isol. from the marine sponge *Halichondria okadai*. Preservative in the food industry. Used in manuf. of preservatives, plasticisers, alkyd resin coatings and caprolactam. Used as alkalimetric standard; in photometric detn. of U and Zr (anionic complexes associated with basic dyes). Reference material used in elemental microanalysis. Antiseptic, expectorant, antifungal, antipyretic, keratolytic agent, phytotoxic, acaricide, antifouling agent. Leaflets or needles (H_2O). Sol. MeOH, C_6H_6; fairly sol. hexane; v. spar. sol. H_2O.
Mp 122°. Bp 249° Bp_{10} 133°. Log P 1.88 (calc). Steam-volatile. λ_{max} 228 (E1%/1cm 728); 273 (E1%/1cm 93.2); 300 (E1%/1cm 46.8) (MeOH) (Berdy).

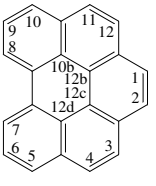
▶ Fl. p. 121°, autoignition temp. 570°. Eye, skin and mucous membrane irritant. Hypersensitivity reactions reported. Low systemic toxicity. Detoxification in humans occurs by conjugation with amino acids (mainly glycine resulting in hippuric acid). DG0875000

[766-76-7, 1079-02-3, 8000-95-1, 43019-90-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 186A; 271B; 291B; 291C; 292D; 340A; 340B; 340C; 380D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1063B; 1199A; 1240A; 1240B; 1241A; 1241B; 1244A; 1337C; 1411A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 181D; 1322C; 1357D; 1358A; 1358B; 1358C; 1360A; 1389D; 1390A; 1390B (*ir*)
Jesson, J.P. *et al., Proc. R. Soc. London, A*, 1962, **268**, 68-78 (*Raman*)
Beynon, J.H. *et al., Z. Naturforsch., A*, 1965, **20**, 883-887 (*ms*)
Moeken, H.H. *et al., Anal. Chim. Acta*, 1967, **37**, 480-483 (*detn, U*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 49; 1004; 1975, **5**, 23; 24; 249; 1979, **7**, 405 (*use*)
Evans, H.B. *et al., J. Phys. Chem.*, 1968, **72**, 2552-2562 (*pmr*)
Escarrilla, A.M. *et al., Anal. Chim. Acta*, 1969, **45**, 199-201 (*use*)
Bel'tyukova, S.V. *et al., Zh. Anal. Khim.*, 1972, **27**, 191-194; *J. Anal. Chem. USSR (Engl. Transl.)*, 1972, **27**, 158-160 (*detn, Zr*)
Dubey, S.C. *et al., Talanta*, 1977, **24**, 266-267 (*detn, U*
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 715-722 (*rev, tox*)
Hassan, M.M.A. *et al., Anal. Profiles Drug Subst.*, 1981, **10**, 55-74 (*rev, benzyl ester*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493-1518 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **4**, 103 (*rev*)
Tremblay, G.C. *et al., Pharmacol. Ther.*, 1993, **60**, 63-90 (*rev, pharmacol, tox*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 7th edn., Akademie-Verlag*, 1994, 3826
Baba, S. *et al., Biol. Pharm. Bull.*, 1995, **18**, 643-647 (*cmr, metab*)
Yamada, A. *et al., Bull. Chem. Soc. Jpn.*, 1997, **70**, 3061-3069 (*isol, sponge*)
Indrayanto, G. *et al., Anal. Profiles Drug Subst.*, 1999, **26**, 1-46 (*rev*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth, pmr, cmr*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2511
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 107
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 117
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BBV250; BCM000; EGR000; IOD000; SFB000; BCQ250; BQK250; BDM500; BCL750; MHA750; PKW760

Benzo[*ghi*]perylene, 9CI B-59

1,12-Benzoperylene
[191-24-2]



$C_{22}H_{12}$ 276.337
Occurs in tar, smoke-polluted atmospheres. Occurs goose barnacles. Yellowish-green fluor. leaflets (C_6H_6).
Mp 272-273°.

▶ Poss. carcinogen (equivocal/insufficient data). DI6200500

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 58C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 969C (*ir*)
Koe, B.K. *et al., Arch. Biochem. Biophys.*, 1952, **41**, 396 (*occur*)
Cooper, R.L. *et al., Chem. Ind. (London)*, 1953, 1364 (*occur*)
Ott, R. *et al., Monatsh. Chem.*, 1953, **84**, 1132 (*synth*)
Aihara, J. *et al., Bull. Chem. Soc. Jpn.*, 1970, **48**, 2435 (*uv*)
Matthews, R.S. *et al., Spectrochim. Acta A*, 1971, **27**, 1185 (*pmr*)
Frycka, J. *et al., J. Chromatogr.*, 1972, **65**, 432 (*glc*)
IARC Monog., 1983, **32**, 195; *Suppl.* 7, 58 (*rev, tox*)
van Dijk, J.T.M. *et al., J.O.C.*, 1996, **61**, 1136 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BCR000

Benzophenone, 8CI B-60

Diphenylmethanone, 9CI. Diphenyl ketone. Phenyl ketone. FEMA 2134
[119-61-9]
PhCOPh
$C_{13}H_{10}O$ 182.221
Constit. of *Pseudomonas putida* and grapes, also occurs in Baltic Sea shale tar. Fixative for heavy perfumes, esp. soaps. Used in the manuf. of antihistamines, hypnotics and insecticides. Flavouring agent. Rhombic prisms (stable form), monoclinic prisms (labile form). Insol. H_2O. d_4^{18} 1.11.
Mp 48.5-49° (stable form) Mp 26° (labile form). Bp_{100} 224° Bp_{10} 157.6°.

▶ LD_{50} (mus, orl) 2895 mg/kg. DI9950000

Oxime: [574-66-3]
$C_{13}H_{11}NO$ 197.236
Cryst. (petrol). Sol. Et_2O, Me_2CO; mod. sol. $CHCl_3$, C_6H_6; spar. sol. H_2O. pK_{a1} 11.18.

▶ DJ1810000

Hydrazone: [5350-57-2]
$C_{13}H_{12}N_2$ 196.251
Mp 98°. Bp_{55} 225-230°.

Phenylhydrazone: [574-61-8]
Needles. Mp 137°.

▶ DJ1817000

2,4-Dinitrophenylhydrazone: [1733-62-6]
Mp 238°.

Semicarbazone: Mp 167°.

Thiosemicarbazone: [7341-60-8]
$C_{14}H_{13}N_3S$ 255.343
Used as EtOH soln. for photometric detn. of Cu (λ_{max} 360 nm, ϵ 13200). Cryst. Sol. DMF, EtOH.

Di-Me acetal: 1,1′-(Dimethoxymethylene)bisbenzene, 9CI. Dimethoxydiphenylmethane
[2235-01-0]
$C_{15}H_{16}O_2$ 228.29
Plates (EtOH). Mp 106-109°. Bp 288-290°.

Di-Et acetal: 1,1′-(Diethoxymethylene)bisbenzene, 9CI. Diethoxydiphenylmethane
[6397-77-9]
$C_{17}H_{20}O_2$ 256.344
Prisms (EtOH). Mp 51-52°. Bp 294-295°.

Azine: See Diphenylketazine in *The Combined Chemical Dictionary.*

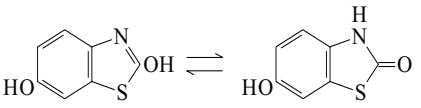
Imine: See Diphenylmethanimine in *The Combined Chemical Dictionary.*

[16592-08-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1264D; **2**, 58A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 884C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1265B (*ir*)
Adv. Chem. Ser., 1955, **15**, 354 (***props***)
Barton, D.H.R. *et al., J.C.S.*, 1962, 470 (*azine, synth, uv, ir*)
Natlis, P. *et al., J. Phys. Chem.*, 1965, **69**, 2943 (*ms*)
Morrison, J.D. *et al., J.O.C.*, 1972, **37**, 1034 (*use*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 873 (*rev, tox*)
Grimaud, M. *et al., Bull. Soc. Chim. Fr.*, 1974, 1935 (*uv*)
Herman, F.L. *et al., Diss. Abstr. Int., B*, 1976, **16**, 6169; *CA*, **85**, 93411c (*use*)
Groebal, B.T. *et al., Chem. Ber.*, 1977, **110**, 854 (*use*)
Loletta, M. *et al., Inorg. Chim. Acta*, 1977, **24**, 195 (*pmr, cmr*)
Vogel, A.I. *et al., Textbook of Practical Organic Chemistry*, 4th Ed., Longman, London, 1978, 775 (*synth*)
Gowda, H.S. *et al., Indian J. Chem., Sect. A*, 1983, **22**, 1086 (*detn, Cu*)
Abraham, R.J. *et al., J.C.S. Perkin 2*, 1988, 1429 (*conformn*)
Zadel, G. *et al., Angew. Chem., Int. Ed.*, 1992, **31**, 1035 (*synth*)
Zhao, D. *et al., Synthesis*, 1994, 915 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 54
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 254-255
Morgan, L.R. *et al., J. Med. Chem.*, 2003, **46**, 4552-4563 (*2,4-dinitrophenylhydrazone, synth, ir, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BCS250

2,6-Benzothiazolediol B-61

*2,6-Dihydroxybenzothiazole. 6-Hydroxy-2(3*H*)-benzothiazolone*
[80567-65-3]



$C_7H_5NO_2S$ 167.188
Mp 233-235°.

*6-Me ether: 6-Methoxy-2(3*H*)-benzothiazolone*
[40925-65-3]
$C_7H_5NO_2S$ 167.188
Mp 163-165°.

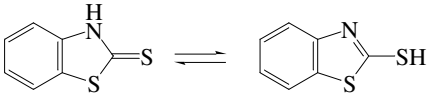
NH-form

N-*Me: 6-Hydroxy-3-methyl-2(3*H*)-benzothiazolone*
[96489-25-7]
$C_8H_7NO_2S$ 181.215
Prod. by a *Micrococcus* sp. found in *Tedania ignis*. Solid (EtOH). Mp 182-183°.

Jones, G.H. *et al., J. Med. Chem.*, 1987, **30**, 295 (*synth*)
Stierle, A.A. *et al., Tet. Lett.*, 1991, **32**, 4847 (*isol, deriv*)
Delhomel, J.F. *et al., J. Het. Chem.*, 2001, **38**, 633-639 (*N-Me*)

2(3*H*)-Benzothiazolethione, 9CI B-62

2-Benzothiazolethiol. 2-Mercaptobenzothiazole. 2-Benzothiazolinethione. Accelerator M. Accel M. Captax. Kaptax. Pneumax MBT. Thiotax. Vulkacit M. Wobezit M
[149-30-4]



$C_7H_5NS_2$ 167.255

NH-form predominates. Isol. from a *Micrococcus* sp. in *Tedania ignis*. Also present in cranberries. Vulcanisation accelerator. Used as 1% $CHCl_3$ soln. for separation pptn. of Au, $I^{\ominus}$; photometric detn. of Pd, Os, Rh, Se, Ni (λ_{max} 750 nm). Needles (MeOH aq.). Spar. sol. EtOH, Et_2O, AcOH; insol. H_2O; sol. alkalis.
Mp 177-179°. Readily oxidised to the disulfide.
▶ LD_{50} (rat, orl) 100 mg/kg. Exp. carcinogen. Exp. reprod. and teratogenic effects. DL6475000

NH-form

N-*Me:* [2254-94-6]
$C_8H_7NS_2$ 181.282
Reagent for stereospecific prepn. of thiirans from oxiranes. Cryst. (petrol). Mp 92° (89-90°). $Bp_{0.5}$ 156°.

N-*Et:* [16407-34-4]
$C_9H_9NS_2$ 195.309
Mp 73-75°.

SH-form

S-*Me: 2-(Methylthio)benzothiazole*
[615-22-5]
$C_8H_7NS_2$ 181.282
Prisms (EtOH aq.). Mp 52°. Bp 291-300° $Bp_{0.5}$ 116°.

S-*Me; hydroiodide:*
Cryst. (EtOH). Mp 128.3°.

S-*Me,* S,S-*dioxide: 2-(Methylsulfonyl)benzothiazole*
[7144-49-2]
$C_8H_7NO_2S_2$ 213.281
Red solid (EtOH). Mp 90°.

S-*Et: 2-(Ethylthio)benzothiazole*
[2757-92-8]
$C_9H_9NS_2$ 195.309
Cryst. (EtOH). Mp 26°. Bp_6 148-150°. n_D^{20} 1.6580.

S-*Butyl:* [2314-17-2]
$C_{11}H_{13}NS_2$ 223.362
Cotton plant defoliant. Bp_6 163-165°.

S-*Benzyl: 2-(Benzylthio)benzothiazole*
[19654-17-2]
$C_{14}H_{11}NS_2$ 257.38
Mp 149-150°.

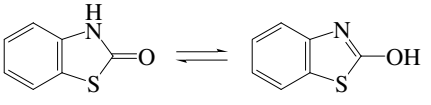
Disulfide: See Di-2-benzothiazolyl disulfide in *The Combined Chemical Dictionary.*

[155-04-4, 2492-26-4, 37437-20-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 701D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 204B; 204C (*nmr*)
Jacobson, P. *et al., Ber.*, 1891, **24**, 1403
Rassow, B. *et al., Chem. Zentralbl.*, 1916, **2**, 394
Reed, F.P. *et al., J.C.S.*, 1939, 473-476 (*N-Me, S-Me, synth*)
Welcher, J.F. *et al., Organic Analytical Reagents*, Van Nostrand, N.Y., 1948, **4**, 109 (*use*)
Morgan, K.I. *et al., J.C.S.*, 1958, 854-858 (*uv*)
Walliczek, E.G. *et al., Talanta*, 1964, **11**, 573 (*detn, Ni*)
Wanzlick, H.W. *et al., Annalen*, 1967, **708**, 155 (*N-Me*)
Bera, C.C. *et al., Analyst (London)*, 1968, **93**, 50 (*detn, Se*)
Sohar, P. *et al., J. Het. Chem.*, 1969, **6**, 163-174 (*N-Me*)
Kujawa, R. *et al., Mikrochim. Acta*, 1969, 193 (*detn, $I^{\ominus}$*)
Chesick, J.P. *et al., Acta Cryst. B*, 1971, **27**, 1441 (*cryst struct*)
DeJongh, D.C. *et al., Adv. Mass Spectrom.*, 1974, **6**, 99 (*ms*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 374 (*N-Me, use*)
Fries, J. *et al., Organic Reagents for Trace Analysis*, E. Merck, Darmstadt, 1977, 302 (*use*)
Uher, M. *et al., Chem. Zvesti*, 1978, **32**, 486; *CA*, **90**, 167746 (*tautom*)
Dou, H.J.M. *et al., Helv. Chim. Acta*, 1978, **61**, 3143-3148 (*S-butyl, synth, pmr*)
Faure, R. *et al., Org. Magn. Reson.*, 1978, **11**, 617 (*cmr, tautom*)
Cristiani, F. *et al., Phosphorus Sulfur Relat. Elem.*, 1984, **20**, 231 (*ir*)
Radha, A. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1985, **171**, 225 (*cryst struct*)
Stierle, A.A. *et al., Tet. Lett.*, 1991, **32**, 4847-4848 (*isol*)
Monge, A. *et al., J. Med. Chem.*, 1994, **37**, 1320 (*deriv, synth, ir, pmr*)
Dalal, D.S. *et al., Org. Prep. Proced. Int.*, 2005, **37**, 539-546 (*S-Me, S-Et*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BDF000; SIG500; BHA750

2-Benzothiazolol B-63

*2(3*H*)-Benzothiazolone, 9CI. 2-Benzothiazolinone. 2-Hydroxybenzothiazole*



C_7H_5NOS 151.189

NH-form predominates. Prod. by a *Micrococcus* sp. found in *Tedania ignis*. Gives colour reaction with Pd (λ_{max} 368 nm). Needles (EtOH).
Mp 138-139°.

NH-form

N-*Ac:* [51360-57-7]
$C_9H_7NO_2S$ 193.226
Needles (EtOH aq.). Mp 50°.

N-*Me: 3-Methyl-2-benzothiazolone*
[2786-62-1]
C_8H_7NOS 165.215
Cryst. (H_2O). Mp 70-71°.

N-*Me, hydrazone: Besthorn's hydrazone. MBTH*
[1128-67-2]
$C_8H_9N_3S$ 179.245
Used as a 0.25% aq. soln. of hydrochloride for photometric detn. of H_2O_2 (λ_{max} 442 nm, ϵ 36000) and aldehydes. Yellow cryst. (EtOH). Sol. dil. acids, EtOH, Me_2CO, C_6H_6. Mp 144°.
▶ LD_{50} (rat, orl) 149-308 mg/kg. LD_{50} (rat, ipr) 135 mg/kg. Mild irritant. DL7160000

N-*Me, hydrazone; hydrochloride:* [14448-67-0] [38894-11-0] Mp 264-266°.

▶DL7160200

OH-form [934-34-9]

Ac: [15456-95-8]
$C_9H_7NO_2S$ 193.226
Mp 60°.

Me ether: 1-Methoxybenzothiazole
[63321-86-8]
C_8H_7NOS 165.215
Cryst. (MeOH) with odour of wintergreen. Mp 34-35°. Bp_{30} 119°.

Et ether: 1-Ethoxybenzothiazole
[70292-64-7]
C_9H_9NOS 179.242
Mp 25°. Bp 360°.

Mills, W.H. *et al., J.C.S.*, 1927, 2738 (*synth*)
Davies, W.H. *et al., J.C.S.*, 1942, 304 (*deriv*)
Sawicke, E. *et al., Anal. Chem.*, 1961, **33**, 93 (*use, deriv*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 672 (*N-Me hydrazone*)
Hauser, T.R. *et al., Anal. Chem.*, 1968, **40**, 231 (*detn, H_2O_2*)
Sohar, P. *et al., J. Het. Chem.*, 1969, **6**, 163
Aboulezz, A.F. *et al., Egypt. J. Chem.*, 1973, **16**, 355; *CA*, **81**, 152075
Joshi, S.R. *et al., Indian J. Chem.*, 1973, **11**, 590 (*detn, Pd*)
Fife, T.H. *et al., J.A.C.S.*, 1975, **97**, 5878 (*synth, deriv*)
Faure, R. *et al., Org. Magn. Reson.*, 1978, **11**, 617 (*tautom, cmr*)
Rudd, S. *et al., Acta Cryst. C*, 1984, **40**, 2118 (*cryst struct, deriv*)
Safanda, J. *et al., Coll. Czech. Chem. Comm.*, 1984, **49**, 1869 (*use, deriv*)
Konishi, K. *et al., Synthesis*, 1984, 254 (*synth*)
D'Amico, J.J. *et al., J. Het. Chem.*, 1986, **23**, 641 (*synth, pmr*)
Ballantyne, B. *et al., Toxicol. Ind. Health*, 1988, **4**, 23 (*N-Me, hydrazone, tox*)
Stierle, A.A. *et al., Tet. Lett.*, 1991, **32**, 4847 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MHJ250

Benzyl methyl sulfide, 8CI B-64

[(Methylthio)methyl]benzene, 9CI. FEMA 3597
[766-92-7]
$PhCH_2SMe$

$C_8H_{10}S$ 138.233
Constit. of the marine sponge *Halichondria panicea*. Liq. with powerful horseradish odour. d^{20} 1.03. Bp 199-201° Bp_{25} 80° Bp_4 70-72°. n_D^{20} 1.5632.

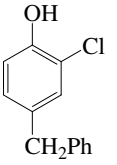
S-*Oxide: [(Methylsulfinyl)methyl]benzene, 9CI. Benzyl methyl sulfoxide*
[824-86-2]
$C_8H_{10}OS$ 154.232
Cryst. (petrol). Mod. sol. H_2O, Et_2O, petrol, sol. EtOH, AcOH. Mp 54°. Opt. active forms known.

S,S-*Dioxide: [(Methylsulfonyl)methyl]benzene. Benzyl methyl sulfone. DMIT*
[3112-90-1]
$C_8H_{10}O_2S$ 170.232
Sol. H_2O. Mp 127°.

Thomson, T. *et al., J.C.S.*, 1932, 69 (*synth, dioxide*)
Hünig, S. *et al., Annalen*, 1953, **579**, 23 (*oxide*)
Doerftel, K. *et al., J. Prakt. Chem.*, 1970, **312**, 701 (*ir*)
Russell, G.A. *et al., J.O.C.*, 1979, **44**, 3990 (*synth*)
Youm, J.R. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2140 (*cmr*)
Luzzio, F.A. *et al., Synth. Commun.*, 1984, **14**, 209 (*synth*)
Fujisaki, S. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 2429 (*synth*)
Langler, R.F. *et al., Can. J. Chem.*, 1987, **65**, 2385 (*synth*)
Comasseto, J.V. *et al., J. Organomet. Chem.*, 1987, **334**, 329 (*synth, pmr*)
Lu, X. *et al., Synthesis*, 1987, 66 (*synth*)
Christophersen, C. *et al., Biochem. Syst. Ecol.*, 1989, **17**, 459 (*occur*)
Torisawa, Y. *et al., Tet. Lett.*, 1990, **29**, 1729 (*synth*)
Olah, G.A. *et al., Synthesis*, 1994, 277 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 63
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 274

4-Benzyl-2-chlorophenol B-65

2-Chloro-4-(phenylmethyl)phenol, 9CI. 2-Chloro-α-phenyl-p-cresol, 8CI. 3-Chloro-4-hydroxydiphenylmethane
[31089-49-3]

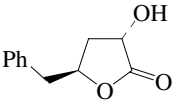


$C_{13}H_{11}ClO$ 218.682
Isol. from the blue-green alga *Anacystis marina*. Bp_{14} 182-185°.

Ger. Pat., 1951, 824 058; *CA*, **49**, 7594i (*synth*)
Alieva, M.K. *et al., Zh. Org. Khim.*, 1983, **19**, 2131-2134 (*synth*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 210 (*occur*)

5-Benzyldihydro-3-hydroxy-2(3*H*)-furanone B-66

Dihydro-3-hydroxy-5-(phenylmethyl)-2(3H)-furanone



(3*S*,5*S*)-*form*

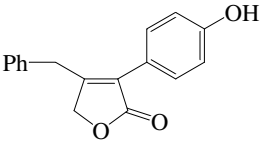
$C_{11}H_{12}O_3$ 192.214

(3*S*,5*S*)-*form*
Harzialactone A
[203243-30-5]
Prod. by a *Trichoderma harzianum* isol. from the sponge *Halichondria okadai*.
Powder.
Mp 82-84°. $[\alpha]_D^{32}$ +33.3 (c, 0.3 in $CHCl_3$). λ_{max} 285 (log ϵ 2.61) (EtOH). λ_{max} 285 (ϵ 407) (MeOH) (Berdy).

Amagata, T. *et al., J. Antibiot.*, 1998, **51**, 33-40 (*isol, uv, ir, cd, pmr, cmr*)

4-Benzyl-3-(4-hydroxyphenyl)-2(5*H*)-furanone B-67

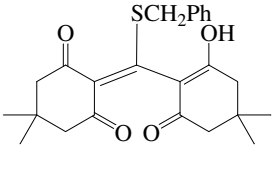
3-(4-Hydroxyphenyl)-4-(phenylmethyl)-2(5H)-furanone.
Eutypoid A



$C_{17}H_{14}O_3$ 266.296
Isol. from a marine fungus *Eutypa* sp. No. 424. Needles.
Mp 160-162°. λ_{max} 238 (ϵ 5850); 276 (ϵ 6800) ($CHCl_3$).

Lin, Y. *et al., Indian J. Chem., Sect. B*, 2002, **41**, 1542-1544 (*isol, pmr, cmr, ms*)

Benzylthiocrellidone B-68



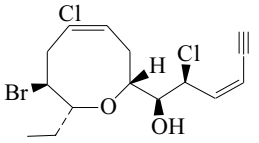
$C_{24}H_{28}O_4S$ 412.549
Enolised β-diketo system. All of the carbonyl groups are structurally equivalent. Isol. from the marine sponge *Crella spinulata*. Bright yellow cryst. (MeOH).

Mp 211° (202-204°). λ_{max} 295 (ϵ 16000); 345 (ϵ 18500) (no solvent reported).

Lam, H.W. *et al., J.C.S. Perkin 1*, 1999, 847-848 (*isol, synth, uv, ir, pmr, cryst struct*)

Bermudenynol B-69

[83474-72-0]



$C_{15}H_{19}BrCl_2O_2$ 382.123
Constit. of *Laurencia intricata*. Cryst. (hexane).
Mp 80-81°. $[\alpha]_D^{25}$ +187 (c, 0.756 in $CHCl_3$).

Ac: [83474-73-1]
$C_{17}H_{21}BrCl_2O_3$ 424.161
Constit. of *Laurencia intricata*. Oil.

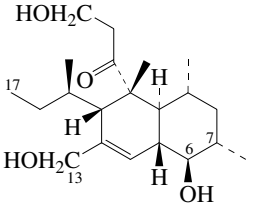
Cordellina, J.H. *et al., Can. J. Chem.*, 1982, **60**, 2675

Berovin B-70

Protein. Isol. from the ctenophore *Beroe ovata*. $Ca^{2\oplus}$-photo-activated protein.

Ward, W.W. *et al., Biochemistry*, 1974, **13**, 1500-1510 (*isol*)

Betaenone G B-71



$C_{21}H_{36}O_4$ 352.513
Prod. by the marine-derived *Microsphaeropsis* sp. Stamm 6288. Amorph. solid. $[\alpha]_D^{20}$ -18 (c, 0.1 in MeOH). λ_{max} 226 (sh) (log ϵ 3.46); 273 (log ϵ 2.51) (MeOH).

6-Deoxy: ***Betaenone H***
$C_{21}H_{36}O_3$ 336.514
Prod. by *Microsphaeropsis* sp. Stamm 6288. Amorph. solid. $[\alpha]_D^{20}$ -18 (c, 0.1 in MeOH). λ_{max} 267 (log ϵ 2.39) (MeOH).

6-Deoxy, 7β-hydroxy: ***Betaenone I***
$C_{21}H_{36}O_4$ 352.513
Prod. by *Microsphaeropsis* sp. Stamm 6288. Amorph. solid. $[\alpha]_D^{20}$ -3 (c, 0.1 in MeOH). λ_{max} 217 (sh) (log ϵ 3.15) (MeOH).

6-Deoxy, 17-hydroxy: ***Betaenone J***
$C_{21}H_{36}O_4$ 352.513
Prod. by *Microsphaeropsis* sp. Stamm 6288. Amorph. solid. $[\alpha]_D^{20}$ -4 (c, 0.1 in MeOH).

Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*isol, cd, pmr, cmr, ms*)

Betaine B-72

Carboxy-N,N,N-*trimethylmethanaminium hydroxide inner salt, 9CI. (Carboxymethyl)trimethylammonium. Glycine betaine. Glycocoll betaine. Lycine. Abromine. Oxyneurine*
[107-43-7]
$Me_3N^{\oplus}CH_2COO^{\ominus}$
$C_5H_{11}NO_2$ 117.147
Prod. by *Aspergillus oryzae, Patella vulgata, Claviceps purpurea* and other fungi. Occurs widely in plants and animals. Alkaloid from *Abroma augusta* (Sterculiaceae). May play a part in cytoplasmic osmoregulation. Causes myoatrophy in combination with Guanidinoacetic acid, G-192. Deliquescent scales or cryst.; cryst. + $1H_2O$ (H_2O). pK_a 3.84 (free acid). Dec. at *ca*. 310° (293-4°) with isom. to Me_2NCH_2COOMe.

▶ LD_{50} (mus, scu) 10800 mg/kg. DS5900000

Monohydrate: Trimethylglycine hydroxide
[17146-86-0] Lipotropic. Cryst. Loses water at 100° to form inner salt.

Hydrochloride: Betaine hydrochloride, USAN. Lycine hydrochloride. Achylin. Acidin. Acidol. Acinorm. Acipepsol. Aciventral forte. Euacid. Muriat. Pepsacid. Pluchine
[590-46-5] Used in solders, fluxes and in org. synth. Lipotropic. Electrolyte replenisher, gastric acidifier. Needles. Mp 243-244° dec. $[\alpha]_D^{20}$ -29.51 (H_2O).

▶ BP3136000

Aspartate (1:1): Hepastyl. Somabet. Somatyl
[52921-08-1] Used in treatment of liver and stomach disorders.

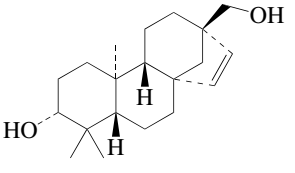
Picrate:
Yellow prisms (H_2O). Mp 181-182°.

Chloride: See 2-Chloro-*N,N,N*-trimethyl-2-oxoethanaminium(1+) in *The Combined Chemical Dictionary.*

[590-47-6]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 482B; 496B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 563D; 588C (*ir*)
Stoltzenberg, H. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1914, **92**, 445 (*synth*)
Edsall, J.T. *et al., J.A.C.S.*, 1943, **65**, 1767 (*synth, spectra*)
Guggenheim, M. *et al., Die Biogenen Amine*, 4th Ed., S. Karger, Basle, 1951, 240 (*occur*)
Gauter, J.A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1955, **241**, 884 (*synth*)
Leifer, A. *et al., J.A.C.S.*, 1957, **79**, 5098 (*struct, ir*)
U.S. Pat., 1957, 2 800 502; *CA*, **51**, 16522 (*synth*)
Fr. Pat., 1964, M2462; *CA*, **61**, 8405 (*salt*)
Dasgupta, B. *et al., Experientia*, 1967, **23**, 989; 1968, **24**, 882; 1970, **26**, 477 (*isol*)
Motohashi, N. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1737 (*cmr*)
Larsen, C. *et al., Biomed. Environ. Mass Spectrom.*, 1988, **17**, 187 (*ms*)
Haussuehl, S. *et al., Z. Kristallogr.*, 1989, **188**, 311 (*derivs, cryst struct*)
Chevalier, Y. *et al., J. Phys. Chem.*, 1990, **94**, 1768 (*conformn*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1303
Merck Index, 13th edn., 2001, No. 1182 (*props, bibl*)
Blunden, G. *et al., Phytochemistry*, 2001, **58**, 451-454 (*occur*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 6th edn., Van Nostrand Reinhold*, 1984, 425

15-Beyerene-3,17-diol B-73



$C_{20}H_{32}O_2$ 304.472

(ent-3β)-form
15-Stachene-3,17-diol
[18449-38-2]
Constit. of *Helichrysum dendroideum*.
Cryst.
Mp 168-170° Mp 190-192°. $[\alpha]_D$ +36 (EtOH). $[\alpha]_D^{25}$ +25.6 (c, 1 in $CHCl_3$).

3-Ketone: 17-Hydroxy-15-beyeren-3-one. ***Rhizophorin C***
[480427-81-4]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Rhizophora mucronata*. Cryst. (MeOH).
Mp 145-148°. $[\alpha]_D^{25}$ -38 (c, 1.5 in $CHCl_3$).

Lloyd, H.A. *et al., Tet. Lett.*, 1967, 4891-4895 (*15-Stachene-3,17-diol*)
Anjaneyulu, A.S.R. *et al., J. Asian Nat. Prod. Res.*, 2002, **4**, 53-61 (*Rhizophorin C*)

BG II B-74

Peptide containing 48 amino acid residues. Isol. from the sea anemone *Bunodosoma granulifera*. Toxin.

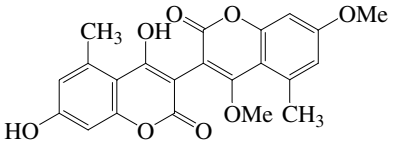
Loret, E.P. *et al., J. Biol. Chem.*, 1994, **269**, 16785-16788 (*isol*)

BgK toxin B-75

Peptide containing 37 amino acid residues and 3 intramol. disulfide bonds. Isol. from the sea anemone *Bunodosoma granulifera*. $K^{\oplus}$-channel-blocking toxin. Genus name incorr. given as Bundosoma.

Aneiros, A. *et al., Biochim. Biophys. Acta*, 1993, **1157**, 86-92 (*isol*)
Dauplais, M. *et al., J. Biol. Chem.*, 1997, **272**, 4302-4309 (*isol, struct*)

Bicoumanigrin B-76



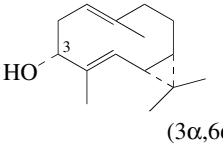
$C_{22}H_{18}O_8$ 410.379

Prod. by *Aspergillus niger* isol. from the sponge *Axinella damicornis*. Shows moderate cytotoxic activity. Amorph. powder.

Hiort, J. *et al., J. Nat. Prod.*, 2004, **67**, 1532-1543 (*isol, pmr, cmr, ms*)

Bicyclogermacren-3-ol B-77

3-Hydroxybicyclogermacrene



(3α,6α,7α)-*form*

$C_{15}H_{24}O$ 220.354

(3α,6α,7α)-*form*

Ac: [74320-15-3]
$C_{17}H_{26}O_2$ 262.391
Constit. of *Plagiochila yokogurensis*.
$[\alpha]_D$ -13.7 (c, 0.7 in $CHCl_3$).

(3β,6α,7α)-*form*

Constit. of *Parerythropodium fulvum*.
Cryst.
Mp 116-117°. $[\alpha]_D$ -49.5 (c, 0.11 in $CHCl_3$).

Ac:
$C_{17}H_{26}O_2$ 262.391
Constit. of *Parerythropodium fulvum*. Oil. $[\alpha]_D$ -25.1 (c, 0.2 in $CHCl_3$).

(3β,6ξ,7ξ)-*form*

Oil. $[\alpha]_D^{24}$ +34.8 (c, 0.77 in $CHCl_3$).

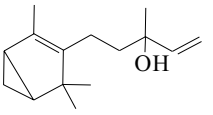
Angeloyl: [54878-84-1]
$C_{20}H_{30}O_2$ 302.456
Isol. from *Othonna* spp. Oil. $Bp_{0.1}$ 130°.

3-(2-Methyl-2-propenoyl):
$C_{19}H_{28}O_2$ 288.429
Constit. of *Euryops* spp. Oil.

Bohlmann, F. *et al., Chem. Ber.*, 1974, **107**, 3928
Bohlmann, K. *et al., Phytochemistry*, 1978, **17**, 1135 (*isol, pmr*)
Asakawa, Y. *et al., Phytochemistry*, 1980, **19**, 2141 (*Ac*)
Bowden, B.F. *et al., Tet. Lett.*, 1980, **21**, 3105-3108 (*isol, Ac, Parerythropodium, pmr, cmr*)

Bicyclolaurencenol B-78

[79373-33-4]

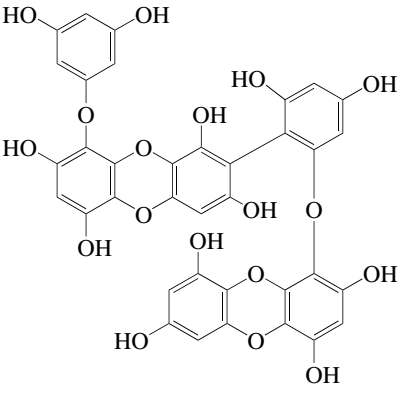


$C_{15}H_{24}O$ 220.354
Constit. of *Laurencia intricata*. Oil. $[\alpha]_D^{25}$ -16.1 (c, 0.67 in $CHCl_3$).

Horsley, S.B. *et al., J.O.C.*, 1981, **46**, 5033

2‴,8-Bieckol B-79

[96820-21-2]

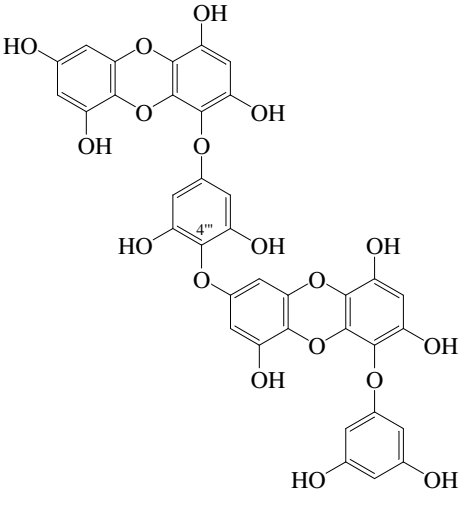


$C_{36}H_{22}O_{18}$ 742.559
Numbering systems vary. Constit. of the brown alga *Eisenia arborea*. Isol. as dodeca-Ac.

Glombitza, K.-W. *et al., Phytochemistry*, 1985, **24**, 543-551 (*isol, pmr, cmr*)

4‴,7-Bieckol B-80

[88095-79-8]

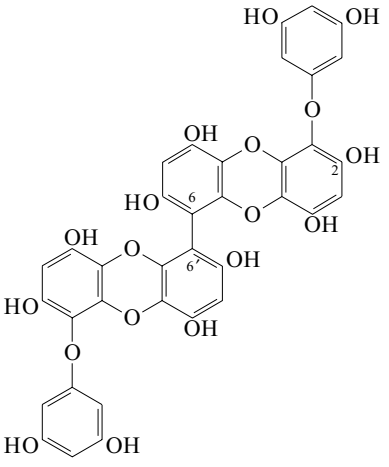


$C_{36}H_{22}O_{18}$ 742.559
Numbering systems vary. Constit. of the brown algae *Ecklonia maxima*, *Eisenia arborea* and *Eisenia bicyclis*. Isol. as undeca-Ac to which CAS no. refers. λ_{max} 233; 278; 290 (sh) (MeCN) (as undeca-Ac).

Glombitza, K.-W. *et al., Phytochemistry*, 1985, **24**, 308-312; 543-551 (*isol, pmr, cmr*)

6,6′-Bieckol B-81

[88095-81-2]



$C_{36}H_{22}O_{18}$ 742.559

Numbering systems vary. Constit. of the brown algae *Ecklonia kurome* and *Eisenia arborea*. Antiplasmin inhibitor. α_2-Macroglobulin inhibitor. Prisms (H_2O).
Mp 300°. λ_{max} 295 (ϵ 11000) (MeOH) (Berdy).

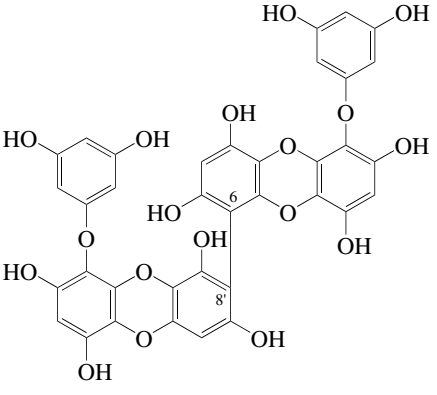
*2-*O*-(2,4,6-Trihydroxyphenyl): 2-*O*-(2,4,6-Trihydroxyphenyl)-6,6′-bieckol.* ***2-Phloro-6,6′-bieckol***
[89079-38-9]
$C_{42}H_{26}O_{21}$ 866.655
Constit. of *Ecklonia kurome*. Antiplasmin inhibitor. α_2-Macroglobulin inhibitor. Amorph. solid. λ_{max} 295 (ϵ 11000) (MeOH) (Berdy).

8,8′-Dihydroxy: ***8,8′-Dihydroxy-6,6′-bieckol***
[96820-22-3]
$C_{36}H_{22}O_{20}$ 774.558
Constit. of the brown alga *Eisenia arborea*. Isol. as tetradeca-Ac.

Glombitza, K.-W. *et al., Phytochemistry*, 1985, **24**, 543-551 (*isol, pmr, cmr, 8,8′-dihydroxy*)
Fukuyama, Y. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2438-2440 (*isol, uv, ir, pmr, cmr, ms*)

6,8′-Bieckol B-82

[99469-09-7]



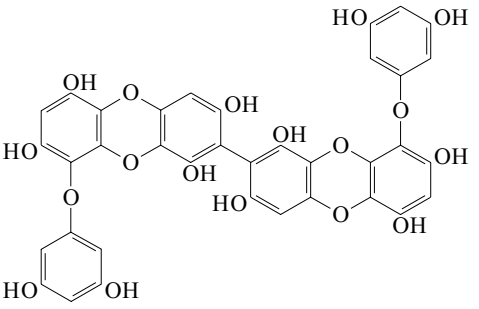
$C_{36}H_{22}O_{18}$ 742.559

Numbering systems vary. Constit. of the brown algae *Eisenia arborea* and *Ecklonia maxima*. Isol. as dodeca-Ac, to which CAS no. refers.

Glombitza, K.-W. *et al., Phytochemistry*, 1985, **24**, 543-551 (*isol, pmr, cmr*)
Glombitza, K.W. *et al., Planta Med.*, 1985, 308-312 (*isol, pmr, cmr*)

8,8′-Bieckol B-83

[89445-12-5]



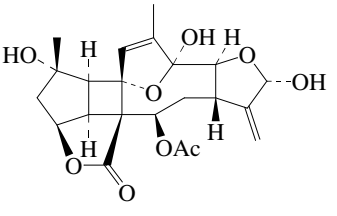
$C_{36}H_{22}O_{18}$ 742.559

Related to Dieckol, D-410. Numbering systems vary. Constit. of the brown algae *Ecklonia kurome* and *Eisenia arborea*. Antiplasmin inhibitor. α_2-Macroglobulin inhibitor. Light brown prisms (H_2O).
Mp 300°. λ_{max} 231 (ϵ 3800); 295 (ϵ 8800) (MeOH) (Berdy).

Glombitza, K.-W. *et al., Phytochemistry*, 1985, **24**, 534-551 (*isol, pmr, cmr*)
Fukuyama, Y. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2438-2440 (*isol, uv, ir, pmr, cmr, ms*)

Bielschowskysin B-84

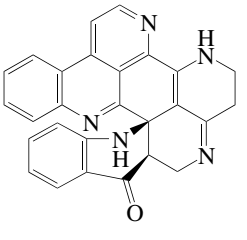
[697298-90-1]



$C_{22}H_{26}O_9$ 434.442
Constit. of *Pseudopterogorgia kallos*. Cryst.
Mp 139-141° dec. $[\alpha]_D^{20}$ -17.3 (c, 1.1 in MeOH).

Marrero, J. *et al., Org. Lett.*, 2004, **6**, 1661-1664 (*isol, pmr, cmr, cryst struct*)

Biemnadin B-85



$C_{27}H_{19}N_5O$ 429.48

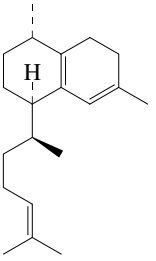
(±)-form [152053-10-6]
Alkaloid from the Okinawan marine sponge *Biemna* sp. and *Biemna fortis*. Cytotoxic. Neuronal differentiation inducer. Yellow cryst. (as hydrochloride).
Mp 300° (hydrochloride). Closely related to Eudistone A, E-888. λ_{max} 229 (ϵ 29000); 256 (ϵ 17000); 370 (ϵ 5000) (MeOH).

Zeng, C.-M. *et al., Tetrahedron*, 1993, **49**, 8337-8342 (*isol, uv, ir, pmr, cmr, cryst struct*)
Aoki, S. *et al., Bioorg. Med. Chem.*, 2003, **11**, 1969-1973 (*isol, pmr, cmr*)

1(6),4,15-Bifloratriene B-86

Isoelisabethatriene

[334022-60-5]



$C_{20}H_{32}$ 272.473

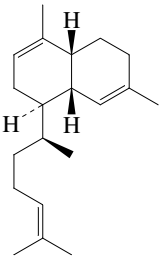
Constit. of *Pseudopterogorgia elisabethae*. λ_{max} 245 (MeOH).

Kohl, A.C. *et al., Mar. Drugs*, 2003, **1**, 54-65 (*isol, pmr*)

4,9,15-Bifloratriene B-87

[251114-02-0]

[173692-41-6 incorrect epimer]



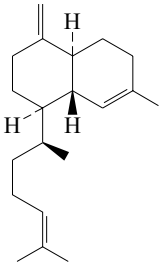
$C_{20}H_{32}$ 272.473

Constit. of a *Cribrochalina* sp. and of *Acanthella cavernosa*. Larval settlement inhibitor, antifouling agent. Oil. $[\alpha]_D^{20}$ +51.4 (c, 0.5 in $CHCl_3$). $[\alpha]_D$ +64 (c, 0.05 in $CHCl_3$). Struct. of *C.* isolate revised in 2005; formerly assigned as a stereoisomer.

Hirota, H. *et al., Tetrahedron*, 1996, **52**, 2359 (*1-epimer*)
Ciavatta, M.L. *et al., Tetrahedron*, 1999, **55**, 12629-12636; 2005, **61**, 8049-8053 (*isol, pmr, cmr, struct*)

4,10(19),15-Bifloratriene B-88

[69636-81-3]



$C_{20}H_{32}$ 272.473

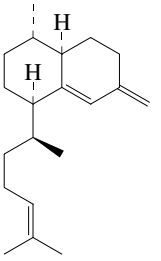
Constit. of defensive secretion of *Cubitermes umbratus* and other *Cubitermes* spp. Also found in the soft coral, *Xenia obscuronata*. Oil. $[\alpha]_D$ -92 (c, 0.13 in MeOH).

Wiemer, D.F. *et al., J.O.C.*, 1980, **45**, 191 (*isol, cryst struct*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1983, **60**, 757 (*synth*)
Groweiss, A. *et al., Tetrahedron*, 1983, **39**, 3385 (*isol*)
Mori, K. *et al., Tetrahedron*, 1984, **40**, 305 (*synth, abs config*)
Kodama, M. *et al., Tet. Lett.*, 1984, **25**, 5781 (*synth*)
Parker, K.A. *et al., J.O.C.*, 1986, **51**, 4023 (*synth*)
Grieco, P.A. *et al., Tet. Lett.*, 1986, **27**, 4813 (*synth*)
Paknikar, S.K. *et al., J. Nat. Prod.*, 1988, **51**, 326 (*synth*)

4(20),5,15-Bifloratriene B-89

Elisabethatriene

[334499-19-3]

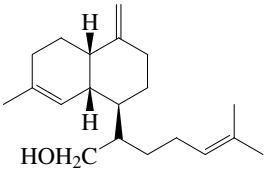


$C_{20}H_{32}$ 272.473

Constit. of *Pseudopterogorgia elisabethae*. Biosynthetic precursor of the pseudopterosins and secopseudopterosins. Oil. λ_{max} 245 (MeOH).

Coleman, A.C. *et al., Tetrahedron*, 2000, **56**, 9569-9574 (*isol, pmr, cmr*)
Kohl, A.C. *et al., Mar. Drugs*, 2003, **1**, 54-65 (*biosynth*)

4,10(19),15-Bifloratrien-12-ol B-90



$C_{20}H_{32}O$ 288.472

12-O-*β*-D-*Xylopyranoside:* ***Lemnaflavoside***
[473299-25-1]
$C_{25}H_{40}O_5$ 420.588
Constit. of *Lemnalia flava*. Amorph. solid. $[\alpha]_D$ +12 (c, 0.9 in MeOH).

12-(2-O-*Acetyl-β-D-xylopyranoside):* [471890-91-2]
$C_{27}H_{42}O_6$ 462.625
Constit. of *Lemnalia flava*. Oil.

12-(3-O-*Acetyl-β-D-xylopyranoside):* [471890-93-4]
$C_{27}H_{42}O_6$ 462.625
Constit. of *Lemnalia flava*. Oil.

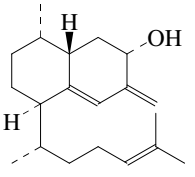
12-(4-O-*Acetyl-β-D-xylopyranoside):* [471890-95-6]
$C_{27}H_{42}O_6$ 462.625
Constit. of *Lemnalia flava*. Oil.

Rudi, A. *et al., J. Nat. Prod.*, 2002, **65**, 1672-1674 (*isol, pmr, cmr*)

4(20),5,15-Bifloratrien-3-ol B-91

Elisabethatrienol

[890153-96-5]

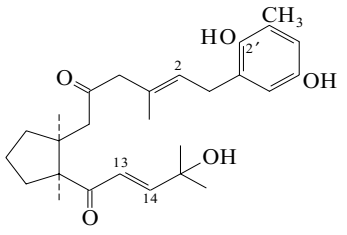


$C_{20}H_{32}O$ 288.472

Constit. of *Pseudopterogorgia elisabethae*. Amorph. solid. $[\alpha]_D^{25}$ -44.8 (c, 0.14 in MeOH). λ_{max} 236 (ϵ 16800) (MeOH).

Duque, C. *et al., Tetrahedron*, 2006, **62**, 4205-4213 (*Elisabethatrienol*)

Bifurcarenone B-92



(2*E*)–*form*

$C_{27}H_{38}O_5$ 442.594

Struct. revised in 1989. λ_{max} 215 (ϵ 15600); 225 (ϵ 16200); 292 (ϵ 3400) (MeOH) (Derep).

(2*E*)-*form* [75872-68-3]
[110351-79-6]
Constit. of the brown alga *Cystoseira stricta* and *Bifurcaria galapagensis*. Antibacterial. Oil. $[\alpha]_D^{20}$ +5.7 (c, 0.24 in $CHCl_3$) $[\alpha]_D^{20}$ +5.5 (c, 8 in EtOH).

2′-Me ether: [110309-19-8]
$C_{28}H_{40}O_5$ 456.621
Constit. of *Cystoseira stricta*. Oil. $[\alpha]_D^{20}$ +5.3 (c, 1.15 in EtOH).

5′-Me ether: [194550-95-3]
$C_{28}H_{40}O_5$ 456.621
Constit. of *Cystoseira amentacea* var. *stricta* and *Cystoseira tamariscifolia*. Oil. $[\alpha]_D^{25}$ +10.7 (c, 1.5 in EtOH). λ_{max} 214 (log ϵ 4.02); 224 (log ϵ 4.07); 289 (log ϵ 3.34) (EtOH).

13,14-Dihydro, 2′,5′-di-Me ether: [93236-29-4]
$C_{29}H_{44}O_5$ 472.664
Constit. of the brown alga *Cystoseira algeriensis* and *Cystoseira jabukae*. Oil. $[\alpha]_D^{20}$ +25 (c, 1.1 in EtOH).

(2*Z*)-*form* [104529-85-3]
Sol. MeOH, C_6H_6; poorly sol. H_2O. λ_{max} 215 (ϵ 15600); 225 (ϵ 16200); 292 (ϵ 3400) (MeOH) (Berdy).

13,14-Dihydro, 2′,5′-di-Me ether: [93380-11-1]
$C_{29}H_{44}O_5$ 472.664
Constit. of *Cystoseira algeriensis*. Oil. $[\alpha]_D^{20}$ +12 (c, 1.3 in EtOH).

Sun, H.H. *et al., Tet. Lett.*, 1980, 3123-3126 (*isol, struct, spectra*)
Amico, V. *et al., Phytochemistry*, 1984, **23**, 2017-2020; 1987, **26**, 1715-1718 (*isol, 13,14-dihydro-2′,5′-di-Me ether*)
Mori, K. *et al., Tetrahedron*, 1989, **45**, 1945-1958; 1990, **46**, 4193-4204 (*synth, abs config*)
Amico, V. *et al., J. Nat. Prod.*, 1991, **54**, 877-881; 1997, **60**, 1088-1093 (*cmr, abs config*)
Mesguiche, V. *et al., Phytochemistry*, 1997, **45**, 1489-1494 (*5′-Me ether*)
Bennamara, A. *et al., Phytochemistry*, 1999, **52**, 37-40 (*5′-Me ether*)

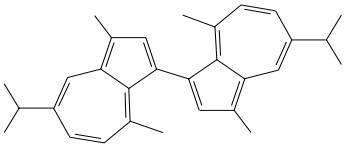
Limulus Big defensin B-93

Horseshoe crab big defensin
Peptide containing 79 amino acid residues. Isol. from haemocytes of the horseshoe crab *Limulus*. Shows antibacterial activity.

Saito, T. *et al., J. Biochem. (Tokyo)*, 1995, **117**, 1131-1137 (*isol, struct*)
Kiwabata, S. *et al., Methods Mol. Biol.*, 1997, **78**, 51-61 (*isol*)

2,2′-Biguaiazulenyl B-94

3,3′,8,8′-Tetramethyl-5,5′-bis(1-methylethyl)-1,1′-biazulene
[17509-79-4]

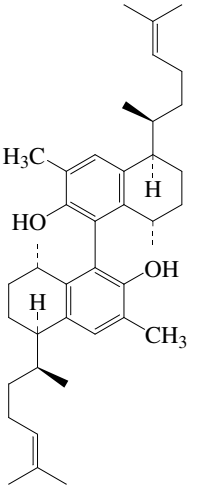


$C_{30}H_{34}$ 394.599
Constit. of *Calicogorgia granulosa*. Blue-green solid.
Mp 88-90°. λ_{max} 250 (ϵ 45770); 283 (ϵ 63100); 309 (ϵ 42280); 354 (ϵ 16220); 374 (ϵ 19520); 626 (ϵ 2795) (MeOH) (Berdy).

Seo, Y. *et al., J. Nat. Prod.*, 1996, **59**, 985-986 (*isol, pmr, cmr*)

8,8′-Bi[7-hydroxyerogorgiaene] B-95

Bis-7-hydroxyerogorgiaene
[318513-15-4]



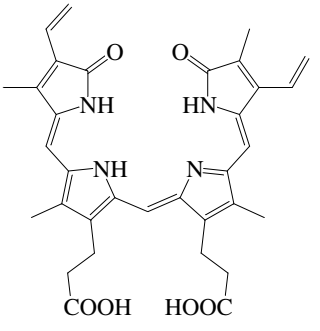
$C_{40}H_{58}O_2$ 570.897

Incorrectly drawn as *meso*-compound in ref. Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{25}$ +61.5 (c, 0.7 in $CHCl_3$). λ_{max} 210 (ϵ 41600); 286 (ϵ 5800) (MeOH).

Rodríguez, A.D. *et al., J. Nat. Prod.*, 2001, **64**, 100-102 (*isol, pmr, cmr*)

Biliverdin B-96

Biliverdin IXα
[114-25-0]



$C_{33}H_{34}N_4O_6$ 582.655

Blue-green pigment of bile, eggshells of birds, dog placenta. Major pigment from the blue coral *Heliopora coerulea*. Primary prod. derived from Haem by oxidative ring fission *in vivo*, also formed by oxidn. of Bilirubin. Dark-blue green cryst. with violet sheen ($CHCl_3$).
Mp 300°. Gives Gmelin reaction with conc. $HNO_3/CHCl_3$.
Reduced to Bilirubin in mammals.

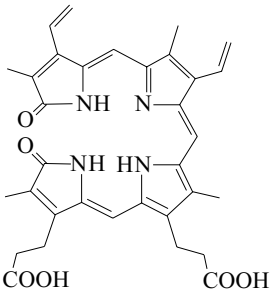
Di-Me ester: [10035-62-8]
$C_{35}H_{38}N_4O_6$ 610.708
Blue-green cryst. ($CHCl_3$/petrol). Mp 220-221°. λ_{max} 379; 656 (no solvent reported).

[55482-27-4]

Lemberg, R. *et al., Haematin Compounds and Bile Pigments*, Interscience, N.Y., 1949,
Rüdiger, W. *et al., Annalen*, 1968, **713**, 209 (*isol, ms*)
Plieninger, H. *et al., Annalen*, 1972, **758**, 195 (*synth*)
Sheldrick, W.S. *et al., J.C.S. Perkin 2*, 1976, 1457 (*cryst struct*)
Stoll, M.S. *et al., Biochem. J.*, 1977, **163**, 59 (*pmr, ms*)
Smit, K. *et al., J. Phys. Chem.*, 1993, **97**, 11887 (*ir, Raman*)

Biliverdin IXδ B-97

[29575-16-4]



$C_{33}H_{34}N_4O_6$ 582.655

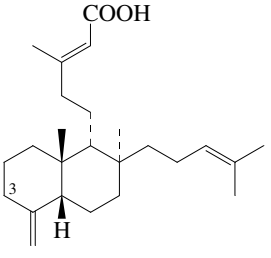
Prod., together with isomers, by oxidative cleavage of Haem. Isol. from ovaries of marine snail *Turbo cornutus*.

Di-Me ester: [26195-58-4]
$C_{35}H_{38}N_4O_6$ 610.708
Blue cryst. Mp 172-174°. λ_{max} 379, 651-7 nm.

Bonnett, R. *et al., J.C.S. Perkin 1*, 1973, 881 (*synth*)
Benedikt, E. *et al., Eur. J. Biochem.*, 1988, **175**, 643 (*isol*)

Bilosespene A B-98

[243971-15-5]



$C_{25}H_{40}O_2$ 372.59

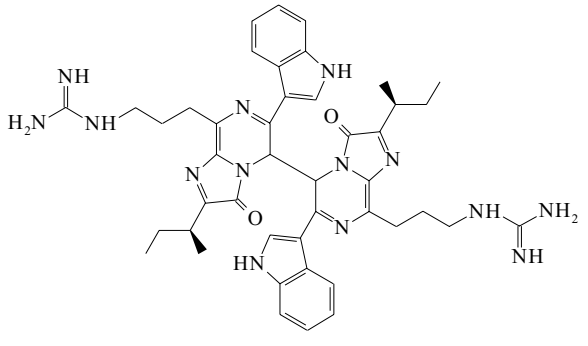
Constit. of *Dysidea cinerea*.

Δ^3-Isomer: ***Bilosespene B***
[243971-16-6]
$C_{25}H_{40}O_2$ 372.59
Constit. of *Dysidea cinerea*.

Rudi, A. *et al., Org. Lett.*, 1999, **1**, 471-472 (*isol, pmr, cmr*)
Hsu, D.-S. *et al., Org. Lett.*, 2003, **5**, 4741-4743 (*synth*)

Cypridina Biluciferyl B-99

Cypridina *Biluciferol*
[96700-80-0]



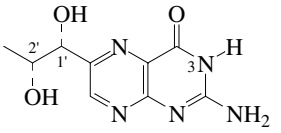
$C_{44}H_{52}N_{14}O_2$ 808.987

Dimer of *Cypridina* Luciferin, L-239. Isol. from *Cypridina* sp. Bioluminescent compd.

Toya, Y. *et al., Tet. Lett.*, 1985, **26**, 239 (*uv, pmr, struct*)

Biopterin B-100

*2-Amino-6-(1,2-dihydroxypropyl)-4(1*H*)-pteridinone, 9CI. 2-Amino-4-hydroxy-6-(1,2-dihydroxypropyl)pterin. Ranachrome 1*



(1'*R*,2'*R*)-*form*

$C_9H_{11}N_5O_3$ 237.218

(1′R,2′R)-form
D-threo-*form*. ***Dictyopterin***
[13019-52-8]
Isol. from *Dictyostelium discoideum*.
Mp 300°. pK_{a1} 2.2; pK_{a2} 7.92.

(1′R,2′S)-form
L-erythro-*form*
[22150-76-1]
Widely distributed in microorganisms, insects, algae, amphibia and mammals. Found in urine. Growth factor. Pale yellow cryst. (AcOH aq.).
Mp 250-280° dec. $[\alpha]_D^{20}$ -66 (c, 0.2 in 0.1*M* HCl). pK_{a1} 2.23; pK_{a2} 7.89.

► UO3506000

1′-O-D-Glucopyranoside: ***Biopterin glucose***
[32838-67-8]
$C_{15}H_{21}N_5O_8$ 399.36
Constit. of a marine plankton.

2′-O-α-D-Glucopyranoside: [235416-12-3]
$C_{15}H_{21}N_5O_8$ 399.36
Isol. from *Spirulina* (*Arthrospira*) *platensis*.

2′-O-(2-Acetamido-2-deoxy-β-D-glucopyranoside): ***Limipterin***
[164803-20-7]
$C_{17}H_{24}N_6O_8$ 440.412
Prod. by *Chlorobium limicola f. thiosulfatophilum*.

3-Me: ***2-Amino-6-(1,2-dihydroxypropyl)-3-methylpterin-4-one***
[111317-37-4]
$C_{10}H_{13}N_5O_3$ 251.244
Isol. from the marine anthozoan *Astroides calycularis*. Pale yellow cryst. powder (MeOH). Sol. MeOH, H_2O.
Mp 229-231°. $[\alpha]_D$ -60 (c, 0.3 in 0.1*M* HCl). λ_{max} 230 (ϵ 28200); 319 (ϵ 11700) (pH 1 H_2O) (Derep). λ_{max} 242 (ϵ 28200); 276 (ϵ 24000); 356 (ϵ 9550) (H_2O pH 7) (Derep).

7,8-Dihydro: 7,8-Dihydrobiopterin
[6779-87-9]
[7644-44-2]
$C_9H_{13}N_5O_3$ 239.233
Hygroscopic needles (H_2O or MeOH aq.). $[\alpha]_D^{22}$ +35 (c, 0.4 in 0.1*M* NaOH).

5,6,7,8-Tetrahydro: See 5,6,7,8-Tetrahydrobiopterin in *The Combined Chemical Dictionary*.

(1′S,2′R)-form
D-erythro-*form*
[13039-62-8]
Mp 300°. pK_{a1} 2.23; pK_{a2} 7.9.

(1′S,2′S)-form
L-threo-*form*. ***Orinapterin***. *Ciliapterin*
[13039-82-2]
Isol. from human urine. Prod. by *Aphanizomenon flos-aquae*.
Pale yellow cryst. (AcOH aq.).
Mp 300°. $[\alpha]_D$ +72 (0.1*M* HCl). pK_{a1} 2.24; pK_{a2} 7.87.

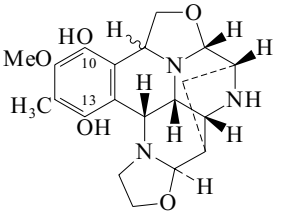
2′-O-(2-Acetamido-2-deoxy-β-D-glucopyranoside): ***Tepidopterin***
[188778-28-1]
$C_{17}H_{24}N_6O_8$ 440.412
Prod. by *Chlorobium tepidum*.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 480B (*nmr*)
Patterson, E.L. *et al., J.A.C.S.*, 1955, **77**, 3167
Kidder, G.W. *et al., J. Biol. Chem.*, 1968, **243**, 826 (*Ciliapterin*)

Kidder, G.W. *et al., Methods Enzymol.*, 1971, **18B**, 739 (*Ciliapterin*)
Rembold, H. *et al., Angew. Chem., Int. Ed.*, 1972, **11**, 1061 (*biochem*)
Blair, J.A. *et al., Tet. Lett.*, 1973, 203-204 (*synth, uv, dihydro*)
Sugimoto, T. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 3767 (*synth*)
Taylor, E.C. *et al., J.A.C.S.*, 1976, **98**, 2301 (*synth*)
Schircks, B. *et al., Helv. Chim. Acta*, 1977, **60**, 211; 1978, **61**, 2731-2738; 1985, **68**, 1639 (*synth, pmr, cmr, derivs*)
Fukushima, T. *et al., Methods Enzymol.*, 1980, **66**, 508-511 (*synth, uv, dihydro*)
Armarego, W.L.F. *et al., Aust. J. Chem.*, 1982, **35**, 785 (*synth*)
Kappel, M. *et al., Annalen*, 1984, 1815 (*synth*)
Aiello, A. *et al., Experientia*, 1987, **43**, 950 (*deriv*)
Mori, K. *et al., Annalen*, 1989, 958; 1212 (*synth, bibl*)
Klein, R. *et al., Eur. J. Biochem.*, 1990, **187**, 665 (*Dictyopterin*)
Ogiwara, S. *et al., Biol. Chem. Hoppe-Seyler*, 1992, **373**, 1061 (*Orinapterin*)
Cha, K.W. *et al., Helv. Chim. Acta*, 1995, **78**, 600-614 (*Limipterin*)
Ikawa, M. *et al., Phytochemistry*, 1995, **38**, 1229 (*isol, pmr, ms*)
Fernandez, A.M. *et al., J.O.C.*, 1996, **61**, 8698 (*synth*)
Cho, S.-H. *et al., Biochim. Biophys. Acta*, 1998, **1379**, 53-60 (*Tepidopterin*)
Noguchi, Y. *et al., Mar. Biotechnol.*, 1999, **1**, 207-210 (*2′-glucoside*)

Bioxalomycin α1 B-101

Antibiotic 31F508α1. 31F508α1
[157207-82-4]



$C_{20}H_{25}N_3O_5$ 387.435
Isol. from the marine-derived *Streptomyces viridostaticus* ssp. *littoralis* (LL-31F508). Exhibits potent antimicrobial and antitumour activity. Powder. Sol. MeOH, H_2O, DMSO, Me_2CO; poorly sol. CH_2Cl_2, Me_2CO, MeCN, $CHCl_3$. λ_{max} 290; 294 (MeOH) (Berdy).

N-*Me:* ***Bioxalomycin α2***. *Antibiotic 31F508α2. 31F508α2*
[157207-83-5]
$C_{21}H_{27}N_3O_5$ 401.461
From *Streptomyces viridostaticus* ssp. *littoralis*. Exhibits potent antimicrobial and antitumour activity. Powder. Sol. MeOH, Me_2CO, DMSO, H_2O; poorly sol. CH_2Cl_2, $CHCl_3$, MeCN, Me_2CO. $[\alpha]_D^{25}$ +31 (MeOH). Unstable in soln. λ_{max} 292 (ε 2729) (MeOH) (Berdy).

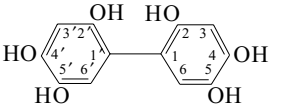
10,13-Quinone: ***Bioxalomycin β1***. *Antibiotic 31F508β1. 31F508β1*
[157207-84-6]
$C_{20}H_{23}N_3O_5$ 385.419
Isol. from *Streptomyces viridostaticus* ssp. *littoralis*. Potent antitumour and antimicrobial agent. Sol. CH_2Cl_2, DMSO, MeOH, $CHCl_3$; poorly sol. H_2O, hexane.

10,13-Quinone, N-*Me:* ***Bioxalomycin β2***. *Antibiotic 31F508β2. 31F508β2*
$C_{21}H_{25}N_3O_5$ 399.446
From *Streptomyces viridostaticus* ssp. *littoralis*. Exhibits potent antitumour and antimicrobial activity. Sol. CH_2Cl_2, $CHCl_3$, DMSO, MeOH; poorly sol. H_2O, hexane. It is proposed that this is the naturally occurring form of Naphthyridinomycin (see Naphthyridinomycin A). λ_{max} 270 (ε 10508); 370 (MeOH) (Berdy). λ_{max} 264; 370 (MeOH-HCl) (Berdy).

Bernan, V.S. *et al., J. Antibiot.*, 1994, **47**, 1417-1424 (*isol, props*)
Zaccardi, J. *et al., J.O.C.*, 1994, **59**, 4045-4047 (*isol, ir, uv, pmr, cmr, ms*)

2,2′,4,4′,5,5′-Biphenylhexol B-102

2,2′,4,4′,5,5′-Hexahydroxybiphenyl
[76625-61-1]



$C_{12}H_{10}O_6$ 250.207
Constit. of the sponge *Axinella polycapella*. Antimicrobial agent. Light-blue-grey solid.
Mp 277-280°.

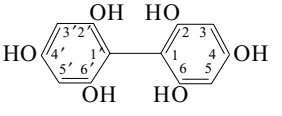
Hexa-Ac:
$C_{24}H_{22}O_{12}$ 502.431
Cryst. (EtOH). Mp 172-174°.

Hexa-Me ether: 2,2′,4,4′,5,5′-Hexamethoxybiphenyl
[1702-67-6]
$C_{18}H_{22}O_6$ 334.368
Needles (AcOH). Mp 180°.

Erdtman, H.G.H. *et al., Proc. R. Soc. London, A*, 1933, **143**, 191
Meerwein, H. *et al., J. Prakt. Chem.*, 1940, **154**, 266
Forrest, J. *et al., J. Pharm. Pharmacol.*, 1952, **4**, 231
Wratten, S.J. *et al., Experientia*, 1981, **37**, 13 (*isol, synth*)

2,2′,4,4′,6,6′-Biphenylhexol B-103

2,2′,4,4′,6,6′-Hexahydroxybiphenyl. ***Difucol***
[4371-20-4]



$C_{12}H_{10}O_6$ 250.207
Occurs in several brown algae, e.g. *Fucus vesiculosus*, *Cystophora retroflexa*, *Carpophyllum angustifolium*.

2-O-*Sulfate:* [123203-15-6]
$C_{12}H_{10}O_9S$ 330.272
Constit. of an alga.

4,4′-Di-O-*sulfate:* [123203-16-7]
$C_{12}H_{10}O_{12}S_2$ 410.336
Isol. from alga *Pleurocarpus gardneri*. Isol. as di-K salt.

Hexa-Me ether: 2,2′,4,4′,6,6′-Hexamethoxybiphenyl
[14262-07-8]
$C_{18}H_{22}O_6$ 334.368
Cryst. (EtOH). Mp 156°.

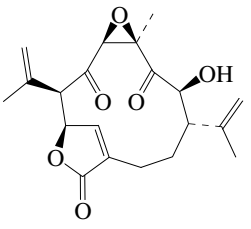
3-Chloro: 3-Chloro-2,2′,4,4′,6,6′-biphenylhexol. ***3-Chlorodifucol***
$C_{12}H_9ClO_6$ 284.652
Isol. from *Carpophyllum angustifolium*. Called 3[A_4]-chloro in the lit. by analogy with phlorotannins having a greater no. of rings.

[57103-39-6, 115834-42-9, 115868-52-5]

Riedl, W. *et al., Annalen*, 1955, **597**, 148 (*synth*)
Wünsche, C. *et al., Tetrahedron*, 1968, **24**, 3407 (*ms*)
Anderson, N.H. *et al., J.C.S.(C)*, 1969, 2403 (*synth*)
Glombitza, K.W. *et al., Phytochemistry*, 1975, **14**, 1403-1405; 1999, **50**, 869-881 (*isol*)
Craigie, J.S. *et al., Can. J. Chem.*, 1977, **55**, 1575 (*pmr, cmr*)
Glombitza, K.-W. *et al., Mar. Nat. Prod. Chem.*, Plenum Press, N.Y., 1977, 191 (*occur*)
Koch, M. *et al., Phytochemistry*, 1984, **23**, 2633
Peter-Katalinic, J. *et al., Biomed. Environ. Mass Spectrom.*, 1988, **15**, 595 (*ms*)
Glombitza, K.W. *et al., Phytochemistry*, 1992, **31**, 279 (*isol, sulfate, disulfate*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*3-Chlorodifucol*)

Bipinnapterolide A B-104

[245681-43-0]

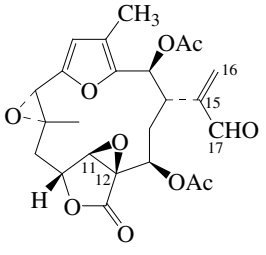


$C_{20}H_{24}O_6$ 360.406
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 153-154°. $[\alpha]_D^{24}$ -7.8 (c, 2.1 in $CHCl_3$). λ_{max} 216 (ϵ 9800) (MeOH).

Rodriguez, A.D. *et al., J. Nat. Prod.*, 1999, **62**, 1228-1237 (*isol, pmr, cmr, cryst struct*)

Bipinnatin B B-105

Lophotoxin-analog I
[99552-24-6]



Absolute Configuration

$C_{24}H_{26}O_{10}$ 474.463
Metab. of *Pseudopterogorgia bipinnata*. Cytotoxic. Irreversibly inhibits the binding of α-toxin to nicotinic acetylcholine receptor. $[\alpha]_D^{20}$ -68.9 (c, 1.2 in CH_2Cl_2). λ_{max} 242 (ϵ 948) ($CHCl_3$) (Derep). λ_{max} 242 (ϵ 948) ($CHCl_3$) (Berdy).

17-Carboxylic acid, Me ester: ***Bipinnatin A***. *Lophotoxin-analog V*
[99552-28-0]
$C_{25}H_{28}O_{11}$ 504.49
Metab. of *Pseudopterogorgia bipinnata*. Cytotoxic. $[\alpha]_D^{20}$ -76.6 (c, 3.5 in $CHCl_3$). λ_{max} 286 (ϵ 10500) ($CHCl_3$) (Derep). λ_{max} 286 (ϵ 10500) ($CHCl_3$) (Berdy).

11,12-Deepoxy(Z-): ***Bipinnatin D***
[123374-33-4]
$C_{24}H_{26}O_9$ 458.464
Metab. of *Pseudopterogorgia bipinnata*. Cytotoxic. $[\alpha]_D^{20}$ +34.2 (c, 0.17 in $CHCl_3$). λ_{max} 242 (ϵ 948) ($CHCl_3$) (Derep). λ_{max} 241 (ϵ 641) ($CHCl_3$) (Berdy).

15S,16-Epoxide, 17-deoxo: ***Bipinnatin C***
[123483-20-5]
$C_{24}H_{28}O_{10}$ 476.479
Metab. of *Pseudopterogorgia bipinnata*. Cryst. (CH_2Cl_2/MeOH/H_2O). $[\alpha]_D^{20}$ -45.6 (c, 0.54 in $CHCl_3$). λ_{max} 242 (ϵ 948) ($CHCl_3$) (Derep).

11,12-Deepoxy(Z-), 17-deoxo: ***Bipinnatin G***
[134455-94-0]
$C_{24}H_{28}O_8$ 444.48
Constit. of *Pseudopterogorgia bipinnata*. Solid. $[\alpha]_D^{24}$ -12.9 (c, 2.1 in $CHCl_3$). λ_{max} 212 (ϵ 18000) (MeOH).

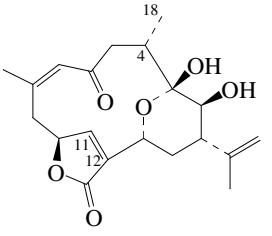
11,12-Deepoxy(Z-), 17-deoxo, 15S,16-epoxide: ***Bipinnatin H***
[134455-95-1]
$C_{24}H_{28}O_9$ 460.48
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 221-222°. $[\alpha]_D^{24}$ -8.8 (c, 2.1 in $CHCl_3$). λ_{max} 214 (ϵ 19000) (MeOH).

11,12-Deepoxy(Z-), 17-carboxylic acid, Me ester: ***Bipinnatin I***
[134455-96-2]
$C_{25}H_{28}O_{10}$ 488.49
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 162-163° dec. $[\alpha]_D^{24}$ +22.9 (c, 2.4 in $CHCl_3$). λ_{max} 228 (ϵ 12500) (MeOH).

Culver, P. *et al., Mol. Pharmacol.*, 1985, **28**, 436 (*pharmacol*)
Abramson, S.N. *et al., J. Biol. Chem.*, 1989, **264**, 12666 (*pharmacol*)
Wright, A.E. *et al., Tet. Lett.*, 1989, **30**, 3491-3494 (*Bipinnatins A-D*)
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1999, **62**, 1228-1237 (*Bipinnatins G-I*)

Bipinnatolide I B-106

[245681-51-0]



$C_{20}H_{26}O_6$ 362.422
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 162-163° (dec.). $[\alpha]_D^{24}$ +22.9 (c, 2.4 in $CHCl_3$). λ_{max} 228 (ϵ 12500) (MeOH).

11α,12α-Epoxide: ***Bipinnatolide H***
[245681-50-9]
$C_{20}H_{26}O_7$ 378.421
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 205-206°. $[\alpha]_D^{24}$ +10 (c, 1.4 in $CHCl_3$). λ_{max} 206 (ϵ 4700); 240 (ϵ 10400) (MeOH).

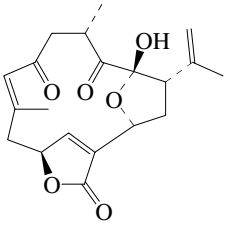
4,5-Didehydro, 11α,12α-epoxide: ***Bipinnatolide F***
[245681-45-2]
$C_{20}H_{24}O_7$ 376.405
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 204-208° (dec.). $[\alpha]_D^{24}$ +25.3 (c, 0.95 in $CHCl_3$). λ_{max} 204 (ϵ 7200) (MeOH).

4,18-Didehydro, 11α,12α-epoxide: ***Bipinnatolide G***
[245681-47-4]
$C_{20}H_{24}O_7$ 376.405
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 234-235°. $[\alpha]_D^{24}$ +3.9 (c, 0.51 in $CHCl_3$). λ_{max} 206 (ϵ 6200); 242 (ϵ 10900) (MeOH).

Rodriguez, A.D. *et al., J. Nat. Prod.*, 1999, **62**, 1228-1237 (*isol, pmr, cmr, cryst struct*)

Bipinnatolide J B-107

[245681-53-2]

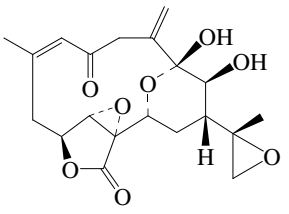


$C_{20}H_{24}O_6$ 360.406
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 180-183° (dec.). $[\alpha]_D^{24}$ +3.9 (c, 1.55 in $CHCl_3$). λ_{max} 212 (ϵ 8000) (MeOH).

Rodríguez, A.D. *et al., J. Nat. Prod.*, 1999, **62**, 1228-1237 (*isol, pmr, cmr*)

Bipinnatolide K B-108

[302925-22-0]

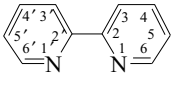


$C_{20}H_{24}O_8$ 392.405
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 199-200°. $[\alpha]_D^{24}$ -9.2 (c, 0.8 in $CHCl_3$). λ_{max} 210 (ϵ 62400) (MeOH).

Rodríguez, A.D. *et al., J. Nat. Prod.*, 2000, **63**, 1548-1550 (*isol, pmr, cmr*)

2,2′-Bipyridine, 9CI B-109

2,2′-Bipyridyl. α,α′-Bipyridyl. Bipy
[366-18-7]
[37275-48-2]



$C_{10}H_8N_2$ 156.187
Used in photometric detn. of Fe(*II*) (λ_{max} 522 nm, ϵ 8700, pH 2-9); as a masking agent for Zn, Cd, Cu. Fe(*II*) chelate is used as a redox indicator. Complexing agent for prepn. of inorganic complexes. Prisms (petrol). Sol. H_2O, EtOH, Et_2O, C_6H_6, $CHCl_3$, dil. acids. Mp 69.5°. Bp 272.5°. pK_{a1} 4.3 (25°, H_2O). Fe^{II} salts → red col.

▶ LD_{50} (rat, orl) 100 mg/kg. Exp. teratogen. DW1750000

Methiodide: [77972-47-5]
Yellow-white needles (Et_2O/MeCN). Mp 143-145°.

Chlorochromate: [76899-34-8]
$C_{10}H_9ClCrN_2O_3$ 292.642
Used to oxidise acid labile primary and secondary alcohols to carbonyl compounds. Yellow cryst.

Mono-N-*oxide:* [33421-43-1]
$C_{10}H_8N_2O$ 172.186
Mp 59°.

▶ DW1840000

N,N′-*Dioxide:* [7275-43-6]
$C_{10}H_8N_2O_2$ 188.185
Mp 310° dec.

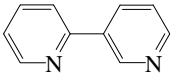
▶ DW1770000

N,N′-*Di-Me:* ***1,1′-Dimethyl-2,2′-bipyridinium (2+)***
$C_{12}H_{14}N_2^{2\oplus}$ 186.256
Isol. from mollusc *Callista chione*.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 731C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 239B; 483B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1513B (*ir*)
Fresenius, W. *et al., Fresenius' Z. Anal. Chem.*, 1965, **209**, 340 (*detn, Fe*)
Schilt, A.A. *et al., Analytical Applications of 1,10-Phenanthroline and Related Compounds*, Pergamon, London, 1969, (*use*)
Nordén, B. *et al., Acta Chem. Scand.*, 1972, **26**, 429 (*spectra*)
French, W.J. *et al., Analyst (London)*, 1972, **97**, 828 (*detn, Fe*)
Org. Synth., Coll. Vol., 5, 1973, 102
Keats, N.G. *et al., J. Het. Chem.*, 1976, **13**, 369 (*ms*)
Guziec, F.S. *et al., Synthesis*, 1980, 691 (*chlorochromate, synth, use*)
Cheng, K.L. *et al., Handbook of Organic Analytical Reagents*, CRC Press, Boca Raton, 1982, 309 (*use*)
Wenkert, D. *et al., J.O.C.*, 1983, **48**, 283 (*oxides*)
Moran, D.B. *et al., J. Het. Chem.*, 1986, **23**, 1071 (*monoxide*)
Almenningen, A. *et al., Acta Chem. Scand.*, 1989, **43**, 932 (*ed, struct, bibl*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 409-410 (*chlorochromate, use*)
Norrby, T. *et al., Acta Chem. Scand.*, 1998, **52**, 77-85 (*monoxide, methiodide*)
Demnitz, F.W.J. *et al., Org. Prep. Proced. Int.*, 1998, **30**, 467-469 (*monoxide*)
Vagias, C. *et al., Nat. Prod. Lett.*, 2000, **14**, 425-428 (*N,N′-di-Me, isol*)
Bowen, R.J. *et al., Acta Cryst. C*, 2004, **60**, o113-o114 (*cryst struct*)
Rajalakshmanan, E. *et al., Synth. Commun.*, 2005, **35**, 891-895 (*synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BGO500

2,3′-Bipyridine, 9CI B-110

2,3′-Dipyridyl. ***Isonicoteine***
[581-50-0]
[37275-48-2]



$C_{10}H_8N_2$ 156.187
Occurs in tobacco (*Nicotiana tabacum*) (Solanaceae) and the marine hoplonemertine *Amphiporus angulatus*. Used for extraction-photometric detn. of Cu(*II*), and for extraction of Sc. Liq. Insol. H_2O. d_{20}^4 1.14. Bp 298°. n_D^{20} 1.6223.

▶ Crustacean convulsant, but weak activity in mice. Mutagenic props. DW1755000

Perchlorate (1:2): Mp 215-216°.

Picrate: Mp 153-154°.

Dipicrate: Mp 165-168°.

Methiodide (1:2): [63095-08-9]
Cryst. (EtOH aq.). Mp 210-214° dec.

1-Oxide: [39182-27-9]
$C_{10}H_8N_2O$ 172.186
Solid. Mp 135-137°. Prepared indirectly, not obt. by direct oxidation.

1′-Oxide: [39182-28-0]
$C_{10}H_8N_2O$ 172.186
Cryst. + $1H_2O$ (Me_2CO/hexane). Mp 78°.

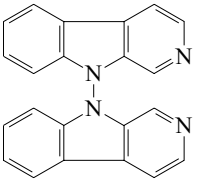
1,1′-Dioxide: [30651-23-1]
$C_{10}H_8N_2O_2$ 188.185
Cryst. (MeOH). Mp 240-243°.

[42907-60-8]

Smith, J.R. *et al., J.A.C.S.*, 1930, **52**, 397 (*synth*)
Morgan, G.T. *et al., J.C.S.*, 1932, 20 (*synth*)
Späth, E. *et al., Ber.*, 1936, **69**, 2448 (*isol*)
Talipov, S.T. *et al., Uzb. Khim. Zh.*, 1963, 22 (*detn, Cu*)
Leete, E. *et al., J.A.C.S.*, 1969, **91**, 1697 (*synth*)
Alimarin, I.P. *et al., CA*, 1973, **78**, 8393m (*sepn, Sc*)
Kem, W.R. *et al., Experientia*, 1976, **32**, 684-686 (*isol, ms, tox*)
Leete, E. *et al., J.A.C.S.*, 1976, **98**, 6326 (*biosynth*)
Moran, D.B. *et al., J. Het. Chem.*, 1986, **23**, 1071 (*oxides*)
Zoltewicz, J.A. *et al., J.O.C.*, 1992, **57**, 2392 (*deriv, synth, pmr*)
Zoltewicz, J.A. *et al., Tetrahedron*, 1995, **51**, 3103 (*1-oxide*)

9,9′-Bi-9*H*-pyrido[3,4-*b*]indole, 9CI B-111

N,N′-*Bi-β-carboline*
[85753-68-0]

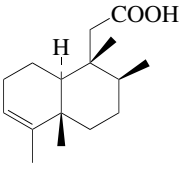


$C_{22}H_{14}N_4$ 334.379
Alkaloid from the ascidian *Didemnum* sp. Also obt. by photochemical dimerisation of β-Carboline, C-93. Needles (EtOAc/hexane).
Mp 209-210° dec.

Erra-Balsells, R. *et al., Tetrahedron*, 1983, **39**, 33-39 (*synth*)
Erra-Balsells, R. *et al., Magn. Reson. Chem.*, 1988, **26**, 1109-1112 (*cmr*)
Kearns, P.S. *et al., J. Nat. Prod.*, 1995, **58**, 1075-1076 (*isol, uv, ir, pmr, cmr, ms*)

14(4 →5),15(10 →9)-Bisabeo-3-drimene-11-carboxylic acid B-112

[193157-88-9]



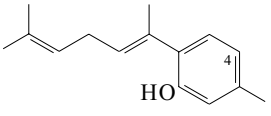
$C_{16}H_{26}O_2$ 250.38

Probably a degradation product of the Aurones, see Avarol, A-766. Constit. of a *Dysidea* sp. Oil. λ_{max} 238; 289; 319 (MeOH).

Stewart, M. *et al., Aust. J. Chem.*, 1997, **50**, 341-347 (*isol, pmr, cmr*)

1,3,5,7,10-Bisabolapentaen-1-ol B-113

2-(1,5-Dimethyl-1,4-hexadienyl)-5-methylphenol, 9CI. 7,8-Dehydrocurcuphenol



(*E*)–*form*

$C_{15}H_{20}O$ 216.322

(*E*)-*form*

Ac: [84753-68-4]
$C_{17}H_{22}O_2$ 258.36
Constit. of a *Halichondria* sp. Oil. $Bp_{0.1}$ 94°.

4-Hydroxy: ***1,3,5,7,10-Bisabolapentaene-1,4-diol***. *2-(1,5-Dimethyl-1,4-hexadienyl)-5-methyl-1,4-benzenediol, 9CI*
[84743-24-8]
$C_{15}H_{20}O_2$ 232.322
Constit. of a *Halichondria* sp. Cryst. (CH_2Cl_2/petrol).
Mp 76-77.5°.

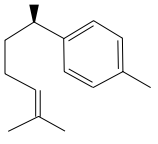
(*Z*)-*form*

4-Hydroxy: [84743-23-7]
Constit. of a *Halichondria* sp.
Oil. $Bp_{0.1}$ 160°.

Capon, R.J. *et al., Aust. J. Chem.*, 1982, **35**, 2583

1,3,5,10-Bisabolatetraene B-114

1-(1,5-Dimethyl-4-hexenyl)-4-methylbenzene, 9CI. 2-Methyl-6-(4-methylphenyl)-2-heptene. ***α-Curcumene****.* ar-*Curcumene*
[644-30-4]



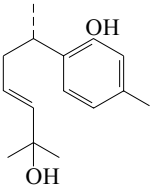
(*R*)–*form*

$C_{15}H_{22}$ 202.339
λ_{max} 254 (ε 450); 259 (ε 490); 265 (ε 530); 273 (ε 500) (EtOH) (Derep).

(*R*)-*form* [4176-17-4]
Widespread occurrence in plants e.g. *Curcuma aromatica, Ambrosia* spp. and *Amorpha fruticosa*. Also isol. from the gorgonian *Muricea elongata*.
Liq. Sol. C_6H_6, hexane; poorly sol. H_2O. Bp_{17} 137°. $[\alpha]_D$ -34.3.
λ_{max} 259; 264; 272 (MeOH) (Berdy).

(*S*)-*form* [4176-06-1]
Liq. Bp_1 105-110° (bath). $[\alpha]_D$ +40 (c, 3.3 in $CHCl_3$).
Naves, Y.-H. *et al., Bull. Soc. Chim. Fr.*, 1951, 987 (*isol*)
Honwad, V.K. *et al., Tetrahedron*, 1965, **21**, 2593 (*abs config*)
Jeffs, P.W. *et al., J. Nat. Prod.*, 1974, **37**, 315-317 (*isol, Muricea*)
Hall, S.S. *et al., J.O.C.*, 1975, **40**, 3306 (*synth*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1976, **53**, 54 (*synth*)
Tamao, K. *et al., Tet. Lett.*, 1979, 2155 (*synth*)
Nabeta, K. *et al., Agric. Biol. Chem.*, 1986, **50**, 2915 (*biosynth*)
Takano, S. *et al., Chem. Comm.*, 1988, 1539 (*synth*)
Nabeta, K. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 792 (*biosynth*)
Meyers, A.I. *et al., J.O.C.*, 1997, **62**, 5219-5221 (*synth*)
Fuganti, C. *et al., J.C.S. Perkin 1*, 1999, 279-282 (*synth*)
Hagiwara, H. *et al., J.C.S. Perkin 1*, 2002, 895-900 (*synth*)
Harmata, M. *et al., Tet. Lett.*, 2003, **44**, 7261-7264 (*synth*)
Du, Z.T. *et al., Chin. Chem. Lett.*, 2004, **15**, 1389-1391 (*synth*)

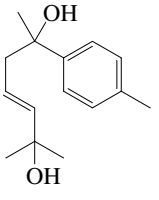
1,3,5,9-Bisabolatetraene-1,11-diol B-115



$C_{15}H_{22}O_2$ 234.338
Constit. of an *Arenochalina* sp. Pale yellow oil. $[\alpha]_D$ +19.6 (c, 1 in $CHCl_3$).

Butler, M.S. *et al., J. Nat. Prod.*, 1991, **54**, 619 (*isol, pmr, cmr*)

1,3,5,9-Bisabolatetraene-7,11-diol B-116



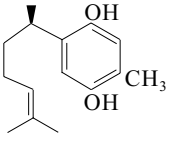
$C_{15}H_{22}O_2$ 234.338

(7ξ,9*E*,11ξ)-*form* [861394-33-4]
Constit. of *Laurencia tristicha*.
Cryst. (MeOH).
Mp 77-79°. $[\alpha]_D^{20}$ +3.6 (c, 0.09 in MeOH).

Sun, J. *et al., J. Nat. Prod.*, 2005, **68**, 915-919 (*Laurencia tristicha constit*)

1,3,5,10-Bisabolatetraene-1,4-diol B-117

2-(1,5-Dimethyl-4-hexenyl)-5-methyl-1,4-benzenediol, 9CI



$C_{15}H_{22}O_2$ 234.338

(*R*)-*form*

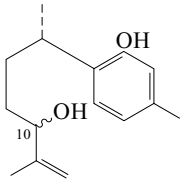
Curcuhydroquinone*. Curcuquinol*
[69301-25-3]
Constit. of *Pseudopterogorgia rigida* (gorgonian sea plume). Has antibiotic props.
Viscous oil. $[\alpha]_D$ -21 (c, 0.9 in $CHCl_3$). λ_{max} 296 (ε 3000) (MeOH) (Derep). λ_{max} 294 (ε 2240) (MeOH) (Berdy).

1-O-*(3-Methylbutanoyl):*
$C_{20}H_{30}O_3$ 318.455
Constit. of *Perezia carpholepis.* Oil. $[\alpha]_D$ -10 (c, 1 in $CHCl_3$).

1-Ac:
$C_{17}H_{24}O_3$ 276.375
Constit. of *Pseudopterogorgia americana*. Oil. $[\alpha]_D$ -3.8 (c, 0.94 in $CHCl_3$).

McEnroe, F.J. *et al., Tetrahedron*, 1978, **34**, 1661 (*isol, ir, pmr, struct*)
Sanchez, I.H. *et al., J.O.C.*, 1981, **46**, 4666 (*synth*)
Joseph-Nathan, P. *et al., Phytochemistry*, 1982, **21**, 669
Garcá, E. *et al., J. Nat. Prod.*, 1987, **50**, 1055 (*synth*)
Ono, M. *et al., Heterocycles*, 1994, **37**, 181 (*synth*)
Ono, M. *et al., Chem. Pharm. Bull.*, 1995, **43**, 553 (*synth*)
Miller, S.L. *et al., J. Nat. Prod.*, 1995, **58**, 1116 (*1-Ac*)
Kad, G.L. *et al., J. Chem. Res., Synop.*, 1999, 164-165 (*synth*)
Yoshimura, T. *et al., ARKIVOC*, 2003, **viii**, 247-255 (*synth*)
Vyvyan, J.R. *et al., J.O.C.*, 2004, **69**, 2461-2468 (*synth*)

1,3,5,11-Bisabolatetraene-1,10-diol B-118



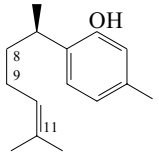
$C_{15}H_{22}O_2$ 234.338
Constit. of an *Arenochalina* sponge. Pale yellow oil. $[\alpha]_D$ -2.6 (c, 0.31 in $CHCl_3$).

10-Epimer:
$C_{15}H_{22}O_2$ 234.338
Constit. of an *Arenochalina* sp. Pale yellow oil. $[\alpha]_D$ +17.7 (c, 0.23 in $CHCl_3$).

Butler, M.S. *et al., J. Nat. Prod.*, 1991, **54**, 619-623 (*isol, pmr, cmr*)

1,3,5,10-Bisabolatetraen-1-ol B-119

2-(1,5-Dimethyl-4-hexenyl)-5-methylphenol, 9CI. ***Curcuphenol***
[17194-58-0]
[69350-75-0]



(*R*)–*form*

$C_{15}H_{22}O$ 218.338
λ_{max} 237 (ϵ 5200); 290 (ϵ 3520) (MeOH/NaOH) (Derep). λ_{max} 217 (ϵ 4690); 276 (ϵ 2400) (MeOH) (Derep).

(*R*)-*form* [69301-27-5]
Constit. of *Pseudopterogorgia rigida* and *Lasianthaea podocephala*.
Oil. $[\alpha]_D$ -7 (c, 3.65 in $CHCl_3$). $[\alpha]_D$ -23.6 ($CHCl_3$). λ_{max} 217 (ϵ 4690); 276 (ϵ 2400) (MeOH) (Berdy). λ_{max} 237 (ϵ 5200); 290 (ϵ 3520) (MeOH/NaOH) (Berdy).

Ac:
Oil. $[\alpha]_D^{24}$ -11 (c, 0.4 in $CHCl_3$).

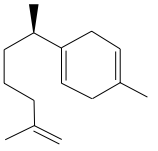
(*S*)-*form* [70878-71-6]
Constit. of the sponge *Epipolasis* sp. and of *Didiscus flavus*. H, K-ATPase inhibitor. Oil. $[\alpha]_D^{23}$ +29.1 (c, 3.13 in $CHCl_3$).

*8,9-Didehydro (*E-*): 1,3,5,8,10-Bisabolapentaen-1-ol.* ***Dehydrocurcuphenol***
[114027-43-9]
$C_{15}H_{20}O$ 216.322
Constit. of *Epipolasis* sp. H, K-ATPase inhibitor. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{23}$ -1.2 (c, 0.48 in $CHCl_3$). λ_{max} 232 (ϵ 9636); 278 (ϵ 2454) (MeOH) (Berdy).

Bohlmann, F. *et al., Chem. Ber.*, 1978, **111**, 843 (*isol*)
McEnroe, F.J. *et al., Tetrahedron*, 1978, **34**, 1661 (*isol, struct*)
Ghisalberti, E. *et al., Aust. J. Chem.*, 1979, **32**, 1627 (*isol*)
Fusetani, N. *et al., Experientia*, 1987, **43**, 1234-1235 (*isol, Dehydrocurcuphenol*)
Wright, A.E. *et al., J. Nat. Prod.*, 1987, **50**, 976 (*isol*)
Joseph-Nathan, P. *et al., J. Nat. Prod.*, 1988, **51**, 1116 (*cmr*)
Ono, M. *et al., Chem. Pharm. Bull.*, 1995, **43**, 553 (*synth*)
Ono, M. *et al., Tetrahedron: Asymmetry*, 1995, **6**, 1829 (*synth*)
Ono, M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1581-1585 (*synth*)
Kimachi, T. *et al., J.O.C.*, 2001, **66**, 2700-2704 (*synth*)
Hagiwara, H. *et al., J.C.S. Perkin 1*, 2002, 895-900 (*synth*)
Singh, V. *et al., J.C.S. Perkin 1*, 2002, 1766-1768 (*synth*)
Harmata, M. *et al., Tet. Lett.*, 2003, **44**, 7261-7264 (*synth*)
Du, Z.-T. *et al., J. Chin. Chem. Soc. (Taipei)*, 2004, **51**, 571-574 (*synth*)
Vyvyan, J.R. *et al., J.O.C.*, 2004, **69**, 2461-2468 (*synth*)
Gaspar, H. *et al., Mar. Drugs*, 2004, **2**, 8-13 (*activity*)
Kim, S.-G. *et al., Tet. Lett.*, 2005, **46**, 2437-2439 (*synth*)

2,5,11-Bisabolatriene B-120

1-(1,5-Dimethyl-5-hexenyl)-4-methyl-1,4-cyclohexadiene, 9CI. ***β-Curcumene***
[451-56-9]



(*R*)–*form*

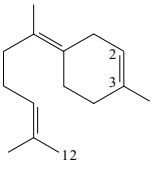
$C_{15}H_{24}$ 204.355

(*R*)-*form* [28976-67-2]
Constit. of the essential oil of *Curcuma aromatica* , *Curcuma amada* (mango-ginger), *Curcuma xanthorrhiza* (Java turmeric) and others.
Liq. Bp_{19} 142°. $[\alpha]_D$ -48.2. The abs. config is as in CA but does not appear to be explicitly stated in the lit.

(*S*)-*form*
Constit. of *Nectandra elaiophora*. $Bp_{2.2}$ 98-100°. $[\alpha]_D^{20}$ +26.7.
Naves, Y.-R. *et al., Bull. Soc. Chim. Fr.*, 1951, 987
Jain, M.K. *et al., Indian J. Chem.*, 1964, **2**, 39 (*isol*)

2,6,10-Bisabolatriene B-121

4-(1,5-Dimethyl-4-hexenylidene)-1-methylcyclohexene, 9CI. ***γ-Bisabolene****. α-Bisabolene (obsol.)†. γ-Limene*
[495-62-5]



(*E*)–*form*

$C_{15}H_{24}$ 204.355
Flavouring agent.

(*E*)-*form* [53585-13-0]
Constit. of *Ayapana amygdalina* and a *Laurencia* sp.
Oil. $[\alpha]_D^{24}$ -18.8 (c, 1 in $CHCl_3$).

2,3-Epoxide: 2,3-Epoxy-6,10-bisaboladiene. ***γ-Bisabolene-2,3-epoxide***
[75744-73-9]
$C_{15}H_{24}O$ 220.354
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D$ +37.3 (c, 2.2 in $CHCl_3$). Called γ-Bisabolene 8,9-epoxide in the reference.

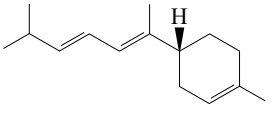
12-Hydroxy: 2,6,10-Bisabolatrien-12-ol. ***12-Hydroxy-γ-bisabolene***
$C_{15}H_{24}O$ 220.354
Isol. from a *Pseudopterogorgia* sp. Oil.

(*Z*)-*form* [13062-00-5]
Constit. of oil of myrrh and oil of lime.
Oil.

Vig, O.P. *et al., Indian J. Chem.*, 1970, **8**, 955 (*synth*)
Giraudi, E. *et al., Recherches*, 1974, **19**, 205 (*synth*)
Overton, K.H. *et al., Chem. Comm.*, 1976, 105 (*biosynth*)
Wolinsky, J.E. *et al., J.O.C.*, 1976, **41**, 697 (*struct*)
Delay, F. *et al., Helv. Chim. Acta*, 1979, **62**, 369 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **80**, 1997 (*isol*)
Suzuki, T. *et al., Chem. Lett.*, 1980, 1267 (*epoxide*)
Buss, A.D. *et al., Tet. Lett.*, 1983, **24**, 111 (*synth*)
Anastasis, P. *et al., Can. J. Chem.*, 1984, **62**, 2079 (*biosynth, bibl*)
Look, S.A. *et al., Experientia*, 1984, **40**, 931 (*12-Hydroxy-γ-bisabolene*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 617 (*synth, deriv*)
Anastasia, L. *et al., Eur. J. Org. Chem.*, 2001, 3039-3043 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 159-160 (*FEMA 3331, use*)

2,7,9-Bisabolatriene B-122

4-(1,5-Dimethyl-1,3-hexadienyl)-1-methylcyclohexene, 9CI. ***Theonelline***
[94663-92-0]

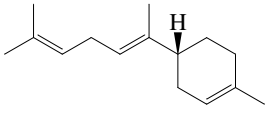


$C_{15}H_{24}$ 204.355
Constit. of the sponge *Theonella* cf. *swinhoei*. Oil. Sol. MeOH, $CHCl_3$, Me_2CO; poorly sol. H_2O. $[\alpha]_D^{25}$ +23 (c, 0.26 in hexane). λ_{max} 238 (ϵ 19000) (MeOH) (Derep). λ_{max} 238 (ϵ 19000) (MeOH) (Berdy).

Nakamura, H. *et al., Tet. Lett.*, 1984, **25**, 5401-5404 (*isol*)

2,7,10-Bisabolatriene B-123

4-(1,5-Dimethyl-1,4-hexadienyl)-1-methylcyclohexene, 9CI. ***α-Bisabolene***†. *α-Limene. FEMA 3331*
[17627-44-0]



(*R,E*)-*form*

$C_{15}H_{24}$ 204.355
Not the same as 2,6,10-Bisabolatriene, B-121 which has been renamed (formerly α-Bisabolene). The FEMA number refers to mixed bisabolenes including 2,7(14),10-Bisabolatriene, B-124 and 2,6,10-Bisabolatriene B-121. Constit. of numerous essential oils, e.g. chamomile, lemon, bergamot, calamus, etc. Flavouring ingredient used singly or as mixed isomers.

(*R,E*)-*form* [70286-31-6]
Isol. from *Halichondria* sp.
Oil. $[\alpha]_D^{20}$ +54.3 (c, 1 in EtOH).

(*R,Z*)-*form* [70286-33-8]
Oil. $[\alpha]_D^{20}$ -12 (c, 1 in EtOH).

(*S,E*)-*form* [70286-32-7]
Oil. $[\alpha]_D^{20}$ -38.9 (c, 1 in EtOH).

(*S,Z*)-*form* [58845-44-6]
Constit. of oil of Opopanax and defence secretion of termite *Amitermes wheeleri*.
Oil. Bp_{12} 155-157°. $[\alpha]_D^{20}$ +8 (c, 1 in EtOH).

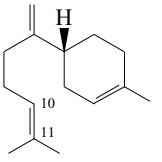
(ξ,*E*)-*form* [25532-79-0]
Constit. of *Athanasia crithmifolia*.
Oil. Abs. config. not detd., no opt. rotn. given.

[29837-07-8, 70286-16-7, 70332-15-9, 73465-96-0]

Delay, F. *et al., Helv. Chim. Acta*, 1979, **62**, 369-377 (*synth, bibl*)
Scheffrahn, R.H. *et al., J. Chem. Ecol.*, 1983, **9**, 1293-1305 (*S,Z-form, isol, pmr*)
Sullivan, B.W. *et al., J.O.C.*, 1986, **51**, 5134-5136 (*R,E-form, isol*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1987, **64**, 756-757 (*synth*)
Buss, A.D. *et al., J.C.S. Perkin 1*, 1987, 2569-2577 (*synth*)
Zdero, C. *et al., Phytochemistry*, 1991, **30**, 1161-1163 (*Athanasia constit*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 283-284 (*use, props*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 159-160 (*FEMA 3331, use*)

2,7(14),10-Bisabolatriene B-124

1-Methyl-4-(5-methyl-1-methylene-4-hexenyl)cyclohexene, 9CI. ***β-Bisabolene***. *β-Limene*
[21902-26-1]



(*R*)−*form*

$C_{15}H_{24}$ 204.355

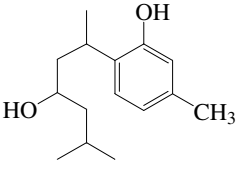
(*R*)-*form* [20377-48-4]
Isol. from *Chamaecyparis nootkatensis*, *Pinus sibirica* and defense secretions of termite *Amitermes wheeleri*, also from gorgonian *Muricea elongata*.
$[\alpha]_D$ +75. n_D^{20} 1.4879.
2β,3β-Epoxide: ***2,3-Epoxy-7(14),10-bisaboladiene***
[733766-73-9]
$C_{15}H_{24}O$ 220.354
Constit. of *Pimpinella corymbosa*. Oil. $[\alpha]_D^{25}$ +43.5 (c, 2.7 in $CHCl_3$). λ_{max} 214 (log ϵ 2.08) (EtOH).

(*S*)-*form* [495-61-4]
Constit. of the essential oils of bergamot, lemon, wild carrot, liverworts, *Artemisia capillaris*, *Psidium guajava* and many other fruits.
Oil. $Bp_{10.5}$ 129-130°. $[\alpha]_D^{20}$ -84.4.
10ξ,11ξ-Epoxide: ***10,11-Epoxy-2,7(14)-bisaboladiene***
[88861-98-7]
$C_{15}H_{24}O$ 220.354
Constit. of *Acritopappus confertus*. Oil. $Bp_{0.1}$ 120°. $[\alpha]_D^{24}$ -89 (c, 11.1 in $CHCl_3$).

Pentegova, V.A. *et al., Coll. Czech. Chem. Comm.*, 1961, **26**, 1362-1372 (*R-form, isol*)
Manjarrez, A. *et al., J.O.C.*, 1966, **31**, 348-349 (*synth*)
Andersen, N.H. *et al., Phytochemistry*, 1970, **9**, 1325-1340 (*R-form, isol*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1971, **48**, 993-999 (*synth*)
Crawford, R.J. *et al., J.A.C.S.*, 1972, **94**, 4298-4306 (*synth*)
Jeffs, P.W. *et al., J. Nat. Prod.*, 1974, **37**, 315-317 (*isol, Muricea*)
Miyazawa, M. *et al., Phytochemistry*, 1977, **16**, 1054-1057 (*S-form, occur*)
Andersen, N.H. *et al., Phytochemistry*, 1977, **16**, 1731-1751 (*S-form, occur*)
Scheffrahn, R.H. *et al., J. Chem. Ecol.*, 1983, **9**, 1293-1305 (*R-form, isol*)
Sakane, S. *et al., J.A.C.S.*, 1983, **105**, 6154-6155 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1983, **22**, 2243-2252 (*10,11-epoxide*)
Sakurai, H. *et al., Tetrahedron*, 1983, **39**, 883-894 (*synth*)
Nabeta, K. *et al., Agric. Biol. Chem.*, 1986, **50**, 2915-2916 (*biosynth*)
Nabeta, K. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 792-798 (*biosynth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 159-160 (*FEMA 3331, use*)
Tabanca, N. *et al., Planta Med.*, 2003, **69**, 933-938 (*2,3-epoxide*)

1,3,5-Bisabolatriene-1,9-diol B-125

Parahigginol A
[224176-17-4]



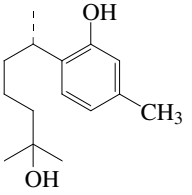
$C_{15}H_{24}O_2$ 236.353

Constit. of a *Parahigginsia* sp. Oil. $[\alpha]_D$ -4.8 (c, 0.075 in $CHCl_3$). λ_{max} 218 (log ϵ 3.4); 276 (log ϵ 3) (MeOH).

9-Ac: 9-Acetoxy-1,3,5-bisabolatrien-1-ol. ***Parahigginol C***
[224176-19-6]
$C_{17}H_{26}O_3$ 278.391
Constit. of a *Parahigginsia* sp. Oil. $[\alpha]_D$ -9.5 (c, 2.1 in $CHCl_3$). λ_{max} 219 (log ϵ 3.8); 278 (log ϵ 3.4); 284 (log ϵ 3.4) (MeOH).
Chen, C.-Y. *et al., J. Nat. Prod.*, 1999, **62**, 573-576 (*isol, pmr, cmr*)

1,3,5-Bisabolatriene-1,11-diol B-126

Curcudiol. *10,11-Dihydro-11-hydroxycurcuphenol*
[109028-15-1]

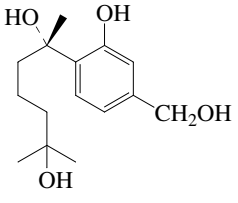


$C_{15}H_{24}O_2$ 236.353
Constit. of the sponges *Didiscus flavus* and an *Epipolasis* sp. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{22}$ +9.2 (c, 10.8 in $CHCl_3$). λ_{max} 278 (ϵ 2033) (EtOH) (Berdy). λ_{max} 240 (ϵ 10476); 290 (ϵ 6349) (MeOH-EtOH) (Berdy).

Wright, A.E. *et al., J. Nat. Prod.*, 1987, **50**, 976
Ono, M. *et al., Tetrahedron: Asymmetry*, 1995, **6**, 1829 (*synth*)
Ono, M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1581-1585 (*synth*)
Gaspar, H. *et al., Mar. Drugs*, 2004, **2**, 8-13 (*activity*)

1,3,5-Bisabolatriene-1,7,11,15-tetrol B-127

Curcutetraol

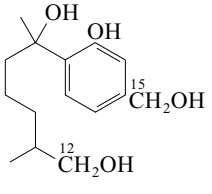


$C_{15}H_{24}O_4$ 268.352

(S)-form [848645-02-3]
Constit. of bacterium CNH-741 isol. from a marine sediment. Oil. $[\alpha]_D^{20}$ +5.24 (c, 7.4 in MeOH). λ_{max} 219 (ϵ 13534); 278 (ϵ 7490) (MeOH).
Mülhaupt, T. *et al., Eur. J. Org. Chem.*, 2005, 334-341 (*Curcutetraol*)

1,3,5-Bisabolatriene-1,7,12,15-tetrol B-128

Waraterpol
[150624-45-6]



$C_{15}H_{24}O_4$ 268.352

Prod. by *Penicillium* sp. FH-A6260. Antibacterial and antifungal agent. Sol. MeOH, Me_2CO, EtOAc, $CHCl_3$, Py; poorly sol. H_2O. $[\alpha]_D^{20}$ +6.7 (c, 1.5 in MeOH). λ_{max} 205 (ϵ 12850); 219; 278 (ϵ 2850) (MeOH) (Berdy). λ_{max} 216 (ϵ 9250); 244 (ϵ 5800); 294 (ϵ 3650) (MeOH/NaOH) (Berdy).

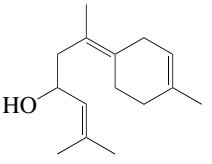
12-Ac: ***12-O-Acetylwaraterpol***
[150370-77-7]
$C_{17}H_{26}O_5$ 310.389
Prod. by *Penicillium* sp. FH-A6260.
$[\alpha]_D^{20}$ +1.9 (c, 1.3 in $CHCl_3$).

15-Ac: ***15-O-Acetylwaraterpol***
[150370-78-8]
$C_{17}H_{26}O_5$ 310.389
Prod. by *Penicillium* sp. FH-A6260.
$[\alpha]_D^{20}$ +14.5 (c, 0.31 in $CHCl_3$).

12-Carboxylic acid: 1,7,15-Trihydroxy-1,3,5-bisabolatrien-12-oic acid
$C_{15}H_{22}O_5$ 282.336

12-Carboxylic acid, amide: ***Curcutriolamide***
[848645-03-4]
$C_{15}H_{23}NO_4$ 281.351
Constit. of fungus CNC-979 isol. from a marine sediment. Oil. $[\alpha]_D^{20}$ -3.8 (c, 0.3 in MeOH). λ_{max} 203 (ϵ 138523); 282 (ϵ 18014) (MeOH).
Henne, P. *et al., Annalen*, 1993, 565
Mülhaupt, T. *et al., Eur. J. Org. Chem.*, 2005, 334-341 (*Curcutriolamide*)

2,6,10-Bisabolatrien-9-ol B-129

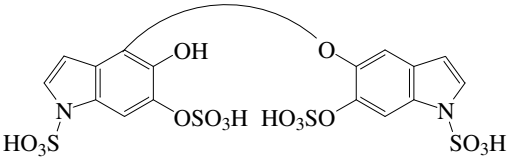


$C_{15}H_{24}O$ 220.354

(E)-form
Ac: 9-Acetoxy-γ-bisabolene
[195823-86-0]
$C_{17}H_{26}O_2$ 262.391
Constit. of *Laurencia rigida*. Oil. $[\alpha]_D^{25}$ +1 (c, 0.56 in $CHCl_3$).
König, G.M. *et al., J. Nat. Prod.*, 1997, **60**, 967-970 (*isol, pmr, cmr*)

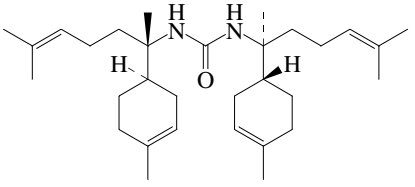
Bisancorinolate B B-130

[471913-82-3]



$C_{16}H_{12}N_2O_{16}S_4$ 616.539
Alkaloid from the sponge *Ancorina* sp. Powder (as tetra-Na salt). CAS no. refers to tetra Na salt. λ_{max} 221 (log ϵ 4.53); 268 (log ϵ 4.07); 301 (log ϵ 3.82) (MeOH) (tetra-Na salt).
Meragelman, K.M. *et al., J.O.C.*, 2002, **67**, 6671-6677 (*isol, pmr, cmr, ms*)

N,N′-Bis(2,10-bisaboladien-7-yl)urea B-131



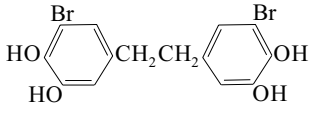
Absolute Configuration

$C_{31}H_{52}N_2O$ 468.765

(6*R*,6′*R*,7*S*,7′*S*)-*form* [105281-45-6]
Isol. from a *Halichondria* sp.
Mp 139-141°. $[\alpha]_D^{20}$ +44 (c, 1.1 in $CHCl_3$).
Sullivan, B.W. *et al., J.O.C.*, 1986, **51**, 5134-5136 (*isol, pmr, cmr*)

1,2-Bis(3-bromo-4,5-dihydroxyphenyl)ethane B-132

4,4′-(1,2-Ethanediylbis[6-bromo-1,2-benzenediol]), 9CI. 3,3′-Dibromo-4,4′,5,5′-tetrahydroxybibenzyl
[60484-69-7]

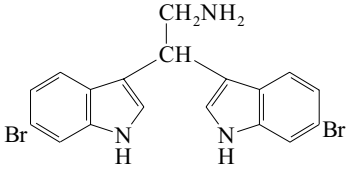


$C_{14}H_{12}Br_2O_4$ 404.054
Isol. from *Polysiphonia urceolata*. Cryst. (C_6H_6/MeOH).
Mp 205-206°.

Kurata, K. *et al., Chem. Lett.*, 1976, 821 (*isol*)

2,2-Bis(6-bromo-3-indolyl)ethylamine B-133

*6-Bromo-β-(6-bromo-1*H*-indol-3-yl)-1*H*-indole-3-ethanamine, 9CI*
[135077-20-2]

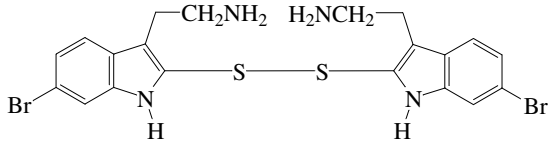


$C_{18}H_{15}Br_2N_3$ 433.145
Alkaloid from the marine tunicate *Didemnum candidum*. Also isol. from the deep-water New Caledonian sponge *Orina* sp. Pale yellow oil.

Fahy, E. *et al., J. Nat. Prod.*, 1991, **54**, 564-569 (*isol, uv, ir, pmr, cmr, ms, struct*)
Bifulco, G. *et al., J. Nat. Prod.*, 1995, **58**, 1254-1260 (*isol*)

Bis(6-bromo-2-tryptaminyl) disulfide B-134

*Bis[3-(2-aminoethyl)-6-bromo-1*H*-indol-2-yl] disulfide*

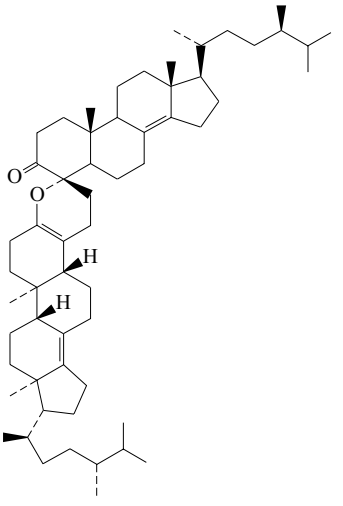


$C_{20}H_{20}Br_2N_4S_2$ 540.345
Alkaloid from the marine snail *Calliostoma canaliculatum*. Potassium channel agonist. Neurotoxin.

Kelley, W.P. *et al., J. Biol. Chem.*, 2003, **278**, 34934-34942 (*isol, pmr, cmr, ms, activity*)
Wolters, A.M. *et al., J. Nat. Prod.*, 2005, **68**, 162-167 (*pmr, anal*)

Bisconicasterone B-135

[154277-93-7]

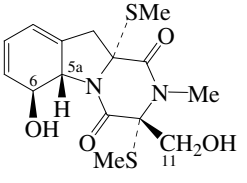


$C_{58}H_{92}O_2$ 821.364
Constit. of *Theonella swinhoei*. Cryst.
Mp 213-216°.

Inouye, Y. *et al., Chem. Lett.*, 1994, 419-420 (*isol, pmr, cmr*)

Bisdethiobis(methylthio)gliotoxin B-136

*2,3,5*a*,6,10,10*a*-Hexahydro-6-hydroxy-3-(hydroxymethyl)-2-methyl-3,10*a*-bis(methylthio)pyrazino[1,2-*a*]indole-1,4-dione, 9CI. FR 49175. Antibiotic FR 49175*
[74149-38-5]



$C_{15}H_{20}N_2O_4S_2$ 356.466
Related to Gliotoxin, G-94. Prod. by *Gliocladium deliquescens* and marine-derived *Aspergillus fumigatus* and *Pseudallescheria* sp. (MFB165). Inhibits PAF induced platelet aggregation. Antibacterial agent. Powder. $[\alpha]_D^{20}$ -51 (c, 1 in MeOH).
▶ LD_{50} (mus, ipr) 500-1500 mg/kg.

*5*a*,6-Didehydro:* ***5*a*,6-Dehydrobisdethiobis(methylthio)gliotoxin***. *Bisdethiobis(methylthio)dehydrogliotoxin*
[74149-39-6]
$C_{15}H_{18}N_2O_4S_2$ 354.45
Prod. by *Gliocladium deliquescens*. Yellow gum.

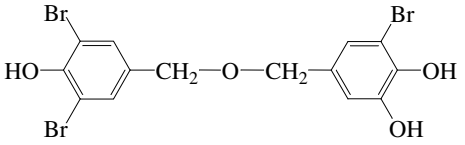
11-Deoxy: ***Deoxybisdethiobis(methylthio)gliotoxin***
$C_{15}H_{20}N_2O_3S_2$ 340.467
Prod. by a marine-derived *Pseudallescheria* sp. (MFB165). Antibacterial agent. Oil. $[\alpha]_D$ -48 (c, 0.3 in MeOH). λ_{max} 271 (log ϵ 4.25) (MeOH).

Kirby, G.W. *et al., J.C.S. Perkin 1*, 1980, 119-121 (*isol, synth, pmr*)
Hanson, J.R. *et al., J.C.S. Perkin 1*, 1981, 218-220 (*didehydro*)
Okamoto, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 340-344 (*isol, pmr, activity*)
Yoshida, K. *et al., Prog. Biochem. Pharmacol.*, 1988, **22**, 66 (*rev, pharmacol*)
Afiyatullov, S.S. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 236-238 (*marine isol, pmr, cmr*)
Li, X. *et al., J. Antibiot.*, 2006, **59**, 248-250 (*marine, isol*)

Bis(3,5-dibromo-4-hydroxybenzyl) ether **B-137**

4,4′-[Oxybis(methylene)]bis[2,6-dibromophenol], 9CI. 3,3′,5,5′-Tetrabromo-4,4′-dihydroxydibenzyl ether

[135658-97-8]



$C_{14}H_{10}Br_4O_3$ 545.847

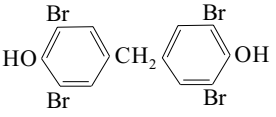
Constit. of *Thelepus cincinnatus, Thelepus extensus* and *Thelepus setosus.*

Goerke, H. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **99**, 203-206 (*isol*)

Bis(3,5-dibromo-4-hydroxyphenyl)methane **B-138**

4,4′-Methylenebis(2,6-dibromophenol), 9CI. 3,3′,5,5′-Tetrabromo-4,4′-dihydroxydiphenylmethane

[21825-03-6]



$C_{13}H_8Br_4O_2$ 515.821

Constit. of *Thelepus setosus.* Cryst. (C_6H_6).

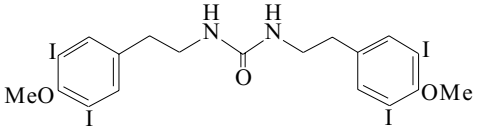
Mp 230-232°.

Higa, T. *et al., J.A.C.S.*, 1974, **96**, 2246 (*isol*)

Higa, T. *et al., Tetrahedron*, 1975, **31**, 2379 (*ir, uv, nmr*)

***N,N′*-Bis[2-(3,5-diiodo-4-methoxyphenyl)ethyl]urea, 9CI** **B-139**

[89631-87-8]



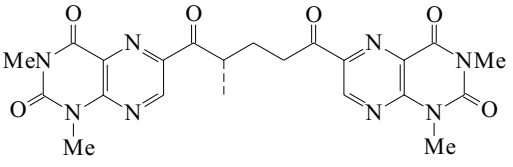
$C_{19}H_{20}I_4N_2O_3$ 831.997

Minor metab. from an unidentified didemnid tunicate *Didemnum* sp.

Mp 224-225°.

Sesin, D.F. *et al., Tet. Lett.*, 1984, **25**, 403-404 (*pmr, cmr, struct*)

1,5-Bis(1,3-dimethyl-6-lumazinyl)-2-methyl-1,5-pentanedione **B-140**



$C_{22}H_{22}N_8O_6$ 494.466

(*S*)-*form* [173324-68-0]

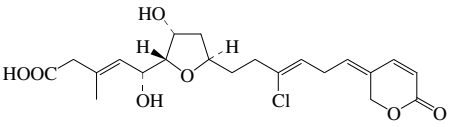
Metab. from the marine polychaete *Odontosyllis undecimdonta*.

Solid (MeOH).

Mp 114-115°. $[\alpha]_D^{25}$ -61.9 (c, 0.21 in $CHCl_3$).

Tanino, H. *et al., Heterocycles*, 1996, **42**, 125-128 (*isol, uv, ir, pmr, ms, synth, struct*)

Biselide E **B-142**



Absolute Configuration

$C_{21}H_{27}ClO_7$ 426.893

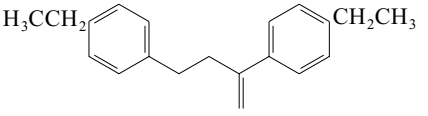
Constit. of a *Didemnum* sp. Oil.

Teruya, T. *et al., Tetrahedron*, 2005, **61**, 6561-6567 (*isol, pmr, cmr*)

2,4-Bis(4-ethylphenyl)-1-butene **B-143**

1,1′-(1-Methylene-1,3-propanediyl)bis[4-ethylbenzene], 9CI

[156251-84-2]



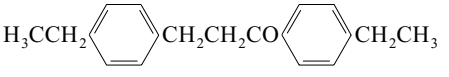
$C_{20}H_{24}$ 264.41

Constit. of the starfish *Pteraster militaris.*

Yayli, N. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 556 (*isol, pmr, cmr*)

1,3-Bis(4-ethylphenyl)-1-propanone **B-144**

[156251-85-3]



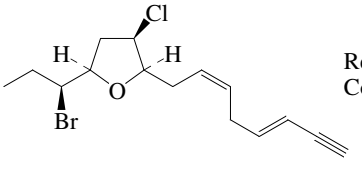
$C_{19}H_{22}O$ 266.382

Constit. of the starfish *Pteraster militaris.*

Yayli, N. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 556 (*isol*)

Bisezakyne A **B-145**

13-Bromo-10-chloro-9,12-epoxy-3,6-pentadecadien-1-yne



Relative Configuration

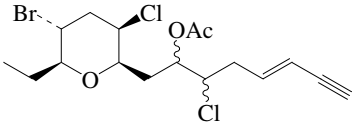
$C_{15}H_{20}BrClO$ 331.679

Constit. of a *Laurencia* sp. Oil. $[\alpha]_D^{22}$ -71.3 (c, 0.33 in $CHCl_3$). λ_{max} 228 (ϵ 14400) (EtOH).

Suzuki, M. *et al., Phytochemistry*, 1999, **51**, 657-662 (*isol, uv, ir, pmr, cmr, ms*)

Bisezakyne B **B-146**

7-Acetoxy-12-bromo-6,10-dichloro-9,13-epoxy-3-pentadecen-1-yne



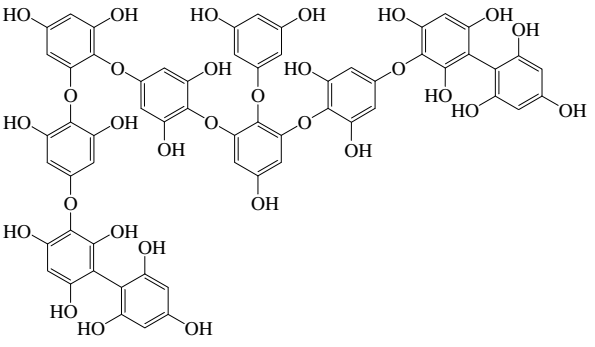
$C_{17}H_{23}BrCl_2O_3$ 426.176

Constit. of a *Laurencia* sp.

Mp 69-70°. $[\alpha]_D^{22}$ -45.1 (c, 0.27 in $CHCl_3$). λ_{max} 223 (ϵ 14440) (EtOH).

Suzuki, M. *et al., Phytochemistry*, 1999, **51**, 657-662 (*isol, uv, ir, pmr, cmr, ms*)

Bisfucoheptaphlorethol A B-147

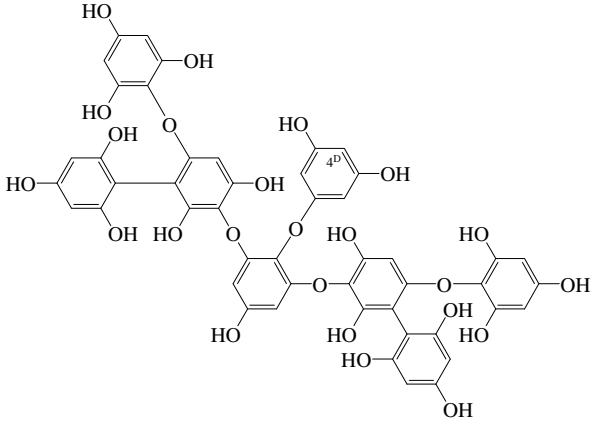


$C_{60}H_{42}O_{30}$ 1242.974
Isol. from brown alga *Cystophora retroflexa*.

Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol, pmr, cmr, ms*)

Bisfucopentaphlorethol A B-148

[88524-53-2]



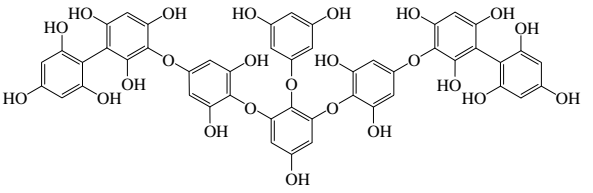
$C_{48}H_{34}O_{24}$ 994.782
Constit. of *Himanthalia elongata*, *Cystophora torulosa* and *Cystophora retroflexa*. Isol. as per-Ac, to which CAS no. refers.

4^D-Chloro: ***Chlorobisfucopentaphlorethol A***
[202211-26-5]
$C_{48}H_{33}ClO_{24}$ 1029.227
Isol. from *Sargassum spinuligerum*. Isol. as per-Ac, to which CAS no. refers.

4^D-Hydroxy: ***Hydroxybisfucopentaphlorethol A***
[199857-67-5]
$C_{48}H_{34}O_{25}$ 1010.782
Isol. from *Cystophora torulosa*. Isol. as per-Ac, to which CAS no. refers.

Grosse-Damhues, J. *et al., Phytochemistry*, 1983, **22**, 2043 (*Bisfucopentaphlorethol A, isol, struct*)
Glombitza, K.W. *et al., Planta Med.*, 1985, **50**, 42-46 (*isol, struct*)
Glombitza, K.W. *et al., Phytochemistry*, 1997, **46**, 735-740 (*Hydroxybisfucopentaphlorethol A*)
Glombitza, K.W. *et al., Phytochemistry*, 1997, **46**, 1417-1422 (*Chlorobisfucopentaphlorethol A*)
Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol*)

Bisfucopentaphlorethol B B-149

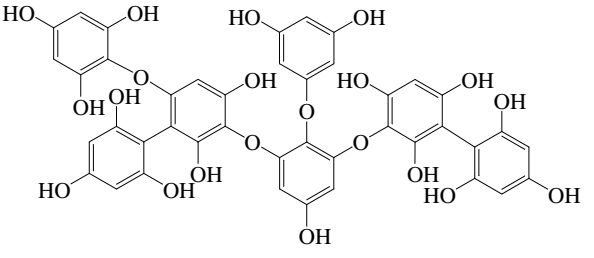


$C_{48}H_{34}O_{24}$ 994.782
Isol. from *Cystophora retroflexa* and *Cystophora torulosa*.

Glombitza, K.W. *et al., Phytochemistry*, 1997, **46**, 1417-1422 (*isol, pmr, ms*)
Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol*)

Bisfucotetraphlorethol A B-150

[96738-80-6]

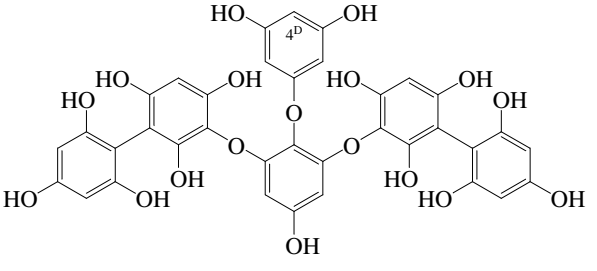


$C_{42}H_{30}O_{21}$ 870.686
Isol. from *Cystophora retroflexa*, *Cystophora torulosa* and *Himanthalia elongata*. Identified as per-Ac, to which CAS no. refers.

Glombitza, K.W. *et al., Planta Med.*, 1985, **50**, 42-46 (*isol, struct*)
Glombitza, K.W. *et al., Phytochemistry*, 1997, **46**, 735-740; 1999, **50**, 869-881 (*isol*)

Bisfucotriphlorethol A B-151

[79003-53-5]

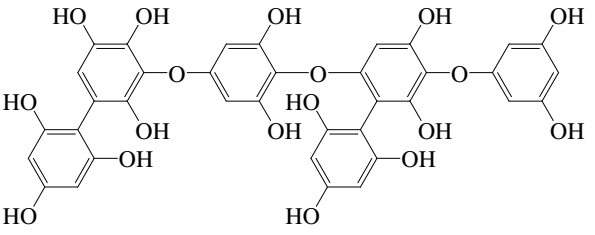


$C_{36}H_{26}O_{18}$ 746.591
Isol. from *Cystophora retroflexa*, *Cystoseira baccata*, *Carpophyllum maschalocarpum*, *Carpophyllum angustifolium*, *Sargassum spinuligerum* and *Himanthalia elongata*. Isol. as per-Ac, to which CAS no. refers.

4^D-Hydroxy: ***Hydroxybisfucotriphlorethol A***
$C_{36}H_{26}O_{19}$ 762.59
Isol. from *Sargassum spinuligerum*.

Glombitza, K.W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1981, **314**, 602-608 (*isol, struct*)
Glombitza, K.W. *et al., Phytochemistry*, 1991, **30**, 3423-3427; 1997, **46**, 735-740; 1999, **50**, 869-881 (*isol, pmr, ms*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

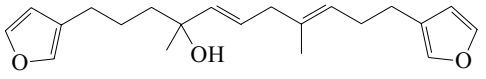
Bisfucotriphlorethol B B-152



$C_{36}H_{26}O_{18}$ 746.591
Isol. from brown alga *Cystophora torulosa*.

Glombitza, K.W. *et al., Phytochemistry*, 1997, **46**, 735-740

1,11-Bis(3-furanyl)-4,8-dimethyl-5,8-undecadien-4-ol B-153



$C_{21}H_{28}O_3$ 328.45

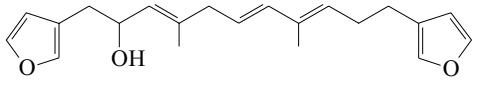
Me ether: 1,11-Bis(3-furanyl)-8-methoxy-4,8-dimethyl-3,6-undecadiene
$C_{22}H_{30}O_3$ 342.477
Constit. of *Fasciospongia cavernosa*. Oil. $[\alpha]_D^{28}$ +12 (c, 0.3 in $CHCl_3$).

[141631-72-3, 141631-89-2]

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 599 (*isol, pmr, cmr*)

1,11-Bis(3-furanyl)-4,8-dimethyl-3,6,8-undecatrien-2-ol B-154

α-[9-(3-Furanyl)-2,6-dimethyl-1,4,6-nonatrienyl]-3-furanethanol, 9CI

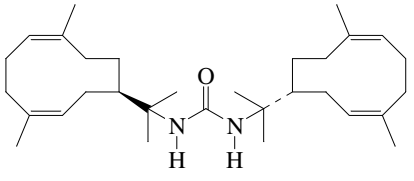


$C_{21}H_{26}O_3$ 326.435

Ac: 2-Acetoxy-1,11-bis(3-furanyl)-4,8-dimethyl-3,6,8-undecatriene
[97530-63-7]
$C_{23}H_{28}O_4$ 368.472
Constit. of nudibranch *Dendrodoris grandiflora*.
$[\alpha]_D$ +12.8 (c, 0.24 in $CHCl_3$).

Cimino, G. *et al., Tetrahedron*, 1985, **41**, 1093

N,N′-Bis[1(10),4-germacradien-11-yl]urea B-155



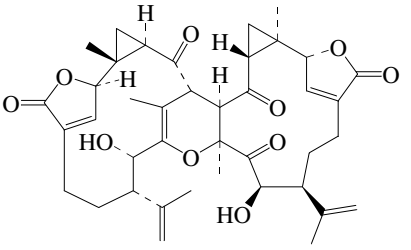
$C_{31}H_{52}N_2O$ 468.765

(1(10)Z,1′(10′)Z,4Z,4′Z)-form [674817-54-0]
Constit. of *Axinyssa* sp.
Cryst. $[\alpha]_D^{25}$ +32.5 (c, 0.2 in $CHCl_3$).

Satitpatipan, V. *et al., J. Nat. Prod.*, 2004, **67**, 503-505 (*isol, pmr, cmr*)

Bisgersolanolide B-156

[240121-10-2]

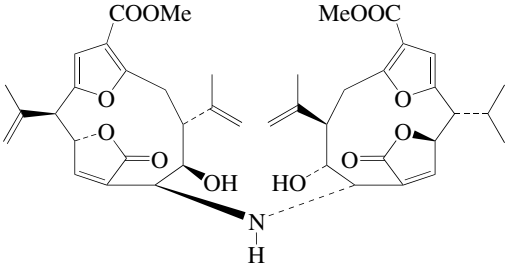


$C_{40}H_{48}O_{10}$ 688.813
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 187-188°. $[\alpha]_D^{24}$ +8.4 (c, 1.3 in $CHCl_3$). λ_{max} 210 (ϵ 51600) (MeOH).

Rodríguez, A.D. *et al., Org. Lett.*, 1999, **1**, 337-340 (*isol, pmr, cmr*)

Bis(gorgiacerol)amine B-157

[138828-03-2]



$C_{42}H_{47}NO_{12}$ 757.833
Constit. of *Pseudopterogorgia acerosa*. Cryst.
Mp 248-249°. $[\alpha]_D$ +40 (c, 0.3 in $CHCl_3$).

Tinto, W.F. *et al., Tetrahedron*, 1991, **47**, 8679-8686 (*isol, pmr, cmr*)

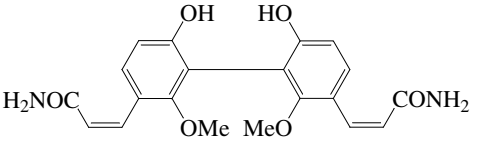
Bis(1-hydroxyethyl) peroxide B-158

1,1′-Dioxybisethanol, 9CI. ***Mozukutoxin B***
[77573-56-9]
$H_3CCH(OH)–O–O–CH(OH)CH_3$
$C_4H_{10}O_4$ 122.121
Isol. from *Sphaerotrichia divarica* and *Cladosiphon okamuranus.*

Fusetani, N. *et al., Nippon Suisan Gakkaishi*, 1981, **47**, 1059-1063; *CA*, **96**, 33523h (*isol, synth*)

3,3′-Bis-3-[(4-hydroxy-2-methoxyphenyl)-2-propenamide] B-159

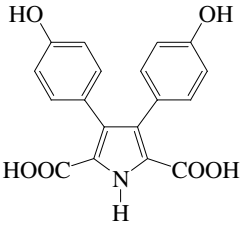
3,3′-(6,6′-Dihydroxy-2,2′-dimethoxy-[1,1′-biphenyl]-3,3′-diyl)-bis[2-propenamide], 9CI. 4,4′-Dihydroxy-2,2′-dimethoxy-3,3′-dicinnamide



$C_{20}H_{20}N_2O_6$ 384.388

(Z,Z)-form [203524-81-6]
Constit. of *Sinularia flexibilis*.
Anjaneyulu, A.S.R. *et al., Nat. Prod. Lett.*, 1997, **11**, 5-11 (*isol*)

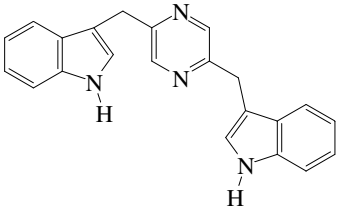
3,4-Bis(4-hydroxyphenyl)-1*H*-pyrrole-2,5-dicarboxylic acid **B-160**



$C_{18}H_{13}NO_6$ 339.304
Prod. by the marine-derived *Halomonas* sp. RK377. Amorph. solid.
Mp 213° dec. λ_{max} 249 (log ϵ 4.27) (MeOH). λ_{max} 252 (log ϵ 4.27) (MeOH/HCl). λ_{max} 251 (log ϵ 4.28) (MeOH/NaOH).

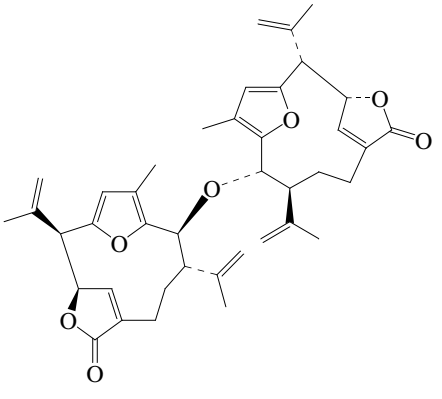
*4′-Deoxy: 3-(4-Hydroxyphenyl)-4-phenyl-1*H*-pyrrole-2,5-dicarboxylic acid*
$C_{18}H_{13}NO_5$ 323.304
Prod. by *Halomonas* sp. RK377. Amorph. solid.
Mp 213° dec. λ_{max} 245 (log ϵ 4.26) (MeOH). λ_{max} 243 (log ϵ 4.26) (MeOH/HCl). λ_{max} 249 (log ϵ 4.27) (MeOH/NaOH).
Liang, L. *et al., Dissertation*, Univ. of Göttingen, 2003, (*isol, uv, pmr, cmr, ms, cryst struct*)

2,5-Bis(1*H*-indol-3-ylmethyl)pyrazine **B-161**



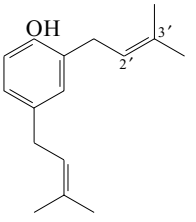
$C_{22}H_{18}N_4$ 338.411
Prod. by *Cytophaga marinoflava* sp. strain AM13.1.
Shaaban, M. *et al., J. Nat. Prod.*, 2002, **65**, 1660-1663 (*isol, pmr, cmr, ms*)

Biskallolide A **B-162**
[275355-75-4]



$C_{40}H_{46}O_7$ 638.799
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 248-266° dec. $[\alpha]_D^{24}$ +88 (c, 0.5 in $CHCl_3$). λ_{max} 220 (ϵ 6400) (MeOH).
Rodríguez, A.D. *et al., J.O.C.*, 2000, **65**, 3192-3199 (*isol, pmr, cmr, synth*)

2,4-Bis(3-methyl-2-butenyl)phenol **B-163**
2,4-Diprenylphenol
[55824-31-2]



$C_{16}H_{22}O$ 230.349
Constit. of *Perithalia caudata*. Also from *Encyothalia cliftonii*. Feeding deterrent. Oil. λ_{max} 280 (ϵ 3300) (MeOH) (Berdy). λ_{max} 297 (MeOH-NaOH) (Berdy).

2′,3′-Dihydro, 3′-hydroxy: ***2-(3-Hydroxy-3-methylbutyl)-4-(3-methyl-2-butenyl)phenol***. *2-(3-Hydroxy-3-methylbutyl)-4-prenylphenol*
[151455-16-2]
$C_{16}H_{24}O_2$ 248.364
Metab. of *Encyothalia cliftonii*. Viscous oil.
Kyogoku, K. *et al., Agric. Biol. Chem.*, 1975, **39**, 133 (*synth*)
Yamada, S. *et al., Synth. Commun.*, 1975, **5**, 181 (*synth*)
Blackmann, A.J. *et al., Phytochemistry*, 1988, **27**, 3686 (*isol*)
Roussis, V. *et al., Phytochemistry*, 1993, **34**, 107-111 (*Encyothalia cliftonii constits*)

Bis(3-oxoundecyl) disulfide **B-164**
1,1′-Dithiodi-3-undecanone, 8CI
[33796-37-1]
$H_3C(CH_2)_7COCH_2CH_2SSCH_2CH_2CO(CH_2)_7CH_3$
$C_{22}H_{42}O_2S_2$ 402.705
Constit. of *Dictyopteris plagiogramma*. Cryst.
Mp 67-67.5°.
Roller, P. *et al., Chem. Comm.*, 1971, 503

Bis(3-oxoundecyl) tetrasulfide **B-165**
1,1′-Tetrathiobis-3-undecanone, 9CI
[34852-29-4]
$H_3C(CH_2)_7COCH_2CH_2SSSSCH_2CH_2CO(CH_2)_7CH_3$
$C_{22}H_{42}O_2S_4$ 466.837
Constit. of *Dictyopteris plagiogramma* and *Dictyopteris australis*.
Mp 32-33°.
Moore, R.E. *et al., Chem. Comm.*, 1971, 1168

Bis(3-oxoundecyl) trisulfide **B-166**
1,1′-Trithiobis-3-undecanone, 9CI
[34852-28-3]
$H_3C(CH_2)_7COCH_2CH_2SSSCH_2CH_2CO(CH_2)_7CH_3$
$C_{22}H_{42}O_2S_3$ 434.771
Constit. of *Dictyopteris plagiogramma* and *Dictyopteris australis*.
Needles (MeOH).
Mp 60.5-61°.
Moore, R.E. *et al., Chem. Comm.*, 1971, 1168

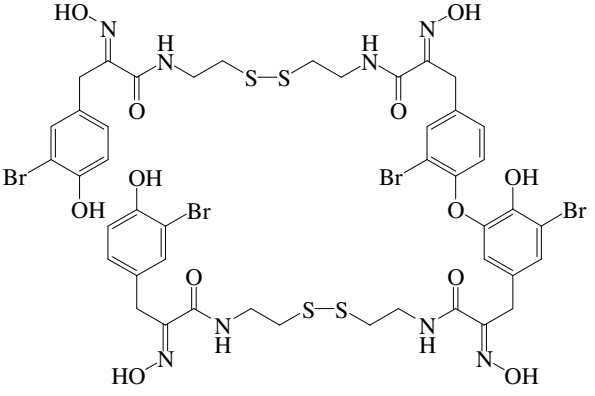
***N*,*N*′-Bis(2-phenylethyl)urea, 9CI** **B-167**
N,N′-Diphenethylurea. AM 2498. Metabolite AM 2498
[5467-84-5]
$PhCH_2CH_2NHCONHCH_2CH_2Ph$
$C_{17}H_{20}N_2O$ 268.358

Metab. from the marine ascidian *Didemnum ternatanum*. Also isol. from a *Streptomyces* sp. strain No. AM-2498. Weak depressant lacking acute toxicity. Needles (MeOH). Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 138-141° (135°). λ_{max} 248 (ϵ 308); 251 (ϵ 411); 253 (ϵ 446); 256 (ϵ 535); 259 (ϵ 549); 262 (ϵ 543); 265 (ϵ 419); 269 (ϵ 351) (MeOH) (Derep).

▶ YS2768000

Iwai, Y. *et al., J. Antibiot.*, 1978, **31**, 375 (*isol, uv, ir, pmr, cmr, struct*)
Ireland, C.M. *et al., J. Nat. Prod.*, 1981, **44**, 360 (*isol, ir, pmr, cmr, ms, synth*)

Bispsammaplin A B-168

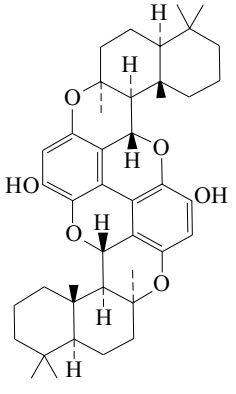


$C_{44}H_{46}Br_4N_8O_{12}S_4$ 1326.774
Isol. from an association of the sponges *Jaspis wondoensis* and *Poecillastra wondoensis*. Yellow oil. $[\alpha]_D^{23}$ -3 (c, 0.21 in MeOH).

Park, Y. *et al., J. Nat. Prod.*, 2003, **66**, 1495-1498 (*isol, pmr, cmr*)

Bispuupehenone B-169

[87734-70-1]

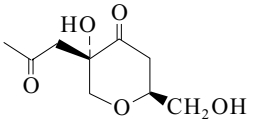


$C_{42}H_{54}O_6$ 654.885
Constit. of *Hyrtios eubamma*. Immunomodulatory agent. Cryst. (CH_2Cl_2).
Mp 234-240°. $[\alpha]_D^{24}$ -98 (c, 2.4 in $CHCl_3$). λ_{max} 230 (ϵ 28200); 284 (ϵ 9550); 295 (ϵ 10700); 341 (ϵ 7080); 353 (sh) (ϵ 5890) (EtOH) (Derep).

Amade, P. *et al., Helv. Chim. Acta*, 1983, **66**, 1672
Urban, S. *et al., J. Nat. Prod.*, 1996, **59**, 900 (*abs config*)

Bissetone B-170

[111718-48-0]

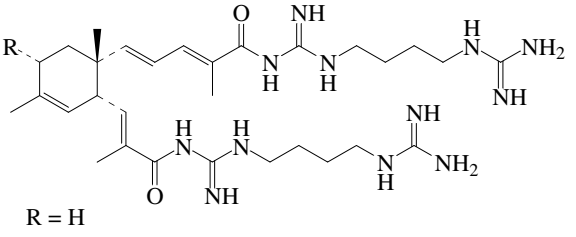


$C_9H_{14}O_5$ 202.207
Constit. of gorgonian *Briareum polyanthes*. Antimicrobial agent. Insecticide. Plant growth regulator. Oil. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D$ -43.6 (c, 4.25 in EtOH).

Cardellina, J.H. *et al., Tet. Lett.*, 1987, **28**, 727 (*cryst struct*)
Brehm, M. *et al., Angew. Chem., Int. Ed.*, 1987, **26**, 1271 (*synth*)

Bistellettadine A B-171

[233766-63-7]



R = H

$C_{30}H_{52}N_{12}O_2$ 612.82
Isol. as a salt tetraprotonated at the guanidino residues. Counterion not specified. Alkaloid from the marine sponge *Stelletta* sp.
$[\alpha]_D^{21}$ +2 (c, 0.72 in MeOH) (salt). λ_{max} 255 (ϵ 13000) (MeOH).

Tsukamoto, S. *et al., J.O.C.*, 1999, **64**, 3794-3795 (*isol, uv, pmr, cmr*)

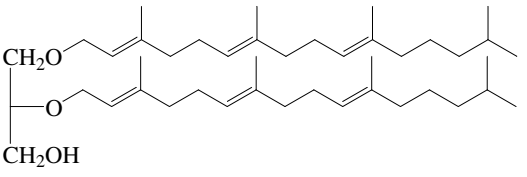
Bistellettadine B B-172

[233766-64-8]
As Bistellettadine A, B-171 with
R = $-CH_2CH{=}C(CH_3)_2$
$C_{35}H_{60}N_{12}O_2$ 680.938
Isol. as a salt tetraprotonated at the guanidino residues. Counterion not specified. Alkaloid from the marine sponge *Stelletta* sp.
$[\alpha]_D^{21}$ +3.9 (c, 0.1 in MeOH) (salt). λ_{max} 255 (ϵ 11000) (MeOH).

Tsukamoto, S. *et al., J.O.C.*, 1999, **64**, 3794-3795 (*isol, uv, pmr, cmr*)

1,2-Bis-*O*-(3,7,11,15-tetramethyl-2,6,10-hexadecatrienyl)glycerol B-173

2,3-Bis[(3,7,11,15-tetramethyl-2,6,10-hexadecatrienyl)oxy]-1-propanol. 1,2-Bis(14,15-dihydrogeranylgeranyl)glycerol
[345260-35-7]

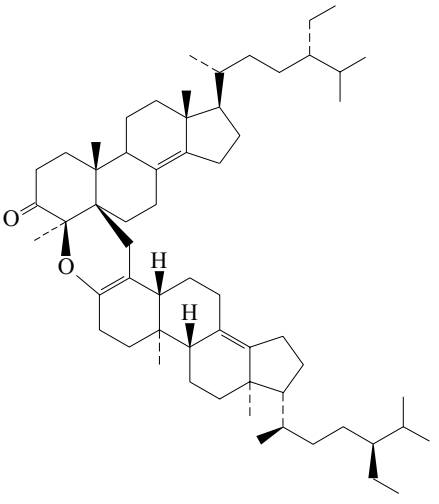


$C_{43}H_{76}O_3$ 641.072
Isol. from the archaeon *Thermococcus* S 557 collected from a deep-sea hydrothermal vent. Oil. $[\alpha]_D^{25}$ +5 (c, 0.28 in $CHCl_3$).

Gonthier, I. *et al., Tet. Lett.*, 2001, **42**, 2795-2797 (*isol, pmr, cmr*)

Bistheonellasterone B-174

[145403-26-5]

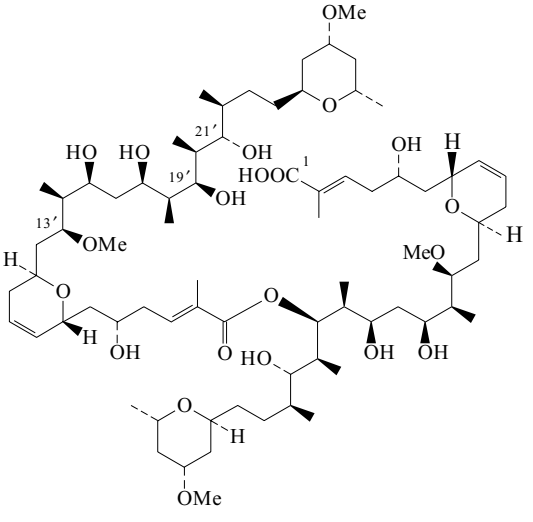


$C_{60}H_{96}O_2$ 849.417
Constit. of *Theonella swinhoei*. Powder. $[\alpha]_D^{26}$ +1.6 (c, 1.45 in $CHCl_3$).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1773-1778 (*isol, pmr, cmr*)

Bistheonellic acid A B-175

[138146-83-5]



$C_{74}H_{130}O_{21}$ 1355.828
Constit. of a *Theonella* sp. Amorph. solid. $[\alpha]_D^{20}$ -20 (c, 0.45 in $CHCl_3$). λ_{max} 232 (ϵ 6310) (MeOH) (Berdy).

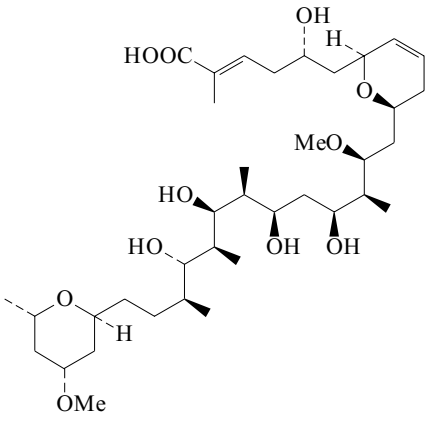
1→21′ Lactone: ***Isobistheonellide A***
[138146-82-4]
$C_{74}H_{128}O_{20}$ 1337.813
Constit. of a *Theonella* sp. Amorph. solid. $[\alpha]_D^{16}$ +43 (c, 0.13 in EtOH). λ_{max} 220 (ϵ 19950) (EtOH) (Berdy).

13′-O-De-Me, 1→19′ lactone: ***Bistheonellide C***
[138146-81-3]
$C_{73}H_{126}O_{20}$ 1323.786
Isol. from a *Theonella* sp. Amorph. solid. $[\alpha]_D^{16}$ -22 (c, 0.68 in EtOH). λ_{max} 222 (ϵ 15850) (EtOH) (Berdy).

Kobayashi, J. *et al., J.C.S. Perkin 1*, 1991, 2379 (*isol, pmr, cmr*)

Bistheonellic acid B B-176

[138146-84-6]

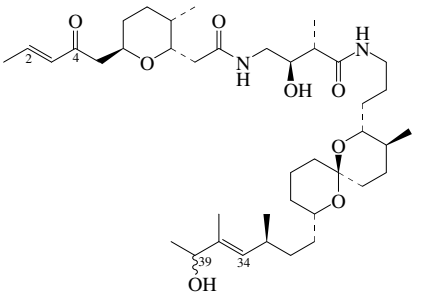


$C_{37}H_{66}O_{11}$ 686.922
Constit. of a *Theonella* sp. Amorph. solid. $[\alpha]_D^{20}$ -7.5 (c, 0.2 in $CHCl_3$). λ_{max} 218 (ϵ 5010) (MeOH) (Berdy).

Kobayashi, J. *et al., J.C.S. Perkin 1*, 1991, 2379-2383 (*isol, pmr, cmr*)

Bistramide A B-177

Bistratene A
[115566-02-4]



Absolute Configuration

$C_{40}H_{68}N_2O_8$ 704.986
Struct. revised in 1992. Isol. from *Lissoclinum bistratum*. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{20}$ +10 (c, 0.05 in CH_2Cl_2). λ_{max} 226 (ϵ 10000) (MeOH) (Derep). λ_{max} 240 (no solvent reported).

39-Ac: ***Bistratene B***
[120853-14-7]
$C_{42}H_{70}N_2O_9$ 747.023
Isol. from *Lissoclinum bistratum*. Cytotoxic agent. λ_{max} 226 (ϵ 10000) (MeOH) (Derep).

39-Ketone: ***Bistramide C***
[160568-16-1]
$C_{40}H_{66}N_2O_8$ 702.97
Isol. from *Lissoclinum bistratum*. Cytotoxic, antiparasitic and antiproliferative agent. Amorph. solid. $[\alpha]_D^{20}$ +10 (c, 0.05 in CH_2Cl_2). λ_{max} 242 (ϵ 31700) (MeOH) (Berdy).

4-Alcohol: ***Bistramide D***
[155660-91-6]
$C_{40}H_{70}N_2O_8$ 707.002
Isol. from *Lissoclinum bistratum*. Antiparasitic agent. Amorph. solid. $[\alpha]_D^{20}$ +8 (c, 0.04 in CH_2Cl_2). λ_{max} 232 (ϵ 490) (MeOH) (Berdy).

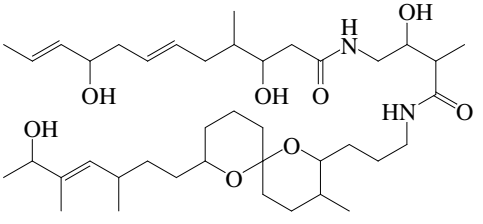
2,3-Dihydro: ***Bistramide B***
[160568-15-0]
$C_{40}H_{70}N_2O_8$ 707.002
Isol. from *Lissoclinum bistratum*. Cytotoxic agent, antiparasitic. $[\alpha]_D^{20}$ +10 (c, 0.01 in CH_2Cl_2). λ_{max} 233 (ϵ 2090) (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 30 mg/kg.

Stereoisomer (?): ***Bistramide L***
[159171-64-9]
$C_{40}H_{68}N_2O_8$ 704.986
Isol. from *Lissoclinum bistratum*.

Gouiffes, D. *et al., Tetrahedron*, 1988, **44**, 451 (*pmr, cmr*)
Degnan, B.M. *et al., J. Med. Chem.*, 1989, **32**, 1354 (*isol*)
Dunkel, R. *et al., Anal. Chem.*, 1992, **64**, 3150 (*pmr*)
Foster, M.P. *et al., J.A.C.S.*, 1992, **114**, 1110 (*pmr, cmr, struct*)
Stanwell, C. *et al., Biochem. Pharmacol.*, 1993, **45**, 1753 (*props*)
Biard, J.F. *et al., J. Nat. Prod.*, 1994, **57**, 1336-1345 (*isol, uv, ir, pmr, cmr*)
Pat. Coop. Treaty (WIPO), 1994, 94 20 503; *CA*, **121**, 292774k (*Bistramide L*)
Wipf, P. *et al., Chem. Eur. J.*, 2002, **8**, 1670-1681 (*synth, abs config*)
Gallagher, P.O. *et al., Tet. Lett.*, 2002, **43**, 531-535 (*config*)
Statsuk, A.V. *et al., J.A.C.S.*, 2004, **126**, 9546-9547 (*synth*)
Wipf, P. *et al., Chem. Comm.*, 2005, 3421-3423 (*Bistramide C, synth*)
Zuber, G. *et al., Org. Lett.*, 2005, **7**, 5269-5272 (*Bistramide C, abs config*)
Rizvi, S.A. *et al., J.A.C.S.*, 2006, **128**, 3882-3883 (*Bistramide A-Actin complex*)
Crimmins, M.T. *et al., J.A.C.S.*, 2006, **128**, 4936-4937 (*synth*)
Bauder, C. *et al., Org. Biomol. Chem.*, 2006, **4**, 1860-1862 (*Bistramide D, cryst struct*)

Bistramide K B-178

[155660-92-7]

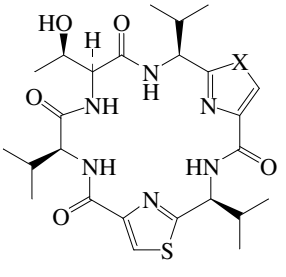


$C_{40}H_{70}N_2O_8$ 707.002
Isol. from *Lissoclinum bistratum*. Cytotoxic agent, antiparasitic. Amorph. solid. $[\alpha]_D^{20}$ +20 (c, 0.02 in CH_2Cl_2). λ_{max} 230 (no solvent reported). λ_{max} 230 (ϵ 130) (MeOH) (Berdy).

Biard, J.-F. *et al., J. Nat. Prod.*, 1994, **57**, 1336-1345

Bistratamide I B-179

[501909-64-4]



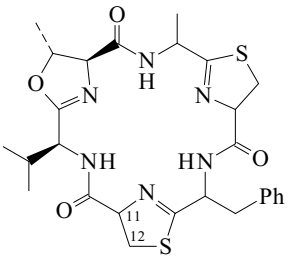
X = O

$C_{25}H_{36}N_6O_6S$ 548.662
Isol. from the ascidian *Lissoclinum bistratum*. Solid. $[\alpha]_D$ -122 (c, 0.5 in MeOH). λ_{max} 243 (sh) (MeOH).

Perez, L.J. *et al., J. Nat. Prod.*, 2003, **66**, 247-250 (*isol, pmr, cmr, ms*)
You, S.-L. *et al., Tetrahedron*, 2005, **61**, 241-249 (*synth*)

Bistratamide A B-180

[120853-13-6]



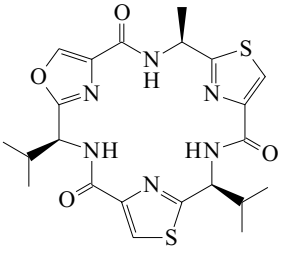
$C_{27}H_{34}N_6O_4S_2$ 570.735
Cyclic hexapeptide from the ascidian *Lissoclinum bistratum* and from *Prochloron* sp. Cytotoxic agent. λ_{max} 232 (ϵ 13000) (CH_2Cl_2) (Derep).

11,12-Didehydro: ***Bistratamide B***
[120881-21-2]
$C_{27}H_{32}N_6O_4S_2$ 568.72
From *Lissoclinum bistratum* and from *Prochloron* sp. Cytotoxic, but less so than Bistratamide A. λ_{max} 232 (ϵ 13000) (CH_2Cl_2) (Derep).

Degnan, B.M. *et al., J. Med. Chem.*, 1989, **32**, 1354-1359 (*isol, pmr, cmr, struct*)

Bistratamide C B-181

[145400-56-2]

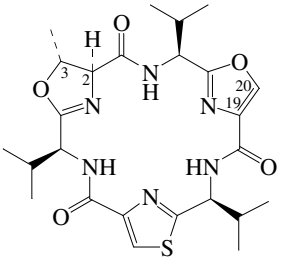


$C_{22}H_{26}N_6O_4S_2$ 502.617
Cyclic hexapeptide from the ascidian *Lissoclinum bistratum*. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{25}$ -65 (c, 0.42 in $CHCl_3$). λ_{max} 233 (ϵ 17000) (CH_2Cl_2) (Derep).

Foster, M.P. *et al., J.O.C.*, 1992, **57**, 6671-6675 (*isol, uv, ir, pmr, cmr, struct*)
Aguilar, E. *et al., Tet. Lett.*, 1994, **35**, 2477 (*synth*)

Bistratamide D B-182

[145427-87-8]



$C_{25}H_{34}N_6O_5S$ 530.647
Cyclic hexapeptide from the ascidian *Lissoclinum bistratum*. Shows sedative and depressant props. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{25}$ -31 (c, 0.33 in $CHCl_3$). λ_{max} 233 (ϵ 17000) (CH_2Cl_2) (Derep).

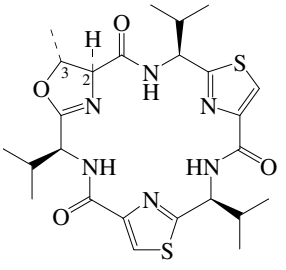
19α,20-Dihydro: ***Bistratamide F***
[501909-61-1]
$C_{25}H_{36}N_6O_5S$ 532.663
Isol. from *Lissoclinum bistratum*. Cream solid. $[\alpha]_D$ +23.2 (c, 1 in MeOH). Incorrect MF in ref. λ_{max} 230 (sh) (MeOH).

2,3-Didehydro: ***Bistratamide G***
[501909-62-2]
$C_{25}H_{32}N_6O_5S$ 528.631
Isol. from *Lissoclinum bistratum*. Solid. $[\alpha]_D$ -73.8 (c, 1 in MeOH). λ_{max} 230 (sh) (MeOH).

Foster, M.P. *et al., J.O.C.*, 1992, **57**, 6671-6675 (*isol, uv, ir, pmr, cmr, struct*)
Downing, S.V. *et al., J.O.C.*, 1999, **64**, 826-831 (*synth, pmr, cmr*)
Perez, L.J. *et al., J. Nat. Prod.*, 2003, **66**, 247-250 (*Bistratamides F,G*)
Shin, C. *et al., Chem. Lett.*, 2004, **33**, 664-665 (*synth*)
You, S.-L. *et al., Tetrahedron*, 2005, **61**, 241-249 (*synth*)

Bistratamide E B-183

[501909-60-0]



$C_{25}H_{34}N_6O_4S_2$ 546.713
Isol. from the ascidian *Lissoclinum bistratum*. Glass. $[\alpha]_D$ -31 (c, 1 in MeOH). λ_{max} 237 (log ϵ 3030) (MeOH).

2,3-Didehydro: ***Bistratamide H***
[501909-63-3]
$C_{25}H_{32}N_6O_4S_2$ 544.698
Isol. from *Lissoclinum bistratum*. Solid. $[\alpha]_D$ -92.9 (c, 1 in MeOH). λ_{max} 237 (sh) (MeOH).

Perez, L.J. *et al., J. Nat. Prod.*, 2003, **66**, 247-250 (*isol, pmr, cmr, ms*)
You, S.-L. *et al., Tetrahedron*, 2005, **61**, 241-249 (*synth*)
Nakamura, Y. *et al., Tet. Lett.*, 2006, **47**, 239-243 (*Bistratamide H, synth*)

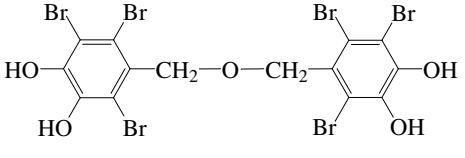
Bistratamide J B-184

[501909-65-5]
As Bistratamide I, B-179 with
X = S
$C_{25}H_{36}N_6O_5S_2$ 564.729
Isol. from *Lissoclinum bistratum*. Solid. $[\alpha]_D$ -25 (c, 0.5 in MeOH). λ_{max} 248 (sh) (MeOH).

Perez, L.J. *et al., J. Nat. Prod.*, 2003, **66**, 247-250 (*isol, pmr, cmr, ms*)
You, S.-L. *et al., Chem. Eur. J.*, 2004, **10**, 71-74 (*synth*)

Bis(2,3,6-tribromo-4,5-dihydroxybenzyl) ether B-185

4,4′-[Oxybis(methylene)]bis[3,5,6-tribromo-1,2-benzenediol]
[73694-38-9]



$C_{14}H_8Br_6O_5$ 735.638
Constit. of the red alga *Symphyocladia latiuscula*. Shows antimicrobial activities. Fine needles (C_6H_6/Me_2CO). Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 177-178°. λ_{max} 297 (log ϵ 3.65) (EtOH).

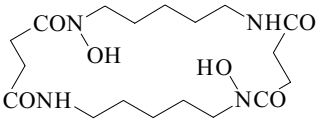
3-Debromo: 2,2′,3,6,6′-Pentabromo-4,4′,5,5′-tetrahydroxydibenzyl ether
$C_{14}H_9Br_5O_5$ 656.742
Isol. from *Symphyocladia latiuscula*. Aldose reductase inhibitor. Pale yellow amorph. solid.
Mp 132-134°.

6,6′-Didebromo: 4,4′-[Oxybis(methylene)]bis[5,6-dibromo-1,2-benzenediol]. Bis(2,3-dibromo-4,5-dihydroxybenzyl) ether
[74849-07-3]
$C_{14}H_{10}Br_4O_5$ 577.846
Isol. from the red alga *Odonthalia corymbifera*. Pale yellow solid. λ_{max} 293 (log ϵ 3.85) (EtOH).

Kurota, K. *et al., Phytochemistry*, 1980, **19**, 141 (*isol, struct*)
Kurihara, H. *et al., J. Nat. Prod.*, 1999, **62**, 882-884 (*6,6′-didebromo*)
Wang, W. *et al., J. Nat. Prod.*, 2005, **68**, 620-622 (*3-debromo*)

Bisucaberine B-186

6,17-Dihydroxy-1,6,12,17-tetraazacyclodocosane-2,5,13,16-tetrone, 9CI
[112972-60-8]

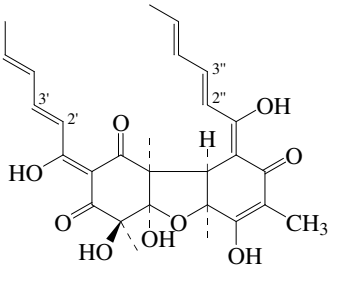


$C_{18}H_{32}N_4O_6$ 400.474
Isol. from a marine *Alteromonas haloplanktis*. Siderophore which sensitizes tumour cells to macrophage-mediated cytolysis. Cryst. Sol. DMSO; fairly sol. MeOH; poorly sol. EtOH, hexane, H_2O.
Mp 180° dec. λ_{max} 215 (ϵ 5740) (MeOH) (Derep). λ_{max} 215 (ϵ 5740) (MeOH) (Berdy). λ_{max} 215 (ϵ 5700) (MeOH-HCl) (Berdy).

Kameyama, T. *et al., J. Antibiot.*, 1987, **40**, 1664-1676; 1671 (*Biscaberine*)
Bergeron, R.J. *et al., Tetrahedron*, 1989, **45**, 4939 (*synth*)

Bisvertinolone B-187

[133683-27-9]



Absolute Configuration

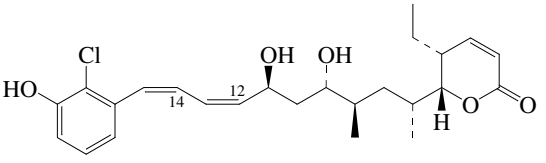
$C_{28}H_{32}O_9$ 512.555
Struct. revised in 1991 and again in 1994. Contains β-enetrione system; other tautomers possible. Prod. by *Verticillium intertextum*, *Acremonium strictum*, *Trichoderma longibrachiatum* and a marine-derived *Penicillium chrysogenum*. β-1,6-Glucan biosynth. inhibitor. Shows DPPH radical scavenging activity. Induces hyphal malformation in fungi. Yellow rosettes (diisopropyl ether).
Mp 156-158.3° dec. $[\alpha]_D^{20}$ -1046 (c, 0.91 in $CHCl_3$). $[\alpha]_D^{25}$ -495 (c, 0.1 in MeOH). λ_{max} 272 (ϵ 23000); 366 (ϵ 24000) (MeOH) (Berdy). λ_{max} 276 (ϵ 32000); 394 (ϵ 17000) (MeOH/NaOH) (Berdy).

2′,3′-Dihydro: ***2′,3′-Dihydrobisvertinolone***
$C_{28}H_{34}O_9$ 514.571
Prod. by a marine-derived *Penicillium terrestre*. Amorph. yellowish powder.
Mp 115-119°. $[\alpha]_D^{20}$ -668 (c, 0.24 in MeOH). λ_{max} 225 (log ϵ 4.57); 271 (log ϵ 4.61); 385 (log ϵ 4.57) (MeOH).

2′,2″,3′,3″-Tetrahydro: ***2′,2″,3′,3″-Tetrahydrobisvertinolone***
$C_{28}H_{36}O_9$ 516.587
Prod. by a marine-derived *Penicillium terrestre*. Amorph. yellowish powder.
Mp 82-87°. $[\alpha]_D^{20}$ -371 (c, 0.36 in MeOH). λ_{max} 228 (log ϵ 4.05); 267 (log ϵ 4.06); 336 (log ϵ 4.01) (no solvent reported).

Trifonov, L.S. *et al., Tetrahedron*, 1986, **42**, 3157 (*isol, pmr, cmr*)
Andrade, R. *et al., Can. J. Chem.*, 1992, **70**, 2526 (*isol, pmr, cmr*)
Kontani, M. *et al., Tet. Lett.*, 1994, **35**, 2577 (*isol, struct, abs config*)
Abe, N. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 661 (*activity*)
Liu, W. *et al., J. Antibiot.*, 2005, **58**, 441-446 (*Dihydrobisvertinolone, Tetrahydrobisvertinolone*)
Bringmann, G. *et al., Tetrahedron*, 2005, **61**, 7252-7265 (*marine isol*)

Bitungolide A B-188



$C_{25}H_{33}ClO_5$ 448.985
Isol. from the Indonesian sponge *Theonella* cf. *swinhoei*. Needles (MeOH aq.).
Mp 179-182°. $[\alpha]_D^{27}$ +30 (c, 0.38 in MeOH). λ_{max} 270 (log ϵ 4.1) (MeOH).

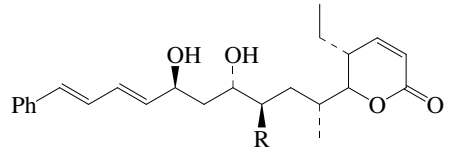
*12*E-*Isomer:* ***Bitungolide D***
$C_{25}H_{33}ClO_5$ 448.985
Isol. from *Theonella* cf. *swinhoei*. Amorph. solid. $[\alpha]_D^{27}$ +66 (c, 0.58 in $CHCl_3$). λ_{max} 270 (log ϵ 4.1) (MeOH).

*14*E-*Isomer:* ***Bitungolide C***
$C_{25}H_{33}ClO_5$ 448.985
Isol. from *Theonella* cf. *swinhoei*. Amorph. solid. $[\alpha]_D^{27}$ +89 (c, 0.11 in $CHCl_3$). λ_{max} 286 (log ϵ 4) (MeOH).

*12*E,*14*E-*Isomer:* ***Bitungolide B***
$C_{25}H_{33}ClO_5$ 448.985
Isol. from *Theonella* cf. *swinhoei*. Amorph. solid. $[\alpha]_D^{27}$ +42 (c, 4.2 in $CHCl_3$). λ_{max} 291 (log ϵ 4) (MeOH).

Sirirath, S. *et al., J. Nat. Prod.*, 2002, **65**, 1820-1823 (*isol, pmr, cmr, ms*)

Bitungolide E B-189



R = CH_3

$C_{25}H_{34}O_4$ 398.541
Isol. from the Indonesian sponge *Theonella* cf. *swinhoei*. Pale yellow glass. $[\alpha]_D^{27}$ +107 (c, 1.3 in $CHCl_3$).

Sirirath, S. *et al., J. Nat. Prod.*, 2002, **65**, 1820-1823 (*isol, pmr, cmr, ms*)

Bitungolide F B-190

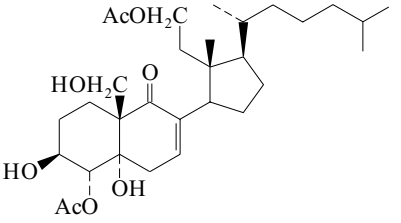
As Bitungolide E, B-189 with
R = H

$C_{24}H_{32}O_4$ 384.514
Isol. from the Indonesian sponge *Theonella* cf. *swinhoei*. Pale yellow glass. $[\alpha]_D^{27}$ +43 (c, 0.85 in $CHCl_3$).

Sirirath, S. *et al., J. Nat. Prod.*, 2002, **65**, 1820-1823 (*isol, pmr, cmr, ms*)

Blancasterol B-191

[152135-67-6]

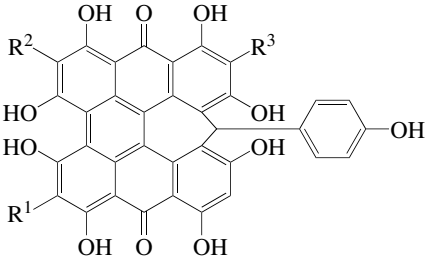


$C_{31}H_{50}O_8$ 550.731
Constit. of a *Pleraplysilla* sp. Amorph. solid. λ_{max} 240 (ϵ 5100); 288 (ϵ 1050) (MeOH) (Berdy).

Pika, J. *et al., Tetrahedron*, 1993, **49**, 8757-8760 (*isol, pmr, cmr*)

Blepharismins B-192

[129898-49-3]



Blepharismin 1 $R^1 = R^2 = CH_2CH_3$, $R^3 = H$
2 $R^1 = CH_2CH_3$, $R^2 = CH(CH_3)_2$, $R^3 = H$
3 $R^1 = R^2 = CH(CH_3)_2$, $R^3 = H$
4 $R^1 = CH_2CH_3$, $R^2 = CH(CH_3)_2$, $R^3 = CH_3$
$R^1 = CH(CH_3)_2$, $R^2 = CH_2CH_3$, $R^3 = CH_3$
5 $R^1 = R^2 = CH(CH_3)_2$, $R^3 = CH_3$

Pigment complex isol. from the ciliate *Blepharisma japonicum*. Photoreceptor molecules. Active against gram-positive bacteria. Red powder.

Blepharismin 1
$C_{39}H_{26}O_{11}$ 670.628

Blepharismin 2
$C_{40}H_{28}O_{11}$ 684.655

Blepharismin 3
$C_{41}H_{30}O_{11}$ 698.681

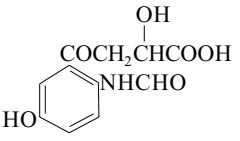
Blepharismin 4
$C_{41}H_{30}O_{11}$ 698.681
Struct. not fully elucidated.

Blepharismin 5
$C_{42}H_{32}O_{11}$ 712.708

Pant, B. *et al., FEMS Microbiol. Lett.*, 1997, **155**, 67-71 (*activity*)
Checcucci, G. *et al., J.A.C.S.*, 1997, **119**, 5762-5763; 9588 (*isol, uv, pmr, cmr*)
Maeda, M. *et al., Tet. Lett.*, 1997, **38**, 7411-7414 (*isol, struct*)

Blepharismone B-193

2-(Formylamino)-α,5-dihydroxy-γ-oxobenzenebutanoic acid, 9CI
[40136-11-6]



$C_{11}H_{11}NO_6$ 253.211
Ciliation-inducing hormone of the ciliate *Blepharisma japonicum*.

(±)-*form*
Yellowish cryst. Mp 250°.

Tokoroyama, T. *et al., Heterocycles*, 1978, **10**, 159 (*synth, bibl*)
Entzeroth, M. *et al., Z. Naturforsch., C*, 1981, **36**, 180 (*synth, pmr, ir, uv, bibl*)
Entzeroth, M. *et al., Annalen*, 1983, 226 (*synth*)

Blood depressing substances B-194

BDS
Isol. from sea anemone *Anemonia sulcata*. Antihypertensive.

BDS I Peptide containing 43 amino acid residues with 3 intramol. disulfide bonds.

BDS II Peptide; differs in 2 positions from BDS I.

Diochot, S. *et al., J. Biol. Chem.*, 1998, **273**, 6744-6749 (*isol, struct*)

Blue copper proteins B-195

Type 1 Copper proteins
$[CuN_2S_2]$

A group of metalloproteins which have a single Cu atom at the active site and three characteristic props.: intense blue colour at *ca*. 600 nm, unusually narrow hyperfine coupling in the epr spectrum of the $Cu^{2\oplus}$ protein, and high reduction potentials (range 184-680 mV).

Amicyanin
Contains 106 amino acids. Isol. from the methylotropic bacteria *Pseudomonas* AMI and *Thiobacillus versutus*. Mediates electron transfer between cytochrome c and methylamine dehydrogenase.

Azurin
Contains 128 or 129 amino acids. Isol. from denitrifying bacteria such as *Alcaligenes denitrificans* and *Pseudomonas aeruginosa*. Functions as electron transport between cytochrome c_{551} and cytochrome oxidase.

Cucumber basic protein
Plantacyanin. CBP
Contains 96 amino acids. Isol. from cucumber.

Plastocyanin
There are a number of Plastocyanins, each containing between 97 and 104 amino acids. Isol. from various higher plants, green algae and blue-green algae. Plastocyanin from *Anabaena variabilis* (blue-green alga) has some different props. Involved in electron transport between photosystems II and I in higher plants and algae.

Pseudoazurin
Contains 123 amino acids. Isol. from *Anabaena faecalis* S-6, *Achromobacter cycloclastes*, *Pseudomonas* sp. and other bacteria. Believed to transfer electrons to a Cu-containing nitrite reductase.

Rusticyanin
Contains 144 amino acids. Isol. from *Thiobacillus ferroxidans*. Respiratory chain component.

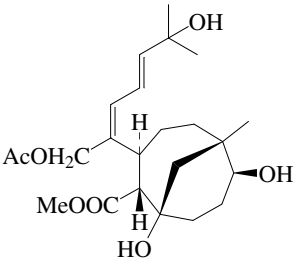
Stellacyanin
Contains 107 amino acids. Isol. from *Rhus vernicifera* (lacquer tree). Biochemical function not v. well studied.

Umecyanin
Contains 125 amino acids. Isol. from roots of *Armoracia laphatifolia* (horseradish). Biochemical function not v. well studied.

Lappin, A.G. *et al., Met. Ions Biol. Syst.*, (Ed. Sigel, H.), Vol. 13, Marcel Dekker, N.Y., 1981, 15 (*rev*)
Copper Proteins Copper Enzymes, (Ed. Lontie, R.), CRC Press, Boca Raton, 1984, (*book*)
Dooley, D.M. *et al., Life Chem. Rep.*, 1987, **5**, 91 (*rev*)
Latour, J.M. *et al., Bull. Soc. Chim. Fr.*, 1988, 508 (*rev*)
Ryden, L. *et al., Prog. Clin. Biol. Res.*, 1988, **274**, 349 (*rev*)
Guss, J.M. *et al., Sciences (N.Y.)*, 1988, 241; 806 (*cryst struct*)
Sykes, A.G. *et al., Adv. Inorg. Chem.*, 1991, **36**, 377 (*rev*)
Gross, E.L. *et al., Adv. Photosynth.*, 1996, **4**, 413-429 (*rev, Plastocyanin*)
Donaire, A. *et al., J.A.C.S.*, 2002, **124**, 13698-13708 (*Pseudoazurin, Rusticyanin, pmr, struct*)
Dennison, C. *et al., J.A.C.S.*, 2004, **126**, 2481-2489 (*Umecyanin, pmr, struct*)
Ralle, M. *et al., J.A.C.S.*, 2004, **126**, 7244-7256 (*Azurin, spectra*)

Blumicin A B-196

[866403-79-4]

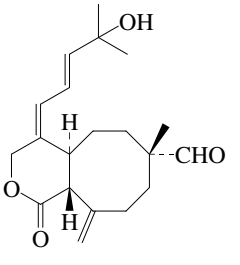


$C_{23}H_{36}O_7$ 424.533
Constit. of *Xenia blumi*. Oil. $[\alpha]_D^{25}$ -23 (c, 0.1 in $CHCl_3$). λ_{max} 235 (log ϵ 4.23) (MeOH).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 1336-1340 (*Blumicin A*)

Blumiolide A B-197

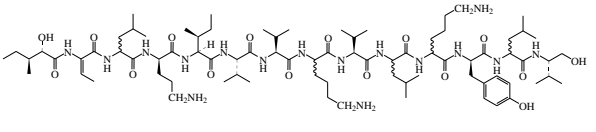
[866403-76-1]



$C_{20}H_{28}O_4$ 332.439
Constit. of *Xenia blumi*. Oil. $[\alpha]_D^{25}$ +18 (c, 0.4 in $CHCl_3$). λ_{max} 226 (log ϵ 3.6) (MeOH).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 1336-1340 (*Blumiolide A*)

Bogorol A B-198

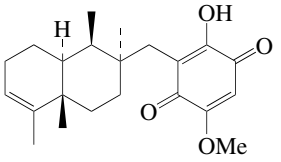


$C_{80}H_{142}N_{16}O_{16}$ 1584.099
Polypeptide antibiotic. Prod. by the marine-derived *Brevibacillus laterosporus* (PNG-276). Active against MRSA and vancomycin-resistant enterococcal strains. Amorph. solid. $[\alpha]_D^{25}$ -38.2 (MeOH).

Barsby, T. *et al., Org. Lett.*, 2001, **3**, 437-440 (*isol, struct*)
Barsby, T. *et al., J.O.C.*, 2006, **71**, 6031-6037 (*struct*)

Bolinaquinone B-199

[216498-95-2]

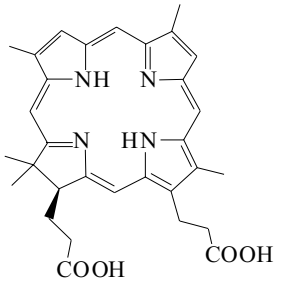


$C_{22}H_{30}O_4$ 358.477
Constit. of a *Dysidea* sp. Cytotoxic agent. Yellow glass. $[\alpha]_D$ -106 (c, 0.4 in $CHCl_3$). λ_{max} 288 (log ϵ 3.7); 424 (log ϵ 2.16) (no solvent reported). λ_{max} 288 (ϵ 5010); 424 (ϵ 144) (MeOH) (Berdy). λ_{max} 290 (ϵ 4677); 518 (ϵ 500) (MeOH/NaOH) (Berdy).

De Guzman, F.S. *et al., J.O.C.*, 1998, **63**, 8042-8044 (*isol, pmr, cmr*)
Giannini, C. *et al., Tet. Lett.*, 2000, **41**, 32-57 (*activity*)

Bonellin B-200

[62888-19-1]



$C_{31}H_{34}N_4O_4$ 526.634
λ_{max} 402; 523; 548 (sh); 587 (sh); 631 (6% HCl) (Derep). λ_{max} 394; 488; 494; 521; 539; 590; 620 (sh); 641 ($CHCl_3$) (Derep).

(S)-form

Green pigment which occurs in the female gephyrean worm *Bonellia viridis*. Also isol. as amino acid conjugates. Sexual differentiation factor. Larvicide. Green needles. Bonellin exists in nature as a peptide deriv. For prod. of acidic treatment see Anhydrobonellin. λ_{max} 396; 488; 494; 521; 539; 590; 641 ($CHCl_3$) (Berdy). λ_{max} 402; 523; 631 (HCl) (Berdy).

Di-Me ester: [62888-20-4]
$C_{33}H_{38}N_4O_4$ 554.688
Dark green cryst. Mp 164-165° (55°).

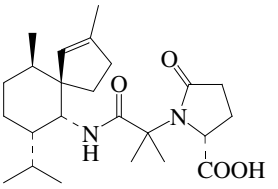
(±)-form

Mp 155-157° (as di-Me ester).

Pelter, A. *et al., Chem. Comm.*, 1976, 999-1000 (*struct*)
Pelter, A. *et al., Tet. Lett.*, 1978, 1881; 2017-2020 (*cryst struct, isol, conjugates*)
Pelter, A. *et al., Pure Appl. Chem.*, 1979, **51**, 1847
Ballantine, J.A. *et al., J.C.S. Perkin 1*, 1980, 1080-1089 (*struct*)
Dutton, C.J. *et al., Chem. Comm.*, 1983, 1237 (*synth*)
Montforts, F.P. *et al., Annalen*, 1990, 415; 1991, 709 (*isol, abs config, bibl, synth*)
Helaja, J. *et al., J.O.C.*, 1999, **64**, 432-437 (*pmr, N-15 nmr, tautom*)

Boneratamide A B-201

[786698-99-5]

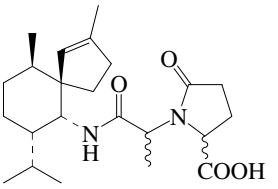


$C_{24}H_{38}N_2O_4$ 418.575
Constit. of *Axinyssa aplysinoides*.

Williams, D.E. *et al., J. Nat. Prod.*, 2004, **67**, 1752-1754 (*isol, pmr, cmr, cryst struct*)

Boneratamide B B-202

[786699-00-1]

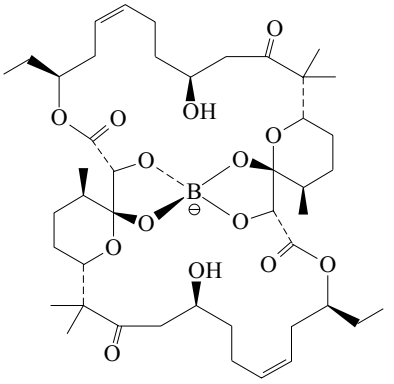


$C_{23}H_{36}N_2O_4$ 404.548
Constit. of *Axinyssa aplysinoides*.

Stereoisomer: ***Boneratamide C***
[786699-02-3]
$C_{23}H_{36}N_2O_4$ 404.548
Constit. of *Axinyssa aplysinoides*.
Williams, D.E. *et al., J. Nat. Prod.*, 2004, **67**, 1752-1754 (*isol, pmr, cmr*)

Borophycin B-203

[156466-52-3]

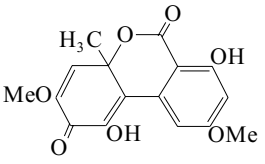


$C_{44}H_{68}BO_{14}^{\ominus}$ 831.824
Tentative stereochem. shown; by analogy with Boromycin. Prod. by the cyanobacteria *Nostoc linckia* and *Nostoc spongiaeformia*. Cytotoxic agent. Cryst. (CH_2Cl_2/MeOH) (as Na salt). $[\alpha]_D$ -23.7 (c, 1.4 in $CHCl_3$) (Na salt). CAS no. refers to Na salt.

Hemscheidt, T. *et al., J.O.C.*, 1994, **59**, 3467 (*isol, pmr, cmr, struct*)

Botrallin B-204

2-Hydroxy-4-methoxy-6-(4-methoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)benzoic acid, 9CI
[19938-10-4]

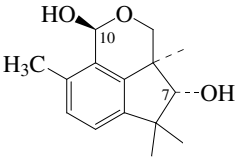


$C_{16}H_{14}O_7$ 318.282
Metab. of *Botrytis allii*, *Microsphaeropsis olivacea* and the marine *Ulocladium botrytis* 193A4. Yellow prisms (EtOH).
Mp 171-172°. Tentative identification only from *U. botrytis* 193A4. λ_{max} 238 (log ϵ 4.36); 273 (log ϵ 4.7); 370 (log ϵ 3.95) (EtOH).

Aoki, H. *et al., Tet. Lett.*, 1974, 103-106 (*struct*)
Höller, U. *et al., Dissertation*, Univ. of Braunschweig, 1999, (*isol, pmr*)
Hormazabal, E. *et al., Z. Naturforsch., C*, 2005, **60**, 11-21 (*isol, pmr, cmr, ms*)

1(9),2,4-Botryatriene-7,10-diol B-205

7-Hydroxydehydrodihydrobotrydial. 7,10-Dihydroxydehydrodihydrobotrydial (incorr.)



$C_{15}H_{20}O_3$ 248.321

(7α,10β)-*form* [850715-14-9]
Metab. of a *Geniculosporium* sp. isol. from a *Polysiphonia* sp. Gum. $[\alpha]_D^{25}$ +37 (c, 0.02 in CH_2Cl_2).

10-Me ether: ***10-Methoxy-1(9),2,4-botryatrien-7-ol***
[850715-15-0]
$C_{16}H_{22}O_3$ 262.348
Metab. of a *Geniculosporium* sp. isol. from a *Polysiphonia* sp. Gum. $[\alpha]_D^{25}$ +64.3 (c, 0.05 in CH_2Cl_2).

10-Et ether: ***10-Ethoxy-1(9),2,4-botryatrien-7-ol***
[850715-16-1]
$C_{17}H_{24}O_3$ 276.375
Metab. of a *Geniculosporium* sp. isol. from a *Polysiphonia* sp. Gum. $[\alpha]_D^{25}$ +67.8 (c, 0.03 in CH_2Cl_2).

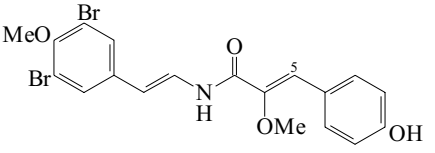
10-Ketone (lactone): ***7-Hydroxy-10-oxodehydrodihydrobotrydial***
[850715-13-8]
$C_{15}H_{18}O_3$ 246.305
Metab. of a *Geniculosporium* sp. isol. from a *Polysiphonia* sp. Gum. $[\alpha]_D^{25}$ +2.5 (c, 0.02 in CH_2Cl_2).

10-Deoxy: 1(9),2,4-Botryatrien-7-ol. ***7-Hydroxy-10-deoxydehydrodihydrobotrydial***
[850715-17-2]
$C_{15}H_{20}O_2$ 232.322
Metab. of a *Geniculosporium* sp. isol. from a *Polysiphonia* sp. Gum. $[\alpha]_D^{25}$ -20.4 (c, 0.03 in CH_2Cl_2).

Krohn, K. *et al., J. Nat. Prod.*, 2005, **68**, 400-405 (*isol, pmr, cmr*)

Botryllamide A B-206

N-*[2-(3,5-Dibromo-4-methoxyphenyl)ethenyl]-3-(4-hydroxyphenyl)-2-methoxy-2-propenamide, 9CI*
[163564-64-5]



$C_{19}H_{17}Br_2NO_4$ 483.156
Isol. from the ascidians *Botrylloides tyreum*, *Botryllus schlosseri* and a *Botryllus* sp. from the Philippines. Needles ($CHCl_3$).
Mp 169-171°.

*4′-*O*-De-Me:* ***Botryllamide G***
[724434-05-3]
$C_{18}H_{15}Br_2NO_4$ 469.129
Isol. from *Botrylloides tyreum*. Gum. λ_{max} 208 (ϵ 22230); 332 (ϵ 22150) (MeOH).

Monodebromo: ***Botryllamide C***
[163564-66-7]
$C_{19}H_{18}BrNO_4$ 404.259
Isol. from *Botrylloides tyreum*, *Botryllus schlosseri* and *Botryllus* sp. Needles ($CHCl_3$).
Mp 173-175°.

Bis(debromo): ***Botryllamide E***
[724434-03-1]
$C_{19}H_{19}NO_4$ 325.363
Isol. from *Botrylloides tyreum*. Gum. λ_{max} 207 (ϵ 15000); 222 (ϵ 12540); 339 (ϵ 29800) (MeOH).

*Bis(debromo), 4′-*O*-de-Me:* ***Botryllamide F***
[724434-04-2]
$C_{18}H_{17}NO_4$ 311.337
Isol. from *Botrylloides tyreum*. Oil. λ_{max} 208 (ϵ 13780); 220 (ϵ 12000); 316 (ϵ 14260) (MeOH).

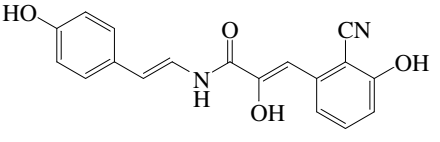
*(5*E*)-Isomer:* ***Botryllamide B***
[163564-65-6]
$C_{19}H_{17}Br_2NO_4$ 483.156
Isol. from *Botryllus schlosseri* and *Botryllus* sp. Gum.

*(5*E*)-Isomer, monodebromo:* ***Botryllamide D***
[163564-67-8]
$C_{19}H_{18}BrNO_4$ 404.259
Isol. from *Botryllus schlosseri*. Shows marginal cytotoxicity against the human cancer cell line HCT 116 but is inactive *in vivo*. Gum. λ_{max} 203 (ϵ 11100); 326 (ϵ 11700) (MeOH) (Berdy).

McDonald, L.A. *et al., Tetrahedron*, 1995, **51**, 5237-5244 (*isol, uv, ir, pmr, cmr, ms, Botryllamides B,C*)
Rao, M.R. *et al., J. Nat. Prod.*, 2004, **67**, 1064-1066 (*isol, pmr, cmr, Botryllamides E-G*)

Botryllamide H B-207

*3-(2-Cyano-3-hydroxyphenyl)-2-hydroxy-*N*-[2-(4-hydroxyphenyl)ethenyl]-2-propenamide, 9CI*
[724434-06-4]

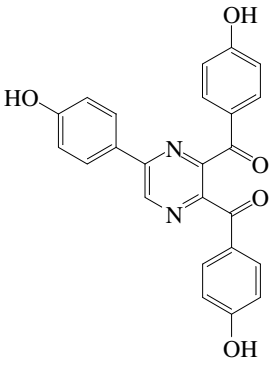


$C_{18}H_{14}N_2O_4$ 322.32
Isol. from the ascidian *Botrylloides tyreum*. Powder. λ_{max} 210 (ϵ 17630); 249 (ϵ 12570); 314 (ϵ 7790) (MeOH).

Rao, M.R. *et al., J. Nat. Prod.*, 2004, **67**, 1064-1066 (*isol, pmr, cmr*)

Botryllazine A B-208

2,3-Bis(4-hydroxybenzoyl)-5-(4-hydroxyphenyl)pyrazine
[252026-23-6]

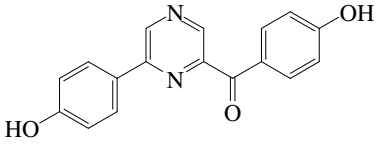


$C_{24}H_{16}N_2O_5$ 412.401
Alkaloid from the red ascidian *Botryllus leachi*. Yellow powder. λ_{max} 228 (ϵ 18500); 310 (ϵ 27500) (MeOH).

Duran, R. *et al., Tetrahedron*, 1999, **55**, 13225-13232 (*isol*)
Buron, F. *et al., J.O.C.*, 2005, **70**, 2616-2621 (*synth*)

Botryllazine B B-209

2-(4-Hydroxybenzoyl)-6-(4-hydroxyphenyl)pyrazine
[252026-25-8]

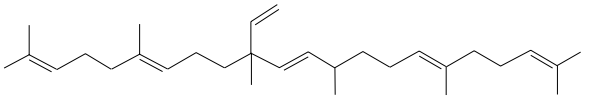


$C_{17}H_{12}N_2O_3$ 292.293
Alkaloid from the red ascidian *Botryllus leachi*. Yellow powder. λ_{max} 228 (ϵ 14700); 298 (ϵ 22800) (MeOH).

Duran, R. *et al., Tetrahedron*, 1999, **55**, 13225-13232 (*isol*)
Mahboobi, S. *et al., Monatsh. Chem.*, 2004, **135**, 333-342 (*synth*)
Buron, F. *et al., J.O.C.*, 2005, **70**, 2616-2621 (*synth*)

C_{30} Botryococcene B-210

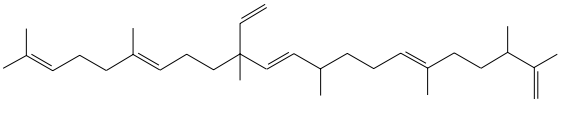
[88361-07-3]



$C_{30}H_{50}$ 410.725
Metab. of the alga *Botryococcus braunii*.

Metzger, P. *et al., Tet. Lett.*, 1983, **24**, 4013 (*struct*)
Metzger, P. *et al., Phytochemistry*, 1985, **24**, 2995 (*ms, pmr, cmr*)
Sato, Y. *et al., Tet. Lett.*, 2003, **44**, 7035-7037 (*biosynth*)

C_{31} Botryococcene B-211

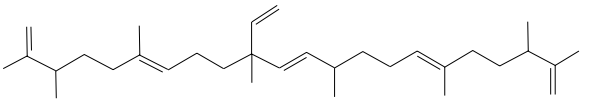


$C_{31}H_{52}$ 424.752
Struct. revised in 1985. Metab. of the alga *Botryococcus braunii*.

Metzger, P. *et al., Tet. Lett.*, 1983, **24**, 4013
Metzger, P. *et al., Phytochemistry*, 1985, **24**, 2995 (*struct*)

C_{32} Botryococcene B-212

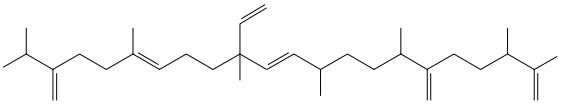
[88361-09-5]



$C_{32}H_{54}$ 438.779
Metab. of the alga *Botryococcus braunii*.

Metzger, P. *et al., Tet. Lett.*, 1983, **24**, 4013
Metzger, P. *et al., Phytochemistry*, 1985, **24**, 2995 (*ms, pmr, cmr*)

C_{33} Botryococcene B-213

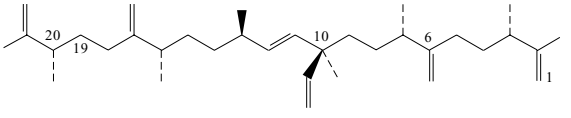


$C_{33}H_{56}$ 452.805
Metab. of alga *Botryococcus braunii*.

Metzger, P. *et al., Phytochemistry*, 1985, **24**, 2995 (*struct*)

C_{34} Botryococcene B-214

10-Ethenyl-2,3,7,10,13,16,20,21-octamethyl-6,17-bis(methylene)-1,11,21-docosatriene, 9CI. Botryococcene
[42719-34-6]



Absolute configuration

$C_{34}H_{58}$ 466.832
Metab. of *Botryococcus braunii*. Oil.

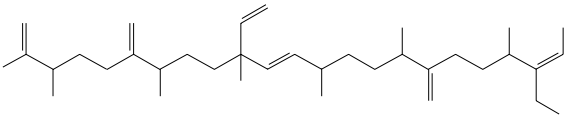
$\Delta^{19,20}$-Isomer: 10-Ethenyl-2,3,7,10,13,16,20,21-octamethyl-6,17-bis(methylene)-1,11,19-docosatriene, 9CI
[100664-64-0]
$C_{34}H_{58}$ 466.832
Metab. of *Botryococcus braunii*.

1,2,6,7,21,22,24,29-Octahydro:
$C_{34}H_{66}$ 474.895
Constit. of lacustrine sediments attributed to algae.

Cox, R.E. *et al., Chem. Comm.*, 1973, 284 (*isol, struct*)
Casadevall, E. *et al., Tet. Lett.*, 1984, **25**, 4123 (*biosynth*)
Wolf, F.R. *et al., Phytochemistry*, 1985, **24**, 733 (*biosynth*)
Metzger, P. *et al., Phytochemistry*, 1985, **24**, 2995 (*isol, ms, pmr, cmr*)
White, J.D. *et al., J.O.C.*, 1992, **57**, 4991 (*abs config, bibl*)
White, J.D. *et al., J.C.S. Perkin 1*, 1993, 759 (*synth*)
Huang, Y. *et al., Tetrahedron*, 1996, **52**, 6973-6982 (*octahydro*)
Sato, Y. *et al., Tet. Lett.*, 2003, **44**, 7035-7037 (*biosynth*)

C_{36} Botryococcene B-215

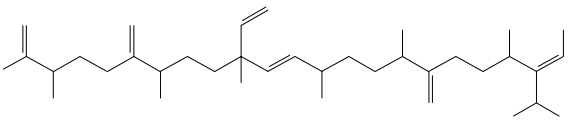
Darwinene
[87946-73-4]



$C_{36}H_{62}$ 494.886
Metab. of green alga *Botryococcus braunii*. Oil.

Galbraith, M.N. *et al., Phytochemistry*, 1983, **22**, 1441 (*struct*)
Metzger, P. *et al., Phytochemistry*, 1985, **24**, 2995 (*isol*)

C_{37} Botryococcene B-216

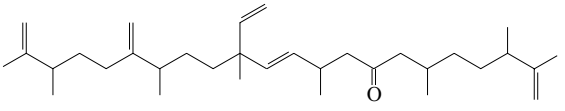


$C_{37}H_{64}$ 508.913
Metab. of alga *Botryococcus braunii*.

Metzger, P. *et al., Phytochemistry*, 1985, **24**, 2995 (*struct*)

Botryococcenone B-217

[133514-81-5]

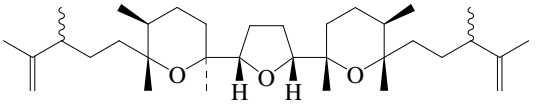


$C_{33}H_{56}O$ 468.805
Constit. of *Botryococcus braunii*. Oil. $[\alpha]_D$ -12 (c, 1.8 in $CHCl_3$).

Summons, R.E. *et al., Aust. J. Chem.*, 1991, **44**, 313 (*isol, pmr, cmr, ms*)

Botryolin A B-218

[443782-82-9]



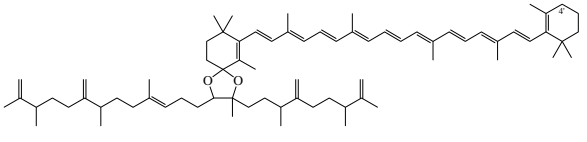
$C_{34}H_{60}O_3$ 516.846
Constit. of *Botryococcus braunii*. Oil. $[\alpha]_D^{25}$ -6 (c, 2.6 in $CHCl_3$).

Diastereoisomer: ***Botryolin B***
[443782-83-0]
$C_{34}H_{60}O_3$ 516.846
Constit. of *Botryococcus braunii*. Oil. $[\alpha]_D^{25}$ -0.6 (c, 3 in $CHCl_3$).

Metzger, P. *et al., Phytochemistry*, 2002, **59**, 839-843 (*isol, pmr, cmr*)

Botryoxanthin A B-219

[173792-78-4]



$C_{74}H_{112}O_2$ 1033.698
Constit. of *Botryococcus braunii*. λ_{max} 274 (ϵ 19000); 426 (sh); 450 (ϵ 104000); 479 (ϵ 92000) (no solent reported).

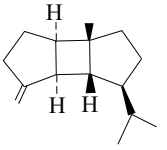
4′-Oxo: ***Botryoxanthin B***
[207594-88-5]
$C_{74}H_{110}O_3$ 1047.681
Constit. of *Botryococcus braunii*. λ_{max} 294 (ϵ 25000); 454 (ϵ 162000) (hexane).

$\Delta^{4'}$-Isomer: ***α-Botryoxanthin A***
[207594-90-9]
$C_{74}H_{112}O_2$ 1033.698
Constit. of *Botryococcus braunii*. λ_{max} 421 (sh) (ϵ 21000); 445 (ϵ 112000); 473 (ϵ 102000) (hexane).

Okada, S. *et al., Tet. Lett.*, 1996, **37**, 1065-1068 (*isol, pmr, cmr*)
Okada, S. *et al., Phytochemistry*, 1998, **47**, 1111-1115 (*Botryoxanthin B, α-Botryoxanthin A*)

4(15)-Bourbonene B-220

β-Bourbonene
[5208-59-3]



$C_{15}H_{24}$ 204.355
Constit. of the essential oil of *Geranium bourbon* and other essential oils. Oil. $[\alpha]_D^{20}$ -92.12.

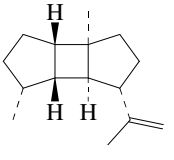
ent-form
(+)-*β*-*Bourbonene*
[68036-15-7]
Constit. of secretion of the scale insect *Ceroplastes ceriferus*.

7-Epimer: **(+)-*β*-*Epibourbonene***
[92998-16-8]
$C_{15}H_{24}$ 204.355
Constit. of *Eunicea succinea*. Oil. $[\alpha]_D$ +94 (c, 1.02 in $CHCl_3$).

Křepinský, J. *et al., Tet. Lett.*, 1966, **7**, 359-367 (*struct*)
Krepinský, J. *et al., Tet. Lett.*, 1966, **7**, 3209-3214 (*abs config*)
White, J.D. *et al., J.A.C.S.*, 1968, **90**, 6171-6177 (*synth*)
Naya, Y. *et al., Experientia*, 1978, **34**, 984-986 (*Ceroplastes ceriferus constit*)
Tomioka, K. *et al., Tet. Lett.*, 1982, **23**, 3401-3404 (*synth*)
Gopichand, Y. *et al., J. Nat. Prod.*, 1984, **47**, 607-614 (*Eunicea succinea constit*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 298-299
Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*biosynth, pmr, cmr*)

11-Bourbonene B-221

Prespatane
[190663-66-2]



Absolute Configuration

$C_{15}H_{24}$ 204.355
Constit. of *Cymbastela hooperi*. Oil. $[\alpha]_D$ -38 (c, 0.55 in $CHCl_3$).

König, G.M. *et al., J.O.C.*, 1997, **62**, 3837-3840 (*isol, pmr, cmr*)
Nabeta, K. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 1772-1776 (*abs config*)
Nabeta, K. *et al., J.C.S. Perkin 1*, 2000, 2703-2708 (*biosynth*)

Boxin B-222

Isol. from the defensive skin secretion of the Red Sea trunkfish *Ostracion cubicus*. Ichthyotoxin.

Kalmanzon, E. *et al., Mar. Biol. (Berlin)*, 2000, **136**, 471-476
Kalmanzon, E. *et al., Cell. Mol. Biol. Lett.*, 2001, **6**, 971-984

Brachyurin B-223

Proteolytic enzymes related to a subfamily of chymotrypsin. Isol. from various crustaceans incl. crabs. Serine collagenolytic agents.

Rudenskaya, G.N. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2003, **29**, 101-111 (*rev*)

Bradykinin B-224

Kallidin I. BRS 640
[58-82-2]
H-Arg-Pro-Pro-Gly-Phe-Ser-Pro-Phe-Arg-OH
$C_{50}H_{73}N_{15}O_{11}$ 1060.221

Isol. from plasma of humans and other mammals. Tissue hormone which produces all four cardinal symptoms of inflammatory response; vasodilation, pain, increased capillary permeability and leucocyte accumulation. Rapidly inactivated by peptidases. Amorph.
Mp 170° dec. $[\alpha]_D^{23}$ -84.1 (c, 1.1 in H_2O). $[\alpha]_D^{25}$ -78.4 (c, 1.4 in 1M AcOH).

N^2-*L-Lysyl:* ***Kallidin II***. N-*Lysylbradykinin*
[342-10-9]
$C_{56}H_{85}N_{17}O_{12}$ 1188.394
Peptide producing the signs of inflammatory response. Amorph.

6-L-Threonine analogue: [6120-63-4]
$C_{51}H_{75}N_{15}O_{11}$ 1074.247
Isol. from plasma of *Alligator mississippiensis* and the turtle *Pseudemys scripta*.

6-L-Threonine, 8-L-leucine analogue: See Ornithokinin in *The Combined Chemical Dictionary.*

1-L-Alanine, 6-L-threonine analogue: [155964-90-2]
$C_{48}H_{68}N_{12}O_{11}$ 989.139
Isol. from plasma of *Python reticulatus.*

5-L-Tryphophan analogue: [77669-54-6]
Isol. from plasma of the bowfin *Amia calva*.

5-L-Tryptophan, 8-L-leucine analogue: [188947-67-3]
$C_{49}H_{76}N_{16}O_{11}$ 1065.24
Isol. from plasma of the trout *Oncorhynchus mykiss* and the cod *Gadus morhua*.

Pless, J. *et al., Helv. Chim. Acta*, 1962, **45**, 394 (*synth*)
Erdos, E.G. *et al., Adv. Pharmacol.*, 1966, **4**, 1 (*rev*)
Schafer, D.J. *et al., J.C.S.(C)*, 1971, 46 (*synth*)
Corley, L. *et al., Biochem. Biophys. Res. Commun.*, 1972, **47**, 1353 (*synth*)
Fujino, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 1021 (*synth*)
Ragnarsson, U. *et al., Int. J. Pept. Protein Res.*, 1975, **7**, 307 (*synth*)
Kahn, S.A. *et al., Synthesis*, 1978, 750 (*synth*)
Erdos, E.G. *et al., Handb. Exp. Pharmacol.*, 1979, **25**, (*book*)
Diz, D. *et al., Clin. Exp. Hypertens.*, Part A, 1984, **A6**, 2085 (*rev*)
Jaouadi, M. *et al., Bull. Soc. Chim. Fr.*, 1988, 870 (*synth*)
Fiedler, F. *et al., Methods Enzymol.*, 1988, **163**, 257 (*hplc*)
Conlon, J.M. *et al., Endocrinology (Baltimore)*, 1990, **126**, 985-991 (*turtle bradykinin*)
Mirmira, S.R. *et al., Magn. Reson. Chem.*, 1990, **28**, 587 (*nmr, conformn*)
Comeau, S. *et al., Am. J. Physiol.*, 1992, **263**, R400-R404 (*alligator bradykinin*)
Conlon, J.M. *et al., FEBS Lett.*, 1993, **334**, 75-78 (*trout bradykinin*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 12451
Conlon, J.M. *et al., Gen. Comp. Endocrinol.*, 1994, **94**, 273-278 (*python bradykinin*)
Conlon, J.M. *et al., Peptides (N.Y.)*, 1995, **16**, 485-489 (*bowfin bradykinin*)
Platzack, B. *et al., Am. J. Physiol.*, 1997, **272**, R710-R717 (*cod bradykinin*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BML500

Oncorhynchus mykiss Bradykinin-related peptides B-225

Arg-Arg-Pro-Pro-Gly-Trp-Ser-Pro-Leu-Arg

Struct. of Trout[Arg0]BK shown. Isol. from plasma of the rainbow trout *Oncorhynchus mykiss.*

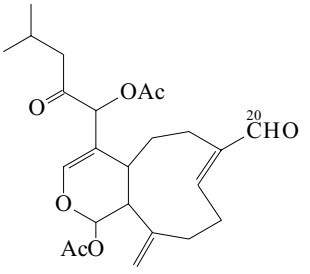
Trout[Arg0]BK
Cod[Arg0]BK. RRPPGWSPLR
[178062-07-2]
$C_{55}H_{88}N_{20}O_{12}$ 1221.427
Also isol. from plasma of the Atlantic cod *Gadus morhua*.

Trout[Lys0]BK
KRPPGWSPLR
[152273-88-6]
$C_{55}H_{88}N_{18}O_{12}$ 1193.414

Conlon, J.M. *et al., FEBS Lett.*, 1993, **334**, 75-78 (*isol*)
Conlon, J.M. *et al., Peptides (N.Y.)*, 1996, **17**, 531-537 (*isol*)
Platzack, B. *et al., Am. J. Physiol.*, 1997, **272**, R710-R717 (*isol*)

Branacenal B-226

[131623-11-5]



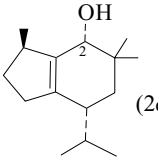
$C_{24}H_{32}O_7$ 432.513
Constit. of *Xenia membranacea*. Amorph.

20-Carboxylic acid: ***Branacenoic acid***
[131643-63-5]
$C_{24}H_{32}O_8$ 448.512
Constit. of *Xenia membranacea*. Amorph. $[\alpha]_D$ +5 (c, 0.67 in $CHCl_3$).

20-Carboxylic acid, Me ester: ***Methyl branacenoate***
$C_{25}H_{34}O_8$ 462.539
Constit. of *Xenia membranacea*. Amorph.

Almourabit, A. *et al., J. Nat. Prod.*, 1990, **53**, 894 (*isol, pmr, cmr*)

1(6)-Brasilen-2-ol B-227



(2α,9β)–*form*

$C_{15}H_{26}O$ 222.37

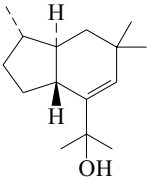
(2α,9β)-*form*
2-Epibrasilenol. *2*-epi-*Brasilenol*
[70000-41-8]
From *Aplysia brasiliana*.
Oil. $[\alpha]_D^{21}$ +96 (c, 1.05 in $CHCl_3$).

(2β,9β)-*form*
Brasilenol
[70000-39-4]
Constit. of *Aplysia brasiliana*.
Cryst.
Mp 55-56°. $[\alpha]_D^{21}$ +33.4 (c, 1.6 in $CHCl_3$).

Ac: Brasilenol acetate
[70000-40-7]
$C_{17}H_{28}O_2$ 264.407
Constit. of *Aplysia brasiliana*. Oil.

Stallard, M.O. *et al., Tetrahedron*, 1978, **34**, 2077-2081 (*isol, struct*)
Greene, A.E. *et al., J.O.C.*, 1986, **51**, 4250; 1987, **52**, 1169 (*synth, abs config*)

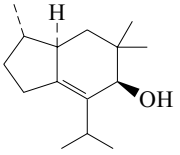
4-Brasilen-10-ol B-228



$C_{15}H_{26}O$ 222.37

(1α,6β,9α)-*form* [136978-51-3]
Constit. of *Laurencia implicata*.
Oil. $[\alpha]_D^{22}$ -3 (c, 0.17 in $CHCl_3$). Struct. revised in 1994.
Wright, A.D. *et al., J. Nat. Prod.*, 1991, **54**, 1025 (*isol, pmr, cmr*)
Tori, M. *et al., Tet. Lett.*, 1994, **35**, 3105 (*synth, struct, abs config*)

5-Brasilen-4-ol B-229



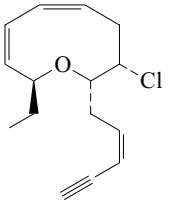
$C_{15}H_{26}O$ 222.37

(1α,4β,9α)-*form* [135448-11-2]
Metab. of *Laurencia obtusa*.
Pale yellow oil. $[\alpha]_D^{25}$ -36.1 (c, 1.6 in EtOH).

(1β,4α,9β)-*form* [136978-49-9]
Constit. of *Laurencia implicata*.
Oil. $[\alpha]_D^{22}$ -45 (c, 0.03 in $CHCl_3$).
[136978-49-9]
Wright, A.D. *et al., J. Nat. Prod.*, 1991, **54**, 1025 (*isol, pmr, cmr*)
Amico, V. *et al., Phytochemistry*, 1991, **30**, 1921 (*isol, pmr, cmr*)

Brasilenyne B-230

3-Chloro-9-ethyl-2,3,4,9-tetrahydro-2-(2-penten-4-ynyl)oxonin, 9CI
[71778-84-2]

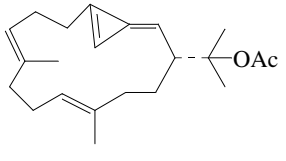


Absolute configuration

$C_{15}H_{19}ClO$ 250.767
Isol. from the sea hare *Aplysia brasiliana*. Cryst. (pentane). Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 37-38°. $[\alpha]_D^{21}$ +216 (c, 0.017 in $CHCl_3$). λ_{max} 224 (ϵ 14000) (MeOH) (Berdy).
Kinnel, R.B. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1979, **76**, 3576-3579 (*isol, pmr, cmr, cryst struct*)
Denmark, S.E. *et al., J.A.C.S.*, 2004, **126**, 12432-12440 (*synth*)

Brassicolene B-231

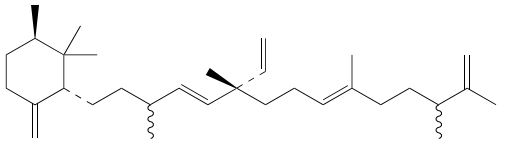
[268558-54-9]



$C_{22}H_{32}O_2$ 328.494
Constit. of *Nephthea brassica*. Oil. $[\alpha]_D^{25}$ +16.2 (c, 0.06 in $CHCl_3$). λ_{max} 226 (log ϵ 4.16) (no solvent reported).
Duh, C.-Y. *et al., Tet. Lett.*, 2000, **41**, 1401-1403 (*isol, pmr, cmr*)

Braunicene B-232

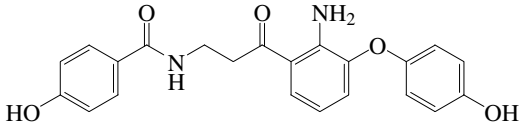
10-Ethenyl-2,3,6,10,13-pentamethyl-15-(2,2,3-trimethyl-6-methylenecyclohexan-1-yl)-1,6,11-pentadecatriene. Meijicoccene
[114066-81-8]



$C_{32}H_{54}$ 438.779
Isol. from the green alga *Botryococcus braunii*. Oil. $[\alpha]_D^{25}$ -29 (c, 3.15 in $CHCl_3$).
Huang, Z. *et al., J.A.C.S.*, 1988, **110**, 3959 (*isol, pmr, cmr, struct*)
Huang, Z. *et al., J.O.C.*, 1988, **53**, 4089 (*abs config*)
Murakami, M. *et al., Phytochemistry*, 1988, **27**, 455

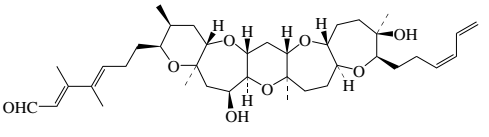
Brefelamide B-234

N-*[3-[2-Amino-3-(4-hydroxyphenoxy)phenyl]-3-oxopropyl]-4-hydroxybenzamide, 9CI*
[868529-07-1]



$C_{22}H_{20}N_2O_5$ 392.41
Isol. from *Dictyostelium brefeldianum* and *Dictyostelium giganteum*. Inhibitor of astrocytoma. Yellow oil.
Kikuchi, H. *et al., J.O.C.*, 2005, **70**, 8854-8858 (*isol, synth, pmr, cmr*)

Brevenal B-235

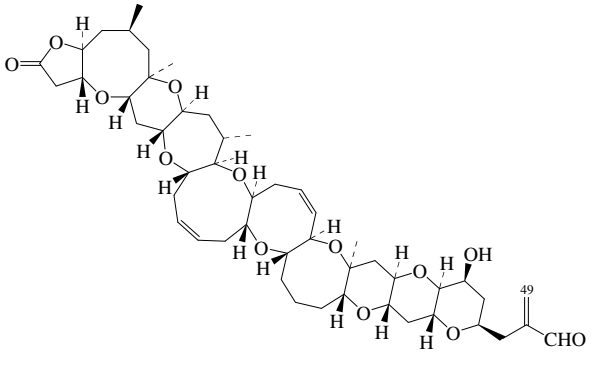


Relative Configuration

$C_{39}H_{60}O_8$ 656.898
Proposed struct. shown to be in need of revision (2006). Isol. from the dinoflagellate *Karenia brevis*. Amorph. solid. λ_{max} 227; 290 (no solvent reported).
Bourdelais, A.J. *et al., J. Nat. Prod.*, 2005, **68**, 2-6 (*isol, pmr, cmr*)
Fuwa, H. *et al., J.A.C.S.*, 2006, **128**, 9648-9650 (*synth*)

Brevetoxin A B-236

Brevetoxin 1. Brevetoxin PbTx1. ***PbTx1****. Toxin GB1. GB1 Toxin†. T46 Toxin*
[85087-27-0]



$C_{49}H_{70}O_{13}$ 867.084

Prod. by *Gymnodinium breve* and *Ptychodiscus brevis*. Potent neuro- and ichthyotoxin. Fine prisms (MeCN). Sol. $CHCl_3$, hexane; poorly sol. H_2O.
Mp 197-199° Mp 218-220° (double Mp). λ_{max} 208 (ϵ 16000) (MeOH) (Derep). λ_{max} 208 (ϵ 11000); 215 (MeOH) (Berdy).

Di-Me acetal: Mp 233-235°.

44-Alcohol: Brevetoxin PbTx7. ***PbTx7***. *Toxin GB7*. *GB7 Toxin*
[99798-30-8]
$C_{49}H_{72}O_{13}$ 869.1
Prod. by *Gymnodinium breve* and *Ptychodiscus brevis*. Neuro- and ichthyotoxin. Sol. Et_2O.

43,49-Dihydro, 44-alcohol: Brevetoxin PbTx10. ***PbTx10***
[148132-90-5]
$C_{49}H_{74}O_{13}$ 871.116
Isol. from *Gymnodinium breve*.

[98112-41-5]

Shimizu, Y. *et al., J.A.C.S.*, 1986, **108**, 514-515 (*struct, bibl*)
Pawlak, J. *et al., J.A.C.S.*, 1987, **109**, 1144 (*abs config*)
Zagorski, M.G. *et al., J.O.C.*, 1988, **53**, 4156 (*cmr*)
Rein, K.S. *et al., J.O.C.*, 1994, **59**, 2101; 2107 (*conformn, props*)
Nicolaou, K.C. *et al., Nature (London)*, 1998, **392**, 264-269 (*synth*)
Nicolaou, K.C. *et al., Chem. Eur. J.*, 1999, **5**, 599-617; 618-627; 628-645; 646-658 (*synth*)
Food Sci. Technol., *Seafood and Freshwater Toxins*, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*revs*)

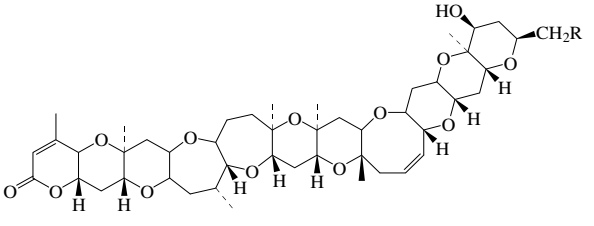
Brevetoxin B_1 B-237

BTXB1
[161434-86-2]
As Brevetoxin B, B-241 with
R = -C(=CH_2)$CONHCH_2CH_2SO_3H$
$C_{52}H_{75}NO_{17}S$ 1018.227
Isol. from the shellfish *Austrovenus stutchburyi*. Neurotoxin. Amorph. solid (as Na salt). λ_{max} 205 (ϵ 27300) (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 0.05 mg/kg.

Ishida, H. *et al., Tet. Lett.*, 1995, **36**, 725-728; 2004, **45**, 29-33 (*isol, pmr, cmr, ms*)

Brevetoxin B_2 B-238

BTXB2
[173691-95-7]



R = -$CH(CH_2OH)CH_2S(O)CH_2CH(NH_2)COOH$

$C_{53}H_{79}NO_{17}S$ 1034.27
Isol. from *Perna canaliculus* (New Zealand green mussel). Na channel blocker, paralytic agent. Amorph. solid. Sol. MeOH. $[\alpha]_D^{25}$ +19 (c, 0.6 in MeCN aq.).
▶ LD_{50} (mus, ipr) 0.306 mg/kg. Paralytic neurotoxin.

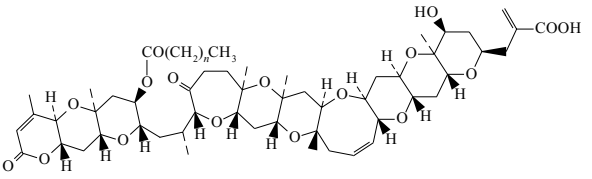
N-*Tetradecanoyl:* ***Brevetoxin B_{4a}***. *BTXB4a*
[260270-43-7]
$C_{67}H_{105}NO_{18}S$ 1244.628
Isol. from *Perna canaliculus* (New Zealand green mussel). Isol. as a mixt. with BTXB4b.

N-*Hexadecanoyl:* ***Brevetoxin B_{4b}***. *BTXB4b*
[260270-44-8]
$C_{69}H_{109}NO_{18}S$ 1272.682
Isol. from *Perna canaliculus* (New Zealand green mussel). Isol. as a mixt. with BTXB4a.

Murata, K. *et al., Tetrahedron*, 1998, **54**, 735-742
Morohashi, A. *et al., Nat. Toxins*, 1999, **7**, 45-48 (*Brevetoxin B_4*)

Brevetoxin B_3 B-239

BTXB3



n = 12 and 14

Isol. from the New Zealand green mussel *Perna canaliculus*. Toxin. Obt. as two homologues. λ_{max} 207 (ϵ 19000) (MeOH) (Berdy).

Brevetoxin B_3 C_{64} component [171527-63-2]
$C_{64}H_{96}O_{17}$ 1137.452
n = 12.

Brevetoxin B_3 C_{66} component [171527-64-3]
$C_{66}H_{100}O_{17}$ 1165.506
n = 14.

Morohashi, A. *et al., Tet. Lett.*, 1995, **36**, 8995-8998 (*isol, pmr, ms*)

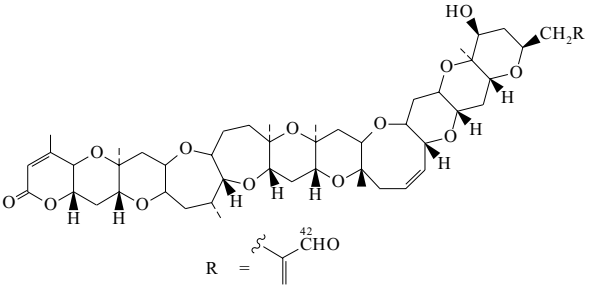
Brevetoxin B_5 B-240

BTXB5
As Brevetoxin B_2, B-238 with
R = -$CH_2C(=CH_2)COOH$
$C_{50}H_{70}O_{15}$ 911.094
Isol. from the New Zealand cockle *Austrovenus stutchburyi*. Neurotoxin. Amorph. solid. λ_{max} 205 (ϵ 27300) (MeOH).

Ishida, H. *et al., Tet. Lett.*, 2004, **45**, 29-33 (*isol, pmr, cmr, ms*)

Brevetoxin B B-241

Brevetoxin PbTx2. *Brevetoxin 2*. ***PbTx2***. *T34 toxin*. *T47 toxin*. *GB2 Toxin*. *Toxin GB2*
[79580-28-2]



$C_{50}H_{70}O_{14}$ 895.095
Constit. of Florida red tide organism *Gymnodinium breve* (*Ptychodiscus brevis*). Ichthyotoxin, cardiotoxic. Sodium channel activator. Cryst. Sol. $CHCl_3$, hexane; poorly sol. H_2O.
Mp 295-297°. λ_{max} 208 (ϵ 16000) (MeOH) (Derep). λ_{max} 213 (EtOH) (Berdy).
▶ XW5886000

37-Ac: Brevetoxin PbTx5. ***PbTx5***. *GB5 Toxin*. *Toxin GB5*
[97958-42-4]
$C_{52}H_{72}O_{15}$ 937.132
Prod. by *Gymnodinium breve*. Ichthyotoxin. Amorph.

42-Alcohol: Dihydrobrevetoxin B. Brevetoxin 3. Brevetoxin PbTx3. ***PbTx3***. *Toxin GB3*. *GB3*
[85079-48-7]
$C_{50}H_{72}O_{14}$ 897.11
From *Gymnodinium breve*. Ichthyotoxin, neurotoxin. Needles (MeCN).
Mp 291-293°. Has R = -$CH(CH_2OH)=CH_2$. λ_{max} 208 (ϵ 16000) (MeOH) (Derep).

►XW5885000

41,43-Dihydro, 42-alcohol: Brevetoxin PbTx9. ***PbTx9***
[142353-09-1]
$C_{50}H_{74}O_{14}$ 899.126
Isol. from *Gymnodinium breve.*

27S,28R-Epoxide: Brevetoxin PbTx6. ***PbTx6****. GB6 Toxin. Toxin GB6*
[97938-23-3]
$C_{50}H_{70}O_{15}$ 911.094
Prod. by *Gymnodinium breve.* Ichthyotoxin, neurotoxin. Cryst. (MeOH).
Mp 295-297°. Sinters at 255°.

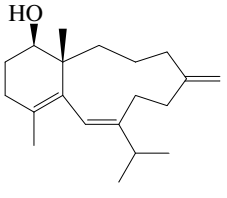
Lin, Y. *et al., J.A.C.S.*, 1981, **103**, 6773-6775 (*cryst struct*)
Chou, H.-N. *et al., Tet. Lett.*, 1982, **23**, 5521-5524; 1985, **26**, 2865-2868 (*37-Ac, 27S,28R-epoxide, 42-alcohol, isol, cryst struct*)
Shimizu, Y. *et al., J.A.C.S.*, 1986, **108**, 514-515 (*struct, bibl*)
Rein, K.S. *et al., J.O.C.*, 1994, **59**, 2101-2106; 2107-2113 (*conformn, props*)
Hua, Y. *et al., Anal. Chem.*, 1995, **67**, 1815-1823 (*hplc-ms*)
Crouch, R.C. *et al., Tetrahedron*, 1995, **51**, 8409-8422 (*PbTx3*)
Nicolaou, K.C. *et al., Angew. Chem., Int. Ed.*, 1996, **35**, 589-607 (*rev, synth*)
Nicolaou, K.C. *et al., Classics in Total Synthesis, Targets, Strategies, Methods*, VCH, 1996, 731 (*bibl, synth*)
Food Sci. Technol., *Seafood and Freshwater Toxins*, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*revs*)
Matsuo, G. *et al., J.A.C.S.*, 2004, **126**, 14374-14376 (*synth*)
Kadota, I. *et al., J.A.C.S.*, 2005, **127**, 9246-9250 (*synth*)

Brevetoxin C B-242

Brevetoxin PbTx8. ***PbTx8***
[82983-92-4]
As Brevetoxin B, B-241 with
R = $-COCH_2Cl$
$C_{49}H_{69}ClO_{14}$ 917.528
Constit. of Florida red tide organism *Gymnodinium breve* (*Ptychodiscus brevis*). Ichthyotoxin, phycotoxin and neurotoxin. Na channel activator. Sol. $CHCl_3$, hexane; poorly sol. H_2O. λ_{max} 208 (ϵ 16000) (MeOH).

Golik, J. *et al., Tet. Lett.*, 1982, **23**, 2535-2538 (*struct*)
Shimizu, Y. *et al., J.A.C.S.*, 1986, **108**, 514-515 (*struct, bibl*)

5(16),8,10-Briaratrien-14-ol B-243

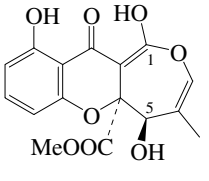


$C_{20}H_{32}O$ 288.472

14β-*form* [282102-32-3]
Constit. of a *Nephthea* sp.
Oil. $[\alpha]_D^{25}$ -77.1 (c, 0.014 in $CHCl_3$). λ_{max} 240 ($CHCl_3$).

Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 2000, **39**, 42-56 (*isol, pmr, cmr*)

Brocaenol A B-244



Absolute Configuration

$C_{16}H_{14}O_8$ 334.282
Isol. from a marine-derived *Penicillium brocae.* Amorph. pale yellow solid. $[\alpha]_D^{25}$ +34 (c, 0.008 in MeOH). λ_{max} 224 (log ϵ 4.49); 238 (log ϵ 4.52); 322 (log ϵ 3.94) (MeOH).

5-Ketone: ***Brocaenol C***
$C_{16}H_{12}O_8$ 332.266
Isol. from a marine-derived *Penicillium brocae.* Amorph. solid. $[\alpha]_D^{25}$ +83 (c, 0.0025 in MeOH). λ_{max} 224 (log ϵ 4.07); 244 (sh) (log ϵ 3.8); 292 (log ϵ 3.82); 308 (sh) (log ϵ 3.78) (MeOH).

5-Ketone, 1-Me ether: ***Brocaenol B***
$C_{17}H_{14}O_8$ 346.293
Isol. from a marine-derived *Penicillium brocae.* Cryst.
Mp 186-190°. $[\alpha]_D^{25}$ +142 (c, 0.009 in MeOH). λ_{max} 236 (log ϵ 3.73); 270 (log ϵ 3.36); 316 (log ϵ 3.15) (MeOH).

Bugni, T.S. *et al., J.O.C.*, 2003, **68**, 2014-2017 (*isol, cd, pmr, cmr*)

Bromine, 11CI B-245

Dibromine
[7726-95-6]
Br_2
Br 79.904

Atomic No. 35. Ground state electron config. $[Ar]3d^{10}4s^24p^5$. Isol. in 1826 by A.J. Balard and C. Löwig. There are 19 isotopes of which ^{79}Br and ^{81}Br are natural and are of importance in nmr spectroscopy. Abundance: 2.5 ppm (earth's crust) and 65 ppm (sea water). Br–Br: 228 pm, 227 pm (solid). Obt. as bromide from natural brines from wells in USA. Oxidation by air gives the element. Synth. from metallic bromides by reaction with oxidants (e.g. $K_2Cr_2O_7/H_2SO_4$). Liberated from brines on chlorination. Occurs naturally in several marine spp. Used in making lead scavenging agents, fumigants, flameproofing agents, water purifn. prods., and many fine chemicals with wide applications. Strong oxidant. Dark brownish-red liq., with a strong disagreeable pungent odour, forming rhombic cryst. Sol. H_2O (3% at r.t.) increased in presence of bromide salts. Misc. most org. solvs. (although it may react). d^{20} 3.12.
Mp -7.3°. Bp 59.5°. Forms adducts with many org. compds. (e.g. ethers such as dioxan, and aromatic hydrocarbons) and also hydrates. Dissociates > 600°. Bond energy 193 kJ mol^{-1}.
►Causes painful burns on skin contact; irritates eyes and throat.
EF9100000

Octahydrate:
Light red cryst. Cubic. May be stored at r.t.

Bromine 75 [14809-47-3]
Radioactive, $t_{½}$ 1.62 h. Prod. from ^{74}Se (d,n), ^{74}Se (p,γ), or ^{65}Cu (^{12}C,2n). Also obt. by proton bombardment of Br or Y. I = -3/2; μ = 0.75(11) μ_N. Decays by orbital electron capture or $\beta^{\oplus}$ emission to ^{75}Se.

Bromine 76 [15765-38-5]
Radioactive, $t_{½}$ 16.0 h. Prod. from ^{75}As (α,3n). Used in diagnostic nuclear medicine.
I = -1; μ = 0.54821 μ_N. Decays by $\beta^{\oplus}$ emission, or orbital electron capture to ^{76}Se.

Bromine 77 [15765-39-6]
Radioactive, $t_{½}$ 2.376 d. Prod. from ^{75}As (α,2n). Used in diagnostic nuclear medicine.
I = -3/2. Decays by orbital electron capture (99%), or $\beta^{\oplus}$ emission (1%) to ^{77}Se.

Bromine 79 [14336-94-8]
Stable. Representative abundance 50.69 atom %. I = -3/2; μ = +2.106399 μ_N. Nmr relative sensitivity (^1H=1.00) 0.0786; receptivity (^{13}C=1.00) 226.

Bromine 80 [14391-61-8]
Radioactive, $t_{½}$ 17.68 min. Prod. from ^{79}Br (n,γ), ^{81}Br (γ,n), or ^{79}Br (d,p). Daughter of ^{80m}Br (4.42 h). I = +1; μ = 0.5140 μ_N. Decays by $\beta^{\ominus}$ emission (91.7%) to ^{80}Kr, or by $\beta^{\oplus}$ emission (8.3%) to ^{80}Se.

Bromine 80m
Radioactive, $t_{½}$ 4.42 h. Prod. from ^{79}Br (n,γ). I = -5; μ = +1.3177 μ_N. Decays by isomeric transition to ^{80}Br.

Bromine 81 [14380-59-7]
Stable. Representative abundance 49.31 atom %. Preferred isotope for nmr spectroscopy.
I = -3/2; μ = +2.270560 μ_N. Nmr relative sensitivity (^{1}H=1.00) 0.0985; receptivity (^{13}C=1.00) 277.

Bromine 82 [14686-69-2]
Radioactive, $t_{1/2}$ 1.471 d. Prod. from ^{81}Br (n,γ). Used in diagnostic nuclear medicine.
I = -5; μ = +1.6270 μ_N. Decays by $\beta^\ominus$ emission to ^{82}Kr.

Bromine 83 [14687-62-8]
Radioactive, $t_{1/2}$ 2.39 h. Daughter of ^{83}Se. I = -3/2. Decays by $\beta^\ominus$ emission to ^{83m}Kr.

Bromine 84 [14331-90-9]
Radioactive, $t_{1/2}$ 31.8 min. Prod. from ^{87}Rb (n,α), or by thermal neutron-induced nuclear fission. I = -2. Decays by $\beta^\ominus$ emission to ^{84}Kr.

Bromine 87 [13982-62-2]
Radioactive, $t_{1/2}$ 55.69 s. Prod. by thermal neutron-induced nuclear fission. I = -3/2. Decays by $\beta^\ominus$ emission to ^{87}Kr, or by neutron emission.

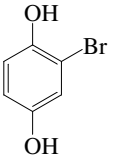
Bromine 88 [14280-22-9]
Radioactive, $t_{1/2}$ 16.7 s. Prod. by thermal neutron-induced nuclear fission. I = -1. Decays by $\beta^\ominus$ emission to ^{88}Kr, or by neutron emission.

[10097-32-2, 11094-39-6, 12595-70-9, 12595-73-2, 14280-22-9, 22541-56-6]

Mellor Compr. Treat. Inorg. Theor. Chem., 1922, **2**, 15; *Suppl. Vol.* 1, 1956, 689 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 7, 1931, ; *Suppl. Vol.*, 1985, 689 (*rev, bibl*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1972, **3**, 34; 1974, **4**, 46; 1975, **5**, 55; 1977, **6**, 70 (*use*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 1107 (*rev, bibl*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 290 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **4**, 226; **24**, 391 (*rev, bibl*)
Lindman, B. *et al., NMR Period. Table. 1978*, (R.K. Harris *et al*, Eds.), Academic Press,London, 1978, 421 (*nmr*)
Soulard, M. *et al., J.C.S. Dalton*, 1981, 2300 (*uv, reactions*)
Johanssen, P.-G. *et al., J. Phys. C: Solid State Phys.*, 1983, **16**, 1961 (*solid, Raman*)
Powell, B.M. *et al., Mol. Phys.*, 1984, **53**, 929 (*cryst struct*)
Greenwood, N.N. *et al., Chemistry of the Elements*, Pergamon, Oxford, 1986, 920 (*rev*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 677-681 (*use*)
Emsley, J. *et al., The Elements*, 3rd edn., Clarendon Press, 1998, 42; 237
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 97 (*haz*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BMP000

2-Bromo-1,4-benzenediol, 9CI B-246

Bromohydroquinone, 8CI. Bromoquinol. Adurol
[583-69-7]



$C_6H_5BrO_2$ 189.008
Isol. from various marine acorn worms. Photographic developer.
Cryst. (toluene). Sol. H_2O.
Mp 110-111°. pK_{a1} 8.67; pK_{a2} 10.68 (22°, KCl). Sublimes.

▶CZ8920000

Di-Ac: [52376-16-6]
$C_{10}H_9BrO_4$ 273.083
Mp 71-73°.

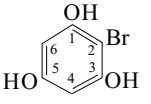
4-Me ether: 2-Bromo-4-methoxyphenol, 9CI
[17332-11-5]
$C_7H_7BrO_2$ 203.035
Liq. Bp_{25} 130°.

Di-Me ether: 2-Bromo-1,4-dimethoxybenzene
[25245-34-5]
$C_8H_9BrO_2$ 217.062
Oil. Bp 262-263°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1048D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 199B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 980B (*ir*)
Bilmann, E. *et al., J.C.S.*, 1925, **127**, 205 (*synth*)
Yanovskaya, L.A. *et al., Zh. Obshch. Khim.*, 1952, **22**, 1594; *CA*, **47**, 8032 (*synth*)
Higa, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **65**, 525 (*isol*)
Pinault, M. *et al., Synthesis*, 1990, 935 (*synth*)
Corgiat, J.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1993, **106**, 83-86 (*acorn worm constit*)
Bloomer, J.L. *et al., Synth. Commun.*, 1998, **28**, 2087-2095 (*di-Me ether*)
Coumbarides, G.S. *et al., Bull. Chem. Soc. Jpn.*, 2001, **74**, 179-180 (*synth, ir, pmr, cmr*)
Chambers, J.J. *et al., J. Med. Chem.*, 2003, **46**, 3526-3535 (*4-Me ether, synth, pmr*)

2-Bromo-1,3,5-benzenetriol, 9CI B-247

2-Bromophloroglucinol
[84743-77-1]



$C_6H_5BrO_3$ 205.008
Isol. from *Rhabdonia verticillata*.
Mp 162.5-163.5°.

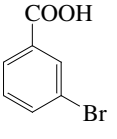
Tri-Ac: [96820-10-9]
$C_{12}H_{11}BrO_6$ 331.119
Isol. from *Eisenia arborea*. Cryst. (EtOH).
Mp 107-108°.

Tri-Me ether: 2-Bromo-1,3,5-trimethoxybenzene, 9CI
[1131-40-4]
$C_9H_{11}BrO_3$ 247.088
Cryst. (Et_2O). Mp 99°.

Blackman, A.J. *et al., Phytochemistry*, 1982, **21**, 2141 (*isol*)
Fischer, A. *et al., Can. J. Chem.*, 1983, **61**, 1045 (*deriv*)
Glombitza, K.W. *et al., Phytochemistry*, 1985, **24**, 543 (*deriv*)
Kiehlmann, E. *et al., Can. J. Chem.*, 1989, **67**, 335-344 (*synth, ms*)
Drake, M.D. *et al., Organometallics*, 2003, **22**, 4158-4162 (*tri-Me ether, synth, pmr, cmr*)

3-Bromobenzoic acid, 9CI B-248

[585-76-2]



$C_7H_5BrO_2$ 201.019
Isol. from the coral *Tubastrea micrantha*. Needles.
Mp 155°. Bp 280°. pK_a 3.81 (25°, H_2O).

Me ester: [618-89-3]
$C_8H_7BrO_2$ 215.046
Plates. Mp 31-32°. Bp_{15} 122.5°.

Et ester: [24398-88-7]
$C_9H_9BrO_2$ 229.073
Liq. Bp 261°.

Chloride: [1711-09-7]
C_7H_4BrClO 219.465
Liq. Bp 243° Bp_{18} 132°.

Amide: [22726-00-7]
C_7H_6BrNO 200.034
Leaflets (H_2O). Mp 155°. pK_a -2.75 (25°, H_2SO_4).

Hydrazide: [39115-96-3]
$C_7H_7BrN_2O$ 215.049
Mp 157-159°.

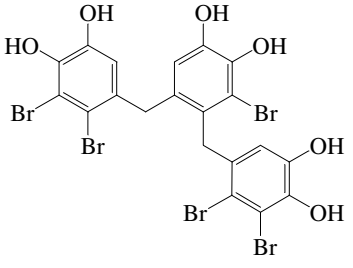
Nitrile: 1-Bromo-3-cyanobenzene
[6952-59-6]
C_7H_4BrN 182.019
Cryst. (EtOH). Mp 38-39°. Bp 225° Bp_{20} 118.5°.

▶ DI2459500

Anhydride:
$C_{14}H_8Br_2O_3$ 384.023
Cryst. by subl. Mp 98°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 191C; 446B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1070A; 1247B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1392C; 1410A (*ir*)
Forbes, W.F. *et al., J.A.C.S.*, 1957, **79**, 6495 (*uv*)
Horton, W.J. *et al., J.O.C.*, 1960, **25**, 1016 (*synth*)
Cox, R.H. *et al., Spectrochim. Acta A*, 1969, **25**, 1189 (*pmr*)
Benoit, F. *et al., Org. Mass Spectrom.*, 1973, **7**, 295 (*ms*)
Bromilow, J. *et al., J.C.S. Perkin 2*, 1981, 753 (*cmr*)
Harrison, J.J. *et al., J.O.C.*, 1981, **46**, 2169 (*synth*)
Sanduja, R. *et al., J. Chem. Res., Synop.*, 1986, 450-451 (*isol*)

3-Bromo-4,5-bis(2,3-dibromo-4,5-dihydroxybenzyl)-1,2-benzenediol B-249

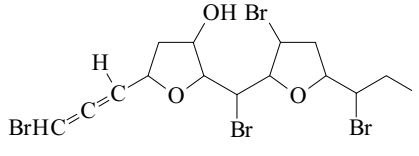


$C_{20}H_{13}Br_5O_6$ 748.839
Isol. from the red alga *Rhodomela confervoides*. Needles (Me_2CO). Mp 237-238°.

Fan, X. *et al., J. Nat. Prod.*, 2003, **66**, 455-458 (*isol, pmr, cmr*)

2-[Bromo[3-bromo-5-(1-bromopropyl)tetrahydro-2-furanyl]methyl]-5-(3-bromo-1,2-propadienyl)tetrahydro-3-furanol B-250

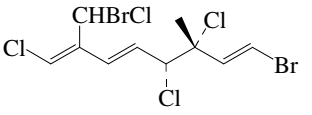
1,8,10,13-Tetrabromo-4,7;9,12-diepoxy-1,2-pentadecadien-6-ol
[176714-53-7]



$C_{15}H_{20}Br_4O_3$ 567.937
Isol. from the alga *Laurencia obtusa*. Cryst. (hexane/Et_2O). Mp 80°. $[\alpha]_D^{21}$ +42.5 (c, 0.6 in $CHCl_3$). Unstable in light at r.t.

Imre, S. *et al., Z. Naturforsch., C*, 1995, **50**, 743-747 (*isol, ir, pmr, cmr*)

8-Bromo-2-(bromochloromethyl)-1,5,6-trichloro-6-methyl-1,3,7-octatriene B-251

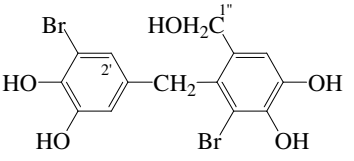


$C_{10}H_{10}Br_2Cl_4$ 431.808

(1*Z*,3*E*,5*R*,6*R*,7*E*)-*form* [260973-21-5]
Constit. of *Plocamium cartilagineum*.
Oil. $[\alpha]_D$ +49.1 (c, 1.12 in CH_2Cl_2). λ_{max} 249 (log ϵ 5.31) (CH_2Cl_2).
Jongaramruong, J. *et al., J. Nat. Prod.*, 2000, **63**, 272-275 (*isol, pmr, cmr*)

3-Bromo-4-[(3-bromo-4,5-dihydroxyphenyl)methyl]-5-(hydroxymethyl)-1,2-benzenediol, 9CI B-252

3-Bromo-2-(3-bromo-4,5-dihydroxybenzyl)-4,5-dihydroxybenzyl alcohol. 5′-Hydroxyisoavrainvilleol. 2,3′-Dibromo-3,4,4′,5′-tetrahydroxy-6-hydroxymethyldiphenylmethane
[111537-53-2]



$C_{14}H_{12}Br_2O_5$ 420.054
Constit. of *Avrainvillea nigricans*. Light yellow oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. λ_{max} 261 (ϵ 2440) (MeOH) (Berdy).

2′-Bromo: 3-Bromo-4-[(2,3-dibromo-4,5-dihydroxyphenyl)-methyl]-5-hydroxymethyl-1,2-benzenediol. 3-Bromo-2-(2,3-dibromo-4,5-dihydroxybenzyl)-4,5-dihydroxybenzyl alcohol. 2,2′,3-Tribromo-3′,4,4′,5-tetrahydroxy-6′-(hydroxymethyl)diphenylmethane
[503609-19-6]
$C_{14}H_{11}Br_3O_5$ 498.95
Constit. of the alga *Rhodomela confervoides*. Yellowish needles (Me_2CO).
Mp 127-129°.

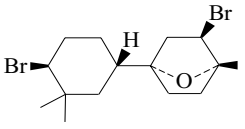
2′-Bromo, 1″-Me ether: 3-Bromo-4-[(2,3-dibromo-4,5-dihydroxyphenyl)methyl]-5-methoxymethyl-1,2-benzenediol, 9CI. 2,2′,3-Tribromo-3′,4,4′,5-tetrahydroxy-6′-(methoxymethyl)diphenylmethane
[65487-77-6]
$C_{15}H_{13}Br_3O_5$ 512.977
Constit. of *Rhodomela larix*. Cryst. (C_6H_6/MeOH). Dec. at ca. 540° without melting (possible error in ref.).

2′-Bromo, 1″-Et ether: 3-Bromo-4-[(2,3-dibromo-4,5-dihydroxyphenyl)methyl]-5-(ethoxymethyl)-1,2-benzenediol. 2,2′,3-Tribromo-6′-(ethoxymethyl)-3′,4,4′,5-tetrahydroxydiphenylmethane
[503609-20-9]
$C_{16}H_{15}Br_3O_5$ 527.004
Constit. of the alga *Rhodomela confervoides*. Yellowish needles (Me_2CO).
Mp 197-199°. Poss. artifact.

Kurata, K. *et al., Chem. Lett.*, 1977, 1435-1438 (*Rhodomela larix constit*)
Colon, M. *et al., J. Nat. Prod.*, 1987, **50**, 368-374 (*5′-Hydroxyisoavrainvilleol*)
Xu, N. *et al., Phytochemistry*, 2003, **62**, 1221-1224 (*Rhodomela confervoides derivs*)

2-Bromo-4-(4-bromo-3,3-dimethylcyclohexyl)-1-methyl-7-oxabicyclo[2.2.1]heptane, 9CI B-253

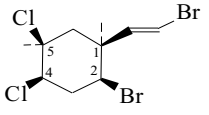
[88556-03-0]



$C_{15}H_{24}Br_2O$ 380.162
Constit. of *Laurencia obtusa*. Cryst. (hexane).
Mp 100-102°. $[\alpha]_D$ -8.7 (c, 2.86 in $CHCl_3$).

González, A.G. *et al., Tet. Lett.*, 1983, **24**, 4143 (*cryst struct*)

2-Bromo-1-(2-bromoethenyl)-4,5-dichloro-1,5-dimethylcyclohexane B-254



$C_{10}H_{14}Br_2Cl_2$ 364.934

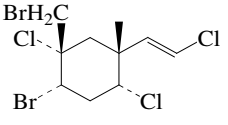
(1*R,2*R**,4*S**,5*R**)-*form*** [68370-29-6]
Constit. of *Plocamium cartilagineum*.
Cryst. (hexane).
Mp 72-73°. $[\alpha]_D$ +18 ($CHCl_3$).

(1*R,2*R**,4*S**,5*S**)-*form*** [105016-85-1]
Constit. of *Aplysia punctata*.

González, A.G. *et al., Phytochemistry*, 1978, **17**, 947-948 (*1R,2R4S,5R-form*)
Quinoa, E. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **92**, 99-101 (*1R,2R,4S,5S-form*)

2-Bromo-1-bromomethyl-1,4-dichloro-5-(2-chloroethenyl)-5-methylcyclohexane B-255

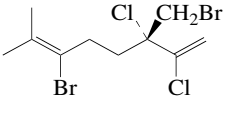
[66321-24-2]



$C_{10}H_{13}Br_2Cl_3$ 399.379
Constit. of *Plocamium cartilagineum*. Metab. of *Aplysia dactylomela*. Shows antifungal and strong algicidal activities. Toxic to brine shrimp.
Mp 74-74.5°. $[\alpha]_D^{20}$ -43.8 (c, 1.01 in $CHCl_3$). $[\alpha]_D$ -67.8.

Higgs, M.D. *et al., Tetrahedron*, 1977, **33**, 2775-2780 (*isol*)
Stierle, D.B. *et al., Tetrahedron*, 1979, **35**, 1261-1265 (*isol, abs config*)
König, G.M. *et al., Phytochemistry*, 1999, **52**, 1047-1053 (*isol, pmr, cmr, cryst struct, abs config*)
Wessels, M. *et al., J. Nat. Prod.*, 2000, **63**, 920-928 (*activity*)

6-Bromo-3-(bromomethyl)-2,3-dichloro-7-methyl-1,6-octadiene B-256



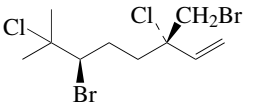
$C_{10}H_{14}Br_2Cl_2$ 364.934

(*S*)-*form* [159125-44-7]
Constit. of *Portieria hornemannii*.
$[\alpha]_D$ -6.7 (c, 1 in $CHCl_3$).

Fuller, R.W. *et al., J. Med. Chem.*, 1994, **37**, 4407-4411 (*isol, pmr, cmr*)

6-Bromo-3-(bromomethyl)-3,7-dichloro-7-methyl-1-octene B-257

[58086-83-2]



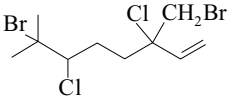
$C_{10}H_{16}Br_2Cl_2$ 366.95

(3*S*,6*R*)-*form* [159125-48-1]
Constit. of *Portieria hornemannii* (*Chondrococcus hornemannii*).
$[\alpha]_D$ +32.3 (c, 1.19 in $CHCl_3$).

Burreson, B.J. *et al., Chem. Lett.*, 1975, 1111 (*isol, pmr*)
Fuller, R.W. *et al., J. Med. Chem.*, 1994, **34**, 4407-4411 (*isol, pmr, cmr*)

7-Bromo-3-bromomethyl-3,6-dichloro-7-methyl-1-octene B-258

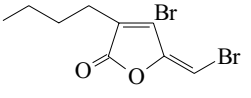
[58086-82-1]



$C_{10}H_{16}Br_2Cl_2$ 366.95
Constit. of *Chondrococcus hornemanni*. Oil.

Burreson, B.J. *et al., Chem. Lett.*, 1975, 1111

4-Bromo-5-(bromomethylene)-3-butyl-2(5*H*)-furanone, 9CI B-259
Fimbrolide
[66042-01-1]


(*E*)–*form*

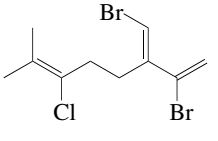
$C_9H_{10}Br_2O_2$ 309.985
► LD_{50} (mus, scu) 12 mg/kg.

(*E*)-*form* [63025-34-3]
Constit. of the red alga *Delisea fimbriata*.

(*Z*)-*form* [63025-35-4]
Constit. of *Delisea fimbriata*.

Kazlauskas, R. *et al., Tet. Lett.*, 1977, 37 (*isol*)
Norton, R.S. *et al., Tetrahedron*, 1977, **33**, 2577 (*cmr*)
Beechan, C.M. *et al., Tet. Lett.*, 1979, 1649 (*synth*)
Caine, D. *et al., J.O.C.*, 1985, **50**, 2195 (*synth*)
De March, P. *et al., J.O.C.*, 1995, **60**, 1815 (*synth*)

2-Bromo-3-(bromomethylene)-6-chloro-7-methyl-1,6-octadiene B-260
2,10-Dibromo-6-chloro-β-myrcene



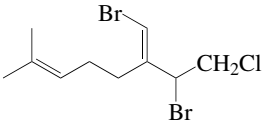
$C_{10}H_{13}Br_2Cl$ 328.473
Config. assigned incorrectly in paper and CAS.

(*E*)-*form* [55498-40-3]
Constit. of *Chondrococcus hornemannii* (*Portieria hornemannii*).
Called (*Z*)- in ref.

Ichikawa, N. *et al., Chem. Lett.*, 1974, 1333-1336 (*isol, pmr, ms*)

7-Bromo-6-(bromomethylene)-8-chloro-2-methyl-2-octene B-261

[58086-85-4]



(*E*)-*form*

$C_{10}H_{15}Br_2Cl$ 330.489

Config. assigned incorrectly in paper.

(*E*)-*form*

Constit. of *Chondrococcus hornemanni*.

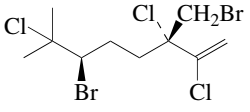
Burreson, B.J. *et al., Chem. Lett.*, 1975, 1111 (*isol*)

6-Bromo-3-bromomethyl-2,3,7-trichloro-7-methyl-1-octene B-262

Halomon

[142439-86-9]

[58086-84-3]



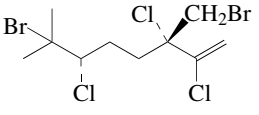
$C_{10}H_{15}Br_2Cl_3$ 401.395

Isol. from red alga *Portieria hornemannii*. Cytotoxic agent. Shows antitumour properties. Cryst. (MeOH).

Mp 49-50°. $[\alpha]_D$ +206 (c, 1.1 in CH_2Cl_2).

Fuller, R.W. *et al., J. Med. Chem.*, 1992, **35**, 3007-3011 (*isol, pmr, cmr, ms, cryst struct*)

7-Bromo-3-(bromomethyl)-2,3,6-trichloro-7-methyl-1-octene B-263



$C_{10}H_{15}Br_2Cl_3$ 401.395

(3*S*,6*S*)-*form*

Isohalomon

[58086-79-6]

Constit. of *Chondrococcus hornemanni*.

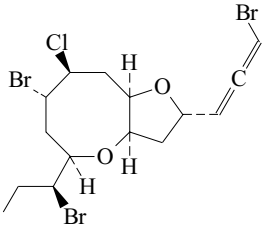
Cryst. $[\alpha]_D$ -25 (c, 1 in $CHCl_3$).

Burreson, B.J. *et al., Chem. Lett.*, 1975, 1111-1114 (*isol*)

Fuller, R.W. *et al., J. Med. Chem.*, 1994, **37**, 4407-4411 (*isol, pmr, cmr, cryst struct, abs config*)

7-Bromo-2-(3-bromo-1,2-propadienyl)-5-(1-bromopropyl)-8-chlorooctahydro-2*H*-furo[3,2-*b*]oxocin B-264

1,10,13-Tribromo-9-chloro-4,7:6,12-diepoxy-1,2-pentadecadiene



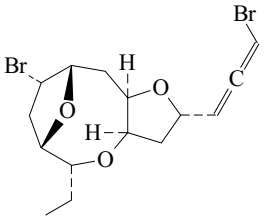
$C_{15}H_{20}Br_3ClO_2$ 507.486

Metab. of *Laurencia implicata*. Oil. $[\alpha]_D^{22}$ +115.9 (c, 0.24 in $CHCl_3$).

Wright, A.D. *et al., J. Nat. Prod.*, 1991, **54**, 1025 (*isol, pmr, cmr*)

8-Bromo-2-(3-bromo-1,2-propadienyl)-6,9-epoxy-5-ethyldecahydrofuro[3,2-*b*]oxonin B-265

1,10-Dibromo-4,7:6,13:9,12-triepoxy-1,2-pentadecadiene



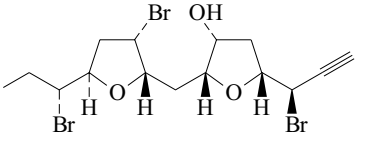
$C_{15}H_{20}Br_2O_3$ 408.129

Metab. of *Laurencia implicata*. Oil. $[\alpha]_D^{22}$ -21.4 (c, 0.19 in $CHCl_3$).

Wright, A.D. *et al., J. Nat. Prod.*, 1991, **54**, 1025 (*isol, pmr, cmr*)

2-[[3-Bromo-5-(1-bromopropyl)tetrahydro-2-furanyl]methyl]-5-(1-bromo-2-propynyl)tetrahydro-3-furanol, 9CI B-266

[126594-25-0]



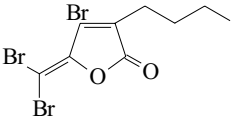
$C_{15}H_{21}Br_3O_3$ 489.041

Metab. of *Laurencia obtusa*. Oil. $[\alpha]_D$ +7.5 (c, 0.03 in $CHCl_3$).

Norte, M. *et al., Tetrahedron*, 1989, **45**, 5987 (*isol, pmr, cmr*)

4-Bromo-3-butyl-5-(dibromomethylene)-2(5*H*)-furanone, 9CI B-267

[63025-36-5]



$C_9H_9Br_3O_2$ 388.881

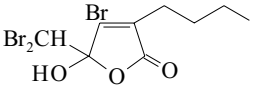
Constit. of the red alga *Delisea elegans*, *Delisea fimbriata* and *Delisea pulchra*. Yellow oil. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. λ_{max} 308 (ϵ 16000) (hexane) (Berdy).

Kazlauskas, R. *et al., Tet. Lett.*, 1977, 37

McCombs, J.D. *et al., Tetrahedron*, 1988, **44**, 1489

4-Bromo-3-butyl-5-(dibromomethyl)-5-hydroxy-2(5*H*)-furanone B-268

[115721-49-8]



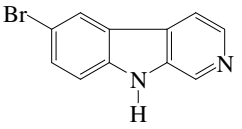
$C_9H_{11}Br_3O_3$ 406.896

Constit. of the red alga *Delisea elegans*. Viscous pale brown-yellow oil. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. λ_{max} 235 (ϵ 10000) (hexane) (Berdy).

McCombs, J.D. *et al., Tetrahedron*, 1988, **44**, 1489 (*isol*)

6-Bromo-β-carboline B-269

*6-Bromo-9*H*-pyrido[3,4-*b*]indole, 9CI.* ***Eudistomin N****. Bromonorharman*
[59444-69-8]



$C_{11}H_7BrN_2$ 247.094
Alkaloid from the Caribbean tunicate *Eudistoma olivaceum*. Mod. active against gram-positive bacteria, yeasts and viruses. Enzyme inhibitor. Yellow needles (MeOH/$CHCl_3$). Sol. MeOH, C_6H_6, $CHCl_3$; poorly sol. H_2O.
Mp 265-268° dec. λ_{max} 233 (ϵ 39600); 251 (ϵ 21000); 283 (ϵ 9200); 291 (ϵ 15800); 342 (ϵ 3800); 357 (ϵ 3900) (MeOH) (Derep). λ_{max} 333; 347; 361; 373 (MeOH) (Berdy). λ_{max} 235 (ϵ 23900); 292 (ϵ 10100); 335 (ϵ 2400); 347 (ϵ 2600) (hexane) (Berdy).

N-*Me:*
$C_{12}H_9BrN_2$ 261.121
Cryst. (Et_2O/hexane). Mp 108-112°.

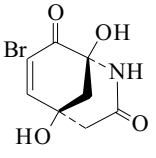
Roques, B.P. *et al., Bull. Soc. Chim. Fr.*, 1975, 2403 (*pmr, struct, synth*)
Rinehart, K.L. *et al., J.A.C.S.*, 1987, **109**, 3378-3387 (*isol, struct, props*)
Ponce, M.A. *et al., J. Het. Chem.*, 2001, **38**, 1087-1095 (*synth, pmr, cmr, ms*)

7-Bromo-β-carboline B-270

*7-Bromo-9*H*-pyrido[3,4-*b*]indole.* ***Eudistomin O***
[88704-40-9]
$C_{11}H_7BrN_2$ 247.094
Alkaloid from *Eudistoma olivaceum* and from the New Zealand ascidian *Ritterella sigillinoides*. Shows mod. activity against bacteria and viruses. Enzyme inhibitor. Pale-yellow cryst. Sol. MeOH, C_6H_6, $CHCl_3$; poorly sol. H_2O.
Mp 208-210°. λ_{max} 333; 347; 361; 373 (MeOH) (Berdy). λ_{max} 235 (ϵ 23900); 292 (ϵ 10100); 335 (ϵ 2400); 347 (ϵ 2600) (hexane) (Berdy). λ_{max} 211 (ϵ 15900); 238 (ϵ 24900); 289 (ϵ 8700); 294 (ϵ 11500); 336 (ϵ 2800) (EtOH) (Berdy).

Rinehart, K.L. *et al., J.A.C.S.*, 1987, **109**, 3378-3387 (*isol, synth*)
Lake, R.J. *et al., Aust. J. Chem.*, 1989, **42**, 1201-1206 (*isol, pmr*)

7-Bromocavernicolenone B-271

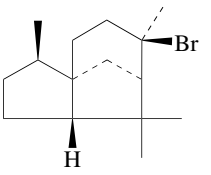


$C_8H_8BrNO_4$ 262.059
Isol. from the Mediterranean sponge *Aplysina cavernicola* (*Verongia cavernicola*). Mildly antibacterial *in vitro*. Needles (MeOH). Sol. MeOH, $CHCl_3$, butanol; poorly sol. H_2O.
Mp 165-170° dec. No observable opt. rotn. from 589 to 365 nm (MeOH). λ_{max} 254 (ϵ 2600) (MeOH) (Berdy).

Chloro analogue: ***7-Chlorocavernicolenone***
$C_8H_8ClNO_4$ 217.608
Metab. from the sponge *Aplysina (Verongia) cavernicola*.
Mp 197-198° dec. No opt. rotn. from 589 to 365 nm. A small excess of one of the enantiomers cannot be ruled out.

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1985, **68**, 1453 (*isol, uv, pmr, cmr, ms, cryst struct*)

3-Bromocedrane B-272

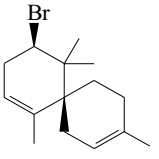


$C_{15}H_{25}Br$ 285.267

3β-*form*
Majusin
[193286-19-0]
Isol. from the red alga *Laurencia majuscula*.
Xu, X.-H. *et al., CA*, 1997, **127**, 146911k (*isol*)

10-Bromo-2,7-chamigradiene B-273

10-Bromo-α-chamigrene
[57473-87-7]

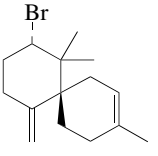


$C_{15}H_{23}Br$ 283.251
Metab. of *Laurencia pacifica* and *Laurencia glandulifera*. Oil. $[\alpha]_D$ -71.1 (c, 0.18 in $CHCl_3$). $[\alpha]_D$ -81 (c, 0.92 in $CHCl_3$).

Howard, B.M. *et al., Tet. Lett.*, 1976, 2519

10-Bromo-2,7(14)-chamigradiene B-274

[195734-65-7]

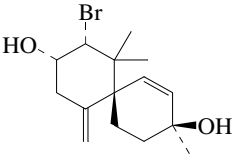


$C_{15}H_{23}Br$ 283.251
Constit. of *Laurencia rigida*. Oil.

König, G.M. *et al., J. Nat. Prod.*, 1997, **60**, 967-970 (*isol, pmr, cmr*)

10-Bromo-1,7(14)-chamigradiene-3,9-diol B-275

Rigidol
[195734-63-5]



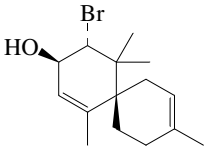
$C_{15}H_{23}BrO_2$ 315.25
Constit. of *Laurencia rigida*. Oil. $[\alpha]_D^{25}$ -6.5 (c, 1.37 in $CHCl_3$).

10-Epimer: ***Isorigidol***
[330583-36-3]
$C_{15}H_{23}BrO_2$ 315.25
Constit. of *Laurencia scoparia*. Cryst.
Mp 138-140°. $[\alpha]_D^{25}$ -115 (c, 0.32 in CH_2Cl_2).

König, G.M. *et al., J. Nat. Prod.*, 1997, **60**, 967-970 (*Rigidol, isol, pmr, cmr*)
Suescun, L. *et al., Acta Cryst. C*, 2001, **57**, 286-288 (*Isorigidol, cryst struct*)
Davyt, D. *et al., J. Nat. Prod.*, 2001, **64**, 1552-1555 (*Isorigidol, pmr, cmr, cryst struct*)

10-Bromo-2,7-chamigradien-9-ol B-276

[195734-61-3]

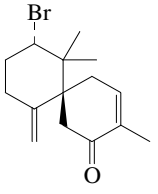


$C_{15}H_{23}BrO$ 299.25
Constit. of *Laurencia rigida*. Oil. $[\alpha]_D^{25}$ -49.4 (c, 0.95 in $CHCl_3$).

König, G.M. *et al., J. Nat. Prod.*, 1997, **60**, 967-970 (*isol, pmr, cmr*)

10-Bromo-2,7(14)-chamigradien-4-one B-277

[124899-51-0]



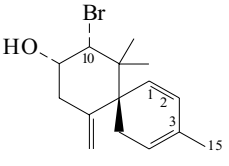
$C_{15}H_{21}BrO$ 297.234
Isol. from an unidentified *Aplysia* sp. and *Aplysia dactylomela*. Cryst.
Mp 134-135°. $[\alpha]_D^{20}$ -145 (c, 0.1 in MeOH).

Fedorov, S.N. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1989, **305**, 877-879 (*Aplysia constit.*)
Shubina, L.K. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2003, **52**, 1022-1026 (*Aplysia dactylomela constit*)

10-Bromo-1,3,7(14)-chamigratrien-9-ol B-278

2-Bromo-1,1,9-trimethylspiro[5.5]undeca-7,9-dien-3-ol, 9CI. ***Obtusadiene***

[113262-62-7]



$C_{15}H_{21}BrO$ 297.234
Constit. of the red alga *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ -52 (c, 2.8 in $CHCl_3$).

$\Delta^{3,15}$-Isomer: 10-Bromo-1,3(15),7(14)-chamigratrien-9-ol. ***Isoobtusadiene***
[113235-90-8]
$C_{15}H_{21}BrO$ 297.234
Constit. of *Laurencia obtusa*, *Laurencia cartilaginea* and *Laurencia majuscula*. Oil. $[\alpha]_D^{25}$ -11.7 (c, 0.7 in $CHCl_3$).

10-Epimer, 1,2-dihydro: ***10-Bromo-2,7(14)-chamigradien-9-ol***
[132342-59-7]
$C_{15}H_{23}BrO$ 299.25
Metab. of *Laurencia nipponica* and *Laurencia majuscula*. Oil. $[\alpha]_D$ -58.9 (c, 0.4 in $CHCl_3$).

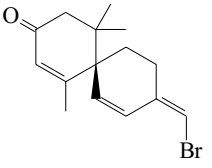
6,10-Diepimer, 1,2-dihydro: ***Dechloroelatol***
[61661-40-3]
$C_{15}H_{23}BrO$ 299.25
Constit. of *Laurencia rigida*. Shows antimycobacterial activity. Oil.

6,10-Diepimer, 1,2-dihydro, Ac: ***Acetyldechloroelatol***
[870480-96-9]
$C_{17}H_{25}BrO_2$ 341.287
Constit. of *Aplysia dactylomela*. Oil. $[\alpha]_D^{20}$ +53 (c, 0.3 in $CHCl_3$).

Gonzalez, A.G. *et al., Tet. Lett.*, 1976, **17**, 3051-3054 (*Dechloroelatol*)
Gerwick, W.H. *et al., J. Nat. Prod.*, 1987, **50**, 1131-1135 (*Obtusadiene, Isoobtusadiene*)
Wright, A.D. *et al., J. Nat. Prod.*, 1990, **53**, 845-861 (*Laurencia majuscula constits*)
König, G.M. *et al., Planta Med.*, 2000, **66**, 337-342 (*activity*)
Xu, X.-H. *et al., Chem. Res. Chin. Univ.*, 2002, **18**, 226-227 (*Isoobtusadiene*)
Dias, T. *et al., J. Nat. Prod.*, 2005, **68**, 1677-1679 (*Acetyldechloroelatol*)

15-Bromo-1,3(15),7-chamigratrien-9-one B-279

[71565-19-0]
[70449-77-3]

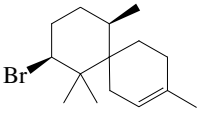


$C_{15}H_{19}BrO$ 295.218
Constit. of *Laurencia majuscula*. λ_{max} 240 (ϵ 30000) (EtOH) (Derep).

Suzuki, M. *et al., Tet. Lett.*, 1978, **19**, 4805-4808 (*isol, pmr*)
Suzuki, M. *et al., Tet. Lett.*, 1979, **20**, 879-882 (*abs config*)

10-Bromo-2-chamigrene B-280

[429683-20-5]

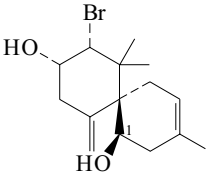


$C_{15}H_{25}Br$ 285.267
Constit. of *Laurencia majuscula*. Cryst. (MeOH).
Mp 124-125°.

Xu, X.-H. *et al., Chem. Res. Chin. Univ.*, 2002, **138**, 3226-227; *CA*, **137**, 182024p (*isol, pmr, cmr*)

10-Bromo-3-chamigrene-1,9-diol B-281

2-Bromo-3,11-dihydroxy-β-chamigrene



$C_{15}H_{23}BrO_2$ 315.249

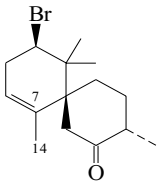
1-Ac: 1-Acetoxy-10-bromo-3-chamigren-9-ol. 11-Acetoxy-2-bromo-3-hydroxy-β-chamigrene
[126005-79-6]
$C_{17}H_{25}BrO_3$ 357.287
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ +49 (c, 0.13 in $CHCl_3$).

Di-Ac: 1,9-Diacetoxy-10-bromo-3-chamigrene. 3,11-Diacetoxy-2-bromo-β-chamigrene
[126005-80-9]
$C_{19}H_{27}BrO_4$ 399.324
Metab. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ +93 (c, 0.36 in $CHCl_3$).

Martin, J.D. *et al., Phytochemistry*, 1989, **28**, 3365 (*isol, pmr, cmr*)

10-Bromo-7-chamigren-2-one B-282

4-Bromo-α-chamigren-8-one



$C_{15}H_{23}BrO$ 299.25
Constit. of *Laurencia glandulifera*. Cryst.(MeOH).
Mp 78-79°. $[\alpha]_D$ -88 (c, 2.46 in $CHCl_3$).

$\Delta^{7(14)}$-Isomer: ***10-Bromo-7(14)-chamigren-2-one****. 4-Bromo-β-chamigren-8-one*
[53767-98-9]
$C_{15}H_{23}BrO$ 299.25
Constit. of the essential oil of *Laurencia glandulifera*.
Mp 116-117°. $[\alpha]_D$ -57.

Suzuki, M. *et al., Tet. Lett.*, 1974, 821 (*isol*)
Suzuki, M. *et al., Tetrahedron*, 1979, **35**, 823 (*abs config*)

Bromochloroacetic acid B-283

[5589-96-8]
ClCHBrCOOH
$C_2H_2BrClO_2$ 173.393
Constit. of the red alga *Asparagopsis taxiformis*.

(±)-form
Mp 31.5°. Bp 215° dec. Bp_{11} 103-104°.

Et ester: [22524-32-9]
$C_4H_6BrClO_2$ 201.447
Liq. Bp 174° dec. Bp_{12} 65°.

Chloride: [38282-29-0]
C_2HBrCl_2O 191.839
Bp 138-139°.

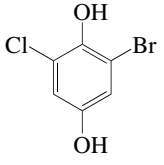
Amide: Bromochloroacetamide
[62872-34-8]
$C_2H_3BrClNO$ 172.408
Constit. of *Asparagopsis taxiformis*. Cryst. Sol. hot H_2O.
Mp 126° (117°).

Nitrile: Bromochloroacetonitrile. Bromochlorocyanomethane
[83463-62-1]
$C_2HBrClN$ 154.393
Detected in drinking water. Bp 138-140°.
▶ Exp. carcinogen. Exp. reprod. effects. AL8010000

Compton, H. *et al., J.C.S.*, 1921, 119; 1874 (*synth*)
Backer, H.J. *et al., J.C.S.*, 1928, 2125 (*synth*)
McBee, E.T. *et al., J.A.C.S.*, 1956, **78**, 4595 (*ester*)
Woolard, F.X. *et al., Tetrahedron*, 1976, **32**, 2843-2846 (*amide, isol*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617-620 (*isol*)
Oliver, B.G. *et al., Environ. Sci. Technol.*, 1983, **17**, 80 (*nitrile*)
Coleman, W.E. *et al., Environ. Sci. Technol.*, 1984, **18**, 674 (*ms, nitrile*)
IARC Monog., 1991, **52**, 269 (*rev, tox, nitrile*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BMY800

2-Bromo-6-chloro-1,4-benzenediol B-284

2-Bromo-6-chlorohydroquinone
[150900-92-8]



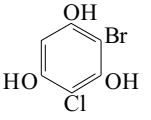
$C_6H_4BrClO_2$ 223.453
Isol. from the marine acorn worm *Ptychodera bahamensis*.

4-Ac: 4-Acetoxy-2-bromo-6-chlorophenol
[150900-93-9]
$C_8H_6BrClO_3$ 265.49
Isol. from *Ptychodera bahamensis*.

Corgiat, J.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1993, **106**, 83-86 (*isol*)

2-Bromo-4-chloro-1,3,5-benzenetriol B-285

Bromochlorophloroglucinol
[84754-06-3]

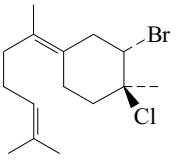


$C_6H_4BrClO_3$ 239.452
Constit. of *Rhabdonia verticillata*.

Blackman, A.J. *et al., Phytochemistry*, 1982, **21**, 2141 (*isol*)

2-Bromo-3-chloro-6,10-bisaboladiene B-286

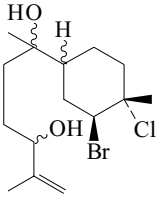
Preintricatol
[58307-76-9]



$C_{15}H_{24}BrCl$ 319.711
Identity with Preintricatol not certain. Constit. of a *Laurencia* sp. Oil. $[\alpha]_D^{25}$ +28.5 (c, 0.48 in $CHCl_3$).

König, G. *et al., J. Nat. Prod.*, 1994, **57**, 477 (*isol, pmr, cmr*)

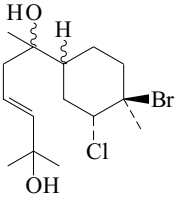
2-Bromo-3-chloro-11-bisabolene-7,10-diol B-287



$C_{15}H_{26}BrClO_2$ 353.726
Constit. of *Laurencia caespitosa*. Oil. $[\alpha]_D^{25}$ +162 (c, 0.14 in $CHCl_3$).

Norte, M. *et al., Phytochemistry*, 1992, **31**, 326 (*isol, pmr, cmr*)

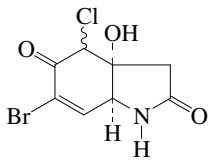
3-Bromo-2-chloro-9-bisabolene-7,11-diol B-288



$C_{15}H_{26}BrClO_2$ 353.726
Constit. of *Laurencia caespitosa*. Oil. $[\alpha]_D^{25}$ -35.2 (c, 0.29 in $CHCl_3$).

Norte, M. *et al., Phytochemistry*, 1992, **31**, 326 (*isol, pmr, cmr*)

5-Bromo-7-chlorocavernicolin B-289



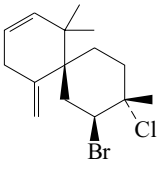
$C_8H_7BrClNO_3$ 280.505
Metab. from the Mediterranean sponge *Aplysina cavernicola (Verongia cavernicola)* (Verongidae). Racemic. Isol. as a mixt. of C(7)-epimerizing monoacetates.

[93253-82-8, 93269-61-5]

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1984, **67**, 1484 (*ms, struct*)

2-Bromo-3-chloro-7(14),9-chamigradiene B-290

Nidifidiene
[54928-02-8]

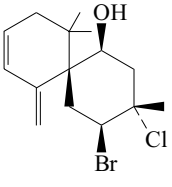


$C_{15}H_{22}BrCl$ 317.695
Constit. of *Laurencia nidifica*. Cryst.

Waraszkiewicz, S.M. *et al., Tet. Lett.*, 1974, 2003

2-Bromo-3-chloro-7(14),8-chamigradien-5-ol B-291

Nidifidienol
[55890-19-2]

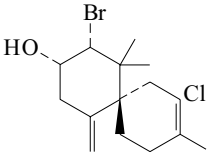


$C_{15}H_{22}BrClO$ 333.695
Constit. of *Laurencia nidifica*. Oil.

Waraszkiewicz, S.M. *et al., Tet. Lett.*, 1975, 281

10-Bromo-2-chloro-2,7(14)-chamigradien-9-ol B-292

Elatol
[55303-97-4]



$C_{15}H_{22}BrClO$ 333.695
Constit. of *Laurencia elata*, *Laurencia scoparia*, *Laurencia rigida*, *Laurencia cartilaginea* and *Aplysia dactylomela*. Shows antimycobacterial activity, cytotoxic agent, antifeeding agent, antimutagenic, antifouling agent. Oil. Sol. hexane. $[\alpha]_D$ +83.5 (c, 0.365 in MeOH).

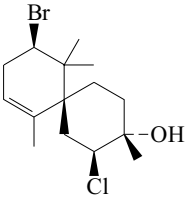
Ac: ***Acetylelatol***
[55196-02-6]
$C_{17}H_{24}BrClO_2$ 375.732
Constit. of *Aplysia dactylomela*. Cryst. (hexane).
Mp 157-158°. $[\alpha]_D^{20}$ +173 (c, 0.086 in $CHCl_3$).

Debromo: 2-Chloro-2,7(14)-chamigradien-9-ol. ***Debromoelatol***
[61661-37-8]
$C_{15}H_{23}ClO$ 254.799
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ +98.

Sims, J.J. *et al., Tet. Lett.*, 1974, 3487-3490 (*Elatol, cryst struct, abs config*)
Gonzalez, A.G. *et al., Tet. Lett.*, 1976, **17**, 3051-3054 (*Elatol, Debromoelatol*)
Schmitz, F.J. *et al., J.A.C.S.*, 1982, **104**, 6415-6423 (*Elatol*)
Martin, J.D. *et al., Phytochemistry*, 1989, **28**, 3365-3367 (*Debromoelatol*)
König, G.M. *et al., J. Nat. Prod.*, 1997, **60**, 967-970 (*isol, pmr, cmr*)
König, G.M. *et al., Planta Med.*, 2000, **66**, 337-342 (*activity*)
Bansemir, A. *et al., Chem. Biodiversity*, 2004, **1**, 463-467 (*Elatol*)
Dias, T. *et al., J. Nat. Prod.*, 2005, **68**, 1677-1679 (*Acetylelatol*)

10-Bromo-2-chloro-7-chamigren-3-ol B-293

Glanduliferol
[54278-86-3]

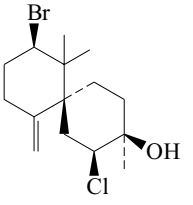


$C_{15}H_{24}BrClO$ 335.711
Constit. of *Laurencia glandulifera*. Gum. $[\alpha]_D$ -21.7 (c, 1.7 in $CHCl_3$).

Suzuki, M. *et al., Tet. Lett.*, 1974, 1807 (*isol*)
Suzuki, M. *et al., Tetrahedron*, 1979, **35**, 823 (*abs config*)

10-Bromo-2-chloro-7(14)-chamigren-3-ol B-294

Hurgadol

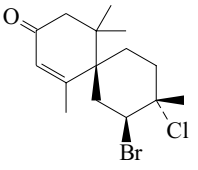


$C_{15}H_{24}BrClO$ 335.711
Metab. of *Laurencia obtusa*. Cryst.
Mp 121°. $[\alpha]_D$ -1.7 (c, 0.71 in $CHCl_3$).

Ayyad, S.-E.N. *et al., Phytochemistry*, 1990, **29**, 3193 (*isol, pmr, cmr, ms, cryst struct*)

2-Bromo-3-chloro-7-chamigren-9-one B-295

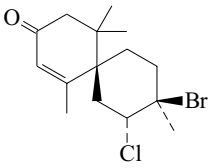
Laurencenone D
[116384-28-2]



$C_{15}H_{22}BrClO$ 333.695
Metab. of *Laurencia obtusa*. Solid.

Kennedy, D.J. *et al., Phytochemistry*, 1988, **27**, 1761

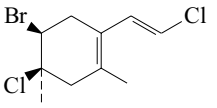
3-Bromo-2-chloro-7-chamigren-9-one B-296
Laurencenone A
[73465-61-9]



$C_{15}H_{22}BrClO$ 333.695
Metab. of *Laurencia obtusa*. Oil.

Kennedy, D.J. *et al., Phytochemistry*, 1988, **27**, 1761

5-Bromo-4-chloro-1-chloroethenyl-2,4-dimethylcyclohexene B-297
[66321-22-0]

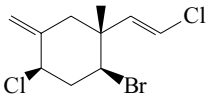


$C_{10}H_{13}BrCl_2$ 284.022
Constit. of *Plocamium cartilagineum*.
Mp 104-105°. $[\alpha]_D^{23}$ -13.2 (c, 1.1 in $CHCl_3$).

1α,2α-Epoxide: ***5-Bromo-4-chloro-1-(chloroethenyl)-1,2-epoxy-2,4-dimethylcyclohexane***
[213995-37-0]
$C_{10}H_{13}BrCl_2O$ 300.022
Constit. of *Plocamium cartilagineum*.
Mp 49-50°. $[\alpha]_D$ -48 (c, 0.4 in $CHCl_3$).

Norton, R.S. *et al., Tet. Lett.*, 1977, 3905 (*isol, cmr*)
Higgs, M.D. *et al., Tetrahedron*, 1977, **33**, 2775 (*isol*)
Abreu, P.M. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 610-611 (*epoxide*)

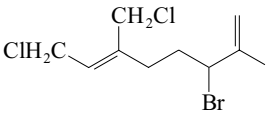
2-Bromo-4-chloro-1-(2-chloroethenyl)-1-methyl-5-methylenecyclohexane, 9CI B-298
[119903-45-6]



$C_{10}H_{13}BrCl_2$ 284.022
Constit. of *Plocamium hamatum*. Oil. $[\alpha]_D$ -34 (c, 0.008 in $CHCl_3$).

Coll, J.C. *et al., Aust. J. Chem.*, 1988, **41**, 1743
Whitney, J.M. *et al., J.O.C.*, 1997, **62**, 8962-8963 (*synth*)

3-Bromo-8-chloro-6-chloromethyl-2-methyl-1,6-octadiene B-299

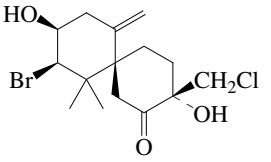


$C_{10}H_{15}BrCl_2$ 286.038

(3ξ,6Z)-form [125537-99-7]
Constit. of *Chondrococcus hornemanni* and *Portieria hornemanni*.
Oil. $[\alpha]_D$ -22.5 (c, 0.008 in $CHCl_3$).

Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1983 (*isol, pmr, cmr*)
Wright, A.D. *et al., J. Nat. Prod.*, 1990, **53**, 845-861 (*isol*)

10-Bromo-15-chloro-3,9-dihydroxy-7(14)-chamigren-2-one B-300
[68370-43-4]

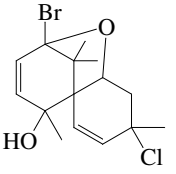


$C_{15}H_{22}BrClO_3$ 365.694
Constit. of *Laurencia obtusa*.

Di-Ac:
$C_{19}H_{26}BrClO_5$ 449.768
Cryst. Mp 217-219°.

González, A.G. *et al., Tet. Lett.*, 1978, **19**, 2035-2036 (*isol, pmr, cryst struct*)

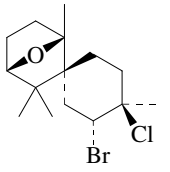
10-Bromo-3-chloro-1,10-epoxy-4,8-chamigradien-7-ol B-301
[168850-82-6]



$C_{15}H_{20}BrClO_2$ 347.679
Constit. of *Aplysia dactylomela*.

Rao, C.B. *et al., CA*, 1995, **123**, 251787q (*isol*)

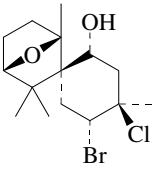
2-Bromo-3-chloro-7,10-epoxychamigrane B-302
Oxachamigrene
[443752-18-9]



$C_{15}H_{24}BrClO$ 335.711
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ -10.2 (c, 0.3 in $CHCl_3$).

Brito, I. *et al., J. Nat. Prod.*, 2002, **65**, 946-948 (*isol, pmr, cmr*)

2-Bromo-3-chloro-7,10-epoxy-5-chamigranol B-303



$C_{15}H_{24}BrClO_2$ 351.71

Ac: ***5-Acetoxyoxachamigrene***
[443785-07-7]
$C_{17}H_{26}BrClO_3$ 393.747
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ -4.3 (c, 0.2 in $CHCl_3$).

Stereoisomer, Ac: ***Cyclodebromoacetoxyintricatol***
[58307-77-0]
$C_{17}H_{26}BrClO_3$ 393.747

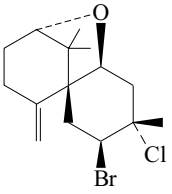
Constit. of *Laurencia intricata*.

White, R.H. *et al., CA*, 1976, **84**, 71515 (*Cyclodebromoacetoxyintricatol*)
Brito, I. *et al., J. Nat. Prod.*, 2002, **65**, 946-948 (*5-Acetoxyoxachamigrene*)

2-Bromo-3-chloro-5,10-epoxy-7(14)-chamigrene B-304

Nidifocene

[60545-17-7]

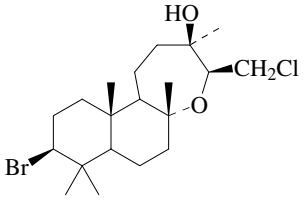


$C_{15}H_{22}BrClO$ 333.695

Constit. of *Laurencia nidifica*. Cryst. (hexane).
Mp 79-81°.

Waraszkiewicz, S.M. *et al., Tet. Lett.*, 1977, 2311 (*isol, cryst struct*)
Miyashita, K. *et al., Chem. Pharm. Bull.*, 1993, **41**, 465 (*synth*)

3-Bromo-15-chloro-8,14-epoxy-13-labdanol B-305



$C_{20}H_{34}BrClO_2$ 421.844

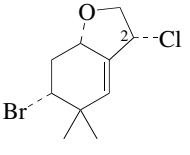
(3β,8α,13β,14*S*)-*form* [611230-86-5]

Constit. of *Laurencia obtusa*.
Oil. $[\alpha]_D^{20}$ +6.2 (c, 0.13 in $CHCl_3$). λ_{max} 230 (log ϵ 2.92) (hexane).

Iliopoulou, D. *et al., J. Nat. Prod.*, 2003, **66**, 1225-1228 (*isol, pmr, cmr*)

6-Bromo-2-chloro-1,4-epoxy-3(8)-ochtodene B-306

6-Bromo-3-chloro-2,3,5,6,7,7a-hexahydro-5,5-dimethylbenzofuran



(2*R**,4*R**,6a*S**)-*form*

$C_{10}H_{14}BrClO$ 265.577

(2*R,4*R**,6a*S**)-*form*** [112710-64-2]

Constit. of the red alga *Chondrococcus hornemanni*.
$[\alpha]_D$ -92.6 (c, 0.005 in $CHCl_3$).

(2*S,4*R**,6a*S**)-*form*** [112642-63-4]

Constit. of the red alga *Chondrococcus hornemanni*.
Yellow oil. $[\alpha]_D$ +7.8 (c, 0.03 in $CHCl_3$).

Coll, J.C. *et al., Aust. J. Chem.*, 1987, **40**, 1893-1900 (*isol, ir, pmr, cmr, ms*)

1-Bromo-2-chloroethane B-307

Ethylene bromochloride

[107-04-0]

$BrCH_2CH_2Cl$

C_2H_4BrCl 143.41

Isol. from the alga *Cytoseira barbata*. Insecticide used to fumigate soil. Now superseded. Liq. d_4^{20} 1.74.
Fp -16.7. Bp 107°.

► Eye, skin and mucous membrane irritant. LD_{50} (rat, orl) 64 mg/kg. Hepatotoxic, nephrotoxic. Fl. p. >107°. KH6500000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 72B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 107B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 104A (*ir*)
Kharasch, M.S. *et al., J.A.C.S.*, 1934, **28**, 712 (*synth*)
Lorenz, J. *et al., Angew. Chem., Int. Ed.*, 1965, **4**, 241 (*synth*)
Pesticide Manual, 9th edn., 1991, No. 1310
Milkova, T. *et al., Phytochemistry*, 1996, **45**, 93 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CES500

2-Bromo-1-chloroethanol B-308

$BrCH_2CHClOH$

C_2H_4BrClO 159.41

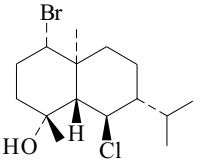
Isol. from the alga *Cytoseira barbata*.

(±)-*form*

Ac: [51483-37-5]
$C_4H_6BrClO_2$ 201.447
Bp_{25} 80-81° Bp_{10} 64-65°.

Negoro, T. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 2111 (*synth, Ac*)
Milkova, T. *et al., Phytochemistry*, 1997, **45**, 93 (*isol*)

1-Bromo-6-chloro-4-eudesmanol B-309



$C_{15}H_{26}BrClO$ 337.726

(1α,4α,5β,6β,7α,10α)-*form*

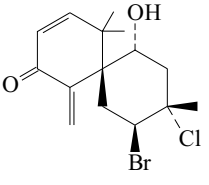
Heterocladol

[65746-13-6]

Constit. of *Laurencia filiformis*.
Cryst. (petrol).
Mp 78-79°. $[\alpha]_D$ +13.8 (c, 1 in $CHCl_3$).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1977, **30**, 2679 (*cryst struct*)

2-Bromo-3-chloro-5-hydroxy-7(14),9-chamigradien-8-one B-310



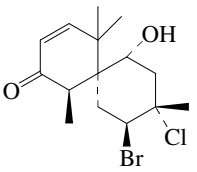
$C_{15}H_{20}BrClO_2$ 347.678

Ac: [102107-17-5]
$C_{17}H_{22}BrClO_3$ 389.716
From *Aplysia dactylomela*. Cryst.
Mp 105-106°. $[\alpha]_D^{20}$ -27.8 (c, 0.54 in $CHCl_3$).

Enantiomer, Ac:
$C_{17}H_{22}BrClO_3$ 389.716
Constit. of *Laurencia majuscula*.

Sakai, R. *et al., Helv. Chim. Acta*, 1986, **69**, 91
Masuda, M. *et al., Phycol. Res.*, 1997, **45**, 59-64; *CA*, **127**, 133150 (*Laurencia majuscula constit*)

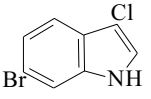
2-Bromo-3-chloro-5-hydroxy-9-chamigren-8-one B-311
Pinnatifinone
[141361-46-8]



$C_{15}H_{22}BrClO_2$ 349.694
Isol. from *Laurencia pinnatifida*.

Ahmad, V.U. *et al., Sci. Pharm.*, 1991, **59**, 243-246 (*isol, struct*)

6-Bromo-3-chloro-1*H*-indole, 9CI B-312
[57916-08-2]



C_8H_5BrClN 230.491
Isol. from the yellow hemichordate *Ptychodera flava laysanica* and from *Ptychodera flava*.
Mp 55-57° (54.5-56.5°).

Ac: Mp 158-159°.

Higa, T. *et al., Naturwissenschaften*, 1975, **62**, 395 (*isol, struct*)
Higa, T. *et al., Heterocycles*, 1976, **4**, 231 (*synth, ir, pmr, ms*)
Higa, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **65**, 525 (*isol*)

Bromochloroiodomethane, 9CI B-313
[34970-00-8]
CHBrClI
CHBrClI 255.28
Occurs in small amounts in the oil of the alga *Asparagopsis taxiformis*. d_4^{24} 2.8.
Mp -24.5°. Bp 163° Bp_{30} 68-69°.

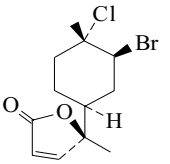
Hine, J. *et al., J.A.C.S.*, 1958, **80**, 4282 (*synth*)
Burreson, B.J. *et al., Tet. Lett.*, 1975, 473 (*occur*)
Somayajulu, G. *et al., J. Magn. Reson.*, 1979, **33**, 559 (*cmr*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)

Bromochloromethane, 9CI, 8CI B-314
Methylene bromochloride. Methylene chlorobromide. Halon 1011. MIL-B 4394B
[74-97-5]
$BrCH_2Cl$
CH_2BrCl 129.384
Isol. from several marine algae. Intermed. for org. synth., fire extinguishant. Liq. with sweet odour. d_{25}^{25} 1.93.
Fp -88. Bp 67.8°.

▶ Eye, skin and respiratory tract irritant. High conc. narcotic. LD_{50} (rat, orl) 5 g/kg. OES: long-term 200 ppm; short-term 250 ppm.
PA5250000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 71B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 105B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 102B (*ir*)
Henry, L. *et al., J. Prakt. Chem.*, 1885, **32**, 431 (*synth*)
Stevens, C.L. *et al., J.A.C.S.*, 1956, **78**, 2264 (*synth*)
Caws, A.C. *et al., J. Pharm. Pharmacol.*, 1957, **9**, 824 (*synth*)
Litchman, W.M. *et al., J.A.C.S.*, 1968, **90**, 1400 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **4**, 569
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 168
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CES650

5-(3-Bromo-4-chloro-4-methylcyclohexyl)-5-methyl-2(5*H*)-furanone B-315

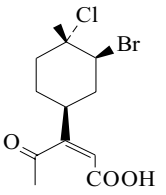


Absolute configuration

$C_{12}H_{16}BrClO_2$ 307.614
Metabolite of red alga *Laurencia caespitosa*.
Mp 122-123°. $[\alpha]_D$ +16 (c, 0.23 in $CHCl_3$).

Estrada, D.M. *et al., Tet. Lett.*, 1987, **28**, 687 (*cryst struct*)

3-(3-Bromo-4-chloro-4-methylcyclohexyl)-4-oxo-2-pentenoic acid, 9CI B-316



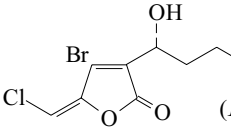
Absolute configuration

$C_{12}H_{16}BrClO_3$ 323.613

Me ester: [112515-90-9]
$C_{13}H_{18}BrClO_3$ 337.64
Metabolite of red alga *Laurencia caespitosa*. Cryst.
Mp 52-53°. $[\alpha]_D$ +37 (c,0.14 in $CHCl_3$).

Estrada, D.M. *et al., Tet. Lett.*, 1987, **28**, 687 (*cryst struct*)

4-Bromo-5-(chloromethylene)-3-(1-hydroxybutyl)-2(5*H*)-furanone B-317



(*R*)–(*E*)–*form*

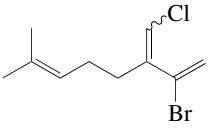
$C_9H_{10}BrClO_3$ 281.533

(*R*)-(*E*)-*form* [63025-31-0]
Constit. of the red alga *Delisea pulchra*.
Yellow oil.

(*R*)-(*Z*)-*form* [63025-32-1]
Constit. of *Delisea pulchra*.
Yellow oil. $[\alpha]_D^{25}$ +9 (c, 0.5 in $CHCl_3$).

de Nys, R. *et al., Tetrahedron*, 1993, **49**, 11213 (*isol, pmr, cmr*)

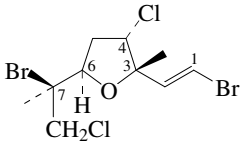
2-Bromo-3-(chloromethylene)-7-methyl-1,6-octadiene B-318
2-Bromo-10-chloro-β-myrcene
[55498-43-6]



$C_{10}H_{14}BrCl$ 249.577
Tentative struct. Constit. of *Chondrococcus hornemanni* (*Portieria hornemannii*).

Ichikawa, N. *et al., Chem. Lett.*, 1974, 1333-1336 (*isol, ms*)

5-(1-Bromo-2-chloro-1-methylethyl)-2-(2-bromoethenyl)-3-chlorotetrahydro-2-methylfuran B-319
1,7-Dibromo-4,8-dichloro-3,6-epoxy-3,7-dimethyl-1-octene

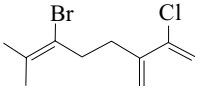


$C_{10}H_{14}Br_2Cl_2O$ 380.933
Terpenoid numbering shown.

(1E,3R*,4R*,6R*,7R*)-form [479072-74-7]
Constit. of *Plocamium cartilagineum*.
Oil. $[\alpha]_D^{25}$ -153 (c, 0.02 in $CHCl_3$).

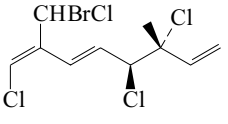
4-Dechloro, 4α-bromo: ***3-Bromo-5-(1-bromo-2-chloro-1-methylethyl)-2-(2-bromoethenyl)tetrahydro-2-methylfuran***. *1,4,7-Tribromo-8-chloro-3,6-epoxy-3,7-dimethyl-1-octene*
[479072-75-8]
$C_{10}H_{14}Br_3ClO$ 425.385
Constit. of *Plocamium cartilagineum*. Oil. $[\alpha]_D^{25}$ -120 (c, 0.01 in $CHCl_3$).
Díaz-Marrero, A.R. *et al., Tetrahedron*, 2002, **58**, 8539-8542 (*isol, pmr, cmr*)

6-Bromo-2-chloro-7-methyl-3-methylene-1,6-octadiene B-320
6-Bromo-2-chloromyrcene
[55498-42-5]



$C_{10}H_{14}BrCl$ 249.577
Constit. of *Chondrococcus hornemanni*. Oil.
Ichikawa, N. *et al., Chem. Lett.*, 1974, 1333-1336 (*isol, ms*)
Burreson, B.J. *et al., Chem. Lett.*, 1975, 1111-1114 (*cmr*)

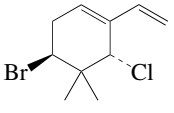
2-(Bromochloromethyl)-1,5,6-trichloro-6-methyl-1,3,7-octatriene, 9CI B-321
[89197-88-6]



$C_{10}H_{11}BrCl_4$ 352.912
Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O.

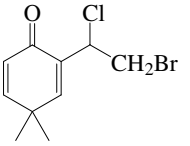
(3R*,4S*,5E,7E)-form
Constit. of *Plocamium cartilagineum*.
Oil.
Crews, P. *et al., J.O.C.*, 1984, **49**, 1371 (*isol, struct, cmr*)

6-Bromo-8-chloro-1,3-ochtodadiene B-322
[159125-50-5]
[67237-07-4]



$C_{10}H_{14}BrCl$ 249.577
Constit. of *Portieria hornemannii*. λ_{max} 233 (ε 15400) (MeOH).
McConnell, O.J. *et al., J.O.C.*, 1978, **43**, 4238-4241 (*synth, pmr*)
Fuller, R.W. *et al., J. Med. Chem.*, 1994, **34**, 4407-4411 (*isol*)

1-Bromo-2-chloro-3(8),5-ochtodadien-4-one B-323
2-(2-Bromo-1-chloroethyl)-4,4-dimethyl-2,5-cyclohexadien-1-one
[104499-91-4]



$C_{10}H_{12}BrClO$ 263.561
Constit. of the red alga *Portieria hornemanni*. Oil. $[\alpha]_D^{24}$ -9.4 (c, 2.49 in CCl_4).
Kuniyoshi, M. *et al., J. Chin. Chem. Soc. (Taipei)*, 2003, **50**, 167-170 (*isol, pmr, cmr*)

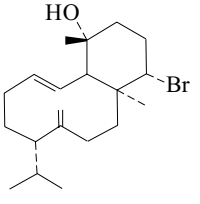
1-Bromo-3-chloro-2-propanone B-324
3-Bromo-1-chloroacetone
[53535-68-5]
$BrCH_2COCH_2Cl$
C_3H_4BrClO 171.421
Isol. from *Asparagopsis taxiformis*.
Mp 34-35°. Bp 178-180°.

2,4-Dinitrophenylhydrazone: Mp 118-119°.

Di-Me acetal: 1-Bromo-3-chloro-2,2-dimethoxypropane
[22089-54-9]
$C_5H_{10}BrClO_2$ 217.489
Mp 69.5-70.5°.
Bankowska, Z. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1959, **33**, 1039; *CA*, **54**, 6525 (*synth*)
Baucom, K.B. *et al., J.O.C.*, 1972, **37**, 1730
Fenical, W. *et al., Tet. Lett.*, 1974, **15**, 4463-4466 (*isol*)

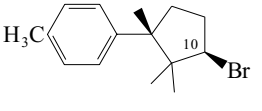
Bromocontryphan B-325
[186821-81-8]
Gly-Cys-Hyp-D-Trp-Glu-Pro-Trp*-Cys-NH_2
$C_{45}H_{54}BrN_{11}O_{11}S_2$ 1069.025
Peptide containing 6-bromotryptophan (Trp*) and 4-hydroxyproline (Hyp) residues. Isol. from venom of *Conus radiatus*.
Jimenez, E.C. *et al., Biochemistry*, 1997, **36**, 989-994 (*isol*)

Bromocorodienol B-326
[92675-10-0]



$C_{20}H_{33}BrO$ 369.384
Constit. of red alga *Sphaerococcus coronopifolius*. Cryst. (MeCN). Mp 89-91°. $[\alpha]_D$ +34.3 (c, 1.5 in $CHCl_3$).
Cafieri, F. *et al., Tet. Lett.*, 1984, **25**, 3141

α-Bromocuparene B-327
1-(3-Bromo-1,2,2-trimethylcyclopentyl)-4-methylbenzene, 9CI. Bromocuparene
[57794-64-6]

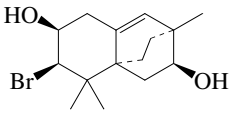


$C_{15}H_{21}Br$ 281.235

Constit. of *Laurencia* spp. Oil. $[\alpha]_D$ +23 (c, 0.95 in $CHCl_3$).

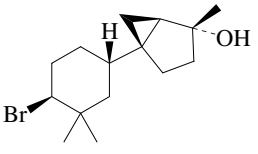
10-Epimer: ***α-Isobromocuparene***
[57766-60-6]
$C_{15}H_{21}Br$ 281.235
Constit. of *Laurencia* spp. Oil. $[\alpha]_D$ +91 (c, 0.87 in $CHCl_3$).
Suzuki, T. *et al., Tet. Lett.*, 1975, 3057

10-Bromo-3,14-cyclo-7(14)-chamigrene-2,9-diol B-328
[488834-25-9]



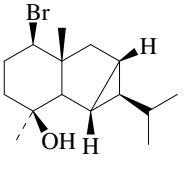
$C_{15}H_{23}BrO_2$ 315.25
Constit. of *Caloglossa leprieurii*. Cryst.
Mp 104-105°.
Xu, X.H. *et al., Chin. Chem. Lett.*, 2002, **13**, 953-954 (*isol, pmr, cmr*)

Bromocyclococanol B-329
[439612-81-4]



$C_{15}H_{25}BrO$ 301.266
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ +7.3 (c, 0.2 in $CHCl_3$).
Brito, I. *et al., Tet. Lett.*, 2002, **43**, 2551-2553 (*isol, pmr, cmr*)

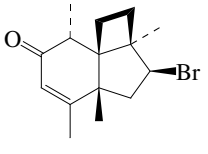
1-Bromo-6,8-cyclo-4-eudesmanol B-330



$C_{15}H_{25}BrO$ 301.266

(1β,4β,6β*H*,8β*H*)-*form* [479633-71-1]
Constit. of *Laurencia microcladia*.
Oil. $[\alpha]_D^{20}$ +10 (c, 0.13 in MeOH).
Guella, G. *et al., Z. Naturforsch., B*, 2002, **57**, 1147-1151 (*isol, pmr, cmr*)

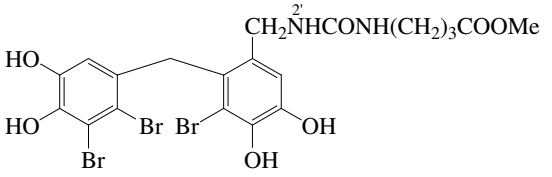
7-Bromo-8,11-cyclo-3-perforen-2-one B-331



$C_{15}H_{21}BrO$ 297.234

(1α,7β,8*R*,11*S*)-*form* [874193-59-6]
Constit. of *Laurencia obtusa*.
Oil. $[\alpha]_D^{20}$ -40.4 (c, 0.14 in CH_2Cl_2). λ_{max} 228 (log ϵ 4.1) (hexane).
Kladi, M. *et al., Tetrahedron*, 2006, **62**, 182-189 (*Laurencia obtusa constit*)

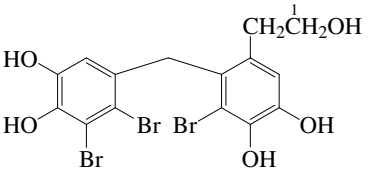
***N*-[3-Bromo-2-(2,3-dibromo-4,5-dihydroxybenzyl)-4,5-dihydroxybenzyl]-*N′*-(3-methoxycarbonylpropyl)urea** B-332
Methyl N′*-[3-bromo-(2,3-dibromo-4,5-dihydroxybenzyl)-4,5-dihydroxybenzyl] γ-ureidobutyrate*



$C_{20}H_{21}Br_3N_2O_7$ 641.107
Constit. of *Rhodomela confervoides*. Brown powder.
Mp 176-178°.

$N^{2'}$*-(2,3-Dibromo-4,5-dihydroxybenzyl):*
$C_{27}H_{25}Br_5N_2O_9$ 921.023
Constit. of *Rhodomela confervoides*. Brown gum.
Ma, M. *et al., J. Nat. Prod.*, 2006, **69**, 206-210 (*isol, pmr, cmr, ms*)

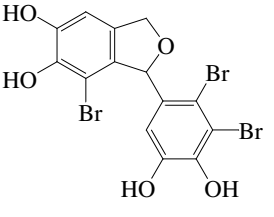
2-(3-Bromo-2-(2,3-dibromo-4,5-dihydroxybenzyl)-4,5-dihydroxyphenyl)ethanol B-333



$C_{15}H_{13}Br_3O_5$ 512.977

1-Sulfate:
$C_{15}H_{13}Br_3O_8S$ 593.041
Constit. of *Rhodomela confervoides*. Brown gum. λ_{max} 209 (log ϵ 4.75); 290 (log ϵ 3.68) (MeOH).
Ma, M. *et al., J. Nat. Prod.*, 2006, **69**, 206-210 (*isol, pmr, cmr, ms*)

7-Bromo-1-(2,3-dibromo-4,5-dihydroxyphenyl)-1,3-dihydro-5,6-isobenzofurandiol B-334
7-Bromo-1-(2,3-dibromo-4,5-dihydroxyphenyl)-1,3-dihydro-5,6-dihydroxyisobenzofuran

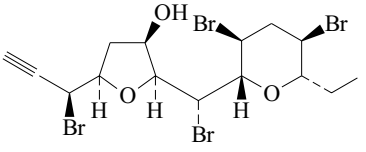


$C_{14}H_9Br_3O_5$ 496.934

(+)-*form*
Constit. of the brown alga *Leathesia nana*.
Brown powder (Me_2CO).
Mp 132-134°. $[\alpha]_D^{20}$ +6 (c, 0.16 in MeOH).
Xu, X. *et al., J. Nat. Prod.*, 2004, **67**, 1661-1666 (*isol, pmr, cmr, ms*)

2-[Bromo(3,5-dibromo-6-ethyltetrahydro-2*H*-pyran-2-yl)methyl]-5-(1-bromo-2-propynyl)tetrahydro-3-furanol, 9CI B-335

3,8,10,12-Tetrabromo-4,7:9,13-diepoxy-1-pentadecyn-6-ol
[132194-44-6]

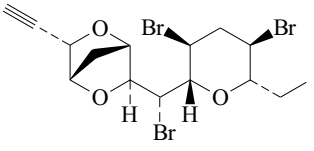


$C_{15}H_{20}Br_4O_3$ 567.937
Isol. from the sponge *Mycale rotalis* and the alga *Laurencia paniculata*. Cryst. (Et_2O/hexane).
Mp 142-143°. $[\alpha]_D^{25}$ +28.9 (c, 0.8 in $CHCl_3$).

Giordano, F. *et al., Chem. Comm.*, 1990, 1559
Imre, S. *et al., Z. Naturforsch., C*, 1995, **50**, 743 (*isol, ir, pmr, cmr*)

3-[Bromo(3,5-dibromo-6-ethyltetrahydro-2*H*-pyran-2-yl)methyl]-6-ethynyl-2,5-dioxabicyclo[2.2.1]heptane, 9CI B-336

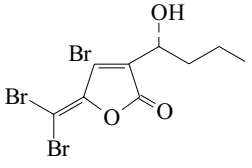
8,10,12-Tribromo-3,6:4,7:9,13-triepoxy-1-pentadecyne
[132194-45-7]



$C_{15}H_{19}Br_3O_3$ 487.025
Isol. from the sponge *Mycale rotalis* and the alga *Laurencia paniculata*. Cryst. (Et_2O/hexane).
Mp 145-147°.

Giordano, F. *et al., Chem. Comm.*, 1990, 1559 (*isol, struct*)
Imre, S. *et al., Z. Naturforsch., C*, 1995, **50**, 743 (*isol*)

4-Bromo-5-(dibromomethylene)-3-(1-hydroxybutyl)-2(5*H*)-furanone B-337



$C_9H_9Br_3O_3$ 404.88

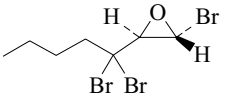
(*R*)-*form* [63025-33-2]
Constit. of the red alga *Delisea pulchra*.
Oil. $[\alpha]_D^{25}$ +16 (c, 1 in $CHCl_3$).

Ac: 3-(1-Acetoxybutyl)-4-bromo-5-(dibromomethylene)-2(5H)-furanone
[63025-26-3]
$C_{11}H_{11}Br_3O_4$ 446.918
Constit. of *Delisea pulchra*. Oil. $[\alpha]_D^{25}$ +6.6 (c, 1 in $CHCl_3$).

de Nys, R. *et al., Tetrahedron*, 1993, **49**, 11213 (*isol, pmr, cmr*)

2-Bromo-3-(1,1-dibromopentyl)oxirane, 9CI B-338

1,3,3-Tribromo-1,2-epoxyheptane. 1,3,3-Tribromo-1-heptene oxide



Relative configuration

$C_7H_{11}Br_3O$ 350.875

(2*R,3*S**)-*form*** [66002-41-3]
Metab. of *Bonnemaisonia nootkana* and *Bonnemaisonia hamifera*. $[\alpha]_D^{20}$ +78.6 (c, 6 in $CHCl_3$).

[69394-14-5]

Jacobsen, N. *et al., Tet. Lett.*, 1978, 3065 (*synth, pmr, ms, isol*)
Young, D.N. *et al., Phytochemistry*, 1981, **20**, 2335 (*biosynth*)

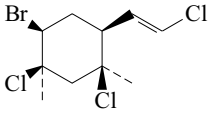
1-Bromo-3,4-dichloro-3-buten-2-one, 9CI B-339

[70442-42-1]
$ClCH{=}CClCOCH_2Br$
$C_4H_3BrCl_2O$ 217.877
Isol. from *Asparagopsis taxiformis*.

Fenical, W. *et al., Proc. Int. Seaweed Symp.*, 1977, **9**, 387-400; *CA*, **91**, 14474y (*synth*)

4-Bromo-1,5-dichloro-2-chloroethenyl-1,5-dimethylcyclohexane B-340

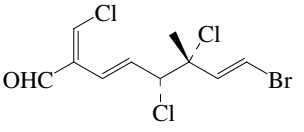
[66389-42-2]



$C_{10}H_{14}BrCl_3$ 320.483
Constit. of *Plocamium cartilagineum*.

Norton, R.S. *et al., Tet. Lett.*, 1977, 3905 (*cmr*)
Crews, P. *et al., J.O.C.*, 1984, **49**, 1371 (*cmr, struct*)

8-Bromo-5,6-dichloro-2-chloromethylene-6-methyl-3,7-octadienal B-341

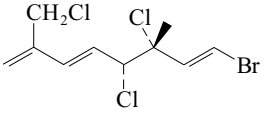


$C_{10}H_{10}BrCl_3O$ 332.451

(2*E*,3*E*,5*R*,6*R*,7*E*)-*form* [260973-20-4]
Constit. of *Plocamium cartilagineum*.
Oil. $[\alpha]_D$ +50.8 (c, 0.128 in CH_2Cl_2). λ_{max} 234 (log ϵ 3.98); 261 (log ϵ 3.98) (CH_2Cl_2).

Jongaramruong, J. *et al., J. Nat. Prod.*, 2000, **63**, 272-275 (*isol, pmr, cmr*)

1-Bromo-3,4-dichloro-7-chloromethyl-3-methyl-1,5,7-octatriene B-342

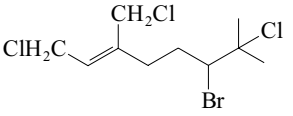


$C_{10}H_{12}BrCl_3$ 318.467
Metab. of *Plocamium cartilagineum*. Yellow oil. $[\alpha]_D^{22}$ +4.4 (c, 0.16 in $CHCl_3$). λ_{max} 228 (ϵ 6600) (hexane) (Berdy).

König, G.M. *et al., J. Nat. Prod.*, 1990, **53**, 1615 (*isol, pmr, cmr*)

6-Bromo-1,7-dichloro-3-chloromethyl-7-methyl-2-octene, 9CI B-343

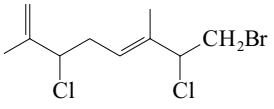
[136980-50-2]



$C_{10}H_{16}BrCl_3$ 322.499
Constit. of *Portieria hornemannii*. Oil. $[\alpha]_D^{25}$ +47 (c, 0.12 in $CHCl_3$).

Wright, A.D. *et al., Tetrahedron*, 1991, **47**, 5717 (*isol, pmr, cmr*)

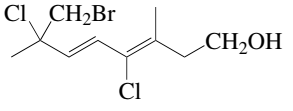
8-Bromo-3,7-dichloro-2,6-dimethyl-1,5-octadiene B-344



$C_{10}H_{15}BrCl_2$ 286.038

(E)-form [73328-38-8]
Constit. of *Plocamium angustum*.
Oil. $[\alpha]_D^{20}$ +19 (c, 0.5 in $CHCl_3$).
Dunlop, R.W. *et al., Aust. J. Chem.*, 1979, **32**, 2735

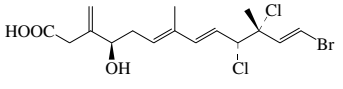
8-Bromo-4,7-dichloro-3,7-dimethyl-3,5-octadien-1-ol B-345



$C_{10}H_{15}BrCl_2O$ 302.037

(3Z,5E)-form
Ac: [188000-16-0]
$C_{12}H_{17}BrCl_2O_2$ 344.075
Constit. of *Aplysia punctata*. Oil. $[\alpha]_D^{25}$ -4.8 (c, 0.2 in $CHCl_3$). λ_{max} 250 (ϵ 9300) (MeOH).
Ortega, M.J. *et al., J. Nat. Prod.*, 1997, **60**, 482-484 (*isol, pmr, cmr*)

13-Bromo-10,11-dichloro-4-hydroxy-7,11-dimethyl-3-methylene-6,8,12-tridecatrienoic acid B-346



(4R,6E,8E,10R,11R,12E)-form

$C_{16}H_{21}BrCl_2O_3$ 412.15

(4R,6E,8E,10R,11R,12E)-form [353754-82-2]
Constit. of *Plocamium cartilagineum*.
$[\alpha]_D$ +30.1 (c, 0.14 in MeOH). λ_{max} 243 (log ϵ 2.37) (EtOH).

4-Ketone: ***13-Bromo-10,11-dichloro-7,11-dimethyl-3-methylene-4-oxo-6,8,12-tridecatrienoic acid***
[353754-81-1]
$C_{16}H_{19}BrCl_2O_3$ 410.134
Constit. of *Plocamium cartilagineum*.
$[\alpha]_D$ +37.6 (c, 0.14 in MeOH). λ_{max} 243 (log ϵ 2.37) (EtOH).

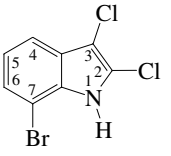
Debromo: ***10,11-Dichloro-4-hydroxy-7,11-dimethyl-3-methylene-6,8,12-tridecatrienoic acid***
$C_{16}H_{22}Cl_2O_3$ 333.253
Constit. of *Plocamium cartilagineum*. Oil. $[\alpha]_D$ +15.4 (c, 0.18 in MeOH). λ_{max} 243 (log ϵ 2.37) (EtOH).

(4R,6E,8E,10S,11R,12E)-form [353754-83-3]
Constit. of *Plocamium cartilagineum*.
$[\alpha]_D$ +15.4 (c, 0.18 in MeOH). Confusion in ref. about presence of Br. λ_{max} 243 (log ϵ 2.37) (EtOH).

4-Ketone: [353754-80-0]
Constit. of *Plocamium cartilagineum*.
$[\alpha]_D$ -43.1 (c, 0.17 in MeOH). λ_{max} 243 (log ϵ 2.37) (MeOH).
Řezanka, T. *et al., Phytochemistry*, 2001, **57**, 607-611 (*isol, pmr, cmr*)

7-Bromo-2,3-dichloro-1*H*-indole, 9CI B-347

[68234-19-5]



$C_8H_4BrCl_2N$ 264.936
Alkaloid from the marine red alga *Rhodophyllis membranacea*.
Mp 82-83°.

Brennan, M.R. *et al., Tet. Lett.*, 1978, 1637 (*isol, pmr, struct*)
Erickson, K.L. *et al., Synth. Commun.*, 1981, **11**, 253 (*synth, ir, pmr, ms*)

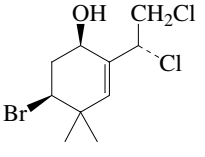
Bromodichloromethane, 9CI B-348

Dichloromethyl bromide. R 20B1. BDCM
[75-27-4]
Cl_2CHBr
$CHBrCl_2$ 163.828
Isol. from several marine algae. Source of dichlorocarbene on treatment with base. d^{15} 2.06.
Mp -57.1°. Bp 88.4-88.6° (89.2 - 90.6°).

▶ Possible human carcinogen. LD_{50} (rat, orl) 916 mg/kg. Exp. carcinogen (large dose). PA5310000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 83C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 122B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 116D (*ir*)
Seyferth, D. *et al., J.A.C.S.*, 1965, **87**, 681 (*synth*)
Fedorynski, M. *et al., Synth. Commun.*, 1977, **7**, 287 (*synth*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
IARC Monog. (Web),
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BND500

6-Bromo-1,2-dichloro-3(8)-ochtoden-4-ol B-349



$C_{10}H_{15}BrCl_2O$ 302.037

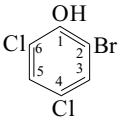
(2R*,4β,6β)-form
Ac: [851473-84-2]
$C_{12}H_{17}BrCl_2O_2$ 344.075
Constit. of *Carpopeltis crispata*. Oil. $[\alpha]_D^{20}$ -68 (c, 0.058 in $CHCl_3$).
Kimura, J. *et al., J. Nat. Prod.*, 2005, **68**, 585-587 (*isol, pmr, cmr*)

1-Bromo-1,2-dichloro-1-octen-3-one B-350

$H_3C(CH_2)_4COCCl{=}CBrCl$
$C_8H_{11}BrCl_2O$ 273.984
Occurs as a 1:1 mixture of *Z* and *E* isomers. Constit. of the seaweed *Bonnemaisonia asparagoides*. Antibacterial agent.
McConnell, O.J. *et al., Tet. Lett.*, 1977, 1851 (*isol, synth, ms*)

2-Bromo-4,6-dichlorophenol, 9CI, 8CI B-351

[4524-77-0]



$C_6H_3BrCl_2O$ 241.899
Isol. from the marine acorn worm *Ptychodera bahamensis*.
Needles.
Mp 68°. Bp_{200} 220°.

4-Methylbenzenesulfonyl:
Cryst. Mp 82-83°.

Fox, D.L. *et al., J.C.S.*, 1930, 1861 (*synth*)
Corgiat, J.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1993, **106**, 83-86 (*isol*)

1-Bromo-1,3-dichloro-2-propanone, 9CI B-352

1-Bromo-1,3-dichloroacetone
[1578-17-2]
$ClCH_2COCHBrCl$
$C_3H_3BrCl_2O$ 205.866

(±)-*form*
Component of the red alga *Asparagopsis armata*.
Liq. Bp_{11} 80-82°. n_D^{25} 1.5296.

Rappe, C. *et al., Ark. Kemi*, 1965, **24**, 105; *CA*, **63**, 5489a (*synth*)
McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367 (*isol, glc*)

3-Bromo-1,1-dichloro-2-propanone, 9CI B-353

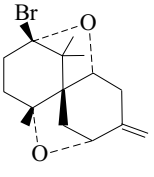
3-Bromo-1,1-dichloroacetone
[1578-16-1]
$Cl_2CHCOCH_2Br$
$C_3H_3BrCl_2O$ 205.866
Component of the red alga *Asparagopsis armata* and tetrasporophyte *Falkenbergia rufolanosa*. Needles.
Mp 30-31°. Bp_{25} 92-93° Bp_9 78°. n_D^{25} 1.5197.

Hydrate: Mp 54-57°.

Semicarbazone:
Prisms (EtOH aq.). Mp 131°.

King, F.E. *et al., J.C.S.*, 1952, 2144 (*synth*)
Polaczkowa, W. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1956, **30**, 119 (*synth*)
Rappe, C. *et al., Ark. Kemi*, 1965, **24**, 105; *CA*, **63**, 5489a (*synth*)
Mironov, V.F. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1965, 2193 (*synth, ir*)
McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367 (*isol, glc, ms*)
Combaut, G. *et al., Phytochemistry*, 1978, **17**, 1661 (*isol, glc, ms*)

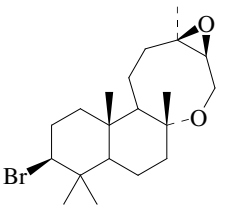
10-Bromo-5,10:2,7-diepoxy-3(15)-chamigrene B-354



$C_{15}H_{21}BrO_2$ 313.234
Constit. of *Laurencia nipponica*. Cryst.
Mp 78-79°. $[\alpha]_D^{21}$ -54.8.

Kikuchi, H. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 2437

3-Bromo-8,15:13,14-diepoxylabdane B-355

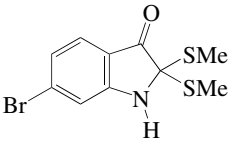


$C_{20}H_{33}BrO_2$ 385.384

(3β,8α,13β,14β)-*form* [611230-85-4]
Constit. of *Laurencia obtusa*.
Oil. $[\alpha]_D^{20}$ +21.9 (c, 0.32 in $CHCl_3$). λ_{max} 229 (log ϵ 2.55) (CH_2Cl_2).
Iliopoulou, D. *et al., J. Nat. Prod.*, 2003, **66**, 1225-1228 (*isol, pmr, cmr*)

6-Bromo-1,2-dihydro-2,2-bis(methylthio)-3*H*-indol-3-one, 9CI B-356

Tyrindolinone
[50630-71-2]

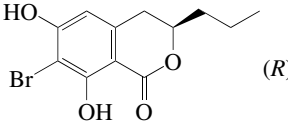


$C_{10}H_{10}BrNOS_2$ 304.231
Alkaloid from the mollusc *Dicathais orbita*. Yellow needles (C_6H_6/petrol).
Mp 117° (dec.). λ_{max} 225 (sh) (ϵ 21000); 248 (ϵ 25000); 270 (sh) (ϵ 8000); 355 (sh) (ϵ 1600); 402 (ϵ 2700) (EtOH).

Baker, J.T. *et al., Aust. J. Chem.*, 1973, **26**, 2153-2157 (*isol, uv, ir, pmr, ms*)
Cooksey, C.J. *et al., Molecules*, 2001, **6**, 736-769 (*rev*)

7-Bromo-3,4-dihydro-6,8-dihydroxy-3-propyl-1*H*-2-benzopyran-1-one B-357

7-Bromo-3,4-dihydro-6,8-dihydroxy-3-propylisocoumarin. ***Hiburipyranone***



(*R*)-*form*

$C_{12}H_{13}BrO_4$ 301.136
λ_{max} 219 (ϵ 15600); 227 (ϵ 12600); 273 (ϵ 8200); 306 (ϵ 3200) (MeOH) (Derep).

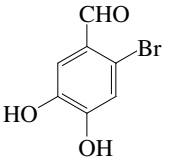
(*R*)-*form* [134419-24-2]
Constit. of *Mycale adhaerens*. Cytotoxic agent. Needles (EtOAc/hexane) (synthetic).
Mp 186-187° (synthetic). $[\alpha]_D$ -2.3 (c, 0.0028 in $CHCl_3$) (natural). $[\alpha]_D$ -30 (c, 0.6 in $CHCl_3$) (synthetic).

(±)-*form*
Cryst. (hexane/EtOAc). Mp 191.5-193° (sealed tube).

Fusetani, N. *et al., J.O.C.*, 1991, **56**, 4971-4974 (*isol, pmr, cmr*)
Uchida, K. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1564-1567 (*synth, ir, pmr, cmr*)
Uchida, K. *et al., Tetrahedron*, 1998, **54**, 8975-8984 (*synth, abs config*)

2-Bromo-4,5-dihydroxybenzaldehyde B-358

[4815-99-0]



$C_7H_5BrO_3$ 217.019
Isol. from the brown alga *Leathesia nana*. Pale-yellow cryst. (EtOH aq.).
Mp 220°.

4-Me ether: 2-Bromo-5-hydroxy-4-methoxybenzaldehyde. 6-Bromoisovanillin
[2973-59-3]
$C_8H_7BrO_3$ 231.045
Needles + $1H_2O$ (EtOH aq.). Mp 112-114°.

5-Me ether: 2-Bromo-4-hydroxy-5-methoxybenzaldehyde. 6-Bromovanillin
[60632-40-8]
$C_8H_7BrO_3$ 231.045
Mp 178°.

Di-Me ether: 2-Bromo-4,5-dimethoxybenzaldehyde. 6-Bromoveratric aldehyde
[5392-10-9]
$C_9H_9BrO_3$ 245.072
Needles (MeOH aq.). Mp 149-151°.

Methylene ether: 6-Bromo-1,3-benzodioxole-5-carboxaldehyde, 9CI. 2-Bromo-4,5-methylenedioxybenzaldehyde
[15930-53-7]
$C_8H_5BrO_3$ 229.03
Needles or plates (EtOH). Mp 129°. Steam-volatile.

▶ TO1576250

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 126A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 128A (*ir*)
Henry, T.A. *et al., J.C.S.*, 1930, 2279-2289 (*synth*)
Parijs, A.H. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1930, **49**, 33-44 (*synth*)
Reitz, A. *et al., J.O.C.*, 1981, **46**, 4859-4863 (*synth*)
Saraf, S.D. *et al., Synth. Commun.*, 1983, **13**, 7-14 (*4-Me ether, synth, pmr*)
Morey, J. *et al., J. Chem. Educ.*, 1988, **65**, 627-628 (*5-Me ether, synth*)
Coltart, D.M. *et al., Can. J. Chem.*, 1996, **74**, 88-94 (*di-Me ether, synth, ir, pmr, cmr, ms*)
Lear, Y. *et al., Can. J. Chem.*, 1997, **75**, 817-824 (*methylene ether, synth, pmr*)
Olivera, R. *et al., J.O.C.*, 2000, **65**, 6398-6411 (*di-Me ether, synth, pmr, cmr, ir*)
Xu, X. *et al., J. Nat. Prod.*, 2004, **67**, 1661-1666 (*isol*)

3-Bromo-4,5-dihydroxybenzaldehyde, 9CI B-359

[16414-34-9]

$C_7H_5BrO_3$ 217.019
Constit. of the red algae *Polysiphonia* spp. and the sponge *Psammaplysilla purpurea*. Antibiotic. Needles (EtOH aq.).
Mp 230°.

4-Me ether: 3-Bromo-5-hydroxy-4-methoxybenzaldehyde, 9CI. 5-Bromoisovanillin
[23354-30-5]
$C_8H_7BrO_3$ 231.046
Mp 116.5-117.5°.

5-Me ether: 3-Bromo-4-hydroxy-5-methoxybenzaldehyde. 5-Bromovanillin
[2973-76-4]
$C_8H_7BrO_3$ 231.045
Mp 164°.

Di-Me ether: 3-Bromo-4,5-dimethoxybenzaldehyde. 5-Bromoveratric aldehyde
[6948-30-7]
$C_9H_9BrO_3$ 245.072
Isol. from the fungus *Lepista nuda*. Needles (petrol or EtOH aq.).
Mp 65-66°.

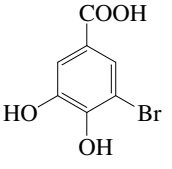
Di-Et ether: 3-Bromo-4,5-diethoxybenzaldehyde
[90109-64-1]
$C_{11}H_{13}BrO_3$ 273.126
Oil. $Bp_{0.3}$ 105-115°.

Methylene ether: 7-Bromo-1,3-benzodioxole-5-carboxaldehyde, 9CI. 3-Bromo-4,5-methylenedioxybenzaldehyde
[19522-96-4]
$C_8H_5BrO_3$ 229.03
Needles (MeOH). Mp 124-125°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 126D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 964B; 966A (*nmr*)
Pschorr, R. *et al., Annalen*, 1912, **391**, 23-39 (*synth*)
Henry, T.A. *et al., J.C.S.*, 1930, 2279-2289 (*synth*)
Eme, M. *et al., Helv. Chim. Acta*, 1950, **33**, 912-916 (*synth*)
Anhoury, M.L. *et al., Bull. Soc. Chim. Belg.*, 1974, **83**, 117-132 (*synth, 4-Me ether*)
Weinstein, B. *et al., Phytochemistry*, 1975, **14**, 2667-2670 (*isol, rev*)
Jacob, P. *et al., J. Med. Chem.*, 1984, **27**, 881-888 (*di-Et ether, synth*)
Yang, Z. *et al., J.O.C.*, 1992, **57**, 7248-7257 (*5-Me ether, synth*)
Hjelm, O. *et al., Chemosphere*, 1996, **32**, 1719-1728 (*di-Me ether, isol*)
Majetich, G. *et al., J.O.C.*, 1997, **62**, 4321-4326 (*5-Me ether, synth*)
Walz, A.J. *et al., J.O.C.*, 2000, **65**, 8001-8010 (*methylene ether, synth, pmr, cmr*)
Furstner, A. *et al., Chem. Eur. J.*, 2002, **8**, 1856-1871 (*Me ether, synth, ir, pmr, cmr*)
Yadav, J.S. *et al., Adv. Synth. Catal.*, 2004, **346**, 77-82 (*5-Me ether*)
Vallejos, G. *et al., Bioorg. Med. Chem.*, 2005, **13**, 4450-4457 (*synth, ir, pmr*)

3-Bromo-4,5-dihydroxybenzoic acid B-360

5-Bromoprotocatechuic acid
[61203-46-1]



$C_7H_5BrO_4$ 233.018
Constit. of Indian algae.
Mp 227-229°.

Me ester:
$C_8H_7BrO_4$ 247.045
Isol. from the red alga *Rhodomela confervoides*. Amorph. powder (Me_2CO).
Mp 176-178°.

Di-Ac:
$C_{11}H_9BrO_6$ 317.093
Mp 187°.

4-Me ether: 3-Bromo-5-hydroxy-4-methoxybenzoic acid. 5-Bromoisovanillic acid
[52783-66-1]
$C_8H_7BrO_4$ 247.045
Isol. from *Rhodomela confervoides*. Cryst.
Mp 201-202°.

5-Me ether: 3-Bromo-4-hydroxy-5-methoxybenzoic acid. 5-Bromovanillic acid
$C_8H_7BrO_4$ 247.045
Mp 236°.

5-Me ether, nitrile: 2-Bromo-4-cyano-6-methoxyphenol
$C_8H_6BrNO_2$ 228.045
Mp 144°.

Di-Me ether: 3-Bromo-4,5-dimethoxybenzoic acid. 5-Bromoveratric acid
[20731-48-0]
$C_9H_9BrO_4$ 261.072
Needles (MeOH or AcOH). Mp 192-193°.

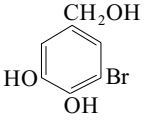
Di-Me ether, Me ester:
$C_{10}H_{11}BrO_4$ 275.099
Prisms (petrol). Mp 71-72°.

[65841-10-3]

Pschorr, R. *et al., Annalen*, 1912, **391**, 32 (*synth*)
Raiford, L. *et al., J.A.C.S.*, 1933, **55**, 1684 (*deriv*)
Piatak, D.M. *et al., J.O.C.*, 1977, **42**, 1068 (*synth, pmr*)
Borchardt, R.T. *et al., J. Med. Chem.*, 1982, **25**, 258-263 (*3-Bromo-5-hydroxy-4-methoxybenzoic acid*)
Pandya, A.C. *et al., Planta Med.*, 1990, **56**, 557
Shepherd, J.A. *et al., Tet. Lett.*, 1996, **37**, 2395-2398 (*synth, ester*)
Fan, X. *et al., J. Nat. Prod.*, 2003, **66**, 455-458 (*Me ester, isol*)
Zhao, J. *et al., J. Nat. Prod.*, 2004, **67**, 1032-1035 (*3-Bromo-5-hydroxy-4-methoxybenzoic acid*)

3-Bromo-4,5-dihydroxybenzyl alcohol B-361

3-Bromo-5-(hydroxymethyl)-1,2-benzenediol, 9CI
[52897-61-7] .



$C_7H_7BrO_3$ 219.034
Isol. from Rhodomelaceae such as *Halopytis pinastroides* and from *Avrainvillea nigricans* and *Polysiphonia* spp. Shows antibiotic activity, algicide. Cryst. (EtOH aq.).
Mp 104-106°. λ_{max} 287 (EtOH) (Berdy).

5-Me ether: 3-Bromo-4-hydroxy-5-methoxybenzenemethanol, 9CI. 5-Bromovanillyl alcohol
[2316-61-2]
$C_8H_9BrO_3$ 233.061
Cryst. (H_2O). Mp 132-134°.

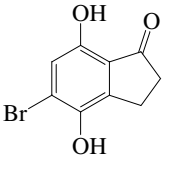
1,5-Di-Me ether: 2-Bromo-6-methoxy-4-methoxymethylphenol
$C_9H_{11}BrO_3$ 247.088
Cryst. by subl. Mp 64-67°.

4,5-Di-Me ether: 3-Bromo-4,5-dimethoxybenzenemethanol, 9CI. 5-Bromoveratryl alcohol
[52783-74-1]
$C_9H_{11}BrO_3$ 247.088
Liq. Bp_{12} 190° Bp_1 140°.

McIvor, R.A. *et al., Can. J. Chem.*, 1953, **31**, 298-302 (*5-Me ether, 1,5-Me ether*)
Pederson, M. *et al., Phytochemistry*, 1974, **13**, 2273 (*isol, ms*)
Glombitza, K.-W. *et al., Planta Med.*, 1974, **25**, 105
Weinstein, B. *et al., Phytochemistry*, 1975, **14**, 2667 (*isol, rev*)
Gerecke, M. *et al., Helv. Chim. Acta*, 1979, **62**, 1549-1558 (*di-Me ether, pmr, ms*)
Colon, M. *et al., J. Nat. Prod.*, 1987, **50**, 368-374 (*Avrainvillea nigricans constit*)
Morey, J. *et al., J. Chem. Educ.*, 1988, **65**, 627-628 (*5-Me ether, synth*)

5-Bromo-4,7-dihydroxy-1-indanone B-362

5-Bromo-2,3-dihydro-4,7-dihydroxy-1H-inden-1-one, 9CI
[181623-65-4]

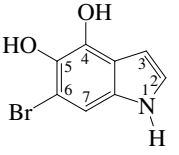


$C_9H_7BrO_3$ 243.057
Isol. from a marine sponge. Antitumour agent.

Japan. Pat., 1996, 96 198 798; *CA*, **125**, 217489a

6-Bromo-4,5-dihydroxyindole B-363

6-Bromo-1H-indole-4,5-diol, 9CI
[211808-67-2]



$C_8H_6BrNO_2$ 228.045
Alkaloid from the gastropod *Drupella fragum*. Amorph. solid.

Ochi, M. *et al., J. Nat. Prod.*, 1998, **61**, 1043-1045 (*isol*)

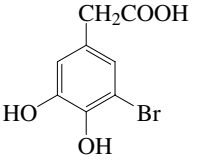
6-Bromo-4,7-dihydroxyindole B-364

6-Bromo-1H-indole-4,7-diol, 9CI
[211808-68-3]
$C_8H_6BrNO_2$ 228.045
Alkaloid from the gastropod *Drupella fragum*. Amorph. solid.

Ochi, M. *et al., J. Nat. Prod.*, 1998, **61**, 1043-1045 (*isol*)

3-Bromo-4,5-dihydroxyphenylacetic acid B-365

3-Bromo-4,5-dihydroxybenzeneacetic acid, 9CI



$C_8H_7BrO_4$ 247.045

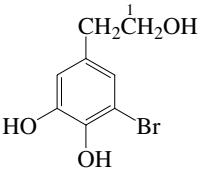
4-Me ether: 3-Bromo-5-hydroxy-4-methoxyphenylacetic acid
[89936-30-1]
$C_9H_9BrO_4$ 261.072
Isol. from the red alga *Rhodomela confervoides*. Protein kinase C inhibitor. Cryst. (toluene).
Mp 159.5-160.5°.

4-Me ether, Me ester:
$C_{10}H_{11}BrO_4$ 275.099
Isol. from *Rhodomela confervoides*. Brown gum.

Weller, D.D. *et al., J.O.C.*, 1984, **49**, 2061-2063 (*synth, pmr*)
Zhao, J. *et al., J. Nat. Prod.*, 2004, **67**, 1032-1035 (*isol, cmr*)

2-(3-Bromo-4,5-dihydroxyphenyl)ethanol B-366

3-Bromo-5-(2-hydroxyethyl)-1,2-benzenediol



$C_8H_9BrO_3$ 233.061

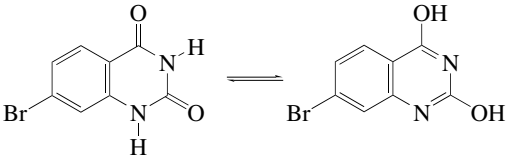
1-Sulfate:
$C_8H_9BrO_6S$ 313.126
Constit. of *Rhodomela confervoides*. Brown gum. λ_{max} 209 (log ε 4.27); 287 (log ε 3.32) (MeOH).

Ma, M. *et al., J. Nat. Prod.*, 2006, **69**, 206-210

7-Bromo-2,4-dihydroxyquinazoline B-367

*7-Bromo-2,4(1*H*,3*H*)-quinazolinedione, 9CI. 7-Bromo-2,4-quinazolinediol*

[114703-12-7]



$C_8H_5BrN_2O_2$ 241.044

Alkaloid from the marine tunicate *Pyura sacciformis*. Cryst. (MeOH).

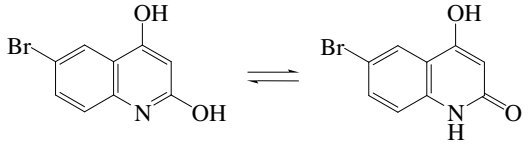
Mp 330°. λ_{max} 225 (ϵ 47000); 310 (ϵ 4600) (EtOH) (Derep).

Niwa, H. *et al., J. Nat. Prod.*, 1988, **51**, 343-344 (*isol, uv, ir, pmr, ms, synth, struct*)

6-Bromo-2,4-dihydroxyquinoline B-368

*6-Bromo-4-hydroxy-2(1*H*)-quinolinone, 9CI. 6-Bromo-2,4-quinolinediol*

[54675-23-9]



$C_9H_6BrNO_2$ 240.056

Isol. from the sponge *Hyrtios erecta*. Yellow powder.

Mp >340°.

Buckle, D.R. *et al., J. Med. Chem.*, 1975, **18**, 726-732 (*synth*)
Aoki, S. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1372-1374 (*isol, pmr, cmr*)

Bromodiiodomethane, 9CI B-369

[557-95-9]

$CHBrI_2$

$CHBrI_2$ 346.732

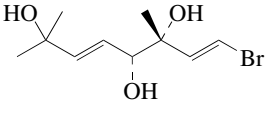
Occurs in the oil of the alga *Asparagopsis taxiformis*.

Mp 60°. Bp_{25} 110°.

Auger, V. *et al., C. R. Hebd. Seances Acad. Sci.*, 1908, **146**, 1037 (*synth*)
Somayajulu, G.M. *et al., J. Magn. Reson.*, 1975, **33**, 559 (*cmr*)
Bunneson, B.J. *et al., Tet. Lett.*, 1975, 473 (*occur*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Novak, I. *et al., J.O.C.*, 2002, **67**, 3510-3513 (*pmr, cmr, pe*)

8-Bromo-2,6-dimethyl-3,7-octadiene-2,5,6-triol B-370

Pantoneurotriol



(3*E*,5*R**,6*R**,7*E*)-*form*

$C_{10}H_{17}BrO_3$ 265.147

Error in struct. in CAS abstract.

(3*E*,5*R*,6*R*,7*E*)-*form* [207130-30-1]

Constit. of *Pantoneura plocamioides*.

Oil. $[\alpha]_D^{25}$ -100 (c, 0.2 in $CHCl_3$).

(3*E*,5*R*,6*S*,7*E*)-*form* [207130-29-8]

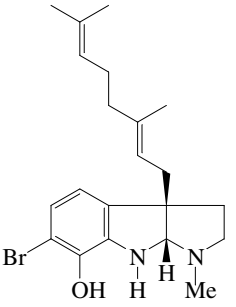
Constit. of *Pantoneura plocamioides*.

Oil. $[\alpha]_D^{25}$ -90 (c, 0.21 in $CHCl_3$).

Cueto, M. *et al., Tetrahedron*, 1998, **54**, 3575-3580 (*isol, pmr, cmr*)

6-Bromo-3*a*-(3,7-dimethyl-2,6-octadienyl)-1,2,3,3*a*,8,8*a*-hexahydro-1-methylpyrrolo[2,3-*b*]indol-7-ol B-371

[474779-13-0]



Relative Configuration

$C_{21}H_{29}BrN_2O$ 405.377

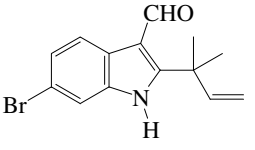
Alkaloid from the marine bryozoan *Flustra foliacea*. Yellow oil. $[\alpha]_D^{22}$ -22 (c, 0.1 in $CHCl_3$). λ_{max} 251 (log ϵ 4.7); 309 (log ϵ 4.5) (no solvent reported).

Peters, L. *et al., J. Nat. Prod.*, 2002, **65**, 1633-1637 (*isol, pmr, cmr, ms*)

6-Bromo-2-(1,1-dimethyl-2-propenyl)-1*H*-indole-3-carboxaldehyde B-372

6-Bromo-3-formyl-2-(1,1-dimethyl-2-propenyl)indole

[474657-70-0]



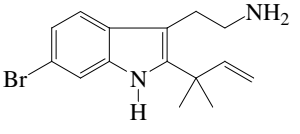
$C_{14}H_{14}BrNO$ 292.175

Alkaloid from the marine bryozoan *Flustra foliacea*. Yellow oil. λ_{max} 222 (log ϵ 4.6); 274 (log ϵ 4); 300 (log ϵ 3.9) (MeOH).

Peters, L. *et al., J. Nat. Prod.*, 2002, **65**, 1633-1637 (*isol, pmr, cmr, ms*)

6-Bromo-2-(1,1-dimethyl-2-propenyl)tryptamine B-373

*6-Bromo-2-(1,1-dimethyl-2-propenyl)-1*H*-indole-3-ethanamine, 9CI. 3-(2-Aminoethyl)-6-bromo-2-(1,1-dimethyl-2-propenyl)-1*H*-indole. 6-Bromo-2-(1,1-dimethylallyl)tryptamine*



$C_{15}H_{19}BrN_2$ 307.233

N^b-*Me:* ***Deformylflustrabromine***

[474657-72-2]

$C_{16}H_{21}BrN_2$ 321.259

Isol. from *Flustra foliacea*. Cytotoxic. Yellow oil. λ_{max} 231 (log ϵ 4.6); 289 (log ϵ 3.9) (MeOH). λ_{max} 204 (ϵ 30190); 230 (ϵ 22730); 282 (ϵ 4770) (MeOH).

N^b-*Me,* N^b-*formyl:* ***Flustrabromine***

[80693-54-5]

$C_{17}H_{21}BrN_2O$ 349.27

Alkaloid from the marine bryozoan *Flustra foliacea*. Amorph. solid. Consists of two rotameric forms reflecting hindered rotation around the formamide C–N bond. Each rotamer also exists in equilib. with a form in which the amide nitrogen atom associates intramolecularly with the benzene ring.

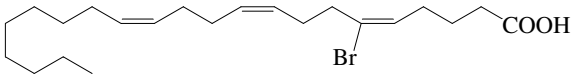
N^b-*Me,* N^b-*(methylsulfonyl):* **N-*[2-[6-Bromo-2-(1,1-dimethyl-2-propenyl)-1*H*-indol-3-yl]ethyl]*-N-*methylmethanesulfonamide**
[474657-71-1]
$C_{17}H_{23}BrN_2O_2S$ 399.351
Isol. from *Flustra foliacea*. Yellow oil. λ_{max} 227 (log ϵ 4.8); 288 (log ϵ 4.3) (MeOH).
Wulff, P. *et al., J.C.S. Perkin 1*, 1981, 2895-2898 (*Flustrabromine, isol, uv, ir, pmr, cmr, ms, struct*)
Peters, L. *et al., J. Nat. Prod.*, 2002, **65**, 1633-1637 (*Deformylflustrabromine, N-Me N-methylsulfonyl*)
Lysek, N. *et al., Z. Naturforsch., C*, 2002, **57**, 1056-1061 (*Deformylflustrabromine*)

6-Bromo-5,9-docosadienoic acid B-374

$H_3C(CH_2)_{11}CH{=}CHCH_2CH_2CBr{=}CH(CH_2)_3COOH$
$C_{22}H_{39}BrO_2$ 415.453

(5*E*,9*Z*)-*form* [161925-95-7]
Isol. from the sea anemone *Stoichactis helianthus*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1994, **57**, 1688-1695 (*isol, ms*)

6-Bromo-5,9,13-docosatrienoic acid B-375

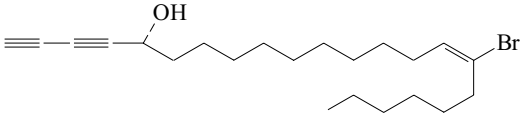


$C_{22}H_{37}BrO_2$ 413.437

(5*E*,9*Z*,13*Z*)-*form*
Isol. from *Stoichactis helianthus*.
Dembitsky, V.M. *et al., Prog. Lipid Res.*, 2002, **41**, 315-367 (*occur*)

16-Bromo-15-docosene-1,3-diyn-5-ol B-376

18-Dihydrorenierin 1

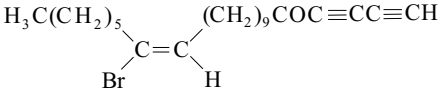


$C_{22}H_{35}BrO$ 395.422
λ_{max} 227 (ϵ 1200); 240 (ϵ 880); 254 (ϵ 430) (MeOH) (Derep).

(*R*,*E*)-*form* [64010-40-8]
Constit. of *Reniera fulva*.
Oil. $[\alpha]_D$ -5.4 (c, 5.4 in $CHCl_3$).
Cimino, G. *et al., Tet. Lett.*, 1977, 1325 (*isol*)

16-Bromo-15-docosene-1,3-diyn-5-one B-377

Renierin 1



$C_{22}H_{33}BrO$ 393.406
λ_{max} 236 (ϵ 5880); 246 (ϵ 9400); 262 (ϵ 12200); 276 (ϵ 8920) (MeOH) (Derep).

(*E*)-*form*
cis-*form*
[63987-87-1]
Constit. of *Reniera fulva*. Oil.
Cimino, G. *et al., Tet. Lett.*, 1977, 1325 (*isol, struct*)

6-Bromo-5,9-eicosadienoic acid B-378

[172806-85-8]
$H_3C(CH_2)_9CH{=}CHCH_2CH_2CBr{=}CH(CH_2)_3COOH$
$C_{20}H_{35}BrO_2$ 387.399
Constit. of the phospholipids of the anemone *Condylactis gigantea* and the zoanthid *Palythoa caribaeorum*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1995, **58**, 1689-1694 (*isol, struct, ms*)

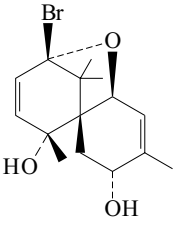
20-Bromo-5,11,15,19-eicosatetraene-9,17-diynoic acid B-379

$BrCH{=}CHC{\equiv}CCH{=}CHCH_2CH_2CH{=}CHC{\equiv}CCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{20}H_{23}BrO_2$ 375.304

(all-E)-form [165128-30-3]
Isol. from *Xestospongia* sp., an association of sponge cells and bacteria.
Amorph. powder. λ_{max} 270 (ϵ 27500); 288 (ϵ 22200) (MeOH).
6-Bromo(Z): 6,20-Dibromo-5,11,15,19-eicosatetraene-9,17-diynoic acid
[165128-31-4]
$C_{20}H_{22}Br_2O_2$ 454.201
Isol. from *Xestospongia* sp. Amorph. powder. λ_{max} 271; 286 (MeOH).
Brantley, S.E. *et al., Tetrahedron*, 1995, **51**, 7667 (*isol, uv, ir, pmr, cmr, ms*)

10-Bromo-5,10-epoxy-3,8-chamigradiene-2,7-diol B-380

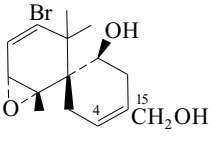
4-Bromo-4,7-epoxy-1,5,5,9-tetramethylspiro[5.5]undeca-2,8-diene-1,10-diol



$C_{15}H_{21}BrO_3$ 329.233
Constit. of *Laurencia nipponica*. Cryst. (Me_2CO/isopropyl ether).
Mp 73-75°. $[\alpha]_D$ -11.7.
Kurata, K. *et al., Chem. Lett.*, 1981, 773

10-Bromo-7,8-epoxy-2,9-chamigradiene-5,15-diol B-381

[86510-25-0]

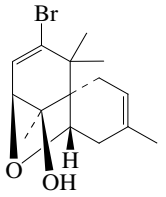


Absolute configuration

$C_{15}H_{21}BrO_3$ 329.233
Constit. of red alga *Laurencia nipponica*. Cryst.
Mp 61-62°. $[\alpha]_D$ +60 (c, 1.00 in $CHCl_3$).

15-Deoxy, 4-bromo: 2,10-Dibromo-7,8-epoxy-2,9-chamigradien-5-ol. ***Dehydrochloroprepacifenol***
[112757-36-5]
$C_{15}H_{20}Br_2O_2$ 392.13
Isol. from *Laurencia majuscula*. Cryst. (CH_2Cl_2/hexane).
Mp 124-125°. $[\alpha]_D^{20}$ +51.7 (c, 1.1 in EtOH).
Kurata, K. *et al., Chem. Lett.*, 1983, 561 (*cryst struct*)
Caccamese, S. *et al., Tetrahedron*, 1987, **43**, 5393-5399 (*Dehydrochloroprepacifenol, cryst struct*)

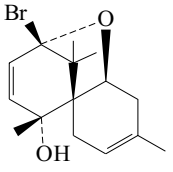
10-Bromo-1,8-epoxy-3,9-chamigradien-7-ol **B-382**
Claviol
[226699-48-5]



$C_{15}H_{21}BrO_2$ 313.234
Constit. of *Laurencia claviformis*. Cryst. (hexane).
Mp 138°. $[\alpha]_D^{25}$ +6.8 (c, 0.97 in $CHCl_3$).

Rovirosa, J. *et al., Phytochemistry*, 1999, **50**, 745-748 (*isol, pmr, cmr*)

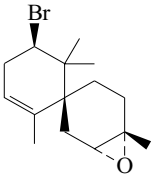
10-Bromo-5,10-epoxy-2,8-chamigradien-7-ol **B-383**
[74173-67-4]



$C_{15}H_{21}BrO_2$ 313.234
Metab. of *Laurencia nipponica*. Cryst.
Mp 103-104°. $[\alpha]_D$ -39.8 (c, 1 in $CHCl_3$).

Suzuki, T. *et al., Chem. Lett.*, 1980, 541-542 (*isol, pmr, cmr*)
Darias, J. *et al., Chem. Lett.*, 1990, 259-262 (*synth*)

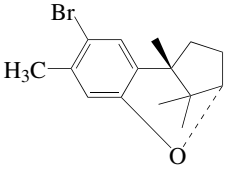
10-Bromo-2,3-epoxy-7-chamigrene **B-384**
4-Bromo-8,9-epoxy-α-chamigrene
[53767-99-0]



$C_{15}H_{23}BrO$ 299.25
Constit. of *Laurencia glandulifera*. Cryst. (MeOH).
Mp 53-54°. $[\alpha]_D$ -92 (c, 0.98 in $CHCl_3$).

Suzuki, M. *et al., Tet. Lett.*, 1974, 821 (*isol*)
Suzuki, M. *et al., Tetrahedron*, 1979, **35**, 823 (*cryst struct, abs config*)

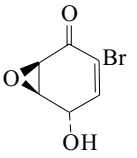
4-Bromo-1,10-epoxy-1,3,5-cuparatriene **B-385**
[864956-87-6]



$C_{15}H_{19}BrO$ 295.219
Constit. of *Laurencia microcladia*. Oil. $[\alpha]_D^{20}$ -29 (c, 0.1 in CH_2Cl_2).
λ_{max} 237 (log ϵ 3.02); 275 (log ϵ 2.42); 285 (log ϵ 2.56); 295 (log ϵ 2.44) (CH_2Cl_2).

Kladi, M. *et al., Tet. Lett.*, 2005, **46**, 5723-5726 (*Laurencia microcladia constit*)

2-Bromo-5,6-epoxy-4-hydroxy-2-cyclohexen-1-one **B-386**
3-Bromo-5-hydroxy-7-oxabicyclo[4.1.0]hept-3-en-2-one, 9CI. ***Bromoxone***

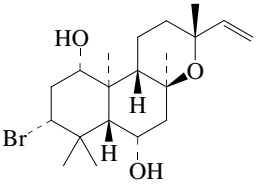


$C_6H_5BrO_3$ 205.008

(4*S*,5*R*,6*R*)-*form* [110786-63-5]
Metab. of sea acorn worms *Ptychodera* sp.
Cryst. ($CHCl_3$/hexane).
Mp 123-127°. $[\alpha]_D^{22}$ +220 (c, 0.09 in $CHCl_3$).
Ac: 4-Acetoxy-2-bromo-5,6-epoxy-2-cyclohexen-1-one
[110786-62-4]
$C_8H_7BrO_4$ 247.045
Metab. of *Ptychodera* sp. Antitumour agent. Needles (EtOAc/hexane). Sol. MeOH, $CHCl_3$.
Mp 93-94°. $[\alpha]_D^{19}$ +265 (c, 0.12 in $CHCl_3$).

Higa, T. *et al., Tetrahedron*, 1987, **43**, 1063-1070 (*isol, cryst struct*)
Corgiat, J.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1993, **106**, 83-86 (*Ptychodera constit*)
Gautier, E.C.L. *et al., Tet. Lett.*, 1994, **35**, 8759-8760 (*synth*)
Johnson, C.R. *et al., J.O.C.*, 1995, **60**, 6674-6675 (*synth*)
Block, O. *et al., J.O.C.*, 2000, **65**, 716-721 (*synth, pmr, cmr*)
Barros, M.T. *et al., Org. Lett.*, 2003, **5**, 4321-4323 (*synth*)
Tachihara, T. *et al., Tetrahedron*, 2003, **59**, 1773-1780; 1773-1780 (*synth*)

3-Bromo-8,13-epoxy-14-labdene-1,6-diol **B-387**

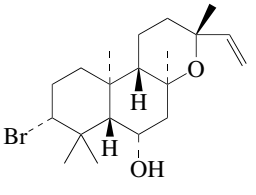


$C_{20}H_{33}BrO_3$ 401.383

(*ent*-1β,3β,6β,8α,13*S*)-*form*
1-Ac: [440680-38-6]
$C_{22}H_{35}BrO_4$ 443.42
Constit. of an Okinawan *Laurencia* sp. Cryst.
Mp 183-184°. $[\alpha]_D^{24}$ +28 (c, 0.27 in $CHCl_3$).
1-Ketone: ***3-Bromo-8,13-epoxy-6-hydroxy-14-labden-1-one***
[440680-39-7]
$C_{20}H_{31}BrO_3$ 399.367
Constit. of an Okinawan *Laurencia* sp. Cryst.
Mp 213-214°. $[\alpha]_D^{24}$ -120 (c, 0.08 in $CHCl_3$).

Suzuki, M. *et al., J. Nat. Prod.*, 2002, **65**, 801-804 (*isol, pmr, cmr, cryst struct*)

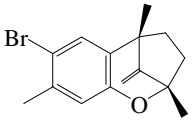
3-Bromo-8,13-epoxy-14-labden-6-ol **B-388**



$C_{20}H_{33}BrO_2$ 385.384

(*ent*-3β,6β,8α,13*S*)-*form*
Paniculatol
[191404-85-0]
Constit. of *Laurencia paniculata*.
Cryst. (hexane).
Mp 172°. $[\alpha]_D$ -12 (c, 0.006 in $CHCl_3$). λ_{max} (MeOH) (Berdy).
Briand, A. *et al., Tet. Lett.*, 1997, **38**, 3399-3400 (*isol, pmr, cmr, cryst struct*)

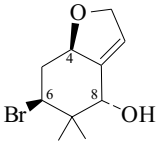
10-Bromo-4,7-epoxy-5(13),6,8,10-lauratetraene **B-389**
4-Bromo-1,10-epoxy-11-laurene



$C_{15}H_{17}BrO$ 293.203

(1*R*,4*R*)-*form* [861251-21-0]
Constit. of *Laurencia tristicha*.
Cryst.
Mp 74-76°. $[\alpha]_D^{20}$ +70.9 (c, 0.16 in MeOH).
Sun, J. *et al., J. Nat. Prod.*, 2005, **68**, 915-919 (*Laurencia tristicha constit*)

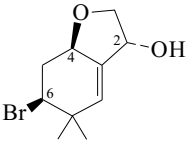
6-Bromo-1,4-epoxy-2-ochtoden-8-ol **B-390**
*6-Bromo-2,3,5,6,7,7*a*-hexahydro-5,5-dimethyl-4-benzofuranol, 9CI*



$C_{10}H_{15}BrO_2$ 247.131

(4*R,6*S**,8*S**)-*form*** [73872-78-3]
Constit. of *Ochtodes crockeri*.
Oil. $[\alpha]_D^{20}$ +30 (c, 2 in $CHCl_3$).
Paul, V.J. *et al., J.O.C.*, 1980, **45**, 3401

6-Bromo-1,4-epoxy-3(8)-ochtoden-2-ol **B-391**
*6-Bromo-2,3,5,6,7,7*a*-hexahydro-5,5-dimethyl-3-benzofuranol, 9CI*



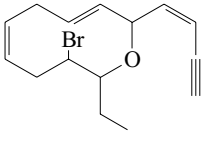
(2*R**,4*R**,6*R**)–*form*
Relative configuration

$C_{10}H_{15}BrO_2$ 247.131

(2*R,4*R**,6*S**)-*form*** [73872-80-7]
Constit. of *Ochtodes crockeri*.
Oil. $[\alpha]_D^{20}$ -55 (c, 1 in $CHCl_3$).

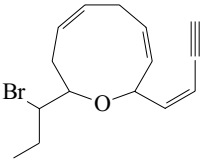
(2*S,4*R**,6*S**)-*form*** [73872-79-4]
Constit. of *Ochtodes crockeri*.
Oil. $[\alpha]_D^{20}$ -64.6 (c, 0.7 in $CHCl_3$).
Paul, V.J. *et al., J.O.C.*, 1980, **45**, 3401

12-Bromo-5,13-epoxy-3,6,9-pentadecatrien-1-yne **B-392**
[125092-22-0]



$C_{15}H_{19}BrO$ 295.218
Metab. of *Laurencia implicata*. Oil. $[\alpha]_D$ +147.4 (c, 0.022 in $CHCl_3$). λ_{max} 240 (ϵ 30000) (EtOH) (Derep).
Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1685 (*isol, pmr, cmr*)

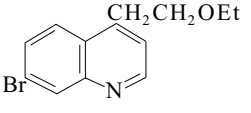
13-Bromo-5,12-epoxy-3,6,9-pentadecatrien-1-yne **B-393**
[125092-23-1]



$C_{15}H_{19}BrO$ 295.218
Metab. of *Laurencia implicata*. Oil. $[\alpha]_D$ -243.7 (c, 0.017 in $CHCl_3$). λ_{max} 240 (ϵ 30000) (EtOH) (Derep).
Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1685 (*isol, pmr, cmr*)

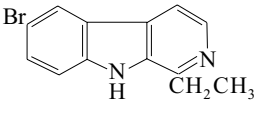
Bromoethane **B-394**
Ethyl bromide
[74-96-4]
H_3CCH_2Br
C_2H_5Br 108.965
Isol. from a marine alga. Liq. d_4^{20} 1.46.
Fp -125.5. Bp 38.4°. n_D^{20} 1.4235.
▶ Preparative haz.; highly flammable, fl. p. 50 (rat, orl) 1350 mg/kg. Exp. carcinogen. OES: long-term 200 ppm; short-term 250 ppm.
KH6475000
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 55B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 81C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 82D (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 29; 36 (*synth*)
McLafferty, F.W. *et al., Anal. Chem.*, 1962, **34**, 2 (*ms*)
Ejchart, A. *et al., Org. Magn. Reson.*, 1980, **13**, 368 (*cmr*)
Kozlowski, R. *et al., Org. Prep. Proced. Int.*, 1988, **20**, 177 (*synth*)
IARC Monog., 1991, **52**, 299 (*rev, tox*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **4**, 570
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0793
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 170
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EGV400

7-Bromo-4-(2-ethoxyethyl)quinoline, 9CI **B-395**
[82503-96-6]



$C_{13}H_{14}BrNO$ 280.164
Minor alkaloid from the marine bryozoan *Flustra foliacea*. Possibly an artifact.
Wulff, P. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **71**, 525-526 (*isol, uv, pmr, ms, struct*)

6-Bromo-1-ethyl-β-carboline **B-396**
*6-Bromo-1-ethyl-9*H*-pyrido[3,4-*b*]indole, 9CI*
[113679-47-3]



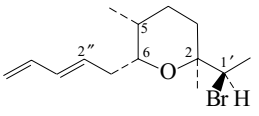
$C_{13}H_{11}BrN_2$ 275.147

Metab. from the marine hydroid *Aglaophenia pluma*. Cryst. (CH_2Cl_2).
Mp 155-157°.

8-Bromo: ***6,8-Dibromo-1-ethyl-β-carboline***
[113679-48-4]
$C_{13}H_{10}Br_2N_2$ 354.043
Major metab. from *Aglaophenia pluma*. Cryst. (CH_2Cl_2).
Mp 150-152°.

Aiello, A. *et al., Tetrahedron*, 1987, **43**, 5929-5932 (*isol, uv, pmr, cmr, struct, synth, deriv*)

2-(1-Bromoethyl)-2,5-dimethyl-6-(2,4-pentadienyl)-tetrahydropyran B-397



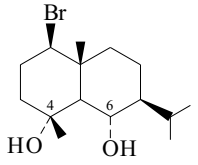
$C_{14}H_{23}BrO$ 287.239

(1′R,2S,2″E,5R,6R)-form
Constit. of *Haliclona* spp.
Oil. $Bp_{0.5}$ 103° (bath). $[\alpha]_D$ +27.3 (c, 0.3 in $CHCl_3$).

2″,3″-Dihydro: Constit. of *Haliclona* spp.
Oil. $Bp_{0.5}$ 82° (bath). $[\alpha]_D$ +25.4 (c, 0.3 in $CHCl_3$).

Capon, R.J. *et al., Tetrahedron*, 1982, **38**, 1699-1703

1-Bromo-4,6-eudesmanediol B-398



(1β,4α,6α,7α*H*)–*form*

$C_{15}H_{27}BrO_2$ 319.281

(1β,4α,6α,7α*H*)-form
6-Ac:
$C_{17}H_{29}BrO_3$ 361.318
Constit. of *Aplysia dactylomela*. Oil.

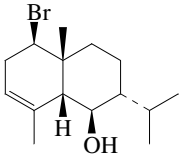
(1β,4α,6α,7β*H*)-form
Austradiol

6-Ac: ***Austradiol acetate***
[82731-83-7]
$C_{17}H_{29}BrO_3$ 361.318
Constit. of *Laurencia filiformis*. Oil. $[\alpha]_D^{22}$ +14.5 (c, 1.75 in $CHCl_3$).

4,6-Di-Ac: ***Austradiol diacetate***
[82731-84-8]
$C_{19}H_{31}BrO_4$ 403.355
Constit. of *Laurencia filiformis*. Cryst.

Brennan, M.R. *et al., J.O.C.*, 1982, **47**, 3917 (*isol, struct*)
Rao, C.B. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 322 (*isol, pmr, cmr, ir, ms*)

1-Bromo-3-eudesmen-6-ol B-399



(1β,5β,6β,7β*H*)-*form*

$C_{15}H_{25}BrO$ 301.266

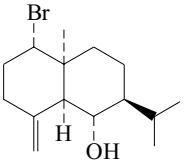
(1β,5β,6β,7β*H*)-form
Lankalapuol A
[117333-13-8]
Constit. of *Aplysia dactylomela*.

Ac:
Cryst. (EtOH aq.). Mp 83.5-84°. $[\alpha]_D$ +96 (c, 0.47 in MeOH).

(1β,6α,7β*H*)-form
Itomanol
[474817-72-6]
Constit. of *Laurencia intricata*.
Oil. $[\alpha]_D^{23}$ -50 (c, 0.31 in $CHCl_3$).

Baker, B. *et al., Tetrahedron*, 1988, **44**, 4695-4701 (*Lankalapuol A*)
Suzuki, M. *et al., Phytochemistry*, 2002, **60**, 861-867 (*Itomanol*)

1-Bromo-4(15)-eudesmen-6-ol B-400



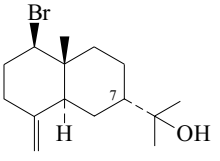
$C_{15}H_{25}BrO$ 301.266

(1α,6α,10α)-form
Lankalapuol B
[117465-31-3]
Constit. of *Aplysia dactylomela*.

Ac:
Cryst. (EtOH aq.). Mp 93.5-94.5°. $[\alpha]_D$ -93 (c, 1 in MeOH).

Baker, B. *et al., Tetrahedron*, 1988, **44**, 4695-4701 (*isol, pmr, cmr*)

1-Bromo-4(15)-eudesmen-11-ol B-401



(1β,7α)–*form*

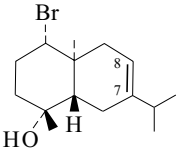
$C_{15}H_{25}BrO$ 301.266

(1β,7α)-form
Isobrasudol
[72154-34-8]
Isol. from *Aplysia brasiliana*. Ichthyotoxin. Antifeedant.
Mp 105-107°. $[\alpha]_D^{26}$ +10.3.

(1β,7β)-form
Brasudol
[72154-35-9]
From *Aplysia brasiliana*. Ichthyotoxin. Exhibits potent fish antifeedant activity.
Mp 105-106°. $[\alpha]_D^{26}$ +16.5.

Dieter, R.K. *et al., Tet. Lett.*, 1979, 1645-1648 (*isol, struct*)

1-Bromo-7-eudesmen-4-ol B-402



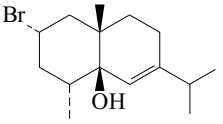
$C_{15}H_{25}BrO$ 301.266
Oil.

(1α,4α,5β,10α)-*form*
ent-*1β-Bromo-4β-hydroxy-7-selinene*
[62264-66-8]
Constit. of *Laurencia* spp.
$[\alpha]_D^{22}$ +52.6 (c, 4.62 in $CHCl_3$).

7,8-Dihydro, 7β-chloro: **ent-*1β-Bromo-7α-chloro-4β-eudesmanol***.
ent-*1β-Bromo-7α-chloro-4β-hydroxyselinane*
[68690-87-9]
$C_{15}H_{26}BrClO$ 337.726
Metab. of *Laurencia* spp. Cryst. (hexane).
Mp 128-131° dec. $[\alpha]_D$ +32.7 (c, 1.07 in $CHCl_3$).
Howard, B.M. *et al., J.O.C.*, 1977, **42**, 2518 (*isol, struct*)
Rose, A.F. *et al., Tet. Lett.*, 1977, 2935; 1978, 2533 (*isol, struct*)

2-Bromo-6-eudesmen-5-ol B-403

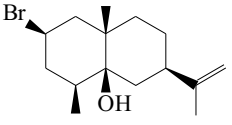
[120637-77-6]



$C_{15}H_{25}BrO$ 301.266

(2α,4α,5β)-*form*
Constit. of *Neomeris annulata*.
Oil. $[\alpha]_D$ -27.3 (c, 1.65 in $CHCl_3$).
Barnekow, D.E. *et al., J.A.C.S.*, 1989, **111**, 3511-3517 (*isol, pmr, cmr*)

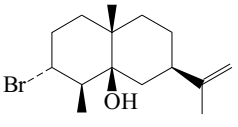
2-Bromo-11-eudesmen-5-ol B-404



$C_{15}H_{25}BrO$ 301.266

(2β,4β,5β)-*form* [151888-87-8]
Isol. from marine green alga *Neomeris annulata*.
Paul, V.J. *et al., J. Chem. Ecol.*, 1993, **19**, 1847-1860
Meyer, K.D. *et al., Mar. Biol. (Berlin)*, 1995, **122**, 537

3-Bromo-11-eudesmen-5-ol B-405

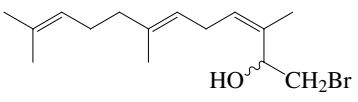


$C_{15}H_{25}BrO$ 301.266

(3α,4β,5β)-*form* [151888-88-9]
Isol. from marine green alga *Neomeris annulata*.
Paul, V.J. *et al., J. Chem. Ecol.*, 1993, **19**, 1847-1860
Meyer, K.D. *et al., Mar. Biol. (Berlin)*, 1995, **122**, 537

1-Bromo-3,6,10-farnesatrien-2-ol B-406

1-Bromo-3,7,11-trimethyl-3,6,10-dodecatrien-2-ol

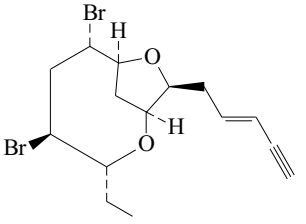


$C_{15}H_{25}BrO$ 301.266

(2ξ,3*Z*,6*E*)-*form* [350483-20-4]
Constit. of *Laurencia luzonensis*.
Oil. $[\alpha]_D^{25}$ +2.9 (c, 0.17 in $CHCl_3$).
Kuniyoshi, M. *et al., J. Nat. Prod.*, 2001, **64**, 696-700 (*isol, pmr, cmr*)

Bromofucin B-407

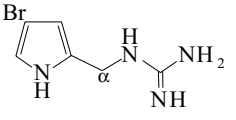
10,12-Dibromo-6,9:7,13-diepoxy-3-pentadecen-1-yne
[125092-24-2]



$C_{15}H_{20}Br_2O_2$ 392.13
Metab. of *Laurencia implicata*. Cryst.
Mp 103-104.5°. $[\alpha]_D$ +1.7 (c, 0.018 in $CHCl_3$).

(Z)-Isomer: ***(Z)-Bromofucin***
$C_{15}H_{20}Br_2O_2$ 392.13
Isol. from *Aplysia parvula*. Amorph. solid. $[\alpha]_D^{24}$ -0.5 (c, 0.25 in $CHCl_3$).
Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1685 (*isol, pmr, cmr*)
McPhail, K.L. *et al., Nat. Prod. Res.*, 2005, **19**, 449-452 (*Z-Bromofucin*)

4-Bromo-2-(guanidinomethyl)pyrrole B-408



$C_6H_9BrN_4$ 217.068
Isol. from the sponge *Agelas* sp.

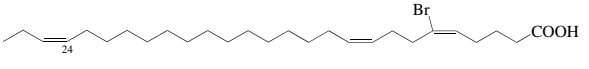
α-Oxo: **N-*(Aminoiminomethyl)-4-bromo-1*H-*pyrrole-2-carboxamide***
$C_6H_7BrN_4O$ 231.051
Isol. from an *Agelas* sp. Not named in the lit., not listed in CA.
Stempien, M.F. *et al., Abstr. Am. Chem. Soc. Natl. Mtg., MEDI Sect., 164th*, 1972, 21 (*α-oxo, isol*)
Christophersen, C. *et al., Alkaloids (N.Y.)*, 1985, **24**, 36 (*occur*)

6-Bromo-5,9-heneicosadienoic acid B-409

$H_3C(CH_2)_{10}CH{=}CHCH_2CH_2CBr{=}CH(CH_2)_3COOH$
$C_{21}H_{37}BrO_2$ 401.426

(5*E*,9*Z*)-*form* [161925-94-6]
Isol. from the sea anemone *Stoichactis helianthus*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1994, **57**, 1688-1695 (*isol, ms*)

6-Bromo-5,9,24-heptacosatrienoic acid, 9CI B-410



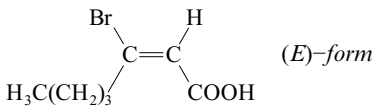
$C_{27}H_{47}BrO_2$ 483.571

(5*E*,9*Z*,24*Z*)-*form*
all-cis-*form*
[162259-49-6]
Isol. from the sponge *Xestospongia* sp.

24,25-Dihydro: 6-Bromo-5,9-heptacosadienoic acid
[149204-39-7]
$C_{27}H_{49}BrO_2$ 485.587
From *Petrosia* sp. and *Xestospongia* sp.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1993, **56**, 739-746 (*isol*)
Li, Y. *et al., J. Chem. Res., Synop.*, 1995, 126-127 (*isol*)

3-Bromo-2-heptenoic acid, 9CI B-411

[66002-54-8]



(*E*)–*form*

$C_7H_{11}BrO_2$ 207.067

(*E*)-*form* [69394-15-6]
Constit. of the red algae *Bonnemaisonia hamifera* and *Bonnemaisonia nootkana*.

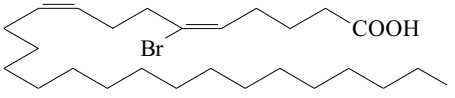
(*Z*)-*form* [74055-83-7]
Isol. from the red alga *Bonnemaisonia nootkana*.

[66002-45-7, 74055-96-2, 154026-90-1]

McConnell, O.J. *et al., Tet. Lett.*, 1977, **18**, 4159-4162 (*isol, pmr*)
Jacobsen, N. *et al., Tet. Lett.*, 1978, 3065 (*isol, pmr*)
McConnell, O.J. *et al., Phytochemistry*, 1980, **19**, 233 (*isol, synth, ir, pmr, ms*)

6-Bromo-5,9-hexacosadienoic acid, 9CI B-412

[121158-15-4]



$C_{26}H_{47}BrO_2$ 471.56

(5*E*,9*Z*)-*form* [121158-12-1]
Isol. from the phospholipids of a marine sponge of the family Hymeniacidonidae.

Me ester: [121158-13-2]
Oil.

Lam, W. *et al., J.O.C.*, 1989, **54**, 3428-3432 (*isol, biosynth, ir, pmr, ms*)
Garson, M.J. *et al., Lipids*, 1993, **28**, 1011-1014

16-Bromo-7,15-hexadecadiene-5,13-diynoic acid, 9CI B-413

$BrCH{=}CHC{\equiv}C(CH_2)_4CH{=}CHC{\equiv}C(CH_2)_3COOH$

$C_{16}H_{19}BrO_2$ 323.229

(7*E*,15*E*)-*form* [111216-67-2]
Isol. from the marine sponge *Xestospongia testudinaria*. Obt. *ca.* 85% pure.

Hirsh, S. *et al., Tetrahedron*, 1987, **43**, 3257 (*isol, struct, ir, uv, pmr, cmr*)

16-Bromo-9,15-hexadecadiene-5,7-diynoic acid B-414

$BrCH{=}CH(CH_2)_4CH{=}CHC{\equiv}CC{\equiv}C(CH_2)_3COOH$

$C_{16}H_{19}BrO_2$ 323.229

(9*E*,15*E*)-*form* [144291-86-1]
Isol. from the marine sponge *Xestospongia muta*.
Amorph. powder.

[144291-92-9]

Patil, A.D. *et al., J. Nat. Prod.*, 1992, **55**, 1170 (*isol, pmr, cmr*)

16-Bromo-11,15-hexadecadiene-3,5,13-triyne-1,2-diol B-415

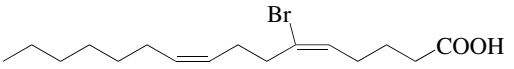
$BrCH{=}CHC{\equiv}CCH{=}CH(CH_2)_4C{\equiv}CC{\equiv}CCH(OH)CH_2OH$

$C_{16}H_{17}BrO_2$ 321.213

(2ξ,11*E*,15*E*)-*form*
Diplyne E
Isol. from the sponge *Diplastrella* sp.
Powder. λ_{max} 215 (ϵ 43300); 272 (ϵ 4120); 287 (ϵ 3410) (MeOH).

Lerch, M.L. *et al., J. Nat. Prod.*, 2003, **66**, 667-670 (*isol, pmr, cmr*)

6-Bromo-5,9-hexadecadienoic acid B-416



$C_{16}H_{27}BrO_2$ 331.292

(5*E*,9*Z*)-*form*
cis,cis-*form*
[162259-47-4]
Isol. from the sponge *Xestospongia* sp.

Li, Y. *et al., J. Chem. Res., Synop.*, 1995, 126-127 (*isol*)

16-Bromo-7,11,15-hexadecatriene-5,13-diynoic acid, 9CI B-417

$BrCH{=}CHC{\equiv}CCH{=}CHCH_2CH_2CH{=}CHC{\equiv}C(CH_2)_3COOH$

$C_{16}H_{17}BrO_2$ 321.213

(7*E*,11*E*,15*E*)-*form* [111216-65-0]
Isol. from the marine sponge *Xestospongia testudinaria*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 234 (ϵ 6300); 246 (ϵ 7600); 285 (ϵ 2800) (MeOH) (Berdy).

(7*E*,11*E*,15*Z*)-*form* [111216-66-1]
Isol. from the marine sponge *Xestospongia testudinaria*.

Hirsh, S. *et al., Tetrahedron*, 1987, **43**, 3257 (*isol, struct, uv, pmr, cmr, ir*)

16-Bromo-15-hexadecene-3,5-diyne-1,2-diol B-418

$BrCH{=}CH(CH_2)_8C{\equiv}CC{\equiv}CCH(OH)CH_2OH$

$C_{16}H_{23}BrO_2$ 327.261

(2ξ,15*E*)-*form*
Diplyne C
Isol. from the sponge *Diplastrella* sp.
Powder. λ_{max} 214 (ϵ 37300) (MeOH).

1-O-*Sulfate:* ***Diplyne C 1-sulfate***
$C_{16}H_{23}BrO_5S$ 407.325
Isol. from *Diplastrella* sp. Powder. Dec. rapidly. λ_{max} 215 (ϵ 48400); 240 (ϵ 5000) (MeOH).

Lerch, M.L. *et al., J. Nat. Prod.*, 2003, **66**, 667-670 (*isol, pmr, cmr*)

16-Bromo-15-hexadecene-3,5,11,13-tetrayne-1,2-diol B-419

$BrCH{=}CHC{\equiv}CC{\equiv}C(CH_2)_4C{\equiv}CC{\equiv}CCH(OH)CH_2OH$

$C_{16}H_{15}BrO_2$ 319.197

(2ξ,15*E*)-*form*
Diplyne D
Isol. from the sponge *Diplastrella* sp.
Powder. λ_{max} 215 (ϵ 61700); 246 (ϵ 6300); 260 (ϵ 11300); 276 (ϵ 16700); 290 (ϵ 13200) (MeOH).

Lerch, M.L. *et al., J. Nat. Prod.*, 2003, **66**, 667-670 (*isol, pmr, cmr*)

16-Bromo-15-hexadecene-3,5,11,13-tetrayn-1-ol B-420

$BrCH{=}CHC{\equiv}CC{\equiv}C(CH_2)_4C{\equiv}CC{\equiv}CCH_2CH_2OH$

$C_{16}H_{15}BrO$ 303.198

(*E*)-*form*
2-Deoxydiplyne D

O-*Sulfate:* ***2-Deoxydiplyne D sulfate***
$C_{16}H_{15}BrO_4S$ 383.262
Isol. from the sponge *Diplastrella* sp. Powder. Dec. rapidly. λ_{max} 246 (ϵ 22400); 259 (ϵ 42300); 274 (ϵ 62700); 290 (ϵ 52400) (MeOH).

Lerch, M.L. *et al., J. Nat. Prod.*, 2003, **66**, 667-670 (*isol, pmr, cmr*)

16-Bromo-15-hexadecene-3,5,13-triyne-1,2-diol B-421

$BrCH{=}CHC{\equiv}C(CH_2)_6C{\equiv}CC{\equiv}CCH(OH)CH_2OH$
$C_{16}H_{19}BrO_2$ 323.229

(2ξ,15*E*)-*form*
Diplyne A
Isol. from the sponge *Diplastrella* sp.
Powder. $[\alpha]_D$ -8.7 (c, 0.33 in MeOH). λ_{max} 217 (ϵ 12500); 238 (ϵ 13300) (MeOH).

1-O-*Sulfate:* ***Diplyne A 1-sulfate***
$C_{16}H_{19}BrO_5S$ 403.293
Isol. from *Diplastrella* sp. Powder. Dec. rapidly.

(2ξ,15*Z*)-*form*
Diplyne B
Isol. from *Diplastrella* sp.
Powder. λ_{max} 215 (ϵ 40900); 235 (ϵ 21400); 246 (ϵ 21000) (MeOH).
Lerch, M.L. *et al., J. Nat. Prod.*, 2003, **66**, 667-670 (*isol, pmr, cmr*)

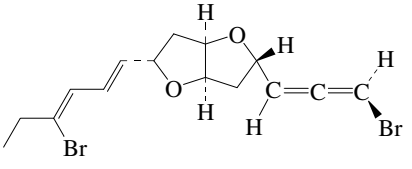
16-Bromo-15-hexadecen-5-ynoic acid B-422

$BrCH{=}CH(CH_2)_8C{\equiv}CCH_2CH_2CH_2COOH$
$C_{16}H_{25}BrO_2$ 329.276

(*E*)-*form* [162259-44-1]
Isol. from the sponge *Xestospongia* sp.
Li, Y. *et al., J. Chem. Res., Synop.*, 1995, 126-127 (*isol*)

2-(4-Bromo-1,3-hexadienyl)-5-(3-bromo-1,2-propadienyl)hexahydrofuro[3,2-*b*]furan, 9CI B-423

Aplysiallene
[99044-96-9]

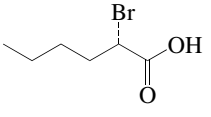


$C_{15}H_{18}Br_2O_2$ 390.114
Constit. of *Aplysia kurodai* and *Laurencia okamurai*. Oil. $[\alpha]_D^{23}$ -215 (c, 0.985 in $CHCl_3$). Shown to be the same as Aplysiallene isol. from *A. kurodai*. λ_{max} 237 (ϵ 27000); 243 (ϵ 28000); 254 (sh) (ϵ 19000) (EtOH).

Suzuki, M. *et al., Phytochemistry*, 1985, **24**, 1999-2002 (*isol, pmr, ms*)
Okamoto, Y. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 474-476; 2003, **67**, 460 (*isol, pmr, cmr*)

2-Bromohexanoic acid, 9CI B-424

[616-05-7]
[38532-59-1]



(*S*)-*form*

$C_6H_{11}BrO_2$ 195.056
▶ MO6650000

(*S*)-*form* [91423-84-6]
$[\alpha]_D^{30}$ -27 (c, 5 in EtOH).
Me ester: [114438-64-1]
$C_7H_{13}BrO_2$ 209.082

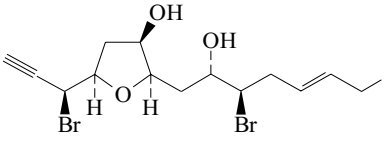
(±)-*form* [2681-83-6]
Mp 4°. Bp 240° Bp_{17} 128-136°.
▶ Fl. p. >66°.
Et ester: [63927-44-6]
$C_8H_{15}BrO_2$ 223.109
Bp 205-210° Bp_1 53°.
Chloride: [42768-46-7]
$C_6H_{10}BrClO$ 213.501
$Bp_{1.5}$ 45-47°.
Bromide: [38532-59-1]
[54971-26-5]
$C_6H_{10}Br_2O$ 257.952
Mp 208-210° dec. Bp_2 54-58°.

(ξ)-*form*
Isol. from the red alga *Bonnemaisonia hamifera*.

[615-96-3, 5445-19-2, 70288-61-8, 91423-83-5, 114438-79-8, 124439-30-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 513A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 801C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 711D (*ir*)
Auwers, K. *et al., J. Prakt. Chem.*, 1923, **106**, 245 (*bromide*)
Levene, P.A. *et al., J. Biol. Chem.*, 1927, **75**, 352; 1937, **117**, 707 (*resoln*)
Levene, P.A. *et al., J.A.C.S.*, 1933, **55**, 1295 (*ester*)
Org. Synth., 1976, **55**, 27 (*chloride*)
Jacobsen, N. *et al., Tet. Lett.*, 1978, **19**, 3065-3068 (*isol, alga*)
Kirchner, G. *et al., J.A.C.S.*, 1985, **107**, 7072 (*resoln*)
Kalaritis, P. *et al., J.O.C.*, 1990, **55**, 812 (*synth*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 433

α-(1-Bromo-3-hexenyl)-5-(1-bromo-2-propynyl)tetrahydro-3-hydroxy-2-furanethanol, 9CI B-425

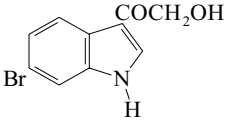


$C_{15}H_{22}Br_2O_3$ 410.145

Ac: 6-Acetoxy-3,10-dibromo-4,7-epoxy-12-pentadecen-1-yne
[94444-24-3]
$C_{17}H_{24}Br_2O_4$ 452.182
Metab. of red alga *Laurencia obtusa*. Oil. $[\alpha]_D$ -14.5 (c, 0.62 in $CHCl_3$).
Gonzalez, A.G. *et al., Tetrahedron*, 1984, **40**, 3443

6-Bromo-3-(hydroxyacetyl)-1*H*-indole B-426

*1-(6-Bromo-1*H*-indol-3-yl)-2-hydroxyethanone, 9CI*
[126235-45-8]

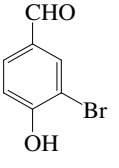


$C_{10}H_8BrNO_2$ 254.083
Alkaloid from the demosponge *Pleroma menouii*. Microcryst. powder (MeOH).
Mp 194-196°. λ_{max} 217 (ϵ 24100); 242 (ϵ 13100); 265 (ϵ 12200); 293 (ϵ 9200) (no solvent reported).

Guella, G. *et al., Z. Naturforsch., C*, 1989, **44**, 914 (*isol, uv, ir, pmr, cmr, ms, struct*)

3-Bromo-4-hydroxybenzaldehyde, 9CI, 8CI B-427

[2973-78-6]



$C_7H_5BrO_2$ 201.019

Isol. from *Asparagopsis taxiformis*, *Psammaplysilla purpurea* and *Rhodomela larix*. Constit. of Indian algae. Leaflets.
Mp 125-126°.

Oxime:
$C_7H_6BrNO_2$ 216.034
Mp 135°.

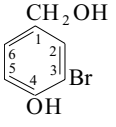
Semicarbazone: Mp 195-196°.

*Me ether: 3-Bromo-4-methoxybenzaldehyde, 9CI. 3-Bromo-*p*-anisaldehyde, 8CI*
[34841-06-0]
$C_8H_7BrO_2$ 215.046
Cryst. (Et_2O). Mp 54°.

Brink, M. *et al., CA*, 1965, **63**, 8240c (*synth*)
Torii, S. *et al., J.O.C.*, 1979, **44**, 3305-3310 (*synth*)
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 2099-2100 (*isol*)
Nagao, Y. *et al., Tet. Lett.*, 1980, **21**, 4931-4934 (*synth*)
de la Mare, P.B.D. *et al., J.C.S. Perkin 2*, 1984, 1797-1802 (*synth*)
Pandya, A.C. *et al., Planta Med.*, 1990, **56**, 557 (*isol*)
Anson, C.E. *et al., J. Organomet. Chem.*, 2003, **668**, 101-122 (*synth*)

3-Bromo-4-hydroxybenzyl alcohol, 8CI B-428

3-Bromo-4-hydroxybenzenemethanol, 9CI. 3-Bromo-4-hydroxyphenylmethanol. 2-Bromo-4-hydroxymethylphenol
[29922-56-3]

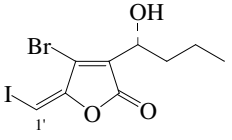


$C_7H_7BrO_2$ 203.035
Isol. from the Rhodomelaceae. Shows antibiotic props.
Mp 128°.

1′-Me ether: 2-Bromo-4-(methoxymethyl)phenol, 9CI
[71119-01-2]
$C_8H_9BrO_2$ 217.062
Constit. of *Odonthalia dentata* and *Rhodomela larix*.
Mp 59-60° (synthetic).

Dunning, B. *et al., J.A.C.S.*, 1936, **58**, 1565
Weinstein, B. *et al., Phytochemistry*, 1975, **14**, 2667 (*isol, rev*)
Torii, S. *et al., J.O.C.*, 1979, **44**, 3305 (*synth*)
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 2099 (*isol, synth*)

4-Bromo-3-(1-hydroxybutyl)-5-(iodomethylene)-2(5*H*)-furanone B-429



(*R*)-(*E*)-*form*

$C_9H_{10}BrIO_3$ 372.985

(R)-(E)-form [63025-29-6]
Constit. of the red alga *Delisea pulchra*.
Oil.

*Ac: 3-(1-Acetoxybutyl)-4-bromo-5-(iodomethylene)-2(5*H*)-furanone. **Acetoxyfimbrolide d***
$C_{11}H_{12}BrIO_4$ 415.022
Constit. of *Delisea fimbriata*.

1′-Deiodo, 1′-bromo: ***Hydroxyfimbrolide a***
[63025-27-4]
$C_9H_{10}Br_2O_3$ 325.984
Constit. of *Delisea fimbriata*. Yellow oil.

*1′-Deiodo, 1′-bromo, Ac: 1-(1-Acetoxybutyl)-4-bromo-4-(bromomethylene)-2(5*H*)-furanone. **Acetoxyfimbrolide a***
[63025-20-7]
$C_{11}H_{12}Br_2O_4$ 368.021
Constit. of *Delisea fimbriata*. Glutamic acid decarboxylase. Gaba inhibitor. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ -4.1 (c, 1.3 in $CHCl_3$). λ_{max} 293 (E1%/1cm 220) (MeOH) (Berdy).
► LD_{50} (mus, scu) 24 mg/kg.

(R)-(Z)-form [63025-30-9]
Constit. of *Delisea pulchra*.
Oil. $[\alpha]_D^{25}$ +3 (c, 0.2 in $CHCl_3$).

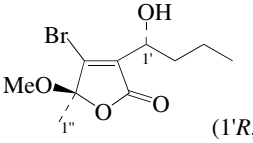
Ac: [63025-23-0]
$C_{11}H_{12}BrIO_4$ 415.022
Constit. of *Delisea pulchra*. Oil. $[\alpha]_D^{25}$ +23.2 (c, 0.5 in $CHCl_3$).

1′-Deiodo, 1′-bromo: ***Hydroxyfimbrolide b***
[63025-28-5]
$C_9H_{10}Br_2O_3$ 325.984
Constit. of *Delisea pulchra*. Yellow oil.

1′-Deiodo, 1′-bromo, Ac: ***Acetoxyfimbrolide b***
[63025-21-8]
$C_{11}H_{12}Br_2O_4$ 368.021
Constit. of *Delisea fimbriata*.
$[\alpha]_D$ +29 (c, 5.8 in $CHCl_3$).

Kazlauskas, R. *et al., Tet. Lett.*, 1977, 37
Pettus, J.A. *et al., Tet. Lett.*, 1977, 41
de Nys, R. *et al., Tetrahedron*, 1993, **49**, 11213
de March, P. *et al., J.O.C.*, 1995, **60**, 1815 (*synth*)

4-Bromo-3-(1-hydroxybutyl)-5-methoxy-5-methyl-2(5*H*)-furanone B-430



(1′*R*,5*R*)-*form*

$C_{10}H_{15}BrO_4$ 279.13

(1′R,5R)-form
Ac: [163936-69-4]
$C_{12}H_{17}BrO_5$ 321.167
Constit. of *Delisea pulchra*. Oil. $[\alpha]_D^{25}$ +3 (c, 1.2 in $CHCl_3$). λ_{max} 231 (ϵ 8500) (MeOH) (Berdy).

1″-Iodo: [163936-66-1]
$C_{10}H_{14}BrIO_4$ 405.027
Constit. of *Delisea pulchra*. Oil. $[\alpha]_D^{25}$ +39 (c, 1 in $CHCl_3$). λ_{max} 230 (ϵ 8500) (MeOH) (Berdy).

1″,1″-Dibromo, Ac: [163936-70-7]
Constit. of *Delisea pulchra*.
$[\alpha]_D$ +27 (c, 0.5 in $CHCl_3$). λ_{max} 208 (ϵ 7100); 233 (ϵ 8500) (MeOH) (Berdy).

(1′R,5S)-form
*Ac: 3-(1-Acetoxybutyl)-4-bromo-5-methoxy-5-methyl-2(5*H*)-furanone*
[163936-68-3]
$C_{12}H_{17}BrO_5$ 321.167
Constit. of the red alga *Delisea pulchra*. Oil. $[\alpha]_D^{25}$ +38 (c, 0.9 in $CHCl_3$). λ_{max} 229 (ϵ 6880) (MeOH) (Berdy).

*1″-Iodo: 4-Bromo-3-(1-hydroxybutyl)-5-(iodomethyl)-5-methoxy-2(5*H*)-furanone*
[163936-67-2]
$C_{10}H_{14}BrIO_4$ 405.027
Constit. of *Delisea pulchra*. Oil. $[\alpha]_D^{25}$ +8 (c, 0.8 in $CHCl_3$). λ_{max} 231 (ϵ 8500) (MeOH) (Berdy).

*1″-Iodo, Ac: 3-(1-Acetoxybutyl)-4-bromo-5-iodomethyl-5-methoxy-2(5*H*)-furanone*
[163936-65-0]
$C_{12}H_{16}BrIO_5$ 447.064
Constit. of *Delisea pulchra*. Oil. $[\alpha]_D^{25}$ +27 (c, 1 in $CHCl_3$). λ_{max} 230 (ϵ 7960) (MeOH) (Berdy).

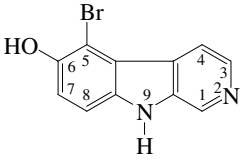
*1″,1″-Dibromo, Ac: 3-(1-Acetoxybutyl)-4-bromo-5-(dibromomethyl)-5-methoxy-2(5*H*)-furanone*
[163936-71-8]
$C_{12}H_{15}Br_3O_5$ 478.959
Constit. of *Delisea pulchra*. Oil. $[\alpha]_D^{25}$ +10 (c, 0.5 in $CHCl_3$). λ_{max} 208 (ϵ 7125); 233 (ϵ 8500) (MeOH) (Berdy).

[87745-25-3, 152195-76-1, 152195-77-2, 152195-78-3]

De Nys, R. *et al., Tetrahedron*, 1993, **49**, 11213-11220 (*isol, uv, ir, pmr, cmr*)
Koenig, G.M. *et al., Helv. Chim. Acta*, 1995, **78**, 758-764 (*isol, cryst struct, abs config*)

5-Bromo-6-hydroxy-β-carboline B-431

*5-Bromo-9*H*-pyrido[3,4-*b*]indol-6-ol, 9CI. 5-Bromo-6-hydroxy-9*H*-pyrido[3,4-*b*]indole.* ***Eudistomin D***
[88704-37-4]



$C_{11}H_7BrN_2O$ 263.093
Alkaloid from the Caribbean tunicate *Eudistoma olivaceum*. Mod. active against gram-positive bacteria and Herpes simplex virus. Yellow amorph. solid.
Mp 280°. λ_{max} 215 (ϵ 14000); 233 (ϵ 24800); 246 (ϵ 19800); 286 (ϵ 8500); 294 (ϵ 15000); 365 (ϵ 4500) (MeOH) (Derep).

N^2-*Me:* ***N*²-Methyleudistomin D***
[380614-17-5]
$C_{12}H_{10}BrN_2O^{\oplus}$ 278.128
Quaternary alkaloid from *Eudistoma gilboverde*. Amorph. yellow powder. Counterion not specified. λ_{max} 214 (log ϵ 4.02); 236 (log ϵ 3.8); 268 (log ϵ 3.96); 303 (sh) (log ϵ 3.71); 314 (log ϵ 3.79); 416 (log ϵ 3.19) (EtOH).

N^9-*Me:* ***Eudistomidin D***
[125422-19-7]
$C_{12}H_9BrN_2O$ 277.12
Alkaloid from the Okinawan tunicate *Eudistoma glaucus*. Cytotoxic. Induces $Ca^{2\oplus}$ release from the sarcoplasmic reticulum. Yellow solid.
Mp 180° dec. λ_{max} 254 (ϵ 7000); 299 (ϵ 8600); 342 (sh); 503 (ϵ 700) (MeOH/KOH) (Derep). λ_{max} 211 (ϵ 13600); 270 (ϵ 9800); 315 (ϵ 6800); 416 (ϵ 1800) (MeOH) (Derep).

Kobayashi, J. *et al., J.A.C.S.*, 1984, **106**, 1526-1528 (*isol, uv, pmr, struct*)
Rinehart, K.L. *et al., J.A.C.S.*, 1987, **109**, 3378-3387 (*isol, struct, props*)
Kobayashi, J. *et al., J.O.C.*, 1990, **55**, 3666-3670 (*Eudistomidin D*)
Rocca, P. *et al., Tet. Lett.*, 1995, **36**, 7085-7088 (*synth*)
Rashid, M.A. *et al., J. Nat. Prod.*, 2001, **64**, 1454-1456 (*N²-Methyleudistomin D*)

7-Bromo-6-hydroxy-β-carboline B-432

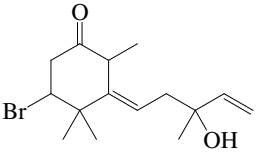
*7-Bromo-9*H*-pyrido[3,4-*b*]indol-6-ol, 9CI.* ***Eudistomin J***
[88704-38-5]
$C_{11}H_7BrN_2O$ 263.093
Alkaloid from the Caribbean tunicate *Eudistoma olivaceum*. Shows modest antibiotic activity. Calcium release inducer. λ_{max} 215 (ϵ 14000); 233 (ϵ 24800); 246 (ϵ 19800); 286 (ϵ 8500); 294 (ϵ 15000); 365 (ϵ 4500) (MeOH) (Derep).

N^2-*Me:* ***N*²-Methyleudistomin J***
[380614-18-6]
$C_{12}H_{10}BrN_2O^{\oplus}$ 278.128
Quaternary alkaloid from *Eudistoma gilboverde*. Yellow gum. λ_{max} 212 (log ϵ 4.04); 236 (log ϵ 3.99); 271 (log ϵ 3.97); 307 (sh) (log ϵ 3.83); 321 (log ϵ 3.96); 412 (log ϵ 3.35) (EtOH).

Rinehart, K.L. *et al., J.A.C.S.*, 1987, **109**, 3378-3387 (*isol*)
Rashid, M.A. *et al., J. Nat. Prod.*, 2001, **64**, 1454-1456 (*N²-Methyleudistomin J*)

2-Bromo-9-hydroxy-6,10-cyclofarnesadien-4-one B-433

[636599-35-4]

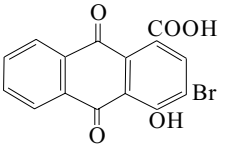


$C_{15}H_{23}BrO_2$ 315.25
Constit. of *Laurencia obtusa*.

Topcu, G. *et al., J. Nat. Prod.*, 2003, **66**, 1505-1508 (*isol, pmr, cmr*)

3-Bromo-4-hydroxy-9,10-dioxo-1-anthracenecarboxylic acid B-434

3-Bromo-4-hydroxyanthraquinone-1-carboxylic acid
[108615-36-7]

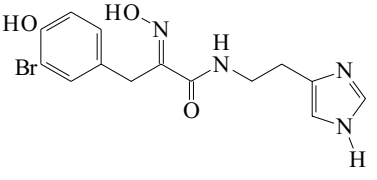


$C_{15}H_7BrO_5$ 347.121
Defence chemical prod. by *Tubastrea micrantha*. Orange needles (EtOH).
Mp 158-160°.

Sanduja, R. *et al., J. Chem. Res., Synop.*, 1986, 450-451 (*isol, struct*)

3-Bromo-4-hydroxy-α-(hydroxyimino)-*N*-[2-(1*H*-imidazol-4-yl)ethyl]benzenepropanamide B-435

Pseudoceratina crassa *Alkaloid*
[165329-94-2]

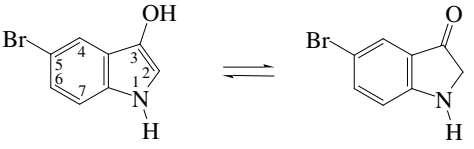


$C_{14}H_{15}BrN_4O_3$ 367.201
Alkaloid from the Caribbean sponge *Pseudoceratina crassa*.

Ciminiello, P. *et al., J. Nat. Prod.*, 1995, **58**, 689 (*isol, uv, ir, pmr, cmr, struct*)

5-Bromo-3-hydroxy-1*H*-indole B-436

*5-Bromo-1*H*-indol-3-ol. 5-Bromo-1,2-dihydro-3*H*-indol-3-one. 5-Bromo-3-indolone*



C_8H_6BrNO 212.045

OH-form

O-*Sulfate:*
$C_8H_6BrNO_4S$ 292.11
Isol. from *Murex trunculus*.

O-*β-D-Galactopyranoside: Z-gal*
[97753-82-7]
$C_{14}H_{16}BrNO_6$ 374.188

Chromogenic substrate for β-galactosidase.

O-*Ac:* [17357-14-1]
$C_{10}H_8BrNO_2$ 254.083
Stout needles (MeOH). Mp 187-188°.

Di-Ac: [33588-54-4]
$C_{12}H_{10}BrNO_3$ 296.12
Needles (MeOH aq./Ac_2O). Mp 125-128°.

Oxo-*form*

Oxime: [76983-85-2]
$C_8H_7BrN_2O$ 227.06
Brown needles (C_6H_6). Mp 233-235°.

Su, H.C.F. *et al., J.A.C.S.*, 1960, **82**, 1187 (*O-Ac*)
Baker, J.T. *et al., Tet. Lett.*, 1968, 43 (*sulfate*)
Fouquet, H. *et al., Angew. Chem., Int. Ed.*, 1971, **10**, 816-817 (*isol, sulfate*)
Baker, J.T. *et al., Tet. Lett.*, 1976, 1233-1234 (*occur, sulfate*)
Torii, S. *et al., J.O.C.*, 1978, **43**, 2882 (*di-Ac*)
Aguzzi, A. *et al., Histochemistry*, 1994, **102**, 477-481 (*O-galactopyranosyl, use*)
Cooksey, C.J. *et al., Molecules*, 2001, **6**, 736-769 (*rev, sulfate*)

6-Bromo-5-hydroxy-1*H*-indole B-437

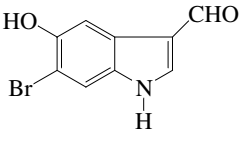
*6-Bromo-1*H*-indol-5-ol*
[211808-66-1]

C_8H_6BrNO 212.046
Alkaloid from the gastropod *Drupella fragum*. Shows antioxidant props. Amorph. solid.

Ochi, M. *et al., J. Nat. Prod.*, 1998, **61**, 1043-1045 (*isol*)

6-Bromo-5-hydroxy-1*H*-indole-3-carboxaldehyde B-438

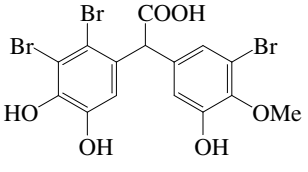
6-Bromo-3-formyl-5-hydroxyindole
[151833-94-2]



$C_9H_6BrNO_2$ 240.056
Isol. from sponge *Oceanapia bartschi*. λ_{max} 255 (ϵ 5800) (no solvent reported).

Cafieri, F. *et al., Z. Naturforsch., B*, 1993, **48**, 1408-1410

(3-Bromo-5-hydroxy-4-methoxyphenyl)(2,3-dibromo-4,5-dihydroxyphenyl)acetic acid B-439



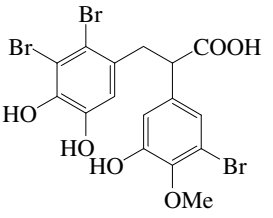
$C_{15}H_{11}Br_3O_6$ 526.96

(ξ)-*form*

Isol. from the red alga *Rhodomela confervoides*.
Brown gum.

Zhao, J. *et al., J. Nat. Prod.*, 2004, **67**, 1032-1035 (*isol, pmr, cmr*)

2-(3-Bromo-5-hydroxy-4-methoxyphenyl)-3-(2,3-dibromo-4,5-dihydroxyphenyl)propanoic acid B-440



$C_{16}H_{13}Br_3O_6$ 540.987

(ξ)-*form*

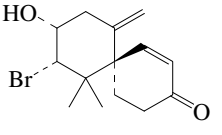
Isol. from the red alga *Rhodomela confervoides*.
Brown gum.

Me ester:
$C_{17}H_{15}Br_3O_6$ 555.014
Isol. from *Rhodomela confervoides*. Brown gum.

Zhao, J. *et al., J. Nat. Prod.*, 2004, **67**, 1032-1035 (*isol, pmr, cmr*)

10-Bromo-9-hydroxy-15-nor-1,7(14)-chamigradien-3-one B-441

Mailione
[185213-74-5]



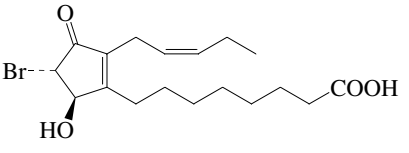
Absolute Configuration

$C_{14}H_{19}BrO_2$ 299.207
Constit. of *Laurencia cartilaginea*. Pale yellow oil. $[\alpha]_D$ -100 (c, 0.2 in $CHCl_3$). λ_{max} 228 (ϵ 8769); 241 (MeOH) (Berdy).

Juagdan, E.G. *et al., Tetrahedron*, 1997, **53**, 521-528 (*isol, pmr, cmr*)
Suescun, L. *et al., Acta Cryst. C*, 2001, **57**, 286-288 (*cryst struct*)

4-Bromo-5-hydroxy-3-oxo-2-(2-pentenyl)-1-cyclopentene-1-octanoic acid B-442

11-Bromo-10-hydroxy-12-oxo-9(13),15-phytodienoic acid. 11-Bromo-10-hydroxychromomoric acid F



$C_{18}H_{27}BrO_4$ 387.313
Misleading synonym.

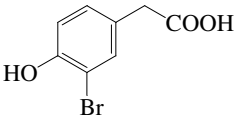
(10*R,11*S**,15*Z*)-*form***

Me ester: [510714-50-8]
$C_{19}H_{29}BrO_4$ 401.34
Isol. from the coral *Dendrophyllia* sp.
$[\alpha]_D^{22}$ +23.8 (c, 0.11 in MeOH). λ_{max} 225 (log ϵ 2.18) (MeOH).

Rezanka, T. *et al., Eur. J. Org. Chem.*, 2003, 309-316 (*isol, cd, pmr, cmr*)

(3-Bromo-4-hydroxyphenyl)acetic acid, 8CI B-443

3-Bromo-4-hydroxybenzeneacetic acid, 9CI. 3-Bromo-4-hydroxy-α-toluic acid
[38692-80-7]



$C_8H_7BrO_3$ 231.045
Needles. Mp 107°.

Me ester: [34918-57-5]
$C_9H_9BrO_3$ 245.072
Mp 41°.

Nitrile: (3-Bromo-4-hydroxyphenyl)acetonitrile. 2-Bromo-4-(cyanomethyl)phenol
[73348-21-7]
C_8H_6BrNO 212.045
Constit. of *Psammaplysilla purpurea* and *Verongia aurea*. Antifungal agent. Pale yellow solid.
Mp 118-119°. λ_{max} 220 (ϵ); 280 (ϵ); 288 (sh) (ϵ) (MeOH) (Derep).

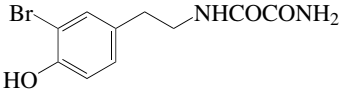
Me ether: (3-Bromo-4-methoxyphenyl)acetic acid, 8CI
[774-81-2]
$C_9H_9BrO_3$ 245.072
Mp 118°.

Me ether, Me ester: [19626-36-9]
$C_{10}H_{11}BrO_3$ 259.099
Mp 48.5°. Bp_3 144-145°.

Tolkachev, O.N. *et al., Zh. Obshch. Khim.*, 1961, **31**, 1540
Coutts, I.G.C. *et al., Aust. J. Chem.*, 1970, **23**, 791 (*deriv*)
D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1984, **67**, 1484 (*synth*)
Pachaly, P. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1989, **322**, 483 (*synth*)
Jimenez, C. *et al., Tetrahedron*, 1991, **47**, 2097 (*nitrile*)
Boehlow, T.R. *et al., J.O.C.*, 2001, **66**, 3111-3118 (*nitrile, synth, pmr, cmr*)

[2-(3-Bromo-4-hydroxyphenyl)ethyl]ethanediamide, 9CI B-444

[182496-50-0]

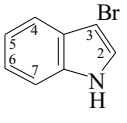


$C_{10}H_{11}BrN_2O_3$ 287.113
Isol. from the Papua New Guinea marine sponge *Ianthella basta*. Amorph. solid. λ_{max} 212 (log ϵ 3.89); 281 (log ϵ 3.14) (MeOH).

Pettit, G.R. *et al., J. Nat. Prod.*, 1996, **59**, 927-934 (*isol, uv, ir, pmr, cmr, ms, struct*)

3-Bromo-1*H*-indole, 9CI B-445

[1484-27-1]



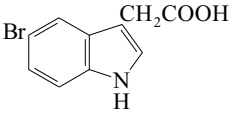
C_8H_6BrN 196.046
Trace odorous component of the marine hemichordate *Ptychodera flava laysanica*. Also isol. from sponge *Oceanapia bartschi*. Cryst. (heptane or EtOH aq.).
Mp 66-67° (65-66° dec.).

N-*(4-Methylbenzenesulfonyl):*
$C_{15}H_{12}BrNO_2S$ 350.235
Needles (EtOH). Mp 119-120°.

Pappalardo, G. *et al., Gazz. Chim. Ital.*, 1958, **88**, 1147 (*uv*)
Jardine, R.V. *et al., Can. J. Chem.*, 1963, **41**, 2067 (*pmr*)
Piers, K. *et al., Can. J. Chem.*, 1963, **41**, 2399 (*synth*)
Higa, T. *et al., Naturwissenschaften*, 1975, **62**, 395 (*isol*)
Cafieri, F. *et al., Z. Naturforsch., B*, 1992, **48**, 1408-1410 (*isol, sponge*)
Hodson, H.F. *et al., Tetrahedron*, 1995, **50**, 1899 (*N-tosyl*)

5-Bromo-1*H*-indole-3-acetic acid B-446

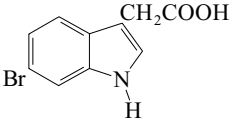
[40432-84-6]



$C_{10}H_8BrNO_2$ 254.083
Constit. of a sponge *Smenospongia* sp.
Mp 143-145°.

Szewezyk, H. *et al., Rocz. Chem.*, 1972, **46**, 2135
Tasdemir, D. *et al., Z. Naturforsch., C*, 2002, **57**, 914-922 (*isol, pmr, cmr, ms*)

6-Bromo-1*H*-indole-3-acetic acid B-447



$C_{10}H_8BrNO_2$ 254.083

*Me ester: Methyl 6-bromo-1*H*-indole-3-acetate, 9CI*
[152213-63-3]
$C_{11}H_{10}BrNO_2$ 268.109
Alkaloid from the marine sponge *Pseudosuberites hyalinus*. Oil.

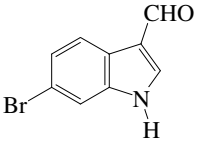
*Amide: 6-Bromo-1*H*-indole-3-acetamide, 9CI*
[152213-62-2]
$C_{10}H_9BrN_2O$ 253.098
Alkaloid from the marine sponge *Pseudosuberites hyalinus*.
Mp 148-150°.

*Nitrile: 6-Bromo-1*H*-indole-3-acetonitrile, 9CI. 6-Bromo-3-(cyanomethyl)indole*
[152213-61-1]
$C_{10}H_7BrN_2$ 235.083
Alkaloid from the marine sponge *Pseudosuberites hyalinus*.
Mp 114-115°.

Rasmussen, T. *et al., J. Nat. Prod.*, 1993, **56**, 1553

6-Bromo-1*H*-indole-3-carboxaldehyde, 9CI B-448

6-Bromo-3-formylindole. 6-Bromoindole-3-carbaldehyde
[17826-04-9]



C_9H_6BrNO 224.056
Isol. from the marine tunicate *Pyura sacciformis*; also from *Pseudosuberites hyalinus*, *Pleroma menoui*, *Tubastrea coccinea*, *Dendrophyllia* spp. and sponges *Oceanapia bartschi*, *Halichondria* spp. and others. From *Acinetobacter sp.* associated with the ascidian *Stomozoa murrayi*. Exhibits antibacterial and antifouling activity; plant growth regulator; algicide. Solid (MeOH).
Mp 203-204°.

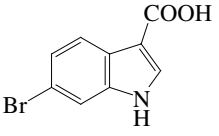
N-*(4-Methylbenzenesulfonyl):* [158991-81-2]
$C_{16}H_{12}BrNO_3S$ 378.246
Solid or cryst. ($CHCl_3$). Mp 115° Mp 146-147°.

Da Settimo, A. *et al., Gazz. Chim. Ital.*, 1967, **97**, 1304-1316 (*synth*)
Dellar, G. *et al., J.C.S. Perkin 1*, 1981, 1679-1680 (*synth, pmr*)

Okuda, R.K. *et al., Pure Appl. Chem.*, 1982, **54**, 1907-1914 (*isol*)
Schmidt, V. *et al., Annalen*, 1985, 1882-1894 (*synth*)
Niwa, H. *et al., J. Nat. Prod.*, 1988, **51**, 343-344 (*isol*)
Guella, G. *et al., Helv. Chim. Acta*, 1989, **72**, 1444-1450 (*isol, hplc*)
Cafieri, F. *et al., Z. Naturforsch., B*, 1992, **48**, 1408-1410 (*isol, sponge*)
Jiang, B. *et al., J.O.C.*, 1994, **59**, 6823-6827 (*synth, ir, pmr, ms*)
Olguin-Uribe, G. *et al., J. Chem. Ecol.*, 1997, **23**, 2507-2521 (*isol, activity*)
Jiang, B. *et al., J.O.C.*, 2001, **66**, 4865-4869 (*tosyl, synth, ir, pmr, cmr, ms*)

6-Bromo-1*H*-indole-3-carboxylic acid, 9CI B-449

[101774-27-0]



$C_9H_6BrNO_2$ 240.056

Early lit. mistakenly reports physical data for both acid and Et ester which actually refer to inseparable equimolar mixt. of 5- and 6-bromo isomers. Isol. from the marine sponge *Pseudosuberites hyalinus*.

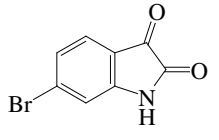
Me ester:
$C_{10}H_8BrNO_2$ 254.083
Alkaloid from *Smenospongia* sp. Yellow solid.

Et ester: [103858-55-5]
$C_{11}H_{10}BrNO_2$ 268.109
Alkaloid from the demosponge *Pleroma menoui* and the sponge *Iotrochota birotulata*. Microcryst. powder (MeOH).
Mp 147-149°.

Leggetter, B.E. *et al., Can. J. Chem.*, 1960, **38**, 1467 (*synth*)
Guella, G. *et al., Z. Naturforsch., C*, 1989, **44**, 914-916 (*Et ester, isol*)
Rasmussen, T. *et al., J. Nat. Prod.*, 1993, **56**, 1553-1558 (*isol, ms, pmr, cmr*)
Segraves, N.L. *et al., J. Nat. Prod.*, 2005, **68**, 1484-1488 (*Me ester*)

6-Bromo-1*H*-indole-2,3-dione, 9CI B-450

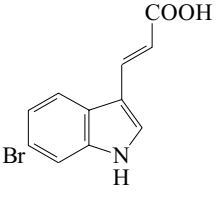
6-Bromoisatin
[6326-79-0]



$C_8H_4BrNO_2$ 226.029
Isol. from many molluscs. Plant growth regulator. Probably a precursor of 6,6′-Dibromoindirubin. Needles, yellow plates (AcOH).
Mp 272.5°. pK_a 10.35.

Inagaki, S. *et al., Yakugaku Zasshi*, 1938, **58**, 961-975; *CA*, **33**, 2516 (*synth*)
Sadler, P.W. *et al., J.O.C.*, 1956, **21**, 169-170 (*synth*)
Budesinsky, Z. *et al., Coll. Czech. Chem. Comm.*, 1977, **42**, 3473-3483 (*synth*)
Clark, R.J.H. *et al., New J. Chem.*, 1999, **23**, 323-328 (*pmr*)
Cooksey, C.J. *et al., Molecules*, 2001, **6**, 736-769 (*rev*)

3-(6-Bromo-1*H*-indol-3-yl)-2-propenoic acid, 9CI B-451



$C_{11}H_8BrNO_2$ 266.094

(E)-form

Penaresin
[135250-41-8]
Alkaloid from the marine sponge *Penares* sp. Powerful Ca-inducer in sarcoplasmic reticulum. Pale yellow solid.
Mp 189-192° dec. λ_{max} 228 (ϵ 27100); 280 (ϵ 18400); 307 (ϵ 18300) (MeOH).

Me ester: [134419-23-1]
[78520-47-5]
$C_{12}H_{10}BrNO_2$ 280.12
Alkaloid from the marine sponges *Hymeniacidon* sp., *Iotrochota* sp. and *Mycale adhaerens*. Clusters of prisms (Et_2O/hexane).
Mp 186°. λ_{max} 226 (ϵ 34200); 283 (ϵ 19900); 324 (ϵ 26200) (MeOH) (Berdy).

Et ester: [226888-27-3]
$C_{13}H_{12}BrNO_2$ 294.147
Alkaloid from the sponge *Hymeniacidon* sp. Cryst. (Me_2CO/petrol) (synthetic).
Mp 147-149° (synthetic).

(Z)-form

Me ester: [419567-80-9]
Alkaloid from *Hymeniacidon* sp.

Et ester: [419567-79-6]
Alkaloid from *Hymeniacidon* sp.

Dellar, G. *et al., J.C.S. Perkin 1*, 1981, 1679-1680 (*isol, ir, pmr, ms, struct, synth, Me ester*)
Kobayashi, J. *et al., Heterocycles*, 1990, **31**, 2205-2208 (*isol, uv, ir, pmr, ms, struct*)
Fusetani, N. *et al., J.O.C.*, 1991, **56**, 4971-4974 (*isol, Me ester*)
Beugelmans, R. *et al., Tetrahedron*, 1999, **55**, 5089-5112 (*Et ester, synth*)
Capon, R.J. *et al., J. Nat. Prod.*, 2002, **65**, 368-370 (*Me esters, Et esters, isol*)

Bromoiodoacetic acid B-452

[71815-43-5]
BrCHICOOH
$C_2H_2BrIO_2$ 264.845
Constit. of the red alga *Asparagopsis taxiformis*.

Et ester: [62874-49-1]
$C_4H_6BrIO_2$ 292.899
Constit. of *Asparagopsis taxiformis* and *Falkenbergia rufolonosa*.

Amide: Bromoiodoacetamide
[62872-36-0]
C_2H_3BrINO 263.86
Constit. of *Asparagopsis taxiformis*.

Woolard, F.X. *et al., Tetrahedron*, 1976, **32**, 2843-2846 (*amide, isol*)
Combaut, G. *et al., Phytochemistry*, 1978, **17**, 1661-1663 (*isol*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617-620 (*isol, ms*)

1-Bromo-2-iodoethane, 9CI B-453

Ethylene bromoiodide
[590-16-9]
$BrCH_2CH_2I$
C_2H_4BrI 234.862
Isol. from the alga *Asparagopsis taxiformis*. Cryst. d_4^{29} 2.52.
Mp 28°. Bp 163°.

Simpson, M. *et al., Ber.*, 1874, **7**, 130 (*synth*)
Gagarin, G. *et al., Ber.*, 1874, **7**, 733 (*synth*)
Morishima, I. *et al., J.A.C.S.*, 1972, **94**, 4812 (*cmr*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)

Bromoiodomethane, 9CI B-454

Methylene bromoiodide
[557-68-6]
CH_2BrI
CH_2BrI 220.835
Isol. from several marine algae. d_4^{17} 2.93. Bp 138-140°.

Henry, L. *et al., J. Prakt. Chem.*, 1885, **32**, 431 (*synth*)
Hine, J. *et al., J.A.C.S.*, 1955, **77**, 3886 (*synth*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)

1-Bromo-3-iodo-2-propanol, 9CI B-455

[62872-30-4]

$BrCH_2CH(OH)CH_2I$

C_3H_6BrIO 264.888

(ξ)-*form*

Present in edible red algae *Asparagopsis taxiformis*.

Yellow liq.

Woolard, F.X. *et al., Tetrahedron*, 1976, **32**, 2843-2846 (*isol, glc, ms*)

Sharghi, H. *et al., Tetrahedron*, 2003, **59**, 8509-8514 (*synth*)

1-Bromo-3-iodo-2-propanone, 9CI B-456

1-Bromo-3-iodoacetone

[59227-98-4]

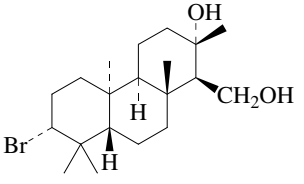
$BrCH_2COCH_2I$

C_3H_4BrIO 262.873

Minor component of the essential oil of the edible Hawaiian red alga *Asparagopsis taxiformis*.

Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*synth, glc, ms, isol*)

3-Bromo-13,15-isocopalanediol B-457



$C_{20}H_{35}BrO_2$ 387.399

Revised struct., formerly assigned *ent*-cleistanthane skeleton. Abs. config. revised in 1984.

(*ent*-3β,8α,13β*OH*,14α)-*form*

Isoaplysin 20

[64854-29-1]

Constit. of *Aplysia kurodai* and *Laurencia perforata*.

Cryst. (MeOH).

Mp 195-198°.

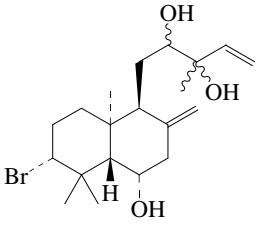
Yamamura, S. *et al., Tet. Lett.*, 1977, 2171-2172 (*isol, Aplysia kurodai constit*)

Nishizawa, M. *et al., J.A.C.S.*, 1984, **106**, 4290-4291 (*cryst struct*)

González, A.G. *et al., J.O.C.*, 1985, **50**, 1261-1264 (*isol, Laurencia perforata constit*)

Nishizawa, M. *et al., J.O.C.*, 1986, **51**, 806-813 (*synth*)

3-Bromo-8(17),14-labdadiene-6,12,13-triol B-458



$C_{20}H_{33}BrO_3$ 401.383

(*ent*-3β,6β,9α,12ξ,13ξ)-*form*

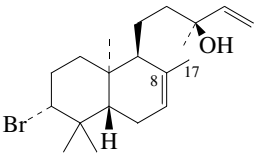
6,12-Di-Ac: [872038-41-0]

$C_{24}H_{37}BrO_5$ 485.457

Constit. of a *Laurencia* sp. Oil. $[\alpha]_D^{24}$ +39.3 (c, 0.25 in $CHCl_3$).

Suzuki, M. *et al., Phytochemistry*, 2005, **66**, 2787-2793 (*Laurencia constit*)

3-Bromo-7,14-labdadien-13-ol B-459



(*ent*-3β,9β*H*,13*R*)-*form*

$C_{20}H_{33}BrO$ 369.384

(*ent*-3β,9β*H*,13*R*)-*form*

Pinnatol C

[98683-36-4]

Constit. of *Laurencia pinnata*.

Oil. $[\alpha]_D$ +110.5 ($CHCl_3$).

Δ^8*-Isomer: 3-Bromo-8,14-labdadien-13-ol*. ***Pinnatol D***

[98683-35-3]

$C_{20}H_{33}BrO$ 369.384

Constit. of *Laurencia pinnata*. Oil. $[\alpha]_D$ -48.2 ($CHCl_3$).

Δ$^{8(17)}$*-Isomer: 3-Bromo-8(17),14-labdadien-13-ol.* ***Pinnatol B***

[98683-37-5]

Constit. of *Laurencia pinnata*.

Cryst.

Mp 106.5-107.5°. $[\alpha]_D$ -7.6 ($CHCl_3$).

(*ent*-3β,13ξ)-*form*

Δ$^{8(17)}$*-Isomer:* ***Isopinnatol B***

[288858-58-2]

$C_{20}H_{33}BrO$ 369.384

Constit. of *Aplysia dactylomela*.

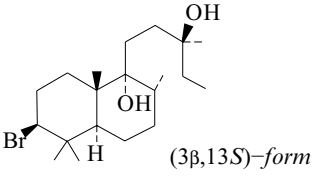
$[\alpha]_D$ +20.2 (c, 0.48 in $CHCl_3$).

Fukuzawa, A. *et al., Chem. Lett.*, 1985, 1259 (*isol, pmr*)

Fujiwara, S. *et al., Chem. Lett.*, 1986, 1763-1786 (*Pinnatol D, synth*)

Wessels, M. *et al., J. Nat. Prod.*, 2000, **63**, 920-928 (*Isopinnatol B*)

3-Bromo-9,13-labdanediol B-460



(3β,13*S*)–*form*

$C_{20}H_{37}BrO_2$ 389.415

(3β,13*S*)-*form*

ent-*13-Epiconcinndiol*

Isol. from *Chondria tenuissima*.

Cryst. ($CHCl_3$/hexane).

Mp 101.5-102°. $[\alpha]_D^{25}$ -17.34 (c, 0.445 in $CHCl_3$).

(*ent*-3β,13*R*)-*form*

Concinndiol

[50326-69-7]

Constit. of *Laurencia concinna*.

Cryst. (hexane).

Mp 212°.

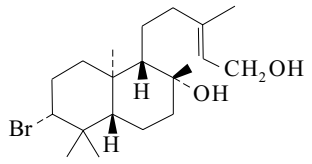
Sims, J.J. *et al., Chem. Comm.*, 1973, 470-471 (*isol, struct*)

Yamaguchi, Y. *et al., Tet. Lett.*, 1985, **26**, 343 (*synth*)

Öztunç, A. *et al., Phytochemistry*, 1989, **28**, 3403 (*isol, pmr, cmr, cryst struct*)

3-Bromo-13-labdene-8,15-diol B-461

[144069-45-4]



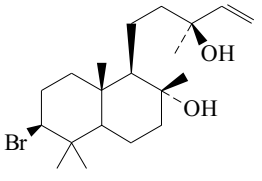
$C_{20}H_{35}BrO_2$ 387.399

(*ent*-3β,8β,13*E*)-*form*
Aplysin 20
[17941-22-9]
Constit. of *Aplysia kurodai*.
Cryst. (MeOH).
Mp 146-147°. $[\alpha]_D^{15}$ -78.1 (c, 1 in MeOH).

(*ent*-3β,8α,13*E*)-*form*
Epiaplysin 20
[144069-44-3]
Constit. of *Aplysia kurodai*.
Needles (MeOH).
Mp 150-152°. $[\alpha]_D^{13}$ -0.69 (c, 0.72 in MeOH).

Matsuda, H. *et al., Chem. Comm.*, 1967, 898-899 (*struct*)
Yamamura, S. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 2560-2562 (*isol*)
Murai, A. *et al., Tet. Lett.*, 1984, **25**, 4955 (*synth*)
Yamaguchi, Y. *et al., Tet. Lett.*, 1985, **26**, 343 (*synth*)
Nishizawa, M. *et al., J.O.C.*, 1986, **51**, 806 (*synth*)
Ojika, M. *et al., Bull. Chem. Soc. Jpn.*, 1992, **65**, 2300-2302 (*isol*)

3-Bromo-14-labdene-8,13-diol B-462



$C_{20}H_{35}BrO_2$ 387.399

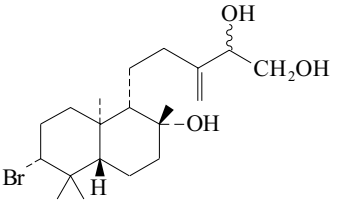
(3β,8α,13*S*)-*form*
Isoconcinndiol
[78012-27-8]
Constit. of *Laurencia snyderae* and *Aplysia dactyomela*.
Cryst. ($CHCl_3$).
Mp 173-174°.

(*ent*-3β,8α,13*S*)-*form*
ent-*Isoconcinndiol*
Constit. of *Aplysia kurodai*.
Plates ($CHCl_3$/hexane).
Mp 171-172°. $[\alpha]_D^{26}$ -4.7 (c, 0.42 in $CHCl_3$).

(*ent*-3β,8β,13*R*)-*form*
Pinnatol A
[98719-41-6]
Constit. of *Laurencia pinnata*.
Cryst.
Mp 49-51°. $[\alpha]_D$ +24.5 ($CHCl_3$).

Howard, B.M. *et al., Phytochemistry*, 1980, **19**, 2774 (*isol*)
Murai, A. *et al., Tet. Lett.*, 1984, **25**, 4955 (*isol*)
Fukuzawa, A. *et al., Chem. Lett.*, 1985, 1259 (*Pinnatol A*)
Rodríguez, M.L. *et al., Acta Cryst. C*, 1989, **45**, 306 (*cryst struct, abs config*)
Ojiki, M. *et al., Bull. Chem. Soc. Jpn.*, 1992, **65**, 2300 (*isol, pmr, cmr*)

3-Bromo-13(16)-labdene-8,14,15-triol B-463



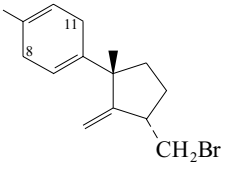
$C_{20}H_{35}BrO_3$ 403.399

(*ent*-3β,8β,14ξ)-*form*
Venustanol
[115346-29-7]
Constit. of *Laurencia venusta*.
Cryst.
Mp 97-99°. $[\alpha]_D^{24}$ -10.8 (c, 0.562 in MeOH).

Suzuki, M. *et al., Phytochemistry*, 1988, **27**, 1209

12-Bromo-5(13),6,9-lauratriene B-464

1-[3-(Bromomethyl)-1-methyl-2-methylenecyclopentyl]-4-methyl-1,4-cyclohexadiene, 9CI
[93395-09-6]

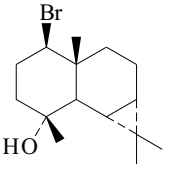


$C_{15}H_{21}Br$ 281.235
Constit. of red alga *Laurencia pinnatifida*. Unstable oil. $[\alpha]_D$ +2.3 (c, 2.15 in $CHCl_3$).

8,11-Didehydro: ***12-Bromo-5(13),6,8,10-lauratetraene****. 1-[3-(Bromomethyl)-1-methyl-2-methylenecyclopentyl]-4-methylbenzene, 9CI*
[93395-10-9]
$C_{15}H_{19}Br$ 279.219
Constit. of *Laurencia pinnatifida*. Oil. $[\alpha]_D$ +4.7 (c, 3.19 in $CHCl_3$).

Gonzalez, A.G. *et al., Tetrahedron*, 1984, **40**, 2751

1-Bromo-4-maalianol B-465



$C_{15}H_{25}BrO$ 301.266

(1β,4α)-*form*
1-Bromomaaliol
[120637-76-5]
Constit. of *Neomeris annulata*.
Oil. $[\alpha]_D$ -45.6 (c, 1.62 in $CHCl_3$).

Barnekow, D.E. *et al., J.A.C.S.*, 1989, **111**, 3511-3517 (*isol, pmr, cmr*)

Bromomethane, 9CI B-466

Methyl bromide, BSI, ISO, JMAF. R 40B1. Dow Fume MC2. Halon 1001. Terabol. Curafume
[74-83-9]
H_3CBr
CH_3Br 94.939
Isol. from various marine sources incl. giant kelp and ice algae.

Used as a solvent for extraction of plant oils and as a refrigerant. Stratospheric ozone depleting agent. Principally used as an insecticidal and nemacidal fumigant, esp. for soil and agricultural produce. Gas with faint chloroform-like odour. Spar. sol. H_2O. Mp -93.7°. Bp 4.5° (3.6°). Forms a hydrate at 0-5°. The signatory countries to the 1995 Montreal Treaty have agreed to phase out the industrial use of methyl bromide by 2010, in the USA its use will be banned after 1st January 2005.

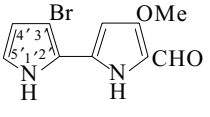
▶ Autoignition temp. 535/537°. Vapour can ignite or explode if strongly heated. Eye irritant and vesicant which can penetrate rubber protection equipment. One of the most toxic organic halides, whose effects are cumulative and may be delayed after exposure. Organs affected after inhalation or percutaneous absorption include nervous system, kidneys and lung. Acute or chronic exposure can be fatal. Exp. carcinogen. OES: long-term 5 ppm; short-term 15 ppm (Sk). PA4900000

[1111-88-2]

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 81D (*ir*)
Dougherty, G. *et al., J.A.C.S.*, 1929, **51**, 576 (*synth*)
Egan, C.J. *et al., J.A.C.S.*, 1938, **60**, 2097 (*props*)
Gallant, R.W. *et al., Hydrocarbon Process.*, 1968, **47**, 128 (*rev*)
Kawaguchi, T. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 53 (*cryst struct*)
Price, C.C. *et al., J.O.C.*, 1973, **38**, 615 (*pmr*)
Ossinger, A.I. *et al., J. Chem. Phys.*, 1976, **65**, 2892 (*ms*)
Jung, M.E. *et al., Tet. Lett.*, 1978, 4483 (*synth*)
Andrews, L. *et al., J.A.C.S.*, 1979, **101**, 7158 (*uv, ir*)
Olah, G.A. *et al., Organometallics*, 1982, **1**, 1485 (*cmr*)
Dangerous Prop. Ind. Mater. Rep., 1985, **5**, 37 (*rev*)
Binbrek, O.S. *et al., J. Phys. Chem.*, 1985, **82**, 1468 (*ir, Raman*)
Bond, J.A. *et al., Toxicol. Appl. Pharmacol.*, 1985, **78**, 259 (*metab*)
IARC Monog., 1986, **41**, 187; *Suppl.* 7, 245; *Suppl.* 6, 386 (*rev, tox*)
Bretherick, L. *et al., Chem. Eng. News*, Dec. 12, 1988, 2 (*haz*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **4**, 567
Pesticide Manual, 9th edn., 1991, No. 8340
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A273
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1129
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 742-744 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 3442, *Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott*, 1988, 322
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0410
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 668
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 173
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MHR200

3′-Bromo-4-methoxy-2,2′-bipyrrole-5-carboxaldehyde B-467

3-Bromo-5′-formyl-4′-methoxy-2,2′-bipyrrole
[85849-99-6]



$C_{10}H_9BrN_2O_2$ 269.097
Isol. from the nembrothid nudibranchs *Roboastra tigris*, *Tambja eliora*, *Tambja abdere* and the bryozoan *Sessibugula translucens*.
Mp 243-245° dec. Artifact.

Carté, B. *et al., J.O.C.*, 1983, **48**, 2314 (*isol, uv, ir, pmr, struct*)

5′-Bromo-4-methoxy-2,2′-bipyrrole-5-carboxaldehyde B-468

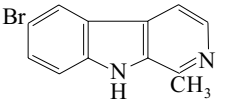
5′-Bromo-5-formyl-4-methoxy-2,2′-bipyrrole
[85849-98-5]

$C_{10}H_9BrN_2O_2$ 269.097
Isol. from the nembrothid nudibranchs *Roboastra tigris*, *Tambja eliora*, *Tambja abdere* and the bryozoan *Sessibugula translucens*.
Mp 235-238° dec. Artifact.

Carté, B. *et al., J.O.C.*, 1983, **48**, 2314 (*isol, uv, ir, pmr, struct*)

6-Bromo-1-methyl-β-carboline B-469

*6-Bromo-1-methyl-9*H*-pyrido[3,4-*b*]indole*
[18813-71-3]

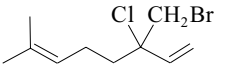


$C_{12}H_9BrN_2$ 261.12
Metab. from the marine hydroid *Aglaophenia pluma*. Cryst. (CH_2Cl_2).
Mp 248-250°.

Aiello, A. *et al., Tetrahedron*, 1987, **43**, 5929-5932 (*isol, uv, pmr, cmr, struct, synth*)
Ponce, M.A. *et al., J. Het. Chem.*, 2001, **38**, 1087-1095 (*synth, pmr, cmr, ms*)

3-Bromomethyl-3-chloro-7-methyl-1,6-octadiene B-470

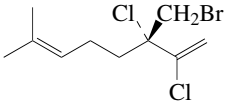
[60696-34-6]



$C_{10}H_{16}BrCl$ 251.593
Constit. of *Chondrococcus hornemanni*. Oil. $[\alpha]_D^{25}$ -3.7 (c, 15 in CH_2Cl_2).

Woolard, F.X. *et al., Phytochemistry*, 1976, **15**, 1069

3-(Bromomethyl)-2,3-dichloro-7-methyl-1,6-octadiene B-471



$C_{10}H_{15}BrCl_2$ 286.038

(3S)-form [58086-81-0]
Constit. of *Chondrococcus hornemannii* (*Portieria hornemannii*).
Oil. $[\alpha]_D$ -1.6 (c, 3 in $CHCl_3$).

Burreson, B.J. *et al., Chem. Lett.*, 1975, 1111-1114 (*isol*)
Fuller, R.W. *et al., J. Med. Chem.*, 1994, **34**, 4407-4411 (*isol, pmr, cmr*)

6-Bromo-21-methyl-5,9-docosadienoic acid B-472

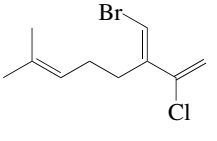
$(H_3C)_2CH(CH_2)_{10}CH{=}CHCH_2CH_2CBr{=}CH(CH_2)_3COOH$
$C_{23}H_{41}BrO_2$ 429.48

(5E,9Z)-form
Homaxinolic acid A
Constit. of a *Homaxinella* sp.
Oil (as Na salt).

Hong, C.-O.L. *et al., Lipids*, 2005, **40**, 981-985 (*isol, pmr, cmr, ms*)

3-(Bromomethylene)-2-chloro-7-methyl-1,6-octadiene B-473

10-Bromo-2-chloro-β-myrcene



(*E*)-*form*

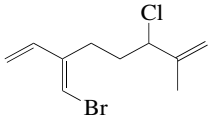
$C_{10}H_{14}BrCl$ 249.577

(*E*)-*form* [55498-39-0]
Constit. of *Chondrococcus hornemanni* (*Portieria hornemannii*).
Called (*Z*)- in ref.

(*Z*)-*form* [55498-38-9]
Constit. of *Chondrococcus hornemanni* (*Portieria hornemannii*).
Called (*E*)- in ref.
Ichikawa, N. *et al., Chem. Lett.*, 1974, 1333-1336 (*isol, ms*)
Burreson, B.J. *et al., Tet. Lett.*, 1975, 2155-2158 (*isol*)

6-(Bromomethylene)-3-chloro-2-methyl-1,7-octadiene B-474

10-Bromo-6-chloro-α-myrcene



(*E*)-*form*

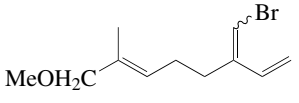
$C_{10}H_{14}BrCl$ 249.577
Config. incorrectly assigned in paper.

(+)-(*E*)-*form* [61263-59-0]
Constit. of *Chondrococcus japonicus.*
$[\alpha]_D^{23}$ +5 (c, 0.1 in Me_2CO).

(-)-(*Z*)-*form* [61263-60-3]
Constit. of *Chondrococcus japonicus.*
$[\alpha]_D^{23}$ -9.3 (c, 0.5 in Me_2CO).
Naya, Y. *et al., Chem. Lett.*, 1976, 839-842 (*isol, pmr, ms*)

3-(Bromomethylene)-8-methoxy-7-methyl-1,6-octadiene B-475

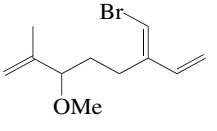
10-Bromo-8-methoxy-β-myrcene
[57593-03-0]



$C_{11}H_{17}BrO$ 245.159
Constit. of *Chondrococcus japonicus.*
Ichikawa, N. *et al., Proc. Jpn. Acad.*, 1975, **51**, 562 (*isol*)

6-(Bromomethylene)-3-methoxy-2-methyl-1,7-octadiene B-476

10-Bromo-6-methoxy-β-myrcene



(*E*)-*form*

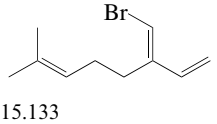
$C_{11}H_{17}BrO$ 245.159

(+)-(*E*)-*form* [57525-03-8]
Constit. of *Chondrococcus japonicus.*

(+)-(*Z*)-*form* [57525-02-7]
Constit. of *Chondrococcus japonicus.*
Ichikawa, N. *et al., Proc. Jpn. Acad.*, 1975, **51**, 562 (*isol*)

3-(Bromomethylene)-7-methyl-1,6-octadiene B-477

10-Bromo-β-myrcene



(*E*)-*form*

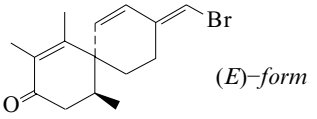
$C_{10}H_{15}Br$ 215.133

(*E*)-*form*
10-Bromomyrcene
[55498-37-8]
Constit. of *Chondrococcus hornemanni* (*Portieria hornemannii*).
Called (*Z*)- in ref.

(*Z*)-*form* [55498-36-7]
Constit. of *Chondrococcus hornemanni* (*Portieria hornemannii*).
Called (*E*)- in ref.
Ichikawa, N. *et al., Chem. Lett.*, 1974, 1333-1336 (*isol, ms*)
Burreson, B.J. *et al., Chem. Lett.*, 1975, 1111-1114 (*biosynth*)
Burreson, B.J. *et al., Tet. Lett.*, 1975, 2155-2158 (*isol*)

9-(Bromomethylene)-1,2,5-trimethylspiro[5.5]undeca-1,7-dien-3-one B-478

[101686-86-6]



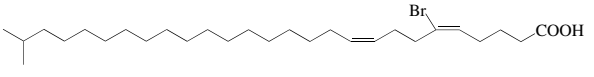
(*E*)–*form*

$C_{15}H_{19}BrO$ 295.218

(*E*)-*form*
Constit. of *Aplysia dactylomela.*
Oil.

(*Z*)-*form*
From *Aplysia dactylomela.*
Cryst.
Mp 97-99.5°. $[\alpha]_D^{20}$ +33.5 (c, 0.074 in $CHCl_3$).
Sakai, R. *et al., Helv. Chim. Acta*, 1986, **69**, 91
Iwata, C. *et al., Chem. Ind. (London)*, 1987, 294 (*synth, struct*)

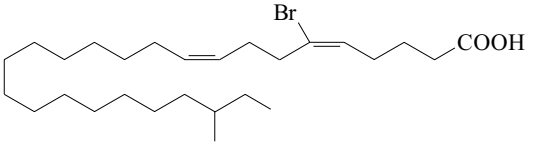
6-Bromo-26-methyl-5,9-heptacosadienoic acid B-479



$C_{28}H_{51}BrO_2$ 499.614

(5*E*,9*Z*)-*form*
cis,cis-*form*
[162259-51-0]
Isol. from the sponge *Xestospongia* sp.
Li, Y. *et al., J. Chem. Res., Synop.*, 1995, 126-127 (*isol*)

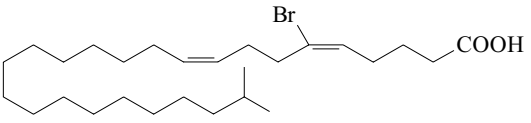
6-Bromo-24-methyl-5,9-hexacosadienoic acid B-480



$C_{27}H_{49}BrO_2$ 485.587

(5*E*,9*Z*)-*form*
cis,cis-*form*
[92313-34-3]
Constit. of the phospholipids of the sponges *Petrosia ficiformis* and *Petrosia hebe.* Incorr. descr. as (*Z,Z*)-.
Wijekoon, W.M.D. *et al., Tet. Lett.*, 1984, **25**, 3285 (*isol*)

6-Bromo-25-methyl-5,9-hexacosadienoic acid B-481

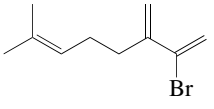


$C_{27}H_{49}BrO_2$ 485.587

(5*E*,9*Z*)-*form*
cis,cis-*form*
[162259-50-9]
[92340-05-1]
Constit. of the phospholipids of the sponges *Petrosia ficiformis*, *Petrosia hebes* and *Xestospongia* sp. Incorr. descr. as (*Z,Z*)-.
Wijekoon, W.M.D. *et al., Tet. Lett.*, 1984, **25**, 3285-3288 (*isol*)
Li, Y. *et al., J. Chem. Res., Synop.*, 1995, 126-127 (*isol*)

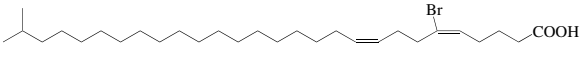
2-Bromo-7-methyl-3-methylene-1,6-octadiene B-482

*2-Bromo-β-myrcene. 7-**Bromomyrcene***
[55498-35-6]



$C_{10}H_{15}Br$ 215.133
Constit. of *Chondrococcus* (*Desmia*) *hornemanni* (*Portieria hornemannii*) and *Chondrococcus japonicus*. Oil.
Ichikawa, N. *et al., Chem. Lett.*, 1974, 1333-1336 (*isol, ms, pmr*)
Ichikawa, N. *et al., Proc. Jpn. Acad.*, 1975, **51**, 562 (*isol*)

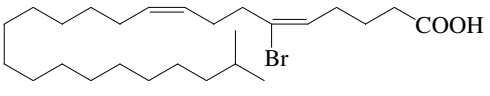
6-Bromo-27-methyl-5,9-octacosadienoic acid B-483



$C_{29}H_{53}BrO_2$ 513.641

(5*E*,9*Z*)-*form*
cis,cis-*form*
[162259-52-1]
Isol. from the sponge *Xestospongia* sp.
Li, Y. *et al., J. Chem. Res., Synop.*, 1995, 126-127 (*isol*)

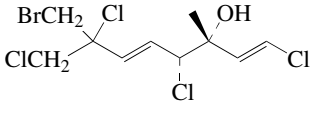
6-Bromo-24-methyl-5,9-pentacosadienoic acid B-484



$C_{26}H_{47}BrO_2$ 471.56

(5*E*,9*Z*)-*form* [150994-72-2]
Constit. of an *Agelas* sp.
Carballeira, N.M. *et al., Lipids*, 1993, **28**, 763-766 (*isol*)

7-Bromomethyl-1,4,7,8-tetrachloro-3-methyl-1,5-octadien-3-ol B-485

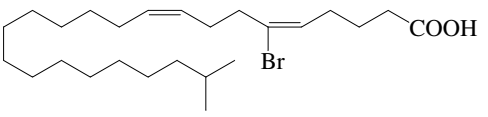


$C_{10}H_{13}BrCl_4O$ 370.927

(1*E*,3*R*,4*R*,5*E*,7ξ)-*form* [130770-03-5]
Constit. of *Pantoneura plocamioides*. Earlier isol. from *Plocamium cartilagineum*, prob. as a mixt. of stereoisomers.
Oil. $[\alpha]_D^{25}$ -28 (c, 0.30 in $CHCl_3$).

(1*E*,3*S*,4*R*,5*E*,7ξ)-*form* [207130-31-2]
Constit. of *Pantoneura plocamioides*.
Oil. $[\alpha]_D^{25}$ -50.8 (c, 0.42 in $CHCl_3$).
Rovirosa, J. *et al., Bol. Soc. Chil. Quim.*, 1990, **35**, 131-135 (*isol*)
Cueto, M. *et al., Tetrahedron*, 1998, **54**, 3575-3580 (*isol, pmr, cmr*)

6-Bromo-23-methyl-5,9-tetracosadienoic acid B-486

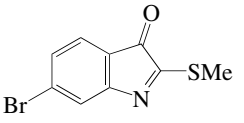


$C_{25}H_{45}BrO_2$ 457.533

(5*E*,9*Z*)-*form* [150994-70-0]
Constit. of an *Agelas* sp.
Carballeira, N.M. *et al., Lipids*, 1993, **28**, 763-766 (*isol*)

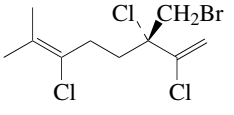
6-Bromo-2-(methylthio)-3*H*-indol-3-one, 9CI B-487

Tyrindoleninone
[50630-70-1]



C_9H_6BrNOS 256.123
Alkaloid from the mollusc *Dicathais orbita*. Red needles.
Mp 109.5°. λ_{max} 217 (ε 8700); 242 (ε 25000); 247 (ε 25000); 278 (ε 11000); 318 (ε 5200); 333 (ε 5000); 355 (ε 2700); 426 (ε 1700); 447 (ε 1700) (hexane).
Baker, J.T. *et al., Aust. J. Chem.*, 1973, **26**, 2153-2157 (*isol, uv, ir, pmr, ms*)
Benkendorff, K. *et al., J. Chem. Ecol.*, 2000, **26**, 1037-1050 (*isol*)

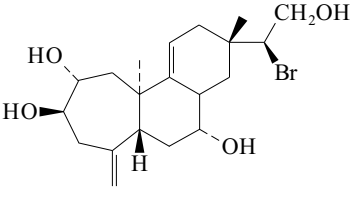
3-(Bromomethyl)-2,3,6-trichloro-7-methyl-1,6-octadiene B-488



$C_{10}H_{14}BrCl_3$ 320.483

(3*S*)-*form* [58086-80-9]
Constit. of *Chondrococcus hornemannii*.
Oil.
Burreson, B.J. *et al., Chem. Lett.*, 1975, 1111-1114 (*isol*)
Fuller, R.W. *et al., J. Med. Chem.*, 1994, **37**, 4407-4411 (*isol, pmr, cmr*)

15-Bromo-4(19),9(11)-neopargueradiene-2,3,7,16-tetrol B-489



$C_{20}H_{31}BrO_4$ 415.366

(2α,3β,7α,15*S*)-*form*
Metab. of red alga *Laurencia obtusa*. Cytotoxic.

2-Ac, 3-O-*palmitoyl: 2α-Acetoxy-15*S*-bromo-7α,16-dihydroxy-3β-palmitoyloxy-4(19),9(11)-neoparguera*diene
[126738-38-3]
$C_{38}H_{63}BrO_6$ 695.816
Metab. of *Laurencia obtusa*. Cytotoxic. Viscous oil. $[\alpha]_D$ -27.2 (c, 2.40 in $CHCl_3$).

Takeda, S. *et al., Chem. Lett.*, 1990, 277 (*isol, struct*)

6-Bromo-5,9-nonacosadienoic acid B-490

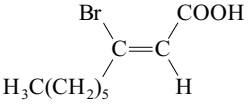
$H_3C(CH_2)_{18}CH{=}CHCH_2CH_2CBr{=}CH(CH_2)_3COOH$
$C_{29}H_{53}BrO_2$ 513.641

(5*E*,9*Z*)-*form*
Constit. of *Cinachyrella alloclada*.

Barnathan, G. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2003, **135**, 297-308 (*isol*)

3-Bromo-2-nonenoic acid B-491

[66002-55-9]



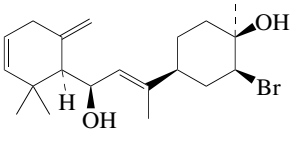
$C_9H_{15}BrO_2$ 235.12

(*Z*)-*form* [74055-84-8]
Constit. of the red alga *Bonnemaisonia nootkana*.

McConnell, O.J. *et al., Tet. Lett.*, 1977, **18**, 4159-4162 (*isol, pmr*)
McConnell, O.J. *et al., Phytochemistry*, 1980, **19**, 233 (*isol, pmr*)

2-Bromo-7,11(18),13-obtusatriene-3,9-diol B-492

Rogioldiol A
[193540-55-5]

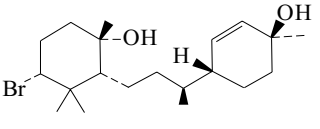


$C_{20}H_{31}BrO_2$ 383.368
Constit. of *Laurencia microcladia*.
$[\alpha]_D^{20}$ -43 (c, 0.1 in MeOH).

Guella, G. *et al., Helv. Chim. Acta*, 1997, **80**, 684-694 (*isol, pmr, cmr*)

14-Bromo-1-obtusene-3,11-diol B-493

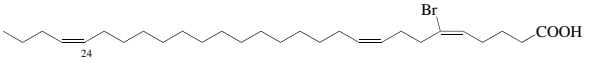
[70145-28-7]



$C_{20}H_{35}BrO_2$ 387.399
Constit. of *Aplysia dactylomela*. Cytotoxic agent. Cryst. Mp 134-135°. $[\alpha]_D$ +20 (c, 0.3 in EtOH).

Schmitz, F.J. *et al., J.O.C.*, 1979, **44**, 2445 (*isol, cryst struct*)

6-Bromo-5,9,24-octacosatrienoic acid, 9CI B-494



$C_{28}H_{49}BrO_2$ 497.598

(5*E*,9*Z*,24*Z*)-*form*
all-cis-*form*
[162259-48-5]
Isol. from the marine sponge *Xestospongia* sp.

24,25-Dihydro: 6-Bromo-5,9-octacosadienoic acid
[149204-40-0]
$C_{28}H_{51}BrO_2$ 499.614
From *Petrosia* sp. and *Xestospongia* sp.

Carballeira, N.M. *et al., J. Nat. Prod.*, 1993, **56**, 739-746 (*isol*)
Li, Y. *et al., J. Chem. Res., Synop.*, 1995, 126-127 (*isol*)

18-Bromo-9,17-octadecadiene-5,7-diynoic acid B-495

$BrCH{=}CH(CH_2)_6CH{=}CHC{\equiv}CC{\equiv}C(CH_2)_3COOH$
$C_{18}H_{23}BrO_2$ 351.282

(9*E*,17*E*)-*form* [144291-87-2]
Isol. from the marine sponge *Xestospongia muta*.
Needles.

[144291-89-4]

Patil, A.D. *et al., J. Nat. Prod.*, 1992, **55**, 1170 (*isol, pmr, cmr*)

18-Bromo-9,17-octadecadiene-7,15-diynoic acid B-496

$BrCH{=}CHC{\equiv}C(CH_2)_4CH{=}CHC{\equiv}C(CH_2)_5COOH$
$C_{18}H_{23}BrO_2$ 351.282
Constit. of sponge *Xestospongia testudinaria*. Cryst. (MeOH aq.). Mp 66-67°.

(9*E*,17*E*)-*form* [96475-42-2]
Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 235 (ϵ 18300) (MeOH) (Berdy).

Me ester:
$C_{19}H_{25}BrO_2$ 365.309
Isol. from the marine sponge *Xestospongia testudinaria*.

(9*Z*,17*E*)-*form*
Me ester: [133084-60-3]
Isol. from the marine sponge *Xestospongia testudinaria*.

Quinn, R.J. *et al., Tet. Lett.*, 1985, **26**, 1671
Hirsch, S. *et al., Tetrahedron*, 1987, **43**, 3257 (*isol*)
Quinn, R.J. *et al., J. Nat. Prod.*, 1991, **54**, 290 (*isol, ms, struct, pmr, cmr*)

18-Bromo-15,17-octadecadiene-5,7-diynoic acid B-497

$BrCH{=}CHCH{=}CH(CH_2)_6C{\equiv}CC{\equiv}C(CH_2)_3COOH$
$C_{18}H_{23}BrO_2$ 351.282

(15*Z*,17*E*)-*form*
Me ester: [147169-58-2]
$C_{19}H_{25}BrO_2$ 365.309
Isol. from the marine sponge *Petrosia volcano*. Oil. λ_{max} 245 (ϵ 8700) (MeOH) (Berdy).

Fusetani, N. *et al., Tetrahedron*, 1993, **49**, 1203 (*isol, pmr*)

18-Bromo-9,15-octadecadiene-5,7,17-triynoic acid B-498

$BrC{\equiv}CCH{=}CH(CH_2)_4CH{=}CHC{\equiv}CC{\equiv}C(CH_2)_3COOH$
$C_{18}H_{19}BrO_2$ 347.251

(9*E*,15*E*)-*form* [144291-88-3]
Isol. from the marine sponge *Xestospongia muta*.
Brown powder. Unstable. λ_{max} 208; 213; 240; 252 (MeOH) (Berdy).

Patil, A.D. *et al., J. Nat. Prod.*, 1992, **55**, 1170 (*isol, pmr, cmr*)

18-Bromo-9,17-octadecadiene-5,7,15-triynoic acid, 9CI B-499

$BrCH{=}CHC{\equiv}C(CH_2)_4CH{=}CHC{\equiv}CC{\equiv}C(CH_2)_3COOH$
$C_{18}H_{19}BrO_2$ 347.251

(9E,17E)-form [144291-85-0]
Isol. from *Xestospongia muta*.
Powder. λ_{max} 234; 252; 275; 285 (MeOH) (Berdy).
Me ester: [133084-61-4]
$C_{19}H_{21}BrO_2$ 361.278
Isol. from the marine sponge *Xestospongia testudinaria*.

(9Z,17E)-form [147169-50-4]
Isol. from the sponge *Petrosia volcano*.
Oil.

(9Z,17Z)-form [147169-51-5]
Isol. from *Petrosia volcano*.
Oil.
Quinn, R.J. *et al., J. Nat. Prod.*, 1991, **54**, 290 (*isol, struct, pmr, cmr*)
Patil, A.D. *et al., J. Nat. Prod.*, 1992, **55**, 1170 (*isol, pmr, cmr*)
Fusetani, N. *et al., Tetrahedron*, 1993, **49**, 1203 (*isol, pmr*)

18-Bromo-13,17-octadecadiene-5,7,15-triynoic acid B-500

$BrCH{=}CHC{\equiv}CCH{=}CH(CH_2)_4C{\equiv}CC{\equiv}C(CH_2)_3COOH$
$C_{18}H_{19}BrO_2$ 347.251

(13E,17E)-form [147169-52-6]
Isol. from the marine sponge *Petrosia volcano*.
Oil. λ_{max} 217 (ϵ 11800); 227 (ϵ 9800); 267 (ϵ 17000); 287 (ϵ 15500) (MeOH) (Berdy).

(13E,17Z)-form [147169-54-8]
Isol. from *Petrosia volcano*.
Oil. λ_{max} 270 (ϵ 5400); 285 (ϵ 4500) (MeOH) (Berdy).

(13Z,17E)-form [147169-53-7]
Isol. from *Petrosia volcano*.
Oil. λ_{max} 267 (ϵ 15100); 283 (ϵ 13100) (MeOH) (Berdy).
Fusetani, N. *et al., Tetrahedron*, 1993, **49**, 1203 (*isol, pmr*)

18-Bromo-5,17-octadecadien-7-ynoic acid B-501

$BrCH{=}CH(CH_2)_8C{\equiv}CCH{=}CHCH_2CH_2CH_2COOH$
$C_{18}H_{27}BrO_2$ 355.314

(5Z,17E)-form [162259-38-3]
Isol. from the sponge *Xestospongia* sp.
Me ester: [162259-40-7]
$C_{19}H_{29}BrO_2$ 369.341
From *Xestospongia* sp.
5,6-Dihydro: 18-Bromo-17-octadecen-7-ynoic acid
[162259-42-9]
$C_{18}H_{29}BrO_2$ 357.33
From *Xestospongia* sp.
Li, Y. *et al., J. Chem. Res., Synop.*, 1995, 126-127 (*isol*)

18-Bromo-7,13,17-octadecatriene-5,15-diynoic acid B-502

$BrCH{=}CHC{\equiv}CCH{=}CH(CH_2)_4CH{=}CHC{\equiv}C(CH_2)_3COOH$
$C_{18}H_{21}BrO_2$ 349.267

(7E,13E,17E)-form [144291-84-9]
Isol. from the marine sponge *Xestospongia muta*.
Powder.
[144291-91-8]
Patil, A.D. *et al., J. Nat. Prod.*, 1992, **55**, 1170 (*isol, pmr, cmr*)

18-Bromo-9,15,17-octadecatriene-5,7-diynoic acid B-503

$BrCH{=}CHCH{=}CH(CH_2)_4CH{=}CHC{\equiv}CC{\equiv}C(CH_2)_3COOH$
$C_{18}H_{21}BrO_2$ 349.267

(9E,15Z,17E)-form
Me ester: [147169-57-1]
$C_{19}H_{23}BrO_2$ 363.293
Isol. from the marine sponge *Petrosia volcano*. Oil. λ_{max} 213 (ϵ 9100); 240 (ϵ 5000); 267 (ϵ 3800); 282 (ϵ 3000) (MeOH) (Berdy).

(9Z,15Z,17E)-form
Me ester: [147169-56-0]
Isol. from *Petrosia volcano*.
Oil. λ_{max} 214 (ϵ 22900); 240 (ϵ 10700); 267 (ϵ 7100); 284 (ϵ 5600) (MeOH) (Berdy).
Fusetani, N. *et al., Tetrahedron*, 1993, **49**, 1203 (*isol, pmr*)

18-Bromo-9,13,17-octadecatriene-5,7,15-triynoic acid B-504

$BrCH{=}CHC{\equiv}CCH{=}CHCH_2CH_2CH{=}CHC{\equiv}CC{\equiv}C(CH_2)_3COOH$
$C_{18}H_{17}BrO_2$ 345.235

(9E,13E,17E)-form [144291-83-8]
Isol. from the marine sponge *Xestospongia muta*.
Amorph. powder.

(9Z,13Z,17E)-form [147169-55-9]
Constit. of the sponge *Petrosia volcano*.
Oil. λ_{max} 214 (ϵ 9550); 240 (ϵ 6600); 267 (ϵ 6500); 284 (ϵ 4600) (MeOH) (Berdy).
Patil, A.D. *et al., J. Nat. Prod.*, 1992, **55**, 1170 (*isol, pmr, cmr*)
Fusetani, N. *et al., Tetrahedron*, 1993, **49**, 1203 (*isol, pmr, struct*)

18-Bromo-17-octadecene-5,7,15-triynoic acid B-505

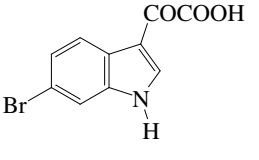
$BrCH{=}CHC{\equiv}C(CH_2)_6C{\equiv}CC{\equiv}C(CH_2)_3COOH$
$C_{18}H_{21}BrO_2$ 349.267

(E)-form
Xestospongic acid
[140423-91-2]
Isol. from the marine sponge *Xestospongia testudinaria*. Possesses antimicrobial activity. Unstable acid, not obt. pure. Characterised as Me ester.
Me ester:
Yellow oil.
Et ester: [140405-24-9]
$C_{20}H_{25}BrO_2$ 377.32
Isol. from *Xestospongia testudinaria*. $Na^{\oplus}/K^{\oplus}$ ATPase inhibitor. Shows weak antimicrobial activity. Pale yellow oil. λ_{max} 223 (ϵ 10000) (EtOH) (Derep).

(Z)-form [147169-49-1]
Isol. from the marine sponge *Petrosia volcano*.
Oil. λ_{max} 233 (ϵ 8300); 245 (ϵ 7900) (MeOH) (Berdy).
Bourguet-Kondracki, M.L. *et al., Tet. Lett.*, 1992, **33**, 225 (*isol, pmr, cmr, struct*)
Fusetani, N. *et al., Tetrahedron*, 1993, **49**, 1203 (*isol, pmr*)

6-Bromo-α-oxo-1*H*-indole-3-acetic acid B-506

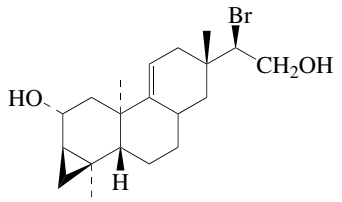
*(6-Bromo-1*H*-indol-3-yl)glyoxylic acid*



$C_{10}H_6BrNO_3$ 268.066

Et ester:
$C_{12}H_{10}BrNO_3$ 296.12
Alkaloid from the sponge *Iotrochota birotulata*. Pale yellow solid. λ_{max} 270; 320 (MeOH).
Li, L. *et al., Pharmazie*, 2003, **58**, 680-681 (*isol, pmr, cmr*)

15-Bromo-9(11)-parguerene-2,16-diol B-507



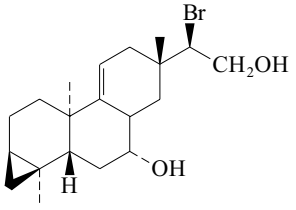
$C_{20}H_{31}BrO_2$ 383.368

(*ent*-2β,15*S*)-*form*

2-Ac: [175990-37-1]
$C_{22}H_{33}BrO_3$ 425.405
Constit. of *Laurencia filiformis*. Oil. $[\alpha]_D$ -16.1 (c, 0.5 in $CHCl_3$).
Rochfort, S.J. *et al., Aust. J. Chem.*, 1996, **49**, 19-26 (*isol, pmr, cmr*)

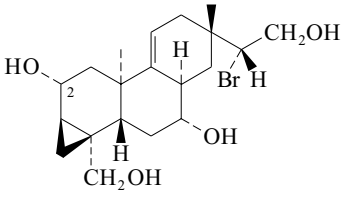
15-Bromo-9(11)-parguerene-7,16-diol B-508

[132435-49-5]



$C_{20}H_{31}BrO_2$ 383.368
Metab. of *Laurencia obtusa*. Cryst. (CH_2Cl_2/diisopropyl ether).
Mp 87-90°. $[\alpha]_D$ -17.8 (c, 1.71 in $CHCl_3$).
Takeda, S. *et al., Bull. Chem. Soc. Jpn.*, 1990, **63**, 3066 (*isol, pmr, cmr*)

15-Bromo-9(11)-parguerene-2,7,16,19-tetrol B-509



$C_{20}H_{31}BrO_4$ 415.366

(*ent*-2β,7β,15*S*)-*form*
Deacetylparguerol
[132342-73-5]
Constit. of *Aplysia punctata*.
Semi-solid. $[\alpha]_D$ -18.4 (c, 0.0049 in MeOH).

2-Ac: Parguerene. ***Parguerol***
[83115-36-0]
$C_{22}H_{33}BrO_5$ 457.404
Metab. of *Aplysia dactylomela*. Cytotoxic agent. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D$ -40 (c, 0.03 in $CHCl_3$).

2,7-Di-Ac: Parguerol 7-acetate
$C_{24}H_{35}BrO_6$ 499.441
Constit. of *Laurencia saitoi*. Oil. $[\alpha]_D^{26}$ -5.41 (c, 0.64 in $CHCl_3$).

2,16-Di-Ac: Parguerol 16-acetate
[83115-43-9]
$C_{24}H_{35}BrO_6$ 499.441
Constit. of *Laurencia saitoi* and *Aplysia dactyomela*. Cytotoxic agent.

2,19-Di-Ac: Parguerol 19-acetate
$C_{24}H_{35}BrO_6$ 499.441
Constit. of *Laurencia saitoi*. Oil. $[\alpha]_D^{20}$ -17.1 (c, 0.81 in $CHCl_3$).

2,7,16-Tri-Ac:
$C_{26}H_{37}BrO_7$ 541.478
Constit. of *Laurencia filiformis*. Waxy solid. $[\alpha]_D$ -13.2 (c, 0.15 in $CHCl_3$).

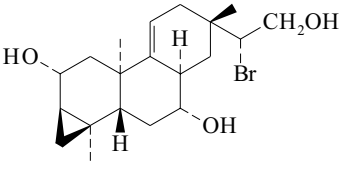
2,16,19-Tri-Ac:
$C_{26}H_{37}BrO_7$ 541.478
Metab. of *Laurencia obtusa*. Viscous oil. $[\alpha]_D$ -37.8 (c, 1.54 in $CHCl_3$).

Tetra-Ac:
$C_{28}H_{39}BrO_8$ 583.515
Constit. of *Laurencia filiformis*. Oil.

2-Ketone: ***15-Bromo-7,16,19-trihydroxy-9(11)-pargueren-2-one***
$C_{20}H_{29}BrO_4$ 413.351
Metab. of *Laurencia obtusa*. Glassy solid. $[\alpha]_D$ -41 (c, 0.89 in MeOH).

Schmitz, F.J. *et al., J.A.C.S.*, 1982, **104**, 6415-6423 (*Parguerol*)
Takeda, S. *et al., Bull. Chem. Soc. Jpn.*, 1990, **63**, 3066-3072 (*Laurencia obtusa constits*)
Rochfort, S.J. *et al., Aust. J. Chem.*, 1996, **49**, 19-26 (*Laurencia filiformis constits*)
Kurata, K. *et al., Phytochemistry*, 1998, **47**, 363-369 (*Laurencia saitoi constits*)
Findlay, J.A. *et al., Can. J. Chem.*, 2002, **80**, 1697-1707 (*Deacetylparguerol*)
Tsukamoto, S. *et al., Mar. Drugs*, 2004, **2**, 170-175 (*Parguerol, pmr, activity*)

15-Bromo-9(11)-parguerene-2,7,16-triol B-510



Absolute configuration

$C_{20}H_{31}BrO_3$ 399.367

(*ent*-2β,7β,15*S*)-*form* [124974-50-1]
Metab. of *Laurencia obtusa*.
Cryst.
Mp 173-174°. $[\alpha]_D$ -36.4 (c, 1.85 in $CHCl_3$).

2-Ac: ***Deoxyparguerene****. Deoxyparguerol*
[83115-44-0]
$C_{22}H_{33}BrO_4$ 441.404
Found in *Aplysia dactylomela* and *Laurencia obtusa*. Cytotoxic. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D$ -35.8 (c, 0.62 in $CHCl_3$).

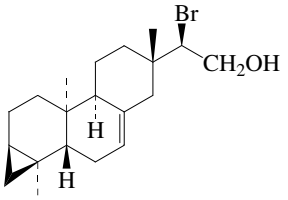
2,16-Di-Ac: [82668-11-9]
$C_{24}H_{35}BrO_5$ 483.441
Metab. of *Laurencia obtusa*. Cryst.
Mp 121-123°. $[\alpha]_D$ -48 (c, 0.1 in MeOH).

2,7-Di-Ac:
$C_{24}H_{35}BrO_5$ 483.441
Constit. of *Laurencia filiformis*. Oil. $[\alpha]_D$ -10 (c, 0.2 in $CHCl_3$).

Tri-Ac:
$C_{26}H_{37}BrO_6$ 525.479
Constit. of *Laurencia filiformis*. Oil.

Schmitz, F.J. *et al., J.A.C.S.*, 1982, **104**, 6415-6423 (*isol, pmr*)
Higgs, M.D. *et al., Phytochemistry*, 1982, **21**, 789-791 (*isol, pmr*)
Suzuki, T. *et al., Chem. Lett.*, 1989, 969-970 (*cryst struct*)
Rochfort, S.J. *et al., Aust. J. Chem.*, 1996, **49**, 19-26 (*isol, pmr, cmr*)

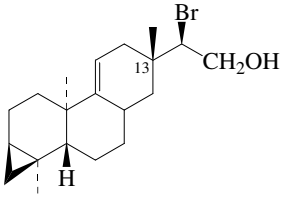
15-Bromo-7-pargueren-16-ol B-511



$C_{20}H_{31}BrO$ 367.368

(*ent*-15*S*)-*form* [798558-05-1]
Constit. of *Laurencia nipponica*.
Oil. $[\alpha]_D^{25}$ +55 (c, 0.14 in $CHCl_3$).
Lyakhova, E.G. *et al., Phytochemistry*, 2004, **65**, 2527-2532 (*isol, pmr, cmr*)

15-Bromo-9(11)-pargueren-16-ol B-512



$C_{20}H_{31}BrO$ 367.368

(*ent*-15*S*)-*form* [175990-38-2]
Constit. of *Laurencia filiformis.*
Oil. $[\alpha]_D$ -12.9 (c, 0.2 in $CHCl_3$).

13-Epimer: ***15-Bromo-13-epi-9(11)-pargueren-16-ol****. 15-Bromo-9(11)-isopargueren-16-ol (incorr.)*
[176199-30-7]
$C_{20}H_{31}BrO$ 367.368
Constit. of *Laurencia filiformis.* Oil. $[\alpha]_D$ +36.7 (c, 0.06 in $CHCl_3$). Tentative struct. Authors' name is misleading as it is not an isoparguerane (see for example Isoparguerol, 2-Ac).

Stereoisomer:
$C_{20}H_{31}BrO$ 367.368
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D^{25}$ -9.1 (c, 0.33 in $CHCl_3$).
Rochfort, S.J. *et al., Aust. J. Chem.*, 1996, **49**, 19-26 (*isol, pmr, cmr*)
Lyakhova, E.G. *et al., Phytochemistry*, 2004, **65**, 2527-2532 (*Laurencia nipponica constit*)

6-Bromo-5,9-pentacosadienoic acid B-513

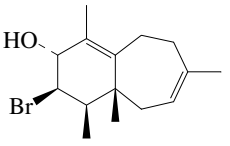
$H_3C(CH_2)_{14}CH{=}CHCH_2CH_2CBr{=}CH(CH_2)_3COOH$
$C_{25}H_{45}BrO_2$ 457.533

(5*E*,9*Z*)-*form* [150994-71-1]
Constit. of the marine sponges *Amphimedon terpenesis* and *Agelas* sp.
Carballeira, N.M. *et al., Lipids*, 1993, **28**, 763 (*isol*)
Garson, M.J. *et al., Lipids*, 1993, **28**, 1011 (*isol*)

1-Bromopentane, 9CI B-514

n-*Amyl bromide. Pentyl bromide*
[110-53-2]
$H_3C(CH_2)_3CH_2Br$
$C_5H_{11}Br$ 151.046
Isol. from a marine alga. Liq. d_4^{15} 1.22.
Fp -95.25. Bp 129.7° Bp_{10} 21°.
▶ Flammable, fl. p. 31/32°. LD_{50} (mus, ipr) 1250 mg/kg. RZ9770000
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 57D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 85A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 85B (*ir*)
Fournier, H. *et al., Bull. Soc. Chim. Fr.*, 1906, **35**, 621 (*synth*)
Oldham, J.W.H. *et al., J.C.S.*, 1950, 100 (*synth*)
Fiaux, A. *et al., Helv. Chim. Acta*, 1974, **67**, 708 (*ms*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 374

3-Bromo-1(11),7-perforadien-2-ol B-515

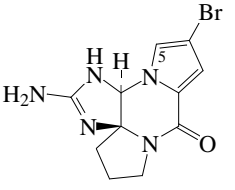


$C_{15}H_{23}BrO$ 299.25

(2α,3β)-*form*
Perforenol B
[874193-57-4]
Constit. of *Laurencia obtusa*.
Oil. $[\alpha]_D^{20}$ -36.7 (c, 0.16 in $CHCl_3$). λ_{max} 202 (log ϵ 3.7); 239 (log ϵ 3.1) (hexane).
Kladi, M. *et al., Tetrahedron*, 2006, **62**, 182-189

4-Bromophakellin B-516

Monobromophakellin



(-)-*form*

$C_{11}H_{12}BrN_5O$ 310.153

(-)-*form* [31955-05-2]
Alkaloid from the marine sponge *Phakellia flabellata*.
Mp 170-180° dec. λ_{max} 227 (ϵ 7140); 277 (ϵ 5540) (as hydrochloride) (Derep). λ_{max} 228 (ϵ 7780); 275 (ϵ 6110) (MeOH) (Derep).

Hydrochloride: Mp 215-220°. $[\alpha]_D^{25}$ -123 (c, 3 in MeOH).

N^7-*Me:* ***4-Bromo-N^7-methylphakellin***. N^7-*Methylmonobromophakellin*
[697284-91-6]
$C_{12}H_{14}BrN_5O$ 324.18
Isol. from an *Agelas* sp. Powder. $[\alpha]_D^{28}$ -35 (c, 1 in MeOH). λ_{max} 238 (ϵ 1700); 280 (ϵ 1280) (MeOH).

5-Bromo: ***(-)-Dibromophakellin***
[31954-96-8]
$C_{11}H_{11}Br_2N_5O$ 389.049
Alkaloid from *Phakellia flabellata*, *Phakellia mauritiana* and *Pseudaxinyssa cantharella*. Sol. MeOH, butanol.
Mp 237-245° dec. λ_{max} 233 (ϵ 8880); 281 (ϵ 8810) (MeOH) (Derep). λ_{max} 211 (ϵ 104000); 237 (ϵ 10700); 285 (ϵ 11000) (EtOH) (Berdy).

5-Bromo; hydrochloride: Mp 220-221°. $[\alpha]_D^{25}$ -205 (c, 2.9 in MeOH).

5-Bromo, N^7-*Me:* ***N^7-Methyldibromophakellin***
[697284-90-5]
$C_{12}H_{13}Br_2N_5O$ 403.076
Isol. from an *Agelas* sp. Powder. $[\alpha]_D^{28}$ -19.8 (c, 1.4 in MeOH). λ_{max} 238 (ϵ 6780); 280 (ϵ 5430) (MeOH).

(+)-*form*

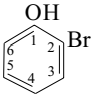
5-Bromo: ***(+)-Dibromophakellin***
$C_{11}H_{11}Br_2N_5O$ 389.049
Metab. of the New Caledonian sponge *Pseudaxinyssa cantharella*.

Mp 220° dec. $[\alpha]_D^{20}$ +159 (c, 1.55 in MeOH). λ_{max} 233 (ε 8880); 281 (ε 8810) (MeOH) (Derep).

Sharma, G. *et al., J.O.C.*, 1977, **42**, 4118 (*isol, uv, ir, pmr, ms, cryst struct, cmr*)
Foley, L.H. *et al., J.A.C.S.*, 1982, **104**, 1776 (*synth*)
Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1985, 578; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 547-548 (*Dibromophakellin, isol*)
De Nanteuil, G. *et al., Tetrahedron*, 1985, **41**, 6019 (*isol, uv, ir, pmr, cmr, cd, cryst struct, deriv*)
Gautschi, J.T. *et al., J. Nat. Prod.*, 2004, **67**, 1256-1261 (N^7-*Methylphakellins*)

2-Bromophenol, 9CI B-517

[95-56-7]



C_6H_5BrO 173.009
Flavour component of marine fish, molluscs and crustaceans. Liq. Bp 194°. pK_a 8.45 (25°).
▶ Fl. p. >66°. LD_{50} (mus, orl) 652 mg/kg. SJ7875000

Ac: [1829-37-4]
$C_8H_7BrO_2$ 215.046
Liq. Bp_{39} 150°.

Benzoyl: [91805-61-7]
$C_{13}H_9BrO_2$ 277.117
Mp 86°.

4-Methylbenzenesulfonyl: [84672-48-0]
$C_{13}H_{11}BrO_3S$ 327.198
Prisms (CH_2Cl_2/hexane). Mp 75.5-76.5° (64-66°).

Me ether: 1-Bromo-2-methoxybenzene. 2-Bromoanisole
[578-57-4]
C_7H_7BrO 187.036
Liq. Bp 210° Bp_{10} 94-96°.
▶ Fl. p. 101°. LD_{50} (mus, orl) 2466 mg/kg. BZ8500000

Trifluoromethyl ether: See 1-Bromo-2-(trifluoromethoxy)benzene in *The Combined Chemical Dictionary.*

Et ether: 1-Bromo-2-ethoxybenzene, 9CI. 2-Bromophenetole
[583-19-7]
C_8H_9BrO 201.062
Liq. Bp 221-224°.
▶ Fl. p. >66°.

Propyl ether: 1-Bromo-2-propoxybenzene, 9CI
[54554-81-3]
$C_9H_{11}BrO$ 215.089
Liq. $Bp_{13.5}$ 116-118° (lit. gives a pressure range).

Butyl ether: 1-Bromo-2-butoxybenzene, 9CI
[54514-30-6]
$C_{10}H_{13}BrO$ 229.116
Liq. Bp 248-250° Bp_{16} 134-135°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1040A; 1072B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 179B; 247A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 967D; 1004B (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 97 (*synth*)
Holmberg, G.A. *et al., CA*, 1951, **45**, 559i (*synth*)
Kolesnikov, G.S. *et al., Zh. Obshch. Khim.*, 1957, **27**, 3009; *J. Gen. Chem. USSR (Engl. Transl.)*, 1957, **27**, 3038 (*synth, ethers*)
Pearson, D.E. *et al., J.O.C.*, 1967, **32**, 2358 (*synth*)
Smith, W.B. *et al., Org. Magn. Reson.*, 1976, **8**, 205 (*cmr*)
Sennikov, P.G. *et al., Zh. Obshch. Khim.*, 1980, **50**, 2761; *J. Gen. Chem. USSR (Engl. Transl.)*, 1980, **50**, 2236 (*uv*)
Brossi, A. *et al., Helv. Chim. Acta*, 1981, **64**, 1672 (*cmr*)
Kim, K. *et al., Chem. Comm.*, 1986, 1159 (*synth*)
Baker, R.W. *et al., J.C.S. Perkin 1*, 1991, 1589 (*synth, tosylate*)
Boyle, J.L. *et al., J. Food Sci.*, 1992, **57**, 918-922 (*occur*)
Whitfield, F.B. *et al., J. Agric. Food Chem.*, 1997, **45**, 4398-4405; 1999, **47**, 2367-2373 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BNV000

4-Bromophenol, 9CI B-518

[106-41-2]

C_6H_5BrO 173.009
Flavour component of marine fish, molluscs and algae. Cryst. Mp 66°. Bp 238°. pK_a 9.37 (24°).
▶ Fl. p. >241°. LD_{50} (mus, orl) 523 mg/kg. SJ7960000

Ac: [1927-95-3]
$C_8H_7BrO_2$ 215.046
Cryst. Mp 21.5°. Bp 235-240° Bp_{15} 129-130°.

Benzoyl: [1523-17-7]
$C_{13}H_9BrO_2$ 277.117
Mp 104°.

Me ether: 1-Bromo-4-methoxybenzene, 9CI. 4-Bromoanisole
[104-92-7]
C_7H_7BrO 187.036
Liq. Mp 11°. Bp 215° Bp_7 60-61°.
▶ Fl. p. 100°. BZ8501000

Et ether: 1-Bromo-4-ethoxybenzene, 9CI. 4-Bromophenetole
[588-96-5]
C_8H_9BrO 201.062
Liq. Mp 4°. Bp 233° Bp_5 91-93°.
▶ Fl. p. >66°.

2-Chloroethyl ether: 4-Bromo-1-(2-chloroethoxy)benzene, 9CI
[55162-34-0]
C_8H_8BrClO 235.507
Mp 58-58.5°. $Bp_{6.5}$ 135°.

Propyl ether: 1-Bromo-4-propoxybenzene, 9CI
[39969-56-7]
$C_9H_{11}BrO$ 215.089
Liq. Bp_4 85-90° (lit. gives a pressure range).

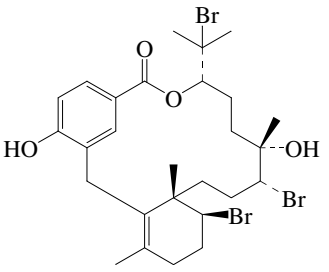
Butyl ether: 1-Bromo-4-butoxybenzene, 9CI
[39969-57-8]
$C_{10}H_{13}BrO$ 229.116
Liq. Bp_4 101-104° (lit. gives a pressure range).
▶ Fl. p. >66°.

Benzyl ether: 1-Bromo-4-(phenylmethoxy)benzene, 9CI
[6793-92-6]
$C_{13}H_{11}BrO$ 263.133
Needles. Mp 63-64° (60-61°). Bp_{50} 226°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1043D; 1044A; 1078C; 1078c (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 187A; 187C; 253C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 972B; 972C; 1011B (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 123 (*synth*)
Palaten, K. *et al., Chem. Listy*, 1957, **51**, 563 (*synth*)
Kolesnikov, G.S. *et al., CA*, 1958, **52**, 12804a (*synth*)
Rowe, E.J. *et al., J.O.C.*, 1958, **23**, 1622-1624 (*benzyl ether*)
Szalecki, W. *et al., Synth. Commun.*, 1976, **6**, 243 (*synth*)
Thorpe, F.G. *et al., J. Organomet. Chem.*, 1977, **128**, 305 (*synth*)
Korzeniowski, S.H. *et al., Tet. Lett.*, 1977, 3519 (*synth*)
Perrin, M. *et al., Cryst. Struct. Commun.*, 1978, **7**, 59 (*cryst struct*)
Takai, H. *et al., Chem. Pharm. Bull.*, 1979, **27**, 1780 (*cmr, Me ether*)
Adam, W. *et al., J.O.C.*, 1979, **44**, 4969 (*synth*)
Sennikov, P.G. *et al., Zh. Obshch. Khim.*, 1980, **50**, 2761; *J. Gen. Chem. USSR (Engl. Transl.)*, 1980, **50**, 2236 (*uv*)
Kim, K. *et al., Chem. Comm.*, 1986, 1159 (*synth*)
Hutton, H.M. *et al., Can. J. Chem.*, 1987, **65**, 1316 (*cmr*)
Percec, V. *et al., J. Polym. Sci., Part A*, 1990, **28**, 1101 (*ethers, synth*)
Akiyama, T. *et al., Bull. Chem. Soc. Jpn.*, 1992, **65**, 1932-1938 (*benzyl ether, synth, ir, pmr*)
Whitfield, F.B. *et al., J. Agric. Food Chem.*, 1997, **45**, 4398-4405; 1999, **47**, 2367-2373 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BNU750

Bromophycolide A B-519

[870474-77-4]

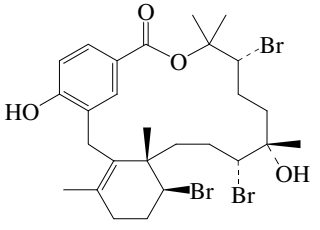


$C_{27}H_{37}Br_3O_4$ 665.299
Constit. of *Callophycus serratus*. Cryst. (MeOH). $[\alpha]_D^{23}$ -35 (c, 0.21 in $CHCl_3$). λ_{max} 229 (log ϵ 3.73) (MeOH).

Kubanek, J. *et al., Org. Lett.*, 2005, **7**, 5261-5264 (*Bromophycolide A, cryst struct*)

Bromophycolide B B-520

[869859-99-4]

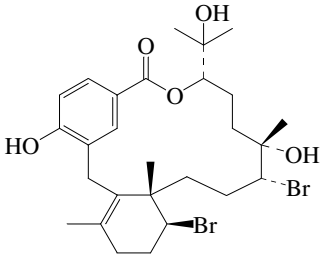


$C_{27}H_{37}Br_3O_4$ 665.299
Constit. of *Callophycus serratus*. Cryst. (MeOH). $[\alpha]_D$ -1 (c, 0.044 in $CHCl_3$). λ_{max} 224 (log ϵ 3.63) (MeOH).

Kubanek, J. *et al., Org. Lett.*, 2005, **7**, 5261-5264 (*Bromophycolide B, cryst struct*)

Bromophycolide C B-521

[889453-94-5]

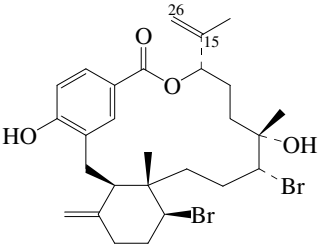


$C_{27}H_{38}Br_2O_5$ 602.402
Constit. of *Callophycus serratus*. Amorph. solid. $[\alpha]_D^{23}$ +12 (c, 0.032 in $CHCl_3$). λ_{max} 265 (log ϵ 3.21) (MeOH).

Kubanek, J. *et al., J. Nat. Prod.*, 2006, **69**, 731-735 (*Bromophycolide C*)

Bromophycolide E B-522

[889453-96-7]



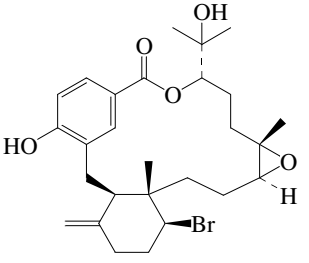
$C_{27}H_{36}Br_2O_4$ 584.387
Constit. of *Callophycus serratus*. Amorph. solid. $[\alpha]_D^{23}$ +35 (c, 0.034 in $CHCl_3$). λ_{max} 263 (log ϵ 3.72) (MeOH).

15,26-Dihydro, 15-bromo: ***Bromophycolide D***
[889453-95-6]
$C_{27}H_{37}Br_3O_4$ 665.299
Constit. of *Callophycus serratus*. Amorph. solid. $[\alpha]_D^{23}$ +47 (c, 0.041 in $CHCl_3$). λ_{max} 263 (log ϵ 3.88) (MeOH).

Kubanek, J. *et al., J. Nat. Prod.*, 2006, **69**, 731-735 (*Bromophycolides D and E*)

Bromophycolide F B-523

[889453-97-8]

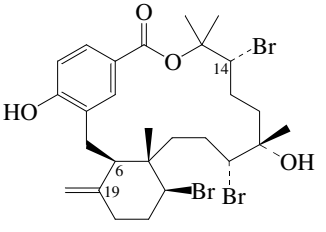


$C_{27}H_{37}BrO_5$ 521.49
Constit. of *Callophycus serratus*. Amorph. solid. $[\alpha]_D^{23}$ +35 (c, 0.034 in $CHCl_3$). λ_{max} 263 (log ϵ 3.72) (MeOH).

Kubanek, J. *et al., J. Nat. Prod.*, 2006, **69**, 731-735 (*Bromophycolide F*)

Bromophycolide H B-524

[889453-99-0]



$C_{27}H_{37}Br_3O_4$ 665.299
Constit. of *Callophycus serratus*. Amorph. solid. $[\alpha]_D^{23}$ +42 (c, 0.049 in $CHCl_3$). λ_{max} 263 (log ϵ 3.68) (MeOH).

14-Debromo, 14β-hydroxy: ***Bromophycolide I***
[888324-01-4]
$C_{27}H_{38}Br_2O_5$ 602.402
Constit. of *Callophycus serratus*. Amorph. solid. $[\alpha]_D^{23}$ +36 (c, 0.011 in $CHCl_3$). λ_{max} 262 (log ϵ 3.7) (MeOH).

14-Debromo, 14β-hydroxy, $\Delta^{6(19)}$-isomer: ***Bromophycolide G***
[889453-98-9]
$C_{27}H_{38}Br_2O_5$ 602.402
Constit. of *Callophycus serratus*. Amorph. solid. $[\alpha]_D^{23}$ -2 (c, 0.013 in $CHCl_3$). λ_{max} 217 (log ϵ 3.95); 262 (log ϵ 3.84) (MeOH).
Kubanek, J. *et al., J. Nat. Prod.*, 2006, **69**, 731-735 (*Bromophycolides G-I*)

1-Bromopropane, 9CI B-525

Propyl bromide
[106-94-5]
$H_3CCH_2CH_2Br$
C_3H_7Br 122.992
Isol. from a marine alga. Liq. d_4^{20} 1.35.
Fp -110. Bp 71°. n_D^{20} 1.4336.
▶ Flammable, fl. p. 50 (rat, ipr) 2950 mg/kg. TX4110000
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 56A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 82C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 83C (*ir*)
Aldrich Library of NMR Spectra, **1**, 49D (*pmr*)
Org. Synth., Coll. Vol., 1, 1932, 36 (*synth*)
Org. Synth., Coll. Vol., 2, 1943, 359 (*synth*)
De Bie, M.J.A. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1978, **97**, 135 (*pmr, cmr*)
Durig, J.R. *et al., J. Chem. Phys.*, 1984, **80**, 5983 (*ir, Raman, conformn*)
Kozlowski, R. *et al., Org. Prep. Proced. Int.*, 1988, **20**, 177 (*synth*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BNX750

1-Bromo-2-propanone B-526

Bromoacetone
[598-31-2]
H_3CCOCH_2Br
C_3H_5BrO 136.976
Isol. from the algae *Asparagopsis taxiformis* and *Falkenbergia rufolanosa*. Liq. which turns violet rapidly. d^{23} 1.63.
Fp -36.5. Bp_{725} 136.5°. pK_{a1} 16.1.
▶ Lachrymator. UC0525000
Oxime: [62116-25-0]
C_3H_6BrNO 151.99
Mp 36.5°. Bp_8 83°.
▶ Explodes on distillation.
Semicarbazone:
Cryst. (C_6H_6). Mp 135° dec.
2,4-Dinitrophenylhydrazone: Mp 120°.
Di-Me ketal: 1-Bromo-2,2-dimethoxypropane
[126-38-5]
$C_5H_{11}BrO_2$ 183.045
Synthetic reagent. Bp_{80} 83-87°.
▶ Lachrymator.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 221C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 361C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 291C (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 88 (*synth*)
Feugeas, Cl. *et al., Bull. Soc. Chim. Fr.*, 1963, 2568
Takahashi, K. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 963 (*pmr*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 692-698 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1128
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 164
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BMS000; BNZ000

3-Bromo-2-propenoic acid, 9CI B-527

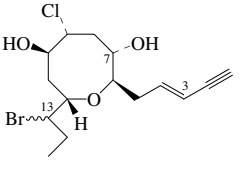
3-Bromoacrylic acid, 8CI
[39773-32-5]
BrCH=CHCOOH
$C_3H_3BrO_2$ 150.959

(E)-form [6213-89-4]
Cryst. (Et_2O). Mp 121°.
Me ester: [6213-87-2]
$C_4H_5BrO_2$ 164.986
Liq. Bp_9 45-50°.
Amide: [72330-65-5]
C_3H_4BrNO 149.975
Mp 153-155°.
Nitrile: 3-Bromoacrylonitrile. 1-Bromo-2-cyanoethylene
[41866-26-6]
C_3H_2BrN 131.959
Cryst. Mp 58-59°.

(Z)-form [1609-92-3]
Isol. from the red alga *Asparagopsis taxiformis*.
Mp 57-58.5°.
Me ester: [6214-22-8] Bp_{11} 60°.
Et ester: [31930-34-4]
$C_5H_7BrO_2$ 179.013
Used in synth. of ethyl *p*-hydroxybenzoate derivatives. Bp_{40} 92-93°.
Amide: [41866-46-0]
Mp 90-90.5°.
Nitrile: [41866-24-4]
Liq. Bp 171°. Sensitive to light and moisture.
[31930-35-5, 42844-38-2]
Gryszkiewicz-Trochimowski, E. *et al., Bull. Soc. Chim. Fr.*, 1948, 593-596 (*E-form, synth*)
Alder, K. *et al., Annalen*, 1955, **593**, 1-22 (*synth*)
Brower, H. *et al., Can. J. Chem.*, 1972, **50**, 601-611 (*cmr*)
McGreer, D.E. *et al., Can. J. Chem.*, 1973, **51**, 1239-1244 (*synth, amide, nitrile, pmr*)
Holy, A. *et al., Coll. Czech. Chem. Comm.*, 1974, **39**, 3177-3186 (*Z-form, Me ester, synth, pmr*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617-620 (*isol, synth, ms*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1988, **13**, 130-131 (*Et ester, use*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1991, 1511-1524 (*E-form, Me ester, ir, pmr*)
Ma, S. *et al., J.O.C.*, 1992, **57**, 709-713 (*Z-form, synth, ir, pmr, ms*)
Keah, H.H. *et al., Aust. J. Chem.*, 1993, **46**, 1413-1419 (*synth, cmr*)
Kotora, M. *et al., Synthesis*, 1997, 121-128 (*Z-form, synth, pmr, cmr, ir*)
Org. Synth., Coll. Vol., 9, 1998, 415-417 (*Z-form, synth, pmr, cmr, ir*)

8-(1-Bromopropyl)-5-chloro-2-(2-penten-4-ynyl)-3,6-oxocanediol B-528

3-Bromo-7-chloro-4,10-epoxy-12-pentadecen-14-yne-6,9-diol



(3*E*,6*R**,7*S**,9*R**,10*R**,12*S**,13ξ)-*form*

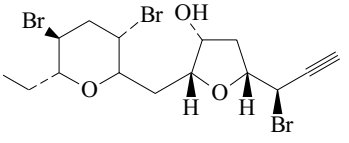
$C_{15}H_{22}BrClO_3$ 365.694
Acetogenin numbering shown.

(3E,6R*,7S*,9R*,10R*,12S*,13ξ)-form
Di-Ac:
$C_{19}H_{26}BrClO_5$ 449.768
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D^{20}$ +11.9 (c, 0.16 in $CHCl_3$). λ_{max} 225 (log ϵ 3.7) (hexane).

(3Z,6R*,7S*,9R*,10R*,12S*,13ξ)-form
Di-Ac: Constit. of *Laurencia obtusa*.
Oil. $[\alpha]_D^{20}$ +48 (c, 0.1 in $CHCl_3$). λ_{max} 224 (log ϵ 3.91) (hexane).
Iliopoulou, D. *et al., Phytochemistry*, 2002, **59**, 111-116 (*isol, pmr, cmr*)

5-(1-Bromo-2-propynyl)-2-[(3,5-dibromo-6-ethyltetrahydro-2*H*-pyran-2-yl)methyl]tetrahydro-3-furanol, 9CI B-529

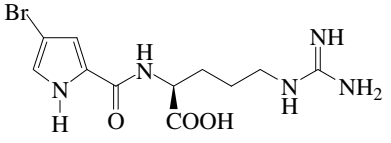
[126618-26-6]



$C_{15}H_{21}Br_3O_3$ 489.041
Metab. of *Laurencia obtusa*. Oil.
Mp 54.5-55°. $[\alpha]_D^{25}$ -4.1 (c, 0.05 in $CHCl_3$).

Shekhani, M.S. *et al., Phytochemistry*, 1990, **29**, 2573 (*isol, pmr, cmr*)

N^2-(4-Bromo-1*H*-pyrrole-2-carbonyl)arginine B-530

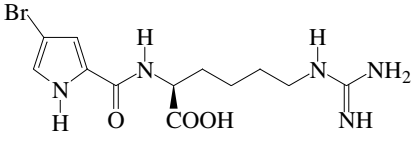


$C_{11}H_{16}BrN_5O_3$ 346.183
Isol. from *Stylissa caribica*. Light yellow oil. $[\alpha]_D^{23}$ -16 (c, 0.25 in MeOH).

Grube, A. *et al., J. Nat. Prod.*, 2006, **69**, 125-127 (*isol, synth, pmr, cmr*)

N^2-(4-Bromo-1*H*-pyrrole-2-carbonyl)homoarginine B-531

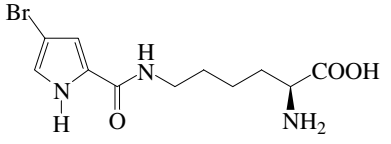
N^6-*(Aminoiminomethyl)*-N^2-*[(4-bromo-1*H*-pyrrol-2-yl)carbonyl]lysine, 9CI*
[242147-75-7]



$C_{12}H_{18}BrN_5O_3$ 360.21
Isol. from *Agelas wiedenmayeri*. λ_{max} 271 (ϵ 11500) (H_2O).

Assmann, M. *et al., Org. Lett.*, 1999, **1**, 455-457 (*isol, struct*)
Lindel, T. *et al., J. Nat. Prod.*, 2000, **63**, 1566-1569 (*synth, uv, ir, pmr, cmr*)

N^6-(4-Bromo-1*H*-pyrrole-2-carbonyl)lysine B-532

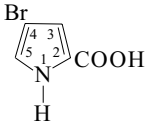


$C_{11}H_{16}BrN_3O_3$ 318.17
Isol. from *Stylissa caribica*. Light yellow oil. $[\alpha]_D^{23}$ +5.2 (c, 0.5 in MeOH).

Grube, A. *et al., J. Nat. Prod.*, 2006, **69**, 125-127 (*isol, synth, pmr, cmr*)

4-Bromo-1*H*-pyrrole-2-carboxylic acid, 9CI B-533

[27746-02-7]



$C_5H_4BrNO_2$ 189.996
Isol. from *Axinella verrucosa*.
Mp 160° dec. pK_a 4.06 (25°,H_2O).

Me ester: [934-05-4]
$C_6H_6BrNO_2$ 204.023
Isol. from sponges *Axinella tenuidigitata* and *Lissodendoryx* sp.
Mp 106-106.5° (98-99°). Struct. of nat. prod. revised in 1993.

Et ester: [433267-55-1]
$C_7H_8BrNO_2$ 218.05
Solid. Mp 55°.

Amide: [196106-96-4]
$C_5H_5BrN_2O$ 189.011
Isol. from the sponge *Acanthella carteri*. λ_{max} 202 (ϵ 13800); 230 (ϵ 9800); 267 (ϵ 16200) (MeOH).

(Methoxymethyl)amide: 4-Bromo-N^2*-methoxymethyl-1*H*-pyrrole-2-carboxamide*
$C_7H_9BrN_2O_2$ 233.064
Alkaloid from *Axinella verrucosa*.

Anderson, H.J. *et al., Can. J. Chem.*, 1965, **43**, 409-414 (*synth*)
Fringuelli, F. *et al., Tetrahedron*, 1969, **25**, 5815-5818 (*synth*)
Bélanger, P. *et al., Tet. Lett.*, 1979, **20**, 2505-2508 (*Me ester*)
Barrow, R.A. *et al., Nat. Prod. Lett.*, 1993, **1**, 243-250 (*Me ester, struct*)
Kitamura, C. *et al., J.C.S. Perkin 1*, 1997, 1443-1447 (*Me ester*)
Mancini, I. *et al., Tet. Lett.*, 1997, **38**, 6271-6274 (*amide, isol, uv, pmr, cmr, ms*)
Reddy, N.S. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 1145-1147 (*Me ester, isol*)
Bergauer, M. *et al., Synthesis*, 2002, 274-278 (*Et ester*)
Aiello, A. *et al., Bioorg. Med. Chem.*, 2006, **14**, 17-24 (*methoxymethylamide, isol*)

5-Bromo-1*H*-pyrrole-2-carboxylic acid, 9CI B-534

[28383-57-5]

$C_5H_4BrNO_2$ 189.996
Mp 138° dec. (block). pK_a 4.17 (25°,H_2O).

Me ester. Methyl 5-bromo-2-pyrrolecarboxylate
[934-07-6]
$C_6H_6BrNO_2$ 204.023
Isol. from the sponge *Lissodendoryx* sp. Cryst. (hexane).
Mp 106.5-108°.

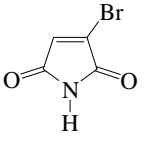
*Amide: 5-Bromo-1*H*-pyrrole-2-carboxamide*
[17543-94-1]
$C_5H_5BrN_2O$ 189.011
Alkaloid from the sponge *Agelas nakamurai*. Needles.
Mp 137-139°. λ_{max} 213 (log ϵ 3.47); 268 (log ϵ 3.93) (MeOH).

(Methoxymethyl)amide: 5-Bromo-N^2*-(methoxymethyl)-1*H*-pyrrole-2-carboxamide*
[213619-56-8]
$C_7H_9BrN_2O_2$ 233.064
Alkaloid from *Agelas nakamurai*. Amorph. solid. λ_{max} 214 (log ϵ 3.6); 271 (log ϵ 4.05) (MeOH).

Anderson, H.J. *et al., Can. J. Chem.*, 1965, **43**, 409-414 (*synth*)
Hodge, P. *et al., J.C.S.*, 1965, 459-470 (*synth, uv, ir*)
Friguelli, F. *et al., Tetrahedron*, 1969, **25**, 5815-5818 (*synth*)
Schmitz, F.J. *et al., J. Nat. Prod.*, 1985, **48**, 47-53 (*Me ester, isol*)
Iwagawa, T. *et al., J. Nat. Prod.*, 1998, **61**, 1310-1312 (*isol, amides*)

3-Bromo-1*H*-pyrrole-2,5-dione B-535

3-Bromomaleimide
[45514-47-4]



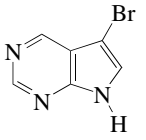
$C_4H_2BrNO_2$ 175.969
Alkaloid from the marine sponge *Axinella brevistyla*. Antifungal and cytotoxic agent. λ_{max} 201 (log ϵ 3.8); 229 (log ϵ 3.7); 245 (sh) (log ϵ 3.5) (MeOH).

N-*Ph:* [72000-67-0]
$C_{10}H_6BrNO_2$ 252.067
Pale yellow solid (EtOH). Mp 150-153°.

Choi, D.S. *et al., J.O.C.*, 1998, **63**, 2646-2655 (*N-Ph, synth*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 2001, **64**, 1576-1578 (*isol, uv, ir, pmr, cmr*)

5-Bromo-7*H*-pyrrolo[2,3-*d*]pyrimidine B-536

[175791-49-8]



$C_6H_4BrN_3$ 198.022
Isol. from a *Hypnea* sp. Scales.
Mp 199-201°. CAS no. refers to 1*H*-form.

Naqvi, S.W.A. *et al., Bot. Mar.*, 1981, **24**, 51-55 (*isol*)
Sakamoto, T. *et al., J.C.S. Perkin 1*, 1996, 459 (*synth, pmr, ir*)

Bromosleeper peptide B-537

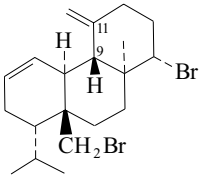
[188735-04-8]

$C_{158}H_{221}BrN_{38}O_{62}S_6$ 3917.001
Peptide containing a 6-bromotryptophan residue at position 1, 4-carboxyglutamate residues at positions 6, 8, 9 and 29, and 4-hydroxyproline residues at positions 21 and 22. Isol. from *Conus radiatus.* Induces a sleep-like state in mice of all ages.

Craig, A.G. *et al., J. Biol. Chem.*, 1997, **272**, 4689-4698 (*isol*)

Bromosphaerene B B-538

[88142-53-4]



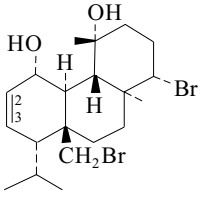
$C_{20}H_{30}Br_2$ 430.265
Constit. of *Sphaerococcus coronopifolius.* Cryst.
Mp 96-98°. $[\alpha]_D^{20}$ -95 (c, 1 in $CHCl_3$).

$\Delta^{9,11}$-Isomer: ***Bromosphaerene A***
[62326-60-7]
$C_{20}H_{30}Br_2$ 430.265
Isol. from *Sphaerococcus coronopifolius.* Cryst.
Mp 101-103°. $[\alpha]_D^{20}$ -143.

Cafieri, F. *et al., Phytochemistry*, 1983, **22**, 1824

Bromosphaerodiol B-539

[65714-67-2]



$C_{20}H_{32}Br_2O_2$ 464.28
Constit. of *Sphaerococcus coronopifolius.* Cryst. (MeOH).
Mp 170-172°. $[\alpha]_D$ -44.3 (c, 1 in $CHCl_3$).

2,3-Dihydro: ***1,2-Dihydro-1-hydroxybromosphaerol***
[85643-75-0]
$C_{20}H_{34}Br_2O_2$ 466.295
Isol. from *Sphaerococcus coronopifolius.* Cryst.
Mp 178-180°. $[\alpha]_D^{20}$ +2.5 (c, 0.8 in $CHCl_3$).

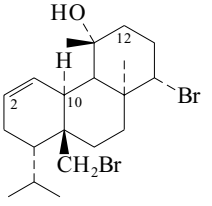
12β-Hydroxy: ***12-Hydroxybromosphaerodiol***
[108925-35-5]
$C_{20}H_{32}Br_2O_3$ 480.279
Constit. of *Sphaerococcus coronopifolius.* Cryst.
Mp 88-90°. $[\alpha]_D$ +39 ($CHCl_3$).

12β-Hydroxy, 1-ketone: ***Bromosphaerone***
[361344-22-1]
$C_{20}H_{30}Br_2O_3$ 478.263
Constit. of *Sphaerococcus coronopifolius.* Amorph. powder.
$[\alpha]_D$ -71 (c, 0.1 in CH_2Cl_2). λ_{max} 205 (log ϵ 3.64); 224 (log ϵ 3.5) (MeOH).

Cafieri, F. *et al., Experientia*, 1977, **33**, 1549 (*Bromosphaerodiol*)
Cafieri, F. *et al., Phytochemistry*, 1982, **21**, 2412; 1987, **26**, 471-473 (*Dihydrohydroxybromosphaerol, 12-Hydroxybromosphaerodiol*)
Etahari, S. *et al., J. Nat. Prod.*, 2001, **64**, 1024-1027 (*Bromosphaerone*)

Bromosphaerol B-540

[62326-56-1]



$C_{20}H_{32}Br_2O$ 448.28
Constit. of *Sphaerococcus coronopifolius.* Viscous oil. $[\alpha]_D$ +0.5.

Ac:
Cryst. Mp 140-142°.

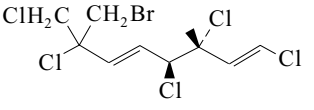
12α-Hydroxy: ***12α-Hydroxybromosphaerol***
[108907-23-9]
Isol. from *Sphaerococcus coronopifolius.*
Cryst.
Mp 89-92°. $[\alpha]_D$ -34 ($CHCl_3$).

12β-Hydroxy: ***12β-Hydroxybromosphaerol***
[81509-31-1]
From *Sphaerococcus coronopifolius.*
Oil.
Mp 88-90°. $[\alpha]_D$ +39 ($CHCl_3$). Formerly descr. as an oil.

$\Delta^{1,10}$-Isomer, 2α-hydroxy:
$C_{20}H_{32}Br_2O_2$ 464.28
Constit. of *Sphaerococcus coronopifolius.* Oil. $[\alpha]_D$ +3.7 ($CHCl_3$).

Fattorusso, E. *et al., Gazz. Chim. Ital.*, 1976, **106**, 779
Cafieri, F. *et al., Experientia*, 1982, **38**, 298-299 (*12β-Hydroxybromosphaerol*)
Cafieri, F. *et al., J.O.C.*, 1985, **50**, 3982 (*abs config*)
Cafieri, F. *et al., Phytochemistry*, 1987, **26**, 471-473 (*12α-Hydroxybromosphaerol*)
Cafieri, F. *et al., Gazz. Chim. Ital.*, 1990, **120**, 139 (*deriv*)

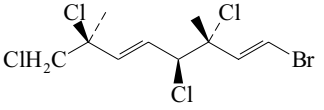
8-Bromo-1,3,4,7-tetrachloro-7-chloromethyl-3-methyl-1,5-octadiene B-541



$C_{10}H_{12}BrCl_5$ 389.372

(1*E*,3*R*,4*S*,5*E*)-*form* [72719-90-5]
Constit. of *Plocamium* spp. Antifungal agent. Oil. $[\alpha]_D$ -20.2 (c, 1.19 in $CHCl_3$).
Stierle, D.B. *et al., Tetrahedron*, 1979, **35**, 2855

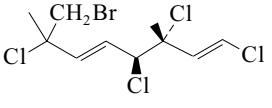
1-Bromo-3,4,7,8-tetrachloro-3,7-dimethyl-1,5-octadiene B-542



$C_{10}H_{13}BrCl_4$ 354.928

(1*E*,3*R*,4*S*,5*E*,7*S*)-*form*
Aplysiaterpenoid B
[101691-08-1]
Constit. of *Aplysia kurodai* and *Plocamium tefairiae*.
Needles. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 47-48°. $[\alpha]_D$ -32.2 (c, 0.37 in $CHCl_3$).
Miyamoto, T. *et al., Annalen*, 1988, 1191 (*isol, pmr, cmr*)
Watanabe, K. *et al., Pestic. Biochem. Physiol.*, 1990, **37**, 275 (*isol, struct*)

8-Bromo-1,3,4,7-tetrachloro-3,7-dimethyl-1,5-octadiene B-543



$C_{10}H_{13}BrCl_4$ 354.928

(1*E*,3*R*,4*S*,5*E*)-*form* [72719-89-2]
Constit. of *Plocamium* spp. Shows antifungal props. Oil. $[\alpha]_D$ -48.8 (c, 0.86 in $CHCl_3$).
Stierle, D.B. *et al., Tetrahedron*, 1979, **35**, 2855

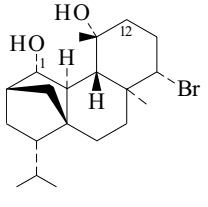
6-Bromo-5,9-tetracosadienoic acid B-544

$H_3C(CH_2)_{13}CH{=}CHCH_2CH_2CBr{=}CH(CH_2)_3COOH$
$C_{24}H_{43}BrO_2$ 443.506

(5*E*,9*Z*)-*form* [150994-69-7]
Constit. of the marine sponges *Amphimedon terpenesis* and *Agelas* sp.
Carballeira, N.M. *et al., Lipids*, 1993, **28**, 763 (*isol*)
Garson, M.J. *et al., Lipids*, 1993, **28**, 1011 (*isol*)

Bromotetrasphaerol B-545

[104900-64-3]

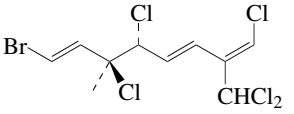


$C_{20}H_{33}BrO_2$ 385.383
Constit. of red alga *Sphaerococcus coronopifolius*. Oil. $[\alpha]_D$ -5.9 (c, 0.5 in $CHCl_3$).

12β-Hydroxy, 1-Me ether:
$C_{21}H_{35}BrO_3$ 415.41
Constit. of *Sphaerococcus coronopifolius*. Oil. $[\alpha]_D$ +0.5 ($CHCl_3$).
Cafieri, F. *et al., Tetrahedron*, 1986, **42**, 4273-4276 (*isol, pmr, cmr, ms, struct, biosynth*)
Cafieri, F. *et al., Gazz. Chim. Ital.*, 1990, **120**, 139 (*deriv*)

8-Bromo-1,5,6-trichloro-2-(dichloromethyl)-6-methyl-1,3,7-octatriene B-546

1-Bromo-7-dichloromethyl-3,4,8-trichloroocta-1,5,7-triene



(1*E*,3*E*,5*R**,6*S**,7*E*)-*form*

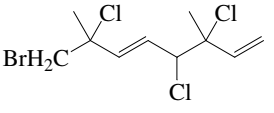
$C_{10}H_{10}BrCl_5$ 387.357

(1*E*,3*E*,5*R,6*S**,7*E*)-*form*** [57766-79-7]
Constit. of *Plocamium cartilagineum*. Metab. of *Aplysia dactylomela*. Shows antibacterial and algicide activity. $[\alpha]_D^{25}$ -22.9 (c, 0.9 in $CHCl_3$).

(1*Z*,3*E*,5*R,6*R**,7*E*)-*form*** [57766-77-5]
Constit. of the red alga *Plocamium cartilagineum*.
$[\alpha]_D^{25}$ +4.7 (c, 1.1 in $CHCl_3$). λ_{max} 244 (pentane).

(1*Z*,3*E*,5*R,6*S**,7*E*)-*form*** [57766-78-6]
Constit. of *Plocamium cartilagineum*.
$[\alpha]_D^{25}$ -4.4 (c, 1.1 in $CHCl_3$). λ_{max} 242 (pentane).
Mynderse, J.S. *et al., Tetrahedron*, 1975, **31**, 1963-1967 (*isol, uv, pmr, ms*)
Wessels, M. *et al., J. Nat. Prod.*, 2000, **63**, 920-928 (*cmr, activity*)

8-Bromo-3,4,7-trichloro-3,7-dimethyl-1,5-octadiene B-547

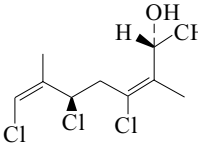


$C_{10}H_{14}BrCl_3$ 320.483

(5*E*)-*form*
Isol. from *Aplysia californica*. Not fully characterised.
Ireland, C. *et al., J.O.C.*, 1976, **41**, 2461-2465 (*isol, pmr*)

1-Bromo-4,6,8-trichloro-3,7-dimethyl-3,7-octadien-2-ol B-548

Costatol
[63023-57-4]

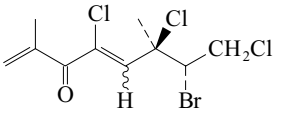


Absolute configuration

$C_{10}H_{14}BrCl_3O$ 336.482
Constit. of *Plocamium costatum*. Cryst. (hexane). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 88-89°. $[\alpha]_D$ -103 (c, 1 in $CHCl_3$).
Kazlauskas, R. *et al., Tet. Lett.*, 1976, 4451

7-Bromo-4,6,8-trichloro-2,6-dimethyl-1,4-octadien-3-one B-549

Plocamenone
[89353-92-4]



$C_{10}H_{12}BrCl_3O$ 334.466

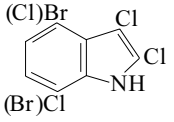
Constit. of the red alga *Plocamium* sp. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ -17.3 ($CHCl_3$). λ_{max} 232 (ϵ 6310) (MeOH) (Derep). λ_{max} 232 (ϵ 6450) (MeOH) (Berdy).

▶ Shows mutagenic props.

Stierle, D.B. *et al., Tet. Lett.*, 1984, **25**, 153 (*isol*)
Naylor, S. *et al., J. Nat. Prod.*, 1985, **48**, 72 (*struct, cmr*)

4(7)-Bromo-2,3,7(2,3,4)-trichloro-1*H*-indole, 9CI B-550

[68124-92-5]



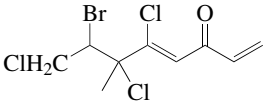
$C_8H_3BrCl_3N$ 299.381

Alkaloid from the marine red alga *Rhodophyllis membranacea*.

Brennan, M.R. *et al., Tet. Lett.*, 1978, 1637 (*isol, pmr, struct*)
Ohta, T. *et al., Heterocycles*, 1989, **29**, 1663 (*synth*)

7-Bromo-5,6,8-trichloro-6-methyl-1,4-octadien-3-one B-551

[73328-39-9]



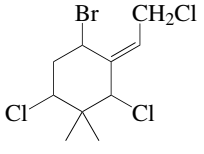
$C_9H_{10}BrCl_3O$ 320.44

Constit. of *Placomium angustum*. Oil. $[\alpha]_D^{21}$ -14.3 (c, 0.8 in $CHCl_3$).

Dunlop, R.W. *et al., Aust. J. Chem.*, 1979, **32**, 2735 (*isol, ir, pmr, cmr*)

4-Bromo-1,6,8-trichloro-2-ochtodene B-552

[159125-45-8]



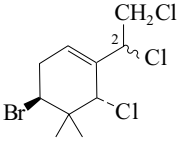
$C_{10}H_{14}BrCl_3$ 320.483

Constit. of *Portieria hornemannii*.
$[\alpha]_D$ +8.1 (c, 5.2 in $CHCl_3$).

Fuller, R.W. *et al., J. Med. Chem.*, 1994, **37**, 4407-4411 (*isol, pmr, cmr*)

6-Bromo-1,2,8-trichloro-3-ochtodene B-553

4-Bromo-6-chloro-1-(1,2-dichloroethyl)-5,5-dimethylcyclohexene, 9CI



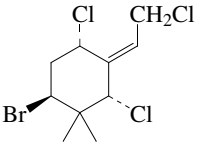
$C_{10}H_{14}BrCl_3$ 320.483

Isol. from *Chondrococcus hornemanni*. Oil. Mixt. of 2-epimers. Called 1,2-dichloro-3-ochtodene in reference.

[94450-32-5, 94450-33-6]

Crews, P. *et al., Phytochemistry*, 1984, **23**, 1449

6-Bromo-1,4,8-trichloro-2-ochtodene B-554



(2*E*,4*S**,6*S**,8*R**)-*form*

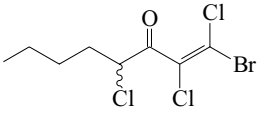
$C_{10}H_{14}BrCl_3$ 320.483

(2*E*,4*S,6*S**,8*R**)-*form***
Apakaochtodene B
[248949-49-7]
Constit. of *Portieria hornemannii*.

(2*Z*,4*S,6*S**,8*R**)-*form***
Apakaochtodene A
[248949-46-4]
Constit. of *Portieria hornemannii*.
Cryst.

Gunatilaka, A.A.L. *et al., J. Nat. Prod.*, 1999, **62**, 1376-1378 (*isol, pmr, cmr, cryst struct*)

1-Bromo-1,2,4-trichloro-1-octen-3-one B-555



(*Z*)–*form*

$C_8H_{10}BrCl_3O$ 308.429

Isolated and synthesised as a 20:1 *E*:*Z* isomer mixture.

(E)-form [64785-87-1]
Constit. of *Bonnemaisonia asparagoides*. Antibacterial agent. Oil.

(Z)-form [64785-86-0]
Constit. of *Bonnemaisonia asparagoides*. Antibacterial agent. Oil.

McConnell, O.J. *et al., Tet. Lett.*, 1977, 1851 (*isol, synth, ms*)

1-Bromo-1,3,3-trichloro-2-propanone, 9CI B-556

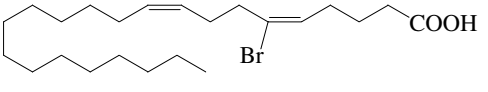
1-Bromo-1,3,3-trichloroacetone
[62874-82-2]
$Cl_2CHCOCHBrCl$
$C_3H_2BrCl_3O$ 240.31

(±)-form
Minor component of the red alga *Asparagopsis armata* and of *Falkenbergia rufolanosa*.
Liq. Bp_{17} 85-95°.

Hydrate:
Scaly cryst. Mp 52-53°.

U.K. Pat., 1959, 823 827; *CA*, **54**, 5713c (*synth*)
McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367 (*isol, glc*)
Combaut, G. *et al., Phytochemistry*, 1978, **17**, 1661 (*isol, glc*)

6-Bromo-5,9-tricosadienoic acid B-557

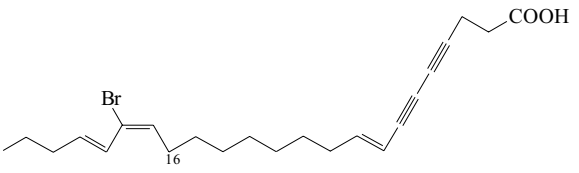


$C_{23}H_{41}BrO_2$ 429.48

(5*E*,9*Z*)-*form*
Isol. from *Siphonochalina siphonella*.

Dembitsky, V.M. *et al., Prog. Lipid Res.*, 2002, **41**, 315-367 (*occur*)

18-Bromo-8,17,19-tricosatriene-4,6-diynoic acid B-558



$C_{23}H_{31}BrO_2$ 419.401

(all-E)-form

Carduusyne B

[158182-76-4]

Constit. of the marine sponge *Phakellia carduus.*

Oil (as Et ester). λ_{max} 207 (ϵ 38500); 214 (ϵ 50100); 240 (ϵ 18000); 252 (ϵ 18400); 267 (ϵ 19300); 282 (ϵ 14800) (MeOH) (Et ester).

16ξ-Hydroxy: 18-Bromo-16-hydroxy-8,17,19-tricosatriene-4,6-diynoic acid. ***Carduusyne D***

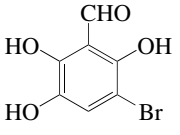
[158182-78-6]

$C_{23}H_{31}BrO_3$ 435.4

Constit. of *Phakellia carduus.* Oil (as Et ester). $[\alpha]_D$ +10.2 (c, 0.1 in $CHCl_3$). λ_{max} 208 (ϵ 43900); 214 (ϵ 57700); 230 (ϵ 18700); 239 (ϵ 21600); 252 (ϵ 19900); 266 (ϵ 19300); 282 (ϵ 14500) (MeOH) (Et ester).

Barrow, R.A. *et al., Aust. J. Chem.*, 1994, **47**, 1901-1918 (*isol, uv, ir, pmr, cmr*)

3-Bromo-2,5,6-trihydroxybenzaldehyde B-559



$C_7H_5BrO_4$ 233.018

λ_{max} 204 (ϵ 12245); 220 (ϵ 9630); 276 (ϵ 4930); 374 (ϵ 1605) (MeOH) (Berdy).

2-Me ether: 3-Bromo-5,6-dihydroxy-2-methoxybenzaldehyde

[151029-40-2]

$C_8H_7BrO_4$ 247.045

Isol. from a marine Verongid sponge. λ_{max} 204 (ϵ 12240); 220 (ϵ 9630); 276 (ϵ 4930); 374 (ϵ 1600) (MeOH).

2,5-Di-Me ether: 3-Bromo-6-hydroxy-2,5-dimethoxybenzaldehyde, 9CI

[65162-35-8]

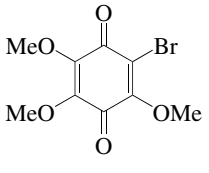
$C_9H_9BrO_4$ 261.072

Solid (MeOH). Mp 73-74°.

Wriede, U. *et al., J.O.C.*, 1987, **52**, 4485-4489 (*2,5-di-Me ether, synth*)
Hamann, M.T. *et al., J.O.C.*, 1993, **58**, 6565-6569 (*isol, uv, ir, pmr, cmr, ms*)

2-Bromo-3,5,6-trimethoxy-1,4-benzoquinone B-560

2-Bromo-3,5,6-trimethoxy-2,5-cyclohexadiene-1,4-dione



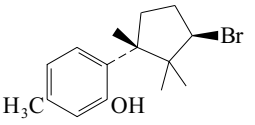
$C_9H_9BrO_5$ 277.071

Isol. from *Ptychodera flava laysanica.*

Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 22 (*occur*)

2-(3-Bromo-1,2,2-trimethylcyclopentyl)-5-methylphenol B-561

[125092-26-4]

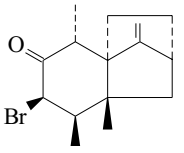


$C_{15}H_{21}BrO$ 297.234

Metab. of *Laurencia implicata*. Oil. $[\alpha]_D$ -9.02 (c, 0.013 in $CHCl_3$).

Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1685 (*isol, pmr, cmr*)

4-Bromo-2,5,6-trimethyl-11-methylenetricyclo[6.2.1.0^{1,6}]undecan-3-one B-562



$C_{15}H_{21}BrO$ 297.234

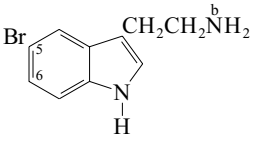
Metab. of *Laurencia tenera*. Unstable cryst. $[\alpha]_D$ -190.2 (c, 0.004 in $CHCl_3$).

Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1695 (*isol, pmr, cmr*)

5-Bromotryptamine B-563

*5-Bromo-1*H*-indole-3-ethanamine, 9CI. 3-(2-Aminoethyl)-5-bromoindole, 8CI*

[3610-42-2]



$C_{10}H_{11}BrN_2$ 239.114

Radioprotective agent. Tryptophan antagonist, 5-Hydroxytryptamine, H-996 antimetabolite displaying vascoconstructive and embryotoxic activity. Amber oil. Biosynth. precursor of Eudistomin H, E-885.

Hydrochloride: [81868-12-4]

Cryst. (EtOH/Et_2O) or solid. Mp 288-289° (286-287°).

N-*Ac:*

$C_{12}H_{13}BrN_2O$ 281.151

Solid. Mp 153.4-153.8°.

N^b*-Hydroxy: 5-Bromo-*N*-hydroxy-1*H*-indole-3-ethanamine. 5-Bromo-*N′*-hydroxytryptamine*

[123475-32-1]

$C_{10}H_{11}BrN_2O$ 255.114

Pale beige resinous material.

N^b,N^b*-Di-Me:* ***5-Bromo-N^b,N^b-dimethyltryptamine.*** *5-Bromo-N,N-dimethyl-1*H*-indole-3-ethanamine, 9CI. 5-Bromo-3-(2-dimethylaminoethyl)indole*

[17274-65-6]

$C_{12}H_{15}BrN_2$ 267.168

Metab. of the marine sponge *Smenospongia aurea* and from *Polyfibrospongia echina*. Major alkaloid from the New Caledonian ascidian *Eudistoma fragum*. Antimicrobial compd. Cryst. (MeOH aq.). Sol. MeOH, EtOAc; poorly sol. H_2O.

Mp 98-99° (90-92°). λ_{max} 225 (ϵ 39000); 285 (ϵ 4400); 305 (ϵ 2700) (MeOH) (Derep). λ_{max} 227 (ϵ 24000); 282 (ϵ 5500); 290 (ϵ 7943); 300 (ϵ 5012) (EtOH) (Berdy).

Quadbeck, G. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1954, **297**, 229; *CA*, **51**, 15795i (*pharmacol*)
Ho, B.-T. *et al., J. Pharm. Sci.*, 1969, **58**, 563 (*pharmacol*)

Djura, P. *et al., J.O.C.*, 1980, **45**, 1435-1441 (*5-Bromo-N,N-dimethyltryptamine, isol, uv, ir, pmr, cmr, struct*)
Landau, M.A. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1981, **69**, 359 (*tox*)
Tymiak, A.A. *et al., Tetrahedron*, 1985, **41**, 1039-1047 (*5-Bromo-N,N-dimethyltryptamine, isol, uv, ir, pmr, ms, synth*)
Kennaway, D.J. *et al., Aust. J. Biol. Sci.*, 1988, **41**, 393 (*synth*)
Debitus, C. *et al., J. Nat. Prod.*, 1988, **51**, 799-801 (*5-Bromo-N,N-dimethyltryptamine, isol, uv, pmr, cmr, ms*)
Still, I.W. *et al., Can. J. Chem.*, 1990, **68**, 1408-1419 (*synth, ir, pmr, cmr, ms*)
Shen, G.Q. *et al., Tet. Lett.*, 1994, **35**, 4923-4926 (*biochem*)
Somei, M. *et al., Heterocycles*, 1995, **40**, 119-122 (*synth, 5-Bromo-N,N-dimethyltryptamine*)

6-Bromotryptamine B-564

*6-Bromo-1*H*-indole-3-ethanamine, 9CI. 3-(2-Aminoethyl)-6-bromoindole*
[96624-18-9]
$C_{10}H_{11}BrN_2$ 239.114
Alkaloid from the encrusting grey marine tunicate *Didemnum candidum*.
Mp 120-120.5°. λ_{max} 225 (ϵ 15800); 286 (ϵ 3100); 294 (ϵ 2700) (MeOH) (Berdy).

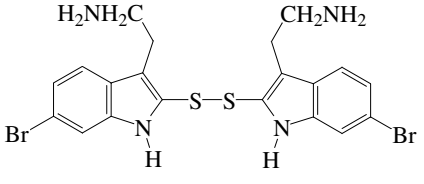
Hydrochloride: [108061-77-4]
Mp 215-217° dec.

N^b*-Me,* N^b*-formyl:* ***6-Bromo-*N^b*-formyl-*N^b*-methyltryptamine***.
N-*[2-(6-Bromo-1*H*-indol-3-yl)ethyl]-*N*-methylformamide, 9CI*
[82503-95-5]
$C_{12}H_{13}BrN_2O$ 281.151
Alkaloid from the marine bryozoan *Flustra foliacea*. Amorph. solid. Shows restricted C–N bond rotn.

N^a*-(3-Methyl-2-butenyl),* N^b*-Me:* ***6-Bromo-*N^b*-methyl-*N^a*-prenyltryptamine***. *Deformylflustrabromine B*
$C_{16}H_{21}BrN_2$ 321.259
Alkaloid from *Flustra foliacea*. Yellow oil. λ_{max} 230 (log ϵ 4.1); 291 (log ϵ 3.3) (MeOH).

Wulff, P. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **71**, 523-524 (*N^b-Me N^b-formyl, isol, pmr, ms, struct*)
Groen, C. *et al., Acta Chem. Scand., Ser. B*, 1984, **38**, 709-711 (*synth, pmr, cmr, ir, uv*)
Rinehart, K.L. *et al., J.A.C.S.*, 1987, **109**, 3378-3387 (*synth, hplc, pmr, cmr, ms, uv, ir*)
Fahy, E. *et al., J. Nat. Prod.*, 1991, **54**, 564-569 (*isol, pmr, cmr*)
Peters, L. *et al., Planta Med.*, 2004, **70**, 883-886 (*Bromomethylprenyltryptamine*)

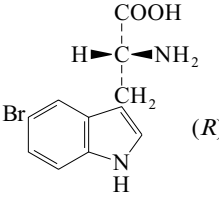
6-Bromotryptamine 2,2′-disulfide B-565



$C_{20}H_{20}Br_2N_4S_2$ 540.345
Isol. from the defensive mucus of *Calliostoma canaliculatum*. K channel antagonist.

Kelley, W.P. *et al., J. Biol. Chem.*, 2003, **278**, 34934-34942 (*isol, pmr, cmr, ms*)

5-Bromotryptophan, 9CI, 8CI B-566



(*R*)–*form*

$C_{11}H_{11}BrN_2O_2$ 283.124
Potent antisickling agent.

(*R*)-*form*

D-form
[93299-40-2]
Cryst. (MeOH aq.). Mp 289-290°. $[\alpha]_D$ +27.1 (c, 1.1 in AcOH).

Me ester: [93299-39-9]
Cryst. (2-propanol/diisopropyl ether). Mp 98-100°. $[\alpha]_D^{20}$ -49.2 (c, 1 in MeOH).

N$^\alpha$*-Ac:* [75816-16-9]
Cryst. + ½ H_2O (MeOH aq.). Mp 120-122° dec. $[\alpha]_D^{26}$ -15.1 (c, 2 in MeOH).

(*S*)-*form*

L-form
[25197-99-3]
Constit. of the sponge *Smenospongia* sp.
Mp 288-291° dec. $[\alpha]_D^{20}$ -28.5 (c, 1 in AcOH). $[\alpha]_D^{20}$ +31.8 (c, 1 in 1*M* HCl). λ_{max} 230 (log ϵ 3.87); 290 (log ϵ 3.47) (MeOH).

Me ester: [93299-38-8]
Cryst. (2-propanol/diisopropyl ether). Mp 100-102°. $[\alpha]_D^{20}$ +48.6 (c, 1 in MeOH).

N$^\alpha$*-Me: 5-Bromo-*N*-methyltryptophan.* ***5-Bromoabrine***
[488827-92-5]
$C_{12}H_{13}BrN_2O_2$ 297.151
Constit. of the sponge *Smenospongia* sp. Light brown powder. $[\alpha]_D^{22}$ -34 (c, 0.05 in MeOH). $[\alpha]_D^{22}$ +45.8 (c, 0.05 in 1*M* HCl). λ_{max} 228 (log ϵ 3.59); 288 (log ϵ 2.92) (MeOH).

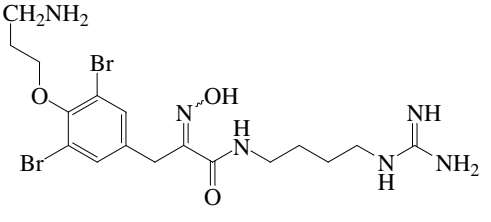
N$^\alpha$,N$^\alpha$*-Di-Me: 6-Bromo-*N,N*-dimethyl-L-tryptophan*
$C_{13}H_{15}Br_2N_2O_2$ 391.082
Isol. from the sponge *Thorectandra* sp. Yellow solid. $[\alpha]_D^{25}$ -19.3 (c, 0.5 in MeOH).

(±)-*form* [6548-09-0]
Mp 273-276° dec. Sinters at 258°.

N$^\alpha$*-Ac:* [75816-15-8]
Cryst. (MeOH aq.). Mp 212-214°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 673A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 145C (*nmr*)
Raverty, W.D. *et al., J.C.S. Perkin 1*, 1977, 1204-1211 (*synth*)
Allen, M.C. *et al., J.C.S. Perkin 1*, 1980, 1928-1932; 1986, 989-1003 (*synth*)
Poillon, W.N. *et al., Biochemistry*, 1982, **21**, 1400-1406 (*pharmacol*)
Irie, K. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2126-2139 (*synth, derivs*)
Prasitpan, N. *et al., Synth. Commun.*, 1990, **20**, 3459-3466 (***synth***)
Nagarathnam, D. *et al., Synth. Commun.*, 1993, **23**, 2011-2017 (*synth*)
Tasdemir, D. *et al., Z. Naturforsch., C*, 2002, **57**, 914-922 (*isol, pmr, cmr, ms, 5-Bromoabrine*)
Segraves, N.L. *et al., J. Nat. Prod.*, 2005, **68**, 1484-1488 (*6-Bromo-N,N-dimethyltryptophan*)

Oceanapia Bromotyrosine alkaloid B-567

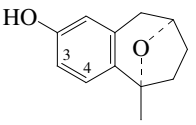


$C_{17}H_{26}Br_2N_6O_3$ 522.239
Isol. from the sponge *Oceanapia* sp. Inhibitor of mycothiol S-conjugate amidase. Related to Purealidin H, P-716.

Nicholas, G.M. *et al., Org. Lett.*, 2001, **3**, 1543-1545 (*isol, pmr, cmr*)
Kende, A.S. *et al., Tet. Lett.*, 2004, **45**, 133-135 (*synth*)
Chanda, B.M. *et al., Tet. Lett.*, 2005, **46**, 6461-6463 (*synth*)

Bruguierol A B-568

[862813-44-3]



$C_{12}H_{14}O_2$ 190.241

Constit. of the stems of the mangrove *Bruguiera gymnorrhiza*. Amorph. solid. $[\alpha]_D^{20}$ +14.4 (c, 0.3 in MeOH). λ_{max} 278 (log ϵ 3.29) (MeOH). λ_{max} 278 (log ϵ 3.07) (MeOH/HCl). λ_{max} 298 (log ϵ 3.46) (MeOH/NaOH).

3-Hydroxy: ***Bruguierol B***
[862813-45-4]
$C_{12}H_{14}O_3$ 206.241

Constit. of the stems of *Bruguiera gymnorrhiza*. Amorph. solid. $[\alpha]_D^{20}$ +8.9 (c, 0.27 in MeOH). λ_{max} 289 (log ϵ 3.86) (MeOH). λ_{max} 289 (log ϵ 3.81) (MeOH/HCl). λ_{max} 302 (log ϵ 3.35) (MeOH/NaOH).

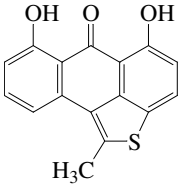
4-Hydroxy: ***Bruguierol C***
[862813-46-5]
$C_{12}H_{14}O_3$ 206.241

Constit. of the stems of *Bruguiera gymnorrhiza*. Antibacterial agent. Amorph. solid. $[\alpha]_D^{20}$ +4 (c, 0.5 in MeOH). λ_{max} 285 (log ϵ 3.09) (MeOH). λ_{max} 284 (log ϵ 2.95) (MeOH/HCl). λ_{max} 293 (log ϵ 3.29) (MeOH/NaOH).

Han, L. *et al., Planta Med.*, 2005, **71**, 160-164 (*isol, uv, pmr, cmr*)

Bryoanthrathiophene B-569

*5,7-Dihydroxy-1-methyl-6*H*-anthra[1,9-*bc*]thiophen-6-one*



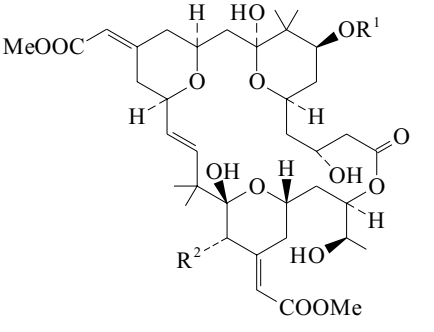
$C_{16}H_{10}O_3S$ 282.319

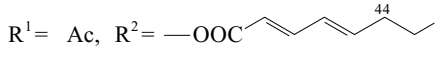
Constit. of the bryozoan *Watersipora subtorquata*. Antiangiogenic agent. Yellow powder. λ_{max} 213 (log ϵ 4.28); 283 (log ϵ 3.81); 324 (log ϵ 3.56); 429 (log ϵ 3.77) (MeOH).

Jeong, S.-J. *et al., J. Nat. Prod.*, 2002, **65**, 1344-1345 (*isol, pmr, cmr, ms*)

Bryostatin 1 B-570

NSC 339555
[83314-01-6]





$C_{47}H_{68}O_{17}$ 905.044

Macrolide antibiotic. Prod. by *Bugula neritina*. Active against M531 murine ovary sarcoma. Protein kinase C modulator. Phase II clin. trials (2002) for a variety of cancer indications, including oesophageal cancer. Cryst. (CH_2Cl_2/MeOH). Sol. MeOH, EtOH, $CHCl_3$, CCl_4; poorly sol. H_2O.
Mp 230-235°. $[\alpha]_D^{25}$ +34.1 (c, 0.044 in MeOH). Log P 1.7 (calc). λ_{max} 232 (ϵ 25700); 263 (ϵ 28700) (MeOH) (Derep).

▶ Mutagenic props. EH9455000

O-*De-Ac:* ***Bryostatin 2***
[87745-28-6]
$C_{45}H_{66}O_{16}$ 863.007

Prod. by *Bugula neritina*. Shows potent antineoplastic props. Fine cryst. (CH_2Cl_2/MeOH). Sol. MeOH, $CHCl_3$, CCl_4; poorly sol. H_2O.
Mp 201-203°. $[\alpha]_D^{25}$ +50 (c, 0.05 in MeOH). Log P 0.75 (calc). λ_{max} 230 (ϵ 36250); 261 (ϵ 35600) (MeOH) (Derep).

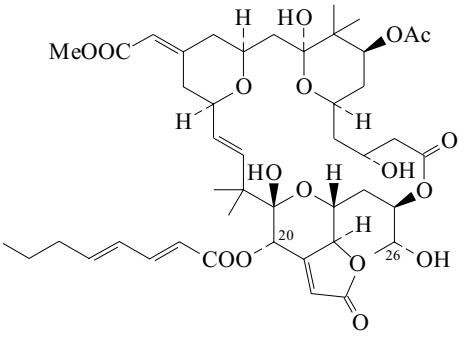
44-Hydroxy: ***Bryostatin 15***
[136448-58-3]
$C_{47}H_{68}O_{18}$ 921.043

From *Bugula neritina*. Cytotoxic agent. $[\alpha]_D^{25}$ +26 (c, 0.3 in MeOH). λ_{max} 227 (ϵ 25995) (MeOH) (Berdy).

Pettit, G.R. *et al., J.A.C.S.*, 1982, **104**, 6846 (*isol, cryst struct, ms, uv, ir*)
Pettit, G.R. *et al., J. Nat. Prod.*, 1983, **46**, 528 (*deriv, pmr*)
Pettit, G.R. *et al., Tetrahedron*, 1985, **41**, 985 (*rev*)
Gschwendt, M. *et al., Carcinogenesis (London)*, 1988, **9**, 555 (*pharmacol*)
Curtis, R.D. *et al., Can. J. Chem.*, 1991, **69**, 834 (*N-15 nmr*)
Mackanos, E.A. *et al., J. Biol. Chem.*, 1991, **266**, 11205 (*pharmacol*)
Pettit, G.R. *et al., J.O.C.*, 1991, **56**, 1337 (*abs config*)
Schaufelberger, D.E. *et al., Magn. Reson. Chem.*, 1991, **29**, 366 (*pmr, cmr*)
Pettit, G.R. *et al., Tetrahedron*, 1991, **47**, 3601 (*Bryostatin 15*)
Prendiville, J. *et al., Br. J. Cancer*, 1993, **68**, 418 (*clin trial*)
Szallasi, Z. *et al., Mol. Pharmacol.*, 1994, **46**, 840 (*pharmacol*)
Zonder, J.A. *et al., Expert Opin. Invest. Drugs*, 1999, **8**, 2189 (*rev*)
Evans, D.A. *et al., J.A.C.S.*, 1999, **121**, 7540-7552 (*Bryostatin 2, synth*)
Mutter, R. *et al., Bioorg. Med. Chem.*, 2000, **8**, 1841-1860 (*rev*)
Manning, T.J. *et al., Nat. Prod. Res.*, 2005, **19**, 467-491 (*rev, occur, ms*)

Bryostatin 3 B-571

[87370-86-3]



$C_{46}H_{64}O_{17}$ 889.001

Macrolide antibiotic. The original isolate called Bryostatin 3 was assigned the incorrect C-20 config. Later the 20-epimer was isolated and called Bryostatin 3- the original compd. was renamed 20-Epibryostatin 3. Isol. from the marine Bryozoan, *Bugula neritina*. Antineoplastic agent. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Log P 0.09 (uncertain value) (calc). λ_{max} 230 (ϵ 36000); 263 (ϵ 35000) (MeOH) (Derep). λ_{max} 230 (ϵ 36000); 261 (ϵ 35000) (MeOH) (Berdy). λ_{max} 229 (ϵ 31700); 264 (ϵ 30600) (EtOH) (Berdy).

20-Epimer: ***20-Epibryostatin 3***
$C_{46}H_{64}O_{17}$ 889.001
Isol. from *Bugula neritina*. Antineoplastic agent. Amorph. solid. $[\alpha]_D^{25}$ +61 (c, 0.26 in MeOH). Formerly known as Bryostatin 3. λ_{max} 228; 266 (MeOH) (Berdy).

26-Ketone: ***Bryostatin 3 26-ketone***
[132564-78-4]
$C_{46}H_{62}O_{17}$ 886.986
Isol. from *Bugula neritina*. The C-20 config. should presumably be reversed (i.e. to correspond with that of Bryostatin 3). λ_{max} 228; 266 (MeCN) (Berdy).

Pettit, G.R. *et al., J.O.C.*, 1983, **48**, 5354 (*isol, ms, uv, ir, pmr, cmr*)
Mackanos, E.A. *et al., J. Biol. Chem.*, 1991, **266**, 11205 (*pharmacol*)
Schaufelberger, D.E. *et al., J.O.C.*, 1991, **56**, 2895 (*cmr, struct*)
Chmurny, G.N. *et al., J.O.C.*, 1992, **57**, 5260 (*struct*)
Ohmori, K. *et al., Bull. Chem. Soc. Jpn.*, 2004, **77**, 875-885 (*synth*)

Bryostatin 4 B-572

NSC 362621
[91523-82-9]
As Bryostatin 1, B-570 with
R^1 = –$COCH_2CH(CH_3)_2$–, R^2 = -$OOCCH_2CH_2CH_3$
$C_{46}H_{70}O_{17}$ 895.049
Macrocyclic lactone antibiotic. Prod. by *Bugula neritina*, *Aplidium californicum* and *Amathia convoluta*. Active against murine lymphocytic leukemia. Protein phosphorylation stimulator, Protein kinase C binding agent, polymorphonuclear leucocyte activator. Amorph. powder. Sol. MeOH, DMSO, $CHCl_3$; poorly sol. H_2O.
Mp 198-200°. λ_{max} 228 (ϵ 36500) (MeOH) (Derep). λ_{max} 226 (ϵ 36500) (MeOH) (Berdy).

Ac:
Needles (CH_2Cl_2/MeOH). Mp 159-162°. $[\alpha]_D^{22}$ +58.71 (c, 0.034 in MeOH).

Deoxy(?): ***Bryostatin B***
[104841-30-7]
$C_{46}H_{70}O_{16}$ 879.049
Isol. from the sponge *Lissodendoryx isodictyalis*. Cryst.
Mp 137-140°. $[\alpha]_D^{27}$ +71.3 (c, 0.03 in MeOH). λ_{max} 227 (ϵ 36000) (MeOH).

Pettit, G.R. *et al., J.A.C.S.*, 1984, **106**, 6768
Pettit, G.R. *et al., Can. J. Chem.*, 1985, **63**, 1204
Pettit, G.R. *et al., Tetrahedron*, 1985, **41**, 985
Pettit, G.R. *et al., Pure Appl. Chem.*, 1986, **58**, 415-421 (*Bryostatin B*)

Bryostatin 5 B-573

NSC 362616
[97850-04-9]
As Bryostatin 1, B-570 with
R^1 = –$COCH_2CH(CH_3)_2$, R^2 = OAc
$C_{44}H_{66}O_{17}$ 866.995
Macrocyclic lactone antibiotic. Found in the marine bryozoan *Bugula neritina*. Active against P388 lymphocytic leukaemia. Needles (CH_2Cl_2/MeOH). Sol. MeOH, DMSO, $CHCl_3$; poorly sol. H_2O.
Mp 169-172°. $[\alpha]_D^{27}$ +106.92 (c, 0.028 in MeOH). λ_{max} 227 (ϵ 36300) (MeOH) (Derep). λ_{max} 226 (ϵ 36300) (MeOH) (Berdy).

Deoxy(?): ***Bryostatin A***
[104841-29-4]
$C_{44}H_{66}O_{16}$ 850.996
Isol. from the sponge *Lissodendoryx isodictyalis*. Cryst.
Mp 142-145°. $[\alpha]_D^{27}$ +74.8 (c, 0.04 in MeOH). λ_{max} 228 (ϵ 36400) (MeOH).

Pettit, G.R. *et al., Can. J. Chem.*, 1985, **63**, 1205
Pettit, G.R. *et al., Tetrahedron*, 1985, **41**, 985
Pettit, G.R. *et al., Pure Appl. Chem.*, 1986, **58**, 415-421 (*Bryostatin A*)
Pettit, G.R. *et al., J.O.C.*, 1991, **56**, 1337 (*abs config*)

Bryostatin 6 B-574

NSC 362617
[97850-06-1]
As Bryostatin 1, B-570 with
R^1 = –$COCH_2CH_2CH_3$, R^2 = -OAc
$C_{43}H_{64}O_{17}$ 852.968
Macrocyclic lactone antibiotic. Found in *Bugula nerihna*. Active against murine lymphocytic leukaemia. Needles (CH_2Cl_2/MeOH). Sol. MeOH, DMSO, $CHCl_3$; poorly sol. H_2O.
Mp 172-175°. $[\alpha]_D^{27}$ +39.92 (c, 0.05 in MeOH). λ_{max} 227 (ϵ 36300) (MeOH) (Derep). λ_{max} 228 (ϵ 36500) (MeOH) (Berdy).

Pettit, G.R. *et al., Can. J. Chem.*, 1985, **63**, 1205 (*isol, struct*)
Pettit, G.R. *et al., J.O.C.*, 1991, **56**, 1337 (*abs config*)

Bryostatin 7 B-575

NSC 362619
[97850-05-0]
As Bryostatin 1, B-570 with
R^1 = Ac, R^2 = OAc
$C_{41}H_{60}O_{17}$ 824.915
Macrocyclic lactone antibiotic. Found in *Bugula neritina*. Active against murine lymphocytic leukaemia. Needles (CH_2Cl_2/MeOH). Sol. MeOH, Et_2O, $CHCl_3$; poorly sol. H_2O.
Mp 176-179°. $[\alpha]_D^{27}$ +39.92 (c, 0.05 in MeOH). λ_{max} 228 (ϵ 36350) (MeOH) (Derep).

Pettit, G.R. *et al., Can. J. Chem.*, 1985, **63**, 1205 (*isol, struct*)
Pettit, G.R. *et al., J.O.C.*, 1991, **56**, 1337 (*abs config*)
Manaviazar, S. *et al., Org. Lett.*, 2006, **8**, 4477-4480 (*synth*)

Bryostatin 8 B-576

[102580-64-3]
As Bryostatin 1, B-570 with
R^1 = –$COCH_2CH_2CH_3$, R^2 = -$OOCCH_2CH_2CH_3$
$C_{45}H_{68}O_{17}$ 881.022
Macrocyclic lactone antibiotic. Constit. of *Amathia convoluta*. Active against murine P388 lymphocytic leukaemia. Amorph. powder. Sol. MeOH, $CHCl_3$, DMSO; poorly sol. H_2O.
Mp 170-173°. $[\alpha]_D^{27}$ +49.9 (c, 0.04 in MeOH). λ_{max} 228 (ϵ 36500) (MeOH) (Derep). λ_{max} 226 (ϵ 37500) (MeOH) (Berdy).

Pettit, G.R. *et al., Tetrahedron*, 1985, **41**, 985 (*isol, struct, rev*)

Bryostatin 9 B-577

[102604-78-4]
As Bryostatin 1, B-570 with
R^1 = Ac, R^2 = –$OOCCH_2CH_2CH_3$
$C_{43}H_{64}O_{17}$ 852.968
Macrocyclic lactone antibiotic. Isol. from *Bugula neritina*. Shows antineoplastic props. Needles. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 159-162°. $[\alpha]_D^{28}$ +87.31 (c, 0.04 in MeOH). λ_{max} 229 (ϵ 36200) (MeOH) (Berdy).

Ac:
Needles (CH_2Cl_2/MeOH). Mp 155-159°. $[\alpha]_D^{27}$ +95.7 (c, 0.5 in MeOH).

Pettit, G.R. *et al., J. Nat. Prod.*, 1986, **49**, 661 (*isol, struct*)
Pettit, G.R. *et al., J.O.C.*, 1991, **56**, 1337 (*abs config*)

Bryostatin 10 B-578

[102580-65-4]
As Bryostatin 1, B-570 with
R^1 = –$COC(CH_3)_3$, R^2 = H
$C_{42}H_{64}O_{15}$ 808.959
Isol. from *Bugula neritina*. Antineoplastic agent. Toxic to brine shrimp. Plates (MeOH/CH_2Cl_2). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 161-164°. $[\alpha]_D^{27}$ +99.8 (c, 0.04 in MeOH). λ_{max} 228 (ϵ 36350) (MeOH) (Derep). λ_{max} 229 (ϵ 36200) (MeOH) (Berdy).

(21Z)-Isomer: ***Bryostatin 18***
[173107-74-9]
Isol. from *Bugula neritina*. Antineoplastic agent. $[\alpha]_D$ +136 (c, 0.7 in MeOH).

19-Deoxy, 19,20-didehydro: ***Bryostatin 16***
[173075-49-5]
$C_{42}H_{62}O_{14}$ 790.943
Isol. from *Bugula neritina*. Antineoplastic agent. $[\alpha]_D$ +84 (c, 0.4 in MeOH).

19-Deoxy, 19,20-didehydro, 21Z-isomer: ***Bryostatin 17***
[173240-55-6]
$C_{42}H_{62}O_{14}$ 790.943
Isol. from *Bugula neritina*. Antineoplastic agent. $[\alpha]_D$ +231 (c, 0.3 in MeOH).

Pettit, G.R. *et al., J.O.C.*, 1987, **52**, 2848; 1991, **56**, 1337 (*isol, struct, props, abs config*)
Kamano, Y. *et al., J. Nat. Prod.*, 1995, **58**, 1868-1875 (*isol, pmr, cmr, conformn*)
Pettit, G.R. *et al., J. Nat. Prod.*, 1996, **59**, 286 (*Bryostatins 16-18*)
Kamano, Y. *et al., Tetrahedron*, 1996, **52**, 2369 (*pmr, conformn*)

Bryostatin 11 B-579

[102580-63-2]
As Bryostatin 1, B-570 with
R^1 = Ac, R^2 = H
$C_{39}H_{58}O_{15}$ 766.878
Isol. from *Bugula neritina*. Antineoplastic agent. Needles (MeOH/CH_2Cl_2). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 171-173°. $[\alpha]_D^{27}$ +42.5 (c, 0.05 in MeOH). λ_{max} 227 (ϵ 35500) (MeOH) (Derep).

Pettit, G.R. *et al., J.O.C.*, 1987, **52**, 2848; 1991, **56**, 1337 (*isol, struct, props, abs config*)

Bryostatin 12 B-580

[107021-10-3]
As Bryostatin 1, B-570 with
R^1 = –$COCH_2CH_2CH_3$, R^2 = -OOCCH=CHCH=$CHCH_2CH_2CH_3$
$C_{49}H_{72}O_{17}$ 933.098
Isol. from *Bugula neritina*. Antineoplastic agent. RNA biosynthesis inhibitor. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{27}$ +39 (c, 0.108 in MeOH). λ_{max} 232 (ϵ 25700); 263 (ϵ 28700) (MeOH) (Derep). λ_{max} 231 (ϵ 28840); 263 (ϵ 29500) (MeOH) (Berdy).

Pettit, G.R. *et al., J.O.C.*, 1987, **52**, 2854; 1991, **56**, 1337 (*isol, struct, props, abs config*)

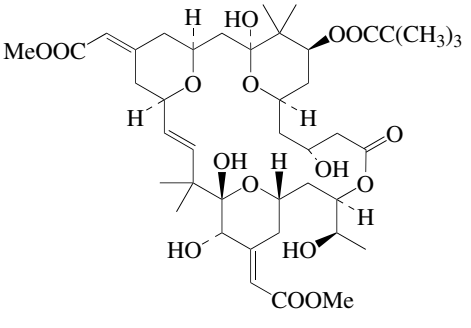
Bryostatin 13 B-581

[107021-11-4]
As Bryostatin 1, B-570 with
R^1 = –$COCH_2CH_2CH_3$, R^2 = H
$C_{41}H_{62}O_{15}$ 794.932
Isol. from *Bugula neritina*. Antineoplastic agent. No phys. props. reported. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 227 (ϵ 35500) (MeOH) (Derep). λ_{max} 229 (ϵ 9120) (MeOH) (Berdy).

Pettit, G.R. *et al., J.O.C.*, 1987, **52**, 2854 (*isol, struct, props*)

Bryostatin 14 B-582

[136448-57-2]

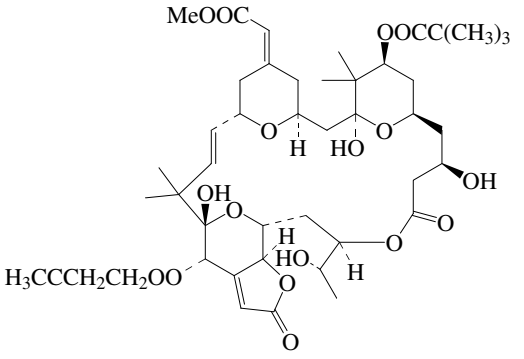


$C_{42}H_{64}O_{16}$ 824.958
Macrolide antibiotic. Isol. from *Bugula neritina*. Cytotoxic agent. Amorph. powder.
Mp 174-176°. $[\alpha]_D^{22}$ +41.3 (c, 0.9 in CH_2Cl_2).

Pettit, G.R. *et al., Tetrahedron*, 1991, **47**, 3601-3610 (*isol, ir, pmr, cmr, ms*)

Bryostatin 19 B-583

[214075-08-8]



$C_{45}H_{66}O_{17}$ 879.006
Polyether antibiotic. Isol. from *Bugula neritina*. Antineoplastic agent.

De(butanoyloxy): ***Bryostatin 20***
$C_{41}H_{60}O_{15}$ 792.916
Isol. from *Bugula neritina*. Oil. $[\alpha]_D^{24}$ +52.1 (c, 0.04 in MeOH). λ_{max} 218 (log ϵ 4.13) (MeOH).

Lin, H. *et al., CA*, 1998, **129**, 272958k (*Bryostatin 19*)
Lopanik, N. *et al., J. Nat. Prod.*, 2004, **67**, 1412-1414 (*Bryostatin 20*)

Buccalin B-584

[116786-35-7]
H-Gly-Met-Asp-Ser-Leu-Ala-Phe-Ser-Gly-Gly-Leu-NH_2
Neuropeptide. Isol. from a neuron of the mollusc *Aplysia californica*. Muscle contraction inhibitor.

[116844-51-0]

Cropper, E.C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1988, **85**, 6177-6181 (*isol, struct*)

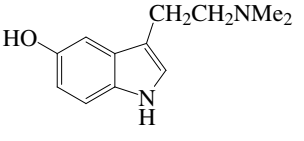
Buccalin B B-585

[147663-31-8]
H-Gly-Leu-Asp-Arg-Tyr-Gly-Phe-Val-Gly-Gly-Leu-NH_2
$C_{53}H_{81}N_{15}O_{14}$ 1152.315
Neuropeptide. Isol. from a neuron of the mollusc *Aplysia californica*. Neuropeptide. Muscle contraction inhibitor.

Vilim, F.S. *et al., Peptides (N.Y.)*, 1994, **15**, 959 (*isol, hplc, ms*)

Bufotenine B-586

*3-(2-Dimethylaminoethyl)-1*H*-indol-5-ol, 9CI. 3-(2-Dimethylaminoethyl)-5-hydroxyindole.* N^b,N^b*-Dimethylserotonin. Cinobufotenine. Mappine. DM SHT*
[487-93-4]



$C_{12}H_{16}N_2O$ 204.271
Alkaloid from poisonous secretion of toads (*Bufo* spp.), from seeds of *Piptadenia peregrina*, many genera in the Leguminosae and Gramineae, and in some mushrooms, e.g. *Amanita citrina*. Also identified spectroscopically in the gorgonian *Paramuricea chamaeleon*. Hallucinogen. Sol. MeOH, acids, EtOH, bases; fairly sol. Et_2O; poorly sol. H_2O.
Mp 146-147°. $Bp_{0.1}$ 320°. λ_{max} 225; 274; 300 (MeOH) (Berdy). λ_{max} 220 (ϵ 10000); 265 (ϵ 3000) (EtOH) (Berdy).
▶ Adverse systemic effects by intravenous route (psychotropic). LD_{50} (mus, ipr) 290 mg/kg. NM2800000

O-*Sulfate:* ***Bufoviridine****. Dihydrobufothionine*
[16369-08-7]
$C_{12}H_{16}N_2O_4S$ 284.335
Isol. from the skins of various amphibia incl. *Bufo viridis.*

O-*β-D-Glucopyranoside:* ***Bufotenine* O-*glucoside***
[64656-15-1]
$C_{18}H_{26}N_2O_6$ 366.413
Alkaloid from the leaves of *Citrus unshiu* (satsuma mandarin). $[\alpha]_D$ -58 (c, 0.5 in H_2O). λ_{max} 224; 274 (No solvent reported).

N^b-*Oxide:* ***Bufotenine* N-*oxide***
[1019-44-9]
$C_{12}H_{16}N_2O_2$ 220.271
Alkaloid from *Desmodium pulchellum* and *Desmodium caudatum* (Leguminosae). Also *Piptadenia macrocarpa* and *Amanita* spp. Constit. of toad venom (*Bufo* spp.). Cryst.
Mp 214-215°.

N^b-*Me, inner salt:* ***Bufotenidine***
[487-91-2]
$C_{13}H_{18}N_2O$ 218.298
Alkaloid from secretions of toad spp.
Mp 209° (as hydriodide).

N^b-*Me, inner salt,* O-*sulfate:* ***Bufotenidine* O-*sulfate***
$C_{13}H_{18}N_2O_4S$ 298.362
Alkaloid from the skin of the toad *Nyctimystes tympanocryptis.* Genus name sometimes given as Nictimystes.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 530D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 663C (*ir*)
Wieland, T. *et al., Annalen*, 1953, **581**, 10-16 (*isol, uv*)
Stromberg, V.L. *et al., J.A.C.S.*, 1954, **76**, 1707 (*isol, uv*)
Harley-Mason, J. *et al., J.C.S.*, 1954, 1165-1171 (*synth*)
Fish, M.S. *et al., J.A.C.S.*, 1955, **77**, 5892-5895 (*oxide*)
Erspamer, V. *et al., Biochem. Pharmacol.*, 1959, **2**, 270 (*Bufoviridine*)
Pachter, I.J. *et al., J.O.C.*, 1959, **24**, 1285-1287 (*isol*)
Ghosal, S. *et al., J.O.C.*, 1966, **31**, 2284-2288 (*isol*)
Paris, R.R. *et al., Ann. Pharm. Fr.*, 1967, **25**, 509 (*oxide*)
Daly, J.W. *et al., J.A.C.S.*, 1967, **89**, 1032-1033 (*pmr*)
Creveling, C.R. *et al., Clin. Chem. (Winston-Salem, N.C.)*, 1968, **14**, 302-309 (*ms*)
Roseghini, M. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1976, **54**, 31-43; 1989, **94**, 455-460 (*Bufoviridine*)
Sanders-Bush, E. *et al., Life Sci.*, 1976, **19**, 1407 (*metab*)
Schultes, R.E. *et al., Planta Med.*, 1976, **29**, 330
Roseghini, M. *et al., Z. Naturforsch., C*, 1976, **31**, 118-120 (*Bufoviridine, Bufotenidine O-sulfate*)
Shaw, G.J. *et al., Biomed. Mass Spectrom.*, 1977, **4**, 348-353 (*ms*)
Cimino, G. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1978, **61**, 361-362 (*occur*)
Barlow, R.B. *et al., Br. J. Pharmacol.*, 1980, **69**, 597-600 (*pharmacol*)
Nishida, R. *et al., Agric. Biol. Chem.*, 1990, **54**, 1853-1855 (*glucoside*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1555
Somei, M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 87-96 (*synth*)
Zhang, P. *et al., Chem. Pharm. Bull.*, 2005, **53**, 1582-1586 (*toad venom constits*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DPG109

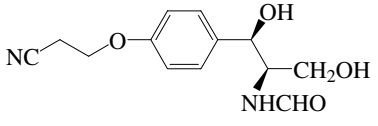
Bursatellanin P B-587

Protein. Isol. from the purple fluid of the sea hare *Bursatella leachii*. Exhibits anti-HIV activity.

Rajaganapathi, J. *et al., Mar. Biotechnol.*, 2002, **4**, 447-453 (*isol*)

Bursatellin B-588

[75347-13-6]



Absolute Configuration

$C_{13}H_{16}N_2O_4$ 264.28
Constit. of *Bursatella leachii pleii, Bursatella leachii leachii* and *Bursatella leachii savignyana*. Oil. $[\alpha]_D$ -8.8 (c, 2.4 in MeOH). λ_{max} 273 (ε 946) (MeOH) (Derep).

Gopichand, Y. *et al., J.O.C.*, 1980, **45**, 5383 (*isol*)
Cimino, G. *et al., J.O.C.*, 1987, **52**, 2301 (*struct*)
Racioppi, R. *et al., Tet. Lett.*, 1990, **31**, 573 (*synth*)
Kawamine, K. *et al., Chem. Pharm. Bull.*, 1991, **39**, 3170 (*synth*)

1,3-Butadiene-1,1,4,4-tetracarboxylic acid B-589

$(HOOC)_2C{=}CHCH{=}C(COOH)_2$

$C_8H_6O_8$ 230.131

Tetra-Et ester:
$C_{16}H_{22}O_8$ 342.345
Cryst. (EtOH). Mp 56°. $Bp_{0.2}$ 170°.

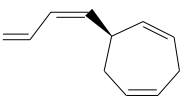
Tetrakis(methylamide): N,N′,N″,N‴-*Tetramethyl-1,3-butadiene-1,1,4,4-tetracarboxamide, 9CI.* ***Chevalieramide***
[124709-40-6]
$C_{12}H_{18}N_4O_4$ 282.299
Alkaloid from the soft coral *Lobophytum chevalieri.*

[64496-11-3]

Baganz, H. *et al., Chem. Ber.*, 1961, **94**, 2132 (*synth, ester*)
Li, R. *et al., CA*, 1990, **112**, 52550e (*Chevalieramide, isol, pmr, cmr, ms*)

6-(1,3-Butadienyl)-1,4-cycloheptadiene B-590

Desmarestene



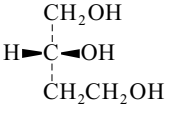
$C_{11}H_{14}$ 146.232

(R)-form [83013-90-5]
Isol. from the brown algae *Desmarestia aculeata* and *Desmarestia viridis.* Algal gamete sex attractant. $[\alpha]_D^{22}$ +168 (c, 1.4 in CH_2Cl_2).

Jaenicke, L. *et al., Angew. Chem., Int. Ed.*, 1982, **21**, 643 (*rev*)
Müller, D.G. *et al., Naturwissenschaften*, 1982, **69**, 290
Pantke-Boecker, S. *et al., Tetrahedron*, 1995, **51**, 7927 (*synth, ir, pmr, cmr, ms, abs config*)

1,2,4-Butanetriol, 9CI B-591

2-Deoxytetritol
[3068-00-6]



(*R*)–*form*

$C_4H_{10}O_3$ 106.121
► EK7176000

(S)-form
D-glycero-*form*
[42890-76-6]
Oil. $Bp_{0.15}$ 130° (bath). $[\alpha]_D^{22}$ -28.2 (c, 2.8 in EtOH).

1-(4-Hydroxybenzoyl):
$C_{11}H_{14}O_5$ 226.229
Prod. by the sponge-derived fungus *Penicillium aurantiogriseum*. Cytotoxic. Amorph. powder. $[\alpha]_D^{22}$ -8.4 (c, 0.01 in MeOH). λ_{max} 224; 254; 262 (MeOH).

[57314-07-5]

Xin, Z.H. *et al., Chin. Chem. Lett.*, 2005, **16**, 1227-1229 (*4-hydroxybenzoate*)

1-Butanol, 9CI B-592

n-*Butyl alcohol, 8CI. FEMA 2178*
[71-36-3]
[35296-72-1]

$H_3CCH_2CH_2CH_2OH$
$C_4H_{10}O$ 74.122

Mainly produced by hydroformylation of 1-Propene with Carbon monoxide and hydrogen in the oxo process, also from Acetaldehyde by aldol condensation. Occurs in essential oils and other plant sources e.g. *Thea sinensis* (tea), *Ribes nigrum* (blackcurrant). Important industrial chemical, 49th in order of volume for USA in 1994 (production 0.72 million tons/year). Industrial solvent, particularly for lacquer coatings. Used in brake fluids and in plasticiser manuf. Anal. derivatisation reagent for carboxylic and amino acids. Liq. Mod. sol. H_2O. d^{15} 0.81.
Fp -90. Bp 117.4°. n_D^{20} 1.3971. Forms constant-boiling mixt. with H_2O, Bp 92°, contg. 37% H_2O.

▶ Flammable, fl. p. 29/35°, autoignition temp. 359°. Eye, skin and respiratory tract irritant. Mild CNS effects by skin absorption and inhalation (headache, dizziness). Can cause dermatitis. LD_{50} (rat, orl) 790 mg/kg. Exp. reprod. effects. OES: short-term 50 ppm. EO1400000

Al salt: See Aluminium butoxide in *The Combined Chemical Dictionary.*

Zr(4+) salt: See Zirconium(*IV*) butoxide in *The Combined Chemical Dictionary.*

Hf(4+) salt: See Hafnium(*IV*) butoxide in *The Combined Chemical Dictionary.*

Nb(5+) salt: See Pentabutoxyniobium in *The Combined Chemical Dictionary.*

α-D-Glucopyranoside: Butyl α-D-glucoside
$C_{10}H_{20}O_6$ 236.264
Isol. from the mollusc *Cryptochiton stelleri.*

Phenylurethane:
Cryst. Mp 61°.

Ac: Butyl acetate. FEMA 2174
[123-86-4]
$C_6H_{12}O_2$ 116.16
Industrial solvent. Component of apple aroma. Used for extraction of Au, Ga, In, Ti (as bromide). Liq. Sol. EtOH, Et_2CO, Me_2CO; insol. H_2O. d_4^{20} 0.88. Fp -77. Bp 125-126°. n_D^{20} 1.3942.

▶ Eye, skin and respiratory tract irritant. High conc. narcotic. Flammable, fl. p. 22°, autoignition temp. 370/425°. OES: long-term 150 ppm; short-term 200 ppm. AF7350000

Methanesulfonyl: [1912-32-9]
$C_5H_{12}O_3S$ 152.214
Liq. Bp_2 81-82°. n_D^{20} 1.4253.

▶ Mutagenic.

4-Methylbenzenesulfonyl: [778-28-9]
$C_{11}H_{16}O_3S$ 228.312
Liq. Bp_2 138-140°.

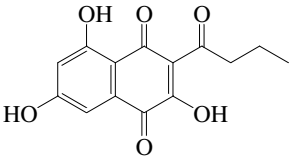
▶ XT6400000

[3999-70-0, 4712-38-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 110A; 601C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 164A; 900A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 156B; 608B (*ir*)
Buchner, E. *et al., Ber.*, 1908, **41**, 1410 (*synth*)
Kagan, M.Ya. *et al., CA*, 1935, **29**, 452 (*synth*)
Vogel, A.I. *et al., J.C.S.*, 1948, 624 (*Ac, synth*)
Chaikin, S.W. *et al., J.A.C.S.*, 1949, **71**, 122 (*synth*)
Bock, R. *et al., Fresenius' Z. Anal. Chem.*, 1953, **138**, 167 (*Ac, use*)
Williams, H.R. *et al., J.A.C.S.*, 1954, **76**, 2984-2987 (*methanesulfonyl*)
Zomzely, C. *et al., Anal. Chem.*, 1962, **34**, 1414 (*use*)
Biddiscombe, D.P. *et al., J.C.S.*, 1963, 1954 (*purifn, props*)
Andersson, J. *et al., Acta Chem. Scand.*, 1966, **20**, 522 (*isol*)
Dorman, D.E. *et al., J.O.C.*, 1975, **40**, 3729 (*cmr, derivs*)
Choudhary, G. *et al., J. Chromatogr.*, 1976, **128**, 261 (*use*)
Crowder, G.A. *et al., J. Mol. Struct.*, 1977, **42**, 27 (*ir, Raman*)
Ejchart, A. *et al., Org. Magn. Reson.*, 1980, **13**, 368 (*cmr*)
Slusarska, E. *et al., Synthesis*, 1981, 155-156 (*methanesulfonyl*)
Colosimo, M. *et al., Org. Mass Spectrom.*, 1982, **17**, 286 (*ms*)
Ullmanns Encykl. Tech. Chem., 5. Aufl., 1985, **A4**, 463 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BPW500; BPU750
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **4**, 691 (*rev, props*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1100
Yamamoto, T. *et al., Org. Prep. Proced. Int.*, 1994, **26**, 555 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 76; 77
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 317-318; 319-320
Kapustina, I.I. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 109-110 (*α-D-glucoside*)
1992, 38; 47 (*tox, rev*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 184; 191
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BPW500; BSP750

2-Butanoyl-3,6,8-trihydroxy-1,4-naphthoquinone B-593

3,6,8-Trihydroxy-2-(1-oxobutyl)-1,4-naphthalenedione, 9CI

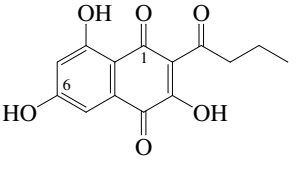


$C_{14}H_{12}O_6$ 276.245
Amorph. orange powder. λ_{max} 234 (ε 12640); 268 (ε 14660); 300 (ε 16180) (AcOH/MeOH).

6-O-Sulfate:
$C_{14}H_{12}O_9S$ 356.309
Constit. of the crinoid *Oxycomanthus japonicus.* Reddish powder. λ_{max} 249 (ε 12740); 295 (ε 11980); 374 (ε 2720) (MeOH aq.).

Takahashi, D. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1609-1612 (*isol, pmr, cmr*)

2-Butanoyl-3,6,8-trihydroxy-1,4-naphthoquinone B-594



$C_{14}H_{12}O_6$ 276.245
Orange amorph. powder. No CAS no. assigned. λ_{max} 234 (ε 12640); 268 (ε 14660); 300 (ε 16180) (1% AcOH/MeOH).

6-O-Sulfate: [557112-76-2]
$C_{14}H_{12}O_9S$ 356.309
Isol. from *Oxycomanthus japonicus.* Reddish amorph. powder. λ_{max} 249 (ε 12740); 295 (ε 11980); 374 (ε 2720) (30% MeOH).

Takahashi, D. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1609-1612 (*6-sulfate, isol, pmr, cmr, uv*)

2-Butenoic acid, 9CI B-595

3-Methylacrylic acid. Ethylideneacetic acid
[3724-65-0]
$H_3CCH{=}CHCOOH$
$C_4H_6O_2$ 86.09
Copolymers with vinyl acetate are used in lacquers and paper sizing.

▶ Skin irritant. LD_{50} (rat, orl) 1000 mg/kg. GQ2800000

(E)-form
Crotonic acid. β-Methacrylic acid. FEMA 3908
[107-93-7]
Isol. from *Streptomyces collinus* (NRC 11). Produced by oxidation of 2-Butenal. Used in manuf. of copolymers such as vinyl acetate-crotonic acid adhesives, fungicides and pharmaceuticals.
Needles (H_2O or petrol). V. sol. H_2O, EtOH; sol. Et_2O, Me_2CO. Mp 71.4°. Bp 185° (189°). n_D^{20} 1.4457. pK_a 4.61 (25°). Q/e values for copolym., Q 0.017, e 0.89.

▶ Fl. p. 89°, autoignition temp. 396°. GQ2900000

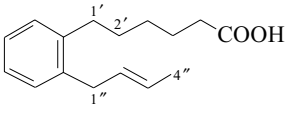
Et ester: Ethyl crotonate. FEMA 3486
[623-70-1]
$C_6H_{10}O_2$ 114.144
Component of strawberry, guava (*Psidium guajava*), pineapple, passionfruit and other fruits. Also present in mussels (*Mytilus edulis*). Fragrance ingredient. Flavouring agent. Liq. Insol. H_2O; sol. EtOH, Et_2O. d_4^{20} 0.92. Bp 137° Bp_{15} 38°. n_D^{20} 1.4243.
▶ Eye, skin and mucous membrane irritant. LD_{50} (rat, orl) 3000 mg/kg. Flammable, fl. p. 28°. GQ3500000

[623-68-7, 3246-27-3, 4786-20-3, 7299-91-4, 10487-71-5, 10544-63-5, 18707-60-3, 20474-93-5, 23350-58-5]

Yasuhara, A. *et al., Chemosphere*, 1987, **16**, 2559-2565 (*mussel, gcms*)
Yasuhara, A. *et al., J. Chromatogr.*, 1987, **409**, 251-258 (*mussel, occur, gc*)

2-(2-Butenyl)benzenehexanoic acid, 9CI B-596

Rubrenoic acid A
[95230-66-3]



$C_{16}H_{22}O_2$ 246.349
Metab. of the marine bacterium *Alteromonas rubra*.

1′,2′-Didehydro: 6-[2-(2-Butenyl)phenyl]-5-hexenoic acid, 9CI. ***Rubrenoic acid B***
[95230-67-4]
$C_{16}H_{20}O_2$ 244.333
From *Alteromonas rubra*.

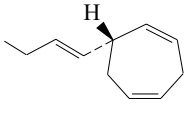
1″,4″-Didehydro: 2-(1,3-Butadienyl)benzenehexanoic acid, 9CI. ***Rubrenoic acid C***
[95230-68-5]
$C_{16}H_{20}O_2$ 244.333
From *Alteromonas rubra*.

$\Delta^{1''}$-Isomer(Z-): 2-(1-Butenyl)benzenehexanoic acid. ***Pseudorubrenoic acid A***
$C_{16}H_{22}O_2$ 246.349
Prod. by the soil bacterium *Pseudomonas fluorescens*.

Holland, G.S. *et al., Chem. Ind. (London)*, 1984, 850-851 (*isol, struct*)
Rickard, R.W. *et al., Tetrahedron*, 2002, **58**, 3793-3800 (*Pseudorubrenoic acid A*)

6-(1-Butenyl)-1,4-cycloheptadiene, 9CI B-597

1-(2,5-Cycloheptadienyl)-1-butene
[38011-59-5]



(R)–(E)–form

$C_{11}H_{16}$ 148.247

(R)-(E)-form
Isol. from *Dictyopteris acrostichoides*.

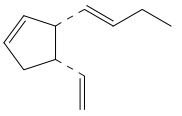
(S)-(Z)-form
Ectocarpene. *Dictyopterene D′*. *Sirenin*†
[33156-92-2]
Constit. of the essential oil of the seaweed *Dictyopteris* spp., e.g. *Dictyopteris acrostichioides*; sex attractant of androgametes of the brown alga *Ectocarpus siliculosus*.
$[\alpha]_D^{25}$ +75 (c, 0.15 in CH_2Cl_2). CAS describes Ectocarpene as the (*R*)-enantiomer, but this appears to be erroneous.

[33156-93-3]

Jaenicke, L. *et al., Annalen*, 1973, 1252 (*synth*)
Pickenhagen, W. *et al., Helv. Chim. Acta*, 1973, **56**, 1868 (*biosynth*)
Jaenicke, L. *et al., J.A.C.S.*, 1974, **96**, 3324 (*isol*)
Moore, R.E. *et al., J.O.C.*, 1974, **39**, 2201 (*isol, abs config*)
Mueller, D.G. *et al., Pure Appl. Chem.*, 1979, **51**, 1885 (*rev*)
Jaenicke, L. *et al., Angew. Chem., Int. Ed.*, 1982, **21**, 643 (*rev*)
Abraham, W.D. *et al., J.A.C.S.*, 1991, **113**, 2313 (*synth*)
Stratmann, K. *et al., Angew. Chem., Int. Ed.*, 1992, **31**, 1246 (*isol*)
Wirth, D. *et al., Helv. Chim. Acta*, 1992, **75**, 734 (*occur*)

3-(1-Butenyl)-4-vinylcyclopentene B-598

3-(1-Butenyl)-4-ethenylcyclopentene, 9CI. ***Multifidene***



(3S,4S)-(E)-form

$C_{11}H_{16}$ 148.247

(3S,4S)-(E)-form [78038-46-7]
Isol. from *Dictyopteris acrostichoides, Cutleria multifida* and *Chorda tomentosa*. Algal gamete sex attractant.

1′,2′-Dihydro: 3-Butyl-4-vinylcyclopentene
[143615-93-4]
$C_{11}H_{18}$ 150.263
Constit. of *Dictyopteris acrostichoides* and *Dictyopteris prolifera*.

(3S,4S)-(Z)-form [52886-04-1]
Isol. from the brown alga *Cutleria multifida*. Algal gamete sex attractant. $[\alpha]_D^{23.5}$ +28 (c, 0.0036 in CCl_4).

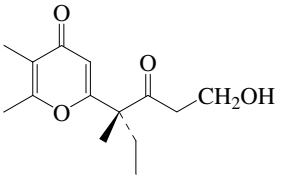
3′,4′-Didehydro: 3-(1,3-Butadienyl)-4-vinylcyclopentene. 3-(1,3-Butadienyl)-4-ethenylcyclopentene. ***Viridiene***
[83013-89-2]
$C_{11}H_{14}$ 146.232
Isol. from the brown algae *Desmarestia aculeata*, *Desmarestia viridis* and *Syringoderma* sp. Algal gamete sex attractant. $[\alpha]_D^{20}$ +255. Has 3*R*-config.

[78038-45-6, 92998-67-9]

Jaenicke, L. *et al., J.A.C.S.*, 1974, **96**, 3324-3325 (*isol, glc, ms, nmr, struct*)
Jaenicke, L. *et al., Angew. Chem., Int. Ed.*, 1982, **21**, 643-653 (*rev*)
Boland, W. *et al., Helv. Chim. Acta*, 1982, **65**, 2355-2362; 1983, **66**, 1905-1913; 1985, **68**, 2062-2073 (*synth, abs config*)
Müller, D.G. *et al., Naturwissenschaften*, 1982, **69**, 290-291 (*Viridiene, isol*)
Paquette, L.A. *et al., J.O.C.*, 1984, **49**, 4516-4518 (*synth, abs config*)
Burks, J.E. *et al., J.O.C.*, 1984, **49**, 4663-4670 (*synth, bibl*)
Wirth, D. *et al., Helv. Chim. Acta*, 1992, **75**, 734-744 (*synth, occur*)
Hemamalini, S. *et al., Helv. Chim. Acta*, 1995, **78**, 447-451 (*synth, ir, pmr, cmr*)
Kajiwara, T. *et al., Phytochemistry*, 1997, **45**, 529-532 (*abs config, Butylvinylcyclopentene*)
Lebreton, J. *et al., Tetrahedron*, 1997, **53**, 145-160 (*synth*)

Butoxylspiciferin B-599

6-(1-Ethyl-4-hydroxy-1-methyl-2-oxobutyl)-2,3-dimethyl-4H-pyran-4-one

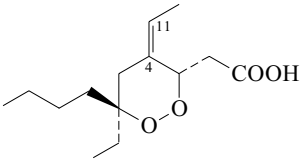


$C_{14}H_{20}O_4$ 252.31
Prod. by *Drechslera hawaiiensis* isol. from the sponge *Callyspongia aerizusa*. Powder. $[\alpha]_D$ -34.8 (c, 0.16 in EtOH). λ_{max} 202 (ϵ 10000); 218 (sh) (ϵ 5200); 252 (ϵ 3400) (EtOH).

Edrada, R.A. *et al., Z. Naturforsch., C*, 2000, **55**, 218-221

1-Butoxy-2-methyl-1-(2-methylpropoxy)-2-propanol B-600

5-(1-Hydroxy-1-methylethyl)-2-methyl-4,6-dioxadecane. 1-[2-Hydroxy-2-methyl-1-(2-methylpropoxy)propoxy]butane



Relative configuration

$C_{12}H_{26}O_3$ 218.336

Prod. by the marine *Vibrio angustum* S14. Oil. $[\alpha]_D^{25}$ +0.1 (c, 0.35 in $CHCl_3$).

De Nys, R. *et al., J. Nat. Prod.*, 2001, **64**, 531-532

Buttonin B-601

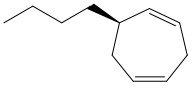
Button-shaped protein. Isol. from sea urchin egg microtubule proteins. Enhances polymerisation of porcine brain tubulin.

Hirokawa, N. *et al., J. Cell Biol.*, 1987, **104**, 1553-1561 (*isol, struct*)

6-Butyl-1,4-cycloheptadiene, 9CI B-602

Dictyopterene C'. *Dictyotene. Dihydroectocarpene*

[22735-58-6]



(*R*)-*form*

$C_{11}H_{18}$ 150.263

(*R*)-*form* [33156-91-1]

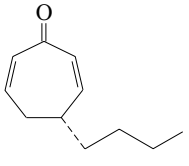
Isol. from brown algae *Dictyopteris* spp. and *Dictyota dichotoma*. Sex hormone attracting spermatozoa of the algae.
Oil. $[\alpha]_D^{25}$ -13 (c, 7.32 in $CHCl_3$).

(±)-*form* [53956-86-8]

Oil.

Pickenhagen, W. *et al., Helv. Chim. Acta*, 1973, **56**, 1868 (*synth*)
Billups, W.E. *et al., Chem. Comm.*, 1974, 252 (*synth*)
Moore, R.E. *et al., J.O.C.*, 1974, **39**, 2201 (*isol*)
Jaenicke, L. *et al., Angew. Chem., Int. Ed.*, 1982, **21**, 643 (*rev*)
Colobert, F. *et al., Tet. Lett.*, 1985, **26**, 2779 (*synth*)
Grandjean, D. *et al., Tetrahedron*, 1991, **47**, 1215 (*synth*)
Wirth, D. *et al., Helv. Chim. Acta*, 1992, **75**, 734 (*isol*)
Stratmann, K. *et al., Tetrahedron*, 1993, **49**, 3755-3766 (*isol, biosynth*)

4-Butyl-2,6-cycloheptadienone, 9CI B-603



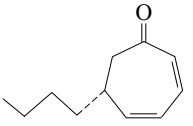
$C_{11}H_{16}O$ 164.247

(*R*)-*form* [52084-28-3]

Present in odoriferous oil from *Dictyopteris* spp.
$[\alpha]_D$ +96 (MeOH/2,3,3-trimethylpentane).

Moore, R.E. *et al., Chem. Comm.*, 1973, 937 (*isol*)

6-Butyl-2,4-cycloheptadienone, 9CI B-604



Probable absolute configuration

$C_{11}H_{16}O$ 164.247

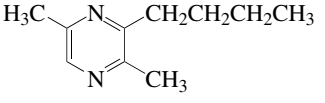
(*R*)-*form* [52084-29-4]

Present in odoriferous oil from *Dictyopteris* spp.
$[\alpha]_D$ +1120 (pentane).

Moore, R.E. *et al., Chem. Comm.*, 1973, 937 (*isol, uv, cmr*)

3-Butyl-2,5-dimethylpyrazine B-605

[40790-29-2]



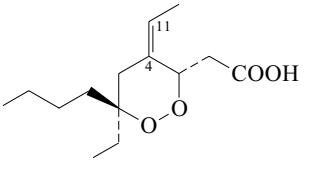
$C_{10}H_{16}N_2$ 164.25

Isol. from the ant *Iridomyrmex purpureus* and the fly *Anastrepha fraterculus*. Prod. by various marine bacteria. Bp_{12} 101°.

Zavylov, S.I. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1973, 707 (*synth*)
Bus, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1973, **92**, 123 (*ir*)
Flament, I. *et al., Bull. Soc. Chim. Belg.*, 1979, **88**, 941 (*synth, ms*)
Cavill, G.W.K. *et al., Insect Biochem.*, 1984, **14**, 505 (*isol*)
Dickschat, J.S. *et al., Eur. J. Org. Chem.*, 2005, 4141-4153 (*marine isol*)
Dickschat, J.S. *et al., J. Chem. Ecol.*, 2005, **31**, 925-947 (*marine isol*)

6-Butyl-6-ethyl-4-ethylidene-1,2-dioxan-3-acetic acid B-606

[153566-06-4]



Relative configuration

$C_{14}H_{24}O_4$ 256.341

Constit. of the sponge *Callyspongia* sp. Cytotoxic agent. Faint yellow gum. $[\alpha]_D$ +50 (c, 0.7 in $CHCl_3$). Related to Plakortic acid, P-472.

4α,11-Dihydro: 6-Butyl-4,6-diethyl-1,2-dioxan-3-acetic acid

[153566-07-5]

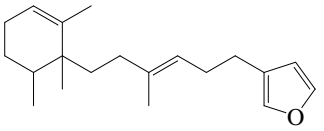
$C_{14}H_{26}O_4$ 258.357

Constit. of *Callyspongia* sp. Cytotoxic agent. Gum. $[\alpha]_D$ +48 (c, 0.5 in $CHCl_3$). C-6 config. not detn.

Toth, S.I. *et al., J. Nat. Prod.*, 1994, **57**, 123

Cacospongin A C-1

[325691-42-7]

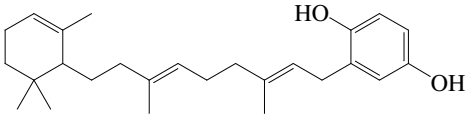


$C_{20}H_{30}O$ 286.456
Constit. of a *Cacospongia* sp. Oil. $[\alpha]_D$ -14 (c, 0.16 in $CHCl_3$). λ_{max} 209 (log ϵ 3.9) (MeOH).

Tasdemir, D. *et al., Tetrahedron*, 2000, **56**, 9025-9030 (*isol, pmr, cmr*)
Tasdemir, D. *et al., Tetrahedron*, 2001, **57**, 5681 (*struct, pmr, cmr*)

Cacospongin B C-2

[325691-43-8]



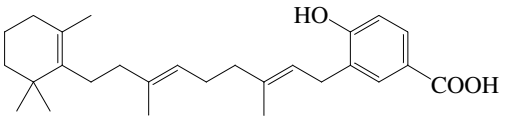
$C_{26}H_{38}O_2$ 382.585
Constit. of a *Cacospongia* sp. Oil. $[\alpha]_D$ -26 (c, 0.63 in $CHCl_3$). λ_{max} 217 (log ϵ 3.2); 290 (log ϵ 3.9) (MeOH).

p-*Quinone:* ***Cacospongin C***
[325691-44-9]
$C_{26}H_{36}O_2$ 380.569
Constit. of a *Cacospongia* sp. Yellow oil. $[\alpha]_D$ -85 (c, 0.24 in $CHCl_3$).

Tasdemir, D. *et al., Tetrahedron*, 2000, **56**, 9025-9030 (*isol, pmr, cmr*)

Cacospongin D C-3

[325691-45-0]

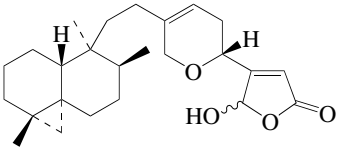


$C_{27}H_{38}O_3$ 410.595
Constit. of a *Cacospongia* sp. and *Strongylophora durissima*. Oil. λ_{max} 254 (log ϵ 3.5); 287 (log ϵ 2.98) (MeOH).

Tasdemir, D. *et al., Tetrahedron*, 2000, **56**, 9025-9030 (*isol, pmr, cmr*)
Shen, Y.-C. *et al., Chin. Pharm. J. (Taipei)*, 2003, **55**, 135-140 (*isol, pmr, cmr, ms*)

Cacospongionolide C-4

[116079-49-3]

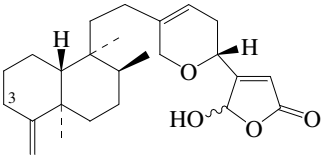


$C_{25}H_{36}O_4$ 400.557
Constit. of *Fasciospongia cavernosa*. Ichthyotoxic and anti-inflammatory agent. Pla_2 enzyme inhibitor. Toxic to brine shrimp. Cryst. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. Mp 163-165°. $[\alpha]_D$ +27 (c, 1.4 in $CHCl_3$). Source originally identified erroneously as *Cacospongia mollior*. λ_{max} 222 (ϵ 4000) (MeOH) (Derep).

De Rosa, S. *et al., J.O.C.*, 1988, **53**, 5020 (*isol, pmr, cmr*)
Puliti, R. *et al., Acta Cryst. C*, 1990, **46**, 1533 (*cryst struct*)
De Rosa, S. *et al., J. Nat. Prod.*, 1998, **61**, 931-935 (*abs config*)

Cacospongionolide B C-5

[172854-76-1]



$C_{25}H_{36}O_4$ 400.557
Constit. of *Fasciospongia cavernosa*. Pla_2 inhibitor. Antiinflammatory agent. Toxic to brine shrimp. Cryst. (MeOH).
Mp 116-118°. $[\alpha]_D$ +28.2 (c, 2.8 in $CHCl_3$). λ_{max} 223 (ϵ 4500) (MeOH) (Berdy).

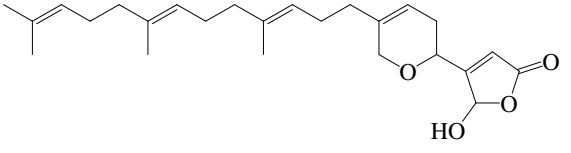
Deoxy: ***25-Deoxycacospongionolide B***
$C_{25}H_{36}O_3$ 384.558
Constit. of *Fasciospongia cavernosa*. Toxic to brine shrimp. Cryst. (MeOH).
Mp 159-161°. $[\alpha]_D$ +10.5 (c, 1.4 in $CHCl_3$).

Δ^3-Isomer: ***Cacospongionolide E***
[211304-16-4]
$C_{25}H_{36}O_4$ 400.557
Constit. of *Fasciospongia cavernosa*. Inhibitor of human secretory phospholipase A_2. $[\alpha]_D$ -85.4 (c, 0.2 in $CHCl_3$). λ_{max} 223 (log ϵ 3.64) (MeOH).

De Rosa, S. *et al., J.A.C.S.*, 1995, **58**, 1776 (*isol, pmr, cmr*)
De Rosa, S. *et al., Tetrahedron*, 1995, **51**, 10731-10736 (*25-Deoxycacospongionolide B*)
De Rosa, S. *et al., J. Nat. Prod.*, 1998, **61**, 931-935 (*Cacospongionolide E, abs config*)
Soriente, A. *et al., Eur. J. Org. Chem.*, 2000, 947-953 (*abs config*)
Cheung, A.K. *et al., J.A.C.S.*, 2002, **124**, 11584-11585 (*synth*)
Cheung, A.K. *et al., J.O.C.*, 2004, **69**, 5712-5719 (*synth*)

Cacospongionolide D C-6

[198208-70-7]

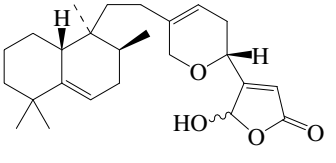


$C_{25}H_{36}O_4$ 400.557
Constit. of *Fasciospongia cavernosa*. Toxic to brine shrimp. Ichthyotoxin. Waxy solid. $[\alpha]_D$ +17.7 (c, 0.2 in $CHCl_3$). λ_{max} 223 (ϵ 4800) (MeOH).

De Rosa, S. *et al., Nat. Prod. Lett.*, 1997, **10**, 267-274 (*isol, pmr, cmr*)

Cacospongionolide F C-7

[247151-66-2]

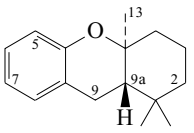


$C_{25}H_{36}O_4$ 400.557
Constit. of *Fasciospongia cavernosa*. Amorph. solid. $[\alpha]_D$ -123 (c, 0.21 in $CHCl_3$). λ_{max} 225 (ϵ 4600) (MeOH).

De Rosa, S. *et al., J. Nat. Prod.*, 1999, **62**, 1316-1318 (*isol, pmr, cmr*)
Demeke, D. *et al., Org. Lett.*, 2003, **5**, 991-994 (*synth*)

Cacoxanthene C-8

2,3,4,4a,9,9a-Hexahydro-1,1,4a-trimethyl-1H-xanthene, 9CI



$C_{16}H_{22}O$ 230.349

Parent compd. unknown. CAS numbering (as used by Garson *et al*) shown.

6-Bromo, 7-hydroxy: ***Debromoisocymobarbatol***
$C_{16}H_{21}BrO_2$ 325.245
Metab. of *Cymopolia barbata*. Feeding deterrent. Viscous oil. λ_{max} 258 (ϵ 4760); 325 (ϵ 6650) (MeOH) (Berdy).

2α,7,13-Tribromo: ***Tribromocacoxanthene***
[122535-68-6]
$C_{16}H_{19}Br_3O$ 467.037
Isol. from a *Cacospongia* sp. Also found in fish and mussels prob. as a pollutant. Cryst. (CH_2Cl_2/Et_2O).
Mp 172-173.5°. $[\alpha]_D$ +8.95 (c, 0.13 in $CHCl_3$).

2α,6-Dibromo, 7-hydroxy: ***Isocymobarbatol***
$C_{16}H_{20}Br_2O_2$ 404.141
Metab. of *Cymopolia barbata*. Antimutagenic agent. Cryst.
Mp 147°. $[\alpha]_D^{23}$ -51.4. Called 4-Isocymobarbatol in the ref. (different numbering scheme). λ_{max} 225; 305 (ϵ 5750) (MeOH) (Berdy). λ_{max} 326 (ϵ 6000) (MeOH/NaOH) (Berdy).

2α,5,7,13-Tetrabromo: Tetrabromocacoxanthene
[122535-69-7]
$C_{16}H_{18}Br_4O$ 545.934
Isol. from a *Cacospongia* sp. Also found in fish and mussels prob. as a pollutant. Cubes (CH_2Cl_2/Et_2O).
Mp 167-168°. $[\alpha]_D$ -169.8 (c, 0.33 in $CHCl_3$).

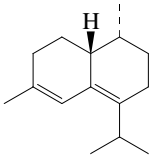
2α,7,13-Tribromo, 9α-hydroxy: ***Tribromo-9α-hydroxycacoxanthene***
[132244-37-2]
$C_{16}H_{19}Br_3O_2$ 483.037
Constit. of a *Cacospongia* sp.
$[\alpha]_D$ -0.83 (c, 0.12 in $CHCl_3$).

2α,7,13-Tribromo, 9β-hydroxy: ***Tribromo-9β-hydroxycacoxanthene***
[132244-36-1]
$C_{16}H_{19}Br_3O_2$ 483.037
Constit. of a *Cacospongia* sp. Needles (CH_2Cl_2/hexane).
Mp 187-189°. $[\alpha]_D$ -11.8 (c, 0.321 in Me_2CO).

2α,6-Dibromo, 7-hydroxy, 9a-epimer: ***Cymobarbatol***
[124962-11-4]
$C_{16}H_{20}Br_2O_2$ 404.141
Metab. of *Cymopolia barbata*. Antimutagenic agent. Cryst.
Mp 166°. $[\alpha]_D^{23}$ -15.4. λ_{max} 225; 306 (ϵ 5260) (MeOH) (Berdy). λ_{max} 327 (ϵ 7000) (MeOH/NaOH) (Berdy).

Garson, M.J. *et al., Aust. J. Chem.*, 1989, **42**, 611; 1990, **43**, 2009 (*Bromohydroxycacoxanthene, Bromocacoxanthenes*)
Wall, M.E. *et al., J. Nat. Prod.*, 1989, **52**, 1092 (*Cymobarbatol, Isocymobarbatol*)
Park, M. *et al., Phytochemistry*, 1992, **31**, 4115 (*Debromoisocymobarbatol*)
Tanaka, A. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 516 (*Cymobarbatol, synth*)
Hiebl, J. *et al., J. Agric. Food Chem.*, 2006, **54**, 2652-2657 (*occur, gc/ms*)

4,6-Cadinadiene C-9



(1β,10α)-*form*

$C_{15}H_{24}$ 204.355

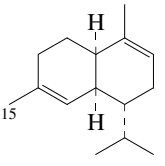
(1β,10α)-*form*
Zonarene
Constit. of *Dictyopteris zonarioides*.
Oil. $[\alpha]_D$ -217.8 (c, 0.46 in cyclohexane).

(1β,10β)-*form*
10-Epizonarene
Constit. of *Cupressus bakeri*.
$[\alpha]_D^{22}$ -229 (c, 2.1 in $CHCl_3$).

Fenical, W. *et al., Phytochemistry*, 1972, **11**, 1161-1163 (*Zonarene*)
Iguchi, M. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 2920 (*synth, abs config*)
Andersen, N.H. *et al., Phytochemistry*, 1973, **12**, 827 (*stereoisomers*)
Williams, J.R. *et al., J.O.C.*, 1983, **48**, 3162 (*synth*)
Kim, Y.-K. *et al., Phytochemistry*, 1994, **36**, 961-965 (*10-Epizonarene*)
Melching, S. *et al., Phytochemistry*, 1997, **44**, 1291-1296 (*Zonarene, isol, pmr, cmr, ms, gc*)
Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*10-Epizonarene, pmr, ms*)

4,9-Cadinadiene C-10

[31983-22-9]



(1α,6α,7α)-*form*

$C_{15}H_{24}$ 204.355
Shows antibacterial activity.

(1α,6α,7α)-*form*
4,9-Muuroladiene. ***(+)-α-Muurolene***
[17627-24-6]
Isol. from various plant oils incl. *Brachylaena hutchinsii*, *Carphephorus odoratissimus*, *Pinus mugo* (dwarf mountain pine) and from the marine sponge *Acanthella cavernosa*. Also from the soft coral *Heteroxenia fuscescens* and gorgonians.
$[\alpha]_D$ +67 ($CHCl_3$) (+58).

9α,10α-Epoxide: ***9,10-Epoxy-4-cadinene****. 9,10-Epoxy-4-muurolene*
$C_{15}H_{24}O$ 220.354
Constit. of *Xenia* spp. Cryst. (Et_2O/petrol).
Mp 47-50°. $[\alpha]_D$ +146 (c, 0.1 in $CHCl_3$).

(1α,6α,7β)-*form*
4,9-Amorphadiene. ***α-Amorphene***
[23515-88-0]
Constit. of *Amorpha fruticosa*.

(1α,6β,7α)-*form*
4,9-Bulgaradiene. ***β$_1$-Bulgarene***
[68000-45-3]
[30021-74-0]
Constit. of berries of *Juniperus oxycedrus*.
Oil. $[\alpha]_D$ -98.5 (c, 0.76 in $CHCl_3$).

(1α,6β,7β)-*form*
α-Cadinene
[24406-05-1]
[29350-73-0]
Constit. of *Humulus lupulus* (hops).
Oil. $[\alpha]_D^{24}$ -62.4 (c, 0.808 in $CHCl_3$).

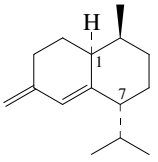
(1β,6β,7β)-*form*
(-)-α-Muurolene
[10208-80-7]
Widespread, e.g. in conifer oils such as turpentine, and other plant oils. Isol. from the gorgonian *Heteroxenia fuscescens*. Bp_{13} 118°.
$[\alpha]_D^{20}$ -52.5. n_D^{22} 1.5051.

[51260-25-4]

Zabza, A. *et al., Coll. Czech. Chem. Comm.*, 1966, **31**, 3373 (*α-Muurolene*)
Naya, Y. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 1468 (*α-Cadinene*)
Gregson, R.P. *et al., Aust. J. Chem.*, 1976, **29**, 2037-2048 (*α-Amorphene, synth*)
De Pascual Teresa, J. *et al., An. Quim.*, 1977, **73**, 1527 (*γ-Bulgarene*)

Kashman, Y. *et al., Tetrahedron*, 1978, **34**, 1227-1229 (*(+)-form, isol, marine animals*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 145-146 (*α-Cadinene, synth*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1986, **39**, 1717-1722 (*9,10-Epoxy-4-muurolene*)
Hirota, H. *et al., Tetrahedron*, 1996, **52**, 2359-2368 (*α-Muurolene*)
Dos Santos, M.H. *et al., Rev. Bras. Cienc. Farm.*, 1999, **35**, 297-300 (*activity*)
Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*α-Cadinene, α-Amorphene, α-Muurolene, pmr, cmr*)

4(15),5-Cadinadiene C-11



(1α,7α,10β)-*form*

$C_{15}H_{24}$ 204.355

(1α,7α,10β)-*form*
4(15),5-Bulgaradiene. ***Nephthene***
Constit. of coral *Nephthea* sp.
Oil. $[\alpha]_D^{20}$ -9 (c, 5.3 in $CHCl_3$).

(1α,7β,10α)-*form*
1-Epibicyclosesquiphellandrene
[54274-73-6]
Constit. of *Ocimum basilicum* (sweet basil).
Oil.

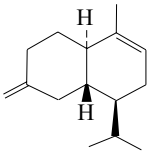
(1β,7β,10α)-*form*
4(15),5-Muuroladiene. ***Bicyclosesquiphellandrene***
[54324-03-7]
Isol. from *Piper cubeba* (cubeb pepper) and a marine *Streptomyces* sp. GWS-BW-H5.
Oil.

(1β,7β,10β)-*form* [157477-72-0]
Constit. of *Cupressus bakeri*.
Oil. $[\alpha]_D^{22}$ +105 (c, 1.7 in $CHCl_3$).

Terhune, S.J. *et al., Phytochemistry*, 1974, **13**, 1183-1185 (*Bicyclosesquiphellandrene, 1-Epibicyclosesquiphellandrene*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1976, **53**, 593 (*synth*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1987, **35**, 124-135 (*Nephthene*)
Kim, Y.K. *et al., Phytochemistry*, 1994, **36**, 961-965 (*4(15), 5-Muuroladiene*)
Melching, S. *et al., Phytochemistry*, 1997, **44**, 1291-1296 (*Bicyclosesquiphellandrene, pmr, ms, gc*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 837-865 (*marine Streptomyces isol*)

4(15),9-Cadinadiene C-12

[29350-73-0]

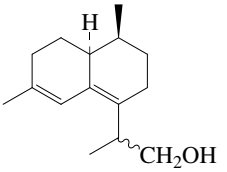


$C_{15}H_{24}$ 204.355

(1α,6β,7β)-*form*
γ$_1$-Cadinene
[66141-11-5]
Constit. of citronella oil (*Cymbopogon nardus*), *Hardwickia pinnata*, *Dictyopteris divaricata* and numerous other plants.
Bp_9 120-121°. $[\alpha]_D$ -19. $n_D^{26.5}$ 1.5155.

Dev, S. *et al., J. Indian Chem. Soc.*, 1949, **26**, 263 (*isol*)
Ghatgey, B.B. *et al., Perfum. Essent. Oil Res.*, 1956, **47**, 157-159 (*isol*)
Irie, T. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 1053-1055 (*isol*)
Andersen, N.H. *et al., Phytochemistry*, 1977, **16**, 1731-1751 (*struct*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 552-554 (*synth*)
Kim, T.C. *et al., Phytochemistry*, 1999, **51**, 793-801 (*occur*)

4,6-Cadinadien-12-ol C-13

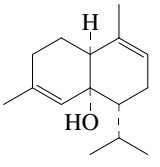


$C_{15}H_{24}O$ 220.354

(1α,10β,11ξ)-*form*
12-Hydroxyzonarene
Constit. of *Lemnalia cervicornis.*
$[\alpha]_D$ +227.6 (c, 0.14 in $CHCl_3$).
Ac: ***12-Acetoxyzonarene***
$C_{17}H_{26}O_2$ 262.391
From *Lemnalia cervicornis.* Oil. $[\alpha]_D$ +241.8 (c, 0.75 in $CHCl_3$).

Bowden, B.F. *et al., Aust. J. Chem.*, 1986, **39**, 103-121

4,9-Cadinadien-6-ol C-14

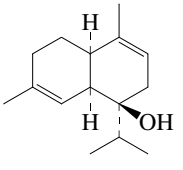


$C_{15}H_{24}O$ 220.354

(1α,6α,7α)-*form*
4,9-Muuroladien-6-ol
[264622-24-4]
Constit. of a soft coral *Heteroxenia* sp.
Yellow oil. $[\alpha]_D$ +23 (c, 1.41 in $CHCl_3$).

Edrada, R.A. *et al., Z. Naturforsch., C*, 2000, **55**, 82-86 (*isol, pmr, cmr*)

4,9-Cadinadien-7-ol C-15

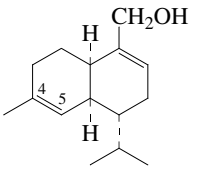


$C_{15}H_{24}O$ 220.354

(1α,6α,7β)-*form*
4,9-Muuroladien-7-ol*. 7-Hydroxy-α-muurolene*
[68354-34-7]
Constit. of *Heteroxenia fuscescens.*
Cryst. (hexane).
Mp 65-70°. $Bp_{0.03}$ 70°. $[\alpha]_D$ -20 ($CHCl_3$).
Ac: [68354-31-4]
[74036-38-7]
$C_{17}H_{26}O_2$ 262.391
Constit. of *Heteroxenia fuscescens.* Oil. $Bp_{0.1}$ 110-120°.

Kashman, Y. *et al., Tetrahedron*, 1978, **34**, 1227-1229 (*isol, pmr, cmr*)

4,9-Cadinadien-14-ol C-16



(1α,6α,7α)-*form*

$C_{15}H_{24}O$ 220.354

(1α,6α,7α)-*form*
4,9-Muuroladien-14-ol
Constit. of *Xenia* spp.
Oil. $[\alpha]_D$ +67 (c, 0.25 in $CHCl_3$).

4α,5α-Epoxide, 15-Ac: ***15-Acetoxy-4,5-epoxy-9-muurolene***
$C_{17}H_{26}O_3$ 278.391
From *Xenia* spp. Oil. $[\alpha]_D$ -19 (c, 0.3 in $CHCl_3$).

14-Aldehyde: 4,9-Cadinadien-14-al. 4,9-Muuroladien-14-al. ***Sclerosporal***
[69394-04-3]
$C_{15}H_{22}O$ 218.338
Constit. of *Sclerotinia fructicola*. Sporogenic agent. Oil. $[\alpha]_D^{20}$ -33.3 (c, 0.62 in $CHCl_3$).

14-Carboxylic acid: 4,9-Cadinadien-14-oic acid. 4,9-Muuroladien-14-oic acid. ***Sclerosporin***
[66419-03-2]
$C_{15}H_{22}O_2$ 234.338
Constit. of *Sclerotinia fructicola*. Sporogenic antifungal agent.
Cryst. (petrol).
Mp 159-160°. $[\alpha]_D^{20}$ +11.1 (c, 0.035 in MeOH).

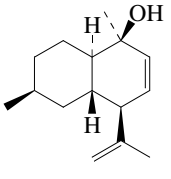
(1β,6β,7α)-*form*
14-Aldehyde: 4,9-Amorphadien-14-al
[394251-65-1]
$C_{15}H_{22}O$ 218.338
Constit. of *Lepidozia fauriana*. Oil.

(1β,6β,7β)-*form*
14-Aldehyde: [97286-74-3]
Oil. $Bp_{1.1}$ 110°. $[\alpha]_D^{19}$ +35.3 (c, 0.69 in $CHCl_3$).

14-Carboxylic acid: ***(-)-Sclerosporin***
[97286-73-2]
$C_{15}H_{22}O_2$ 234.338
From *Diplocarpon mali* and *Sclerotinia fructicola*. Shows antifungal props. Sporogenic agent. Cryst. (petrol). Sol. MeOH, $CHCl_3$; fairly sol. hexane; poorly sol. H_2O.
Mp 163°. $[\alpha]_D^{26}$ -17 (c, 3.7 in $CHCl_3$). λ_{max} 233 (ϵ 7400) (MeOH) (Berdy).

Katayama, M. *et al., Tet. Lett.*, 1979, **20**, 1773-1776; 1983, **24**, 1703-1706; 1984, **25**, 4685-4688 (*Sclerosporin, Sclerosporal, isol, synth, struct, abs config*)
Sawai, K. *et al., Agric. Biol. Chem.*, 1985, **49**, 2501-2503 (*Sclerosporin*)
Kitahara, T. *et al., Tetrahedron*, 1985, **41**, 5475-5485 (*Sclerosporin, Sclerosporal, synth*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1986, **39**, 1717-1722 (*Xenia constits*)
Paul, C. *et al., Phytochemistry*, 2001, **58**, 789-798 (*4,9-Amorphadien-14-al*)

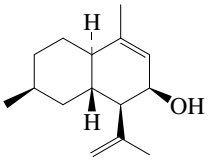
8,11-Cadinadien-10-ol C-17



$C_{15}H_{24}O$ 220.354

(1α,4β,6β,7β,10β)-*form*
Xenitorin C
[479199-46-7]
Constit. of *Xenia puerto-galerae*.
Oil. $[\alpha]_D^{25}$ -5.1 (c, 0.12 in $CHCl_3$). λ_{max} 206 (log ϵ 3.3) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1853-1856 (*isol, pmr, cmr*)
Chang, W.-S. *et al., Org. Biomol. Chem.*, 2006, **4**, 3751-3753 (*synth*)

9,11-Cadinadien-8-ol C-18



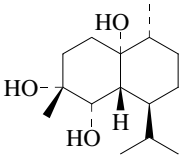
$C_{15}H_{24}O$ 220.354

(1α,4β,6β,7β,8β)-*form*
Xenitorin A
[479199-44-5]
Constit. of *Xenia puerto-galerae*.
Oil. $[\alpha]_D^{25}$ -39 (c, 0.21 in $CHCl_3$). λ_{max} 206 (log ϵ 3.6) (MeOH).

Ketone: 9,11-Cadinadien-8-one. ***Xenitorin B***
[479199-45-6]
$C_{15}H_{22}O$ 218.338
Constit. of *Xenia puerto-galerae*. Amorph. solid. $[\alpha]_D^{25}$ -5.7 (c, 0.2 in $CHCl_3$). λ_{max} 239 (log ϵ 3.9) (MeOH).

9β,10β-Epoxide: 9,10-Epoxy-11-cadinen-8-ol. ***Xenitorin D***
[479199-47-8]
$C_{15}H_{24}O_2$ 236.353
Constit. of *Xenia puerto-galerae*. Oil. $[\alpha]_D^{25}$ -39 (c, 0.16 in $CHCl_3$). λ_{max} 209 (log ϵ 3.7) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1853-1856 (*isol, pmr, cmr*)
Chang, W.-S. *et al., Org. Biomol. Chem.*, 2006, **4**, 3751-3753 (*synth*)

1,4,5-Cadinanetriol C-19



(1α,4α,5α,10α)-*form*

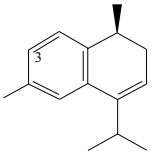
$C_{15}H_{28}O_3$ 256.384

(1α,4α,5α,10α)-*form* [785793-97-7]
Constit. of *Dictyopteris divaricata*.
Cryst. (Me_2CO).
Mp 146-147°. $[\alpha]_D^{20}$ -4 (c, 0.77 in $CHCl_3$).

(1α,4β,5α,6β,7β,10α)-*form*
4,5-Dihydroxycubenol
[162602-03-1]
Constit. of *Dictyopteris delicatula*.
Cryst.
Mp 126.5° (subl.). $[\alpha]_D^{25}$ +7.4 (c, 0.78 in $CHCl_3$).
König, G.M. *et al., Magn. Reson. Chem.*, 1995, **33**, 178-183 (*isol, pmr, cmr*)
Song, F. *et al., J. Nat. Prod.*, 2004, **67**, 1644-1649 (*isol, pmr, cmr*)

1,3,5,7-Cadinatetraene, 8CI C-20

1,2-Dihydro-1,6-dimethyl-4-(1-methylethyl)naphthalene, 9CI.
γ-Calacorene*. 1,2-Dihydro-4-isopropyl-1,6-dimethylnaphthalene.*
9,10-Dihydrocadalene
[24048-45-1]
[38599-17-6]



$C_{15}H_{20}$ 200.323

The (*S*)-Config is given in CA but does not appear to be clearly stated in the lit.

(*S*)-*form*

Constit. of *Juniperus rigida* and *Humulus lupulus* (hops).
Oil.

3-Methoxy: 3-Methoxy-1,3,5,7-cadinatetraene. ***3-Methoxy-9,10-dihydrocadalene***
$C_{16}H_{22}O$ 230.349
Isol. from *Lemnalia cervicornis.* Oil. $[\alpha]_D$ -54.9 (c, 0.69 in $CHCl_3$).

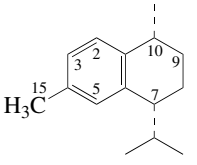
(±)-*form*

Bp_9 125-126°.

Naya, Y. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 2088
Adachi, K. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 651 (*synth*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1986, **39**, 103 (*deriv*)
Nabeta, K. *et al., J.C.S. Perkin 1*, 1994, 3277; 1995, 3111 (*biosynth*)

1,3,5-Cadinatriene C-21

1,2,3,4-Tetrahydro-1,6-dimethyl-4-(1-methylethyl)naphthalene, 9CI. 1,2,3,4-Tetrahydro-4-isopropyl-1,6-dimethylnaphthalene. 4-Isopropyl-1,6-dimethyltetralin. ***Calamenene****. 7,8,9,10-Tetrahydrocadalane*



(7*R*,10*R*)-*form*

$C_{15}H_{22}$ 202.339

Two numbering systems have been used for calamenenes. Only synonyms numbered according to the usual cadinane system, illus., are given here.

(7*R*,10*R*)-*form* [22339-23-7]

Constit. of *Eremophila drummondii*.
Oil. $[\alpha]_D$ +41.3 (c, 1.2 in $CHCl_3$).

3-Hydroxy: 5,6,7,8-Tetrahydro-5-isopropyl-3,8-dimethyl-2-naphthalenol. 1,3,5-Cadinatrien-3-ol. ***3-Hydroxy-10-epicalamenene***
[69126-74-5]
$C_{15}H_{22}O$ 218.338
Constit. of *Osteospermum barberiae* and *Eremophila drummondii*.
$[\alpha]_D$ +27.

5-Hydroxy: 5,6,7,8-Tetrahydro-8-isopropyl-2,5-dimethyl-1-naphthalenol. 1,3,5-Cadinatrien-5-ol. 5-Hydroxycalamenene
[81275-80-1]
$C_{15}H_{22}O$ 218.338
Constit. of *Bazzania tricrenata* and *Bazzania trilobata*. Oil.
$[\alpha]_D$ +33.4 (c, 0.39 in $CHCl_3$).

(7*R*,10*S*)-*form*

Oil. $[\alpha]_D$ +82.

2-Hydroxy: 5,6,7,8-Tetrahydro-5-isopropyl-3,8-dimethyl-1-naphthalenol. 1,3,5-Cadinatrien-2-ol. 2-Calamenenol. ***2-Hydroxycalamenene***†
[88642-92-6]
$C_{15}H_{22}O$ 218.338
Isol. from dried seeds of *Dysoxylum acutangulum*, *Dysoxylum alliaceum* and *Dysoxylum soliffneri*. Fish-poison also showing antibacterial activity. Liq. $Bp_{0.1}$ 150-155°. $[\alpha]_D^{15}$ +38 ($CHCl_3$).

2-Methoxy: 2-Methoxy-1,3,5-cadinatriene. ***2-Methoxycalamenene***
[71306-08-6]
$C_{16}H_{24}O$ 232.365
Constit. of the horny coral *Subergorgia hicksonii*. Oil. $Bp_{0.1}$ 110°. $[\alpha]_D^{25}$ +30 (c, 0.1 in $CHCl_3$).

2-Hydroxy, 5-methoxy: 5-Methoxy-1,3,5-cadinatrien-2-ol. ***2-Hydroxy-5-methoxycalamenene***
[71306-09-7]
$C_{16}H_{24}O_2$ 248.364
Constit. of *Subergorgia hicksonii*. Cryst by subl.
Mp 84°. $[\alpha]_D^{25}$ +58 (c, 0.1 in $CHCl_3$).

3-Hydroxy: ***3-Hydroxycalamenene***†*. 3-Calamenenol*
[88198-96-3]
$C_{15}H_{22}O$ 218.338
From roots of *Osteospermum* spp. and from *Heteroscyphus planus.*
Oil. $[\alpha]_D^{22}$ +59 (c, 0.53 in $CHCl_3$).

3-Methoxy: ***3-Methoxycalamenene***
[146389-49-3]
$C_{16}H_{24}O$ 232.365
Constit. of *Heteroscyphus planus.* Oil. $[\alpha]_D^{22}$ +42 (C, 0.18 in $CHCl_3$).

2,5-Dihydroxy: 1,3,5-Cadinatriene-2,5-diol. ***2,5-Dihydroxycalamenene***
[161873-11-6]
$C_{15}H_{22}O_2$ 234.338
Constit. of *Heteroscyphus planus.* Oil. $[\alpha]_D$ +45.6 (c, 0.31 in $CHCl_3$).

(7*S*,10*R*)-*form* [35943-92-1]

From *Cedrela toona*.
Oil. $[\alpha]_D$ -80.

(7*S*,10*S*)-*form* [483-77-2]

Constit. of *Ulmus thomasii*.
Oil. Bp_{13} 126°. $[\alpha]_D$ -47 ($CHCl_3$).

3-Hydroxy: [76465-67-3]
Constit. of *Ulmus thomasii* and from *Tilia europea* infected with *Ganoderma applanatum*.
Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -30 (c, 1 in $CHCl_3$). λ_{max} 281 (MeOH) (Berdy).

2-Hydroxy, 3-acetoxy: ***3-Acetoxy-2-hydroxycalamenene***
[131984-96-8]
$C_{17}H_{24}O_3$ 276.375
Isol. from the liverwort *Lophocolea heterophylla*. Oil.

15-Hydroxy: 1,3,5-Cadinatrien-15-ol. ***15-Hydroxycalamenene***
[153408-93-6]
$C_{15}H_{22}O$ 218.338
Isol. from *Juniperus formosana*. Amorph. solid. $[\alpha]_D^{20}$ -46.5 (c, 0.8 in $CHCl_3$).

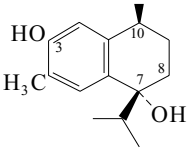
[24406-03-9, 73209-42-4, 87302-52-1, 89015-45-2]

Plattier, M. *et al., Recherches*, 1974, **19**, 214 (*synth*)
Andersen, N.H. *et al., Phytochemistry*, 1977, **16**, 1731-1751 (*Bazzania constit*)
Croft, K.D. *et al., J.C.S. Perkin 1*, 1978, 1267-1270 (*isol, cryst struct*)
Kashman, Y. *et al., Tetrahedron*, 1979, **35**, 263-266 (*Subergorgia hicksoni constit*)
Bunko, J.D. *et al., Aust. J. Chem.*, 1981, **34**, 2237 (*synth, struct, abs config*)
Sangaiah, R. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 13 (*synth*)
Adachi, K. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 651 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1983, **22**, 1645-1651 (*Osteospermum constit*)
Nishigawa, M. *et al., Phytochemistry*, 1983, **22**, 2083-2085 (*8-Hydroxycalamene*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1984, **23**, 992 (*synth*)
Uemura, M. *et al., Tetrahedron*, 1985, **41**, 5771 (*synth, derivs*)
Tanaka, J. *et al., Bull. Chem. Soc. Jpn.*, 1990, **63**, 272 (*5-Hydroxycalamenene, synth, struct*)
Toyota, M. *et al., Phytochemistry*, 1990, **29**, 2334 (*3-Acetoxy-2-hydroxycalamenene*)
Nabeta, K. *et al., Phytochemistry*, 1993, **32**, 117 (*isol, pmr, cmr, 3-Hydroxycalamenene, 3-Methoxycalamenene*)
Nabeta, K. *et al., Phytochemistry*, 1994, **35**, 915-920 (*biosynth*)
Hashimoto, T. *et al., Phytochemistry*, 1995, **38**, 119 (*2,5-Dihydroxycalamenene*)

Kuo, Y.H. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2150-2152 (*15-Hydroxycalamenene*)
Nagashima, F. *et al., Phytochemistry*, 1996, **42**, 1361-1366 (*5-Hydroxycalamenene, cryst struct, abs config*)
Melching, S. *et al., Phytochemistry*, 1997, **44**, 1291-1296 (*Calamenene, pmr, ms, gc*)
Mulholland, D.A. *et al., Phytochemistry*, 1998, **47**, 1421-1422 (*2-Calamenenol, pmr, cmr*)
Hashimoto, M. *et al., Phytochemistry*, 1999, **51**, 389-394 (*biosynth*)
Serra, S. *et al., Tet. Lett.*, 2005, **46**, 4769-4772 (*synth*)

1,3,5-Cadinatriene-3,7-diol C-22

3,7-Calamenenediol



(7α(*OH*),10β)–*form*

$C_{15}H_{22}O_2$ 234.338

Two numbering systems have been used for calamenenes. The numbering given here is based on the usual system of cadalanes.

(7α(*OH*),10β)-*form*

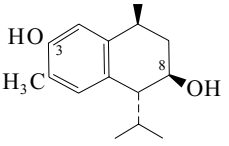
3-Me ether: 3-Methoxy-1,3,5-cadinatrien-7-ol. 3-Methoxy-7-calamenenol
$C_{16}H_{24}O_2$ 248.364
Constit. of *Lemnalia cervicornis*. Oil. $[\alpha]_D$ -1.2 (c, 2.26 in $CHCl_3$).

(7β(*OH*),10β)-*form*

3-Me ether: From *Lemnalia cervicornis*.
Oil. $[\alpha]_D$ +33.5 (c, 0.33 in $CHCl_3$).
Bowden, B.F. *et al., Aust. J. Chem.*, 1986, **39**, 103-121

1,3,5-Cadinatriene-3,8-diol C-23

3,8-Calamenenediol



$C_{15}H_{22}O_2$ 234.338

Two numbering systems have been used for calamenenes. Synonyms are given here only according to the usual numbering system of cadinanes, illus.

(7α,8β,10β)-*form*

Constit. of *Lemnalia cervicornis*.
Oil. $[\alpha]_D$ +23.3 (c, 0.3 in $CHCl_3$).

3-Me ether: 3-Methoxy-1,3,5-cadinatrien-8-ol. ***3-Methoxy-8-calamenenol***
$C_{16}H_{24}O_2$ 248.364
From *Lemnalia cervicornis*. Oil. $[\alpha]_D$ +22 (c, 0.25 in $CHCl_3$).

3-Me ether, 8-Ac:
$C_{18}H_{26}O_3$ 290.402
From *Lemnalia cervicornis*. Oil. $[\alpha]_D$ +22.3 (c, 0.57 in $CHCl_3$).

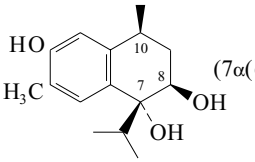
8-Ketone: 3-Hydroxy-1,3,5-cadinatrien-8-one. 3-Hydroxy-8-calamenenone
$C_{15}H_{20}O_2$ 232.322
From *Lemnalia cervicornis*. Cryst. (MeCN).
Mp 121-123°. $[\alpha]_D$ +178.1 (c, 0.18 in $CHCl_3$).

8-Ketone, 3-Ac:
$C_{17}H_{22}O_3$ 274.359
From *Lemnalia cervicornis*. Oil. $[\alpha]_D$ +173.6 (c, 1.24 in $CHCl_3$).

8-Ketone, 3-Me ether: 3-Methoxy-1,3,5-cadinatrien-8-one. 3-Methoxy-8-calamenenone
$C_{16}H_{22}O_2$ 246.349
From *Lemnalia cervicornis*. Oil. $[\alpha]_D$ +136.6 (c, 0.2 in $CHCl_3$).
Bowden, B.F. *et al., Aust. J. Chem.*, 1986, **39**, 103-121

1,3,5-Cadinatriene-3,7,8-triol C-24

3,7,8-Calamenenetriol



(7α(*OH*),8β,10β)–*form*

$C_{15}H_{22}O_3$ 250.337

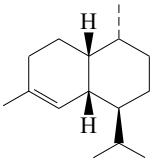
(7α(*OH*),8β,10β)-*form*

Isol. from *Lemnalia cervicornis*.
Cubes ($CHCl_3$).
Mp 160-162°. $[\alpha]_D$ +21.6 (c, 0.21 in MeOH).

(7β(*OH*),8β,10β)-*form*

From *Lemnalia cervicornis*.
Cubes ($CHCl_3$).
Mp 162-164°. $[\alpha]_D$ +89.3 (c, 0.1 in MeOH).
Bowden, B.F. *et al., Aust. J. Chem.*, 1986, **39**, 103

4-Cadinene C-25

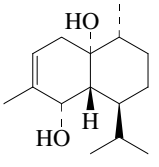


$C_{15}H_{26}$ 206.37

(1β,6β,7β,10α)-*form*

4-Muurolene
[160796-91-8]
Constit. of *Taonia atomaria*.
$[\alpha]_D$ -23 (c, 0.01 in $CHCl_3$).
De Rosa, S. *et al., Phytochemistry*, 1994, **37**, 1327-1330 (*isol, pmr, cmr*)

3-Cadinene-1,5-diol C-26



(1α,5α,6β,10α)-*form*

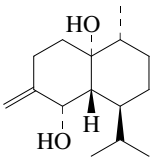
$C_{15}H_{26}O_2$ 238.369

(1α,5α,6β,10α)-*form* [785793-93-3]
Constit. of *Dictyopteris divaricata*.
Gum. $[\alpha]_D^{20}$ +29 (c, 0.15 in MeOH).

5-Ketone: ***1-Hydroxy-3-cadinen-5-one***
[785793-92-2]
$C_{15}H_{24}O_2$ 236.353
Constit. of *Dictyopteris divaricata*. Cryst. (Me_2CO).
Mp 179-180°. $[\alpha]_D^{20}$ -47 (c, 0.18 in MeOH).

(1α,5β,6β,10α)-*form* [785793-94-4]
Constit. of *Dictyopteris divaricata*.
Cryst. (Me_2CO).
Mp 154-156°. $[\alpha]_D^{20}$ +54 (c, 0.15 in MeOH).
Song, F. *et al., J. Nat. Prod.*, 2004, **67**, 1644-1649 (*isol, pmr, cmr, cryst struct*)

4(15)-Cadinene-1,5-diol C-27

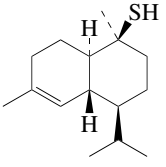


$C_{15}H_{26}O_2$ 238.369

(1α,5α,6β,10α)-*form* [785793-95-5]
Constit. of *Dictyopteris divaricata*.
Cryst. (Me_2CO).
Mp 139-140°. $[\alpha]_D^{20}$ +51 (c, 0.17 in MeOH).
Song, F. *et al., J. Nat. Prod.*, 2004, **67**, 1644-1649 (*isol, pmr, cmr, cryst struct*)

4-Cadinene-10-thiol C-28

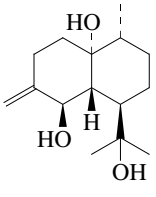
10-Mercapto-4-cadinene



$C_{15}H_{26}S$ 238.436

10β-*form*
T-*Cadinthiol*
[190663-68-4]
Constit. of *Cymbastela hooperi*.
Oil. $[\alpha]_D$ -24.3 (c, 1.1 in $CHCl_3$).
König, G.M. *et al., J.O.C.*, 1997, **62**, 3837-3840 (*isol, pmr, cmr*)

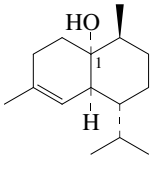
4(15)-Cadinene-1,5,11-triol C-29



$C_{15}H_{26}O_3$ 254.369

(1α,5β,6β,10α)-*form* [785793-96-6]
Constit. of *Dictyopteris divaricata*.
Gum. $[\alpha]_D^{20}$ +55 (c, 0.29 in MeOH).
Song, F. *et al., J. Nat. Prod.*, 2004, **67**, 1644-1649 (*isol, pmr, cmr*)

4-Cadinen-1-ol C-30



(1α,6α,7α,10β)-*form*

$C_{15}H_{26}O$ 222.37

(1α,6α,7α,10β)-*form*
4-Muurolen-1-ol. ***Epicubenol***
[19912-67-5]
Constit. of cubeb pepper (*Piper cubeba*) oil, *Cedrus atlantica* and *Satureja gilliesii*. Isol. from *Dictyopteris divaricata* and *Gymnodinium nagasakiense*.
Oil. $Bp_{2.5}$ 170-180° (bath). $[\alpha]_D^{30}$ -100.6 ($CHCl_3$).

(1α,6α,7β,10α)-*form*
6-Epicubenol
[442853-35-2]
Constit. of *Solidago canadensis*.
Oil.
Me ether: 1-Methoxy-4-cadinene
[744265-66-5]
$C_{16}H_{28}O$ 236.397
Constit. of *Cryptomeria japonica*. Oil. $[\alpha]_D^{25}$ -65.2 (c, 0.11 in $CHCl_3$).

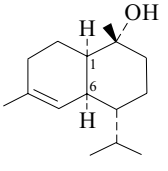
(1α,6β,7β,10α)-*form*
Cubenol
[21284-22-0]
Constit. of oil of cubeb pepper (*Piper cubeba*) and many other plant spp. Also from *Gymnodinium nagasakiense* and ferns *Dictyopteris deliculata* and *Dictyopteris divaricata*. Algicide. Oil. $Bp_{2.5}$ 170-180° (bath). $[\alpha]_D^{20}$ -33 (c, 0.13 in $CHCl_3$).

(1β,6α,7α,10α)-*form* [352457-23-9]
Constit. of Haitian vetiver oil.

(1β,6α,7β,10β)-*form*
4-Bulgaren-1-ol
Constit. of *Fitzroya cupressoides*.

(1β,6β,7β,10α)-*form*
ent-*Epicubenol*
Constit. of *Scapania undulata* and metab. of a *Streptomyces* sp.
Oil. $[\alpha]_D^{24}$ +111.6 (c, 4.7 in $CHCl_3$).
Ohta, Y. *et al., Tet. Lett.*, 1967, **8**, 2073-2075 (*Cubenol, Epicubenol*)
Gerber, N.N. *et al., Phytochemistry*, 1971, **10**, 185-189 (*Streptomyces metab*)
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 2366-2368 (*isol*)
Connolly, J.D. *et al., Phytochemistry*, 1982, **21**, 233-234 (*ent-Epicubenol, isol, struct*)
Kajiwara, T. *et al., Phytochemistry*, 1992, **31**, 783-785 (*isol*)
Labbé, C. *et al., Phytochemistry*, 1993, **34**, 441-444 (*Cubenol*)
Cane, D.E. *et al., Tet. Lett.*, 1994, **35**, 5351-5354; 5355-5358 (*synth, biosynth*)
Gijsen, H.J.M. *et al., Tetrahedron*, 1994, **50**, 4745-4754 (*Cubenol, synth*)
Nabeta, K. *et al., J.C.S. Perkin 1*, 1995, 1935; 1997, 2065-2070 (*biosynth*)
König, G.M. *et al., Magn. Reson. Chem.*, 1995, **33**, 178-183 (*isol, pmr, cmr*)
Cool, L.G. *et al., Phytochemistry*, 1996, **42**, 1015-1019 (*4-Bulgaren-1-ol*)
Weyerstahl, P. *et al., Flavour Fragrance J.*, 2000, **15**, 395-412 (*vetiver oil constit*)
Kasali, A.A. *et al., Phytochemistry*, 2002, **59**, 805-810 (*6-Epicubenol*)
Arihara, S. *et al., Chem. Pharm. Bull.*, 2004, **52**, 463-465 (*Me ether*)

4-Cadinen-10-ol C-31



(1α,6α,7α,10α)–*form*

$C_{15}H_{26}O$ 222.37

(1α,6α,7α,10α)-*form*
4-Muurolen-10-ol. **ent-T-*Muurolol***
Constit. of *Scapania undulata*.
$[\alpha]_D$ +83.4 (c, 2.42 in $CHCl_3$).

(1α,6α,7α,10β)-*form*
Cedrelanol. *Brown-algae cadinol. Pilgerol*
[5937-11-1]
Constit. of *Pinus albicaulis, Pinus armandii, Juniperus communis* (juniper) and *Pilgerodendron uniferum*. Also from *Cedrela odorata,*

Chamaecyparis lawsoniana, Athrotaxis selaginoides, Cryptomeria japonica, Dictyopteris divaricata and others (some earlier identifications prob. erroneous in view of uncertainty over struct.).
Mp 139-140°. $[\alpha]_D^{20}$ -102 (c, 3.2 in EtOH).

(1α,6β,7β,10α)-*form*
α-Cadinol
[481-34-5]
Constit. of *Chamaecyparis lawsoniana* and *Juniperus communis* (juniper). Also from *Chamaecyparis obtusa, Chamaecyparis pisifera, Juniperus horizontalis, Juniperus scopulorum, Athrotaxis* spp. and *Neocallitropsis araucaroides*. Shows cytotoxic activity.
Cryst.
Mp 74.5-75°. $[\alpha]_D$ -47 (-38.5).

Me ether: ***α-Cadinol methyl ether***
$C_{16}H_{28}O$ 236.397
Constit. of *Senecio adenophyllus*. Oil. $[\alpha]_D^{24}$ -49 (c, 3.42 in $CHCl_3$).

(1α,6β,7β,10β)-*form*
T-*Cadinol*
Isol. from the sponge *Acanthella cavernosa*. Constit. of *Taiwania cryptomeroides*, *Commiphora guidottii*, *Teucrium yemense*, *Athrotaxis selaginoides* and *Satureja gilliesii*. Leukotriene biosynthesis inhibitor.
Mp 64-64.5°. $[\alpha]_D$ +3.4 (c, 1.2 in $CHCl_3$).

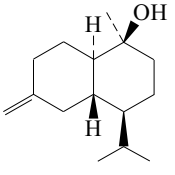
(1β,6β,7β,10α)-*form*
***Torreyol*. δ-Cadinol. Sesquigoyol. Cedreanol**
[36564-42-8]
Constit. of *Pinus parviflora*, *Pinus formosana*, *Juniperus communis* and *Xylopia* sp.
Cryst.
Mp 139-140°. $[\alpha]_D^{20}$ +102 (c, 3.2 in EtOH). First thought to be a cadinene and therefore appropriately named but since shown to be a muurolane.

(1β,6β,7β,10β)-*form*
T-*Muurolol*
[19912-62-0]
Constit. of *Taiwania cryptomeroides*, *Athrotaxis selaginoides*, *Chamaecyparis obtusa* and *Cedrela toona*.
Cryst.
Mp 80.5-81.5°. $[\alpha]_D^{23}$ -114 (c, 1 in $CHCl_3$).

[19435-97-3]

Cheng, Y.S. *et al., Chem. Comm.*, 1967, 565-566 (*T-Cadinol, T-Muurolol*)
Nagasampagi, B.A. *et al., Tet. Lett.*, 1968, **9**, 1913-1918 (*Cedrela toona constits, isol, synth*)
Caine, D. *et al., Tet. Lett.*, 1977, **18**, 3107-3110 (*synth*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 552 (*synth*)
Borg-Karlson, A.-K. *et al., Tetrahedron*, 1981, **37**, 425-430 (*struct, stereochem*)
Rodriguez-Avial Franke, L.R. *et al., Tetrahedron*, 1984, **40**, 3491-3498 (*Torreyol, synth*)
Bottini, A.T. *et al., J. Nat. Prod.*, 1987, **50**, 732 (*cmr*)
Tkachev, A.V. *et al., Khim. Prir. Soedin.*, 1990, **26**, 635; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 539 (*pmr, cmr*)
Dupré, S. *et al., Phytochemistry*, 1991, **30**, 1211-1220 (*α-Cadinol methyl ether*)
Claeson, P. *et al., Planta Med.*, 1991, **57**, 352-356 (*T-Cadinol, pmr, cmr*)
Labbé, C. *et al., Phytochemistry*, 1993, **34**, 441-444 (*T-Cadinol, pmr, cmr*)
Nagashima, F. *et al., Phytochemistry*, 1994, **37**, 1323-1325 (*ent-T-Muurolol*)
Chang, S.-T. *et al., Phytochemistry*, 2000, **55**, 227-232 (*activity*)
Nogata, Y. *et al., Biofouling*, Suppl., 2003, **19**, 193-196 (*Acanthella, isol*)

4(15)-Cadinen-10-ol C-32



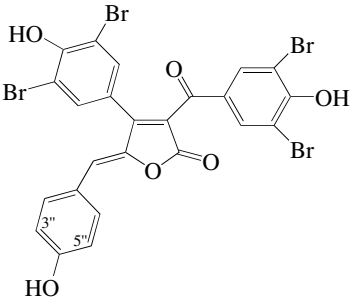
$C_{15}H_{26}O$ 222.37

(1α,6β,7β,10β)-*form*
Millecrol B
[154524-44-4]
Constit. of *Leminda millecra*.
Oil.

Pika, J. *et al., Tetrahedron*, 1994, **50**, 3065-3070 (*isol, pmr, cmr*)

Cadiolide A C-33

[206763-40-8]



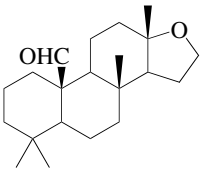
$C_{24}H_{12}Br_4O_6$ 715.971
Isol. from the ascidian *Botryllus* sp. Orange amorph. solid.
λ_{max} 254 (ϵ 10100); 406 (ϵ 16100) (MeOH).

3'',5''-Dibromo: ***Cadiolide B***
[206763-42-0]
$C_{24}H_{10}Br_6O_6$ 873.763
Isol. from a *Botryllus* sp. Orange amorph. solid. λ_{max} 270 (ϵ 16400); 388 (ϵ 24900) (MeOH).

Smith, C.J. *et al., J.O.C.*, 1998, **63**, 4147-4150 (*isol, uv, pmr, cmr, ms*)

Cadlinaldehyde C-34

[194020-35-4]

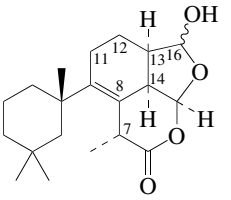


$C_{21}H_{34}O_2$ 318.498
Constit. of *Cadlina luteomarginata*. Needles (MeOH).
Mp 65°. $[\alpha]_D^{25}$ +25 ($CHCl_3$).

Dumdei, E.J. *et al., Can. J. Chem.*, 1997, **75**, 773-789 (*isol, pmr, cmr, cryst struct*)
Kubanek, J. *et al., J.O.C.*, 1997, **62**, 7239-7246 (*biosynth*)

Cadlinolide B C-35

[130221-21-5]



$C_{20}H_{30}O_4$ 334.455
Constit. of *Aplysilla glacialis*. Oil.

Ac (16α-): ***Aplysulphuride***. *Tetrahydroaplysulphurin 1*
[91236-89-4]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Cadlina luteomarginata* and *Darwinella oxeata*. Cryst. (CH_2Cl_2/hexane).

Mp 109°. $[\alpha]_D$ +169 (c, 1 in $CHCl_3$).

16-Me ether: ***Cadlinolide D***
[676154-32-8]
$C_{21}H_{32}O_4$ 348.481
Constit. of *Chelonaplysilla violacea*. Solid.

16-Ketone: ***Cadlinolide A***
[130246-91-2]
$C_{20}H_{28}O_4$ 332.439
Constit. of *Aplysilla glacialis* and *Cadlina luteomarginata*. Cryst. (hexane).
Mp 126-127°. $[\alpha]_D$ +19 (c, 8 in $CHCl_3$).

11,12,13,14-Tetradehydro, Ac (16α-): ***Aplysulphurin***
[91236-90-7]
$C_{22}H_{28}O_5$ 372.46
Constit. of *Aplysilla sulphurea*. Cryst. (hexane).
Mp 195°. $[\alpha]_D^{25}$ +110 (c, 1 in $CHCl_3$).

16-Deoxy: ***Cadlinolide C***
[676154-31-7]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Chelonaplysilla violacea*. Yellow solid. $[\alpha]_D^{20}$ +27.3 (c, 0.68 in CH_2Cl_2).

12-Acetoxy, 16-Ac(16α-): ***12-Acetoxytetrahydrosulphurin I***
$C_{24}H_{34}O_7$ 434.528
Isol. from an *Aplysilla* sp. Phospholipase A2 inhibitor.

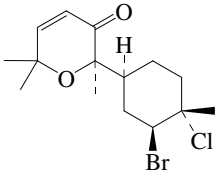
$\Delta^{7,8}$-Isomer, Ac (16α-): ***Tetrahydroaplysulphurin 3***
[106009-85-2]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Darwinella oxeata*. Oil. $[\alpha]_D^{20}$ +11.6 (c, 0.5 in $CHCl_3$).

$\Delta^{8,14}$-Isomer, Ac (16α-): ***Tetrahydroaplysulphurin 2***
[106009-84-1]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Darwinella oxeata*. Cryst. (petrol).
Mp 181-183°.

Karuso, P. *et al., Aust. J. Chem.*, 1984, **37**, 1081; 1986, **39**, 1643-1653 (*Aplysulphurin, Aplysulphuride, Tetrahydroaplysulphurins*)
Buckleton, J.S. *et al., Acta Cryst. C*, 1987, **43**, 2430-2432 (*cryst struct, Aplysulphuride*)
Tischler, M. *et al., J.O.C.*, 1991, **56**, 42-47 (*isol, pmr, cmr, cryst struct*)
Potts, B.C.M. *et al., J. Nat. Prod.*, 1992, **55**, 1701-1717 (*12-Acetoxytetrahydroaplysulphurin I*)
Keyzers, R.A. *et al., Eur. J. Org. Chem.*, 2004, 419-425 (*Cadlinolides C and D*)

Caespitenone† C-36

[124193-10-8]

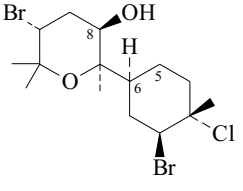


$C_{15}H_{22}BrClO_2$ 349.694
Constit. of *Aplysia dactylomela*.
$[\alpha]_D$ +36.3 (c, 0.47 in $CHCl_3$).

Wessels, M. *et al., J. Nat. Prod.*, 2000, **63**, 920-928 (*isol, pmr, cmr*)

Caespitol C-37

[50656-64-9]



$C_{15}H_{25}Br_2ClO_2$ 432.622
Constit. of *Laurencia caespitosa*. Metab. of *Aplysia dactylomela*. Toxic to brine shrimp. Shows algicidal props. Cryst. (hexane). Poorly sol. hexane.
Mp 109-111°. $[\alpha]_D$ +4.3 (c, 0.44 in $CHCl_3$).

Ac: ***Caespitol acetate****. 8-Acetylcaespitol*
[73410-30-7]
$C_{17}H_{27}Br_2ClO_3$ 474.659
Constit. of *Aplysia dactylomela*.
$[\alpha]_D$ 0 (c, 0.34 in $CHCl_3$).

6-Hydroxy: ***6-Hydroxycaespitol***
$C_{15}H_{25}Br_2ClO_3$ 448.621
Constit. of *Laurencia caespitosa*. Cryst.
Mp 152-153°. $[\alpha]_D$ +11.7 (c, 0.29 in $CHCl_3$).

5β,6-Dihydroxy, 8-Ac: ***Dihydroxydeodactol monoacetate***
[72926-49-9]
$C_{17}H_{27}Br_2ClO_5$ 506.658
Constit. of *Aplysia dactylomela*. Cryst. (hexane/C_6H_6).
Mp 168-169°. $[\alpha]_D$ +40.5 ($CHCl_3$).

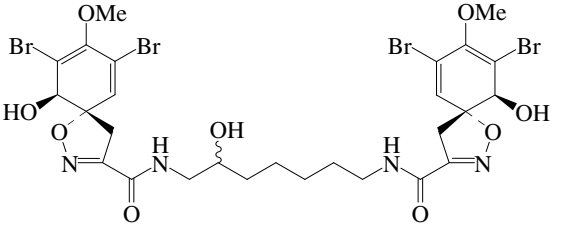
8-Deoxy: ***Caespitane***
[124264-63-7]
$C_{15}H_{25}Br_2ClO$ 416.623
Constit. of *Laurencia caespitosa*. Metab. of *Aplysia dactylomela*. Toxic to brine shrimp. Shows algicidal props. Cryst.
Mp 82-84°. $[\alpha]_D$ +39.8 (c, 0.89 in $CHCl_3$).

8-Deoxy, 5β-hydroxy: ***Deodactol***
[71679-25-9]
$C_{15}H_{25}Br_2ClO_2$ 432.622
Constit. of *Aplysia dactylomela*. Shows antineoplastic props. Cryst. (hexane). Sol. H_2O; poorly sol. MeOH, hexane.
Mp 134-135°. $[\alpha]_D$ +40 (c, 0.2 in EtOH).

8-Deoxy, 6-hydroxy: ***Isodeodactol***
[79373-31-2]
$C_{15}H_{25}Br_2ClO_2$ 432.622
Isol. from *Aplysia dactylomela*. Cryst. (hexane).
Mp 158-160°. $[\alpha]_D$ +18.9 (c, 0.37 in $CHCl_3$).

Gonzales, A.G. *et al., Tet. Lett.*, 1974, 1249-1250; 1976, 3051; 1979, 2719-2722 (*struct, biosynth, cmr*)
Hollenbeak, K.H. *et al., Tetrahedron*, 1979, **35**, 541-545 (*isol, cryst struct, abs config, Deodactol*)
Schmitz, F.J. *et al., J.O.C.*, 1980, **45**, 1525 (*Dihydroxydeodactol monoacetate*)
Gopichand, Y. *et al., J.O.C.*, 1981, **46**, 5192-5197 (*Isodeodactol*)
Chang, M. *et al., Phytochemistry*, 1989, **28**, 1417-1424 (*isol, cryst struct, abs config*)
Wessels, M. *et al., J. Nat. Prod.*, 2000, **63**, 920-928 (*acetate, activity*)

Caissarine B C-38



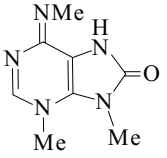
Relative Configuration

$C_{27}H_{32}Br_4N_4O_9$ 876.187
Isol. from the Brazilian sponge *Aplysina caissara*. Glassy solid.
λ_{max} 234 (ϵ 9000); 283 (ϵ 4300) (MeOH).

Saeki, B.M. *et al., J. Nat. Prod.*, 2002, **65**, 796-799; 2003, **66**, 1039 (*isol, pmr, cmr, ms*)

Caissarone C-39

[106145-23-7]



$C_8H_{11}N_5O$ 193.208

Alkaloid from the sea anemone *Bunodosoma caissarum*. Inducer of anomalous growth in sea urchin eggs, increases muscle contraction. λ_{max} 228 (ϵ 21600); 302 (ϵ 17700) (MeOH) (Derep).

▶ Teratogen.

Hydrochloride:

Needles (MeOH aq.). Mp 285-290°.

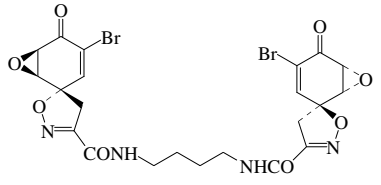
Picrate:

Cryst. (EtOH). Mp 245-250°.

Zelnik, R. *et al., J.C.S. Perkin 1*, 1986, 2051 (*isol, uv, ir, pmr, cmr, cryst struct*)
Fujii, T. *et al., Tet. Lett.*, 1991, **32**, 97 (*synth*)
Itaya, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1601-1607; 1867-1869 (*synth*)

Calafianine C-40

[267876-68-6]



Absolute Configuration

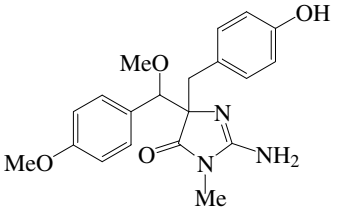
$C_{22}H_{20}Br_2N_4O_8$ 628.23

Related to Aerothionin, A-128. Stereochem. revised in 2005. Isol. from the sponge *Aplysina gerardogreeni*. Solid. λ_{max} 210 (sh); 230 (sh); 260 (sh) (EtOH).

Encarnacion, R.D. *et al., J. Nat. Prod.*, 2000, **63**, 874-875 (*isol, pmr, cmr*)
Ogamino, T. *et al., Tet. Lett.*, 2005, **46**, 1083-1086 (*synth, struct*)
Bardhan, S. *et al., Org. Lett.*, 2006, **8**, 927-930 (*synth, abs config*)

Calcaridine A C-41

[568561-14-8]



$C_{20}H_{23}N_3O_4$ 369.419

Isol. from a calcareous sponge *Leucetta* sp.

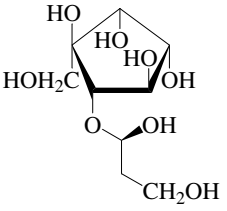
Yellow oil. $[\alpha]_D$ +1.6 (c, 0.12 in MeOH).

Edrada, R.A. *et al., J. Nat. Prod.*, 2003, **66**, 939-942 (*isol, pmr, cmr*)

Calditol C-42

5-(2,3-Dihydroxypropoxy)-1-(hydroxymethyl)-1,2,3,4-cyclohexanetetrol, 9CI

[164300-76-9]



$C_9H_{18}O_8$ 254.236

Originally assigned a branched chain nonitol struct. Correct struct established by synthesis in 1999. Degradation prod. of a complex of macrocyclic tetraether lipids isol. from membranes of thermoacidophilic archaebacteria of the *Caldariella* group and *Methanospirillum* species, e.g. *Sulfolobus solfataricus*. Also found in methanobacteria.

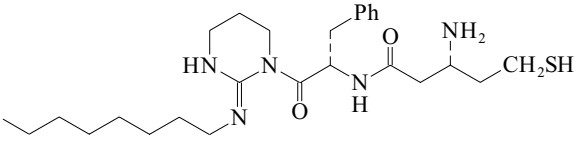
$[\alpha]_D$ -8.72 (c, 1.3 in H_2O).

[74554-26-0, 74578-16-8, 248263-78-7]

De Rosa, M. *et al., Phytochemistry*, 1980, **19**, 249-254; 827-831 (*isol, cmr*)
Nicolaus, B. *et al., Biochem. J.*, 1990, **266**, 785-791 (*biosynth*)
Jeganathan, S. *et al., Tet. Lett.*, 1990, **31**, 1717-1720
Sugai, A. *et al., Lipids*, 1995, **30**, 339-344 (*isol, struct, cmr, pmr*)
Fairbanks, A.J. *et al., Tet. Lett.*, 1995, **36**, 893-896 (*bibl*)
Blériot, Y. *et al., Chem. Eur. J.*, 2002, **8**, 240-246; 1512 (*synth, struct*)
Gambacorta, A. *et al., Tet. Lett.*, 2002, **43**, 451-453 (*biosynth*)
Yamauchi, N. *et al., Bull. Chem. Soc. Jpn.*, 2004, **77**, 771-778 (*biosynth*)

Caledonin C-43

[171675-03-9]



$C_{26}H_{43}N_5O_2S$ 489.724

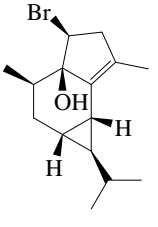
Modified peptide. Isol. from the marine tunicate *Didemnum rodriguesi*. Strongly binds Zn^{II} and Cu^{I} ions. Sol. MeOH, CH_2Cl_2; poorly sol. H_2O.

Mp 170-172°. $[\alpha]_D^{20}$ +24 (c, 0.145 in MeOH). λ_{max} 234 (ϵ 2816) (MeOH) (Berdy).

Vázquez, M.J. *et al., Tet. Lett.*, 1995, **36**, 8853-8856 (*isol, uv, ir, pmr, cmr, struct*)

Calenzanol C-44

[334021-86-2]

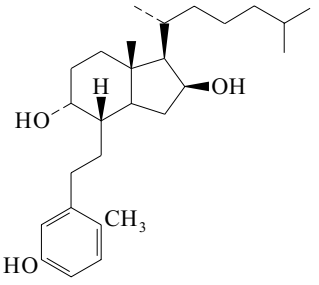


$C_{15}H_{23}BrO$ 299.250

Constit. of *Laurencia microcladia*.

Guella, G. *et al., Tet. Lett.*, 2001, **42**, 723-725 (*isol, pmr, cmr*)

Calicoferol B C-45

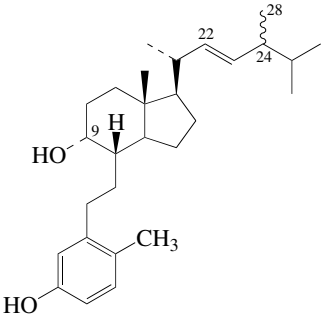


$C_{27}H_{44}O_3$ 416.643
Constit. of a *Calicogorgia* sp. Toxic to brine shrimp. Oil. $[\alpha]_D^{21}$ -16.2 (c, 0.09 in $CHCl_3$).

Ochi, M. *et al., Chem. Lett.*, 1991, 427 (*isol, pmr, cmr*)
Taber, D.F. *et al., J.O.C.*, 2002, **67**, 4821-4827 (*synth*)

Calicoferol F C-46

9,10-Secoergosta-1,3,5(10),22-tetraene-3,9-diol
[214962-73-9]



$C_{28}H_{44}O_2$ 412.654
Constit. of gorgonian *Muricella* sp. Oil. $[\alpha]_D^{25}$ +13.7 (c, 0.1 in $CHCl_3$). λ_{max} 219 (log ϵ 3.81); 279 (log ϵ 3.38) (MeOH).

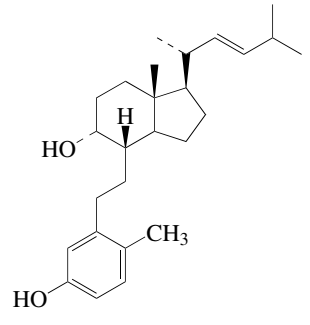
9-Ketone: ***Calicoferol D***
[134387-51-2]
$C_{28}H_{42}O_2$ 410.639
Constit. of a *Muricella* sp. Cryst. (Me_2CO/hexane).
Mp 76-79°. $[\alpha]_D^{25}$ +13.5 (c, 0.4 in $CHCl_3$).

22,23-Dihydro, 24,28-didehydro: 9,10-Secoergost-1,3,5(10),24(28)-tetraene-3,9-diol. ***Calicoferol C***
[169217-41-8]
$C_{28}H_{44}O_2$ 412.654
Constit. of a *Muricella* sp. Oil. $[\alpha]_D^{25}$ -9.5 (c, 0.3 in $CHCl_3$).

Seo, Y. *et al., J. Nat. Prod.*, 1995, **58**, 1291-1295; 1998, **61**, 1441-1443

Calicoferol H C-47

[214962-75-1]

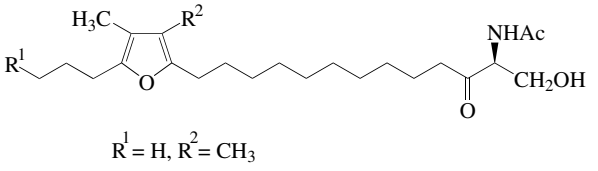


$C_{26}H_{40}O_2$ 384.601
Constit. of a *Muricella* sp. Oil. $[\alpha]_D^{25}$ -6.6 (c, 0.1 in $CHCl_3$). λ_{max} 219 (log ϵ 3.84); 281 (log ϵ 3.32) (MeOH).

Seo, Y. *et al., J. Nat. Prod.*, 1998, **61**, 1441-1443 (*isol, pmr, cmr*)

Calicogorgin A C-48

[134394-71-1]



R^1 = H, R^2 = CH_3

$C_{24}H_{41}NO_4$ 407.592
Sphingadienine analogue. Isol. from the gorgonian *Calicogorgia* sp. Molluscicide. Viscous oil. $[\alpha]_D^{22}$ +7.2 (c, 0.2 in $CHCl_3$). λ_{max} 224 (ϵ 7150); 281 (ϵ 970) (MeOH) (Berdy).

Ochi, M. *et al., Tet. Lett.*, 1992, **33**, 7531-7534 (*isol, uv, ir, pmr, cmr*)
MaGee, D.I. *et al., Tet. Lett.*, 1997, **38**, 1289-1292 (*synth*)

Calicogorgin B C-49

[134381-19-4]
As Calicogorgin A, C-48 with
R^1=-CH_2CH_3, R^2=CH_3
$C_{26}H_{45}NO_4$ 435.646
Sphingadienine analogue. Isol. from the gorgonian *Calicogorgia* sp. Molluscicide. Oil. $[\alpha]_D^{21}$ +7.6 (c, 0.05 in $CHCl_3$). λ_{max} 224 (ϵ 7150); 281 (ϵ 970) (MeOH) (Berdy).

Ochi, M. *et al., Tet. Lett.*, 1992, **33**, 7531-7534 (*isol, pmr, cmr*)

Calicogorgin C C-50

[134381-20-7]
As Calicogorgin A, C-48 with
R^1=-CH_2CH_3, R^2=H
$C_{25}H_{43}NO_4$ 421.619
Sphingadienine analogue. Isol. from the gorgonian *Calicogorgia* sp. Molluscicide. Oil. $[\alpha]_D^{22}$ +5 (c, 0.2 in $CHCl_3$). λ_{max} 224 (ϵ 7150); 281 (ϵ 970) (MeOH) (Berdy).

Ochi, M. *et al., Tet. Lett.*, 1992, **33**, 7531-7534 (*isol, pmr, cmr*)
MaGee, D.I. *et al., Tet. Lett.*, 1997, **38**, 1289-1292 (*synth*)

Califin C-51

Consists of three peptides, designated Califins A, B and C. Structs. comprise a 36-residue subunit bound by a single disulfide bond to an 18 residue subunit. The large subunits of Califins A-C differ from each other by 1 or 2 residues whereas the small subunits are identical. Isol. from the atrial gland of the marine mollusc *Aplysia californica*. Inducer of egg-laying.

[99575-94-7, 99575-95-8, 99575-96-9, 101695-21-0, 101795-07-7, 101800-38-8, 101800-39-9]

Rothman, B.S. *et al., J. Biol. Chem.*, 1986, **261**, 1616 (*isol, struct*)
Nagle, G.T. *et al., J. Biol. Chem.*, 1986, **261**, 7853 (*isol, struct*)

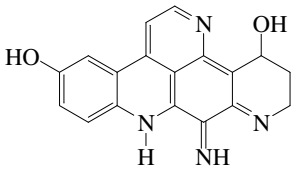
Calitoxin C-52

[118354-83-9]

Peptide. Polypeptide chain containing 46 AA residues. Isol. from the sea anemone *Calliactis parasitica*. Neurotoxin.

Coriello, L. *et al., Biochemistry*, 1989, **28**, 2484 (*isol, struct*)

Calliactine C-53



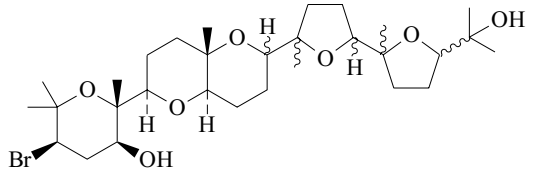
$C_{18}H_{14}N_4O_2$ 318.334

Preferred struct. shown. An isomeric struct. cannot be ruled out. Pigment from the sea anemone *Calliactis parasitica*. λ_{max} 267 (ϵ 12000); 272 (ϵ 11700); 299 (ϵ 9200); 454 (ϵ 8500) (MeOH) (Berdy). λ_{max} 580 (MeOH/NaOH) (Berdy).

Lederer, E. *et al., Bull. Soc. Chim. Fr.*, 1940, **7**, 608-615 (*isol*)
Cimino, G. *et al., Pure Appl. Chem.*, 1986, **58**, 375-386 (*rev, bibl*)
Cimino, G. *et al., Tetrahedron*, 1987, **43**, 4023-4030 (*struct, uv, pmr, cmr*)

Callicladol C-54

[171370-51-7]



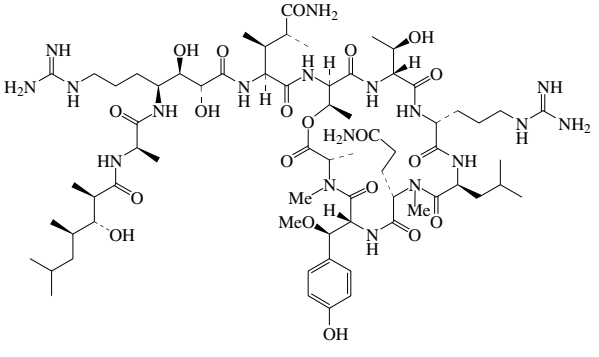
$C_{30}H_{51}BrO_7$ 603.633

Constit. of *Laurencia calliclada*. Cryst. (EtOH). Mp 198-199°. $[\alpha]_D^{23}$ +75.1 (c, 0.6 in $CHCl_3$).

Suzuki, M. *et al., Chem. Lett.*, 1995, 1045 (*isol, pmr, cmr*)

Callipeltin A C-55

[177743-08-7]



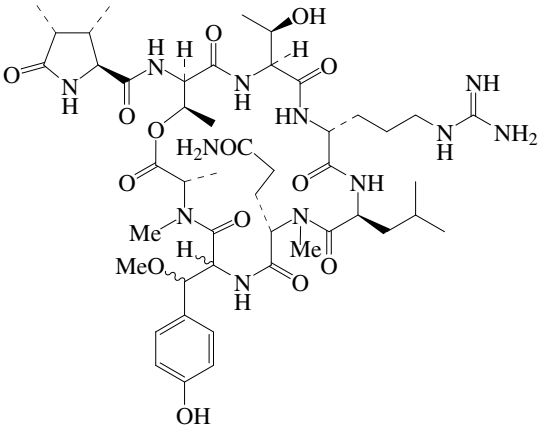
$C_{68}H_{116}N_{18}O_{20}$ 1505.773

Depsipeptide antibiotic. Stereochem. revised in 2002 and full assignment made in 2005; although a 2006 paper suggests a possible revision for one amino acid residue is required. Isol. from the sponges *Callipelta* sp. and *Latrunculia* sp. Protects cells infected by HIV virus. Shows positive inotropic effect. $[\alpha]_D$ +3.6 (MeOH). λ_{max} 232 (ϵ 6919); 274 (ϵ 1272) (MeOH).

Zampella, A. *et al., J.A.C.S.*, 1996, **118**, 6202-6209 (*isol, uv, ir, pmr, cmr*)
Trevisi, L. *et al., Biochem. Biophys. Res. Commun.*, 2000, **279**, 219-222 (*activity*)
Zampella, A. *et al., Tet. Lett.*, 2002, **43**, 6163-6166 (*isol, struct*)
Zampella, A. *et al., Org. Lett.*, 2005, **7**, 3585-3588 (*config*)
Calimsiz, S. *et al., J.O.C.*, 2006, **71**, 6351-6356 (*config*)

Callipeltin B C-56

[178495-02-8]



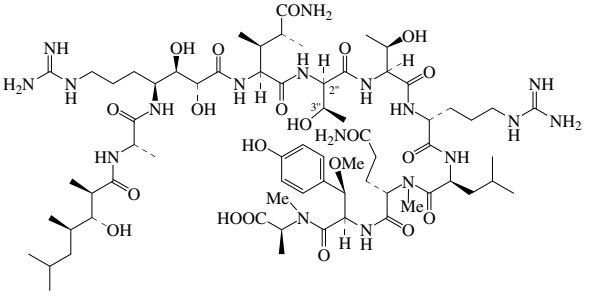
$C_{47}H_{74}N_{12}O_{14}$ 1031.174

Depsipeptide antibiotic. Stereochem. revised in 2002; although a 2006 paper suggests a revision of one amino acid residue is required. Isol. from the sponges *Callipelta* sp. and *Latrunculia* sp. Cytotoxic. $[\alpha]_D$ +11.3 (MeOH). λ_{max} 230 (ϵ 7023); 274 (ϵ 1300) (MeOH).

D'Auria, M.V. *et al., Tetrahedron*, 1996, **52**, 9589-9596 (*isol, uv, ir, pmr, cmr*)
Zampella, A. *et al., Tet. Lett.*, 2002, **43**, 6163-6166 (*isol, struct*)
Calimsiz, S. *et al., J.O.C.*, 2006, **71**, 6351-6356 (*config*)

Callipeltin C C-57

[178495-03-9]



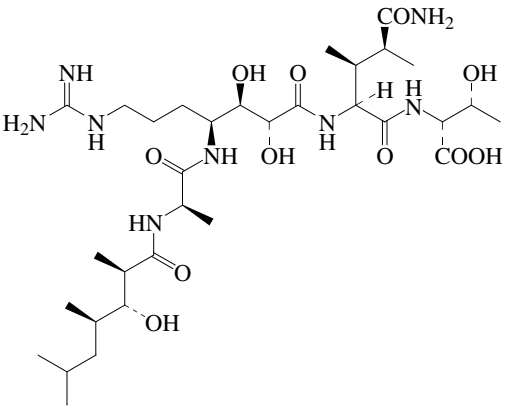
$C_{68}H_{118}N_{18}O_{21}$ 1523.788

Peptide antibiotic. Acyclic struct. of Callipeltin A, C-55. Stereochem. revised in 2002. Isol. from the sponges *Callipelta* sp. and *Latrunculia* sp. Cytotoxic. Antifungal agent. $[\alpha]_D$ -15.3 (MeOH). λ_{max} 230 (ϵ 6890); 274 (ϵ 1320) (MeOH).

3″-Deoxy, 2″,3″-didehydro(Z-): ***Callipeltin H***
[876012-50-9]
$C_{68}H_{116}N_{18}O_{20}$ 1505.773
Isol. from a *Latrunculia* sp. Amorph. solid. $[\alpha]_D^{25}$ -4.5 (c, 0.71 in MeOH).

D'Auria, M.V. *et al., Tetrahedron*, 1996, **52**, 9589-9596 (*isol, uv, ir, pmr, cmr*)
Zampella, A. *et al., Tet. Lett.*, 2002, **43**, 6163-6166 (*isol, struct*)
Sepe, V. *et al., Tetrahedron*, 2006, **62**, 833-840 (*Callipeltin H*)

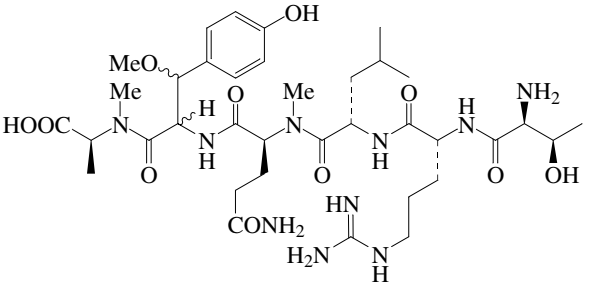
Callipeltin D C-58



$C_{32}H_{60}N_8O_{11}$ 732.873
Isol. from the sponge *Latrunculia* sp. Amorph. solid. $[\alpha]_D^{25}$ -9 (c, 0.14 in MeOH).

Zampella, A. *et al., Tet. Lett.*, 2002, **43**, 6163-6166 (*isol, pmr, cmr*)
Cranfill, D.C. *et al., Org. Lett.*, 2005, **7**, 5881-5883 (*synth*)

Callipeltin E C-59

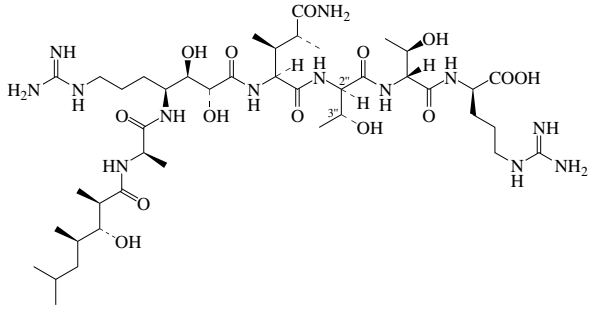


$C_{36}H_{60}N_{10}O_{11}$ 808.93
Stereochem. revised in 2006. Isol. from the sponge *Latrunculia* sp. Amorph. solid. $[\alpha]_D^{25}$ -46 (c, 0.1 in MeOH).

Zampella, A. *et al., Tet. Lett.*, 2002, **43**, 6163-6166 (*isol, pmr, cmr*)
Calimsiz, S. *et al., J.O.C.*, 2006, **71**, 6351-6356 (*synth, config*)

Callipeltin F C-60

[876012-48-5]



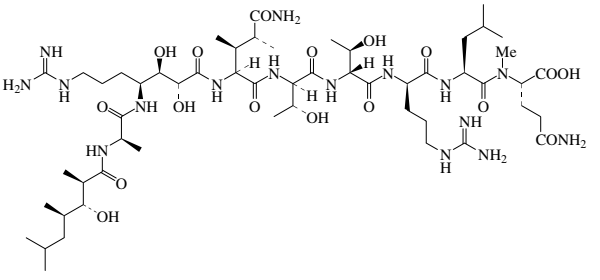
$C_{42}H_{79}N_{13}O_{14}$ 990.165
Isol. from a *Latrunculia* sp. Antifungal agent. Amorph. solid. $[\alpha]_D^{25}$ -4.3 (c, 0.35 in MeOH).

3″-Deoxy, 2″,3″-didehydro(Z-): ***Callipeltin I***
[876012-51-0]
$C_{42}H_{77}N_{13}O_{13}$ 972.15
Isol. from a *Latrunculia* sp. Amorph. solid. $[\alpha]_D^{25}$ +1.3 (c, 0.37 in MeOH).

Sepe, V. *et al., Tetrahedron*, 2006, **62**, 833-840 (*isol, pmr, cmr, ms*)

Callipeltin G C-61

[876012-49-6]

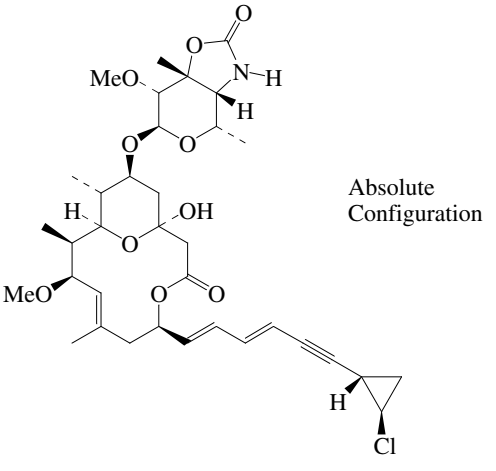


$C_{54}H_{100}N_{16}O_{17}$ 1245.481
Isol. from a *Latrunculia* sp. Antifungal agent. Amorph. solid. $[\alpha]_D^{25}$ -5.3 (c, 0.26 in MeOH).

Sepe, V. *et al., Tetrahedron*, 2006, **62**, 833-840 (*isol, pmr, cmr, ms*)

Callipeltoside A C-62

[183671-13-8]

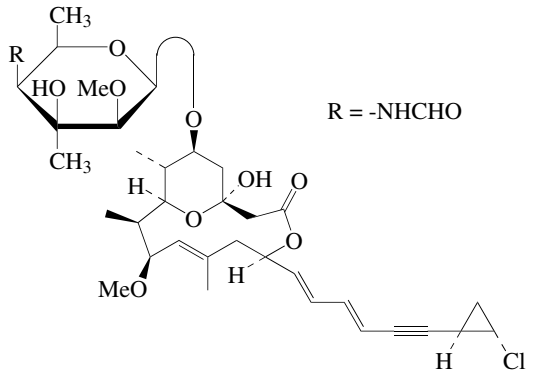


$C_{35}H_{48}ClNO_{10}$ 678.218
Macrolide antibiotic. Isol. from the sponge *Callipelta* sp. Cytotoxic agent, cell proliferation inhibitor. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -17.6 (c, 0.04 in MeOH). λ_{max} 250 (ϵ 6730); 272 (ϵ 8030); 286 (ϵ 6270) (MeOH). λ_{max} 250; 272 (ϵ 6727); 286 (MeOH) (Berdy).

Zampella, A. *et al., J.A.C.S.*, 1996, **118**, 11085-11088 (*isol, uv, ir, pmr, cmr*)
Trost, B.M. *et al., Angew. Chem., Int. Ed.*, 2002, **41**, 841-843 (*synth, abs config*)
Evans, D.A. *et al., J.A.C.S.*, 2002, **124**, 5654-5655 (*synth*)
Trost, B.M. *et al., J.A.C.S.*, 2002, **124**, 10396-10415 (*synth, abs config*)
Paterson, I. *et al., Org. Lett.*, 2003, **5**, 4477-4480 (*synth*)
Huang, H. *et al., Org. Lett.*, 2004, **6**, 4383-4385 (*synth*)

Callipeltoside B C-63

[188713-38-4]



$C_{35}H_{50}ClNO_{10}$ 680.233
Isol. from the sponge *Callipelta* sp. Cytotoxic agent. Cell proliferation inhibitor. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 250 (ϵ 6000); 272 (ϵ 8132); 286 (ϵ 6340) (MeOH).

Zampella, A. *et al., Tetrahedron*, 1997, **53**, 3243 (*isol, uv, pmr, cmr*)

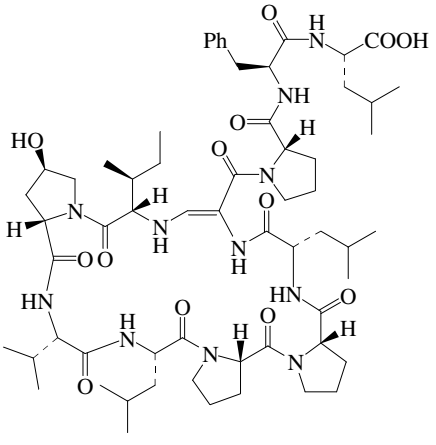
Callipeltoside C C-64

[188713-54-4]
As Callipeltoside B, C-63 with
R = OH

$C_{34}H_{49}ClO_{10}$ 653.208
Isol. from the sponge *Callipelta* sp. Cytotoxic agent. Cell proliferation inhibitor. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Zampella, A. *et al., Tetrahedron*, 1997, **53**, 3243 (*isol, uv, pmr, cmr*)

Callynormine A C-65

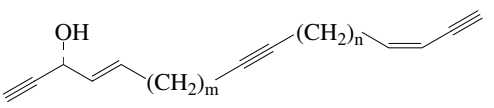


$C_{61}H_{93}N_{11}O_{13}$ 1188.472
Cyclic endiaminopeptide. Isol. from the sponge *Callyspongia abnormis*. Cryst. (MeCN). $[\alpha]_D$ -19 (c, 0.01 in MeOH). Mp >300°.

Berer, N. *et al., Org. Lett.*, 2004, **6**, 2543-2545 (*isol, pmr, cmr, cryst struct*)

Callyspongyne A C-66

4,30-Tritriacontadiene-1,32,?-triyn-3-ol
[211321-74-3]



m + n = 22

$C_{33}H_{52}O$ 464.773
Isol. from the sponge *Callyspongia* sp.

Rooney, F. *et al., Lipids*, 1998, **33**, 639-642

Callyspongyne B C-67

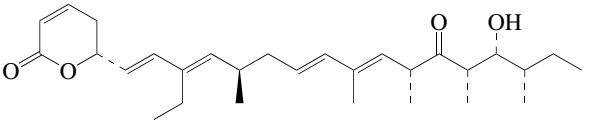
4,32-Pentatriacontadiene-1,34,?-triyn-3-ol
[211321-76-5]
As Callyspongyne A, C-66 with
m + n = 24

$C_{35}H_{56}O$ 492.827
Isol. from the sponge *Callyspongia* sp.

Rooney, F. *et al., Lipids*, 1998, **33**, 639-642

Callystatin A C-68

[189883-16-7]



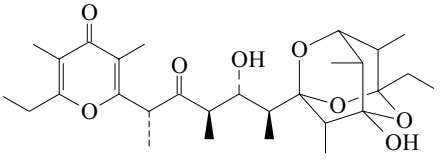
Absolute configuration

$C_{29}H_{44}O_4$ 456.664
Isol. from *Callyspongia truncata*. Cytotoxic agent. Oil. $[\alpha]_D$ -107 (c, 0.1 in MeOH). λ_{max} 243 (ϵ 30900); 300 (ϵ 1300) (no solvent reported). λ_{max} 243 (ϵ 30900); 300 (ϵ 1300) (MeOH) (Berdy).

Kobayashi, M. *et al., Tet. Lett.*, 1997, **38**, 2859-2862 (*isol, uv, pmr, cmr*)
Murakami, N. *et al., Tet. Lett.*, 1997, **38**, 5533-5536; 1998, **39**, 2349-2352 (*abs config, cd, pmr*)
Crimmins, M.T. *et al., J.A.C.S.*, 1998, **120**, 9084-9085 (*synth*)
Smith, A.B. *et al., Org. Lett.*, 2001, **3**, 1685-1688 (*synth*)
Enders, D. *et al., Chem. Eur. J.*, 2002, **8**, 4272-4284 (*synth*)
Marshall, J.A. *et al., J.O.C.*, 2002, **67**, 2751-2754 (*synth*)
Vicario, J.L. *et al., Org. Lett.*, 2002, **4**, 1023-1026 (*synth*)
Lautens, M. *et al., Synthesis*, 2002, 1993-2012 (*synth, ir, pmr, cmr*)
Kalesse, M. *et al., Chem. Eur. J.*, 2003, **9**, 1129-1136 (*synth*)
Langille, N.F. *et al., Org. Lett.*, 2004, **6**, 3203-3206 (*synth*)
Dias, L.C. *et al., J.O.C.*, 2005, **70**, 4762-4773 (*synth*)

Caloudrin B C-69

[160098-73-7]

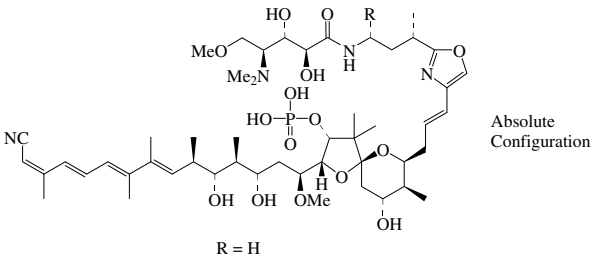


$C_{29}H_{44}O_8$ 520.662
Isol. from the mollusc *Siphonaria zelandica*.
$[\alpha]_D$ -19 ($CHCl_3$). λ_{max} 261 (ϵ 2648) (no solvent reported).

Blanchfield, J.T. *et al., Aust. J. Chem.*, 1994, **47**, 2255-2269 (*isol, uv, ir, pmr, cmr*)
Garson, M.J. *et al., Tet. Lett.*, 1994, **35**, 6929-6932 (*config*)

Calyculin A C-70

[101932-71-2]



R = H

$C_{50}H_{81}N_4O_{15}P$ 1009.181

Isol. from the marine sponge *Discodermia calyx* and from *Lamellomorpha strongylata*. Inhibitor of protein phosphatases. Apoptosis inducer. Needles (Me_2CO/Et_2O/hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 247-249°. $[\alpha]_D^{15}$ +59.8 (c, 0.12 in EtOH). Major metab. The opt. rotn., uv data and yield reported in the original paper were incorr. λ_{max} 230 (ϵ 12000); 341 (ϵ 19000) (EtOH) (Derep).

O-*Dephosphono:* ***Dephosphonocalyculin A***

[191421-64-4]

$C_{50}H_{80}N_4O_{12}$ 929.202

Isol. from *Dysidea calyx*. Protein phosphatase inhibitor. Solid.

15-Amide: ***Calyculinamide A***

[187991-80-6]

$C_{50}H_{83}N_4O_{16}P$ 1027.197

Isol. from *Dysidea calyx* and *Lamellomorpha strongylata*. $[\alpha]_D$ -41 (c, 0.5 in EtOH). $[\alpha]_D$ -18 (c, 0.005 in MeOH). Isol. by two groups of workers. Uv data not in agreement.

N-*De-Me:* **N-*Demethylcalyculin A***

[187944-08-7]

$C_{49}H_{79}N_4O_{15}P$ 995.155

Isol. from *Discodermia calyx*. Amorph. solid. $[\alpha]_D^{20}$ -18 (c, 0.01 in MeOH). λ_{max} 220 (ϵ 9000); 340 (ϵ 8000) (EtOH).

(9Z)-Isomer: ***Calyculin E***

[133445-05-3]

$C_{50}H_{81}N_4O_{15}P$ 1009.181

Isol. from *Discodermia calyx* and *Lamellomorpha strongylata*. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{23}$ -83 (c, 0.2 in EtOH). λ_{max} 230; 325 (ϵ 22000) (MeOH) (Berdy). λ_{max} 227 (ϵ 13800); 321 (ϵ 16400) (EtOH) (Berdy).

(13E)-Isomer: ***Calyculin B***

[107537-44-0]

$C_{50}H_{81}N_4O_{15}P$ 1009.181

From *Discodermia calyx* and *Lamellomorpha strongylata*. Anti-tumour agent. Amorph. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -61 (c, 0.05 in EtOH). λ_{max} 230 (ϵ 12000); 341 (ϵ 19000) (EtOH) (Derep). λ_{max} 230 (ϵ 18000); 341 (ϵ 25000) (EtOH) (Berdy).

(13E)-Isomer, 15-amide: ***Calyculinamide B***

[188292-66-2]

$C_{50}H_{83}N_4O_{16}P$ 1027.197

Isol. from *Lamellomorpha strongylata*. Protein phosphatase inhibitor. Amorph. solid. $[\alpha]_D^{20}$ -27 (c, 0.1 in EtOH). λ_{max} 227 (ϵ 26000); 335 (ϵ 45600) (EtOH). λ_{max} 227 (ϵ 26000); 335 (ϵ 45600) (MeOH) (Berdy).

(9Z,13E)-Isomer: ***Calyculin F***

[133445-06-4]

$C_{50}H_{81}N_4O_{15}P$ 1009.181

Isol. from *Discodermia calyx* and *Lamellomorpha strongylata*. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{23}$ -33 (c, 0.2 in EtOH). λ_{max} 230; 323 (ϵ 24000) (MeOH) (Berdy). λ_{max} 227 (ϵ 15200); 321 (ϵ 18400) (EtOH) (Berdy).

(9Z,13E)-Isomer, 15-amide: ***Calyculinamide F***

[187991-81-7]

$C_{50}H_{83}N_4O_{16}P$ 1027.197

Isol. from *Dysidea calyx*. Protein phosphatase inhibitor. Amorph. solid. $[\alpha]_D^{20}$ -23 (c, 0.01 in MeOH). λ_{max} 228 (ϵ 11000); 236 (ϵ 10000); 315 (ϵ 14000) (EtOH). λ_{max} 228 (ϵ 11000); 236 (ϵ 10000); 315 (ϵ 14000) (MeOH) (Berdy).

Kato, Y. *et al., J.A.C.S.*, 1986, **108**, 2780 (*isol, uv, ir, pmr, cmr, cryst struct*)
Kato, Y. *et al., J.O.C.*, 1988, **53**, 3930 (*isol, pmr, cmr*)
Okada, A. *et al., Agric. Biol. Chem.*, 1991, **55**, 2765-2771 (*Calyculins E-F*)
Matsunaga, S. *et al., Tetrahedron*, 1991, **47**, 2999
Evans, D.A. *et al., J.O.C.*, 1992, **57**, 1958; 1961; 1964 (*synth*)
Evans, D.A. *et al., Spec. Publ. - R. Soc. Chem.*, 1993, **119**, 117 (*rev*)
Tanimoto, N. *et al., Angew. Chem., Int. Ed.*, 1994, **33**, 673 (*synth*)
Dumdei, E.J. *et al., J.O.C.*, 1997, **62**, 2636 (*Calyculinamides*)
Matsunaga, S. *et al., J.O.C.*, 1997, **62**, 2640 (*Calyculinamides*)
Matsunaga, S. *et al., Tet. Lett.*, 1997, **38**, 3763 (*Dephosphonocalyculin A*)
Smith, A.B. *et al., J.O.C.*, 1998, **63**, 7596-7597 (*synth*)
Volter, K.E. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 717-722 (*pmr, cryst struct*)
Smith, A.B. *et al., J.A.C.S.*, 1999, **121**, 10468-10477; 10478-10486 (*synth*)

Calyculin C C-71

[107537-45-1]

As Calyculin A, C-70 with

R = CH_3

$C_{51}H_{83}N_4O_{15}P$ 1023.208

Isol. from *Discodermia calyx*. Antitumour agent. Smooth muscle contractor. Inhibitor of protein phosphatases. Amorph. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -65 (c, 0.05 in EtOH). λ_{max} 230 (ϵ 12000); 341 (ϵ 19000) (EtOH) (Derep). λ_{max} 230 (ϵ 15000); 340 (ϵ 19000) (EtOH) (Berdy).

(13*E*)-*form*

Calyculin D

[107447-09-6]

From *Discodermia calyx*. Antitumour agent. Smooth muscle contractor. Inhibitor of protein phosphatases. Amorph. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -41 (c, 0.05 in EtOH). λ_{max} 230 (ϵ 12000); 341 (ϵ 19000) (EtOH) (Derep).

(9Z)-Isomer: ***Calyculin G***

[135212-39-4]

$C_{51}H_{83}N_4O_{15}P$ 1023.208

Isol. from *Discodermia calyx*. Protein phosphatase inhibitor. Smooth muscle contractor. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{23}$ -81 (c, 0.1 in EtOH). λ_{max} 227 (ϵ 19000); 321 (ϵ 20800) (EtOH) (Berdy).

(9Z,13E)-Isomer: ***Calyculin H***

[135212-40-7]

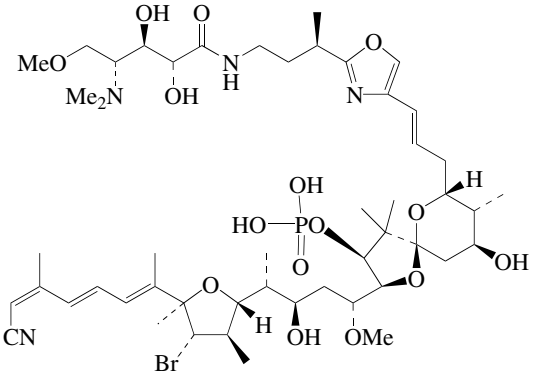
$C_{51}H_{83}N_4O_{15}P$ 1023.208

Isol. from *Discodermia calyx*. Protein phosphatase inhibitor. Smooth muscle contractor. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{23}$ -36 (c, 0.05 in EtOH). λ_{max} 227 (ϵ 22800); 321 (ϵ 28000) (EtOH) (Berdy).

Kato, Y. *et al., J.O.C.*, 1988, **53**, 3930 (*isol, pmr, cmr, struct*)
Matsunaga, S. *et al., Tetrahedron*, 1991, **47**, 2999 (*Z-isomers, isol*)
Scarlato, G.R. *et al., J.O.C.*, 1996, **61**, 6139; 6153 (*synth*)
Ogawa, A.K. *et al., J.A.C.S.*, 1998, **120**, 12435-12442 (*synth*)

Calyculin J C-72

[187991-79-3]



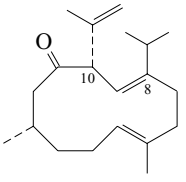
$C_{50}H_{80}BrN_4O_{15}P$ 1088.078

Isol. from the sponge *Discodermia calyx*. Protein phosphatase inhibitor. Yellow solid. $[\alpha]_D^{20}$ -10 (c, 0.08 in MeOH). λ_{max} 228 (ϵ 11000); 291 (ϵ 14000); 304 (ϵ 20000) (EtOH). λ_{max} 228 (ϵ 11000); 291 (ϵ 14000); 304 (ϵ 20000); 318 (ϵ 19000) (MeOH) (Berdy).

Matsunaga, S. *et al., J.O.C.*, 1997, **62**, 2640 (*isol, uv, pmr, cmr*)

Calyculone D C-73

[130575-02-9]



$C_{20}H_{32}O$ 288.472
Constit. of *Eunicea calyculata*. Oil. $[\alpha]_D$ +198 (c, 1 in $CHCl_3$).

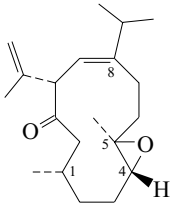
10-Epimer: ***Calyculone E***
[130694-34-7]
$C_{20}H_{32}O$ 288.472
Constit. of *Eunicea calyculata*. Oil. $[\alpha]_D$ -359 (c, 0.5 in $CHCl_3$).

*8*E*-Isomer:* ***Calyculone F***
[130694-35-8]
$C_{20}H_{32}O$ 288.472
Constit. of *Eunicea calyculata*. Oil. $[\alpha]_D$ +143 (c, 0.4 in $CHCl_3$).

*8*E*-Isomer, 10-epimer:* ***Calyculone G***
[130694-36-9]
$C_{20}H_{32}O$ 288.472
Constit. of *Eunicea calyculata*. Oil. $[\alpha]_D$ -107 (c, 0.5 in $CHCl_3$).

Shin, J. *et al., J.O.C.*, 1991, **56**, 1227 (*isol, pmr, cmr*)

Calyculones C-74



(4α,5β,8*E*)*–form*
Relative configuration

$C_{20}H_{32}O_2$ 304.472

(4α,5β,8*E*)-*form*
Calyculone A
[89088-38-0]
Constit. of *Eunicea calyculata*.
Cryst. (Et_2O).
Mp 101-102°. $[\alpha]_D^{20}$ +76 (c, 0.61 in $CHCl_3$).

7α-Acetoxy: ***7-Acetoxycalyculone A***
[656251-65-9]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Eunicea laciniata*. Cryst.
Mp 78-80°. $[\alpha]_D$ +140.3 (c, 0.06 in $CHCl_3$). λ_{max} 212 (log ϵ 3.42) (MeOH).

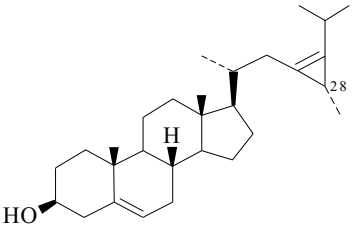
(4α,5α,8*E*)-*form*
Calyculone B
[89163-38-2]
From *Eunicea calyculata*.
Oil. $[\alpha]_D^{20}$ -28 (c, 1.1 in $CHCl_3$).

(4β,5α,8*Z*)-*form*
Calyculone C
[89163-39-3]
From *Eunicea calyculata*.
Oil. $[\alpha]_D^{20}$ +95 (c, 0.99 in $CHCl_3$).

Look, S.A. *et al., J.O.C.*, 1984, **49**, 1417
Marville, K.I. *et al., Heterocycles*, 2004, **63**, 107-113 (*7-Acetoxycalyculone A*)

Calysterol C-75

[57331-04-1]



Absolute configuration

$C_{29}H_{46}O$ 410.682
Constit. of *Calyx nicaeensis* and *Petrosia ficiformis*. Cryst.
Mp 114-116°. $[\alpha]_D$ -29.3 (c, 1 in $CHCl_3$).

5α,6-Dihydro: ***5α-Calystanol***
[117064-35-4]
$C_{29}H_{48}O$ 412.698
Isol. from the sponge *Calyx podatypa*.

5β,6-Dihydro: ***Calystanol***
[123238-26-6]
$C_{29}H_{48}O$ 412.698
Minor sterol from sponge *Calyx nicaeensis*, prob. as an endobacterial metab.

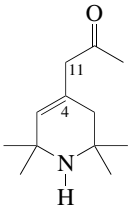
3-Epimer, 5β,6-dihydro: ***5β-Calystan-3α-ol***
[123238-74-4]
$C_{29}H_{48}O$ 412.698
Minor sterol from *Calyx nicaeensis*, prob. as endobacterial metab.

[85798-18-1]

Fattorusso, E. *et al., Tetrahedron*, 1975, **31**, 1715-1716 (*isol, struct*)
Minale, L. *et al., Experientia*, 1977, **33**, 1550-1552 (*biosynth*)
Li, L.N. *et al., J.A.C.S.*, 1982, **104**, 6726-6732 (*abs config*)
Margot, C. *et al., Chem. Comm.*, 1987, 1441-1442 (*biosynth*)
Proudfoot, J.R. *et al., J.C.S. Perkin 1*, 1987, 1283-1290 (*synth, struct*)
Doss, G.A. *et al., J.A.C.S.*, 1988, **110**, 8124-8128 (*5α-Calystanol*)
Ha, T.B.T. *et al., Steroids*, 1989, **53**, 487-499 (*dihydro*)

Calyxamine A C-76

[199105-62-9]



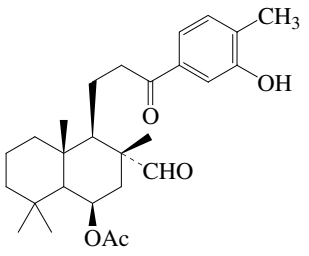
$C_{12}H_{21}NO$ 195.304
Alkaloid from the sponge *Calyx podatypa*. Needles ($CHCl_3$/hexane) (as trifluoroacetate salt). λ_{max} 205 (ϵ 1000) (MeOH) (TFA salt).

$\Delta^{4,11}$-Isomer: ***Calyxamine B***
[150710-72-8]
$C_{12}H_{21}NO$ 195.304
Alkaloid from *Calyx podatypa*. Cryst. (as trifluoroacetate salt). Possible artifact. λ_{max} 231 (ϵ 10400) (MeOH) (TFA salt).

Rodriguez, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 1331-1333 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)

Caminatal C-77

[588725-02-4]



Relative Configuration

$C_{27}H_{38}O_5$ 442.594
Isol. from the sponge *Suberites caminatus*. Oil. $[\alpha]_D^{20}$ +167 (c, 0.12 in $CHCl_3$).

Diaz-Marrero, A.R. *et al., Tet. Lett.*, 2003, **44**, 5939-5942 (*isol, pmr, cmr, ms*)

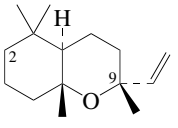
Cangitoxin C-78

Peptide containing 48 amino acid residues incl. 6 cysteines. Isol. from the sea anemone *Bunodosoma cangicum*. Epileptogenic.

Cunha, R.B. *et al., Toxicon*, 2005, **45**, 207-217 (*struct*)

Caparrapioxide C-79

[20303-73-5]
[57345-37-6]



$C_{15}H_{26}O$ 222.37
Isol. from the frontal gland of *Amitermes evuncifer*. Also isol. from the sponge *Dysidea fragilis*. Oil.

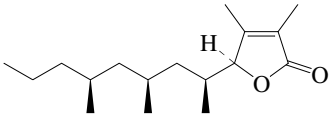
9-Epimer: ***9-Epicaparrapioxide***
[57345-36-5]
[62107-46-4 (*+-form*)]
$C_{15}H_{26}O$ 222.37
Isol. from *Amitermes evuncifer*. Called 8-epi in the lit.

9-Epimer, 2β-bromo: ***3β-Bromo-8-epicaparrapioxide***
[62078-13-1]
$C_{15}H_{25}BrO$ 301.266
Metab. of *Laurencia obtusa*. Oil solidifying at -20°. Sol. MeOH, hexane. $[\alpha]_D^{21}$ +30.4 (c, 1.46 in EtOH). Relative stereochem. known only.

Wadhams, L.J. *et al., Tet. Lett.*, 1974, **15**, 1697-1700 (*9-Epicaparrapioxide*)
Cookson, R.C. *et al., Helv. Chim. Acta*, 1976, **59**, 1158 (*synth, pmr*)
Faulkner, D.J. *et al., Phytochemistry*, 1976, **15**, 1992-1993 (*3-Bromo-8-epicaparrapioxide*)
Baker, R. *et al., Tet. Lett.*, 1978, 4073 (*isol*)
Hoye, T.R. *et al., J.O.C.*, 1979, **44**, 3461 (*synth*)
Barrero, A.F. *et al., Tet. Lett.*, 1998, **39**, 9543-9544 (*synth*)
Shen, Y.C. *et al., Chin. Pharm. J. (Taipei)*, 1999, **51**, 213-218; *CA*, **132**, 47791t (*isol, Dysidea*)
Carter-Franklin, J.N. *et al., J.A.C.S.*, 2004, **126**, 15060-15066 (*biosynth*)
Uyanik, M. *et al., Bioorg. Med. Chem.*, 2005, **13**, 5055-5065 (*synth*)

Capensifuranone C-80

*3,4-Dimethyl-5-(1,3,5-trimethyloctyl)-2(5*H*)-furanone*



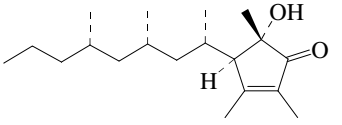
Absolute Configuration

$C_{17}H_{30}O_2$ 266.423
Isol. from the marine mollusc *Siphonaria capensis*. Oil. $[\alpha]_D^{21}$ -15.1 (c, 0.29 in $CHCl_3$).

Beukes, D.R. *et al., Tetrahedron*, 1999, **55**, 4051-4056 (*isol, ir, pmr, cmr, ms*)
Williams, D.R. *et al., J.O.C.*, 2004, **69**, 5374-5382 (*synth, abs config*)

Capensinone C-81

5-Hydroxy-2,3,5-trimethyl-4-(1,3,5-trimethyloctyl)-2-cyclopenten-1-one

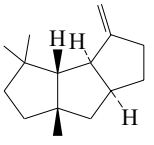


$C_{19}H_{34}O_2$ 294.476
Isol. from the marine mollusc *Siphonaria capensis*. Yellow oil. $[\alpha]_D^{21}$ -65 (c, 0.42 in $CHCl_3$).

Beukes, D.R. *et al., Tetrahedron*, 1999, **55**, 4051-4056 (*isol, ir, pmr, cmr, ms*)

9(12)-Capnellene C-82

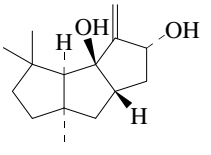
[68349-51-9]



$C_{15}H_{24}$ 204.355
Constit. of *Capnella imbricata*. Oil. $[\alpha]_D^{20}$ -145 (c, 0.4 in $CHCl_3$).

Ayanoglu, E. *et al., Tet. Lett.*, 1978, 1671 (*isol*)
Stevens, K.E. *et al., Tet. Lett.*, 1981, **22**, 4393 (*synth*)
Fujita, T. *et al., Tet. Lett.*, 1982, **23**, 4091 (*synth*)
Oppolzer, W. *et al., Tet. Lett.*, 1982, **23**, 4669 (*synth*)
Mehta, G. *et al., Chem. Comm.*, 1983, 824 (*synth*)
Little, D.R. *et al., J.A.C.S.*, 1983, **105**, 928 (*synth*)
Paquette, L.A. *et al., Can. J. Chem.*, 1984, **62**, 2415 (*synth*)
Iyoda, M. *et al., Chem. Comm.*, 1987, 1607 (*synth*)
Meyers, A.I. *et al., J.O.C.*, 1990, **55**, 791; 3966 (*synth*)
Stille, J.R. *et al., J.O.C.*, 1990, **55**, 843 (*synth*)
Wang, Y. *et al., J.O.C.*, 1990, **55**, 4504 (*synth*)
Sonowane, H.R. *et al., Tetrahedron*, 1991, **47**, 8259 (*synth*)
Ihara, M. *et al., J.C.S. Perkin 1*, 1992, 865 (*synth*)
Gambacorta, A. *et al., Tetrahedron*, 1992, **48**, 4559 (*synth*)
Balme, G. *et al., Tetrahedron*, 1994, **50**, 403 (*synth*)
Asaoka, M. *et al., Tetrahedron*, 1994, **50**, 655 (*synth*)
Tanaka, K. *et al., Chem. Comm.*, 1996, 1839 (*synth*)
Nicolaou, K.C. *et al., Classics in Total Synthesis, Targets, Strategies, Methods*, VCH, 1996, 382 (*bibl, synth*)
Ohshima, T. *et al., J.A.C.S.*, 1996, **118**, 7108 (*synth*)
Singh, V. *et al., J.O.C.*, 1998, **63**, 4011-4017 (*synth*)
Samajdar, S. *et al., Tetrahedron*, 1998, **54**, 1789-1800 (*synth*)

9(12)-Capnellene-8,10-diol C-83

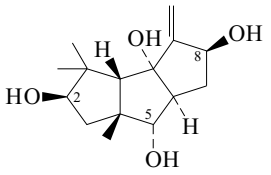


$C_{15}H_{24}O_2$ 236.353

(ent*-8β,10α)-*form [61228-59-9]
Constit. of *Capnella imbricata*. Algicidal. Cryst. (hexane). Mp 113-114°. $[\alpha]_D^{21}$ +41 (c, 0.15 in $CHCl_3$).

Sheikh, Y.M. *et al., Tetrahedron*, 1976, **32**, 1171-1178 (*isol, struct*)
Mak, T.C.W. *et al., Zhongshan Daxue Xuebao Ziran Kexueban*, 1985, 22-27; *CA*, **106**, 33340w (*cryst struct, abs config*)
Pattenden, G. *et al., J.C.S. Perkin 1*, 1988, 1077-1083 (*synth*)
Morris, L.A. *et al., Tetrahedron*, 1998, **54**, 12953-12958 (*isol, pmr, cmr*)

9(12)-Capnellene-2,5,8,10-tetrol C-84



$C_{15}H_{24}O_4$ 268.352

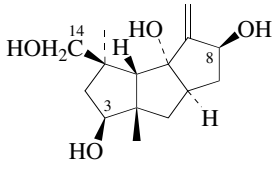
(2β,5α,8β,10α)-*form* [71596-73-1]
Constit. of *Capnella imbricata*.
Cryst. (EtOH).
Mp 219°. $[\alpha]_D^{22}$ +17 (c, 0.9 in MeOH).

8-Ac: ***8β-Acetoxy-9(12)-capnellene-2β,5α,10α-triol***
[97480-34-7]
$C_{17}H_{26}O_5$ 310.389
Constit. of *Capnella imbricata*.

2,5-Di-Ac: ***2β,5α-Diacetoxy-9(12)-capnellene-8β,10α-diol***
[97480-29-0]
$C_{19}H_{28}O_6$ 352.427
Constit. of *Capnella imbricata*. Cryst. (Et_2O/hexane).
Mp 65-66°.

Kaisin, M. *et al., Bull. Soc. Chim. Belg.*, 1979, **88**, 253-258 (*isol, struct*)
Kaisin, M. *et al., Tetrahedron*, 1985, **41**, 1067-1072 (*isol, deriv*)

9(12)-Capnellene-3,8,10,14-tetrol C-85



$C_{15}H_{24}O_4$ 268.352

(3β,8β,10α)-*form* [65563-83-9]
Constit. of *Capnella imbricata*.
Cryst.
Mp 192-195°.

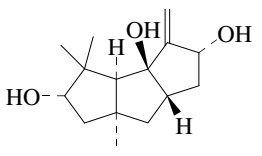
3-Ac:
$C_{17}H_{26}O_5$ 310.389
Constit. of *Capnella imbricata*. Yellow oil. $[\alpha]_D$ +39.7 (c, 0.1 in $CHCl_3$).

8-Ac: [97480-32-5]
$C_{17}H_{26}O_5$ 310.389
Constit. of *Capnella imbricata*.

3,14-Di-Ac:
$C_{19}H_{28}O_6$ 352.427
Constit. of *Capnella imbricata*.

Sheikh, Y.M. *et al., Tetrahedron*, 1977, **33**, 2115 (*isol*)
Kaisin, M. *et al., Tetrahedron*, 1985, **41**, 1067 (*isol*)
Mase, T. *et al., Tet. Lett.*, 1986, **27**, 5245 (*synth*)
Morris, L.A. *et al., Tetrahedron*, 1998, **54**, 12953-12958 (*isol, pmr, cmr*)

9(12)-Capnellene-2,8,10-triol C-86



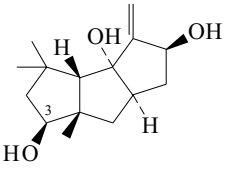
$C_{15}H_{24}O_3$ 252.353

(*ent*-2β,8β,10α)-*form* [61228-61-3]
Constit. of *Capnella imbricata*.
Oil.

2-Ac: ***2-Acetoxy-9(12)-capnellene-8,10-diol***
[97480-31-4]
$C_{17}H_{26}O_4$ 294.39
Constit. of *Capnella imbricata*.

Sheikh, Y.M. *et al., Tetrahedron*, 1976, **32**, 1171-1178 (*isol*)
Kaisin, M. *et al., Tetrahedron*, 1985, **41**, 1067-1072 (*2-Ac*)
Li, R. *et al., Zhongshan Daxue Xuebao Ziran Kexueban*, 1985, 17-21; *CA*, **105**, 187928k (*cryst struct, abs config*)

9(12)-Capnellene-3,8,10-triol C-87



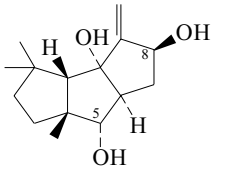
$C_{15}H_{24}O_3$ 252.353

(3β,8β,10α)-*form* [54928-07-3]
Constit. of *Capnella imbricata*.
Cryst. (Et_2O).
Mp 114-117°. $[\alpha]_D$ +2 (c, 0.31 in $CHCl_3$).

3-Ac: ***3β-Acetoxy-9(12)-capnellene-8β,10α-diol***
[97480-26-7]
$C_{17}H_{26}O_4$ 294.39
Constit. of *Capnella imbricata*.

Sheikh, Y.M. *et al., Tetrahedron*, 1976, **32**, 1171 (*isol, struct*)
Karlsson, R. *et al., Acta Cryst. B*, 1977, **33**, 1143 (*cryst struct*)
Kaisin, M. *et al., Tetrahedron*, 1985, **41**, 1067 (*deriv*)

9(12)-Capnellene-5,8,10-triol C-88



$C_{15}H_{24}O_3$ 252.353

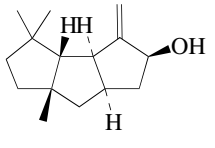
(5α,8β,10α)-*form* [61228-60-2]
Constit. of *Capnella imbricata*.
Cryst. (Et_2O).
Mp 132-133°. $[\alpha]_D^{21}$ +34.02 (c, 1.3 in $CHCl_3$).

5-Ac: ***5α-Acetoxy-9(12)-capnellene-8β,10α-diol***
[97480-27-8]
$C_{17}H_{26}O_4$ 294.39
Constit. of *Capnella imbricata*. Cryst. (hexane).
Mp 94-96°.

8-Ac: ***8β-Acetoxy-9(12)-capnellene-5α,10α-diol***
[97480-30-3]
$C_{17}H_{26}O_4$ 294.39
Constit. of *Capnella imbricata*.

Sheikh, Y.M. *et al., Tetrahedron*, 1976, **32**, 1171 (*isol*)
Kaisin, M. *et al., Tetrahedron*, 1985, **41**, 1067 (*deriv*)

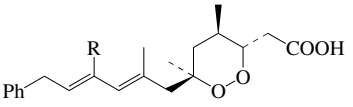
9(12)-Capnellen-8-ol C-89



$C_{15}H_{24}O$ 220.354

8β-*form* [215650-33-2]
Constit. of *Capnella imbricata*.
Amorph. powder. $[\alpha]_D$ +19.5 (c, 0.2 in $CHCl_3$).
Morris, L.A. *et al., Tetrahedron*, 1998, **54**, 12953-12958 (*isol, pmr, cmr*)

Capucinoic acid A C-90



Relative Configuration

R = H

$C_{21}H_{28}O_4$ 344.45
Isol. from *Plakinastrella onkodes*. Cytotoxic. Oil (as Me ester). $[\alpha]_D^{25}$ -44.8 (c, 0.67 in CH_2Cl_2) (Me ester). λ_{max} 227 (ϵ 5330) (CH_2Cl_2).

Williams, D.E. *et al., J. Nat. Prod.*, 2001, **64**, 281-285

Capucinoic acid B C-91

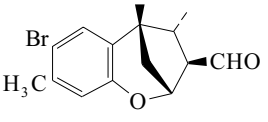
As Capucinoic acid A, C-90 with
R = CH_3

$C_{22}H_{30}O_4$ 358.477
Isol. from *Plakinastrella onkodes* and a *Plakortis* sp. Cytotoxic. Oil (as Me ester). $[\alpha]_D^{25}$ -48.7 (c, 0.37 in CH_2Cl_2) (Me ester). λ_{max} 229 (ϵ 3830) (CH_2Cl_2) (Me ester).

Williams, D.E. *et al., J. Nat. Prod.*, 2001, **64**, 281-285

Caraibical C-92

[79383-37-2]

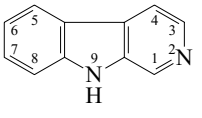


$C_{15}H_{17}BrO_2$ 309.202
Constit. of *Laurencia caraibica*. Cryst.
Mp 106-108°. $[\alpha]_D$ +42 (c, 1.01 in $CHCl_3$). λ_{max} 209 (ϵ 3550); 289 (ϵ 1120); 297 (ϵ 1120) (EtOH) (Derep).

Izac, R.R. *et al., Tet. Lett.*, 1981, 1799

β-Carboline C-93

*9H-Pyrido[3,4-*b*]indole, 9CI. 2,9-Diazafluorene. Norharman. 2-Carboline. Carbazoline*†
[244-63-3]



$C_{11}H_8N_2$ 168.198
Alkaloid from *Chrysophyllum lacourtianum*, *Nocardia* sp., *Catharanthus roseus* leaves, *Lolium perenne*, *Strychnos johnsonii*, *Strychnos potatorum*, and *Festuca arundinacea*. Prod. by *Streptomyces* sp., a metab. from the New Zealand ascidian *Ritterella sigillinoides*. Also a trace constit. of the fluorescent dinoflagellate *Noctiluca miliaris*. Plant growth and enzyme inhibitor. Potentiator of benzo[*a*]pyrene induced mutagenicity, antiparasitic, antirypanosomal agent. A comutagen with aromatic amines active towards bacteria. Needles (EtOH). Sol. hot H_2O; spar. sol. C_6H_6, petrol. Mp 198.5°. Blue fluor. in dil. acid soln. λ_{max} 235 (ϵ 31000); 290; 350 (ϵ 4600) (MeOH) (Berdy).
▶ Exp. nephrotoxic at high doses. A comutagen. UU9350000

N^2-*Oxide:* [24223-07-2]
$C_{11}H_8N_2O$ 184.197
Mp 256°.

N^2-*Me: 2-Methyl-9*H*-pyrido[3,4-*b*]indolium. **Normelinonine F***
[17994-14-8]
[5667-11-8, 21951-87-1]
$C_{12}H_{11}N_2^{\oplus}$ 183.232
Quaternary alkaloid from *Strychnos usambarensis* (Strychnaceae). Antimitotic agent. Poorly sol. hexane.

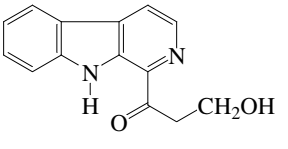
*3,4-Dihydro, 9-Ac: 9-Acetyl-4,9-dihydro-3*H*-pyrido[3,4-*b*]indole, 9CI. 9-Acetyl-3,4-dihydro-β-carboline*
[76528-83-1]
$C_{13}H_{12}N_2O$ 212.251
Alkaloid from the roots of *Adhatoda vasica* (Acanthaceae). Mp 165-166° Mp 187-188° (as hydrochloride).

[244-66-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 681D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 164C (*nmr*)
Kermack, W.O. *et al., J.C.S.*, 1921, **119**, 1602-1642 (*synth*)
Späth, E. *et al., Ber.*, 1940, **73**, 719-723 (*synth*)
Pruckner, F. *et al., Annalen*, 1943, **554**, 127-144 (*uv*)
Poindexter, E.H. *et al., Phytochemistry*, 1961, **1**, 215 (*isol, uv, ir*)
Coutts, R.T. *et al., Org. Mass Spectrom.*, 1970, **3**, 879 (*ms*)
Balkau, F. *et al., Aust. J. Chem.*, 1973, **26**, 1501 (*pmr*)
Bush, L.P. *et al., J. Chromatogr.*, 1975, **111**, 165 (*isol*)
Deumie, M. *et al., J. Photochem.*, 1979, **10**, 365 (*uv*)
Inoue, S. *et al., Chem. Lett.*, 1980, 297-298 (*isol, dinoflagellate*)
Bobbitt, J.M. *et al., J.O.C.*, 1980, **45**, 1978 (*synth*)
Jain, M.P. *et al., Phytochemistry*, 1980, **19**, 1880 (*9-Ac-3,4-dihydro*)
Sugimura, T. *et al., Biol. React. Intermed. 2, Chem. Mech. Biol. Eff.*, Snyder, R. *et al* (ed.), (see *Adv. Exp. Med. Biol.* v136A-136B), Plenum Press, 1982, 1011 (*comutagenicity*)
Caprasse, M. *et al., J. Pharm. Belg.*, 1983, **38**, 135-139 (*Normelinonine F*)
Nakagawa, M. *et al., Tet. Lett.*, 1983, **24**, 2171 (*synth*)
Hiemstra, H.C. *et al., Tetrahedron*, 1983, **39**, 3981 (*synth*)
Becalski, A. *et al., Acta Pol. Pharm.*, 1984, **41**, 601 (*synth*)
Koike, K. *et al., Org. Magn. Reson.*, 1984, **22**, 471 (*cmr*)
Atta-ur-Rahman, *et al., Planta Med.*, 1985, 287 (*isol, uv, ir, pmr, cmr, ms*)
Rommelspacher, H. *et al., Prog. Drug Res.*, 1985, **29**, 415 (*rev*)
Yomosa, K. *et al., Agric. Biol. Chem.*, 1987, **51**, 921 (*isol, bibl*)
Lake, R.J. *et al., Aust. J. Chem.*, 1989, **42**, 1201 (*isol, uv, ir, pmr, cmr*)
Hagiwara, A. *et al., Toxicol. Pathol.*, 1992, **20**, 197 (*tox*)
Rocca, P. *et al., Tetrahedron*, 1993, **49**, 49 (*synth*)
Nakano, K. *et al., Mutat. Res.*, 2000, **470**, 141-146 (*comutagenicity, pmr*)
Kast, O. *et al., Synth. Commun.*, 2003, **33**, 3843-3850 (N^2-*oxide*)
Lewis, R.J. *et al., J.C.S.*, 1937, 466-473 (*synth*)
Braestrup, C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1980, **77**, 2288-2292 (*isol, ms, pmr, cmr*)
Cain, M. *et al., J. Med. Chem.*, 1982, **25**, 1081-1091 (*9-Me Me ester*)
Lippke, K.P. *et al., J. Med. Chem.*, 1983, **26**, 499-503 (*synth, propyl ester, pharmacol*)
Coutts, R.T. *et al., Heterocycles*, 1984, **22**, 131-142 (*amides*)
Moody, C.J. *et al., J.C.S. Perkin 1*, 1984, 2895-2901 (*synth*)
Plate, R. *et al., J.O.C.*, 1986, **51**, 309-314 (*synth*)
Maclaren, J.A. *et al., Aust. J. Chem.*, 1989, **42**, 813-821 (*synth, bibl*)
Koike, K. *et al., Phytochemistry*, 1990, **29**, 3060-3061 (*Et ester*)
Dekhane, M. *et al., Tetrahedron*, 1994, **50**, 6299-6306 (*synth*)
Cabrera, G.M. *et al., J. Nat. Prod.*, 1999, **62**, 759-760 (*3-Carboxy-2-methyl-β-carbolinium*)
Kubicki, M. *et al., Acta Cryst. C*, 2001, **57**, 728-729 (*Me ester, cryst struct*)
Leu, Y.-L. *et al., Chem. Pharm. Bull.*, 2003, **51**, 599-601 (*Taraxacine B*)

1-(β-Carbolin-1-yl)-3-hydroxy-1-propanone C-95

*3-Hydroxy-1-(9*H*-pyrido[3,4-*b*]indol-1-yl)-1-propanone. 1-(3-Hydroxypropanoyl)-β-carboline*



$C_{14}H_{12}N_2O_2$ 240.261
Prod. by the marine bacterium strain Bio215. Yellowish-green solid.

Shaaban, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*isol, pmr, ms*)

Carbon tetrabromide C-96

Tetrabromomethane, 9CI. Carbon bromide†

[558-13-4]

CBr_4

CBr_4 331.627

Isol. from various marine algae. Monoclinic cryst. (below 46.8°). Sol. EtOH, Et_2O, $CHCl_3$; insol. H_2O. $d_4^{99.5}$ 2.96.

Mp 94.3° (90-91°). Bp_{50} 102°. $n_D^{99.5}$ 1.5942. Dimorphic; crystals transformed at 46.8° to cubic form.

▶ High vapour conc. narcotic. Eye and skin irritant. LD_{50} (mus, scu) 298 mg/kg. Hepatotoxic. OES: long-term 0.1 ppm; short-term 0.3 ppm. FG4725000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 86B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 122A (*ir*)
Wallach, O. *et al., Annalen*, 1893, **275**, 145 (*synth*)
Kendall, J. *et al., J.A.C.S.*, 1923, **45**, 973 (*synth*)
Schaum, K. *et al., Annalen*, 1928, **462**, 194 (*props*)
Nonez, F.G. *et al., CA*, 1936, **30**, 5556 (*synth*)
Kaposi, O. *et al., Acta Chim. Acad. Sci. Hung.*, 1976, **89**, 221 (*ms*)
Rudman, R. *et al., J. Chem. Phys.*, 1980, **72**, 1629 (*cryst struct*)
Dostovalova, V.I. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1985, 2467; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 2282 (*cmr*)
Torrie, B.H. *et al., J. Raman Spectrosc.*, 1988, **19**, 79 (*Raman, ir*)
Chizhov, O.S. *et al., Org. Mass Spectrom.*, 1992, **27**, 699 (*ms*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **2**, 997-999 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Smirnov, V.V. *et al., Zh. Org. Khim.*, 2002, **38**, 1004-1008; *Russ. J. Org. Chem. (Engl. Transl.)*, 2002, **38**, 962-966 (*use*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 2; 3478
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0300
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 258
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CBX750

Carbon tetrachloride C-97

Tetrachloromethane, 9CI. Carbon chloride (CCl_4). Carbon chloride†*. Perchloromethane. Tetra. F10. Halon 1040. R10*

[56-23-5]

CCl_4

CCl_4 153.822

Produced by chlorination of hydrocarbons or of Carbon disulfide. Isol from several plants and marine algae. Solv. for org. compds., formerly used in fire extinguishers, as a dry-cleaning solv. and as a grain fumigant. Used in manuf. of chlorofluoromethanes. Chlorinating agent, source of $:CCl_2$. Reference material used in elemental microanalysis. Anthelmintic. Liq. Sol. EtOH, Et_2O; prac. insol. H_2O. d_4^0 1.63.

Mp 21.2° Mp 23.8° Mp 28.6° (trimorph.). Bp 76.74°. n_D^{15} 1.4631.

▶ Toxic by inhalation and skin contact. Dec. to highly toxic Carbonyl chloride if strongly heated in the presence of air. Production controlled by environmental legislation, illegal in EU from 1996. Eye and skin irritant. Repeated skin exposure can cause dermatitis. Acute and chronic exposure cause gastrointestinal and CNS disturbances. High vapour conc. narcotic. Hepatotoxic and nephrotoxic. Poss. human carcinogen. LD_{50} (rat, orl) 2350 mg/kg. LC_{50} (rat, ihl) 8000 ppm (4h exposure). Exp. carcinogen. Exp. reprod. and teratogenic effects. Non-flammable, autoignition temp. >1000°. OES: long-term 2 ppm (Sk). FG4900000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 84C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 125B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 121B (*ir*)
Analyst (London), 1972, **97**, 740 (*microanal*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 69 (*use*)
Causley, G.C. *et al., J. Electron Spectrosc. Relat. Phenom.*, 1977, **11**, 383 (*uv*)
IARC Monog., 1979, **20**, 371; *Suppl.* 6, 136; *Suppl.* 7, 143 (*rev, tox*)
Dostovalova, V.I. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1985, 2467; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1985, 2282 (*cmr*)
Organo-chlorine Solvents, Royal Society of Chemistry, 1986, 225 (*tox, rev*)
Kalf, G.F. *et al., Annu. Rev. Pharmacol. Toxicol.*, 1987, **27**, 399 (*tox*)
Holmes, J.L. *et al., Int. J. Mass Spectrom. Ion Processes*, 1988, **83**, 285 (*ms*)
Andrews, L. *et al., J. Mol. Struct.*, (*Theochem*), 1989, **200**, 325 (*ms, spectra*)
Chumaevskii, N.A. *et al., Zh. Neorg. Khim.*, 1989, **34**, 1416; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1989, **34**, 798 (*Raman*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **5**, 1062 (*rev, synth, props*)
Stevenson, R. *et al., Chem. Br.*, 1992, **28**, 208 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1100
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*rev, occur*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0316
Luxon, S.G. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CBY000

Carbonyl iodide C-98

Carbonic diiodide. Diiodoformaldehyde. Iodophosgene

[13353-01-0]

I_2CO

CI_2O 281.819

Reported from the marine alga *Asparagopsis taxiformis*. Existence may be considered dubious. Ir and ms data have been reported.

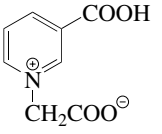
Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*occur*)
Barnes, I. *et al., Chem. Phys. Lett.*, 1995, **246**, 594-599 (*ir*)
Parkington, M.J. *et al., J.C.S. Dalton*, 1997, 251-256 (*attempted synth*)

3-Carboxy-1-(carboxymethyl)pyridinium betaine C-99

1-Carboxymethylnicotinic acid

[137591-89-0]

[148717-05-9, 148717-06-0]



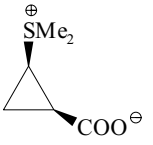
$C_8H_7NO_4$ 181.148

Alkaloid from the sponge *Anthosigmella* cf. *raromicrosclera*. Cysteine protease inhibitor. λ_{max} 267 (ϵ 5000) (H_2O).

Chen, X.-M. *et al., J. Mol. Struct.*, 1991, **249**, 135-140 (*synth, cryst struct*)
Chen, X.-M. *et al., J. Crystallogr. Spectrosc. Res.*, 1993, **23**, 291-296 (*cryst struct*)
Matsunaga, S. *et al., J. Nat. Prod.*, 1998, **61**, 671-672 (*isol, synth, uv, pmr, cmr*)

(2-Carboxycyclopropyl)dimethylsulfonium, 9CI C-100

2-(Dimethylsulfonio)cyclopropanecarboxylate. ***Gonyauline***



(1*R*,2*R*)–*form*

$C_6H_{10}O_2S$ 146.21

(1*R*,2*R*)-*form*

(+)-cis-*form*

[125559-51-5]

Isol. from the dinoflagellate *Gonyaulax polyedra*. Shortens the period of the circadian clock for the host organism. $[\alpha]_D$ +214 (c, 0.83 in MeOH).

(1*RS*,2*RS*)-*form*

(±)-cis-form

[132905-34-1]

Needles. Mp 141-143°.

(1*RS*,2*SR*)-*form*

(±)-trans-*form*

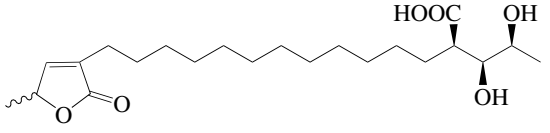
[132905-35-2]

Amorph. solid. Mp 146-151°.

[125559-53-7, 125559-58-2]

Roenneberg, T. *et al., Experientia*, 1990, **47**, 103-106 (*isol, pmr, cmr*)
Nakamura, H. *et al., J.C.S. Perkin 1*, 1990, 3219-3220 (*synth*)
Nakamura, H. *et al., Tet. Lett.*, 1992, **33**, 2821-2822 (*synth, abs config*)
Nakamura, H. *et al., Tetrahedron*, 1997, **53**, 9067-9074 (*biosynth, cmr*)

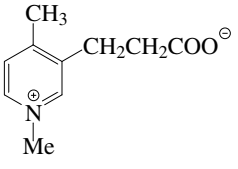
3-(13-Carboxy-14,15-dihydroxyhexadecyl)-5-methyl-2(5*H*)-furanone C-101



$C_{22}H_{38}O_6$ 398.539

*Di-Ac: 3-(14,15-Diacetoxy-13-carboxyhexadecyl)-5-methyl-2(5*H*)-furanone*
[27261-77-4]
$C_{26}H_{42}O_8$ 482.613
Isol. from the gorgonian *Pterogorgia guadalupensis*. Cryst. (2-propanol aq.).
Mp 81.1-82.9°. $[\alpha]_D$ -8.3 (c, 0.47 in $CHCl_3$). λ_{max} 204 (ϵ 17440) (EtOH aq.).
Schmitz, F.J. *et al., J.O.C.*, 1971, **36**, 719-721 (*isol, uv, ir, pmr*)

3-(2-Carboxyethyl)-1,4-dimethylpyridinium, 9CI C-102
Sulcatine
[264870-65-7]



$C_{10}H_{13}NO_2$ 179.218
Zwitterionic. Isol. from the ascidian *Microcosmus vulgaris*. Shows antiproliferative activity. Amorph. solid.
Aiello, A. *et al., J. Nat. Prod.*, 2000, **63**, 517-519 (*isol, pmr, cmr*)

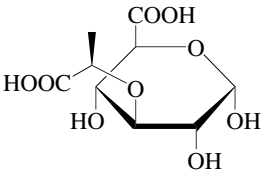
(2-Carboxyethyl)dimethylsulfonium(1+) C-103
Dimethyl-β-propiothetin
[6708-36-7]
[4337-33-1]

$Me_2S^{\oplus}CH_2CH_2COOH$
$C_5H_{11}O_2S^{\oplus}$ 135.207
Isol. from green and red algae, e.g. *Enteromorpha intestinalis, Ulva lactuca*. Also from *Spartina anglica*. Biol. precursor of Dimethyl sulfide, D-894. Fish feeding stimulant. Needles (EtOH) (as chloride).
Mp 134° dec. (129°). pK_a 3.35.

Betaine: 3-Dimethylsulfonio propanoate. Dimethylpropiothetin. DMSP. (2-Carboxyethyl)dimethylsulfonium betaine
[7314-30-9]
[20986-22-5, 44743-29-5]
$C_5H_{10}O_2S$ 134.199
Isol. from numerous marine sources. Biochemical source of dimethyl sulfide. Growth stimulant for fish. Cryst. (EtOH).
Mp 112-114°. Zwitterion.

Challenger, F. *et al., J.C.S.*, 1948, 1591-1597 (*isol, synth*)
Greene, R.C. *et al., J. Biol. Chem.*, 1962, **237**, 2251 (*biosynth*)
Ishida, Y. *et al., Agric. Biol. Chem.*, 1967, **31**, 756-757 (*betaine, isol, pmr*)
Klee, W.A. *et al., Biochemistry*, 1967, **6**, 988 (*conformn, ir*)
Larher, F. *et al., Phytochemistry*, 1977, **16**, 2019 (*isol*)
Blunden, G. *et al., Magn. Reson. Chem.*, 1986, **24**, 965 (*nmr*)
Sciuto, S. *et al., J. Nat. Prod.*, 1988, **51**, 322-325 (*isol*)
Simo, R. *et al., Anal. Chem.*, 1996, **68**, 1493-1498 (*betaine, anal*)

3-*O*-(1-Carboxyethyl)glucuronic acid C-104

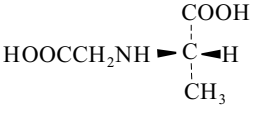


$C_9H_{14}O_9$ 266.204

D-(1′*R*)-*form*
Component of the exopolysaccharide of bacterium *Alteromonas* sp. from a deep sea hydrothermal vent.
Dubureucq, G. *et al., Carbohydr. Res.*, 1996, **290**, 175-181 (*isol, struct*)

(2-Carboxyethyl)trimethylarsonium betaine C-105
(2-Carboxyethyl)trimethylarsonium hydroxide inner salt, 9CI. 3-Trimethylarsoniopropanoic acid. Homoarsenobetaine
[117929-08-5]
$Me_3As^{\oplus}CH_2CH_2COO^{\ominus}$
$C_6H_{13}AsO_2$ 192.089
Zwitterion. Constit. of fish muscle tissue and probably occurs in many other marine animals. Cryst. (Me_2CO/MeOH).
Mp 178°.
Kaise, T. *et al., Appl. Organomet. Chem.*, 1988, **2**, 339-347 (*synth, pmr, cmr*)
Francesconi, K.A. *et al., Chem. Comm.*, 2000, 1083-1084 (*occur*)

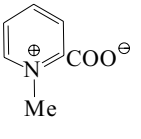
N-(Carboxymethyl)alanine, 9CI C-106
Strombine



$C_5H_9NO_4$ 147.13

(*S*)-*form* [56857-47-7]
Isol. from molluscs *Strombus gigas* and *Crassostrea gigas* and from annelid *Arenicola marina*. Fish attractant.
Mp 131° (as hydrochloride).
Sangster, A.W. *et al., Tetrahedron*, 1975, **31**, 1135
Fields, J.H.A. *et al., Arch. Biochem. Biophys.*, 1980, **20**, 110-114 (*isol, mollusc*)
Kihlberg, J. *et al., Acta Chem. Scand., Ser. B*, 1983, **37**, 911 (*synth*)
Siegmund, B. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **82**, 337-345 (*isol, annelid*)

2-Carboxy-1-methylpyridinium betaine C-107
2-Carboxy-1-methylpyridinium hydroxide inner salt, 9CI. N-*Methylpicolinic betaine.* ***Homarine***
[445-30-7]



$C_7H_7NO_2$ 137.138
Alkaloid from fungus *Polyporus sulphureus*, lobsters *Homarus vulgaris* and *Homarus americanus*, Antarctic soft coral *Gersemia antarctica*, Antarctic gastropod *Marseniopsis mollis*, red alga *Pterocladia capillacea* and other spp. Shows antibacterial activity. Feeding deterrent in marine organisms. Cryst. (EtOH). Dec. on heating, deliquescent.

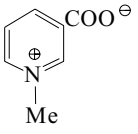
Hydrochloride: Mp 170-175° dec.

Picrate: Mp 158-160°.
Hantzsch, A. *et al., Ber.*, 1886, **19**, 31 (*synth*)

Hoppe-Seyler, F. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1933, **222**, 105-115 (*isol*)
Green, R.W. *et al., J.A.C.S.*, 1956, **78**, 4896 (*uv, tautom*)
Leonard, G.J. *et al., Nature (London)*, 1963, **200**, 78 (*isol*)
Groenneberg, T. *et al., Chem. Scr.*, 1972, **2**, 17 (*ms*)
Sciuto, S. *et al., J. Nat. Prod.*, 1988, **51**, 322-325 (*isol, red alga*)
McClintock, J.B. *et al., J. Chem. Ecol.*, 1994, **20**, 2539-2549 (*isol, activity*)
Slattery, M. *et al., Marine Ecol.: Progr. Ser.*, 1997, **161**, 133-144; *CA*, **128**, 119209b (*isol, activity*)
Polychronopoulos, P. *et al., Nat. Prod. Lett.*, 2001, **15**, 411-418 (*Homarine, pmr, cmr, ms*)

3-Carboxy-1-methylpyridinium betaine C-108

3-Carboxy-1-methylpyridinium hydroxide inner salt. N-*Methylnicotinic betaine*. ***Trigonelline***. *Gynesis*. *Coffearin*
[535-83-1]



$C_7H_7NO_2$ 137.138
Alkaloid from fenugreek (*Trigonella foenum-graecum*) (Leguminosae), *Schumanniophyton magnificum* (Rubiaceae), *Mappia foetida*, *Strophanthus* sp., *Cannabis sativa* and very many other spp.; also present in coffee beans, in many animals, the sponge *Calyx nicaeensis*, the soft coral *Gersemia antarctica*, and the red seaweed *Pterocladia capillacea*. Prisms + $1H_2O$ (EtOH aq.). V. sol. H_2O; sol. MeOH, EtOH; poorly sol. $CHCl_3$, Et_2O.
Mp 218° dec. (anhyd.).

▶ LD_{50} (rat, orl) 5000 mg/kg. YF6825000

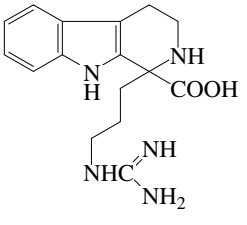
Hydrochloride: [6138-41-6]
Cryst. (EtOH aq.). Mp 257-258° (250°, 245-250° dec.).

Picrate: Mp 205-206° (198-200°).

Gorter, K. *et al., Annalen*, 1910, **372**, 237-246 (*isol*)
Späth, E. *et al., Ber.*, 1944, **77**, 362-369 (*synth*)
Ackermann, D. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1961, **326**, 197-199 (*occur*)
Wang, S.Y. *et al., Biochemistry*, 1968, **7**, 3740-3744 (*uv*)
Wehrli, F.W. *et al., Helv. Chim. Acta*, 1971, **54**, 229-243 (*pmr, cmr*)
Ghosal, S. *et al., Planta Med.*, 1973, **23**, 321-329 (*isol, uv, ir, pmr*)
Houghton, P.J. *et al., Planta Med.*, 1987, **53**, 262-264 (*isol*)
Slattery, M. *et al., Marine Ecol.: Progr. Ser.*, 1997, **161**, 133-144; *CA*, **128**, 119209e (*isol, activity*)
Merck Index, 13th edn., 2001, No. 9765 (*bibl*)
Blunden, G. *et al., Phytochemistry*, 2001, **58**, 451-454 (*occur*)

1-Carboxytrypargine C-109

[227935-85-5]

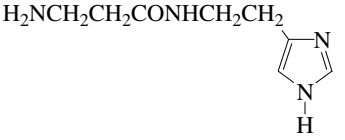


$C_{16}H_{21}N_5O_2$ 315.374
Abs stereochem. not determined. Alkaloid from a *Eudistoma* sp. Amorph. solid. λ_{max} 204 (log ϵ 4); 226 (log ϵ 4.3); 274 (log ϵ 3.7); 282 (log ϵ 3.7); 290 (log ϵ 3.6) (MeOH).

Van Wagoner, R.M. *et al., J. Nat. Prod.*, 1999, **62**, 794-797 (*isol, uv, cd, pmr, cmr*)

Carcinine C-110

3-Amino-N-*[2-(1*H*-imidazol-4-yl)ethyl]propanamide, 9CI*. N-*β-Alanylhistamine*
[56897-53-1]



$C_8H_{14}N_4O$ 182.225
Occurs in cardiac tissue of *Carcinus maenas* and other crustacea. Lowers blood pressure; shows antioxidant props.
Mp 67-68° Mp 114-117°.

Hydrochloride (1:2): [57022-38-5]
Cryst. Mp 94° Mp 195°.

N-tert-*Butoxycarbonyl:* [143885-59-0]
$C_{13}H_{22}N_4O_3$ 282.342
Mp 147-148°.

Arnould, J.-M. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1975, **50**, 59-66; **51**, 301-307 (*synth*)
Arnould, J.-M. *et al., Arch. Int. Physiol. Biochim.*, 1977, **85**, 339-350 (*synth*)
Nanasawa, M. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 1101-1104 (*synth*)
Babizhayev, M.A. *et al., Biochem. J.*, 1994, **304**, 509-516 (*props, ir, pmr, cmr*)
Impellizzeri, G. *et al., Eur. J. Org. Chem.*, 2000, 1065-1076 (*N-tert-butoxycarbonyl, synth*)

Carcinoscorpin C-111

Carcinoscorpius rotunda *Lectin*

Protein, MW *ca*. 420000. Isol. from the Indian horseshoe crab *Carcinoscorpius rotunda cauda*. Sialic acid-binding lectin.

Bishayee, S. *et al., Biochim. Biophys. Acta*, 1980, **623**, 89-97 (*isol*)
Dorai, D.T. *et al., Arch. Biochem. Biophys.*, 1981, **209**, 325-333 (*composition*)

Carcinustatins C-112

H-Tyr-Ala-Phe-Gly-Leu-NH_2

A family of 20 peptides of the allatostatin superfamily with the common C-terminal pentapeptide sequence -YXFGL-NH_2; struct. of Carcinustatin 1 shown. Isol. from the cerebral and thoracic ganglia of the shore crab *Carcinus maenas*. Neuropeptides.

Carcinustatin 1
Penaeustatin 13
[172846-10-5]
$C_{29}H_{40}N_6O_6$ 568.672
Also isol. from the tiger prawn *Penaeus monodon*.

Carcinustatin 2 [204909-50-2]
$C_{37}H_{52}N_8O_{10}$ 768.865

Carcinustatin 3 [204909-51-3]
$C_{39}H_{54}N_8O_{10}$ 794.903

Carcinustatin 4 [204909-52-4]
$C_{38}H_{52}N_8O_{10}$ 780.876

Carcinustatin 5 [204909-53-5]
$C_{38}H_{53}N_9O_9$ 779.892

Carcinustatin 6 [204909-54-6]
$C_{37}H_{52}N_8O_9$ 752.866

Carcinustatin 7 [204909-55-7]
$C_{40}H_{57}N_9O_{10}$ 823.945

Carcinustatin 8
Penaeustatin 6
[204909-56-8]
$C_{39}H_{55}N_9O_9$ 793.918
Also isol. from the crayfish *Orconectes limosus* and the tiger prawn *Penaeus monodon*.

Carcinustatin 9 [204909-57-9]
$C_{38}H_{53}N_9O_9$ 779.892

Carcinustatin 10 [204909-58-0]
$C_{47}H_{67}N_{11}O_{11}$ 962.113

Carcinustatin 11 [204909-59-1]
$C_{43}H_{63}N_{11}O_{12}$ 926.037

Carcinustatin 12 [204909-60-4]
$C_{43}H_{61}N_9O_{11}S$ 912.075

Carcinustatin 13 [204909-61-5]
$C_{102}H_{150}N_{24}O_{30}S$ 2224.516

Carcinustatin 14
Penaeustatin 35
[172846-11-6]
$C_{29}H_{40}N_6O_7$ 584.671
Also isol. from the tiger prawn *Penaeus monodon*.

Carcinustatin 15 [204909-62-6]
$C_{39}H_{55}N_9O_{10}$ 809.918

Carcinustatin 16 [204909-63-7]
$C_{38}H_{53}N_9O_{11}$ 811.89

Carcinustatin 17 [204909-64-8]
$C_{39}H_{56}N_{10}O_{12}$ 856.931

Carcinustatin 18 [204909-65-9]
$C_{41}H_{59}N_9O_{13}S$ 918.036

Carcinustatin 19 [204909-66-0]
$C_{50}H_{73}N_{11}O_{15}S$ 1100.257

Carcinustatin 20 [204909-67-1]
$C_{142}H_{208}N_{38}O_{44}$ 3151.433

Lombarska-Sliwinska, D. *et al., Bull. Pol. Acad. Sci., Chem.*, 1995, **43**, 33-40 (*Carcinustatin 1, Carcinustatin 14, synth*)
Duve, H. *et al., Eur. J. Biochem.*, 1997, **250**, 727-734 (*isol*)
Dircksen, H. *et al., Peptides (N.Y.)*, 1999, **20**, 695-712 (*Carcinustatin 8*)
Duve, H. *et al., Peptides (N.Y.)*, 2002, **23**, 1039-1051 (*isol, Penaeus monodon constits*)

Octopus Cardioactive peptides C-113

H-Gly-D-Phe-Gly-Asp-OH
Struct. of peptide 1 shown. Isol. from the brain of *Octopus minor*.

***Octopus* Cardioactive peptide 1**
GFGD
[134562-90-6]
$C_{17}H_{22}N_4O_7$ 394.383
Cardioactive. *Octopus* Cardioactive peptide 2 in which L-Phe replaces D-Phe shows very low cardioactive activity.

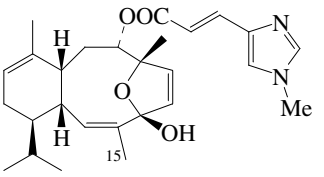
***Octopus* Cardioactive peptide 3**
GSWD
[277317-24-5]
$C_{20}H_{25}N_5O_8$ 463.446
Cardioactive. *Octopus* Cardioactive peptide 4, in which D-Ser replaces L-Ser shows very low cardioactive activity.

[277317-21-2, 277317-28-9]

Iwakoshi, E. *et al., Peptides (N.Y.)*, 2000, **21**, 623-630 (*isol*)

Caribaeorane C-114

[346406-75-5]



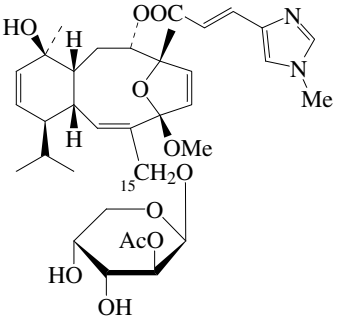
$C_{27}H_{36}N_2O_4$ 452.592
Constit. of *Erythropodium caribaeorum*.

15-Hydroxy: ***15-Hydroxycaribaeorane***
[216317-92-9]
$C_{27}H_{36}N_2O_5$ 468.592
Constit. of *Erythropodium caribaeorum*.

Britton, R. *et al., Tet. Lett.*, 2001, **42**, 2953-2956 (*isol, pmr, cmr*)

Caribaeoside C-115

[259728-79-5]



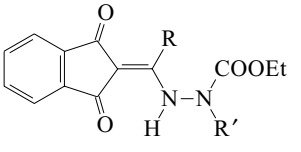
$C_{35}H_{48}N_2O_{11}$ 672.771
Constit. of *Erythropodium caribaeorum*. Related to Eleutherobin, in E-68.

Aglycone, 15-Ac: ***Caribaeolin***
[259728-87-5]
$C_{30}H_{40}N_2O_7$ 540.655
Constit. of *Erythropodium caribaeorum*.

Cinel, B. *et al., Org. Lett.*, 2000, **2**, 257-260 (*isol, pmr, cmr*)

Caribbazoin A C-116

[130518-25-1]



R = CH_3, R′ = Ac

$C_{16}H_{16}N_2O_5$ 316.313
Constit. of *Cliona caribboea*. Cryst. (C_6H_6).
Mp 165-167° Mp 172-173° (synthetic).

Lemke, T.L. *et al., J. Pharm. Sci.*, 1990, **79**, 840 (*isol, pmr, cmr*)

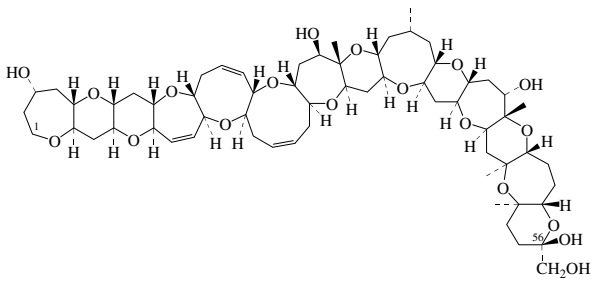
Caribbazoin B C-117

[130518-26-2]
As Caribbazoin A, C-116 with
R = H, R′ = Me
$C_{14}H_{14}N_2O_4$ 274.276
Constit. of *Cliona caribboea*. Shows hypotensive props.

Lemke, T.L. *et al., J. Pharm. Sci.*, 1990, **79**, 840; 1126 (*isol, pmr, cmr*)

Caribbean ciguatoxin 1 C-118

Ciguatoxin (Caribbean). C-CTX 1
[193363-37-0]

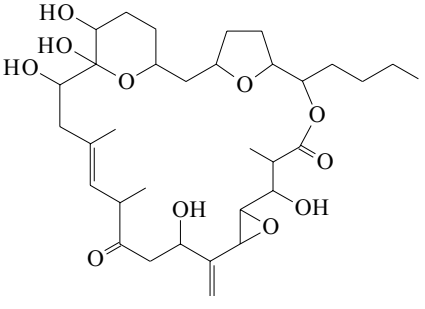


$C_{62}H_{92}O_{19}$ 1141.397
Isol. from *Caranx latus*. Causes ciguatera food poisoning.
Amorph. solid.

56-Epimer: C-CTX 2
[193363-38-1]
$C_{62}H_{92}O_{19}$ 1141.397
Isol. from *Caranx latus*.
Lewis, R.J. *et al., J.A.C.S.*, 1998, **120**, 5914-5920

Caribenolide I C-119

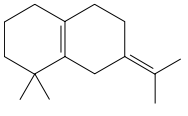
[161505-24-4]



$C_{33}H_{52}O_{11}$ 624.767
Macrolide antibiotic. Isol. from the dinoflagellate *Amphidinium* sp. S1-36-5. Cytotoxic agent. Microcryst. powder (isooctane/2-propanol). $[\alpha]_D^{25}$ +91 (c, 0.1 in CH_2Cl_2).
Bauer, I. *et al., J.O.C.*, 1995, **60**, 1084 (*isol, pmr, cmr, ms*)

Caridiene C-120

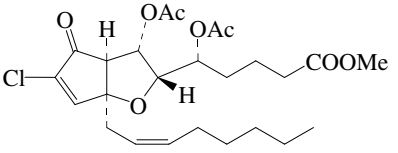
1,2,3,4,5,6,7,8-Octahydro-1,1-dimethyl-7-(1-methylethenyl)-naphthalene. 1,2,3,4,5,6,7,8-Octahydro-7-isopropylidene-1,1-dimethylnaphthalene
[132055-18-6]



$C_{15}H_{24}$ 204.355
Rearranged eremophilane. Constit. of *Pseudopterogorgia americana*. Oil.
Rivero, R.B. *et al., Z. Naturforsch., B*, 1990, **45**, 1571 (*isol, pmr, cmr*)

Carijenone C-121

[719296-43-2]



$C_{25}H_{35}ClO_8$ 498.999
Isol. from the octocoral *Carijoa multiflora*. Oil. $[\alpha]_D^{25}$ +22.2 (c, 0.1 in $CHCl_3$).
Dorta, E. *et al., Org. Lett.*, 2004, **6**, 2229-2232 (*isol, pmr, cmr, ms*)

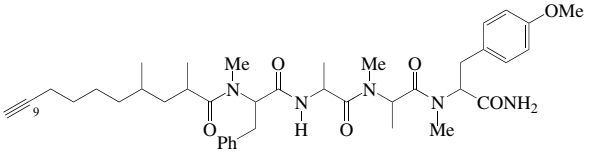
Caritoxins C-122

Actinia cari *Toxins. CTX*

Three basic proteins (Caritoxins I-III) lacking cysteine. Isol. from the sea anemone *Actinia cari*. Show high haemolytic activity.
Macek, P. *et al., Toxicon*, 1982, **20**, 181-185 (*isol*)
Sencic, L. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1990, **97**, 687-693 (*isol*)

Carmabin A C-123

[205492-50-8]



$C_{40}H_{57}N_5O_6$ 703.92
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{27}$ -109 (c, 0.4 in MeOH). λ_{max} 222 (ϵ 6900); 278 (ϵ 1400) (MeOH). λ_{max} 222 (ϵ 6900); 278 (ϵ 1400) (MeOH) (Berdy).

9,9,10,10-Tetrahydro, 9-oxo: ***Carmabin B***
[205492-52-0]
$C_{40}H_{59}N_5O_7$ 721.935
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{27}$ -102 (c, 0.2 in MeOH). λ_{max} 222 (ϵ 7000); 278 (ϵ 1200) (MeOH). λ_{max} 222 (ϵ 7000); 278 (ϵ 1200) (MeOH) (Berdy).
Hooper, G.J. *et al., J. Nat. Prod.*, 1998, **61**, 529-533 (*isol, uv, ir, pmr, cmr, ms*)

Carnocins C-124

Polypeptide bacteriocins.

Carnocin CP 5 [149983-81-3]
Prod. by *Carnobacterium piscicola* CP5.

Carnocin UI 49 [142540-01-0]
Prod. by *Carnobacterium piscicola* UI49 isol. from fish.

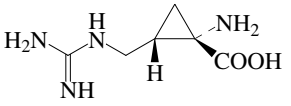
Carnocin H
Peptide containing approx. 75 amino acid residues. Prod. by *Carnobacterium* sp. 377.

Carnocin KZ213
Prod. by *Carnobacterium piscicola* 213.
Stoffels, G. *et al., J. Appl. Bacteriol.*, 1992, **73**, 309-316 (*Carnocin UI 49*)
Mathieu, F. *et al., Biotechnol. Lett.*, 1993, **15**, 587-590 (*Carnocin CP 5*)
Stoffels, G. *et al., Int. J. Food Microbiol.*, 1993, **20**, 199-210 (*Carnocin UI 49*)
Blom, H. *et al., Curr. Microbiol.*, 2001, **43**, 227-231 (*Carnocin H*)
Zhouiti, Z. *et al., J. Ind. Microbiol. Biotechnol.*, 2004, **31**, 5-10 (*Carnocin KZ213*)

Carnosadine C-125

1-Amino-2-[[(aminoiminomethyl)amino]methyl]cyclopropanecarboxylic acid, 9CI. 1-Amino-2-(guanidinomethyl)-1-cyclopropanecarboxylic acid

[93961-20-7]



$C_6H_{12}N_4O_2$ 172.186

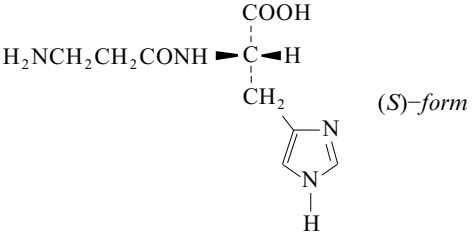
Amino acid from red alga *Grateloupia carnosa*. Antiinflammatory agent. Hygroscopic powder. Sol. H_2O; poorly sol. butanol, hexane.

*Bis(*p*-hydroxyazobenzenesulfonate):* [94061-93-5]
Mp 226-232° dec. (no clear Mp).

Wakamiya, T. *et al., Tet. Lett.*, 1984, **25**, 4411-4412; 1986, **27**, 2143-2144 (*isol, pmr, cmr, struct, synth*)
Stammer, H. *et al., Tetrahedron*, 1990, **46**, 2231-2254 (*rev*)
Burgess, K. *et al., J.O.C.*, 1994, **59**, 2179-2185 (*synth, pmr, cmr*)

Carnosine C-126

N-*β-Alanylhistidine, 9CI*



(S)–form

$C_9H_{14}N_4O_3$ 226.235
Log P -4.13 (calc).

(*R*)-*form*

D-form
[5853-00-9]
No depressor activity on blood pressure. Mp 260°.
$[\alpha]_D^{28}$ -20.4 (c, 1.5 in H_2O).

Hydrochloride: Mp 245°.

N-*Benzyloxycarbonyl:*
$C_{17}H_{20}N_4O_5$ 360.369
Mp 161°. $[\alpha]_D^{24}$ -11 (H_2O).

(*S*)-*form*

L-form
[305-84-0]
Occurs in the skeletal muscles of many animals and man. Isol. from the green alga *Spongomorpha saxatilis*. Also present in high concns. in olfactory bulb tissue. No biochemical role has yet been assigned although it exerts a depressor effect on blood pressure. Appears to be involved in regulation of anaerobic glycolysis, olfactory transmission and other physiol. functions. Has strong pH-buffering, antioxidant and membrane-stabilising props. Needles. Sol. EtOH; fairly sol. MeOH; poorly sol. butanol, hexane.
Mp 246-250° dec. $[\alpha]_D^{20}$ +24.1 (c, 1.5 in H_2O). pK_{a1} 2.62; pK_{a2} 6.66; pK_{a3} 9.24 (25°). Log P -4.13 (calc).
▶ LD_{50} (mus, ipr) 9087 mg/kg. Exp. reprod. and teratogenic effects. MS3080000

Hydrochloride: [5852-99-3]
Mp 245°.

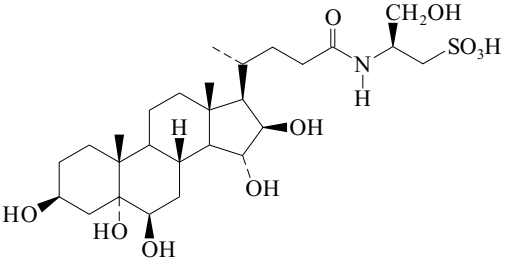
Nitrate: [5852-98-2]
Needles. Mp 219° (222° dec.).

*Sulfate:*Dec. at 238-40°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 622A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 86A (*nmr*)
Rinderknecht, H. *et al., J.O.C.*, 1964, **29**, 1968-1970 (*synth*)
Pietta, P.G. *et al., Ann. Chim. (Rome)*, 1968, **58**, 1431-1434 (*synth*)
Barrons, Y. *et al., J. Mol. Struct.*, 1976, **30**, 225-242 (*cryst struct*)
Itoh, H. *et al., Acta Cryst. B*, 1977, **33**, 2959-2961 (*cryst struct*)
Friedrich, J.O. *et al., Can. J. Chem.*, 1986, **64**, 2132-2138 (*cmr, pmr*)
Boldyrev, A.A. *et al., Adv. Enzyme Regul.*, 1990, **30**, 175-194 (*rev, biol activity*)
Boldyrev, A.A. *et al., Int. J. Biochem.*, 1990, **22**, 129-132 (*rev*)
Gaggelli, E. *et al., J.C.S. Perkin 2*, 1990, 401-406 (*pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, CCK665

Carolisterol A C-127

[151171-32-3]



$C_{27}H_{47}NO_{10}S$ 577.735
Constit. of *Styracaster caroli*.

6-Ketone: ***Carolisterol B***
[151171-33-4]
$C_{27}H_{45}NO_{10}S$ 575.719
Constit. of *Styracaster caroli*.

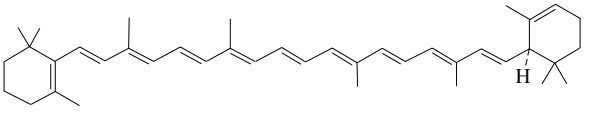
6-Epimer, 5-deoxy: ***Carolisterol C***
[151171-34-5]
$C_{27}H_{47}NO_9S$ 561.736
Constit. of *Styracaster caroli*.

De Riccardis, F. *et al., Tet. Lett.*, 1993, **34**, 4381 (*isol, pmr, cmr*)

α-Carotene C-128

β,ε-Carotene, 9CI

[432-70-2]



$C_{40}H_{56}$ 536.882
Log P 15.2 (uncertain value) (calc).

(*R*)-*form* [7488-99-5]

Widespread carotenoid, e.g. in carrots and palm oil. Present in sponges. Has vitamin A activity but less than that of β-Carotene. Shows tumour inhibitory props. Violet prisms (petrol).
Mp 187°. $[\alpha]_{643}^{18}$ +385 (C_6H_6). λ_{max} 446; 478; 511 (CS_2). λ_{max} 418; 442; 471 (hexane). λ_{max} 424; 448; 476 (Me_2CO).

5,6-Epoxide: See α-Carotene 5,6-epoxide in *The Combined Chemical Dictionary*.

(±)-*form*

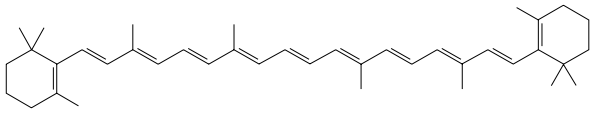
Violet platelets (C_6H_6). Mp 160-162°.

Karrer, P. *et al., Helv. Chim. Acta*, 1933, **16**, 975 (*struct*)
Karrer, P. *et al., Helv. Chim. Acta*, 1950, **33**, 1952 (*synth*)
Tscharner, C. *et al., Helv. Chim. Acta*, 1957, **40**, 1676 (*synth*)
Rüegg, R. *et al., Helv. Chim. Acta*, 1961, **44**, 985 (*synth*)
Strain, H.H. *et al., J.O.C.*, 1961, **26**, 5061 (*ir*)
Goodwin, T.W. *et al., Biochem. J.*, 1965, **97**, 28c (*biosynth*)
Eugster, C.H. *et al., Helv. Chim. Acta*, 1969, **52**, 1729 (*abs config*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1971, **54**, 327 (*uv, cd*)
Kjoesen, H. *et al., Acta Chem. Scand.*, 1972, **26**, 3053 (*pmr, ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 1824 (*occur*)

Liaaen-Jensen, S. *et al., Biochem. Syst. Ecol.*, 1982, **10**, 167-174 (*occur, sponges*)
Bjornland, T. *et al., Phytochemistry*, 1984, **23**, 1711-1715 (*abs config, pmr*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 7 (*bibl*)
Broszeit, G. *et al., Liebigs Ann./Recl.*, 1997, 2205-2213 (*synth, pmr, cmr, ir*)

β-Carotene C-129

Betacarotene, INN, USAN. *Carotaben. Phenoro. Solatene. β,β-Carotene. Provatene. E160a*
[7235-40-7]
[116-32-5]



$C_{40}H_{56}$ 536.882
Widespread in plant and animal kingdoms. In plants it is almost always associated with chlorophyll. Occurs in marine organisms, e.g. sponges, esp. of the Poecilosclerida and Axinellida. Prod. commercially biosynthetically by *Dunaliella salina* growing in highly saline medium. Used in ultraviolet sunscreen preparations. Yellow food colour. Exhibits strong vitamin A activity; dietary supplement, nutrient, vitamin A precursor, antihistamine. Deep purple prisms (C_6H_6/MeOH); red rhombs. (petrol). Sol. CS_2, hexane, C_6H_6; fairly sol. MeOH, Et_2O, $CHCl_3$; poorly sol. H_2O. Mp 183° (sealed tube). Log P 15.23 (uncertain value) (calc). Air-sensitive. λ_{max} 452; 484; 520 (CS_2). λ_{max} 425; 450; 477 (hexane). λ_{max} 429; 452; 478 (Me_2CO). λ_{max} 450; 478 (EtOH).
▶ Produces yellow skin discolouration when used therapeutically.
FI0329500

7,8-Dihydro: ***7,8-Dihydro-β,β-carotene***
[58218-99-8]
$C_{40}H_{58}$ 538.898
Isol. from *Parasilurus asotus*, *Cercospora cruenta* and other catfish. λ_{max} 405 (ε 73600); 427 (ε 111000); 453 (ε 101000) (hexane).

7,7′,8,8′-Tetrahydro: 7,7′,8,8′-Tetrahydro-β,β-carotene. ***η-Carotene***
[40772-88-1]
$C_{40}H_{60}$ 540.914
Isol. from the flavedo of Sinton citrangequat (a *Citrus-Poncirus-Fortunella* hybrid). Constit. of the catfish *Parasilurus asotus*. Poorly characterised. λ_{max} 376; 397; 422 (petrol).

7,8,9,10-Tetrahydro: ***7,8,9,10-Tetrahydro-β,β-carotene***
[496931-98-7]
$C_{40}H_{60}$ 540.914
Isol. from *Parasilurus asotus* and other catfish.

5,6-Epoxide: See β-Carotene epoxide in *The Combined Chemical Dictionary.*

5,6:5′,6-Diepoxide: See β-Carotene diepoxide in *The Combined Chemical Dictionary.*

(9*Z*)-*form* [19361-58-1]
[13312-52-2]
Isol. from *Dunaliella bardawil*. λ_{max} 276; 350; 455 (CH_2Cl_2).

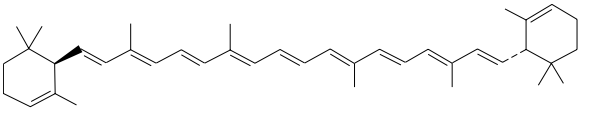
(13*Z*)-*form*
Neo-β-carotene. Pseudo-α-carotene. β,β-Carotene neo B
[6811-73-0]
Constit. of carrots and other plant spp.

[1465-77-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 54A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 71C (*nmr*)
Willstätter, R. *et al., Annalen*, 1907, **355**, 1 (*struct*)
Willstätter, R. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1910, **64**, 47 (*isol*)
Karrer, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1950, **250**, 1920 (*synth*)
Surmatis, J.D. *et al., J.O.C.*, 1961, **26**, 1171 (*synth*)
Sterling, C. *et al., Acta Cryst.*, 1964, **17**, 1224 (*cryst struct*)
Schweiter, U. *et al., Chimia*, 1965, **19**, 294 (*props*)
Yokoyama, H. *et al., Phytochemistry*, 1966, **5**, 1159 (*tetrahydro*)
Yokoyama, H. *et al., J. Agric. Food Chem.*, 1967, **15**, 693 (*tetrahydro*)
Surmatis, J.D. *et al., J.O.C.*, 1969, **34**, 559 (*synth*)
Schweiter, U. *et al., Pure Appl. Chem.*, 1969, **20**, 365 (*pmr, cmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 1821 (*occur*)
Johannes, B. *et al., Org. Mass Spectrom.*, 1974, **9**, 1095 (*ms*)
Fischli, A. *et al., Helv. Chim. Acta*, 1975, **58**, 1584 (*synth*)
Ishida, A. *et al., Chem. Lett.*, 1976, 1127 (*synth*)
Bickel, H. *et al., Phytochemistry*, 1976, **15**, 1253 (*biosynth*)
Bramley, P.M. *et al., Phytochemistry*, 1976, **15**, 1913 (*biosynth*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97 (*pmr*)
Ninet, L. *et al., Microb. Technol.*, 2nd edn., (eds. Peppler, H.J. *et al*), Academic Press, 1979, **1**, 529 (*manuf, rev*)
Liaaen-Jensen, S. *et al., Biochem. Syst. Ecol.*, 1982, **10**, 167-174 (*occur, sponges*)
Wernly, J. *et al., Chem. Comm.*, 1985, 1221 (*pmr, cmr*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987,
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CCK685
Koyama, Y. *et al., J. Mol. Struct.*, 1989, **193**, 185 (*pmr*)
Bjonland, T. *et al., Phytochemistry*, 1989, **28**, 3347 (*isol, pmr*)
Bernhard, K. *et al., Pure Appl. Chem.*, 1991, **63**, 35 (*synth*)
Senge, M.O. *et al., Z. Naturforsch., C*, 1992, **47**, 474 (*cryst struct*)
Ebenezer, W.J. *et al., J.C.S. Perkin 1*, 1993, 1869 (*9Z-form*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1036
Doering, W. von E. *et al., J.A.C.S.*, 1995, **117**, 2747 (*synth, bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 497-500 (*use, props*)
Nabeta, K. *et al., J.C.S. Perkin 1*, 1997, 269 (*biosynth*)
Rauchschwalbe, G. *et al., Eur. J. Org. Chem.*, 2001, 3903-3909 (*synth*)
Tsushima, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2002, **133**, 331-336; 2003, **136**, 147-148 (*Parasilurus asotus constits*)
Inomata, M. *et al., Biosci., Biotechnol., Biochem.*, 2004, **68**, 2571-2580 (*isol, Cercospora cruenta constit*)
Kim, D. *et al., J. Nat. Prod.*, 2004, **67**, 1067-1069 (*biosynth*)
Jeong, Y.C. *et al., Tetrahedron*, 2004, **60**, 10181-10185 (*synth*)
Eguchi, T. *et al., Tetrahedron*, 2005, **61**, 2027-2035 (*synth*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 194
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCK685

ε-Carotene C-130

ϵ_1-Carotene. ε,ε-Carotene
[38894-81-4]



(*R,R*)–*form*

$C_{40}H_{56}$ 536.882

(*R,R*)-*form* [472-89-9]
Constit. of *Navicula torquatum*, *Bryopsis corticulans*, *Codium fragile* and *Cryptomonas ovata*.
Red cryst.
Mp 199-201° Mp 196° (sealed tube). $[\alpha]_D^{27}$ +806 (C_6H_6). λ_{max} 415; 440; 470 (petrol).

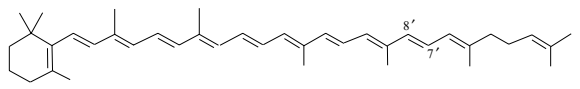
(*S,S*)-*form*
Constit. of *Pelagococcus subviridis* and *Ulva lactuca*.
Mp 197-198° (sealed tube). $[\alpha]_D^{27}$ -786 (C_6H_6). λ_{max} (Me_2CO).

(*RS,RS*)-*form*
Orange platelets (C_6H_6/MeOH). Mp 190° (sealed tube).

Tscharner, C. *et al., Helv. Chim. Acta*, 1958, **41**, 32 (*synth*)
Manchand, P.S. *et al., J.C.S.*, 1965, 2019 (*synth*)
Eugster, C.H. *et al., Helv. Chim. Acta*, 1969, **52**, 1729; 1732 (*abs config*)
Gerhard, E. *et al., Helv. Chim. Acta*, 1975, **58**, 2367 (*cmr*)
Bjornland, T. *et al., Phytochemistry*, 1989, **28**, 3347 (*isol, pmr, cd*)

γ-Carotene C-131

β,ψ-Carotene. Sphaerobolin
[472-93-5]



$C_{40}H_{56}$ 536.882
Widespread carotenoid found esp. in *Gonocaryum pyriforme* and from marine strain of the cyanobacterium *Synechococcus* spp. Exhibits vitamin A activity. Violet prisms (C_6H_6/petrol). Mp 178° (154°). Log P 15.04 (uncertain value) (calc). λ_{max} 437; 462; 494 (hexane). λ_{max} 439; 461; 491 (Me_2CO). λ_{max} 439; 461; 491 ($CHCl_3$).

1′,2′-Dihydro: 1′,2′-Dihydro-β,ψ-carotene. ***1′,2′-Dihydro-γ-carotene***
[198413-30-8]
$C_{40}H_{58}$ 538.898
Constit. of *Chlorobium tepidum*. λ_{max} 439 (sh); 461; 490 (Me_2CO/MeOH/THF).

1′,2′-Dihydro, 1′-hydroxy, O-*β*-D-*glucopyranoside: 1′-Glucosyloxy-1′,2′-dihydro-β,ψ-carotene*
[36473-46-8]
$C_{46}H_{68}O_6$ 717.04
Isol. from a gliding filamentous organism. λ_{max} 462; 490 (Me_2CO) (as per-Ac).

7′,8′-Dihydro: ***β-Zeacarotene****. Carotene X. 7′,8′-Dihydro-β,ψ-carotene*
[514-90-9]
$C_{40}H_{58}$ 538.898
Isol. from sweet corn (*Zea mays*) grains, *Citrus* spp., cultures of *Phycomyces blakesleeanus* etc. Orange-yellow platelets (Me_2CO). Mp 96-97°. λ_{max} 403; 427; 451 (petrol). λ_{max} 406; 428; 454 (EtOH).

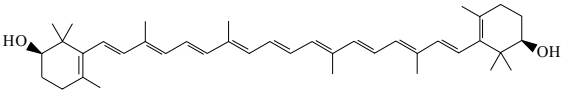
3′,4′-Didehydro: 3′,4′-Didehydro-β,ψ-carotene. 3′,4′-Didehydro-γ-carotene. ***Torulin***†*. Torulene*
[547-23-9]
$C_{40}H_{54}$ 534.867
Constit. of yeasts *Rhodotorula rubra*, *Rhodotorula minuta* and the ladybird beetle *Coccinella septempunctata*. Fine red needles (EtOAc) or violet cryst.(C_6H_6/EtOH). Mp 183-184°. λ_{max} 460 (sh); 484; 518 (petrol). λ_{max} 467; 501; 537 ($CHCl_3$).

3′,4′-Didehydro, 1′,2′-dihydro, 2′-hydroxy: 3′,4′-Didehydro-1′,2′-dihydro-β,ψ-caroten-2′-ol. 2′-Hydroxy-1′,2′-dihydrotorulene. 1,2′-Dihydro-2′-hydroxytorulene
$C_{40}H_{56}O$ 552.882
Minor carotenoid from the asporogenous yeast *Cryptococcus laurentii*. Tentative struct.

3′,4′-Didehydro, 1′,2′-dihydro, 1′-hydroxy, O-*β*-D-*glucopyranoside:*
[36210-85-2]
$C_{46}H_{66}O_6$ 715.024
Isol. from a gliding filamentous organism and from the myxobacterium *Sorangium compositum*. λ_{max} 448; 473; 503 (Me_2CO) (as per-Ac).

Goodwin, T.W. *et al., Annu. Rev. Biochem.*, 1955, **24**, 497 (*rev*)
Petzold, E.N. *et al., Arch. Biochem. Biophys.*, 1959, **82**, 117-124 (*β-Zeacarotene, isol*)
Rüegg, R. *et al., Helv. Chim. Acta*, 1961, **44**, 994 (*synth, β-Zeacarotene*)
Schweiter, U. *et al., Chimia*, 1965, **19**, 294 (*ms*)
Manchand, P.S. *et al., J.C.S.*, 1965, 2019 (*synth*)
Williams, R.J.H. *et al., Phytochemistry*, 1965, **4**, 759 (*β-Zeacarotene*)
Liaen-Jensen, S. *et al., Phytochemistry*, 1965, **4**, 975 (*Torulin*)
Bodea, C. *et al., Rev. Roum. Chim.*, 1966, **11**, 1123 (*synth*)
Weedon, B.C.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1969, **27**, 81 (*pmr*)
Schmidt, K. *et al., Acta Chem. Scand.*, 1971, **25**, 2476 (*uv*)
Kleinig, H. *et al., Arch. Mikrobiol.*, 1971, **78**, 224-233 (*1′,2′-Dihydro-1′-hydroxytorulene glycosides*)
Bae, M. *et al., Phytochemistry*, 1971, **10**, 625 (*1′,2′-Dihydro-2′-hydroxytorulene*)
Halfen, L.N. *et al., Arch. Mikrobiol.*, 1972, **82**, 240 (*1-Glucosyloxy-1′,2′-dihydro-β,ψ-carotene*)
Brittton, G. *et al., Insect Biochem.*, 1977, **7**, 337 (*isol, Torulin*)
Tada, M. *et al., Plant Cell Physiol.*, 1982, **23**, 607 (*isol, Torulin*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 12 (*bibl*)
Takaichi, S. *et al., Arch. Microbiol.*, 1997, **168**, 270-276 (*1′,2′-Dihydro-γ-carotene*)
Zeng, F. *et al., Org. Lett.*, 2001, **3**, 719-722 (*synth*)
Montero, O. *et al., J. Agric. Food Chem.*, 2005, **53**, 9701-9707 (*Synechococcus constit*)

β,β-Carotene-2,2′-diol C-132



(2*R*,2′*R*)*-form*

$C_{40}H_{56}O_2$ 568.881

2′-Deoxy, 5β,6β-epoxide: ***5,6-Epoxy-5,6-dihydro-β,β-caroten-2-ol***
[53120-11-9]
$C_{40}H_{56}O_2$ 568.881
Isol. from *Trentepohlia iolithus*. λ_{max} 423; 443; 472 (Et_2O).

3,3′,4,4′-Tetradehydro, mono-Me ether: ***3,3′,4,4′-Tetradehydro-2′-methoxy-β,β-caroten-2-ol***
[83332-06-3]
$C_{41}H_{54}O_2$ 578.876
Isol. from *Rhaphidophlus typicus.*

3,3′,4,4′-Tetradehydro, di-Me ether: ***3,3′,4,4′-Tetradehydro-2,2′-dimethoxy-β,β-carotene***
[83332-05-2]
$C_{42}H_{56}O_2$ 592.903
Isol. from *Rhaphidophlus typicus.*

(2R,2′R)-form [39668-26-3]
Constit. of *Trentepohlia iolithus* and *Ectatosoma tiaratum.* Purple cryst. ($CHCl_3$/MeOH). Mp 167°. Kayser repts. *ca*. 54% ee 2*S* ex *Ectatosoma tiaratum*.

Monoketone: ***2′-Hydroxy-β,β-caroten-2-one***
$C_{40}H_{54}O_2$ 566.865
Isol. from adult specimens of *Ectatosoma tiaratum* as partial racemate: also isol. from other stick insects as material of undetd. abs. config. CD: λ_{max} 222 nm, Δε + 1.1. λ_{max} 450; 477 (Me_2CO).

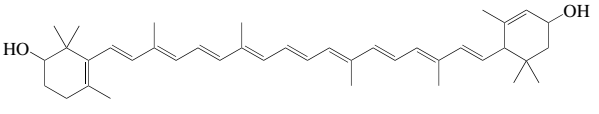
Monodeoxy: ***β,β-Caroten-2-ol***
[58501-76-1]
$C_{40}H_{56}O$ 552.882
Constit. of *Trentepohlia iolithus* and *Cerura vinula*. Isol. from *Idotea* spp. and *Ligia exotica*. Blue cryst. ($CHCl_3$/MeOH). Mp 177-178°. Kayser repts. *ca*. 48% ee 2*S* ex *Cerura vinula*.

[63596-37-2, 88822-91-7]

Kjoesen, H. *et al., Acta Chem. Scand.*, 1972, **26**, 3053 (*pmr, ms, uv*)
Buchecker, R. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 449 (*struct*)
Nybraaten, G. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 483 (*5,6-Epoxy-5,6-dihydro-β,β-caroten-2-ol*)
Tsukida, K. *et al., J. Nutr. Sci. Vitaminol.*, 1975, **21**, 147 (*synth*)
Ito, M. *et al., Tet. Lett.*, 1977, 2767 (*synth*)
Kayser, H. *et al., Z. Naturforsch., C*, 1977, **32**, 327; 1981, **36**, 755; 1982, **37**, 13 (*isol, biosynth, deriv*)
Liaaen-Jensen, S. *et al., Biochem. Syst. Ecol.*, 1982, **10**, 167-174 (*Me ethers*)
Kayser, H. *et al., Insect Biochem.*, 1984, **14**, 51; *CA*, **100**, 83019v (*isol, deriv*)
Gut, S. *et al., Helv. Chim. Acta*, 1989, **72**, 496 (*synth, pmr*)
Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1990, **95**, 759-761 (*Ligia exotica, isol*)

β,ε-Carotene-2,3′-diol C-133

Tilefishxanthin I
[70858-55-8]



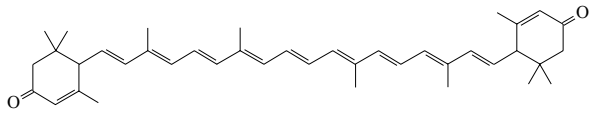
$C_{40}H_{56}O_2$ 568.8813

Isol. from red tile fish, *Branchiostegus japonicus*.

Asahara, M. *et al., Nippon Suisan Gakkaishi*, 1979, **45**, 485 (*isol, uv, struct*)

ϵ,ϵ-Carotene-3,3′-dione C-134

[28840-14-4]



$C_{40}H_{52}O_2$ 564.85

Constit. of *Sebastes flavidus* and other fish. Also found in chitons. Light red cryst. (CH_2Cl_2/Et_2O).

Mp 194°.

(6*S*,6′*S*)-*form* [97169-05-6]

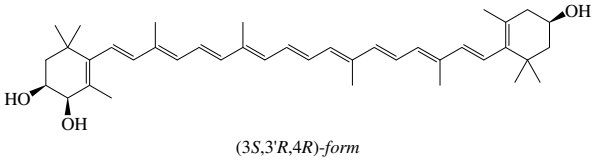
Isol. from marine fish-eggs and egg yolk. Biosynth. precursor of Tunaxanthin, T-795. λ_{max} 415; 438; 468 (petrol).

[57545-55-8, 82880-34-0, 82915-88-6, 97169-05-6]

Surmatis, J.D. *et al., Helv. Chim. Acta*, 1970, **53**, 974 (*synth, uv, pmr*)
Widmer, E. *et al., Helv. Chim. Acta*, 1982, **65**, 958 (*synth*)
Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 779 (*isol*)
Ikuno, Y. *et al., J. Chromatogr.*, 1985, **328**, 387 (*resoln*)
Ikuno, Y. *et al., Nippon Suisan Gakkaishi*, 1985, **51**, 2033 (*occur*)
Tsushima, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **93**, 665 (*occur*)

β,β-Carotene-3,3′,4-triol C-135

[70800-74-7]



(3*S*,3′*R*,4*R*)-*form*

$C_{40}H_{56}O_3$ 584.881

(3*S*,3′*R*,4*R*)-*form* [123122-22-5]

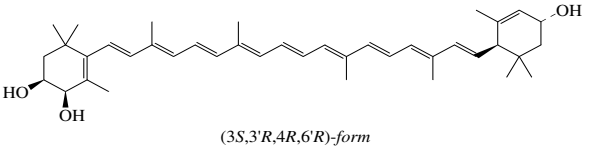
Isol. from chitons incl. *Acanthochiton defilippii* and *Liolophura japonica*.

(3*S*,3′*R*,4ξ)-*form* [97134-07-1]

Isol. as a minor constit. from the crustacean *Euchaeta russelli* and from eggs of mackerel, yellowtail and flying fish. Also from dolphin tissues. λ_{max} 423; 450; 473 (hexane). λ_{max} 425; 450; 475 (EtOH).

Bandaranayake, W.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **72**, 409 (*isol*)
Matsumo, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 779 (*occur, biosynth*)
Tsushima, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **93**, 665-671 (*isol, pmr*)

β,ϵ-Carotene-3,3′,4-triol C-136



(3*S*,3′*R*,4*R*,6′*R*)-*form*

$C_{40}H_{56}O_3$ 584.881

Possibly a naturally occurring carotenoid.

(3*S*,3′*R*,4*R*,6′*R*)-*form* [123163-67-7]

Isol. from chitons incl. *Acanthochiton defilippii* and *Liolophura japonica*.

(3*S*,3′*S*,4*R*,6′*R*)-*form*

4-Hydroxylutein

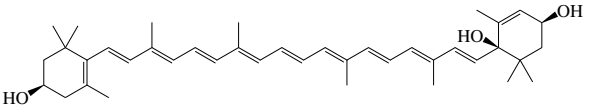
[253264-73-2]

Constit. of the goldfish *Carassius auratus*.

[68420-68-8, 68474-24-8, 68474-25-9, 78739-19-2]

Buchecker, R. *et al., Helv. Chim. Acta*, 1978, **61**, 1962-1968 (*synth*)
Tsushima, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **93**, 665-671 (*isol, pmr*)
Ohkubo, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1999, **124**, 333-340 (*isol, pmr*)

β,ϵ-Carotene-3,3′,6-triol C-137



$C_{40}H_{56}O_3$ 584.881

(3*R*,3′*S*,6′*R*)-*form*

Deepoxysalmoxanthin

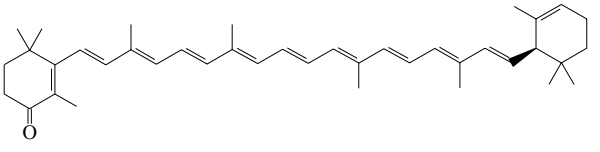
[342425-09-6]

Isol. from the salmon *Oncorhynchus keta*. λ_{max} 420 (sh); 444; 473 (no solvent reported).

Matsuno, T. *et al., J. Nat. Prod.*, 2001, **64**, 507-510 (*isol, pmr, cmr, cd, uv, abs config*)

β,ϵ-Caroten-4-one C-138

4-Keto-α-carotene. Phoenicopterone



$C_{40}H_{54}O$ 550.866

(*R*)-*form* [3297-23-2]

Partially synthesised from BF_3 complex of α-carotene; isol. from the Red Sea crinoid *Lamprometra klunzingeri*.

Salmon-pink platelets (C_6H_6/MeOH).

Mp 189-190°. λ_{max} 452 (hexane).

4-Alcohol: β,ϵ-Caroten-4-ol. 4-Hydroxy-α-carotene

[2213-16-3]

$C_{40}H_{56}O$ 552.882

Presumed to be naturally occurring, but lit. citations are inaccessible. Large rectangular orange plates (C_6H_6/MeOH).

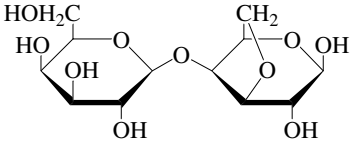
Mp 177°. λ_{max} 446; 474 (hexane).

Entschel, R. *et al., Helv. Chim. Acta*, 1958, **41**, 983 (*synth*)
Bush, W.V. *et al., J.A.C.S.*, 1958, **80**, 2991 (*synth, alcohol*)
Grob, E.C. *et al., Helv. Chim. Acta*, 1965, **48**, 930 (*synth, alcohol*)
Gross, J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1975, **52**, 459 (*isol, occur*)

Carrabiose C-139

3,6-Anhydro-4-O-β-D-galactopyranosyl-D-galactose, 9CI. Carrobiose

[19253-99-7]



β-Pyranose-*form*

$C_{12}H_{20}O_{10}$ 324.284

Produced by partial methanolysis of the polysaccharide from marine alga *Chondrus crispus* (κ-carrageenan) and the red alga

Furcellaria fastigiata. Amorph. solid. $[\alpha]_D^{17}$ +15.2 (c, 1.25 in H_2O).

Phenylosazone: Mp 214-215°. $[\alpha]_D^{10}$ +68.2 → +45 (c, 0.6 in EtOH/Py).

Phenylhydrazone:
Yellow cryst. (EtOH/Et_2O). Mp 211-213°. $[\alpha]_D^{21}$ +110 (c, 0.4 in MeOH).

Di-Et dithioacetal:
$C_{16}H_{30}O_9S_2$ 430.54
Cryst. (EtOH/Et_2O). Mp 116-117°. $[\alpha]_D^{25}$ +4 (c, 1.8 in H_2O).

Di-Et dithioacetal, hexa-Ac:
$C_{28}H_{42}O_{15}S_2$ 682.763
Cryst. (EtOH aq.). Mp 118-119°. $[\alpha]_D$ -4 (c, 1.2 in $CHCl_3$).

α-Pyranose-*form*

Me glycoside: Methyl α-carrabioside
$C_{13}H_{22}O_{10}$ 338.311
Cryst. (MeOH/EtOH). Mp 203-204°. $[\alpha]_D^{17}$ +36 (c, 1.0 in H_2O).

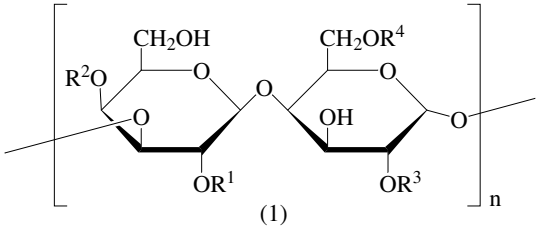
β-Pyranose-*form*

Me glycoside: Methyl β-carrabioside
$C_{13}H_{22}O_{10}$ 338.311
Needles (EtOH/Me_2CO). Mp 136-138° (as monohydrate).
$[\alpha]_D$ -78.6 (c, 0.70 in H_2O).

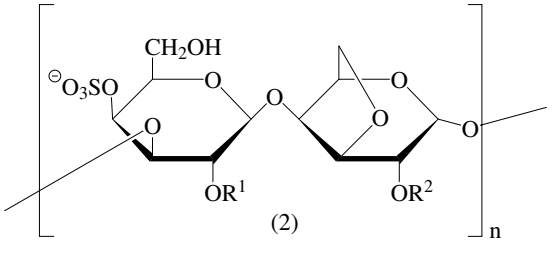
O'Neill, A.N. *et al., J.A.C.S.*, 1955, **77**, 6324 (*occur, struct, di-Et dithioacetal, di-Et dithioacetal hexa Ac*)
Araki, C. *et al., Bull. Chem. Soc. Jpn.*, 1956, **29**, 770 (*β-D-Me pyr*)
Painter, T.J. *et al., J.C.S.*, 1964, 1396 (*struct*)
Hirase, S. *et al., Bull. Chem. Soc. Jpn.*, 1967, **40**, 2627 (*synth, α-D-Me pyr*)
Lambda, D. *et al., Carbohydr. Res.*, 1986, **155**, 11 (*cryst struct, deriv*)
Parra, E. *et al., Carbohydr. Res.*, 1990, **208**, 83 (*synth, α-D-Me pyr*)
Storz, C.A. *et al., Carbohydr. Res.*, 2002, **337**, 2311-2323 (*conformn*)

Carrageenan C-140

Carrageenin. Carragheen. Genuvisco J. FEMA 2596. E407
[9000-07-1]



(1)



(2)

A complex mixt. of polysaccharides composed of galactans, the proportions of which vary with spp., season and environment. The major structural feature is β(1→3) and α(1→4) linked galactose units with various degrees and sites of sulfation (sulfate ester content 15-40%). The Greek prefixes denote the idealised constitution of different disaccharide units although native carrageenans show variation from these idealised structs. The struct. also varies during life-cycle of the alga. Obt. from red seaweeds in the families Furcellariaceae, Gigartinacaceae, Phyllophorraceae and Solieraceae. Used for gelling, thickening and emulsion stabilisation of foods (salts may also be used). Sol. H_2O; fairly sol. DMSO; poorly sol. oils, MeOH, hexane. ν component also referred to in the lit. alongside those descr. below.

▶ FI0700000

Ethyldimethyl(1-methyl-3,3-diphenylpropyl)ammonium salt:
Emepronium carrageenate, BAN. *Cetiprin novum*
Anticholinergic agent. Muscarinic antagonist. Consists mainly of κ and λ fractions.

μ-*form* [51311-96-7]
Isol. from *Furcellaria fastigiata*. Structure (1) with $R^1 = R^3 = H$, $R^2 = R^4 = SO_3^{\ominus}$. Minor fraction of carrageenan samples.

λ-*form*
Picnin A
[9064-57-7]
Isol. from *Chondrus crispus*. Present particularly in algal tetrasporophytes. Structure (1) with $R^1 = R^3 = R^4 = SO_3^{\ominus}$, $R^2 = H$. Major fraction.

▶ FI0704000

ε-*form* [51311-95-6]
Isol. from *Furcellaria fastigiata*. Structure (1) with $R^1 = R^3 = SO_3^{\ominus}$, $R^2 = R^4 = H$.

ι-*form* [9062-07-1]
Isol. from *Eucheuma spinosum* and *Agardhiella tenera* red seaweeds. Structure (2) with $R^1 = H$, $R^2 = SO_3^{\ominus}$. Major fraction.

κ-*form* [11114-20-8]
Isol. from *Chondrus crispus*. Present particularly in algal gametophytes. Structure (2) with $R^1 = R^2 = H$. Major fraction.

▶ FI0703000

ξ-*form* [70431-33-3]
Isol. from *Gigartina* spp. tetrasporophytes. Structure (1) with $R^1 = R^3 = SO_3^{\ominus}$, $R^2 = R^4 = H$.

π-*form* [71078-00-7]
Structure (1) with $R^1 = R^3 = SO_3^{\ominus}$, $R^4 = H$, C_4-C_6 pyruvate bridge in left-hand residue.

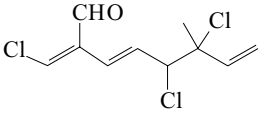
θ-*form*
Structure (2) with $R^1 = R^2 = SO_3^{\ominus}$.

[8015-95-0, 8036-85-9, 60063-90-3, 64366-24-1]

O'Neill, A.N. *et al., J.A.C.S.*, 1955, **77**, 2837-2839; 6324-6326 (*κ-form, isol, struct*)
Dolan, T.C.S. *et al., J.C.S.*, 1965, 3534-3539 (*λ-form, struct*)
Painter, T.J. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 98-100 (*κ-form, isol*)
Rees, D.A. *et al., Adv. Carbohydr. Chem.*, 1969, **24**, 267-332 (*rev*)
Penman, A. *et al., J.C.S. Perkin 1*, 1973, 2191-2196 (*κ-form, struct*)
Massey, J.A. *et al., Br. J. Urol.*, 1986, **58**, 125-128 (*emepronium carrageenan*)
Hallen, B. *et al., Arzneim.-Forsch.*, 1988, 1482-1485 (*emepronium carrageenan*)
Millane, R.P. *et al., Carbohydr. Res.*, 1988, **182**, 1-17 (*κ-form, struct, bibl*)
Falshaw, R. *et al., Carbohydr. Res.*, 1995, **276**, 155-165 (*ξ-form, isol, bibl*)
Chiovitti, A. *et al., Carbohydr. Res.*, 1997, **299**, 229-243 (*isol*)
Arndt, E.R. *et al., Carbohydr. Res.*, 1997, **303**, 73-78 (*cd, struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 500-516 (*props, use*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 461 (*emepronium carrageenan*)
Janaswamy, S. *et al., Carbohydr. Res.*, 2001, **335**, 181-194 (*ι-form, struct*)
Yu, G. *et al., Carbohydr. Res.*, 2002, **337**, 433-440 (*κ-form, purifn, struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCL250; CCL350

Cartilagineal C-141

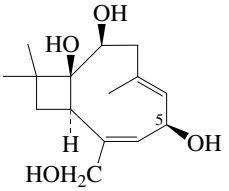
5,6-Dichloro-2-(chloromethylene)-6-methyl-3,7-octadienal, 9CI
[53915-35-8]



$C_{10}H_{11}Cl_3O$ 253.554
Constit. of *Plocamium cartilagineum*. Viscous liq. $Bp_{0.1}$ 130°.
λ_{max} 245 (ε 15800) (EtOH) (Berdy).

Crews, P. *et al., J.O.C.*, 1974, **39**, 3303
Faulkner, D.J. *et al., Tetrahedron*, 1977, **33**, 1421-1443

3,6-Caryophylladiene-5,9,10,15-tetrol C-142



$C_{15}H_{24}O_4$ 268.352

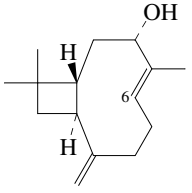
(3*E*,5β,6*E*,9β,10β)-*form*

5-Me ether: ***Fuscoatrol A***
[855780-05-1]
$C_{16}H_{26}O_4$ 282.379
Metab. of the marine fungus *Humicola fuscoatra*.

(3*Z*,5β,6*E*,9β,10β)-*form*

5-Me ether, 9-Ac: ***Pestalotiopsin B***
[173428-99-4]
$C_{18}H_{28}O_5$ 324.416
Metab. of an *Pestalotiopsis* sp, an endophytic fungus from *Taxus brevifolia*. Cryst. (EtOAc).
Mp 156°. $[\alpha]_D^{22}$ -240.5 (c, 0.49 in MeOH). Error in struct. diag. in 1996 paper; cryst. struct. diag is correct.
Pulici, M. *et al., J.O.C.*, 1996, **61**, 2122-2124; 1997, **62**, 1564 (*Pestalotriopsin B, cryst struct*)
Pulici, M. *et al., Phytochemistry*, 1997, **46**, 313-319 (*Pestalotiopsin B*)
Smetanina, O.F. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2004, **53**, 2643-2646 (*Fuscoatrol A*)

3(15),6-Caryophylladien-8-ol C-143



(6*E*,8α)-*form*

$C_{15}H_{24}O$ 220.354

(6*E*,8α)-*form*

6β,7β-Epoxide: 6,7-Epoxy-3(15)-caryophyllen-8-ol. ***Suberosol A***
[444593-60-6]
$C_{15}H_{24}O_2$ 236.353
Constit. of *Subergorgia suberosa*. Oil. $[\alpha]_D^{29}$ -17.4 (c, 0.13 in $CHCl_3$).

(6*E*,8β)-*form*

Suberosol C
[444593-62-8]
Constit. of *Subergorgia suberosa*.
Oil. $[\alpha]_D^{29}$ -67.9 (c, 0.14 in $CHCl_3$).

6β,7β-Epoxide: ***Suberosol B***
[444593-61-7]
$C_{15}H_{24}O_2$ 236.353
Constit. of *Subergorgia suberosa*. Oil. $[\alpha]_D^{29}$ -10.7 (c, 0.24 in $CHCl_3$).

(6*Z*,8α)-*form*

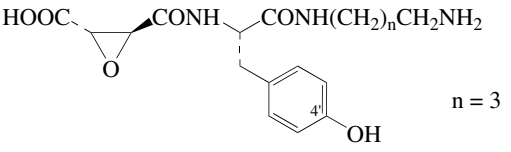
Suberosol D
[444593-63-9]
Constit. of *Subergorgia suberosa*.
Oil. $[\alpha]_D^{29}$ +2.5 (c, 0.045 in $CHCl_3$).
Wang, G.-H. *et al., J. Nat. Prod.*, 2002, **65**, 887-891 (*isol, pmr, cmr*)

Catch-releasing peptide C-144

*1-L-Alanine-3-L-prolinemyomodulin A (*Aplysia californica*), 9CI. AMPMLRL amide*
[111846-40-3]
H-Ala-Met-Pro-Met-Leu-Arg-Leu-NH_2
Isol. from pedal ganglion extracts of the mussel *Mytilus edulis*. Relaxes catch-tension of the anterior byssus retractor muscle.
Hirata, T. *et al., Brain Res.*, 1987, **422**, 374 (*isol, struct*)

Cathestatin B C-145

PF 1126B. Antibiotic PF 1126B
[162112-42-7]
[167818-23-7, 169735-72-2]



$C_{17}H_{23}N_3O_6$ 365.385
Prod. by *Aspergillus terricola*, *Penicillium citrinum* and the sponge-derived *Microascus longirostris*. Inhibitor of cysteine protease. Amorph. solid. Stereochemical identity with PF 1126 antibiotics not certain.

4′-Deoxy: ***Cathestatin A***. *PF 1126A. Antibiotic PF 1126A*
[162112-41-6]
[167818-22-6, 169735-71-1, 169735-75-5, 169735-77-7]
$C_{17}H_{23}N_3O_5$ 349.386
Prod. by *Aspergillus terricola*, *Microascus longirostris* and *Penicillium citrinum*. Inhibitor of cysteine protease. Amorph. solid. Sol. H_2O, MeOH.
Woo, J.-T. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 350-352 (*isol, pmr, cmr*)
Japan. Pat., 1995, 95 157 479; *CA*, **123**, 196747z (*PF 1126B*)
Yu, C.-M. *et al., J. Antibiot.*, 1996, **49**, 395-397 (*isol, pmr, cmr*)

Cathestatin C C-146

PF 1138B. Antibiotic PF 1138B
[176486-11-6]
[172940-60-2]
As Cathestatin B, C-145 with

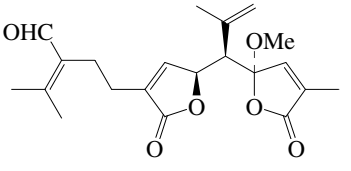
n = 4

$C_{18}H_{25}N_3O_6$ 379.412
Prod. by *Chaetomium globosum* and the sponge-derived *Microascus longirostris*. Inhibitor of cysteine protease. Sol. H_2O. Stereochemical identity with PF 1138 antibiotics not certain.

4′-Deoxy: ***Antibiotic PF 1138A***. *PF 1138A*
[172940-59-9]
$C_{18}H_{25}N_3O_5$ 363.413
Prod. by *Chaetomium globosum*. Thiol protease inhibitor.
Japan. Pat., 1995, 95 252 245; *CA*, **124**, 117071u (*PF 1138*)
Yu, C.-M. *et al., J. Antibiot.*, 1996, **49**, 395 (*isol, pmr, cmr*)

Caucanolide A C-147

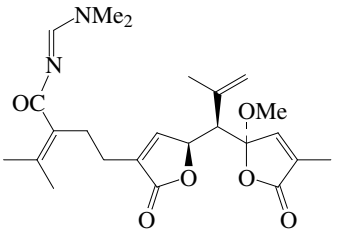
[869801-88-7]



$C_{21}H_{26}O_6$ 374.433
Constit. of *Pseudopterogorgia bipinnata*. Oil. $[\alpha]_D^{20}$ -42 (c, 0.7 in $CHCl_3$). λ_{max} 204 (ε 26200); 246 (ε 15500) (MeOH).
Ospina, C.A. *et al., J. Nat. Prod.*, 2005, **68**, 1519-1526 (*Caucanolide A*)

Caucanolide B C-148

[869801-89-8]



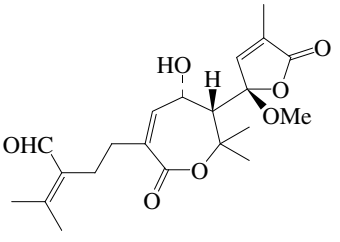
$C_{24}H_{32}N_2O_6$ 444.527

Constit. of *Pseudopterogorgia bipinnata*. Oil. $[\alpha]_D^{20}$ -20.8 (c, 0.6 in $CHCl_3$). λ_{max} 195 (ϵ 17200); 205 (ϵ 16200) (MeOH).

Ospina, C.A. *et al., J. Nat. Prod.*, 2005, **68**, 1519-1526 (*Caucanolide B*)

Caucanolide C C-149

[869801-90-1]



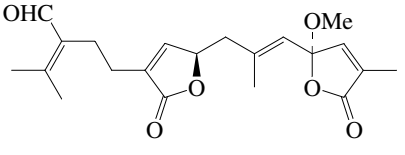
$C_{21}H_{28}O_7$ 392.448

Constit. of *Pseudopterogorgia bipinnata*. Oil. $[\alpha]_D^{20}$ -7.1 (c, 1.1 in $CHCl_3$). λ_{max} 210 (ϵ 16100); 244 (ϵ 6000) (MeOH).

Ospina, C.A. *et al., J. Nat. Prod.*, 2005, **68**, 1519-1526 (*Caucanolide C*)

Caucanolide D C-150

[869801-91-2]



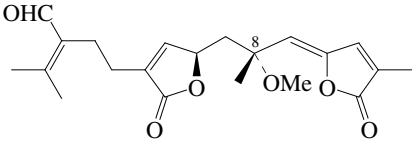
$C_{21}H_{26}O_6$ 374.433

Constit. of *Pseudopterogorgia bipinnata*. Oil. $[\alpha]_D^{20}$ -16.2 (c, 1.4 in $CHCl_3$). λ_{max} 205 (ϵ 16600); 240 (ϵ 12800) (MeOH).

Ospina, C.A. *et al., J. Nat. Prod.*, 2005, **68**, 1519-1526 (*Caucanolide D*)

Caucanolide E C-151

[869801-92-3]



$C_{21}H_{26}O_6$ 374.433

Constit. of *Pseudopterogorgia bipinnata*. Oil. $[\alpha]_D^{20}$ +72.2 (c, 1.3 in $CHCl_3$). λ_{max} 206 (ϵ 16500); 261 (ϵ 16100) (MeOH).

8-Epimer: ***Caucanolide F***

[869801-93-4]

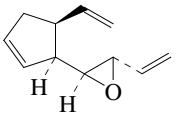
$C_{21}H_{26}O_6$ 374.433

Constit. of *Pseudopterogorgia bipinnata*. Oil. $[\alpha]_D^{20}$ +34.5 (c, 1.3 in $CHCl_3$). λ_{max} 209 (ϵ 19900); 261 (ϵ 21500) (MeOH).

Ospina, C.A. *et al., J. Nat. Prod.*, 2005, **68**, 1519-1526 (*Caucanolides E and F*)

Caudoxirene C-152

[117415-46-0]



Absolute Configuration

$C_{11}H_{14}O$ 162.231

Metab. of *Perithalia caudata*. Gamete releasing factor (threshold conc. = 30 pmol). Oil. $[\alpha]_D$ +238.3 (CH_2Cl_2).

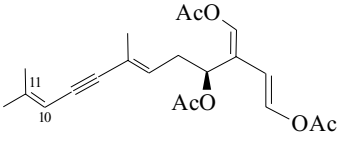
Muller, D.G. *et al., Biol. Chem. Hoppe-Seyler*, 1988, **369**, 655 (*ms, pharmacol*)

Wirth, D. *et al., Helv. Chim. Acta*, 1990, **73**, 916; 1992, **75**, 751 (*isol, pmr, cmr, ms, ir, synth, abs config*)

Lebreton, J. *et al., Tetrahedron*, 1997, **53**, 145 (*synth*)

Caulerpenyne C-153

[70000-22-5]



$C_{21}H_{26}O_6$ 374.433

Constit. of *Caulerpa prolifera*, *Caulerpa vanbosseae*, *Caulerpa taxifolia* and *Volvatella* sp. Inhibitor of prenyl transferase, 5-lipoxygenase and phospholipase A2. Ichthyotoxin. Cryst. Sol. $CHCl_3$, MeOH; poorly sol. H_2O.

Mp 57-58°. $[\alpha]_D^{20}$ +7.1 (c, 1 in EtOH). λ_{max} 252 (ϵ 33100); 265 (ϵ 27900); 280 (ϵ 1700) (MeOH) (Berdy). λ_{max} 252 (ϵ 33100) (EtOH) (Berdy).

10ξ,11ξ-Epoxide: ***10,11-Epoxycaulerpenyne***

$C_{21}H_{26}O_7$ 390.432

Constit. of *Caulerpa taxifolia*. Oil. $[\alpha]_D$ -12.3 (c, 0.56 in EtOH).

▶ Mutagenic.

1,2-Dihydro: 1,2-Dihydrocaulerpenyne

$C_{21}H_{28}O_6$ 376.449

Isol. as a mixt. of higher acyl homologues (1-Ac replaced by long chain acyl groups) from green alga *Caulerpa prolifera*.

Amico, V. *et al., Tet. Lett.*, 1978, 3593-3596 (*isol*)

De Napoli, L. *et al., Experientia*, 1983, **39**, 141-143 (*Dihydrocaulerpenyne analogues*)

Guerriero, A. *et al., Helv. Chim. Acta*, 1992, **75**, 689 (*isol, pmr, cmr*)

Jung, V. *et al., Tetrahedron*, 2001, **57**, 7169-7172 (*bibl*)

Pohnert, G. *et al., Org. Lett.*, 2003, **5**, 5091-5093 (*biosynth*)

Commeiras, L. *et al., Tet. Lett.*, 2003, **44**, 2311-2314 (*synth*)

Cutignano, A. *et al., Org. Biomol. Chem.*, 2004, **2**, 3167-3171 (*metab*)

Caulerpicin C-154

[11003-42-2]

$C_{43}H_{87}NO_2$ 650.166

Consists of a mixt. of ceramides derived from 2-Amino-1,3-octadecanediol, A-376 with $C_{18} \rightarrow C_{26}$ saturated fatty acids. Toxic principle, isol. from the green alga *Caulerpa racemosa* and other *Caulerpa* spp. Concentrates in crabs, shrimps and other

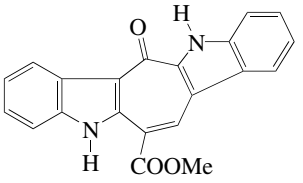
organisms in the marine food chain. Cryst. Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 95°.

▶ Toxic agent causing sensory numbness.

Doty, M.S. *et al., Nature (London)*, 1966, **211**, 990
Nielsen, P.G. *et al., Phytochemistry*, 1982, **21**, 1643 (*pmr, ms, struct*)

Caulersin C-155

[196803-51-7]

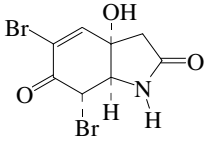


$C_{21}H_{14}N_2O_3$ 342.353
Alkaloid from the alga *Caulerpa serrulata*. Bright yellow cryst. (MeOH).
Mp 269-270°. λ_{max} 206 (log ϵ 4.51); 220 (log ϵ 3.62); 265 (log ϵ 2.02); 273 (log ϵ 1.1); 311 (log ϵ 1.36) (EtOH).

Su, J.-Y. *et al., J. Nat. Prod.*, 1997, **60**, 1043-1044 (*isol, uv, ir, pmr, cmr, ms*)
Wahlström, N. *et al., Tetrahedron*, 2004, **60**, 2147-2153 (*synth, pmr, cmr*)
Miki, Y. *et al., Tet. Lett.*, 2006, **47**, 5215-5218 (*synth*)

Cavernicolin 1 C-156

[84590-04-5]



Absolute Configuration

$C_8H_7Br_2NO_3$ 324.956
Alkaloid from the sponges *Aplysina cavernicola* and *Suberea* aff. *praetensa*. λ_{max} 200 (sh) (MeOH/NaOH) (Derep). λ_{max} 257 (ϵ 8300) (MeOH) (Derep).

5-Debromo, 5-chloro: ***7-Bromo-5-chlorocavernicolin***
$C_8H_7BrClNO_3$ 280.505
Metab. from *Aplysina cavernicola*. Racemic. Isol. as a mixt. of C(7)-epimerising monoacetates.

7-Debromo: ***5-Bromocavernicolin***
$C_8H_8BrNO_3$ 246.06
Isol. from the sponge *Suberea* aff. *praetensa*.

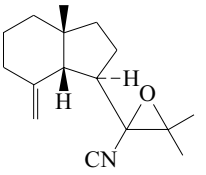
5,7-Bisdebromo, 5-chloro: ***5-Chlorocavernicolin***
$C_8H_8ClNO_3$ 201.609
Alkaloid from *Aplysina cavernicola* and *Suberea* aff. *praetensa*. Nearly racemic.

7-Epimer: ***Cavernicolin 2***
[84590-06-7]
$C_8H_7Br_2NO_3$ 324.956
Alkaloid from *Aplysina cavernicola* and *Suberea* aff. *praetensa*. λ_{max} 200 (sh) (MeOH/NaOH) (Derep). λ_{max} 257 (ϵ 8300) (MeOH) (Derep).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1984, **67**, 1484-1492 (*isol, uv, pmr, cmr, ms, struct*)
Kijjoa, A. *et al., Z. Naturforsch., C*, 2002, **57**, 732-738 (*Suberea aff. praetensa alkaloids*)

Cavernoisonitrile C-157

[145543-56-2]

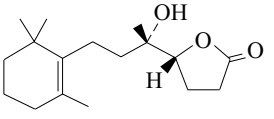


$C_{16}H_{23}NO$ 245.364
Constit. of *Acanthella* cf. *cavernosa* and *Phyllidia ocellata*. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D$ +27 (c, 0.17 in MeOH).

Fusetani, N. *et al., Tet. Lett.*, 1992, **33**, 6823-6836 (*isol, pmr, cmr*)

Cavernosine C-158

[84316-05-2]

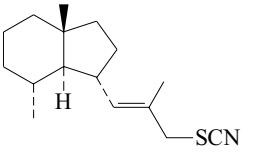


$C_{17}H_{28}O_3$ 280.406
Constit. of sponge *Fasciospongia cavernosa*. Ichthyotoxin. Oil. $[\alpha]_{435}$ -1.8 (c, 1.19 in $CHCl_3$).

Braekman, J.C. *et al., Bull. Soc. Chim. Belg.*, 1982, **91**, 791 (*isol*)
Jefford, C.W. *et al., Tet. Lett.*, 1987, **28**, 4041 (*synth*)

Cavernothiocyanate C-159

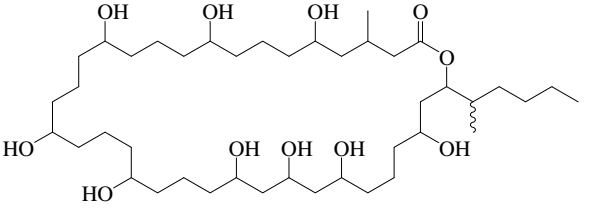
12-Thiocyanato-7(11)-oppositene
[145543-57-3]



$C_{16}H_{25}NS$ 263.446
Constit. of *Acanthella* cf. *cavernosa* and *Phyllidia ocellata*. Larval metamorphosis inhibitor. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D$ -37.8 (c, 0.037 in $CHCl_3$).

Fusetani, N. *et al., Tet. Lett.*, 1992, **33**, 6823-6836 (*isol, pmr, cmr*)
Hirota, H. *et al., Tetrahedron*, 1996, **52**, 2359 (*isol, pmr, cmr*)

Caylobolide A C-160

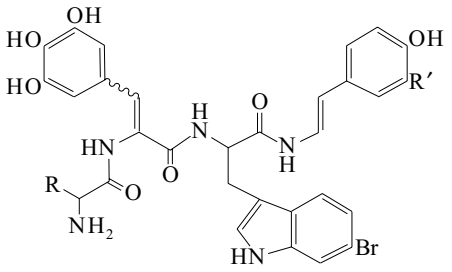


$C_{42}H_{82}O_{11}$ 763.103
Isol. from *Lyngbya majuscula*. Cytotoxic. $[\alpha]_D$ -9.7 (c, 0.25 in MeOH).

MacMillan, J.B *et al., Org. Lett.*, 2002, **4**, 1535-1538 (*isol*)

Celenamide A C-161

[74144-98-2]



R = $CH_2CH(CH_3)_2$, R′ = OH

$C_{34}H_{36}BrN_5O_8$ 722.591
Alkaloid from the sponge *Cliona celata*.
$[\alpha]_D^{25}$ +40 (c, 1.1 in Me_2CO) (as hexa-Ac).

Stonard, R.J. *et al., J.O.C.*, 1980, **45**, 3687 (*isol, uv, ir, pmr, ms, struct*)

Celenamide B C-162

[74144-99-3]
As Celenamide A, C-161 with
R = $-CH(CH_3)_2$, R′ = OH
$C_{33}H_{34}BrN_5O_8$ 708.564
Metab. from the sponge *Cliona celata*.
$[\alpha]_D^{25}$ +22 (c, 1.1 in Me_2CO) (as hexa-Ac). Isol. and elucidated as the Hexa-Ac deriv.

Stonard, R.J. *et al., J.O.C.*, 1980, **45**, 3687 (*isol, uv, ir, pmr, ms, struct*)

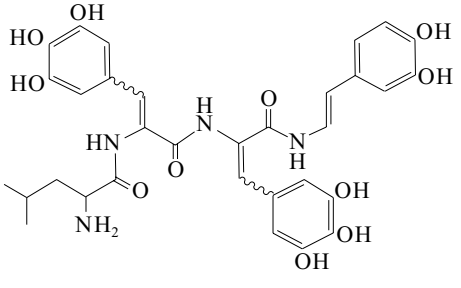
Celenamide C C-163

[75472-51-4]
As Celenamide A, C-161 with
R = $-CH_2CH(CH_3)_2$, R′ = H
$C_{34}H_{36}BrN_5O_7$ 706.592
Minor metab. from the sponge *Cliona celata*.
$[\alpha]_D^{25}$ +14 (c, 0.30 in Me_2CO) (as penta-Ac). Isol. and elucidated as the Penta-Ac deriv.

Stonard, R.J. *et al., Can. J. Chem.*, 1980, **58**, 2121 (*isol, ir, pmr, ms, struct*)

Celenamide D C-164

[75472-50-3]

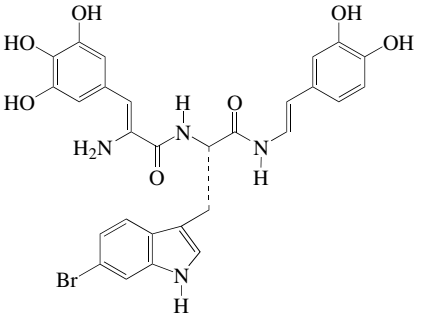


$C_{32}H_{34}N_4O_{11}$ 650.641
Minor metab. from the sponge *Cliona celata*.
$[\alpha]_D^{25}$ -25 (c, 0.54 in Me_2CO) (as nona-Ac). Isol. and elucidated as the Nona-Ac deriv.

Stonard, R.J. *et al., Can. J. Chem.*, 1980, **58**, 2121 (*isol, ir, pmr, ms, struct*)

Celenamide E C-165

[202855-03-6]

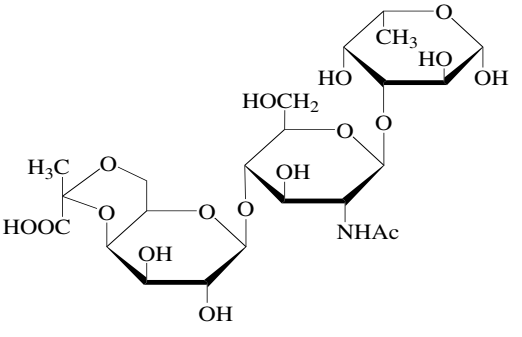


$C_{28}H_{25}BrN_4O_7$ 609.432
Metab. of the sponge *Cliona chilensis*. Amorph. yellow solid (MeOH aq.).
Mp 212-218° dec. $[\alpha]_D^{25}$ -25 (c, 0.25 in MeOH). λ_{max} 226 (log ϵ 4.5); 296 (log ϵ 4.17); 340 (log ϵ 4.3) (MeOH).

Palermo, J.A. *et al., J. Nat. Prod.*, 1998, **61**, 488-490 (*isol, uv, ir, pmr, cmr*)

Microciona Cell aggregation factor C-166

[149635-87-0]



$C_{23}H_{37}NO_{17}$ 599.542
Aggregation factor of the sponge *Microciona prolifera*.

Spillmann, D. *et al., J. Biol. Chem.*, 1993, **268**, 13378-13387 (*isol, pmr, hplc*)
Ziegler, T. *et al., Annalen*, 1995, 949-955 (*synth*)

Cellulose synthases C-167

Hexosyltransferase enzymes. Present in plants, most algae and some bacteria and fungi.

Cellulose synthase (UDP-forming)

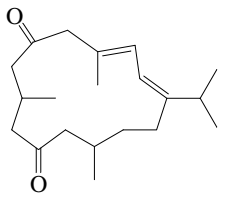
E.C. 2.4.1.12. UDP-glucose:1,4-β-D-glucan 4-β-D-glucosyltransferase. UDP-glucose-cellulose glucosyltransferase
[9027-19-4]
Catalyses transfer of glucose from UDP-glucose to cellulose thus causing elongation of the cellulose chain.

Cellulose synthase (GDP-forming)

E.C. 2.4.1.29. GDP-glucose:1,4-β-D-glucan 4-β-D-glucosyltransferase
[9027-18-3]
Catalyses transfer of glucose from GDP-glucose to cellulose thus causing elongation of the cellulose chain.

Elbein, A.D. *et al., Methods Enzymol.*, 1966, **8**, 416-418 (*E.C. 2.4.1.29, Phaseolus aureus*)
Potter, J.L. *et al., Methods Enzymol.*, 1972, **28**, 581-583 (*Acanthamoeba*)
Delmer, D.P. *et al., Annu. Rev. Plant Physiol. Plant Mol. Biol.*, 1999, **50**, 245-276 (*rev*)
Richmond, T.A. *et al., Plant Physiol.*, 2000, **124**, 495-498 (*rev*)
Perrin, R.M. *et al., Curr. Biol.*, 2001, **11**, R213-R216 (*rev*)

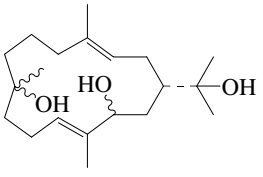
1,3-Cembradiene-6,10-dione C-168



$C_{20}H_{32}O_2$ 304.472

(1*Z*,3*E*,8ξ,12ξ)-*form* [603089-60-7]
Constit. of *Eunicea tourniforti*.
Cryst.
Mp 95-96°. $[\alpha]_D$ -2.5 (c, 0.22 in $CHCl_3$). λ_{max} 239 (log ϵ 3.2) (MeOH).
Marville, K.I. *et al., J. Nat. Prod.*, 2003, **66**, 1284-1287 (*isol, pmr, cmr*)

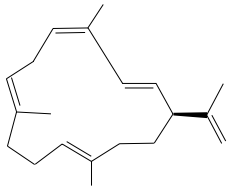
3,11-Cembradiene-8,13,15-triol C-169



$C_{20}H_{36}O_3$ 324.503

(1*S*,3*E*,8ξ,11*E*,13ξ)-*form* [210828-06-1]
Constit. of the coral *Lobophytum catalai*.
Oil. $[\alpha]_D$ +35.6 (c, 1.1 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 267-274

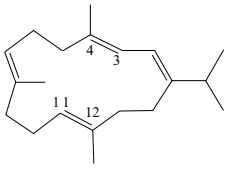
2,4,7,11,15-Cembrapentaene C-170



$C_{20}H_{30}$ 270.457

(2*E*,4*Z*,7*E*,11*E*)-*form*
Cembrenene
[79296-91-6]
Constit. of *Sinularia mayi*.
Oil. $[\alpha]_D$ +78.1 ($CHCl_3$).
Uchio, Y. *et al., Tet. Lett.*, 1981, 1689 (*isol*)
Aoki, M. *et al., Chem. Lett.*, 1983, 1121 (*abs config*)
Forkas, I. *et al., Helv. Chim. Acta*, 1990, **73**, 1980 (*synth*)
Pattenden, G. *et al., J.C.S. Perkin 1*, 1996, 57 (*synth*)

1,3,7,11-Cembratetraene C-171



(*all–E*)–*form*

$C_{20}H_{32}$ 272.473

(1*E*,3*E*,7*E*,11*E*)-*form*
Cembrene C. *Isoneocembrene A*. *α-Pinacene*
[64363-64-0]
Constit. of *Sarcophyton ehrenbergi*, *Armina maculata* and *Nephthea* spp.
Oil.

*7*R,*8*R-*Epoxide:* [75222-56-9]
$C_{20}H_{32}O$ 288.472
Constit. of *Sarcophyton crassocaule*. Oil. $[\alpha]_D$ -22.5 (c, 0.19 in $CHCl_3$).

*7*S,*8*S-*Epoxide:* ***7,8-Epoxy-1,3,11-cembratriene***
$C_{20}H_{32}O$ 288.472
Constit. of *Sarcophyton molle*.
$[\alpha]_D^{25}$ +99 (c, 1.9 in MeOH).

*11*S,*12*S-*Epoxide: 11,12-Epoxy-1,3,7-cembratriene*. ***Epoxyisoneocembrene A***. *11,12-Epoxycembrene C*
[68043-37-8]
$C_{20}H_{32}O$ 288.472
Constit. of *Sinularia grayi*. Oil. $[\alpha]_D$ +117.

*3*S,*4*S:*11*S,*12*S-*Diepoxide:* ***3,4:11,12-Diepoxy-1,7-cembradiene***
$C_{20}H_{32}O_2$ 304.472
Constit. of a *Lobophytum* sp. Cryst.
Mp 109-110°. $[\alpha]_D$ +53.5 (c, 0.56 in $CHCl_3$).

*7*S,*8*S:*11*S,*12*S-*Diepoxide:* ***7,8:11,12-Diepoxy-1,3-cembradiene***
$C_{20}H_{32}O_2$ 304.472
Constit. of a *Eunicea* sponge. Cryst. (CH_2Cl_2).
Mp 99-101°. $[\alpha]_D$ -76.4 (c, 0.4 in MeOH). λ_{max} 242 (ϵ 25000); 249 (ϵ 27000) (MeOH) (Derep).

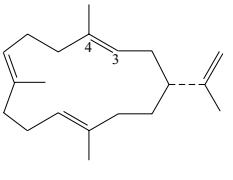
(1*Z*,3*E*,7*E*,11*E*)-*form*
γ-Pinacene
[37905-11-6]
Constit. of *Pinus koraiensis* (Korean pine) and *Pinus sibirica*.
Oil.

(1*Z*,3*Z*,7*E*,11*E*)-*form*
β-Pinacene
[37905-10-5]
Constit. of *Pinus koraiensis* (Korean pine) and *Pinus sibirica*.
Oil.

[69743-88-0]

Raldugin, V.A. *et al., Khim. Prir. Soedin.*, 1971, **7**, 604; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 582 (*isol, ir, pmr*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1978, **31**, 2707 (*isol*)
Vanderah, D.J. *et al., J.O.C.*, 1978, **43**, 1614 (*isol*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1980, **33**, 879-884; 1983, **36**, 2289 (*7R,8R-epoxide, 3,4:11,12-diepoxide*)
Raldugin, V.A. *et al., CA*, 1985, **102**, 149548s (*pmr, cmr, struct*)
Guerriero, A. *et al., Helv. Chim. Acta*, 1990, **73**, 277 (*isol*)
Shin, J. *et al., Tetrahedron*, 1993, **49**, 515 (*7,8:11,12-diepoxide*)
Rao, Z.-G. *et al., Youji Huaxue*, 1997, **17**, 252-255; *CA*, **127**, 119673c (*7S,8S-epoxide*)
Liu, Z. *et al., J.C.S. Perkin 1*, 2000, 4250-4257 (*7,8-epoxide, 11,12-epoxide, synth, abs config*)
Li, Y. *et al., Tet. Lett.*, 2000, **41**, 7465-7470 (*11,12-Epoxycembrene C, synth*)

3,7,11,15-Cembratetraene C-172



$C_{20}H_{32}$ 272.473

(*all-E*)-*form*
Cembrene A. *Neocembrene. Neocembrene A*
[31570-39-5]
Widespread in nature. Mainly found in higher plants but also in insects and corals. Component of the paracloacal gland secretion of the Chinese alligator *Alligator sinensis*. Cytotoxic to P388 and

KB cell lines. Oil. Poorly sol. hexane. $Bp_{0.8}$ 150-152°. $[\alpha]_D$ -19.7 ($CHCl_3$). n_D^{20} 1.5110.

3S,4S-Epoxide: ***3,4-Epoxy-7,11,15-cembratriene***
[79897-31-7]
$C_{20}H_{32}O$ 288.472
Isol. from *Sinularia facile* and a *Scleronephthya* sp. Cytotoxic to P388 and KB cell lines. Oil. $[\alpha]_D$ +49 (c, 0.22 in $CHCl_3$).

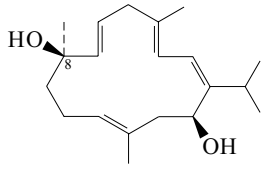
3R,4R:15ξ,16-Diepoxide: ***3,4:15,16-Diepoxy-7,11-cembradiene***
$C_{20}H_{32}O_2$ 304.472
Constit. of *Eunicea mammosa*. Oil. $[\alpha]_D^{25}$ -23.97 (c, 1.46 in $CHCl_3$). λ_{max} 242 (ϵ 25000); 249 (ϵ 27000) (MeOH) (Derep).

(3*Z*,7*E*,11*E*)-*form* [71213-92-8]
Isol. from *Cubitermes umbratus.*

[65622-51-7]

Shmidt, E.N. *et al., Khim. Prir. Soedin.*, 1970, **6**, 694; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 705 (*isol, pmr, ms, struct*)
Kitahara, Y. *et al., Chem. Lett.*, 1976, 219 (*synth*)
Ravi, B.N. *et al., J.O.C.*, 1978, **43**, 2127 (*isol, pmr, cmr*)
Wiemer, D.F. *et al., J.O.C.*, 1979, **44**, 3950 (*struct*)
Kato, T. *et al., J.O.C.*, 1980, **45**, 1126 (*synth*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1981, **34**, 1551 (*epoxide*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 918 (*synth*)
Ghisalberti, E.L. *et al., Aust. J. Chem.*, 1986, **39**, 1703 (*synth*)
Schwabe, R. *et al., Helv. Chim. Acta*, 1988, **71**, 292 (*synth*)
Forkas, I. *et al., Helv. Chim. Acta*, 1990, **73**, 1980 (*synth*)
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 1101 (*diepoxide*)
Mattern, D.L. *et al., J. Nat. Prod.*, 1997, **60**, 828-831 (*isol, alligator, cmr*)
Duh, C.-Y. *et al., J. Nat. Prod.*, 1999, **62**, 1518 (*isol, activity*)
Liu, Z. *et al., Tetrahedron: Asymmetry*, 2001, **12**, 95-100 (*synth*)
Yan, X.-H. *et al., Youji Huaxue*, 2004, **24**, 1233-1238; *CA*, **142**, 71702 (*epoxide*)

1,3,6,11-Cembratetraene-8,14-diol C-173



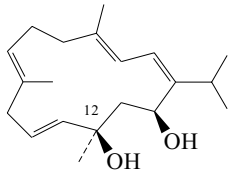
(1*Z*,3*E*,6*E*,8*R*,11*E*,14*S*)–*form*

$C_{20}H_{32}O_2$ 304.472

(1*Z*,3*E*,6*E*,8*R*,11*E*,14*S*)-*form*
Sarcophytol R
[123853-58-7]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D^{22}$ +12 (c, 0.6 in $CHCl_3$).

(1*Z*,3*E*,6*E*,8*S*,11*E*,14*S*)-*form*
Sarcophytol S
[123930-90-5]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D^{20}$ +57 (c, 0.60 in $CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2053 (*isol, pmr, cmr*)

1,3,7,10-Cembratetraene-12,14-diol C-174



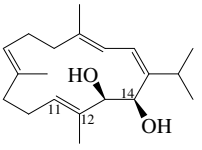
(1*Z*,3*E*,7*E*,10*E*,12*R*,14*S*)–*form*

$C_{20}H_{32}O_2$ 304.472

(1*Z*,3*E*,7*E*,10*E*,12*R*,14*S*)-*form*
Sarcophytol D
[77394-00-4]
Constit. of *Sarcophyton glaucum*.
Cryst.
Mp 131-134°. $[\alpha]_D$ +125 (c, 0.94 in $CHCl_3$).

(1*Z*,3*E*,7*E*,10*E*,12*S*,14*S*)-*form*
Sarcophytol G
[121421-64-5]
Constit. of *Sarcophyton glaucum*.
Cryst.
Mp 122-123°. $[\alpha]_D$ +109 (c, 3.17 in $CHCl_3$).
Nakagawa, T. *et al., Chem. Pharm. Bull.*, 1981, **29**, 82
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 631 (*Sarcophytol G*)

1,3,7,11-Cembratetraene-13,14-diol C-175



(1*Z*,3*E*,7*E*,11*E*,13*R*,14*R*)-*form*

$C_{20}H_{32}O_2$ 304.472

(1*Z*,3*E*,7*E*,11*E*,13*R*,14*R*)-*form*
Sarcophytol B
[72629-68-6]
Constit. of *Sarcophyton glaucum* and the coral *Alcyonium flaccidum*. Antiinflammatory and antipsoriatic agent. Histamine release inhibitor. Antitumour promoter. Cryst. (Me_2CO). Poorly sol. hexane.
Mp 125-126.5°. $[\alpha]_D$ +164 (c, 1 in $CHCl_3$). λ_{max} 253 (ϵ 17400) (EtOH) (Derep). λ_{max} 252 (MeOH) (Berdy).

14-Ac: ***14-Acetylsarcophytol B***
[145900-94-3]
$C_{22}H_{34}O_3$ 346.509
Constit. of a *Sinularia* sp. Oil. $[\alpha]_D$ +235.2 (c, 0.6 in $CHCl_3$). λ_{max} 252 (ϵ 12000) (MeOH) (Berdy).

(1*Z*,3*E*,7*E*,13*S*,14*R*)-*form*
11S,12R-Epoxide, 14-Ac: 14-Acetoxy-11,12-epoxy-1,3,7-cembratrien-13-ol. ***Flaccidoxide***
[77965-78-7]
$C_{22}H_{34}O_4$ 362.508
Isol. from *Alcyonium flaccidum*. Toxic to brine shrimp. Oil. $[\alpha]_D^{24}$ +118 (c, 2.4 in $CHCl_3$).

11S,12R-Epoxide, 13,14-di-Ac: ***Flaccidoxide acetate***
[303966-02-1]
$C_{24}H_{36}O_5$ 404.545
Constit. of *Cladiella kashmani*. Oil. $[\alpha]_D^{21}$ +157.8 (c, 0.78 in $CHCl_3$). λ_{max} 252 (log ϵ 4.3) (MeOH).

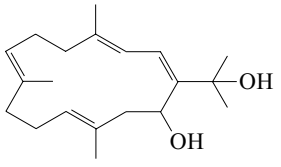
(1*Z*,3*Z*,7*E*,11*E*,13*R*,14*R*)-*form*
Sarcophytol J
[121421-67-8]
Constit. of *Sarcophyton glaucum*.
Cryst.
Mp 115-116°. $[\alpha]_D$ -277 (c, 1.5 in $CHCl_3$).

14-Ac: ***14-Acetylsarcophytol J***
[145986-76-1]
$C_{22}H_{34}O_3$ 346.509
Constit. of a *Sinularia* sp.
$[\alpha]_D$ -85.6 (c, 0.21 in $CHCl_3$).

(1*E*,3*Z*,7*E*,11*E*,13*R*,14*R*)-*form*
Sarcophytol K
[123931-78-2]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D^{20}$ +20 (c, 0.77 in $CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1979, **27**, 2382; 1989, **37**, 631; 2053 (*Sarcophytols*)
Kashman, Y. *et al., J.O.C.*, 1981, **46**, 3592 (*isol*)
Czarkie, D. *et al., Tetrahedron*, 1985, **41**, 1049 (*isol*)
McMurry, J.E. *et al., Tet. Lett.*, 1989, **30**, 1173 (*synth, cryst struct*)
Iguchi, K. *et al., J. Nat. Prod.*, 1992, **55**, 1779-1782 (*14-Acetylsarcophytol B*)

Li, W.-D.Z. *et al., Tet. Lett.*, 1999, **40**, 965-968 (*synth*)
Gray, C.A. *et al., J. Nat. Prod.*, 2000, **63**, 1551-1553 (*Flaccidoxide, Flaccidoxide acetate, abs config, activity*)

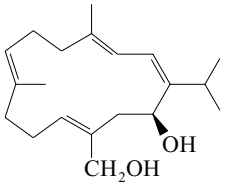
1,3,7,11-Cembratetraene-14,15-diol C-176



$C_{20}H_{32}O_2$ 304.472

(1*E*,3*E*,7*E*,11*E*,14ξ)-*form* [177714-92-0]
Constit. of *Sinularia gibberosa*.
Oil. $[\alpha]_D^{25}$ +59.1 (c, 0.015 in $CHCl_3$). λ_{max} 205 (log ϵ 4); 245 (log ϵ 3.7) (MeOH). λ_{max} 205 (ϵ 10000); 245 (ϵ 7940) (MeOH) (Berdy).
Duh, C.-Y. *et al., J. Nat. Prod.*, 1996, **59**, 595-598 (*isol, pmr, cmr*)

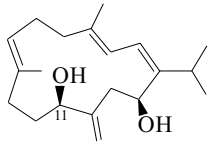
1,3,7,11-Cembratetraene-14,20-diol C-177



$C_{20}H_{32}O_2$ 304.472

(1*Z*,3*Z*,7*E*,11*Z*,14*S*)-*form*
Sarcophytol P
[123853-57-6]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D^{28}$ -66 (c, 0.84 in $CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2053 (*isol, pmr, cmr*)

1,3,7,12(20)-Cembratetraene-11,14-diol C-178



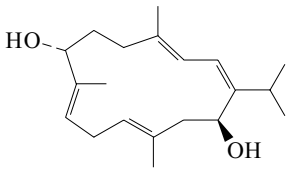
(1*Z*,3*E*,7*E*,11*R*,14*S*)–*form*

$C_{20}H_{32}O_2$ 304.472

(1*Z*,3*E*,7*E*,11*R*,14*S*)-*form*
Sarcophytol I
[121421-65-6]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D$ -31 (c, 1.3 in $CHCl_3$).

(1*Z*,3*E*,7*E*,11*S*,14*S*)-*form*
Sarcophytol E
[77393-99-8]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D$ +160 (c, 1 in $CHCl_3$).
Nakagawa, T. *et al., Chem. Pharm. Bull.*, 1981, **29**, 82 (*Sarcophytol E*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 631 (*Sarcophytol I*)

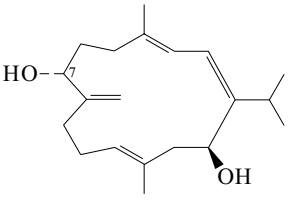
1,3,8,11-Cembratetraene-7,14-diol C-179



$C_{20}H_{32}O_2$ 304.472

(1*E*,3*E*,7*R*,8*E*,11*E*,14*S*)-*form* [159405-63-7]
Constit. of *Sarcophyton trocheliophorum*.
Oil. $[\alpha]_D$ +49 (c, 1.1 in $CHCl_3$). λ_{max} 208 (ϵ 11800); 254 (ϵ 13570) (MeOH) (Berdy).
Greenland, G.J. *et al., Aust. J. Chem.*, 1994, **47**, 2013 (*isol, pmr, cmr, abs config*)

1,3,8(19),11-Cembratetraene-7,14-diol C-180



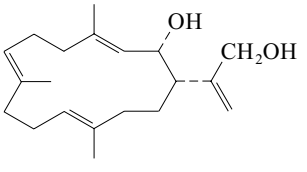
(1*Z*,3*E*,7*R*,11*E*,14*S*)–*form*

$C_{20}H_{32}O_2$ 304.472

(1*Z*,3*E*,7*R*,11*E*,14*S*)-*form*
Sarcophytol H
[121421-66-7]
Constit. of *Sarcophyton glaucum*.
Cryst.
Mp 143-145°. $[\alpha]_D$ +147 (c, 0.86 in $CHCl_3$).
Di-Ac:
$C_{24}H_{36}O_4$ 388.546
Constit. of *Sarcophyton glaucum*. Oil. $[\alpha]_D$ +195 (c, 0.85 in $CHCl_3$).

(1*Z*,3*E*,7*S*,11*E*,14*S*)-*form*
Sarcophytol O
[121340-71-4]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D$ +124 (c, 1.02 in $CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 631 (*isol, pmr, cmr*)

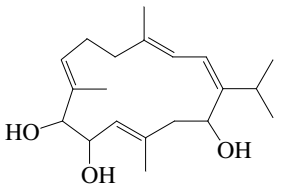
3,7,11,15(17)-Cembratetraene-2,16-diol C-181



$C_{20}H_{32}O_2$ 304.472

(1*S*,2*S*,3*E*,7*E*,11*E*)-*form*
Sinulariol A
[81780-84-9]
Constit. of *Sinularia mayi*.
Cryst.
Mp 116-117.5°. $[\alpha]_D$ +101 (c, 0.99 in $CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 2314 (*isol, pmr*)

1,3,7,11-Cembratetraene-9,10,14-triol C-182

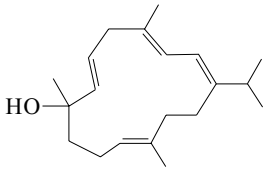


$C_{20}H_{32}O_3$ 320.471

(1*Z*,3*E*,7*E*,9ξ,10ξ,11*E*,14ξ)-*form*

14-Ac: [603089-61-8]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Eunicea tourniforti*. Oil. $[\alpha]_D$ +42.9 (c, 0.06 in $CHCl_3$). λ_{max} 248 (log ϵ 3.42) (MeOH).
Marville, K.I. *et al., J. Nat. Prod.*, 2003, **66**, 1284-1287 (*isol, pmr, cmr*)

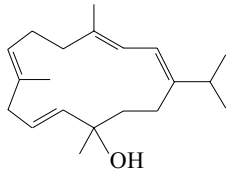
1,3,6,11-Cembratetraen-8-ol C-183



$C_{20}H_{32}O$ 288.472

(1*E*,3*E*,6*E*,11*E*)-*form*
Alcyonol B
[86302-89-8]
Constit. of coral *Alcyonium utinomii*.
Oil.
Kinamoni, Z. *et al., Tetrahedron*, 1983, **39**, 1643

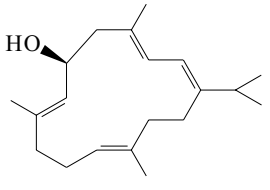
1,3,7,10-Cembratetraen-12-ol C-184



$C_{20}H_{32}O$ 288.472

(1*E*,3*E*,7*E*,10*E*)-*form*
Alcyonol A
[86302-90-1]
Constit. of coral *Alcyonium utinomii*.
Oil.
Kinamoni, Z. *et al., Tetrahedron*, 1983, **39**, 1643

1,3,7,11-Cembratetraen-6-ol C-185

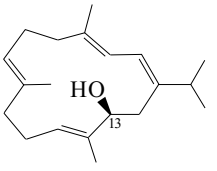


$C_{20}H_{32}O$ 288.472

(1*E*,3*E*,6*S*,7*E*,11*E*)-*form*

Ac: ***Preverecynarmin***
[128083-10-3]
$C_{22}H_{34}O_2$ 330.509
Constit. of *Armina maculata* and *Veretillum cynomorium*. Oil. $[\alpha]_D$ +116.2 (c, 0.16 in EtOH).
Guerriero, A. *et al., Helv. Chim. Acta*, 1990, **73**, 277-283 (*isol, pmr, cmr*)
Lan, J. *et al., Tet. Lett.*, 1999, **40**, 1963-1966 (*synth*)

1,3,7,11-Cembratetraen-13-ol C-186



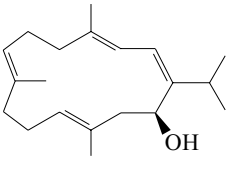
$C_{20}H_{32}O$ 288.472
λ_{max} 257 (ϵ 31000) (hexane) (Derep).

(1*E*,3*E*,7*E*,11*E*,13*S*)-*form* [81575-69-1]
Constit. of *Nephthea brassica*.
Cryst. (MeCN) (also descr. as foam).
Mp 66-68°. $[\alpha]_D$ -8.5 (-34.6).

Ac: ***Isosarcophytol A***
$C_{22}H_{34}O_2$ 330.509
Constit. of *Nephthea brassica*. Oil. $[\alpha]_D$ -1.4.

*7*R,*8*R-*Epoxide, Ac:* ***Epoxysartone B***
[237755-18-9]
$C_{22}H_{34}O_3$ 346.509
Constit. of a *Sarcophyton* sp. Oil. $[\alpha]_D$ +50.7 (c, 0.18 in MeOH). Trivial name is misleading since it is not an epoxide of Sartone B, in C-206 and it is not a ketone. λ_{max} 250 (log ϵ 4.33) (MeOH).
Poet, S.E. *et al., Aust. J. Chem.*, 1982, **35**, 77 (*isol*)
Blackman, A.J. *et al., Aust. J. Chem.*, 1982, **35**, 1873 (*isol*)
Li, Y. *et al., J.C.S. Perkin 1*, 1993, 2953 (*synth*)
Li, W.D. *et al., Chin. Chem. Lett.*, 1994, **5**, 97 (*synth*)
Iwagawa, T. *et al., J. Nat. Prod.*, 1999, **62**, 1046-1049 (*Epoxysartone B*)

1,3,7,11-Cembratetraen-14-ol C-187



(1*Z*,3*E*,7*E*,11*E*,14*S*)–*form*

$C_{20}H_{32}O$ 288.472

(1*Z*,3*E*,7*E*,11*E*,14*S*)-*form*
Sarcophytol A
[72629-69-7]
Constit. of *Sarcophyton* sp. and *Sinularia* sp. Antitumour promoter. Ornithine decarboxylase inhibitor. Hyperplasia and histamine release inhibitor. Antiinflammatory, cytotoxic and antipsoriatic agent. Oil. Poorly sol. hexane. $[\alpha]_D$ +115. $[\alpha]_D$ +206.5 ($CHCl_3$). λ_{max} 253 (ϵ 17400) (EtOH) (Derep).

Ac: [72629-72-2]
$C_{22}H_{34}O_2$ 330.509
Constit. of *Sarcophyton* spp. Oil. $[\alpha]_D$ +206.5 (c, 1.72 in $CHCl_3$) (+127). λ_{max} 252 (ϵ 20000) (EtOH) (Derep).

7α,8α-Epoxide: 7,8-Epoxy-1,3,11-cembratrien-14-ol. ***7,8-Epoxy-sarcophytol A***
[159309-65-6]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Sarcophyton trocheliophorum*. Oil. $[\alpha]_D$ +87 (c, 1.11 in $CHCl_3$).

7α,8α-Epoxide, Ac: 14-Acetoxy-7,8-epoxy-1,3,11-cembratriene
[159572-49-3]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Sarcophyton trocheliophorum*. Oil. $[\alpha]_D$ +136 (c, 1.1 in $CHCl_3$).

11α,12α-Epoxide: 11,12-Epoxy-1,3,7-cembratrien-14-ol. ***11,12-Epoxysarcophytol A***
[88924-81-6]
$C_{20}H_{32}O_2$ 304.472
Constit. of a *Lobophytum* sp. and *Cladiella kashmani*. Toxic to brine shrimp. Needles (MeCN).
Mp 75-76°. $[\alpha]_D$ +229 (c, 0.95 in $CHCl_3$).

11α,12α-Epoxide, Ac: 14-Acetoxy-11,12-epoxy-1,3,7-cembratriene
[88924-80-5]
$C_{22}H_{34}O_3$ 346.509
Constit. of a *Lobophytum* sp. Oil. $[\alpha]_D$ +296 (c, 0.36 in $CHCl_3$).

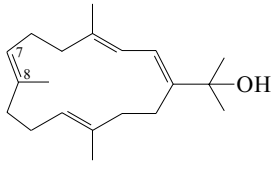
(1*Z*,3*E*,7*E*,11*E*,14*R*)-*form* [137894-82-7]
Constit. of *Plexaura flexuosa*.
Oil. $[\alpha]_D^{29}$ -190.4 (c, 1 in $CHCl_3$).

(1*Z*,3*Z*,7*E*,11*E*,14*S*)-*form*
Sarcophytol N
[121421-68-9]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D$ -280 (c, 0.77 in $CHCl_3$).

(1*E*,3*E*,7*E*,11*E*,14*S*)-*form*
Sarcophytol F
[123930-91-6]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D$ +57 (c, 0.99 in $CHCl_3$).

(1*E*,3*Z*,7*E*,11*E*,14*S*)-*form* [125710-44-3]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D^{19}$ -12 (c, 0.84 in $CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1979, **27**, 2387-2382; 1988, **36**, 2331-2341; 1989, **37**, 631-636; 2053-2057; 1990, **38**, 815-817 (*isol, struct, abs config, Sarcophytols*)
Blackman, A.J. *et al., Aust. J. Chem.*, 1982, **35**, 1873-1880 (*isol*)
Bawden, B.F. *et al., Aust. J. Chem.*, 1983, **36**, 2289-2295 (*11,12-Epoxysarcophytol A*)
Kobayashi, M. *et al., J.O.C.*, 1990, **55**, 1947-1951 (*isol, pmr, cmr*)
Takayanagi, H. *et al., Tet. Lett.*, 1990, **31**, 3317-3320 (*synth*)
Peniston, M. *et al., J. Nat. Prod.*, 1991, **54**, 1009-1016 (*isol, pmr, cmr*)
Takahashi, T. *et al., J.O.C.*, 1992, **57**, 3521-3523 (*synth*)
Kodama, M. *et al., Tet. Lett.*, 1993, **34**, 8453-8456 (*synth*)
Greenland, G.J. *et al., Aust. J. Chem.*, 1994, **47**, 2013-2021 (*7,8-Epoxysarcophytol A, cmr*)
Takayanagi, H. *et al., J.O.C.*, 1994, **59**, 2700-2706 (*synth*)
Takayanagi, H. *et al., J.C.S. Perkin 1*, 1995, 751-756 (*synth*)
Shen, J.-H. *et al., J. Chin. Chem. Soc. (Taipei)*, 1999, **46**, 253-257 (*isol, activity*)
Li, W.-D.Z. *et al., Tet. Lett.*, 1999, **40**, 965-968 (*synth*)
Koh, M. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 858-861 (*Sarcophytol A, occur*)
Gray, C.A. *et al., J. Nat. Prod.*, 2000, **63**, 1551 (*activity*)
Lan, J. *et al., Tet. Lett.*, 2000, **41**, 2181-2184 (*11,12-Epoxysarcophytol A, synth*)

1,3,7,11-Cembratetraen-15-ol C-188



$C_{20}H_{32}O$ 288.472

(All-*E*)-*form*
Constit. of *Lobophytum pauciflorum*.
Cryst. (hexane).
Mp 81-83°.

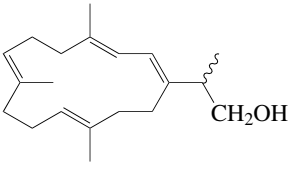
*7*R,*8*S-*Epoxide:* ***7,8-Epoxy-1,3,11-cembratrien-15-ol***
[64285-82-1]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Sarcophyton* spp. Cryst. (petrol).
Mp 105-106°. $[\alpha]_D$ +61.8 (c, 0.5 in EtOH).

11,12-Epoxide: ***11,12-Epoxy-1,3,7-cembratrien-15-ol***
[177770-69-3]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Sinularia gibberosa*. Oil. $[\alpha]_D^{25}$ -8.6 (c, 0.17 in $CHCl_3$). λ_{max} 202 (ϵ 12590); 244 (ϵ 10000) (MeOH) (Berdy).

Me ether, 3β,4β:11β,12β-diepoxide: ***3,4:11,12-Diepoxy-15-methoxy-1,7-cembradiene***
[177714-91-9]
$C_{21}H_{34}O_3$ 334.498
Constit. of *Sinularia gibberosa*. Prisms.
Mp 98-100°. $[\alpha]_D^{25}$ +138.9 (c, 0.24 in $CHCl_3$). λ_{max} 205 (ϵ 25119) (MeOH) (Berdy).

*3*R*,4*S*:11*R*,12*S*-Diepoxide: 3,4:11,12-Diepoxy-17-cembradien-15-ol.* ***Sinugibberol***
[167709-44-6]
$C_{20}H_{32}O_3$ 320.471
Constit. of *Sinularia gibberosa*. Cryst.
Mp 142-144°. $[\alpha]_D$ +30.6 (c, 0.011 in $CHCl_3$). λ_{max} 210 (ϵ 20000) (MeOH) (Berdy).
Coll, J.C. *et al., Aust. J. Chem.*, 1977, **30**, 1305 (*cryst struct, epoxide*)
Bowden, B.F. *et al., J. Nat. Prod.*, 1987, **50**, 650
Hoa, R.-S. *et al., J. Nat. Prod.*, 1995, **56**, 1126 (*Sinugibberol, isol, pmr, cmr, cryst struct*)
Duh, C.-Y. *et al., J. Nat. Prod.*, 1996, **59**, 595 (*isol, pmr, cmr*)

1,3,7,11-Cembratetraen-16-ol C-189



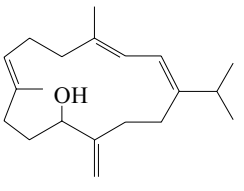
$C_{20}H_{32}O$ 288.472

(1*E*,3*E*,7*E*,11*E*,15ξ)-*form*
Carboxylic acid, Me ester: Methyl 1,3,7,11-cembratetraen-16-oate
$C_{21}H_{32}O_2$ 316.483
Constit. of *Sinularia mayi*. Oil. $[\alpha]_D$ +43.4 (c, 0.09 in $CHCl_3$).

*(11*R*,12*R*)-Epoxide, Ac:* ***16-Acetoxy-11,12-epoxy-1,3,7-cembratriene***
[204252-45-9]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Sarcophyton ehrenbergi*. Oil. $[\alpha]_D^{25}$ +54.6 (c, 0.5 in $CHCl_3$). λ_{max} 245 (ϵ 8550); 249 (ϵ 8810); 259 (sh) (ϵ 5710) (EtOH).

*(3*R*,4*S*:11*R*,12*R*)-Diepoxide, Ac: 16-Acetoxy-3,4:11,12-diepoxy-1,7-cembradiene*
[204252-46-0]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Sarcophyton ehrenbergi*. Oil. $[\alpha]_D^{25}$ +1.8 (c, 0.5 in $CHCl_3$).
Kusumi, T. *et al., Chem. Lett.*, 1990, 1315 (*acid*)
König, G.M. *et al., J. Nat. Prod.*, 1998, **61**, 494-496 (*epoxide derivs*)

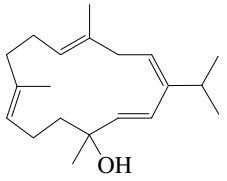
1,3,7,12(20)-Cembratetraen-11-ol C-190



$C_{20}H_{32}O$ 288.472

(1*E*,3*E*,7*E*)-*form*
Alcyonol C
[86302-88-7]
Constit. of coral *Alcyonium utinomii*.
Oil.
Kinamoni, Z. *et al., Tetrahedron*, 1983, **39**, 1643

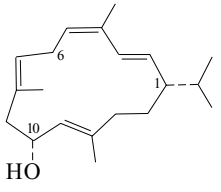
1,4,8,13-Cembratetraen-12-ol C-191



$C_{20}H_{32}O$ 288.472

(1*Z*,4*E*,8*E*,12ξ,14*E*)-*form*
Acutanol
[421547-05-09]
Constit. of *Sarcophyton acutangulum*.
Mada, K. *et al., Spectroscopy (Amsterdam)*, 2001, **15**, 177-182 (*isol*)

2,4,7,11-Cembratetraen-10-ol C-192

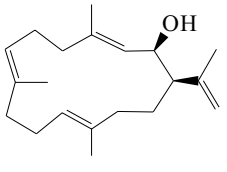


Absolute configuration

$C_{20}H_{32}O$ 288.472

(1*S*,2*E*,4*Z*,7*E*,10*R*,11*E*)-*form*
10-Hydroxycembrene
[81522-05-6]
Constit. of the soft corals *Sarcophyton elegans* and *Sarcophyton glaucum*.
Cryst. (Et_2O/petrol).
Mp 126-127°. $[\alpha]_D$ +155 (c, 0.94 in $CHCl_3$).
Me ether: ***10-Methoxycembrene***
[81499-19-6]
$C_{21}H_{34}O$ 302.499
Constit. of *Sarcophyton elegans*. Oil. $[\alpha]_D$ +130.6 (c, 1.0 in $CHCl_3$).
10-Ketone: 2,4,7,11-Cembratetraen-10-one. ***10-Oxocembrene***
[88210-49-5]
$C_{20}H_{30}O$ 286.456
Constit. of *Sarcophyton elegans*. Oil. $[\alpha]_D$ +313.9 (c, 2.0 in $CHCl_3$).
Uchio, Y. *et al., Chem. Lett.*, 1983, 1719 (*cryst struct*)

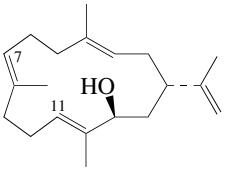
3,7,11,15-Cembratetraen-2-ol C-193



$C_{20}H_{32}O$ 288.472

(1*R*,2*R*,3*E*,7*E*,11*E*)-*form*
Mayol
[79355-94-5]
Constit. of *Sinularia mayi*.
Oil. $[\alpha]_D$ +138.5 ($CHCl_3$).
Ac: ***Mayol acetate***
[79355-95-6]
$C_{22}H_{34}O_2$ 330.509
Constit. of *Sinularia hirta*. Oil. $[\alpha]_D^{25}$ +77.2 (c, 0.9 in $CHCl_3$).
Uchio, Y. *et al., Tet. Lett.*, 1981, 1689 (*isol*)
Aoki, M. *et al., Chem. Lett.*, 1983, 1121 (*abs config*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 815 (*acetate*)

3,7,11,15-Cembratetraen-13-ol C-194



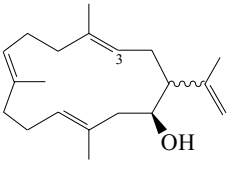
$C_{20}H_{32}O$ 288.472

(1*S*,3*E*,7*E*,11*E*,13*S*)-*form*
13-Hydroxyneocembrene
[117854-31-6]
Constit. of *Sarcophyton trocheliophorum*.
Oil. $[\alpha]_D^{20}$ -150 (c, 0.2 in MeOH).
*11*S*,12*S*-Epoxide: 11,12-Epoxy-3,7,15-cembratrien-13-ol.* ***11,12-Epoxy-13-hydroxyneocembrene***
[117872-28-3]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Sarcophyton trocheliophorum*. Oil. $[\alpha]_D^{20}$ -85 (c, 0.5 in MeOH).
13-Ketone: ***3,7,11,15-Cembratetraen-13-one***
[65622-49-3]
$C_{20}H_{30}O$ 286.456
Constit. of an unidentified soft coral. λ_{max} 233 (ϵ 11000) (hexane) (Derep).

(1*R*,3*E*,11*E*,13*R*)-*form*
*7*S,8*S-*Epoxide:* [198559-59-0]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Eunicea succinea*. Oil. $[\alpha]_D^{25}$ -8.1 (c, 4.2 in $CHCl_3$).

(1*S*,3*E*,7*E*,11*Z*)-*form*
13-Ketone: [65622-47-1]
Constit. of an unidentified soft coral.
Oil. $[\alpha]_D$ -20.56 (c, 5.3 in CCl_4).
Ravi, B.N. *et al., J.O.C.*, 1978, **43**, 2127-2131 (*ketones*)
Suleimenova, A.M. *et al., Khim. Prir. Soedin.*, 1988, **24**, 535-540; *Chem. Nat. Compd. (Engl. Transl.)*, 1988, **24**, 453-458 (*Sarcophyton trocheliophorum constits, isol, pmr, cmr, cryst struct*)
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 1134-1138 (*7,8-epoxide*)
Xing, Y. *et al., J. Chin. Chem. Soc. (Taipei)*, 1999, **46**, 595-600 (*synth*)
Zhang, T. *et al., Synthesis*, 2001, 393-398 (*13-Hydroxyneocembrene, 11,12-Epoxy-13-hydroxyneocembrene*)
Liu, Z. *et al., Tet. Lett.*, 2001, **42**, 275-277 (*synth*)

3,7,11,15-Cembratetraen-14-ol C-195



(1α,3*E*,7*E*,11*E*,14β)–*form*

$C_{20}H_{32}O$ 288.472

(1α,3*E*,7*E*,11*E*,14β)-*form*

14-Ketone: 3,7,11,15-Cembratetraen-14-one. ***Sinularone A***
[118628-94-7]
$C_{20}H_{30}O$ 286.456
Constit. of *Sinularia mayi*. Oil. $[\alpha]_D$ -410 (c, 1.59 in $CHCl_3$).

3α,4α-Epoxide: ***3,4-Epoxy-7,11,15-cembratrien-14-ol***
[65622-50-6]
$C_{20}H_{32}O_2$ 304.472
Constit. of an unidentified soft coral.

3α,4α-Epoxide, 14-ketone: ***3,4-Epoxy-7,11,15-cembratrien-14-one***
[65622-48-2]
$C_{20}H_{30}O_2$ 302.456
Constit. of an unidentified soft coral. Cryst. (Et_2O).
Mp 66°. $[\alpha]_D$ +38.65 (c, 4.16 in $CHCl_3$). λ_{max} 217 (ϵ 1070) (hexane) (Derep).

11,12-Epoxide, 14-ketone: 11,12-Epoxy-3,7,15-cembratrien-14-one. ***Sinularone B***
[118583-95-2]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Sinularia mayi*. Oil. $[\alpha]_D$ -108 (c, 1.46 in $CHCl_3$).

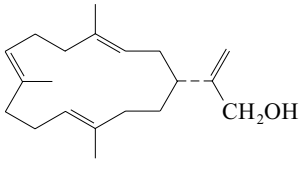
(All-*E*,14*S*)-*form*
Sinulariol C
[118628-93-6]
Constit. of *Sinularia mayi*.
Oil. $[\alpha]_D$ +12.2 (c, 1.5 in $CHCl_3$).

(1ξ,3*E*,7*E*,11*E*,14ξ)-*form*
14-Hydroxyneocembrene
[95772-53-5]
Constit. of *Sinularia mayi*.
Oil. $[\alpha]_D$ -30.3 (c, 0.9 in $CHCl_3$).

[118628-95-8]

Ravi, B.N. *et al., J.O.C.*, 1978, **43**, 2127 (*epoxides*)
Aoki, M. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 779
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3780 (*isol, pmr, cmr, Sinulariol C, Sinularones*)

3,7,11,15(17)-Cembratetraen-16-ol C-196



$C_{20}H_{32}O$ 288.472

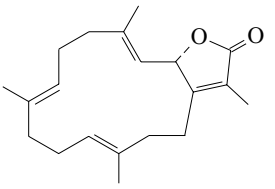
(1*R*,3*E*,7*E*,11*E*)-*form*
Sinulariol D
[118583-93-0]
Constit. of *Sinularia mayi* and *Sarcophyton glaucum*.
Oil. $[\alpha]_D$ +14 (c, 0.84 in $CHCl_3$).

16-Aldehyde: 3,7,11,15(17)-Cembratetraen-16-al. ***Sinularial A***
[118607-64-0]
$C_{20}H_{30}O$ 286.456
Constit. of *Sinularia mayi*. Oil. $[\alpha]_D$ +12.5 (c, 0.64 in $CHCl_3$).

16-Carboxylic acid: 3,7,11,15(17)-Cembratetraen-16-oic acid. ***Sinularic acid A***
[118583-94-1]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Sinularia mayi*. Oil. $[\alpha]_D$ +19.7 (c, 0.71 in $CHCl_3$).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3780; 1989, **37**, 631-636 (*isol, pmr, cmr*)
Yue, X. *et al., Bull. Soc. Chim. Belg.*, 1996, **105**, 373-375 (*synth*)

1(15),3,7,11-Cembratetraen-16,2-olide C-197

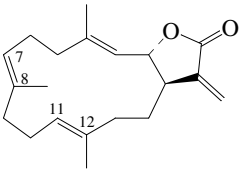


$C_{20}H_{28}O_2$ 300.44

(3*E*,7*E*,11*E*)-*form*
Sarcophytonin B
[131614-81-8]
Constit. of a *Sarcophyton* coral.
Oil. $[\alpha]_D^{21}$ +160 (c, 0.97 in $CHCl_3$).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2442 (*isol, pmr, cmr*)
Nishitani, K. *et al., Heterocycles*, 1994, **37**, 679 (*synth*)

3,7,11,15(17)-Cembratetraen-16,2-olide C-198
Cembranolide



(1*R*,2*S*,3*E*,7*E*,11*E*)-*form*

$C_{20}H_{28}O_2$ 300.44

(1*R*,2*S*,3*E*,7*E*,11*E*)-*form* [473700-48-0]
Constit. of *Clavularia koellikeri*.
Oil. $[\alpha]_D^{25}$ +28.9 (c, 1.25 in $CHCl_3$). λ_{max} 219 (log ϵ 2.19) (EtOH).

(1*S*,2*R*,3*E*,7*E*,11*E*)-*form*
Constit. of *Sinularia mayi*.
Oil. $[\alpha]_D$ -29 (c, 3.4 in $CHCl_3$).

*7*R*,8*R*-Epoxide:* ***7,8-Epoxy-3,11,15(17)-cembratrien-16,2-olide***
$C_{20}H_{28}O_3$ 316.439
Isol. from *Efflatounaria variabilis.* Oil. $[\alpha]_D$ +48.1 (c, 1.4 in $CHCl_3$).

(1*S*,2*S*,3*E*,7*E*,11*E*)-*form*
Constit. of *Sinularia mayi* and *Lobophytum michaelae.*
Cryst.
Mp 98-99°. $[\alpha]_D$ +89.9 (c, 1.9 in $CHCl_3$).

*7*R*,8*R*-Epoxide:* [158513-22-5]
$C_{20}H_{28}O_3$ 316.439
Constit. of a *Lobophytum* sp. Cryst. (EtOAc/petrol).
Mp 151-152°.

*7*S*,8*S*-Epoxide:*
$C_{20}H_{28}O_3$ 316.439
Isol. from *Efflatounaria* sp. G12651. Cryst. (Et_2O/petrol).
Mp 171-172°. $[\alpha]_D$ +3 (c, 0.55 in $CHCl_3$).

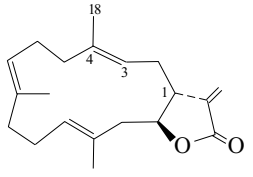
(1ξ,2ξ,3*E*,7*E*)-*form*

11ξ,12ξ-Epoxide: ***11,12-Epoxy-3,7,15(17)-cembratrien-16,2-olide***
[75077-41-7]
$C_{20}H_{28}O_3$ 316.439
Isol. from *Lobophytum pauciflorum*. Cryst. (MeOH).
Mp 121-124°.

Coll, J.C. *et al., Aust. J. Chem.*, 1977, **30**, 1859-1863 (*isol, Lobophytum*)
Yamada, Y. *et al., Chem. Pharm. Bull.*, 1980, **28**, 2035 (*11,12-epoxide*)
Uchio, Y. *et al., Chem. Lett.*, 1982, 277 (*isol*)
Kodama, M. *et al., Tet. Lett.*, 1982, **23**, 5175 (*synth*)
Aoki, M. *et al., Chem. Lett.*, 1984, 695 (*synth*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1986, **39**, 123 (*7,8-epoxides*)
Marshall, J.A. *et al., Tet. Lett.*, 1987, **28**, 5081 (*synth*)

Nishitani, K. *et al., Heterocycles*, 1993, **36**, 1957; 1994, **37**, 679 (*synth*)
Rao, C.B. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 1004-1005 (*7,8-epoxide*)
Taber, D.F. *et al., J.O.C.*, 1997, **62**, 6603-6607 (*synth*)
Iwashima, M. *et al., J. Nat. Prod.*, 2002, **65**, 1441-1446 (*Clavularia koellikeri constit*)

3,7,11,15(17)-Cembratetraen-16,14-olide C-199



(1*R*,3*E*,7*E*,11*E*,14*S*)–*form*

$C_{20}H_{28}O_2$ 300.44

(1*R*,3*E*,7*E*,11*E*,14*S*)-*form*
Constit. of soft coral *Lobophytum crassospiculatum*.
Oil. $[\alpha]_D$ +61 (c, 0.16 in $CHCl_3$).

*3*R,*4*R-*Epoxide: 3,4-Epoxy-7,11,15(17)-cembratrien-16,14-olide.* ***Isolobophytolide***
[66275-29-4]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Lobophytum crassospiculatum* and *Lobophytum crassum*. Cryst. (pentane) or oil.
Mp 59-60°. $[\alpha]_D$ -139 (c, 0.7 in $CHCl_3$). $[\alpha]_D$ -103 (c, 0.04 in $CHCl_3$). λ_{max} 210 (ϵ 6540) (EtOH) (Derep).

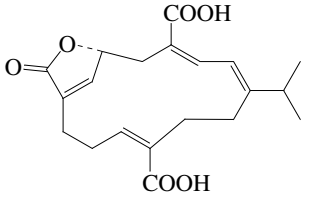
(1*S*,3*E*,7*E*,11*E*,14*R*)-*form*
*3*S,*4*S-*Epoxide:* ***Sarcocrassolide***
[313674-25-8]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Sarcophyton crassocaule*. Oil. $[\alpha]_D^{25}$ +7.8 (c, 0.1 in $CHCl_3$). λ_{max} 235 (log ϵ 4.2) (MeOH).

(1*S*,3*E*,7*E*,11*E*,14*S*)-*form*
*3*R,*4*R-*epoxide:* ***Euniolide***
$C_{20}H_{28}O_3$ 316.439
Isol. from gorgonians *Eunicea succinea* and *Eunicea mammosa*.
Cryst. ($CHCl_3$/MeOH).
Mp 122-125°. $[\alpha]_D^{26}$ +30 (c, 0.15 in $CHCl_3$). λ_{max} 242 (ϵ 350) ($CHCl_3$) (Berdy).

(1ξ,3*E*,7*E*,11*E*,14ξ)-*form*
3ξ,4ξ-Epoxide, 18-acetoxy: 18-Acetoxy-3,4-epoxy-7,11,15(17)-cembratrien-16,14-olide. ***Lobolide***
[64180-71-8]
$C_{22}H_{30}O_5$ 374.476
Isol. from a *Lobophytum* sp. Ichthyotoxin. Cryst.
Mp 114-115°. $[\alpha]_D$ -58 (c, 2.7 in $CHCl_3$). λ_{max} 209 (ϵ 7000) (MeOH) (Berdy).

Kashman, Y. *et al., Tet. Lett.*, 1977, 1159 (*Lobolide*)
Bowden, B.F. *et al., Tet. Lett.*, 1977, 3661 (*isol, struct*)
Ahond, A. *et al., Aust. J. Chem.*, 1979, **32**, 1273 (*isol, struct*)
Marshall, J.A. *et al., J.O.C.*, 1987, **52**, 2378 (*struct, synth*)
McMurry, J.E. *et al., J.A.C.S.*, 1990, **112**, 6942 (*synth*)
Morales, J.J. *et al., Tetrahedron*, 1990, **46**, 5889 (*Euniolide*)
Duh, C.Y. *et al., J. Nat. Prod.*, 2000, **63**, 1634-1637 (*Sarcocrassolide*)

1,3,7,11-Cembratetraen-19,6-olide-18,20-dioic acid C-200

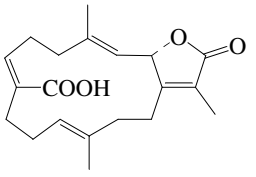


$C_{20}H_{24}O_6$ 360.406

(1*E*,3*Z*,6α,11*Z*)-*form*
Di-Me ester: [467430-39-3]
$C_{22}H_{28}O_6$ 388.46
Constit. of a *Sarcophyton* sp. Oil.
1β,2β-Epoxide, di-Me ester: [467430-40-6]
$C_{22}H_{28}O_7$ 404.459
Constit. of a *Sarcophyton* sp. Oil.

Longeon, A. *et al., Tet. Lett.*, 2002, **43**, 5937-5939 (*isol, pmr, cmr*)

1(15),3,7,11-Cembratetraen-16,2-olid-19-oic acid C-201

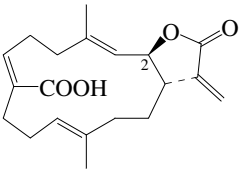


$C_{20}H_{26}O_4$ 330.423

(2*S*,3*E*,7*Z*,11*E*)-*form*
Me ester: ***13-Dehydroxysarcoglaucol-16-one***
[541509-68-6]
$C_{21}H_{28}O_4$ 344.45
Constit. of *Sarcophyton chebonnieri*. Solid. $[\alpha]_D^{23}$ +79 (c, 0.1 in MeOH). λ_{max} 211 (ϵ 8040) (MeOH).

Gross, H. *et al., Org. Biomol. Chem.*, 2003, **1**, 944-949 (*isol, pmr, cmr*)

3,7,11,15(17)-Cembratetraen-16,2-olid-19-oic acid C-202



(1*S*,2*R*,3*E*,7*Z*,11*E*)-*form*

$C_{20}H_{26}O_4$ 330.423
Confusion in lit. concerning C-7 double bond configs.

(1*S*,2*R*,3*E*,7*Z*,11*E*)-*form*
Anisomelic acid. *Anisomelide. Anisomelolide*
[59632-76-7]
Isol. from *Anisomeles malabarica* and *Anisomeles indica*.
Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 155° (142-143°). $[\alpha]_D^{25}$ -35 ($CHCl_3$). λ_{max} 206 (EtOH) (Berdy).

(1*S*,2*R*,3*E*,7*Z*,11*Z*)-*form*
11Z-2-Epilobohedleolide. *11Z-Anisomelic acid*
[158513-21-4]
Constit. of a *Lobophytum* sp.
Cryst. (Me_2CO/petrol).
Mp 190-192°. λ_{max} 219 (ϵ 9850) (MeOH).

(1*S*,2*S*,3*E*,7*E*,11*E*)-*form*
7E-Lobohedleolide
From *Lobophytum hedleyi*. Shows HIV-inhibitory activity, growth inhibitor. Cryst. (EtOH).
Mp 183-184°. $[\alpha]_D$ +61.4 (c, 1.01 in $CHCl_3$). $[\alpha]_D$ +35 (c, 0.07 in $CHCl_3$).

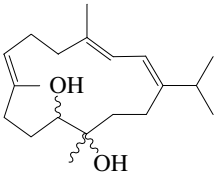
p-*Bromophenacyl ester:*
Cryst. (EtOH). Mp 130-131°.

19-Alcohol: 19-Hydroxy-3,7,11,15(17)-cembratetraen-16,2-olide
$C_{20}H_{28}O_3$ 316.439

19-Alcohol, 19-Ac: ***Lobocrassolide***
[286432-47-1]
$C_{22}H_{30}O_4$ 358.477
Constit. of *Lobophytum crassum*. Cryst.
Mp 98-100°. $[\alpha]_D^{25}$ +81.6 (c, 1.2 in $CHCl_3$).

(1*S*,2*S*,3*E*,7*Z*,11*E*)-*form*
Lobohedleolide
[81026-38-2]
Isol. from *Lobophytum hedleyi* and *Lobophytum crassum*.
Cytotoxic agent. HIV-inhibitory activity. Oil. Poorly sol. hexane.
$[\alpha]_D$ +104.2 (c, 1.12 in $CHCl_3$). λ_{max} 217 (ϵ 9800) (EtOH) (Berdy).
Purushothaman, K.K. *et al., Indian J. Chem.*, 1975, **13**, 1357 (*isol*)
Devi, G. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 441 (*isol, struct*)
Uchio, Y. *et al., Tet. Lett.*, 1981, **22**, 4089-4092 (*cryst struct, activity*)
Marshall, J.A. *et al., Tetrahedron*, 1987, **43**, 4849-4860 (*synth*)
Rao, C.B. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 1004-1005 (*1S,2R,3E,7Z,11Z-form*)
Rashid, M.A. *et al., J. Nat. Prod.*, 2000, **63**, 531-533 (*isol, activity*)
Duh, C.Y. *et al., J. Nat. Prod.*, 2000, **63**, 884-885 (*Lobocrassolide*)

1,3,7-Cembratriene-11,12-diol C-203

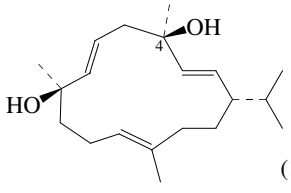


$C_{20}H_{34}O_2$ 306.487

(1*E*,3*E*,7*E*,11ξ,12ξ)-*form* [210828-05-0]
Constit. of the coral *Lobophytum catalai*.
Oil. $[\alpha]_D$ +15.2 (c, 1.2 in $CHCl_3$). λ_{max} 252 ($CHCl_3$).
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 267-274

2,6,11-Cembratriene-4,8-diol C-204

3,8,13-Duvatriene-1,5-diol



(1*S*,2*E*,4*R*,6*E*,8*R*,11*E*)-*form*

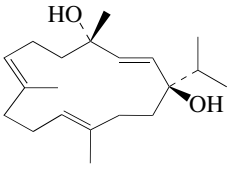
$C_{20}H_{34}O_2$ 306.487

(1*S*,2*E*,4*R*,6*E*,8*R*,11*E*)-*form*
11S,12S-Epoxide: ***11,12-Epoxy-2,6-cembradiene-4,8-diol***
[95404-30-1]
$C_{20}H_{34}O_3$ 322.487
Constit. of a *Sarcophyton* sp. Powder. $[\alpha]_D^{25}$ -6.5 (c, 0.26 in $CHCl_3$).
λ_{max} 208 (ϵ 1600) (MeOH).

(1*S*,2*E*,4*R*,6*E*,8*S*,11*E*)-*form* [84367-92-0]
Constit. of tobacco.
Cryst. (Et_2O).
Mp 150-152° (146-148°). $[\alpha]_D^{25}$ +40. $[\alpha]_D$ +38 (c, 0.37 in $CHCl_3$).
11S,12S-Epoxide: [84284-67-3]
Constit. of a *Sarcophyton* sp.
Powder. $[\alpha]_D^{25}$ -8.2 (c, 0.28 in $CHCl_3$). λ_{max} 208 (ϵ 1400) (MeOH).

(1*S*,2*E*,4*S*,6*E*,8*S*,11*E*)-*form* [84367-90-8]
Constit. of tobacco.
Cryst. (hexane).
Mp 118-120° (116-119°). $[\alpha]_D^{25}$ +100. $[\alpha]_D$ +72 (c, 0.57 in $CHCl_3$).
Rowland, R.L. *et al., J.O.C.*, 1963, **28**, 1165-1169 (*isol*)
Colledge, A. *et al., Ann. Tab., Sect. 2*, 1974, 159 (*isol*)
Wahlberg, I. *et al., Acta Chem. Scand., Ser. B*, 1982, **36**, 443-449 (*isol, pmr, struct, bibl, cryst struct*)
Pham, N.B. *et al., J. Nat. Prod.*, 2002, **65**, 1147-1150 (*epoxides*)

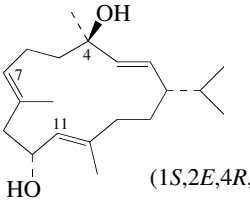
2,7,11-Cembratriene-1,4-diol C-205



$C_{20}H_{34}O_2$ 306.487

(1*S*,2*E*,4*R*,7*E*,11*E*)-*form*
Sarcophytol T
[204251-32-1]
Constit. of *Sarcophyton ehrenbergi*.
Oil. $[\alpha]_D^{25}$ -6.5 (c, 1 in $CHCl_3$).
König, G.M. *et al., J. Nat. Prod.*, 1998, **61**, 494-496 (*isol, pmr, cmr*)

2,7,11-Cembratriene-4,10-diol C-206



(1*S*,2*E*,4*R*,7*E*,10*R*,11*E*)-*form*

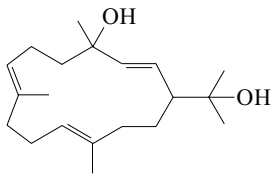
$C_{20}H_{34}O_2$ 306.487

(1*S*,2*E*,4*R*,7*E*,10*R*,11*E*)-*form*
Sartol A
[185117-70-8]
Constit. of *Sarcophyton* sp.
Oil. $[\alpha]_D^{27}$ +24.7 (c, 0.75 in MeOH). λ_{max} 208 (ϵ 5370) (MeOH).
4-Me ether: ***4-O-Methylsartol A***
[185102-32-3]
$C_{21}H_{36}O_2$ 320.514
Constit. of *Sarcophyton* sp. Oil. $[\alpha]_D^{27}$ +16.7 (c, 0.87 in MeOH).
10-Ketone: 4-Hydroxy-2,7,11-cembratrien-10-one. ***Sartone A***
[185117-77-5]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Sarcophyton* sp. Oil. $[\alpha]_D^{27}$ +134.6 (c, 0.69 in MeOH).
λ_{max} 246 (ϵ 7300) (MeOH). λ_{max} 246 (ϵ 7300) (MeOH) (Berdy).
10-Ketone, 11α,12β-epoxide: 11,12-Epoxy-4-hydroxy-2,7-cembradien-10-one. ***Epoxysartone A***
[185102-34-5]
$C_{20}H_{32}O_3$ 320.471
Constit. of *Sarcophyton* sp. Oil. $[\alpha]_D^{27}$ +30.4 (c, 0.49 in MeOH).
Error in struct. diag. in ref. λ_{max} 206 (ϵ 3840) (MeOH).

(1*S*,2*E*,4*R*,7*E*,10*R*,11*Z*)-*form*
10-Ketone: ***Sartone B***
[185117-79-7]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Sarcophyton* sp. Oil. $[\alpha]_D^{27}$ -2.7 (c, 0.22 in MeOH).
λ_{max} 245 (ϵ 5380) (MeOH). λ_{max} 245 (ϵ 5390) (MeOH) (Berdy).
10-Ketone, 4-Me ether: ***4-O-Methylsartone B***
[185102-33-4]
$C_{21}H_{34}O_2$ 318.498
Constit. of *Sarcophyton* sp. Oil. $[\alpha]_D^{27}$ -6.4 (c, 0.09 in MeOH).
λ_{max} 245 (ϵ 5600) (MeOH). λ_{max} 245 (ϵ 5600) (MeOH) (Berdy).

(1*S*,2*E*,4*R*,7*Z*,10*R*,11*Z*)-*form*
10-Ketone: ***Sartone C***
[185117-80-0]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Sarcophyton* sp. Oil. $[\alpha]_D^{27}$ -8.2 (c, 0.085 in MeOH).
λ_{max} 272 (ϵ 7500) (MeOH). λ_{max} 239 (ϵ 5100) (MeOH) (Berdy).
Iwagawa, T. *et al., Bull. Chem. Soc. Jpn.*, 1996, **69**, 3543-3549 (*isol, pmr, cmr*)

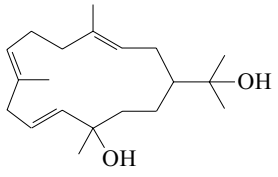
2,7,11-Cembratriene-4,15-diol C-207



$C_{20}H_{34}O_2$ 306.487

(2*E*,7*E*,11*E*)-*form*
Pauciflorol A
[86334-87-4]
Constit. of coral *Lobophytum pauciflorum*.
Oil.
Kinamoni, Z. *et al., Tetrahedron*, 1983, **39**, 1643

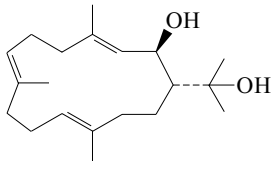
3,7,10-Cembratriene-12,15-diol C-208



$C_{20}H_{34}O_2$ 306.487

(3*E*,7*E*,10*E*)-*form*
Pauciflorol B
[86302-87-6]
Constit. of coral *Lobophytum pauciflorum*.
Oil.
Kinamoni, Z. *et al., Tetrahedron*, 1983, **39**, 1643

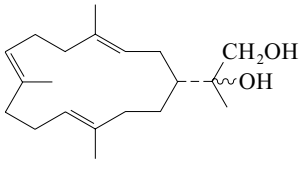
3,7,11-Cembratriene-2,15-diol C-209



$C_{20}H_{34}O_2$ 306.487

(1*R*,2*R*,3*E*,7*E*,11*E*)-*form*
2-Hydroxynephthenol
[56987-39-4]
Constit. of *Litophyton viridis*.
Cryst. (hexane).
Mp 98-99°. $[\alpha]_D$ -104 (c, 0.4 in $CHCl_3$).
Suzuki, M. *et al., Chem. Lett.*, 1978, 759

3,7,11-Cembratriene-15,16-diol C-210

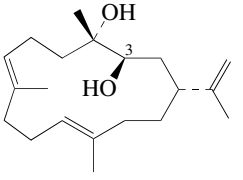


$C_{20}H_{34}O_2$ 306.487

(1*R*,3*E*,7*E*,11*E*,16ξ)-*form*
Sinulariol B
[110202-75-0]
Constit. of *Sinularia mayi*.
Cryst.
Mp 61-63°. $[\alpha]_D$ -52 (c, 1.12 in $CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 2314 (*isol, pmr*)
Yue, X. *et al., Tet. Lett.*, 1996, **37**, 671 (*synth*)
Yue, X. *et al., Tetrahedron*, 1999, **55**, 133-140 (*synth*)

7,11,15-Cembratriene-3,4-diol C-211

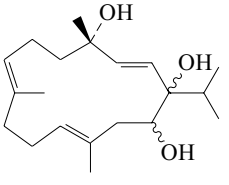
[178955-59-4]



$C_{20}H_{34}O_2$ 306.487

(1*R*,3*R*,4*S*,7*E*,11*E*)-*form*
3-Me ether: ***3-Methoxy-7,11,15-cembratrien-4-ol***
[180000-92-4]
$C_{21}H_{36}O_2$ 320.514
Constit. of the soft coral *Sinularia conferta*. Oil.
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 826-831 (*isol, ir, pmr, cmr*)
Yue, X. *et al., Synthesis*, 1996, 736 (*synth*)

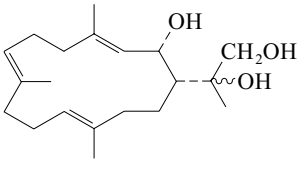
2,7,11-Cembratriene-1,4,14-triol C-212



$C_{20}H_{34}O_3$ 322.487

(1ξ,2*E*,4*S*,7*E*,11*E*,14ξ)-*form*
Sarcophytol Q
[123931-77-1]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D^{26}$ +79 (c, 4.18 in $CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2053 (*isol, pmr, cmr*)

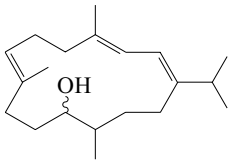
3,7,11-Cembratriene-2,15,16-triol C-213



$C_{20}H_{34}O_3$ 322.487

(1*R*,2*S*,3*E*,7*E*,11*E*,15ξ)-*form*
Sinulariol E
[157622-53-2]
Constit. of *Sinularia mayi*.
Oil. $[\alpha]_D$ +4 (c, 1.45 in $CDCl_3$).
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1993, 458 (*isol, pmr, cmr*)

1,3,7-Cembratrien-11-ol C-214



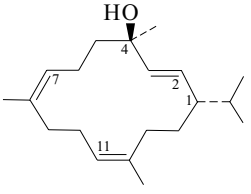
$C_{20}H_{34}O$ 290.488

(1*E*,3*E*,7*E*,11ξ)-*form*

Ac: 11-Acetoxy-1,3,7-cembratriene
$C_{22}H_{36}O_2$ 332.525
Constit. of a *Lobophytum* coral. Oil. $[\alpha]_D^{30}$ -15 (c, 0.5 in $CHCl_3$).

Bowden, B.F. *et al., Aust. J. Chem.*, 1978, **31**, 2707 (*synth*)
Subrahmanyam, C. *et al., Tetrahedron*, 1992, **48**, 3111 (*isol, pmr, cmr*)

2,7,11-Cembratrien-4-ol C-215



(1*S*,2*E*,4*R*,7*Z*,11*Z*)–*form*

$C_{20}H_{34}O$ 290.488

(1*S*,2*E*,4*R*,7*Z*,11*Z*)-*form*

Thunbergol. *Isocembrol. Trocheliophoral*
[25269-17-4]
Constit. of *Pseudotsuga menziesii*, *Pinus sibirica*, *Picea obovata* and the mollusc *Phyllodesmium longicirra*.
Oil. $[\alpha]_D$ +74.4 (c, 0.3 in $CHCl_3$). n_D^{20} 1.5020.

Hexahydro: 4-Cembranol. 4-Isopropyl-1,7,11-trimethylcyclotetradecanol
Cryst. Mp 89-91°. $[\alpha]_D$ -14 (c, 0.6 in $CHCl_3$).

(1*S*,2*E*,4*S*,7*Z*,11*Z*)-*form*

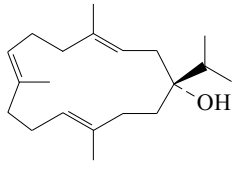
Epiisocembrol. 4-epi-*Isocembrol*
[80126-41-6]
Isol. from *Pinus* spp.

(1*R*,4*R*,2*E*,7*E*,11*E*)-*form*

Constit. of *Sinularia facile.*
Oil. $[\alpha]_D$ -118 (c, 0.09 in $CHCl_3$).

Erdtman, H. *et al., Acta Chem. Scand.*, 1968, **22**, 938 (*isol*)
Kimland, B. *et al., Acta Chem. Scand.*, 1968, **22**, 943 (*struct*)
Raldugin, V.A. *et al., Khim. Prir. Soedin.*, 1976, **12**, 609; 1977, **13**, 577; *Chem. Nat. Compd. (Engl. Transl.)*, 483; 545 (*isol, abs config*)
Kodama, M. *et al., Tet. Lett.*, 1977, 2763 (*synth*)
Weinheimer, A.J. *et al., Prog. Chem. Org. Nat. Prod.*, 1979, **36**, 285
Bowden, B.F. *et al., Aust. J. Chem.*, 1981, **34**, 1551 (*isol*)
Coll, J.C. *et al., Tetrahedron*, 1985, **41**, 1085
Astles, P.C. *et al., J.C.S. Perkin 1*, 1997, 845 (*synth*)

3,7,11-Cembratrien-1-ol C-216



(1*R*,3*E*,7*E*,11*E*)–*form*

$C_{20}H_{34}O$ 290.488

(1*R*,3*E*,7*E*,11*E*)-*form*

Sarcophytol M
[66648-97-3]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D$ +57 (c, 0.94 in $CHCl_3$).

(1*S*,3*E*,7*E*,11*E*)-*form*

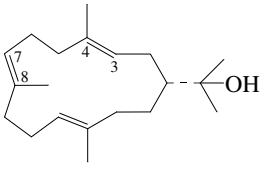
Serratol. *Cembrenol*
[67814-27-1]
Constit. of *Boswellia carteri* and *Boswellia serrata* (Indian olibanum).
Oil. Bp_1 150°. $[\alpha]_D^{20}$ -152.2 (c, 0.4 in EtOH).

[67921-02-2]

Pardhy, R.S. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 171 (*isol*)
Klein, E. *et al., Tet. Lett.*, 1978, 349 (*abs config*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 631 (*Sarchophytol M*)
Li, Y. *et al., Tet. Lett.*, 1993, **34**, 2799 (*synth*)
Yue, X. *et al., Bull. Soc. Chim. Belg.*, 1994, **103**, 35 (*synth*)

3,7,11-Cembratrien-15-ol C-217

[53915-41-6]



(1*R*,3*E*,7*E*,11*E*)-*form*

$C_{20}H_{34}O$ 290.488

(1*R*,3*E*,7*E*,11*E*)-*form*

Nephthenol†
Constit. of *Nephthea* spp. and *Litophyton viridis.* Hypotensive agent. Oil. $Bp_{0.03}$ 96°. $[\alpha]_D$ -36 (c, 0.2 in $CHCl_3$).

Ac:
$C_{22}H_{36}O_2$ 332.525
Constit. of *Nephthea brassica*. Oil. $[\alpha]_D$ -57.

3,4-Epoxide: 3,4-Epoxy-7,11-cembradien-15-ol. ***3,4-Epoxynephthenol***
[78039-86-8]
$C_{20}H_{34}O_2$ 306.487
Constit. of *Sarcophyton decaryi*. Oil. $[\alpha]_D^{24}$ +7 (c, 1.3 in $CHCl_3$).

7,8-Epoxide: 7,8-Epoxy-3,11-cembradien-15-ol. ***7,8-Epoxynephthenol***. *Epoxynephthenol*
[53915-40-5]
$C_{20}H_{34}O_2$ 306.487
Cryst. Mp 58.7-61.8°.

7,8-Epoxide, Ac: [53840-43-0]
$C_{22}H_{36}O_3$ 348.525
Isol. from *Nephthea* spp. Oil. $Bp_{0.03}$ 96°. $[\alpha]_D$ -20.7.

(1*S*,3*E*,7*E*,11*E*)-*form* [385809-55-2]
Constit. of a *Eunicea* sp.
Oil. $[\alpha]_D^{22}$ +25.3 (c, 2.1 in $CHCl_3$).

O-*(6*-O-*Acetyl-β-*D*-glucopyranoside):* ***Calyculaglycoside E***
[386211-75-2]
$C_{28}H_{46}O_7$ 494.667
Constit. of a *Eunicea* sp. Oil. $[\alpha]_D^{24}$ +11.5 (c, 2.5 in $CHCl_3$). λ_{max} 204 (log ϵ 3.97); 220 (log ϵ 3.72) (MeOH).

O-*(6*-O-*Acetyl-β-*D*-galactopyranoside):* ***Calyculaglycoside D***
[386211-74-1]
$C_{28}H_{46}O_7$ 494.667
Constit. of a *Eunicea* sp. Oil. $[\alpha]_D^{24}$ +10 (c, 4.3 in $CHCl_3$). λ_{max} 204 (log ϵ 3.79); 230 (log ϵ 3.4) (MeOH).

O-*(3,6-Di*-O-*acetyl-β-*D*-galactopyranoside):* ***Calyculaglycoside A***
[197231-68-8]
$C_{30}H_{48}O_8$ 536.704

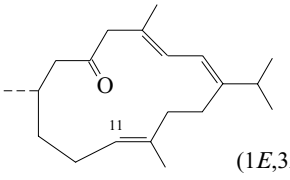
Constit. of a *Eunicea* sp. Antiinflammatory agent. Prostaglandin-Leukotriene biosynthesis inhibitor. Oil. $[\alpha]_D^{24}$ +9.2 (c, 0.6 in $CHCl_3$). Struct. revised in 2001. λ_{max} 214 (log ϵ 3.88) (MeOH).

O-*(4,6-Di*-O-*acetyl-β-*D*-glucopyranoside):* ***Calyculaglycoside B***
[197231-81-5]
$C_{30}H_{48}O_8$ 536.704
Constit. of a *Eunicea* sp. Antiinflammatory , Prostaglandin-Leukotriene Biosynthesis Inhibitor. PLA2 inhibitor. Oil. $[\alpha]_D^{26}$ +11.4 (c, 0.5 in $CHCl_3$). Struct. revised in 2001. λ_{max} 210 (log ϵ 3.67) (MeOH).

O-*(4,6-Di*-O-*acetyl-β-*D*-galactopyranoside):* ***Calyculaglycoside C***
[197231-89-3]
$C_{30}H_{48}O_8$ 536.704
Constit. of a *Eunicea* sp. Antiinflammatory , Prostaglandin-Leukotriene Biosynthesis Inhibitor. PLA2 inhibitor. Oil. $[\alpha]_D^{24}$ +7.8 (c, 0.5 in $CHCl_3$). Struct. revised in 2001. λ_{max} 212 (log ϵ 3.67) (MeOH).

Schmitz, F.J. *et al., Chem. Comm.*, 1974, 407 (*Epoxynephthenol*)
Tursche, B. *et al., Bull. Soc. Chim. Belg.*, 1975, **84**, 767 (*struct*)
Carmely, S. *et al., J.O.C.*, 1981, **46**, 4279 (*isol*)
Blackman, A.J. *et al., Aust. J. Chem.*, 1982, **35**, 1873 (*isol*)
Schwabe, R. *et al., Helv. Chim. Acta*, 1988, **71**, 292 (*synth*)
Cóbar, O.M. *et al., J.O.C.*, 1997, **62**, 7183-7188 (*Calyculaglycosides*)
Shi, Y.P. *et al., J. Nat. Prod.*, 2001, **64**, 1439-1443 (*Calyculaglycosides*)

1,3,11-Cembratrien-6-one C-218



(1*E*,3*E*,8*S*,11*E*)*–form*

$C_{20}H_{32}O$ 288.472

(1*E*,3*E*,8*S*,11*E*)-*form* [130575-03-0]
Constit. of *Eunicea calyculata.*
Oil. $[\alpha]_D$ +353 (c, 0.6 in $CHCl_3$).

*11S,12*S-*Epoxide:* [824957-46-2]
$C_{20}H_{32}O_2$ 304.472
Constit. of a *Eunicea* sp. Oil. $[\alpha]_D^{20}$ +27 (c, 1 in $CHCl_3$). λ_{max} 202 (ϵ 12100); 245 (ϵ 5898) (MeOH).

(1*E*,3*E*,8ξ,11*E*)-*form*
11ξ,12ξ-Epoxide: 11,12-Epoxy-1,3-cembradien-6-one
[603089-59-4]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Eunicea tourniforti.* Oil. $[\alpha]_D$ -14.4 (c, 0.24 in $CHCl_3$). λ_{max} 240 (log ϵ 4.27) (MeOH).

(1*E*,3*Z*,8*S*,11*E*)-*form* [130575-05-2]
Constit. of *Eunicea calyculata.*
Oil. $[\alpha]_D$ +283 (c, 0.8 in $CHCl_3$).

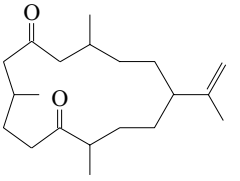
(1*E*,3*Z*,8ξ,11*E*)-*form*
11ξ,12ξ-Epoxide: [603089-58-3]
Constit. of *Eunicea tourniforti.*
Oil. $[\alpha]_D$ +150.9 (c, 0.21 in $CHCl_3$). λ_{max} 240 (log ϵ 4.33) (MeOH).

(1*Z*,3*Z*,8*S*,11*E*)-*form* [130575-04-1]
Constit. of *Eunicea calyculata.*
Oil. $[\alpha]_D$ +23 (c, 0.1 in $CHCl_3$).

Shin, J. *et al., J.O.C.*, 1991, **56**, 1227 (*isol, pmr, cmr*)
Li, J. *et al., Bull. Soc. Chim. Belg.*, 1996, **105**, 297 (*synth*)
Li, J. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 2851 (*synth*)
Marville, K.I. *et al., J. Nat. Prod.*, 2003, **66**, 1284-1287 (*epoxides*)
Wei, X. *et al., Tetrahedron*, 2004, **60**, 11813-11819 (*Eunicea epoxide*)

15-Cembrene-6,11-dione C-219

[151694-01-8]

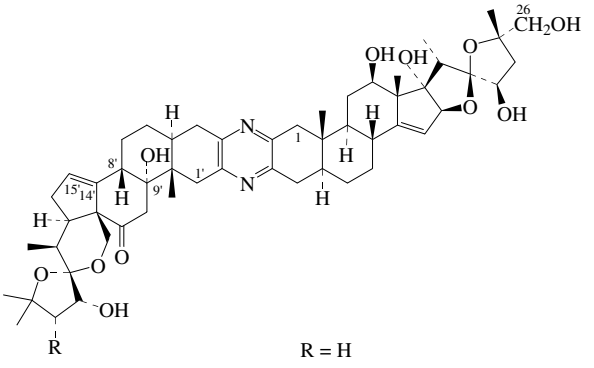


$C_{20}H_{34}O_2$ 306.487
Constit. of *Eunicea mammosa.* Semisolid. $[\alpha]_D^{25}$ -9.09 (c, 0.44 in $CHCl_3$).

Rodríguez, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 1101 (*isol, pmr, cmr*)

Cephalostatin 2 C-220

[116199-48-5]



R = H

$C_{54}H_{74}N_2O_{11}$ 927.185
Disteroidal alkaloid from the hemichordate marine worm *Cephalodiscus gilchristi.* Powerful cell growth inhibitor. Needles (EtOAc/MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 350°. $[\alpha]_D$ +111 (c, 0.07 in MeOH). λ_{max} 290 (ϵ 13700); 308 (sh) (EtOH) (Derep).

14′β,15′β-Epoxide: ***Cephalostatin 4***
[116229-58-4]
$C_{54}H_{74}N_2O_{12}$ 943.185
Alkaloid from *Cephalodiscus gilchristi.* Powerful cell growth inhibitor. Solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 350°. $[\alpha]_D$ +89 (c, 0.11 in MeOH). λ_{max} 290 (ϵ 13700); 308 (sh) (EtOH) (Derep).

9′-Deoxy: ***Cephalostatin 1***
[112088-56-9]
$C_{54}H_{74}N_2O_{10}$ 911.186
Alkaloid from *Cephalodiscus gilchristi.* Powerful cell growth inhibitor. Needles (EtOAc/MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 326° dec. $[\alpha]_D$ +102 (c, 0.04 in MeOH). λ_{max} 290 (ϵ 13700); 308 (sh) (EtOH) (Derep). λ_{max} 289 (ϵ 15233) (EtOH) (Berdy).

9′-Deoxy, 8′-hydroxy, 9′,11′-didehydro, 14′α,15′α-epoxide: ***Cephalostatin 14***
[159602-64-9]
$C_{54}H_{72}N_2O_{12}$ 941.169
Constit. of *Cephalodiscus gilchristi.* Cell growth inhibitor. Amorph. powder. $[\alpha]_D$ +80.9 (c, 0.11 in MeOH). λ_{max} 230 (log ϵ 3.69); 288 (log ϵ 3.9); 305 (sh) (MeOH).

26-Deoxy: ***Cephalostatin 17***
[170591-44-3]
$C_{54}H_{74}N_2O_{10}$ 911.186

Constit. of *Cephalodiscus gilchristi*. Cell growth inhibitor. Amorph. solid. $[\alpha]_D$ +70 (c, 0.7 in MeOH). λ_{max} 288 (ϵ 15000); 305 (sh) (MeOH).

1α-Methoxy: ***Cephalostatin 10***
[153698-88-5]
$C_{55}H_{76}N_2O_{12}$ 957.212
Alkaloid from *Cephalodiscus gilchristi*. Powerful cell growth inhibitor.
Mp >300°. $[\alpha]_D$ +80 (c, 0.17 in MeOH). λ_{max} 289 (log ϵ 4.08); 304 (sh) (MeOH).

1α-Methoxy, 9′-deoxy: ***Cephalostatin 18***
[211050-18-9]
$C_{55}H_{76}N_2O_{11}$ 941.212
Alkaloid from *Cephalodiscus gilchristi*. Cell growth inhibitor. Amorph. solid.
Mp >300°. $[\alpha]_D^{25}$ +95 (c, 0.06 in MeOH). λ_{max} 288 (log ϵ 4.06); 308 (MeOH).

1′α-Methoxy: ***Cephalostatin 11***
[153698-87-4]
$C_{55}H_{76}N_2O_{12}$ 957.212
Alkaloid from *Cephalodiscus gilchristi*. Powerful cell growth inhibitor.
Mp >300°. $[\alpha]_D$ +75 (c, 0.13 in MeOH). λ_{max} 288 (log ϵ 3.96); 305 (sh) (MeOH).

1′α-Methoxy, 9′-deoxy: ***Cephalostatin 19***
[211050-19-0]
$C_{55}H_{76}N_2O_{11}$ 941.212
Alkaloid from *Cephalodiscus gilchristi*. Amorph. solid.
Mp >320°. $[\alpha]_D^{25}$ +67 (c, 0.05 in MeOH). λ_{max} 288 (log ϵ 3.99); 308 (MeOH).

Pettit, G.R. *et al., Chem. Comm.*, 1988, 865-867; 1440 (*Cephalostatins 2-4*)
Pettit, G.R. *et al., J.A.C.S.*, 1988, **110**, 2006 (*Cephalostatin 1*)
Pat. Coop. Treaty (WIPO), 1989, 89 08 655 (*Cephalostatins 1,2,3,4*)
Pettit, G.R. *et al., Can. J. Chem.*, 1994, **72**, 2260-2267 (*Cephalostatin 14*)
Pettit, G.R. *et al., J. Nat. Prod.*, 1994, **57**, 52; 1998, **61**, 955-958 (*Cephalostatins 10,11,18,19*)
Pettit, G.R. *et al., Bioorg. Med. Chem. Lett.*, 1995, **5**, 2027-2032 (*Cephalostatin 17*)
Pettit, G.R. *et al., J.O.C.*, 1995, **60**, 608-613 (*Cephalostatin 14*)

Cephalostatin 3 C-221

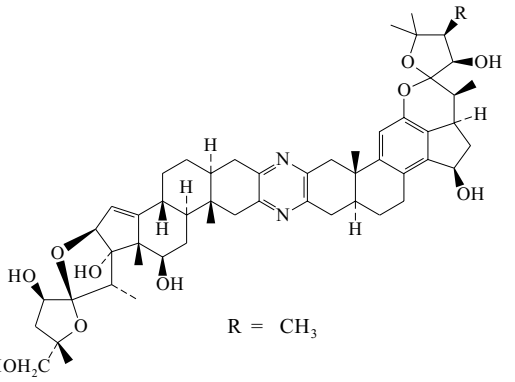
[116199-49-6]
As Cephalostatin 2, C-220 with
R = CH_3
$C_{55}H_{76}N_2O_{11}$ 941.212
Disteroidal alkaloid from the hemichordate marine worm *Cephalodiscus gilchristi*. Powerful cell growth inhibitor. Shows antitumour activity. Needles (EtOAc/MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 350°. $[\alpha]_D$ +99 (c, 0.15 in MeOH). λ_{max} 290 (ϵ 13700); 308 (sh) (ϵ) (EtOH) (Derep).

9′-Deoxy, 8′-hydroxy, 9′,11′-didehydro, 14′α,15′α-epoxide: ***Cephalostatin 15***
[159602-65-0]
$C_{55}H_{74}N_2O_{12}$ 955.196
Constit. of *Cephalodiscus gilchristi*. Shows antitumour activity. Amorph. powder.
Mp >300°. $[\alpha]_D$ +71.5 (c, 0.34 in MeOH). λ_{max} 202 (log ϵ 4.25); 228 (sh); 288 (log ϵ 3.96); 305 (sh) (MeOH).

Pettit, G.R. *et al., Chem. Comm.*, 1988, 865-867 (*uv, ir, cmr, struct*)
Pat. Coop. Treaty (WIPO), 1989, 89 08 655 (*Cephalostatin 3*)
Pettit, G.R. *et al., Can. J. Chem.*, 1994, **72**, 2260-2267 (*Cephalostatin 15*)

Cephalostatin 5 C-222

[121071-11-2]



$C_{54}H_{72}N_2O_{10}$ 909.17
Disteroidal alkaloid from the Indian Ocean (South African) marine worm *Cephalodiscus gilchristi*. Possesses lymphocytic leukaemia (murine P388) cell growth inhibitory activity (less potent than cephalostatins 1-4).
Mp 350°. $[\alpha]_D$ +100 (c, 0.02 in MeOH). λ_{max} 289 (ϵ 10000); 310 (sh) (MeOH) (Derep).

Pettit, G.R. *et al., Can. J. Chem.*, 1989, **67**, 1509-1513 (*isol, uv, struct*)

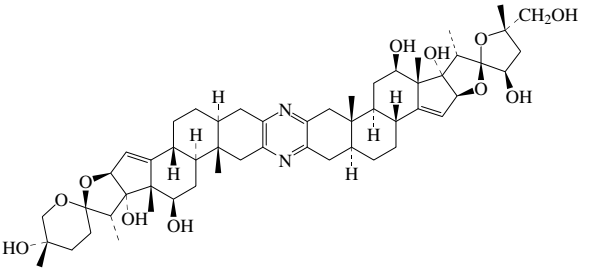
Cephalostatin 6 C-223

[121038-34-4]
As Cephalostatin 5, C-222 with
R = H
$C_{53}H_{70}N_2O_{10}$ 895.143
Disteroidal alkaloid from the Indian Ocean marine worm *Cephalodiscus gilchristi*. Possesses lymphocytic leukaemia (murine P388) cell growth inhibitory activity (less potent than cephalostatins 1-4).
Mp 350°. $[\alpha]_D$ +100 (c, 0.01 in MeOH). λ_{max} 289 (ϵ 10000); 310 (sh) (ϵ) (MeOH) (Derep).

Pettit, G.R. *et al., Can. J. Chem.*, 1989, **67**, 1509-1513 (*isol, uv, pmr, cmr, struct*)

Cephalostatin 7 C-224

[138605-82-0]

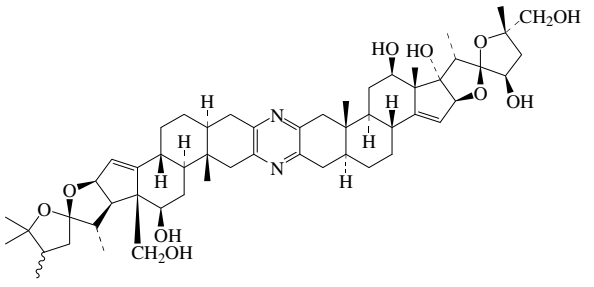


$C_{54}H_{76}N_2O_{11}$ 929.201
Constit. of *Cephalodiscus gilchristi*. Cytotoxic agent. Amorph. powder.
Mp 315° dec. $[\alpha]_D$ +106 (c, 0.244 in MeOH). λ_{max} 286 (ϵ 17400) (MeOH).

Pettit, G.R. *et al., J.O.C.*, 1992, **57**, 429-431 (*isol, pmr, cmr*)
Jeong, J.U. *et al., J.A.C.S.*, 1999, **121**, 2071-2084 (*synth*)

Cephalostatin 8 C-225

[138605-83-1]

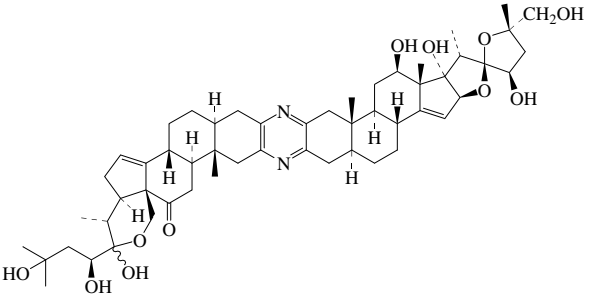


$C_{55}H_{78}N_2O_{10}$ 927.229
Constit. of *Cephalodiscus gilchristi*. Cytotoxic agent. Amorph. powder.
Mp 313° (dec.). $[\alpha]_D$ +110 (c, 0.1 in MeOH). λ_{max} 286 (ϵ 20800); 310 (sh) (MeOH).

Pettit, G.R. *et al., J.O.C.*, 1992, **57**, 429-431 (*isol, pmr, cmr*)

Cephalostatin 9 C-226

[138628-96-3]

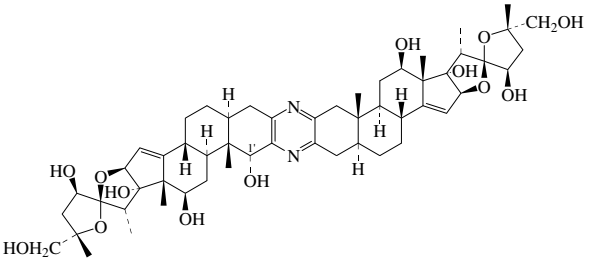


$C_{54}H_{76}N_2O_{11}$ 929.201
Constit. of *Cephalodiscus gilchristi*. Amorph. powder.
Mp 307° (dec.). $[\alpha]_D$ +105 (c, 0.5 in MeOH). λ_{max} 286 (ϵ 18600); 310 (sh) (MeOH).

Pettit, G.R. *et al., J.O.C.*, 1992, **57**, 429-431 (*isol, pmr, cmr*)

Cephalostatin 13 C-227

[158371-97-2]



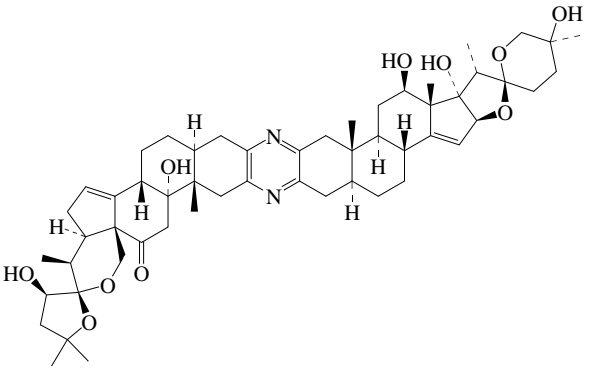
$C_{54}H_{76}N_2O_{13}$ 961.2
Alkaloid from the marine worm *Cephalodiscus gilchristi*. Antineoplastic agent. Amorph. solid.
Mp >300°. $[\alpha]_D^{20}$ +108.1 (c, 0.07 in MeOH). λ_{max} 287 (log ϵ 3.89); 308 (sh) (log ϵ 3.46) (MeOH).

1′-Deoxy: ***Cephalostatin 12***
[158371-96-1]
$C_{54}H_{76}N_2O_{12}$ 945.201
Alkaloid from *Cephalodiscus gilchristi*. Antineoplastic agent. Amorph. solid.
Mp >300°. $[\alpha]_D^{20}$ +157.5 (c, 0.4 in MeOH). λ_{max} 288 (log ϵ 4.16); 308 (sh) (log ϵ 3.89) (MeOH).

Pettit, G.R. *et al., Bioorg. Med. Chem. Lett.*, 1994, **4**, 1507-1512 (*isol, pmr, cmr, uv*)
Jeong, J.U. *et al., J.A.C.S.*, 1999, **121**, 2071-2084 (*synth*)

Cephalostatin 16 C-228

[170591-43-2]



$C_{54}H_{74}N_2O_{10}$ 911.186
Alkaloid from the marine worm *Cephalodiscus gilchristi*. Antineoplastic agent. Amorph. powder.
Mp >300°. $[\alpha]_D$ +55 (c, 1.73 in MeOH). λ_{max} 288 (ϵ 11600); 305 (sh) (MeOH).

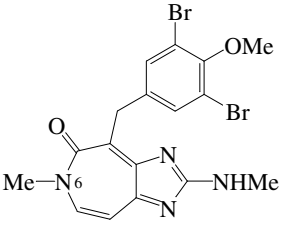
Pettit, G.R. *et al., Bioorg. Med. Chem. Lett.*, 1995, **5**, 2027-2032 (*isol, pmr, cmr*)

Cephalotocin C-229

CYFRNCPIG amide
[139545-42-9]
Cys-Tyr-Phe-Arg-Asn-Cys-Pro-Ile-Gly-NH_2
$C_{47}H_{68}N_{14}O_{11}S_2$ 1069.273
Peptide of the oxytocin/vasopressin family; struct. of reduced form shown. Isol. from the nerves of *Octopus vulgaris*. Neuropeptide.

Reich, G. *et al., Neurosci. Lett.*, 1992, **134**, 191-194 (*isol, struct*)

Ceratamine A C-230



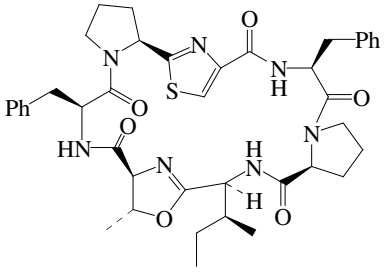
$C_{17}H_{16}Br_2N_4O_2$ 468.147
Alkaloid from the marine sponge *Pseudoceratina* sp. Antimitotic agent. Yellow cryst. (MeOH).
Mp 236°.

N^6*-De-Me:* ***Ceratamine B***
$C_{16}H_{14}Br_2N_4O_2$ 454.12
Alkaloid from a *Pseudoceratina* sp. Yellow cryst. (MeOH).
Mp 242°.

Manzo, E. *et al., Org. Lett.*, 2003, **5**, 4591-4594 (*isol, pmr, cmr*)

Ceratospongamide C-231

[259794-28-0]



$C_{41}H_{49}N_7O_6S$ 767.947

Isol. as two stable conformational isomers. Isol. from the red alga *Ceratodictyon spongiosum* containing the symbiotic sponge *Sigmadocia symbiotica*. Antiinflammatory agent.

cis,cis-form

Amorph. solid. $[\alpha]_D$ -190 (c, 0.13 in $CHCl_3$). λ_{max} 246 (ϵ 11830) ($CHCl_3$).

trans,trans-form

Amorph. solid. $[\alpha]_D$ -39.2 (c, 0.52 in $CHCl_3$). λ_{max} 246 (ϵ 11270) ($CHCl_3$).

Tan, L.T. *et al., J.O.C.*, 2000, **65**, 419-425 (*isol, pmr, cmr*)
Yokokawa, F. *et al., Synlett*, 2001, 986-988 (*synth*)
Kutsumura, N. *et al., Bull. Chem. Soc. Jpn.*, 2002, **75**, 847-850 (*synth*)
Yokokawa, F. *et al., Tetrahedron*, 2002, **58**, 8127-8143 (*synth, conformn*)
Chen, Z. *et al., ARKIVOC*, 2003, **vii**, 268-285 (*synth*)
Doi, M. *et al., Acta Cryst. C*, 2003, **59**, 323-325 (*cryst struct*)

Aplysia californica Cerebral peptide 1 C-232

[180461-30-7]

H-Phe-Ser-Gly-Leu-Met-Ser-Glu-Gly-Ser-Ser-Leu-Glu-Ala-OH

$C_{55}H_{87}N_{13}O_{22}S$ 1314.432

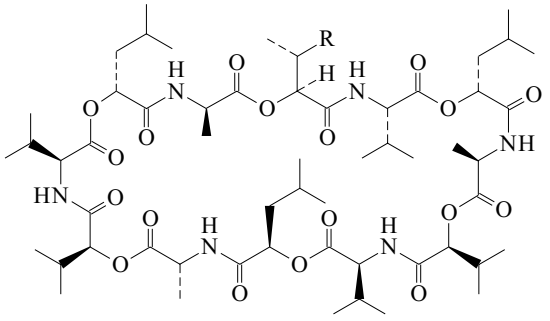
Isol. from the cerebral ganglia of *Aplysia californica*. Neuropeptide. *Aplysia californica* Cerebral peptide 2 is an amidated peptide comprising 41 amino acid residues.

[175419-50-8]

Phares, G.A. *et al., Biochemistry*, 1996, **35**, 5921-5927 (*Cerebral peptide 2*)
Phares, G.A. *et al., Peptides (N.Y.)*, 1996, **17**, 753-761 (*isol, struct*)

Cereulide C-233

[157232-64-9]



R = CH_3

$C_{57}H_{96}N_6O_{18}$ 1153.415

Depsipeptide antibiotic. Prod. by *Bacillus cereus*. Rb and K selective ionophore. Emetic toxin. Cytotoxic. Powder. $[\alpha]_D$ +10.4 (c, 0.2 in MeOH). Similar to Valinomycin.

Homologue (R = CH_2CH_3): ***Homocereulide***

[170034-95-4]

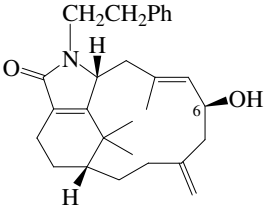
$C_{58}H_{98}N_6O_{18}$ 1167.442

Prod. by *Bacillus cereus*. Emetic toxin. Cytotoxic. Powder. $[\alpha]_D$ +10.5 (c, 0.1 in MeOH).

[169338-32-3]

Isobe, M. *et al., Bioorg. Med. Chem. Lett.*, 1995, **5**, 2855 (*synth*)
Wang, G.-Y.-S. *et al., Chem. Lett.*, 1995, 791 (*isol, pmr, cmr*)
Suwan, S. *et al., J.C.S. Perkin 1*, 1995, 765 (*isol, pmr, cmr, cryst struct*)
Kuse, M. *et al., Bioorg. Med. Chem. Lett.*, 2000, **10**, 735-739 (*biosynth*)

Cespitulactam A C-234



$C_{28}H_{37}NO_2$ 419.606

Constit. of *Cespitularia taeniata*. Amorph. powder. $[\alpha]_D$ -196 (c, 1 in CH_2Cl_2). λ_{max} 217; 230; 257 (MeOH).

6-Ketone: ***Cespitulactam B***

$C_{28}H_{35}NO_2$ 417.59

Constit. of *Cespitularia taeniata*. Amorph. powder. $[\alpha]_D^{25}$ -110 (c, 0.05 in CH_2Cl_2).

4′-Hydroxy: ***Cespitulactam C***

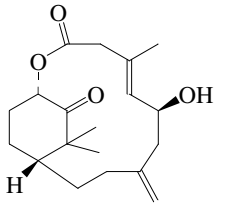
$C_{28}H_{37}NO_3$ 435.605

Constit. of *Cespitularia taeniata*. Amorph. powder. $[\alpha]_D^{25}$ -255 (c, 0.2 in CH_2Cl_2). C-4′ position on Ph. λ_{max} 224; 279 (MeOH).

Shen, Y.-C. *et al., Tet. Lett.*, 2005, **46**, 7893-7897 (*isol, cd, pmr, cmr, ms*)

Cespitulactone A C-235

[886984-47-0]



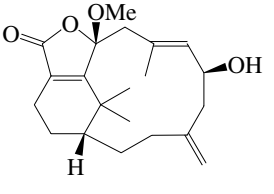
$C_{19}H_{28}O_4$ 320.428

Constit. of *Cespitularia taeniata*. Amorph. powder. $[\alpha]_D^{25}$ -122 (c, 1 in CH_2Cl_2). λ_{max} 235 (MeOH).

Shen, Y.-C. *et al., Bioorg. Med. Chem. Lett.*, 2006, **16**, 2369-2372 (*Cespitulactone A*)

Cespitulactone B C-236

[886984-48-1]



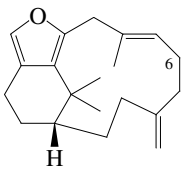
$C_{21}H_{30}O_4$ 346.466

Constit. of *Cespitularia taeniata*. Amorph. powder. $[\alpha]_D^{25}$ -61 (c, 2 in CH_2Cl_2). λ_{max} 222 (MeOH).

Shen, Y.-C. *et al., Bioorg. Med. Chem. Lett.*, 2006, **16**, 2369-2372 (*Cespitulactone B*)

Cespitularin B C-237

[473911-37-4]



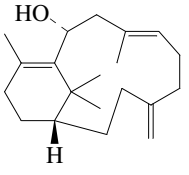
$C_{20}H_{28}O$ 284.441
Constit. of *Cespitularia hypotentaculata*. Amorph. solid.
Mp 62-63°. $[\alpha]_D^{25}$ -20.6 (c, 0.08 in $CHCl_3$). λ_{max} 204 (log ϵ 3.9) (MeOH).

6-Hydroxy: ***Cespitularin A***
[473911-35-2]
$C_{20}H_{28}O_2$ 300.44
Constit. of *Cespitularia hypotentaculata*. Amorph. solid.
Mp 71-72°. $[\alpha]_D^{25}$ -140.1 (c, 0.12 in $CHCl_3$). λ_{max} 202 (log ϵ 2.8) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1429-1433 (*isol, pmr, cmr*)

Cespitularin C C-238

[473911-39-6]

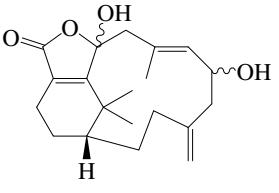


$C_{20}H_{32}O$ 288.472
Constit. of *Cespitularia hypotentaculata*. Amorph. solid.
Mp 66-68°. $[\alpha]_D^{25}$ -62.3 (c, 0.1 in $CHCl_3$).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1429-1433 (*isol, pmr, cmr*)

Cespitularin D C-239

[473911-40-9]

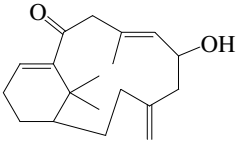


$C_{20}H_{28}O_4$ 332.439
Constit. of *Cespitularia hypotentaculata*. Oil. $[\alpha]_D^{25}$ -169.6 (c, 0.23 in $CHCl_3$). λ_{max} 220 (log ϵ 4.1) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1429-1433 (*isol, pmr, cmr*)

Cespitularin E C-240

[473911-42-1]

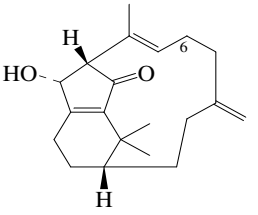


$C_{19}H_{28}O_2$ 288.429
Constit. of *Cespitularia hypotentaculata*. Oil. $[\alpha]_D^{25}$ +122.3 (c, 0.22 in $CHCl_3$). λ_{max} 232 (log ϵ 4.2) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1429-1433 (*isol, pmr, cmr*)

Cespitularin G C-241

[473911-46-5]



Relative Configuration

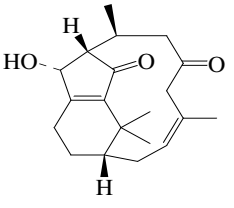
$C_{20}H_{28}O_2$ 300.44
Constit. of *Cespitularia hypotentaculata*. Oil. $[\alpha]_D^{25}$ -63.6 (c, 0.16 in $CHCl_3$). λ_{max} 234 (log ϵ 4.2) (MeOH).

6-Hydroxy: ***Cespitularin F***
[473911-44-3]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Cespitularia hypotentaculata*. Oil. $[\alpha]_D^{25}$ +39.8 (c, 0.21 in $CHCl_3$). λ_{max} 236 (log ϵ 4.3) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1429-1433 (*isol, pmr, cmr*)

Cespitularin H C-242

[473911-48-7]



Relative Configuration

$C_{20}H_{28}O_3$ 316.439
Constit. of *Cespitularia hypotentaculata*. Amorph. solid.
Mp 120-121°. $[\alpha]_D^{25}$ -93.6 (c, 0.19 in $CHCl_3$). λ_{max} 235 (log ϵ 4) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1429-1433 (*isol, pmr, cmr*)

CFI C-243

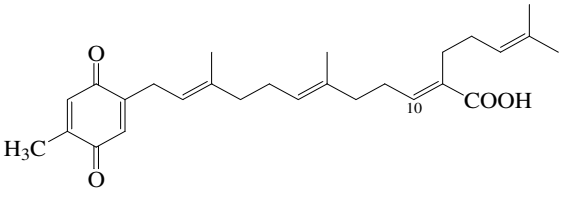
Coelomic fluid protease inhibitor

Monomeric protein. Isol. from *Holothuria polii*. Protease inhibitor for trypsin and rubtilisin but not for α-chymotrypsin.

Canicatti, C. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **98**, 593-596 (*isol*)

Chabrolobenzoquinone A C-244

[827038-33-5]



$C_{27}H_{36}O_4$ 424.579
Constit. of *Nephthea chabrolii*. Oil. λ_{max} 251 (log ϵ 4) (MeOH).

Me ester: ***Chabrolobenzoquinone B***
[827038-34-6]
$C_{28}H_{38}O_4$ 438.606
Constit. of *Nephthea chabrolii*. Oil. λ_{max} 252 (log ϵ 4.02) (MeOH).

10Z-Isomer: ***Chabrolobenzoquinone C***
[827038-35-7]
$C_{27}H_{36}O_4$ 424.579

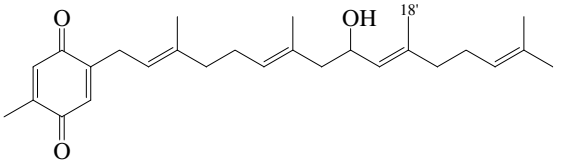
Constit. of *Nephthea chabrolii*. Oil. λ_{max} 251 (log ϵ 4.06) (MeOH).

10Z-Isomer, Me ester: [827038-36-8]
$C_{28}H_{38}O_4$ 438.606
Constit. of *Nephthea chabrolii*. Oil. λ_{max} 251 (log ϵ 4.03) (MeOH).

Sheu, J.-H. *et al., J. Nat. Prod.*, 2004, **67**, 2048-2052 (*isol, pmr, cmr*)

Chabrolobenzoquinone G C-245

[871915-32-1]



$C_{27}H_{38}O_3$ 410.595
Constit. of *Nephthea chabrolii*. Pale yellow oil. $[\alpha]_D^{25}$ +6.4 (c, 0.5 in $CHCl_3$). λ_{max} 251 (log ϵ 3.99) (MeOH).

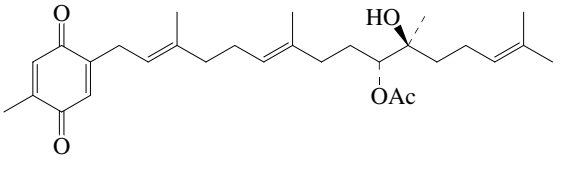
Deoxy, 18′-hydroxy: ***Chabrolobenzoquinone E***
[871915-30-9]
$C_{27}H_{38}O_3$ 410.595
Constit. of *Nephthea chabrolii*. Pale yellow oil. λ_{max} 252 (log ϵ 3.89) (MeOH).

Deoxy, 18′-acetoxy: ***Chabrolobenzoquinone F***
[871915-31-0]
$C_{29}H_{40}O_4$ 452.633
Constit. of *Nephthea chabrolii*. Pale yellow oil. λ_{max} 251 (log ϵ 3.95) (MeOH).

Su, J.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1651-1655

Chabrolobenzoquinone H C-246

[871915-33-2]

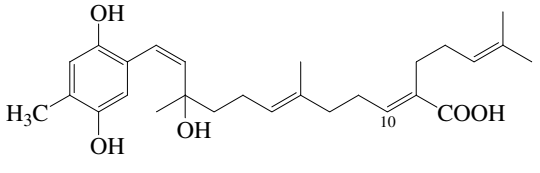


$C_{29}H_{42}O_5$ 470.648
Constit. of *Nephthea chabrolii*. Pale yellow oil. $[\alpha]_D^{25}$ -20.5 (c, 0.5 in $CHCl_3$). λ_{max} 252 (log ϵ 3.95) (MeOH).

Su, J.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1651-1655 (*Chabrolobenzoquinone H*)

Chabrolohydroxybenzoquinone A C-247

[827038-29-9]



$C_{27}H_{38}O_5$ 442.594
Constit. of *Nephthea chabrolii*. Oil. λ_{max} 266 (log ϵ 3.65); 332 (log ϵ 3.69) (MeOH).

Me ester: ***Chabrolohydroxybenzoquinone B***
[827038-30-2]
$C_{28}H_{40}O_5$ 456.621
Constit. of *Nephthea chabrolii*. Oil. λ_{max} 266 (log ϵ 3.7); 331 (log ϵ 3.72) (MeOH).

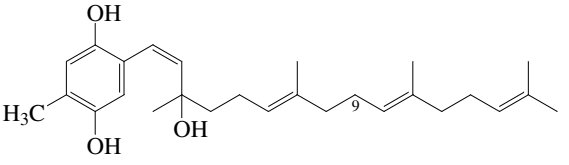
10Z-Isomer: ***Chabrolohydroxybenzoquinone C***
[827038-31-3]
$C_{27}H_{38}O_5$ 442.594
Constit. of *Nephthea chabrolii*. Oil. λ_{max} 267 (log ϵ 3.8); 330 (log ϵ 3.77) (MeOH).

10Z-Isomer, Me ester: ***Chabrolohydroxybenzoquinone D***
[827038-32-4]
$C_{28}H_{40}O_5$ 456.621
Constit. of *Nephthea chabrolii*. Oil. λ_{max} 267 (log ϵ 3.7); 331 (log ϵ 3.67) (MeOH).

Sheu, J.-H. *et al., J. Nat. Prod.*, 2004, **67**, 2048-2052 (*isol, pmr, cmr*)

Chabrolohydroxybenzoquinone E C-248

[871915-34-3]



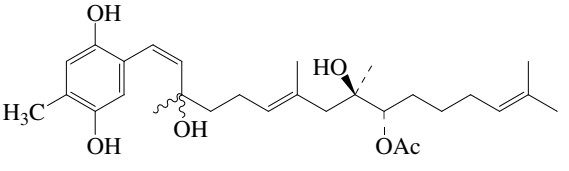
$C_{27}H_{40}O_3$ 412.611
Constit. of *Nephthea chabrolii*. Pale yellow oil. λ_{max} 266 (log ϵ 3.77); 331 (log ϵ 3.77) (MeOH).

9-Hydroxy: ***Chabrolohydroxybenzoquinone F***
[871915-35-4]
$C_{27}H_{40}O_4$ 428.611
Constit. of *Nephthea chabrolii*. Pale yellow oil. $[\alpha]_D^{25}$ +1.6 (c, 1 in $CHCl_3$). λ_{max} 267 (log ϵ 3.62); 330 (log ϵ 3.63) (MeOH).

Su, J.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1651-1655 (*Chabrolohydroxybenzoquinones E and F*)

Chabrolohydroxybenzoquinone G C-249

[871915-36-5]

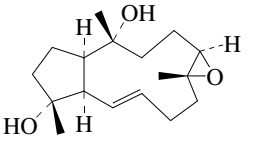


$C_{29}H_{44}O_6$ 488.663
Constit. of *Nephthea chabrolii*. Pale yellow oil. $[\alpha]_D^{25}$ -6.5 (c, 1.08 in $CHCl_3$). λ_{max} 267 (log ϵ 3.65); 331 (log ϵ 3.64) (MeOH).

Su, J.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1651-1655 (*Chabrolohydroxybenzoquinone G*)

Chabrolol B C-250

[356558-95-7]

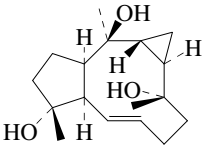


$C_{17}H_{28}O_3$ 280.406
Constit. of *Nephthea chabroli*. Cryst. ($CHCl_3$).
Mp 224-225°. $[\alpha]_D^{25}$ +23.5 (c, 0.047 in $CHCl_3$).

Zhang, W.-H. *et al., Tet. Lett.*, 2001, **42**, 4681-4685 (*isol, pmr, cmr, cryst struct*)

Chabrolol C C-251

[356558-96-8]

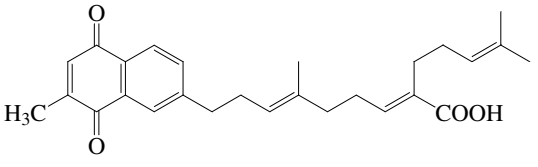


$C_{17}H_{28}O_3$ 280.406
Constit. of *Nephthea chabroli*. Cryst. ($CHCl_3$/MeOH). Mp 195-196°. $[\alpha]_D^{25}$ -278.2 (c, 0.052 in MeOH).

Zhang, W.-H. *et al., Tet. Lett.*, 2001, **42**, 4681-4685 (*isol, pmr, cmr, cryst struct*)

Chabrolonaphthoquinone A C-252

[827038-28-8]

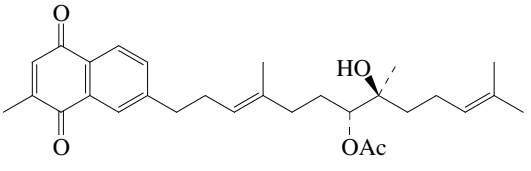


$C_{27}H_{32}O_4$ 420.547
Constit. of *Nephthea chabrolii*. Yellow oil. λ_{max} 257 (log ϵ 3.69); 266 (log ϵ 3.63); 343 (log ϵ 2.79) (MeOH).

Sheu, J.-H. *et al., J. Nat. Prod.*, 2004, **67**, 2048-2052 (*isol, pmr, cmr*)

Chabrolonaphthoquinone B C-253

[871915-29-6]

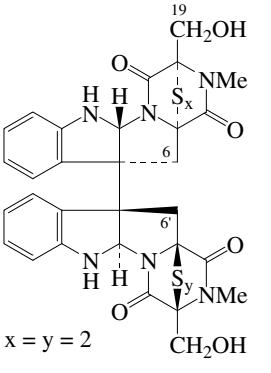


$C_{29}H_{38}O_5$ 466.616
Constit. of *Nephthea chabrolii*. Pale yellow oil. $[\alpha]_D^{25}$ -19.3 (c, 0.88 in $CHCl_3$). λ_{max} 257 (log ϵ 3.64); 265 (log ϵ 3.49); 348 (log ϵ 2.64) (MeOH).

Su, J.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1651-1655

Chaetocin C-254

Chetocin, 9CI
[28097-03-2]



Absolute Configuration

$C_{30}H_{28}N_6O_6S_4$ 696.852

Epithiodioxopiperazine antibiotic. Stereoisomeric with the series represented by Verticillin A, V-37. The original publication incorrectly shows the stereochem. of Chaetocin as a *meso*-form. The struct. has C_2-symmetry with the bridgehead *H*s *cis*- to the bond linking the two C_{15} residues. CAS numbering shown. Metab. of *Chaetomium minutum*, *Chaetomium thielavioideum and Farrowia* sp. Sol. Py, EtOAc, DMSO, MeOH; poorly sol. H_2O. $[\alpha]_D^{20}$ +379 (c, 1 in Py). λ_{max} 203 (ϵ 50100); 240 (sh) (ϵ 14100); 301 (ϵ 5370) (Ac_2O/MeOH) (Derep). λ_{max} 306 (ϵ 6030) (DMSO) (Derep).

▶ LD_{50} (mus, ipr) 1.7 mg/kg , LD_{50} (mus, orl) 1200 mg/kg. FM3032000

O,O′-Di-Ac: Mp 220-225° dec. $[\alpha]_D^{20}$ +679 (c, 1 in $CHCl_5$).

6S-Hydroxy: ***Melinacidin III***
[12794-84-2]
$C_{30}H_{28}N_6O_7S_4$ 712.851
Prod. by *Acrostalagmus cinnabarinus* var. *melinacidinus* NRRL3291 and the marine-derived *Corollospora pulchella*. Shows similar activity to Melinacidin II. Cryst. Sol. $CHCl_3$, DMF, DMSO; fairly sol. MeOH, EtOH, Me_2CO; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ +776 (c, 0.5 in $CHCl_3$). λ_{max} 241 (sh) (ϵ 15300); 300 (ϵ 5310) (MeOH) (Derep).

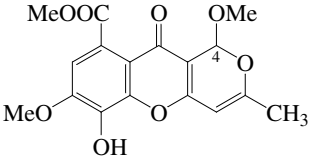
19-Deoxy, 6 or 6′S-hydroxy: ***Melinacidin II***
[12794-85-3]
$C_{30}H_{28}N_6O_6S_4$ 696.852
Epithiodioxopiperazine antibiotic. Prod. by *Acrostalagmus cinnabarinus* var. *melinacidinus* NRRL13291 and *Verticillium tererum*. Shows antibacterial and antitumour activity but is highly toxic. Cryst. Sol. $CHCl_3$, DMSO, DMF; fairly sol. MeOH, EtOH, Me_2CO; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ +726 (c, 0.5 in $CHCl_3$). λ_{max} 203 (ϵ 50100); 240 (sh) (ϵ 14100); 301 (ϵ 5370) (Ac_2O/MeOH) (Derep). λ_{max} 306 (ϵ 6030) (DMSO) (Derep). λ_{max} 300 (E1%/1cm 73) (MeOH) (Berdy).

6S,6′S-Dihydroxy: ***Melinacidin IV***
[37934-52-4]
$C_{30}H_{28}N_6O_8S_4$ 728.851
Prod. by *Acrostalagmus cinnabarinus* var. *melinacidinus* NRRL13291 and the marine-derived *Corollospora pulchella*. Shows similar activity to Melanicidin II. Cryst. $[\alpha]_D^{25}$ +718 (c, 0.5 in $CHCl_3$). λ_{max} 241 (sh) (ϵ 15300); 300 (ϵ 5310) (MeOH) (Derep).

▶ FM3036000

Hauser, D. *et al., Helv. Chim. Acta*, 1970, **53**, 1061-1073 (*isol, uv, cd, ir, pmr, ms, cryst struct*)
Argoudelis, A.D. *et al., J. Antibiot.*, 1972, **25**, 171-178; 1977, **30**, 468 (*Melinacidins*)
Nagarajan, R. *et al., J.A.C.S.*, 1973, **95**, 7212-7222 (*cd*)
Sekita, S. *et al., Chem. Pharm. Bull.*, 1980, **28**, 2428-2435 (*isol*)

Chaetocyclinone A C-255



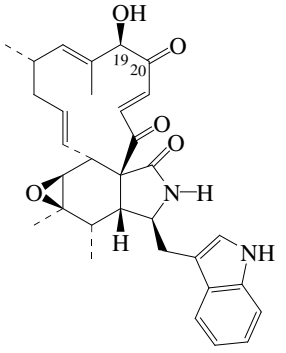
$C_{17}H_{16}O_8$ 348.309
Prod. by the marine-derived *Chaetomium* sp. Gö 100/2.

4-Demethoxy: ***Chaetocyclinone B***
$C_{16}H_{14}O_7$ 318.282
Prod. by *Chaetomium* sp. Gö 100/2.

Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*biosynth*)

Chaetoglobosin A C-256

[50335-03-0]



Absolute Configuration

$C_{32}H_{36}N_2O_5$ 528.647

Isoindole antibiotic. Metab. of *Chaetomium cochliodes*, *Chaetomium globosum* NRRL12718, *Chaetomium subaffine*, other *Chaetomium* spp., *Penicillium aurantiogriseum*, *Cylindrocladium floridanum* and *Ascotricha chartarum*. Cytotoxic to HeLa cells; fibrinolysis enhancer; mycotoxin; phytotoxin; microtubule protein assembly inhibitor; urokinase prodn. inducer. Pale yellow prisms (CH_2Cl_2). Sol. MeOH; poorly sol. H_2O.
Mp 188° (168-170°). $[\alpha]_D$ -270 (MeOH). λ_{max} 222 (ϵ 36300); 273 (ϵ 6760); 281 (ϵ 6760); 291 (ϵ 5750) (MeOH) (Derep). λ_{max} 196 (ϵ 42700); 220 (ϵ 41600); 271 (ϵ 6600); 280 (ϵ 6600); 290 (ϵ 5360) (MeOH) (Berdy). λ_{max} 223 (ϵ 40740); 274 (ϵ 6610); 282 (ϵ 6607); 292 (ϵ 5370) (EtOH) (Berdy).

▶ Teratogen. HA5305000

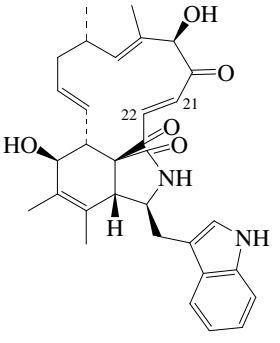
21,22-Dihydro: ***Penochalasin F***
[345642-82-2]
$C_{32}H_{38}N_2O_5$ 530.663
Prod. by a marine *Penicillium* sp. Cytotoxic. Oil. $[\alpha]_D$ -80 (c, 0.13 in $CHCl_3$). λ_{max} 220 (log ϵ 4.68); 240 (sh) (log ϵ 4.28); 280 (log ϵ 4.17); 291 (log ϵ 4.1) (EtOH).

19-Epimer, 21,22-dihydro: ***Penochalasin E***
[345642-81-1]
$C_{32}H_{38}N_2O_5$ 530.663
Prod. by a marine *Penicillium* sp. Cytotoxic. Oil. $[\alpha]_D$ +73 (c, 0.14 in $CHCl_3$). λ_{max} 221 (log ϵ 4.43); 241 (sh) (log ϵ 3.97); 280 (log ϵ 3.84); 291 (log ϵ 3.77) (EtOH).

Iwamoto, C. *et al., Tetrahedron*, 2001, **57**, 2997-3004 (*Penochalasins*)

Chaetoglobosin B C-257

[50335-04-1]



$C_{32}H_{36}N_2O_5$ 528.647
Prod. by *Chaetomium cochliodes*, *Chaetomium rectum, Chaetomium mollipilum* and *Chaetomium globosum*. Cytotoxic to HeLa cells. Mycotoxin. Pale yellow needles (C_6H_6). Sol. MeOH; poorly sol. H_2O.
Mp 186-187°. $[\alpha]_D$ -176 (c, 0.1 in MeOH). λ_{max} 222 (ϵ 36300); 273 (ϵ 6760); 281 (ϵ 6760); 291 (ϵ 5750) (MeOH) (Derep). λ_{max} 222 (ϵ 43650); 274 (ϵ 7940); 281 (ϵ 7950); 290 (ϵ 6760) (EtOH) (Berdy).

19-Ac: ***19-O-Acetylchaetoglobosin B***
[80375-18-4]
$C_{34}H_{38}N_2O_6$ 570.684
Prod. by *Chaetomium globosum*. Mycotoxin. Yellow needles (C_6H_6). Poorly sol. hexane.
Mp 154-157°. $[\alpha]_D^{20}$ -148 (c, 0.5 in $CHCl_3$). λ_{max} 221 (log ϵ 4.64); 272 (log ϵ 3.83); 279 (log ϵ 3.83); 289 (log ϵ 3.74) (EtOH).

21,22-Dihydro: ***Chaetoglobosin O***
[52645-09-7]
$C_{32}H_{38}N_2O_5$ 530.663
Prod. by *Cylindrocladium floridanum*. Phytotoxin. Mycotoxin. Oil. $[\alpha]_D$ -168 ($CHCl_3$).

21,22-Dihydro, 19-ketone: ***Chaetoglobosin G***
[65773-98-0]
$C_{32}H_{36}N_2O_5$ 528.647
Prod. by *Chaetomium cochliodes* and *Chaetomium subaffine* ATCC22132. Cytotoxic to HeLa cells. Mycotoxin. Leaflets (MeOH).
Mp 251-253°. $[\alpha]_D$ +89 (c, 0.10 in MeOH). λ_{max} 222 (ϵ 36300); 273 (ϵ 6760); 281 (ϵ 6760); 291 (ϵ 5750) (MeOH) (Derep). λ_{max} 222; 275; 282; 291 (EtOH) (Berdy).

21,22-Dihydro, 19-ketone, 20β-alcohol: ***Chaetoglobosin E***
[55945-74-9]
$C_{32}H_{38}N_2O_5$ 530.663
Prod. by *Chaetomium cochliodes*, *Chaetomium subaffine* ATCC22132, *Chaetomium mollipilum* and *Chaetomium globosum*. Cytotoxic to HeLa cells. Needles (MeOH). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 279-280°. $[\alpha]_D$ +158 (c, 0.1 in MeOH). λ_{max} 222 (ϵ 36300); 273 (ϵ 6760); 281 (ϵ 6760); 291 (ϵ 5750) (MeOH) (Derep). λ_{max} 221 (ϵ 56200); 275 (ϵ 7080); 281 (ϵ 7080); 291 (ϵ 6800) (EtOH) (Berdy).

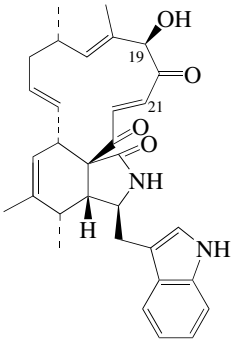
19-Deoxy: ***Prochaetoglobosin III***
[146426-37-1]
$C_{32}H_{36}N_2O_4$ 512.647
Metab. of *Chaetomium subaffine*. Pale yellow cryst. ($CHCl_3$).
Mp 153-155°. $[\alpha]_D$ -15.3 (c, 0.06 in $CHCl_3$). λ_{max} 222 (log ϵ 4.43); 282 (log ϵ 3.66); 291 (log ϵ 3.6) (MeOH).

19-Epimer, 21,22-dihydro: ***Penochalasin H***
[345642-84-4]
$C_{32}H_{38}N_2O_5$ 530.663
Prod. by a marine *Penicillium* sp. Powder.
Mp 180-182°. $[\alpha]_D$ -72.7 (c, 0.18 in $CHCl_3$). λ_{max} 220 (log ϵ 4.16); 243 (sh) (log ϵ 3.97); 281 (log ϵ 3.52); 290 (log ϵ 3.5) (EtOH).

Umeda, M. *et al., Experientia*, 1975, **31**, 435-438 (*Chaetomium globosum constits*)
Sekita, S. *et al., Chem. Pharm. Bull.*, 1980, **30**, 1609-1617; 1618-1628; 1629-1638 (*isol, ir, uv, pmr, ms, struct, Chaetoglobosins E,G*)
Probst, A. *et al., Helv. Chim. Acta*, 1981, **64**, 2056-2064 (*19-Ac*)
Oikawa, H. *et al., J.C.S. Perkin 1*, 1992, 2949-2953; 2955-2959 (*Prochaetoglobosin III*)
Ichihara, A. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 360-361 (*Chaetoglobosin O*)
Iwamoto, C. *et al., Tetrahedron*, 2001, **57**, 2997-3004 (*Penochalasin H*)

Chaetoglobosin J C-258

[65745-47-3]



$C_{32}H_{36}N_2O_4$ 512.647

Prod. by *Chaetomium cochliodes*, *Chaetomium globosum* and *Chaetomium subaffine*. Cytotoxic to HeLa cells. Pale yellow prisms.
Mp 149-151°. $[\alpha]_D$ +41 (c, 0.1 in MeOH). λ_{max} 222 (ϵ 36300); 273 (ϵ 6760); 281 (ϵ 6760); 291 (ϵ 5750) (MeOH) (Derep). λ_{max} 224; 270; 280; 290 (EtOH) (Berdy).

6β,7β-Epoxide: See Chaetoglobosin A, C-256

21,22-Dihydro: ***Penochalasin G***
$C_{32}H_{38}N_2O_4$ 514.663
Prod. by a marine *Penicillium* sp. Cytotoxic. Powder.
Mp 124-126°. $[\alpha]_D$ -143.6 (c, 0.19 in $CHCl_3$). λ_{max} 220 (log ϵ 4.42); 240 (sh) (log ϵ 3.82); 280 (log ϵ 3.8) (EtOH).

21,22-Dihydro, 19-ketone: ***Isochaetoglobosin J***
[146426-38-2]
$C_{32}H_{36}N_2O_4$ 512.647
Metab. of *Chaetomium subaffine*. Pale yellow cryst. ($CHCl_3$).
Mp 117-119°. $[\alpha]_D$ -20 (c, 0.07 in MeOH). λ_{max} 221 (log ϵ 4.59); 291 (log ϵ 3.74) (MeOH).

19-Deoxy: ***Prochaetoglobosin II***
[133625-26-0]
$C_{32}H_{36}N_2O_3$ 496.648
Metab. of *Chaetomium subaffine*. Pale yellow cryst. (MeOH).
Mp 187-189°. $[\alpha]_D$ -204.2 (c, 0.4 in MeOH). λ_{max} 221 (log ϵ 4.45); 273 (log ϵ 3.59) (MeOH).

19-Deoxy, 20ξ-alcohol: ***20-Dihydroprochaetoglobosin II***
[149439-83-8]
$C_{32}H_{38}N_2O_3$ 498.664
Metab. of *Chaetomium subaffine*. Proposed biosynth. intermediate of Chaetoglobosin A, C-256. Oil. $[\alpha]_D$ -68.6 (c, 0.07 in MeOH). λ_{max} 221 (log ϵ 4.34); 291 (log ϵ 3.38) (MeOH).

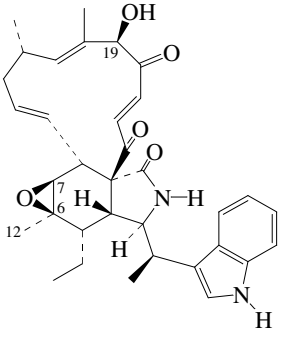
20-Deoxo: ***Chaetoglobosin T***
$C_{32}H_{38}N_2O_3$ 498.664
Prod. by *Chaetomium globosum*. Solid. $[\alpha]_D^{20}$ -80 (c, 0.1 in MeOH). λ_{max} 220 (log ϵ 4.39); 283 (log ϵ 3.58); 290 (log ϵ 3.54) (MeOH).

20-Deoxo, 19-deoxy: ***Prochaetoglobosin I***
[133613-77-1]
$C_{32}H_{38}N_2O_2$ 482.664
Metab. of *Chaetomium subaffine*. Cryst. (MeOH).
Mp 214-216°. $[\alpha]_D$ -101.3 (c, 0.3 in MeOH). λ_{max} 223 (log ϵ 4.45); 291 (log ϵ 3.5) (MeOH).

Sekita, S. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1609; 1618; 1629 (*isol, ir, uv, pmr, ms, struct*)
Oikawa, H. *et al., J.C.S. Perkin 1*, 1992, 2949; 2955 (*isol, uv, ir, pmr, cmr, ms, biosynth, derivs*)
Oikawa, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 628-631 (*20-Dihydroprochaetoglobosin II*)
Iwamoto, C. *et al., Tetrahedron*, 2001, **57**, 2997-3004 (*Penochalasin G*)
Jiao, W. *et al., J. Nat. Prod.*, 2004, **67**, 1722-1725 (*isol, pmr, cmr*)

Chaetoglobosin K C-259

[72509-61-6]



$C_{34}H_{40}N_2O_5$ 556.7

Cytochalasan antibiotic. Obt. from cultures of *Diplodia macrospora*. Plant growth inhibitor, toxic to chickens. Mycotoxin. Yellow prisms (Me_2CO).
Mp 235-240° Mp 264-266°. λ_{max} 221 (ϵ 43700); 273 (ϵ 9120); 281 (ϵ 9120); 290 (ϵ 7590) (EtOH) (Derep). λ_{max} 219 (ϵ 44800) (EtOH) (Berdy).

▶ JF7954000

19-Ketone: ***Chaetoglobosin M***
[119212-28-1]
$C_{34}H_{38}N_2O_5$ 554.685
Isol. from *Diplodia macrospora* DM7. Mycotoxin. Sl. yellow gum. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{22}$ -18.3 (c, 0.92 in CH_2Cl_2). λ_{max} 230 (ϵ 12300); 290 (ϵ 3980) (CH_2Cl_2) (Derep).

Deepoxy, 6,7-didehydro: ***Chaetoglobosin 540***
$C_{34}H_{40}N_2O_4$ 540.701
Prod. by a marine-derived *Phomopsis asparagi* incubated with Jaspamide, J-4. Pale yellow powder. $[\alpha]_D^{25}$ -118 (c, 0.009 in MeOH). λ_{max} 221 (log ϵ 4.43); 289 (log ϵ 3.36) (MeOH).

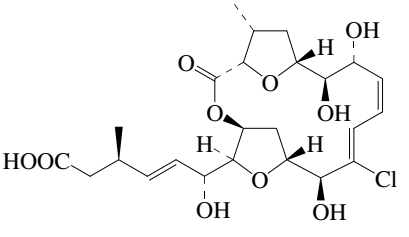
Deepoxy, 6,7-didehydro, 20β-alcohol: ***Chaetoglobosin 542***
$C_{34}H_{42}N_2O_4$ 542.717
Prod. by a marine-derived *Phomopsis asparagi* incubated with Jaspamide, J-4. Cytotoxic. Amorph. powder. $[\alpha]_D^{25}$ -44 (c, 0.01 in MeOH). λ_{max} 222 (log ϵ 4.21); 281 (log ϵ 3.43); 290 (log ϵ 3.35) (MeOH).

Deepoxy, 6,7-didehydro, 19-deoxy, 20-deoxo: ***Chaetoglobosin 510***
$C_{34}H_{42}N_2O_2$ 510.718
Prod. by a marine-derived *Phomopsis asparagi* incubated with Jaspamide, J-4. Amorph. powder. $[\alpha]_D^{25}$ -100 (c, 0.02 in MeOH). λ_{max} 222 (log ϵ 4.37); 281 (log ϵ 3.57); 290 (log ϵ 3.5) (MeOH).

Deepoxy, 6,12-didehydro, 7β-hydroxy: ***Chaetoglobisin L***
[83481-23-6]
$C_{34}H_{40}N_2O_5$ 556.7
Obt. from cultures of *Diplodia macrospora*. Yellow gum. Not obt. completely pure.

Cutler, H.G. *et al., CA*, 1980, **92**, 141619 (*props*)
Cutler, H.G. *et al., J. Agric. Food Chem.*, 1980, **28**, 139 (*isol, cryst struct*)
Springer, J.P. *et al., Tet. Lett.*, 1980, **21**, 1905 (*cryst struct*)
Probst, A. *et al., Helv. Chim. Acta*, 1982, **65**, 1543 (*isol, pmr, struct*)
Cox, R.H. *et al., J. Agric. Food Chem.*, 1983, **31**, 405 (*pmr, cmr, use*)
Spoendlin, C. *et al., Helv. Chim. Acta*, 1988, **71**, 1881 (*deriv*)
Christian, O.E. *et al., J. Nat. Prod.*, 2005, **68**, 1592-1597 (*Chaetoglobosins 510,540,542*)

Chagosensin C-260



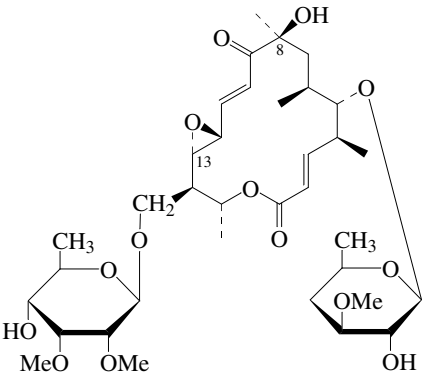
Absolute Configuration

$C_{24}H_{33}ClO_{10}$ 516.971
Isol. from the sponge *Leucetta chagosensis*. Powder. $[\alpha]_D^{23}$ -131 (c, 0.01 in CH_2Cl_2). λ_{max} 230 (log ϵ 4.16) (MeOH).

Rezanka, T. *et al., Eur. J. Org. Chem.*, 2003, 4073-4079 (*isol, pmr, cmr*)

Chalcomycin C-261

[20283-48-1]



$C_{35}H_{56}O_{14}$ 700.819

Macrolide antibiotic. Prod. by some strains of *Streptomyces bikiniensis*. Possesses broad spectrum of antimicrobial activity. Cryst. (butanol).
Mp 121-123°. $[\alpha]_D^{27}$ -43.5 (c, 1 in EtOH). Possibly identical with Myconomycin and Aldgamycin D. λ_{max} 218 (ϵ 22800) (MeOH) (Derep).

4″-O-Propanoyl: ***Chalcomycin B***
$C_{38}H_{60}O_{15}$ 756.883
Prod. by the marine *Streptomyces* sp. B7064. Amorph. solid.
Mp 98°. $[\alpha]_D^{20}$ +186 (c, 5.9 in MeOH).

8-Deoxy: ***8-Deoxychalcomycin***
[125225-83-4]
[102851-26-3]
$C_{35}H_{56}O_{13}$ 684.82
Prod. by *Streptomyces hirsutus*. Active against gram-positive bacteria.

10,11-Dihydro: ***10,11-Dihydrochalcomycin, 9CI***. *GERI 155*. *Antibiotic GERI 155*
[182495-48-3]
$C_{35}H_{58}O_{14}$ 702.835
Prod. by *Streptomyces* sp. GERI 155; KCTC0041BP. Antibacterial agent. Powder. Sol. Me_2CO, MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 98.5° dec. $[\alpha]_D^{23}$ -75.5 (c, 0.1 in MeOH). λ_{max} 217 (ϵ 18350); 290 (sh) (MeOH).

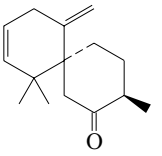
10,11-Dihydro, 8-deoxy, 12,13-deepoxy, 12,13-didehydro: ***Antibiotic 250-144C***. *250-144C*
[189760-01-8]
$C_{35}H_{58}O_{12}$ 670.836
Prod. by a *Streptomyces* sp. SNUS-9011-250. Amorph. solid. Sol. MeOH, Et_2O, $CHCl_3$, EtOH; poorly sol. H_2O, hexane.
Mp 74-76°. $[\alpha]_D^{26}$ -16 (c, 0.05 in EtOH). λ_{max} 216 (ϵ 3050); 282 (ϵ 450) (EtOH).

6-Demethyl: See Neutramycin in *The Combined Chemical Dictionary*.

Woo, P.W.K. *et al., J.A.C.S.*, 1962, **84**, 1512; 1964, **86**, 2724; 2726 (*struct*)
Celmer, W.D. *et al., J.A.C.S.*, 1965, **87**, 1801 (*struct*)
Omura, S. *et al., J.A.C.S.*, 1975, **97**, 4001 (*nmr*)
Neszmelyi, A. *et al., Chem. Comm.*, 1976, 97 (*nmr*)
Jardim, M.E. *et al., Int. J. Mass Spectrom. Ion Phys.*, 1983, **48**, 189 (*ms, struct*)
Hauske, J.R. *et al., J.O.C.*, 1986, **51**, 2808 (*8-Deoxychalcomycin, nmr, ms*)
Kim, S.D. *et al., J. Antibiot.*, 1996, **49**, 955-957 (*10,11-Dihydrochalcomycin*)
Woo, P.W.K. *et al., Tetrahedron*, 1996, **52**, 3857 (*cryst struct, abs config*)
Goo, Y.M. *et al., J. Antibiot.*, 1997, **50**, 85-88 (*cmr, 250-144C*)
Asolkar, R.N. *et al., J. Antibiot.*, 2002, **55**, 893-898 (*cmr, Chalcomycin B*)

7(14),9-Chamigradien-2-one C-262

2,5(14)-Chamigradien-8-one

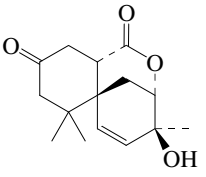


$C_{15}H_{22}O$ 218.338
Constit. of *Laurencia flexilis*. Oil. $[\alpha]_D^{25}$ -28 (c, 0.25 in $CHCl_3$).

de Nys, R. *et al., Phytochemistry*, 1993, **34**, 725-728 (*isol, pmr, cmr, ms*)

Chamigrenelactone C-263

[777093-36-4]

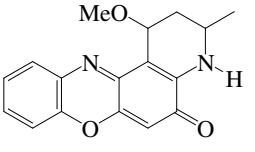


$C_{15}H_{20}O_4$ 264.321
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ -150 (c, 0.1 in $CHCl_3$).

Dorta, E. *et al., Tet. Lett.*, 2004, **45**, 7065-7068 (*isol, pmr, cmr*)

Chandrananimycin C C-264

[664355-11-7]

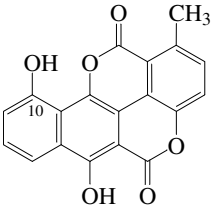


$C_{17}H_{16}N_2O_3$ 296.325
Prod. by a marine bacteria *Actinomadura* sp. M045 and *Halomonas* sp. GWS-BW-H8hM. Antibiotic. Orange solid. λ_{max} 243 (log ϵ 4.49); 282 (log ϵ 4.19); 366 (log ϵ 4.16); 433 (log ϵ 4.2) (MeOH).

Maskey, R.P. *et al., J. Antibiot.*, 2003, **56**, 622-629 (*isol, ir, pmr, cmr*)
Bitzer, J. *et al., J. Antibiot.*, 2006, **59**, 86-92 (*isol, pmr, ms*)

Chartarin C-265

*6,10-Dihydroxy-1-methylbenzo[*h*][1]benzopyrano[5,4,3-*cde*][1]-benzopyran-5,12-dione, 9CI*
[34170-23-5]



$C_{19}H_{10}O_6$ 334.284
Synthetic. Needles. Mp 315-316° (309-310°).

10-O-[6-Deoxy-α-D-galactopyranosyl-(1→2)-6-deoxy-β-D-galactopyranoside]: ***3″-O-Demethylchartreusin***
[128229-64-1]
$C_{31}H_{30}O_{14}$ 626.57

From *Streptomyces chartreusis* IFO1275. Antineoplastic agent. Yellow powder. Sol. MeOH, EtOAc; fairly sol. $CHCl_3$, Et_2O; poorly sol. H_2O.
Mp 251-254°. Log P 0.24 (uncertain value) (calc). λ_{max} 239 (ϵ 48800); 310 (ϵ 5240); 357 (ϵ 7620); 438 (ϵ 13300) (MeOH/KOH) (Derep). λ_{max} 236 (ϵ 39700); 260 (sh) (ϵ); 264 (ϵ 39200); 274 (sh) (ϵ); 334 (ϵ 6140); 380 (ϵ 8640); 400 (ϵ 14300); 423 (ϵ 15800) (MeOH) (Derep). λ_{max} 235 (ϵ 9000); 265 (ϵ 7300); 332 (ϵ 1700); 380 (ϵ 1500); 400 (ϵ 230); 422 (ϵ 2500) (MeOH) (Berdy).

*10-*O*-[2-*O*-Acetyl-6-deoxy-3-*O*-methyl-α-D-galactopyranosyl-(1→2)-6-deoxy-β-D-galactopyranoside]:* ***2''-O-Acetylchartreusin***
$C_{34}H_{34}O_{15}$ 682.634
Prod. by the marine isolate *Streptomyces* sp. B5525. Yellow solid.

*10-*O*-[4-*O*-Acetyl-6-deoxy-3-*O*-methyl-α-D-galactopyranosyl-(1→2)-6-deoxy-β-D-galactopyranoside]:* ***4''-O-Acetylchartreusin***
$C_{34}H_{34}O_{15}$ 682.634
Prod. by the marine isolate *Streptomyces* sp. B5525. Yellow solid. λ_{max} 265 (log ϵ 4.42); 399 (log ϵ 3.45); 418 (log ϵ 3.48) (MeOH).

*10-*O*-[6-Deoxy-3-C-methyl-β-D-galactopyranoside]:* ***Elsamicin B***. *BBM 2478B. Antibiotic BBM 2478B*
[97068-31-0]
$C_{26}H_{22}O_{10}$ 494.454
Isol. from actinomycete *Actinomadura* J907-21. Shows antibacterial, antimelanoma and antileukaemia activities. Sol. DMF, dioxan, DMSO; fairly sol. MeOH, EtOH, $CHCl_3$; poorly sol. C_6H_6, H_2O, Et_2O, hexane.
Mp 271-272° dec. $[\alpha]_D^{26}$ -8 (Py). λ_{max} 236 (ϵ 36600); 266 (ϵ 34600); 333 (ϵ 5830); 378 (ϵ 8350); 398 (ϵ 12600); 422 (ϵ 14300) (MeOH) (Derep). λ_{max} 240; 269; 435 (MeOH/NaOH) (Berdy).

*10-*O*-[6-Deoxy-3-*O*-methyl-α-D-galactopyranosyl-(1→2)-6-deoxy-β-D-galactopyranoside]:* ***Chartreusin***. *NSC 5159. X 465A. Antibiotic 747. Antibiotic 1293. Antibiotic X 465A. Antibiotic G 261A. G 261A. Lambdamycin*
[6377-18-0]
[128229-64-1]
$C_{32}H_{32}O_{14}$ 640.596
Isol. from *Streptomyces chartreusis* and the marine-derived Streptomyces sp. B5525. Antineoplastic antibiotic. Yellow plates (Me_2CO aq. or CH_2Cl_2/EtOH).
Mp 184-186°. $[\alpha]_D^{25}$ +127.5 (c, 0.3 in Py). $[\alpha]_D$ -36.2 (c, 0.3 in AcOH). Log P 0.91 (uncertain value) (calc). λ_{max} 239 (ϵ 48800); 310 (ϵ 5240); 357 (ϵ 7620); 438 (ϵ 13300) (MeOH/KOH) (Derep). λ_{max} 236 (ϵ 39700); 260 (sh) (ϵ); 264 (ϵ 39200); 274 (sh) (ϵ); 334 (ϵ 6140); 380 (ϵ 8640); 400 (ϵ 14300); 423 (ϵ 15800) (MeOH) (Derep).
▶ LD_{50} (mus, ipr) 300 mg/kg. FL7350000

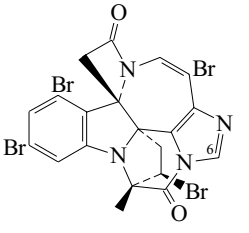
*10-*O*-[6-Deoxy-3-*O*-methyl-α-D-galactopyranosyl-(1→2)-6-deoxy-β-D-galactopyranosyl-(1→2)-6-deoxy-β-D-galactopyranoside]:* ***Antibiotic D 329C***. *D 329C*
[146644-96-4]
$C_{38}H_{42}O_{18}$ 786.739
Prod. by a mutant of *Streptomyces chartreusis*. Antitumour agent. Yellow powder.
Mp 194-199°. $[\alpha]_D^{20}$ -61.8 (c, 0.5 in MeOH). λ_{max} 235 (ϵ 43000); 264 (ϵ 42000); 332 (ϵ 7100); 376 (ϵ 9400); 399 (ϵ 16000); 422 (ϵ 17000) (MeOH) (Derep).

*10-*O*-[2-Amino-2,6-dideoxy-3-*O*-methyl-α-D-galactopyranosyl-(1→2)-6-deoxy-3-C-methyl-β-D-galactopyranoside]:* ***Elsamicin A***. *Antibiotic BBM 2478A. Elsamitrucin. Antibiotic BMY 28090. BBM 2478A*
[97068-30-9]
[123303-94-6, 123303-95-7]
$C_{33}H_{35}NO_{13}$ 653.638
Isol. from actinomycete *Actinomadura* J907-21. Possesses antibacterial, antimelanoma and antileukaemia activities. Antitumour antibiotic. Sol. DMF, DMSO, dioxan; fairly sol. MeOH, $CHCl_3$, EtOH; poorly sol. C_6H_6, H_2O, Et_2O, hexane.
Mp 225-226°. $[\alpha]_D^{26}$ +124 (c, 0.5 in Py). λ_{max} 240 (ϵ); 268 (ϵ); 435 (ϵ) (MeOH/NaOH) (Derep). λ_{max} 236 (ϵ 38530); 266 (ϵ 35915); 333 (ϵ 6350); 378 (ϵ 8620); 398 (ϵ 13387); 422 (ϵ 14693) (MeOH) (Derep).
▶ LD_{50} (mus, ipr) 38mg/kg. DE5410000

Leach, B.E. *et al., J.A.C.S.*, 1953, **75**, 4011 (*Chartreusin, isol*)
Berger, J. *et al., J.A.C.S.*, 1958, **80**, 1636; 1639 (*Chartreusin, props*)
Simonitsch, E. *et al., Helv. Chim. Acta*, 1960, **43**, 58; 1964, **47**, 1459 (*Chartreusin, struct*)
Eisenhuth, W. *et al., Helv. Chim. Acta*, 1964, **47**, 1475 (*Chartreusin, struct*)
Canham, P.L. *et al., Can. J. Chem.*, 1977, **55**, 2450 (*biosynth*)
Strauss, D.G. *et al., Z. Allg. Mikrobiol.*, 1977, **29**, 362 (*Chartreusin, isol, props*)
Hauser, F.M. *et al., J.O.C.*, 1980, **45**, 4071 (*Chartarin*)
Beisler, J.A. *et al., Prog. Med. Chem.*, 1982, **19**, 247 (*Chartreusin, rev, pharmacol*)
Belg. Pat., 1985, 900 735; *CA*, **103**, 36177 (*Elsamicins A,B, isol, props*)
Konishi, M. *et al., J. Antibiot.*, 1986, **39**, 784 (*Elsamicins A,B, isol, props*)
Sugawara, K. *et al., J.O.C.*, 1987, **52**, 996 (*Chartreusin, Elsamicins A,B, pmr, cmr*)
Schurig, J.E. *et al., Invest. New Drugs*, 1989, **7**, 173 (*Elsamicins A,B, pharmacol*)
Lam, K.S. *et al., J. Nat. Prod.*, 1989, **52**, 1015 (*biosynth*)
Salas, X. *et al., FEBS Lett.*, 1991, **292**, 223 (*Elsamicins A,B, pharmacol*)
Sakuda, S. *et al., Tet. Lett.*, 1991, **32**, 1817 (*Elsamicins A,B, abs config*)
Aoyama, Y. *et al., J. Antibiot.*, 1992, **45**, 875 (*Demethylchartreusin*)
Uchida, H. *et al., J. Antibiot.*, 1993, **46**, 1611 (*D 329C*)
Maskey, R.P. *et al., Z. Naturforsch., B*, 2002, **57**, 823-829 (*Acetylchartreusins*)
Kamitori, S. *et al., Carbohydr. Res.*, 2003, **338**, 1523-1525 (*crys struct, benzylidenechartreusin*)
Xu, Z. *et al., Chem. Biol.*, 2005, **12**, 579-588 (*Chartreusin, biosynth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CDK250 (*Chartreusin*)

Chartellamide A C-266

[111268-63-4]



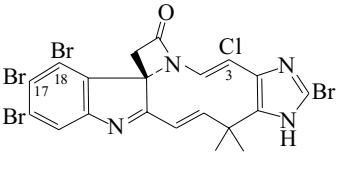
$C_{20}H_{12}Br_4N_4O_2$ 659.956
Alkaloid from the marine bryozoan *Chartella papyracea* and from *Flustra papyracea*. Sol. MeOH, EtOH; poorly sol. H_2O. λ_{max} 212 (log ϵ 4.28); 230 (log ϵ 4.41); 258 (log ϵ 4.03); 294 (log ϵ 3.76); 303 (log ϵ 3.74); 318 (log ϵ 3.53) (EtOH).

6-Bromo: ***Chartellamide B***
[111268-64-5]
$C_{20}H_{11}Br_5N_4O_2$ 738.852
From *Chartella papyracea*. Sol. MeOH, EtOH; poorly sol. H_2O. λ_{max} 213 (log ϵ 3.7); 231 (log ϵ 3.81); 260 (log ϵ 3.46); 293 (log ϵ 3.19); 303 (log ϵ 3.15); 318 (log ϵ 2.85) (EtOH).

Anthoni, U. *et al., J.O.C.*, 1987, **52**, 5638-5639 (*isol, uv, ir, cd, pmr, cmr, ms, struct*)

Chartelline A C-267

[96845-55-5]



$C_{20}H_{13}Br_4ClN_4O$ 680.418
Alkaloid from the marine bryozoan *Chartella papyracea* and from *Flustra papyracea*. Cryst. (EtOAc). Sol. MeOH, $CHCl_3$.
Mp 214-216° dec. $[\alpha]_D^{20}$ -421 (c, 0.038 in EtOH). Shows imidazole tautomerism in soln. λ_{max} 230 (ϵ 38900); 243 (ϵ 37200) (EtOH) (Derep). λ_{max} 230 (ϵ 38900) (MeOH) (Berdy).

17-Debromo: ***Chartelline B***
[110271-21-1]
$C_{20}H_{14}Br_3ClN_4O$ 601.521
Alkaloid from *Chartella papyracea* and *Flustra papyracea*.
$[\alpha]_D^{20}$ -339.1 (c, 0.023 in EtOH). λ_{max} 225 (ϵ 27500); 235 (ϵ 26900) (EtOH) (Derep).

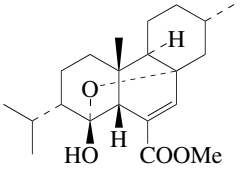
17,18-Didebromo: ***Chartelline C***
[110271-22-2]
$C_{20}H_{15}Br_2ClN_4O$ 522.625
Alkaloid from *Chartella papyracea* and *Flustra papyracea*.
$[\alpha]_D^{20}$ -217.4 (c, 0.023 in EtOH). λ_{max} 227 (ϵ 25700); 234 (ϵ 25700) (EtOH) (Derep).

3-Dechloro, 3-methoxy: ***Methoxydechlorochartelline A***
[110271-23-3]
$C_{21}H_{16}Br_4N_4O_2$ 675.999
Alkaloidal artifact from *Chartella papyracea* and *Flustra papyracea*.
$[\alpha]_D^{20}$ -196.3 (c, 0.055 in EtOH). λ_{max} 230 (ϵ 31622); 245 (ϵ 25700) (EtOH) (Berdy).

Chevolot, L. *et al., J.A.C.S.*, 1985, **107**, 4542-4543 (*isol, uv, ir, pmr, cmr, cryst struct*)
Anthoni, U. *et al., J.O.C.*, 1987, **52**, 4709-4712 (*derivs, isol*)

Chatancin C-268

[129895-81-4]

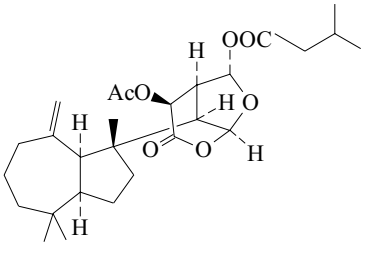


$C_{21}H_{32}O_4$ 348.481
Isol. from a soft coral. *Sarcophyton* sp. Platelet activating factor antagonist. Needles (MeOH aq.).
Mp 106-108°. $[\alpha]_D$ +10.5 (c, 1 in $CHCl_3$). λ_{max} 218 (ϵ 7500) (MeCN).

Sugano, M. *et al., J.O.C.*, 1990, **55**, 5803-5805 (*isol, ir, cd, pmr, cmr, ms, cryst struct*)
Toró, A. *et al., Org. Lett.*, 2000, **2**, 2737-2740 (*synth*)
Soucy, P. *et al., J.O.C.*, 2003, **68**, 9983-9987 (*synth*)

Chelonaplysin A C-269

[133587-15-2]

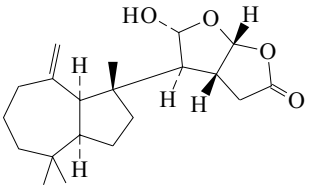


$C_{27}H_{40}O_7$ 476.609
Metab. of *Chelonaplysilla* spp. Oil. $[\alpha]_D$ -45.8 (c, 0.24 in $CHCl_3$).

Bobzin, S.C. *et al., J. Nat. Prod.*, 1991, **54**, 225 (*isol, pmr, cmr*)

Chelonaplysin B C-270

[133587-16-3]

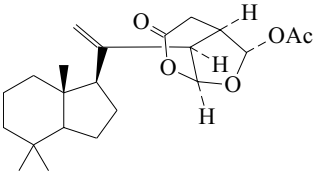


$C_{20}H_{30}O_4$ 334.455
Metab. of *Chelonaplysilla* spp. Oil. $[\alpha]_D$ +4.5 (c, 0.11 in $CHCl_3$).

Bobzin, S.C. *et al., J. Nat. Prod.*, 1991, **54**, 225 (*isol, pmr, cmr*)

Chelonaplysin C C-271

[133587-17-4]

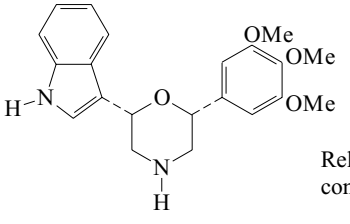


$C_{22}H_{32}O_5$ 376.492
Metab. of *Chelonaplysilla* spp. Ichthyotoxin. Cryst. (hexane/Et_2O).
Mp 148°. $[\alpha]_D$ -6.1 (c, 0.23 in $CHCl_3$).

Bobzin, S.C. *et al., J. Nat. Prod.*, 1991, **54**, 225 (*isol, pmr, cmr*)
Bergquist, P.R. *et al., Aust. J. Chem.*, 1993, **46**, 623 (*isol, pmr, cmr*)

Chelonin A C-272

2-(3-Indolyl)-6-(3,4,5-trimethoxyphenyl)morpholine
[133985-26-9]



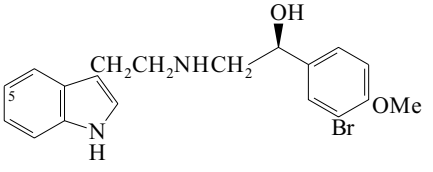
Relative configuration

$C_{21}H_{24}N_2O_4$ 368.432
Alkaloid from the marine sponge *Chelonaplysilla* sp. Possesses antiflammatory and antibacterial activities. Cryst. (MeOH).
Mp 182°. $[\alpha]_D$ -11.7 (c, 0.32 in $CHCl_3$). λ_{max} 213 (ϵ 37100); 272 (ϵ 6300); 278 (ϵ 6400); 288 (ϵ 5100) (MeOH) (Derep).

Bobzin, S.C. *et al., J.O.C.*, 1991, **56**, 4403 (*isol, uv, ir, pmr, cmr, ms, struct*)
Somei, M. *et al., Heterocycles*, 1995, **41**, 5 (*synth*)

Chelonin B C-273

*3-Bromo-α-[[[2-(1*H*-indol-3-yl)ethyl]amino]methyl]-4-methoxybenzenemethanol, 9CI. 3-[2-[[2-(3-Bromo-4-methoxyphenyl)-2-hydroxyethyl]amino]ethyl]indole.* N*-(3-Bromo-β-hydroxy-4-methoxyphenethyl)tryptamine*
[133985-27-0]



$C_{19}H_{21}BrN_2O_2$ 389.291

λ_{max} 208 (ϵ 29000); 221 (ϵ 30600); 280 (ϵ 6400); 288 (sh) (ϵ) (MeOH) (Derep).

(S)-form

Alkaloid from the marine sponge *Chelonaplysilla* sp. Shows antibacterial activity. Solid.
Mp 260° dec.

5-Bromo: ***Bromochelonin B***

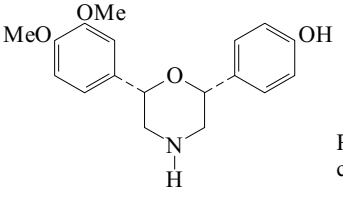
[134004-59-4]
$C_{19}H_{20}Br_2N_2O_2$ 468.187
From the sponge *Chelonaplysilla* sp. and *Dendrilla* sp. Shows antibacterial activity. Gum. $[\alpha]_D$ +3.7 (c, 0.27 in DMSO). λ_{max} 208 (ϵ 29000); 221 (ϵ 30600); 279 (sh) (ϵ); 287 (ϵ 2500); 299 (sh) (ϵ) (DMSO) (Derep).

Bobzin, S.C. *et al., J.O.C.*, 1991, **56**, 4403-4407 (*isol, pmr, cmr, struct*)
Lawrence, N.J. *et al., Tet. Lett.*, 2001, **42**, 7671-7674 (*synth, abs config*)

Chelonin C C-274

4-[6-(3,4-Dimethoxyphenyl)-2-morphinolinyl]phenol, 9CI. 2-(4-Hydroxyphenyl)-6-(3,4-dimethoxyphenyl)morpholine

[133985-28-1]



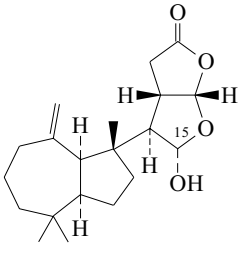
Relative configuration

$C_{18}H_{21}NO_4$ 315.368
Alkaloid from the marine sponge *Chelonaplysilla* sp. Solid.
Mp 238° dec. $[\alpha]_D$ +5.8 (c, 0.53 in $CHCl_3$). λ_{max} 210 (ϵ 18200); 236 (ϵ 12900); 279 (ϵ 3800); 295 (sh) (MeOH/NaOH) (Derep). λ_{max} 208 (ϵ 15100); 227 (ϵ 13800); 277 (ϵ 3600) (MeOH) (Derep).

Bobzin, S.C. *et al., J.O.C.*, 1991, **56**, 4403 (*isol, uv, ir, pmr, cmr, ms, struct*)

Cheloviolene A C-275

[135886-54-3]



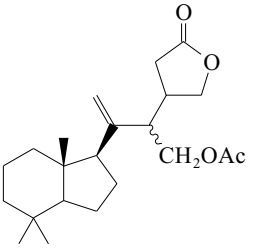
$C_{20}H_{30}O_4$ 334.455
Constit. of *Chelonaplysilla violacea*. Cryst. (EtOAc/hexane).
Mp 161-163°. $[\alpha]_D$ +6 (c, 1 in $CHCl_3$).

15-Epimer: ***Cheloviolene B***

[149952-32-9]
$C_{20}H_{30}O_4$ 334.455
Constit. of *Chelonaplysilla violacea*. Cryst. (hexane).
Mp 200°.

Buckleton, J.S. *et al., Acta Cryst. C*, 1993, **47**, 1438 (*cryst struct*)
Bergquist, P.R. *et al., Aust. J. Chem.*, 1993, **46**, 623 (*isol, pmr, cmr*)

Cheloviolene C C-276

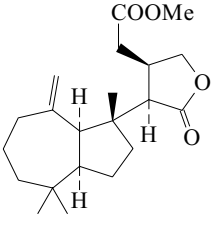


$C_{22}H_{34}O_4$ 362.508
Constit. of *Chelonaplysilla violacea*. Gum.

Bergquist, P.R. *et al., Aust. J. Chem.*, 1993, **46**, 623 (*isol, pmr, cmr*)

Cheloviolene D C-277

[149864-70-0]

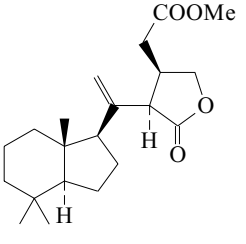


$C_{21}H_{32}O_4$ 348.481
Constit.of *Chelonaplysilla violacea*. Gum.

Bergquist, P.R. *et al., Aust. J. Chem.*, 1993, **46**, 623 (*isol, pmr, cmr*)

Cheloviolene E C-278

[149952-33-0]

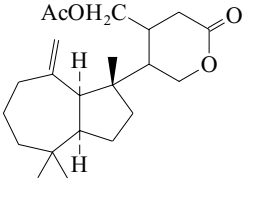


$C_{21}H_{32}O_4$ 348.481
Constit. of *Chelonaplysilla violacea*. Oil.

Bergquist, P.R. *et al., Aust. J. Chem.*, 1993, **46**, 623 (*isol, pmr, cmr*)

Cheloviolene F C-279

[149952-34-1]

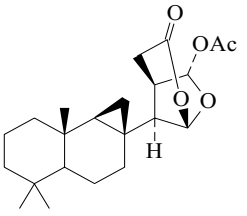


$C_{22}H_{34}O_4$ 362.508
Constit. of *Chelonaplysilla violacea*. Oil.

Bergquist, P.R. *et al., Aust. J. Chem.*, 1993, **46**, 623 (*isol, pmr, cmr*)

Cheloviolin C-280

[149864-71-1]

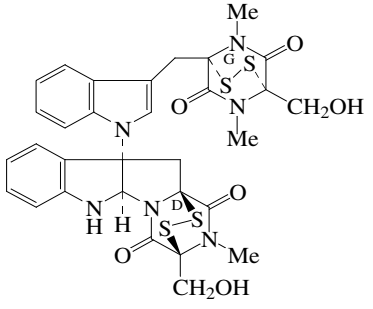


$C_{22}H_{32}O_5$ 376.492
Constit. of *Chelonaplysilla violacea*. Oil.

Bergquist, P.R. *et al., Aust. J. Chem.*, 1993, **46**, 623 (*isol, pmr, cmr*)

Chetomin C-281

Chaetomin
[1403-36-7]



Absolute Configuration

$C_{31}H_{30}N_6O_6S_4$ 710.879
Metab. of *Chaetomium cochliodes*, *Chaetomium globosum*, *Chaetomium seminudum*, *Chaetomium subglobosum* and *Chaetomium teniussimum*. Antibacterial agent and immunosuppressant. Cytotoxic. Powder. Sol. Me_2CO, EtOAc, $CHCl_3$, C_6H_6, Py, dioxan; fairly sol. MeOH, EtOH, Et_2O; poorly sol. H_2O, hexane.
Mp 218-220°. $[\alpha]_D^{25}$ +278 (c, 0.12 in $CHCl_3$). λ_{max} 276 (log ϵ 3.8); 287 (log ϵ 3.83); 295 (log ϵ 3.82) (EtOH).

▶ LD_{50} (rat, orl) 75 mg/kg. FM3038000

O,O′-Di-Ac: Mp 175-177°.

O,O′-Di-Ac, N-*Me:* Mp 112-114°.

Ring D trithia homologue: ***Chetoseminudin A***
$C_{31}H_{30}N_6O_6S_5$ 742.945
Prod. by *Chaetomium seminudum* 72-S-204-1. Immunosuppressant. Amorph. solid. $[\alpha]_D^{24}$ +279 (c, 0.05 in $CHCl_3$). λ_{max} 277 (log ϵ 3.88); 285 (log ϵ 3.89); 295 (log ϵ 3.87) (EtOH).

Ring G trithia homologue: ***Chetomin B***. *Chaetomin B*
$C_{31}H_{30}N_6O_6S_5$ 742.945
Prod. by the marine-derived *Chaetomium* sp. Gö 100/9. Amorph. solid.
Mp >200°. $[\alpha]_D^{20}$ +270 (c, 0.1 in $CHCl_3$). λ_{max} 205 (sh) (log ϵ 4.18); 290 (log ϵ 3.53) (MeOH).

Safe, S. *et al., J.C.S. Perkin 1*, 1972, 472 (*isol, uv, pmr, cd, struct*)
McInnes, A.G. *et al., J.A.C.S.*, 1976, **98**, 6741 (*cmr, nmr, struct*)
Brewer, D. *et al., J.C.S. Perkin 1*, 1978, 1248 (*nmr*)
Jeu, W.C. *et al., Can. J. Microbiol.*, 1983, **29**, 1399 (*props*)
Fujimoto, H. *et al., J. Nat. Prod.*, 2004, **67**, 98-102; 526 (*isol, pmr, cmr, Chetoseminudin A*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 601

Chicken gonadotrophin-releasing hormones C-282

Chicken GnRH. *cGnRH*

5-OxoPro-His-Trp-Ser-Tyr-Gly-Leu-Gln-Pro-Gly-NH_2

Struct. of cGnRH I shown.

cGnRH-I

Alligator GnRH-I
[47922-48-5]

$C_{54}H_{71}N_{15}O_{14}$ 1154.247
Isol. from brains of chicken and alligator. Shows one substitution (Gln for ^{8}Arg) as compared with Gonadorelin.

cGnRH-II

Alligator GnRH-II. *Catfish GnRH-II*. *Sea bream GnRH-II*. *Ratfish GnRH*
[91097-16-4]

$C_{60}H_{69}N_{17}O_{13}$ 1236.311
Isol. from brains of chicken, alligator, catfish (*Clarias* sp.), sea bream (*Sparus aurata*), ratfish (*Hydrolagus colliei*) and Pacific herring (*Clupea harengus pallasi*).

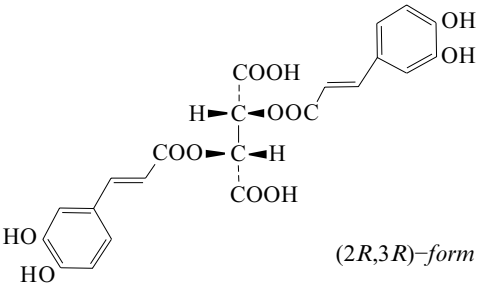
Herring gonadotrophin-releasing hormone

Herring GnRH. *hrGnRH*. Clupea pallasi *Gonadotrophin-releasing hormone*
[260780-12-9]
Isol. from brain of Pacific herring *Clupea harengus pallasi*.

King, J.A. *et al., J. Biol. Chem.*, 1982, **257**, 10729-10732 (*isol, struct, chicken*)
Lovejoy, D. *et al., Gen. Comp. Endocrinol.*, 1991, **82**, 152-161 (*isol, catfish*)
Lovejoy, D.A. *et al., Regul. Pept.*, 1991, **33**, 105-116 (*isol, alligator*)
Bogerd, J. *et al., Biochem. Biophys. Res. Commun.*, 1992, **187**, 127-134 (*isol, catfish*)
Ngamvongghon, S. *et al., Gen. Comp. Endocrinol.*, 1992, **87**, 266-274 (*isol, catfish*)
Powell, J.F. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1994, **91**, 12081-12085 (*isol, sea bream*)
Carolsfeld, J. *et al., Endocrinology (Baltimore)*, 2000, **141**, 505-512 (*isol, herring*)

Chicoric acid C-283

2,3-Bis[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]butanedioic acid, 9CI. *Dicaffeoyltartaric acid*. *Cichoric acid*
[6537-80-0]
[52248-48-3]



(2*R*,3*R*)–*form*

$C_{22}H_{18}O_{12}$ 474.377

(2*R*,3*R*)-*form*

L-Chicoric acid
[70831-56-0]
Constit. of leaves of chicory (*Cichorium intybus*), *Onychium japonicum* and *Echinacea purpurea*. Also found in the marine aquatic plant *Posidonia oceanica*. Immunostimulator and HIV-1 integrase inhibitor. Silky needles. Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 206°. $[\alpha]_D$ -384 (c, 1.07 in MeOH). λ_{max} 318 (MeOH) (Berdy).

3-Me ether: ***Caffeoylferuloyltartaric acid***
[99119-75-2]
$C_{23}H_{20}O_{12}$ 488.404
Isol. from *Echinacea pallida* and *Echinacea purpurea*. Stereochem. not confirmed.

3,3′-Di-Me ether: ***Chicoric acid dimethyl ether***
[99119-76-3]
$C_{24}H_{22}O_{12}$ 502.431
Isol. from *Echinacea* spp. Stereochem. not confirmed.

(2S,3S)-form

Isol. from chicory (*Cichorium intybus*) and *Cichorium endivia* (endive).
Needles (H_2O).
Mp 206°. $[\alpha]_D$ +384 (c, 1.55 in MeOH).

(2RS,3RS)-form

(±)-form
Cryst. (H_2O). Mp 206°.

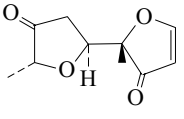
(2RS,3SR)-form

Mesochicoric acid
[133520-29-3]
[53797-30-1]
Constit. of *Equisetum arvense.*
Cryst. (H_2O).
Mp 225°.

Scarpati, M.L. *et al., Tetrahedron*, 1958, **4**, 43-48 (*isol, struct, synth*)
Woeldecke, M. *et al., Z. Naturforsch., C*, 1974, **29**, 360-361 (*isol*)
Cariello, L. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1979, **62**, 159 (*isol*)
Becker, H. *et al., Z. Naturforsch., C*, 1985, **40**, 585-587 (*isol*)
Soicke, H. *et al., Planta Med.*, 1988, **54**, 175-176 (*isol*)
Veit, M. *et al., Phytochemistry*, 1991, **30**, 527-529 (*isol, struct*)
Robinson, W.E. *et al., Antiviral Res.*, 1998, **39**, 101-111 (*activity*)
Zhao, H. *et al., Synth. Commun.*, 1998, **28**, 737-740 (*synth, pmr*)
Lamidey, A.-M. *et al., Helv. Chim. Acta*, 2002, **85**, 2328-2334 (*synth*)

Chilenone A C-284

[87746-82-5]

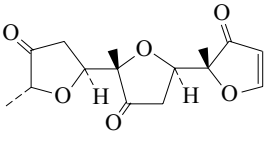


$C_{10}H_{12}O_4$ 196.202
Constit. of *Laurencia chilensis.* Cryst.
Mp 51°. Racemic.

Martin, A.S. *et al., Tet. Lett.*, 1983, **24**, 4063 (*cryst struct*)

Chilenone B C-285

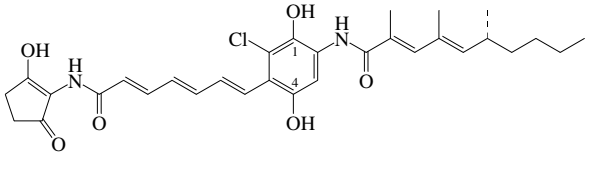
[113394-05-1]



$C_{15}H_{18}O_6$ 294.304
Constit. of red alga *Laurencia chilensis.* Cryst. (Et_2O/hexane).
Mp 111°. Racemate.

San-Martin, A. *et al., Tet. Lett.*, 1987, **28**, 6013 (*cryst struct*)

Chinikomycin A C-286

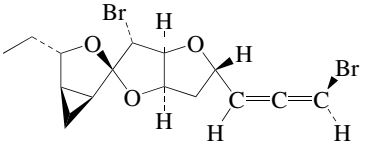


$C_{31}H_{37}ClN_2O_6$ 569.096
Related to Manumycin A, M-89. Prod. by the marine-derived *Streptomyces* sp. M 045. Yellow-brown solid. λ_{max} 260 (log ϵ 4.46); 335 (sh) (log ϵ 4.46); 395 (log ϵ 4.62) (MeOH).

1,4-Quinone: ***Chinikomycin B***
$C_{31}H_{35}ClN_2O_6$ 567.08
Prod. from *Streptomyces* sp. MO45. Red solid. Artifact. λ_{max} 261 (log ϵ 4.68); 344 (log ϵ 4.72); 500 (log ϵ 3.98) (MeOH).

Li, F. *et al., J. Nat. Prod.*, 2005, **68**, 349-353 (*isol, pmr, cmr, ms*)

Chinzallene C-287

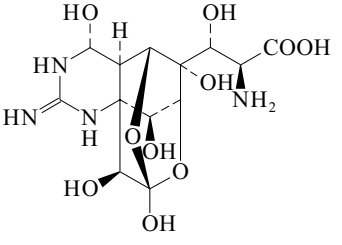


$C_{15}H_{18}Br_2O_3$ 406.113
Constit. of *Laurencia* sp.
$[\alpha]_D^{21}$ +184 (c, 0.57 in $CHCl_3$).

Suzuki, M. *et al., Phytochemistry*, 2005, **66**, 2787-2793 (*isol, pmr, cmr, ms*)

Chiriquitoxin C-288

11-(Aminocarboxymethyl)tetrodotoxin, 9CI
[61132-15-8]

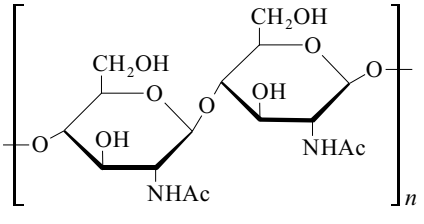


$C_{13}H_{20}N_4O_{10}$ 392.322
Toxin from skin and eggs of *Atelopus chiriquiensis.* Amorph. solid. Sol. H_2O. $[\alpha]_D^{22}$ -17.3 (c, 0.075 in AcOH aq.).
▶ FM6102600

Yotsu, M. *et al., Tet. Lett.*, 1990, **31**, 3187-3190 (*isol, pmr, cmr, struct*)

Chitin, 9CI, 8CI C-289

[1398-61-4]



$C_8H_{13}NO_5$ 203.194
A linear polymer of 2-Acetamido-2-deoxyglucose. Minimum formula given. Occurs in shells of crustacea, most fungi, mycelial yeast, green algae and some brown and red algae. Antihaemorrhagic. Used as a wound healant. $[\alpha]_D^{20}$ -14 → +56 (HCl). The fully *N*-deacetylated prod. is called Chitan.
▶ LD_{50} (rat, ivn) 50 mg/kg. FM6125000

Partially deacylated deriv.: See Chitosan in *The Combined Chemical Dictionary.*

[39280-86-9, 87582-10-3, 88650-88-8]

Foster, A.B. *et al., Adv. Carbohydr. Chem.*, 1960, **15**, 371 (*rev*)
BeMiller, J.N. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 103 (*synth*)
Jeuniaux, C. *et al., Compr. Biochem.*, (eds. Florkin, M. et al), 1971, **26C**, 595
Pervaiz, S.M. *et al., Z. Naturforsch., C*, 1975, **30**, 571 (*struct*)
Muzzarelli, R.A.A. *et al., Chitin*, Pergamon, N.Y., 1977,
Austin, P.R. *et al., Science (Washington, D.C.)*, 1981, **212**, 749 (*rev*)
Encyclopaedia of Polymer Science and Engineering, 1985, **3**, 430 (*rev*)

Chitin Nat. Technol. Proc. Int. Conf. Chitin Chitosan, 3rd, 1985, (Eds. Muzzarelli, R.A.A. *et al*), Plenum Press, 1986, (*book*)
Chitin and Chitosan: Biochem. Phys. Props., Applications, (Eds. Skjåk-Braek, G. *et al*), Elsevier, Amsterdam, 1989, (*book*)
Brine, C.J. *et al., Adv. Chitin Chitosan*, Elsevier Applied Science, 1992,
Nishimura, Y. *et al., Hoshasen Kagaku (Tokyo)*, 1992, **35**, 13 (*rev*)
Perfect, J.R. *et al., Clin. Dermatol.*, 1993, **7**, 365 (*pharmacol*)
Tanioka, S.-I. *et al., Front. Biomed. Biotechnol.*, 1993, **1**, 153 (*rev, use*)
Winterowd, J.G. *et al., Food Sci. Technol.*, 1995, **67**, 441 (*rev, use, activity*)
Chang, K.L.B. *et al., Carbohydr. Res.*, 1997, **303**, 327-332 (*synth, Chitosan*)
Muzzarelli, R. *et al., Carbohydrates in Europe*, 1997, **19**, 10-17 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CDM750

Chitin synthase C-290

*E.C. 2.4.1.16. UDP-*N*-acetyl-D-glucosamine:chitin 4β-*N*-acetylglucosaminyltransferase*
[9030-18-6]
Hexosyltransferase enzyme. Present in yeast, fungi, arthropods, nematodes and insects. Catalyses the transfer of *N*-acetyl-D-glucosamine from UDP-*N*-acetyl-D-glucosamine to chitin thus causing elongation of the chitin chain.

Glaser, L. *et al., J. Biol. Chem.*, 1957, **228**, 729-742 (*Neurospora crassa*)
Carib, E. *et al., Methods Enzymol.*, 1972, **28**, 572-580 (*Saccharomyces cerevisiae*)
Kang, M.S. *et al., J. Biol. Chem.*, 1984, **259**, 14966-14972 (*Saccharomyces cerevisiae*)
Carib, E. *et al., Adv. Enzymol. Relat. Areas Mol. Biol.*, 1987, **59**, 59-101 (*rev*)
Marchida, S. *et al., J. Biol. Chem.*, 1993, **268**, 1702-1707 (*Absidia glauca*)
Ruiz-Herrera, J. *et al., FEMS Yeast Res.*, 2002, **1**, 247-256 (*rev, yeasts, fungi*)
Merzendorffer, H. *et al., J. Exp. Biol.*, 2003, **206**, 4393-4312 (*rev, insects*)

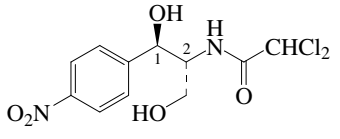
Chitovibrin C-291

Protein. Secreted by the marine bacterium *Vibrio parahemolyticus*. Chitin-binding lectin.

Gildemeister, O.S. *et al., Glycoconjugate J.*, 1994, **11**, 518-526 (*isol*)

Chloramphenicol, BAN, INN, JAN, USAN C-292

*2,2-Dichloro-*N*-[2-hydroxy-1-(hydroxymethyl)-2-(4-nitrophenyl)ethyl]acetamide, 9CI. 2-Dichloroacetamido-1-*p*-nitrophenyl-1,3-propanediol.* N*-(1,1′-Dihydroxy-1-*p*-nitrophenylisopropyl)dichloroacetamide. Alficetyn. Chemicetin. Chlorcetin. Chlorocid. Chloramphenicol C. Chloromycetin. Chloronitrin. Chloroptic. Detreomycin. Enteromycetin. Flamycin. Gloveticol. Halcetin. Kemicetine. Levomycetin. Normimycin V. Ophthochlor. Paraxin. Sintomicetin. Synthomycin. Umimycin. I 337A. NCI C55709. NSC 3069. Antibiotic I 337A. Antibiotic NCI C55709*



(1*R*,2*R*)-*form*

$C_{11}H_{12}Cl_2N_2O_5$ 323.132
Log P 0.69 (calc). λ_{max} 273 (ϵ 9630) (EtOH) (Derep).

(1*R*,2*R*)-*form*
(+)-threo-*form*
[56-75-7]
Isol. from *Streptomyces venezuelae* (Isp5230, Atcc10712), *Streptomyces phaeochromogenes-chloromyceticus*, *Streptomyces omiyaensis*, *Streptosporangium* Sp. , *Corynebacterium* Sp. , *Nocardia* Sp. *Kitasatoa kanaensis* (I377), *Arthrobacter* Sp., *Streptomyces sphaeroides* (Nrrl15600), *Micromonospora carbonacea-africana*, *Streptomyces purpureus combacillus* and various other bacteria. Antibacterial and antirickettsial antibiotic, now used mainly for ophthalmic and veterinary purposes and for life-threatening acute bacterial infections, e.g. meningitis. Smooth muscle relaxant. Pale yellow needles (H_2O or 1,2-dichloroethane). Sol. EtOH, EtOAc, Me_2CO, MeOH, H_2O, Et_2O; insol. C_6H_6, petrol.
Mp 150.5-151.5°. $[\alpha]_D^{25}$ +18.6 (c, 4.86 in EtOH). $[\alpha]_D^{25}$ -25.4 (c, 0.57 in EtOAc). Sublimes in high vacuum. Sign of optical rotation is solvent dependent. λ_{max} 278 (E1%/1cm 298) (H_2O) (Berdy). λ_{max} 278 (E1%/1cm 350) (EtOH) (Berdy). λ_{max} 279 (NaOH) (Berdy).
▶ Haemopoietic and other adverse effects reported when used therapeutically. Probable human carcinogen. Exp. reprod. and teratogenic effects; LD_{50} (mus, ivn) 245 mg/kg , LD_{50} (mus, ipr) 1320 mg/kg , LD_{50} (mus, orl) 2640 mg/kg. AB6825000

Compd. with calcium pantothenate (4:1): ***Chloramphenicol pantothenate****. Pantofenicol. Pantophenicol*
[31342-36-6]
$C_{20}H_{27}Cl_2N_3O_9$ 524.353
Antibacterial agent. Hygroscopic cryst. Log P 1.15 (calc). Sinters at 93°.

3-Ac: ***3-O-Acetylchloramphenicol***
$C_{13}H_{14}Cl_2N_2O_6$ 365.169
Prod. by *Streptomyces venezuelae*.

*3-*O*-Hexadecanoyl:* ***Chloramphenicol palmitate, USAN****. Detreopal*
[530-43-8]
$C_{27}H_{42}Cl_2N_2O_6$ 561.544
Used to circumvent bitter taste of Chloramphenicol. Cryst. (C_6H_6). Mp 90°. $[\alpha]_D^{26}$ +24.6 (c, 5 in EtOH). Log P 8.86 (uncertain value) (calc).
▶ LD_{50} (mus, orl) 2640 mg/kg. Exp. reprod. and teratogenic effects. RT4735000

*3-*O*-(3-Carboxypropanoyl): Kemicetine succinate. Protophenicol.* ***Chloramphenicol succinate***
[3544-94-3]
$C_{15}H_{16}Cl_2N_2O_8$ 423.205
Antibacterial agent. Chloramphenicol prodrug. Cryst. (C_6H_6); hygroscopic white or yellowish-white powder, as Na salt. Sol. H_2O (0.35 g per 100 cm^3 at 27°). Mp 126-128°. $[\alpha]_D^{25}$ +12.8 (c, 5.0 in EtOH). Normally used as Na salt. λ_{max} 276 (H_2O).

*3-*O*-(Carboxypropanoyl), Na salt: Globenicol. Chlorocid S*
[982-57-0] Sol. H_2O.

*3-*O*-(Carboxypropanoyl), arginine salt: Chloramphenicol arginine succinate. Paraxin succinate A*
[34327-18-9]
$C_{21}H_{30}Cl_2N_6O_{10}$ 597.408
Mp 134-135° dec.

Dibromo analogue: See Bromamphenicol in *The Combined Chemical Dictionary.*

(1*S*,2*R*)-*form*
(+)-erythro-*form*
[7384-89-6]
Mp 179-180°. $[\alpha]_D^{20}$ +13.9 (EtOH).

(1*S*,2*S*)-*form*
(-)-threo-*form*
[134-90-7]
Mp 151.5-152.5°. $[\alpha]_D^{20}$ -20 (EtOH).

(1*RS*,2*RS*)-*form*
(±)-threo-*form*
[2787-09-9]
Cryst. (EtOH). Mp 141-142°.

(1*RS*,2*SR*)-*form*
(±)-erythro-*form*
[3419-87-2]
Mp 173-174°.

[7387-98-6, 50762-99-7, 140694-65-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 362D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1380A (*nmr*)
Bartz, Q.R. *et al., J. Biol. Chem.*, 1948, **172**, 445-450 (*Chloromycetin, isol*)
Long, L.M. *et al., J.A.C.S.*, 1949, **71**, 2473-2475 (*synth*)
U.S. Pat., 1950, (*Rhone-Poulenc*)2 586 661; *CA*, **46**, 9126 (*Kemicetine*)
U.K. Pat., 1953, (*Parke-Davis*)687 749; *CA*, **48**, 2102 (*Kemicetine*)
Honjo, M. *et al., Yakugaku Zasshi*, 1953, **73**, 368-371 (*abs config*)
Cerriotti, G. *et al., Farmaco*, 1954, **9**, 21; *CA*, **48**, 6571h (*3-carboxypropanoyl*)
Edgerton, W.H. *et al., J.A.C.S.*, 1955, **77**, 27-29 (*palmitate*)
U.S. Pat., 1958, 2 852 430; *CA*, **53**, 1651 (*Kemicetine*)
U.S. Pat., 1963, 3 078 300; *CA*, **59**, 3834 (*pantothenate*)

East Ger. Pat., 1964, 42 166; *CA*, **64**, 17483d (*Kemicetine*)
Mitscher, L.A. *et al., J. Med. Chem.*, 1973, **16**, 93-97; 98-101 (*cd*)
Weinstein, L. *et al., Pharmacol. Basis Ther., 5th edn.*, 5th Ed., 1975, 1183 (*rev*)
Muro, M.H.G. *et al., Tet. Lett.*, 1975, 2659-2662 (*biosynth*)
IARC Monog., 1976, **10**, 85; *Suppl.* 6, 142; *Suppl.* 7, 145 (*tox, rev*)
Acharya, K. *et al., Acta Cryst. B*, 1979, **35**, 1360-1363 (*struct*)
Pongs, O. *et al., Antibiotics (N.Y.)*, 1979, **5**, 26-42 (*rev*)
Fuglesang, J. *et al., Antibiot. Chemother. (Basel, 1954-70)*, 1982, **31**, 1-21 (*pharmacol, rev*)
Malik, V. *et al., Biotechnol. Ser.*, 1983, **2**, 293-309 (*rev*)
Ambrose, P.J. *et al., Clin. Pharmacokinet.*, 1984, **9**, 222-238 (*succinate, pharmacol, rev*)
Vining, L.C. *et al., Drugs Pharm. Sci.*, 1984, **22**, 387-411 (*rev*)
Al-Badr, A.A. *et al., Anal. Profiles Drug Subst.*, 1986, **15**, 701-760 (*rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 1901 (*synonyms*)
Yunis, A.A. *et al., Annu. Rev. Pharmacol. Toxicol.*, 988, **28**, 83 (*tox, rev*)
Gal, J. *et al., J. Pharm. Sci.*, 1988, **77**, 1062-1065 (*hplc, resoln*)
Hazra, B.G. *et al., Synth. Commun.*, 1989, **19**, 1763-1770 (*synth*)
Chenevert, R. *et al., Synthesis*, 1989, 444-446 (*synth, pmr*)
Ottolina, G. *et al., J.O.C.*, 1990, **55**, 2366-2369 (*3-carboxypropanoyl, synth, pmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **2**, 961 (*rev*)
Rao, A.V.R. *et al., Chem. Comm.*, 1992, 859-860 (*synth*)
Lou, B. *et al., Chem. Ind. (London)*, 1993, 249-250 (*synth*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 203
Hazra, B.G. *et al., Synth. Commun.*, 1997, **27**, 1857-1864 (*synth*)
Corey, E.J. *et al., Tet. Lett.*, 2000, **41**, 2765-2768 (*synth*)
Merck Index, 13th edn., 2001, No. 2087 (*props, bibl*)
Loncaric, C. *et al., Org. Lett.*, 2001, **3**, 3675-3678 (*synth*)
Gross, F. *et al., Bioorg. Med. Chem. Lett.*, 2002, **12**, 283-286 (*3-Acetylchloramphenicol*)
Bhaskar, G. *et al., Tetrahedron: Asymmetry*, 2004, **15**, 1279-1283 (*2R,3R-form, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CDP250; CDP700

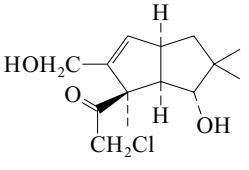
Chlorellin C-293

Struct. unknown. Prod. by *Chlorella vulgaris, Chlorella pyrenoidosa* and *Chlorella ellipsoideus.*

Pratt, R. *et al., Science (Washington, D.C.)*, 1944, **99**, 351 (*isol*)
Suda, S. *et al., CA*, 1958, **52**, 17409; 1961, **55**, 9556 (*isol, props*)

Chloriolin A C-294

[158402-63-2]



$C_{14}H_{21}ClO_3$ 272.771
Metab. of a fungus separated from a *Jaspis* marine sponge. Chemoprotective agent. Cryst. $[\alpha]_D$ -35 (c, 0.01 in $CHCl_3$).

Cheng, Y.-C. *et al., J.O.C.*, 1994, **59**, 6344 (*isol, pmr, cmr, cryst struct*)

Chloroacetic acid, 9CI C-295

Monochloroacetic acid
[79-11-8]
$ClCH_2COOH$
$C_2H_3ClO_2$ 94.497
Prod. by catalytic chlorination of Acetic acid. Constit. of the red alga *Asparagopsis taxiformis.* Used for manuf. of CMC (carboxymethylcellulose), Glycine and Mercaptoacetic acid. Postemergence contact herbicide (usually as Na salt). Cryst. in three forms. V. sol. H_2O; sol. org. solvs.
Mp 61.3° (α-form) Mp 56.2° (β-form) Mp 52.5° (γ-form). Bp 189°. pK_a 2.87 (25°).

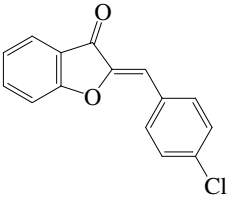
▶ Corrosive skin, eye and mucous membrane irritant. LD_{50} (mus, orl) 165 mg/kg. Toxic in contact with skin. Contamination of 5 to 10% of skin area can be fatal. Fl. p. 150°, autoignition temp. >500°. AF8575000

[3926-62-3, 14526-03-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 508A; 650C; 652A; 713B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 790B; 1007A; 1013A; 1171C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 591B; 700A; 701C (*ir*)
Sadtler Standard C-13 NMR Spectra, 472 (*cmr*)
Pickering, S.U. *et al., J.C.S.*, 1895, **67**, 664 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 86; 129; 130; 1972, **3**, 36 (*tert-butyl ester, anhydride, use*)
Kanters, J.A. *et al., Acta Cryst. B*, 1976, **32**, 3328; 3331 (*cryst struct*)
Szyper, M. *et al., Anal. Chim. Acta*, 1976, **85**, 357 (*uv*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617-620 (*isol*)
Dillon, K.B. *et al., J. Magn. Reson.*, 1980, **39**, 499 (*pmr*)
Ullmann's Encycl. Ind. Chem., VCH, Weinheim, 1985, **A6**, 537 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 165 (*rev*)
Merck Index, 13th edn., 2001, No. 2129 (*bibl, props*)
Hiegel, G.A. *et al., Synth. Commun.*, 2004, **34**, 889-893 (*synth*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 281
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BEE500; CEA000; SFU500; MIF775

4′-Chloroaurone C-296

*2-[(4-Chlorophenyl)methylene]-3(2*H*)-benzofuranone. 2-(4-Chlorobenzylidene)-3(2*H*)-benzofuranone*



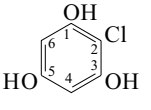
$C_{15}H_9ClO_2$ 256.688

(Z)-form
Isol. from the brown alga *Spatoglossum variabile.*
Solid.
Mp 206°. λ_{max} 204 (log ε 4.9) ($CHCl_3$).

Atta-ur-Rahman, *et al., Chem. Pharm. Bull.*, 2001, **49**, 105-107

2-Chloro-1,3,5-benzenetriol C-297

Chlorophloroglucinol
[84743-76-0]



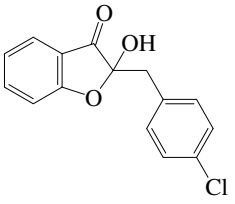
$C_6H_5ClO_3$ 160.556
Constit. of *Rhabdonia verticillata* and from brown algae *Eisenia arborea* (as mixt. with 2-Iodo-1,3,5-benzenetriol, I-80) and *Carpophyllum angustifolium*. Cryst. (EtOAc/petrol).
Mp 219-220°.

Tri-Me ether: 2-Chloro-1,3,5-trimethoxybenzene
[67827-56-9]
$C_9H_{11}ClO_3$ 202.637
Plates. Mp 93° (72-74°).

Lloyd, G. *et al., J.C.S.*, 1956, 3209-3212 (*tri-Me ether*)
Blackman, A.J. *et al., Phytochemistry*, 1982, **21**, 2141 (*isol*)
Elix, J.A. *et al., Aust. J. Chem.*, 1992, **45**, 845-855 (*synth*)
Leonard, K.A. *et al., Organometallics*, 1996, **15**, 4285-4292 (*tri-Me ether*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

2-(4-Chlorobenzyl)-2-hydroxy-3(2*H*)-benzofuranone C-298

4′-Chloro-2-hydroxybenzylcoumaranone



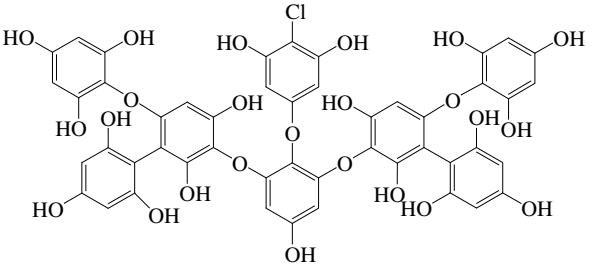
$C_{15}H_{11}ClO_3$ 274.703

(±)-*form*

Isol. from the brown alga *Spatoglossum variabile*.
Solid.
Mp 225°. λ_{max} 202 (log ϵ 5.02) ($CHCl_3$).

Atta-ur-Rahman, *et al., Chem. Pharm. Bull.*, 2001, **49**, 105-107

Chlorobisfucopentaphlorethol B C-299



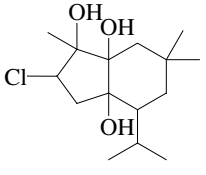
$C_{48}H_{33}ClO_{24}$ 1029.227

Different skeleton from Bisfucopentaphlorethol B, B-149. Isol. from brown alga *Sargassum spinuligerum*.

Glombitza, K.W. *et al., Phytochemistry*, 1997, **46**, 1417-1422

8-Chloro-1,6,9-brasilanetriol C-300

[778637-06-2]



$C_{15}H_{27}ClO_3$ 290.829

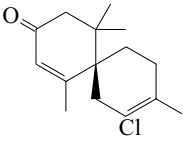
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D^{20}$ -2.21 (c, 0.08 in $CHCl_3$).

Aydoğmus, Z. *et al., Nat. Prod. Res.*, 2004, **18**, 43-49 (*isol, pmr, cmr*)

4-Chloro-3,7-chamigradien-9-one C-301

Laurencenone B

[108925-15-1]



$C_{15}H_{21}ClO$ 252.783

Metab. of *Laurencia obtusa*. Oil.

Dechloro: 3,7-Chamigradien-9-one. 1,5,5,9-Tetramethylspiro[5.5]undeca-1,8-dien-3-one, 9CI. ***Laurencenone C***. ent-*9-Oxo-α-chamigrene*

[61661-47-0]

$C_{15}H_{22}O$ 218.338

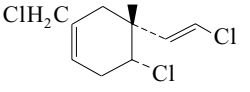
Metab. of *Laurencia obtusa* and *Marchantia polymorpha*. Oil. $[\alpha]_D$ -43 (c, 1 in $CHCl_3$).

[61661-46-9, 116907-14-3]

Gonzalez, A.G. *et al., Tet. Lett.*, 1976, 3051
Kennedy, D.J. *et al., Phytochemistry*, 1988, **27**, 1761
Asakawa, Y. *et al., Phytochemistry*, 1990, **29**, 1577
Srikrishna, A. *et al., Tet. Lett.*, 2006, **47**, 2103-2106 (*synth*)

4-Chloro-5-(2-chloroethenyl)-1-chloromethyl-5-methylcyclohexane C-302

[73191-61-4]



$C_{10}H_{13}Cl_3$ 239.571

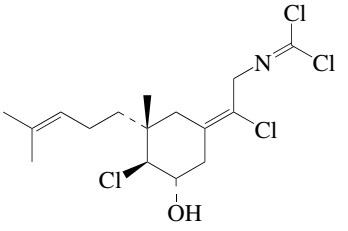
Constit. of *Plocamium cartilagineum*. Antifungal agent. Oil. $[\alpha]_D$ -110 (c, 0.91 in $CHCl_3$).

Stierle, D.B. *et al., Tetrahedron*, 1979, **35**, 1261 (*isol, abs config*)

[2-Chloro-2-[4-chloro-5-hydroxy-3-methyl-3-(4-methyl-3-pentenyl)cyclohexylidene]ethyl]carbonimidic dichloride, 9CI C-303

6,14-Dichloro-5-hydroxy-3(14),9-axinyssadien-15-yl carbonimidic dichloride

[64789-88-4]



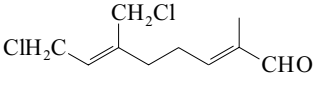
$C_{16}H_{23}Cl_4NO$ 387.175

Isol. from the sponge *Pseudaxinyssa pitys*. Oil. $[\alpha]_D^{20}$ +36 (c, 1.1 in $CHCl_3$).

Wratten, S.J. *et al., J.A.C.S.*, 1977, **99**, 7367-7368 (*isol, uv, pmr, cmr*)

8-Chloro-6-chloromethyl-2-methyl-2,6-octadienal, 9CI C-304

[136980-51-3]

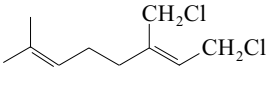


$C_{10}H_{14}Cl_2O$ 221.125

Constit. of *Portieria hornemannii*. Oil.

Wright, A.D. *et al., Tetrahedron*, 1991, **47**, 5717 (*isol, pmr, cmr*)

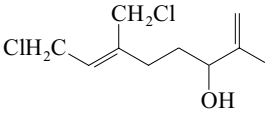
1-Chloro-3-chloromethyl-7-methyl-2,6-octadiene, 9CI C-305



$C_{10}H_{16}Cl_2$ 207.142

(*Z*)-*form* [112642-61-2]
Constit. of *Chondrococcus hornemannii*.
Oil.
Coll, J.C. *et al., Aust. J. Chem.*, 1987, **40**, 1893

8-Chloro-6-chloromethyl-2-methyl-1,6-octadien-3-ol C-306

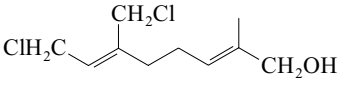


$C_{10}H_{16}Cl_2O$ 223.141

(*Z*)-*form* [125538-02-5]
Constit. of *Chondrococcus hornemannii*.
Oil. $[\alpha]_D$ -12.3 (c, 0.002 in $CHCl_3$).

3-Me ether: 8-Chloro-6-chloromethyl-3-methoxy-2-methyl-1,6-octadiene
[125538-01-4]
$C_{11}H_{18}Cl_2O$ 237.168
Constit. of *Chondrococcus hornemannii*. Oil. $[\alpha]_D$ -16.5 (c, 0.017 in $CHCl_3$).
Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1983 (*isol, pmr, cmr*)

8-Chloro-6-chloromethyl-2-methyl-2,6-octadien-1-ol C-307

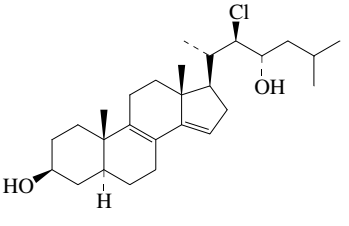


$C_{10}H_{16}Cl_2O$ 223.141

(2*E*,6*Z*)-*form* [125538-04-7]
Constit. of *Chondrococcus hornemannii*.
Oil.

Me ether: 1-Chloro-3-chloromethyl-8-methoxy-7-methyl-2,6-octadiene
[125538-03-6]
$C_{11}H_{18}Cl_2O$ 237.168
Constit. of *Chondrococcus hornemannii*. Oil. λ_{max} 217 (EtOH) (Berdy).
Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1983 (*isol, pmr, cmr*)

22-Chlorocholesta-8,14-diene-3,23-diol, 9CI C-308



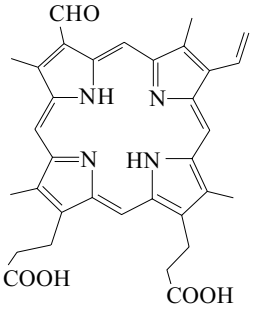
(3β,5α,22*R*,23*S*)-*form*

$C_{27}H_{43}ClO_2$ 435.088

(3β,5α,22*R*,23*S*)-*form* [71268-93-4]
Constit. of the starfish *Echinaster sepositus*.
Oil.
Minale, L. *et al., Tet. Lett.*, 1979, 645 (*isol, cmr*)

Chlorocruoroporphyrin C-309

Spirographis porphyrin. Photoprotoporphyrin
[24869-67-8]



$C_{33}H_{32}N_4O_5$ 564.64
Prosthetic group of the oxygen-carrying pigment of certain polychaete worms, e.g., *Spirographis spallanzanii*. Violet cryst. (Et_2O).

Di-Me ester:
$C_{35}H_{36}N_4O_5$ 592.693
Violet cryst. ($CHCl_3$/MeOH). Mp 285°. Isochlorocruoroporphyrin di-Me ester (the isomer with the formyl and vinyl groups transposed) has also been synthesised. λ_{max} 421; 520; 560; 585; 644 (No solvent reported).

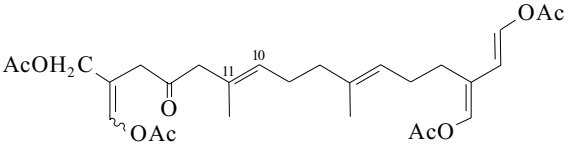
*Fe complex: **Chlorocruorohaem**. Spirographishaem*
$C_{33}H_{30}FeN_4O_5$ 618.471
Found in polychaete worms. Oxygen transport pigment. Analogous to Haem.

[34268-29-6]

Inhoffen, H.H. *et al., Tet. Lett.*, 1966, 3779 (*synth*)
Jackson, A.H. *et al., Chem. Comm.*, 1967, 1027; *J.C.S. Perkin 1*, 1974, 480 (*struct, synth, pmr, ms*)
Bamfield, P. *et al., J.C.S.(C)*, 1968, 1259 (*synth*)
Clezy, P.S. *et al., Aust. J. Chem.*, 1975, **28**, 2703 (*synth*)
Kenner, G.W. *et al., Tetrahedron*, 1976, **32**, 2753 (*synth*)

Chlorodesmin C-310

1,16,17,20-Tetraacetoxy-1,3(20),6,10,15-phytapentaen-13-one
[72877-82-8]

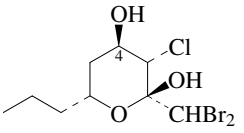


$C_{28}H_{38}O_9$ 518.603
Constit. of *Chlorodesmis fastigiata*, *Cyerce nigricans* and mollusc *Elysia* sp. Ichthyotoxic. Oil.

*10,11-Dihydro: 1,16,17,20-Tetraacetoxy-1,3(20),6,15-phytatetraen-13-one. **10,11-Dihydrochlorodesmin***
$C_{28}H_{40}O_9$ 520.619
Constit. of *Chlorodesmis fastigiata*. Oil.
Wells, R.J. *et al., Experientia*, 1979, **35**, 1544
Paul, V.J. *et al., Bioorganic Mar. Chem.*, 1987, **1**, 1

3-Chloro-2-(dibromomethyl)tetrahydro-6-propyl-2*H*-pyran-2,4-diol C-311

3-Chloro-2-(dibromomethyl)-2,4-dihydroxy-6-propyltetrahydropyran. 1,1-Dibromo-3-chloro-2,6-epoxy-2,4-nonanediol



$C_9H_{15}Br_2ClO_3$ 366.476

(2*R,3*S**,4*R**,6*R**)-*form***

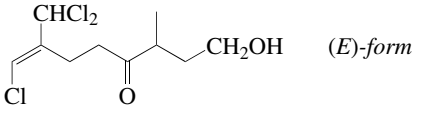
Pyranosylmagellanicus A

Constit. of the red alga *Ptilonia magellanica*.
Oil. $[\alpha]_D^{25}$ +2 (c, 1.5 in CH_2Cl_2).

4-Ac: ***Pyranosylmagellanicus B***

$C_{11}H_{17}Br_2ClO_4$ 408.514
Constit. of *Ptilonia magellanica*. Oil. $[\alpha]_D^{25}$ +2 (c, 2 in CH_2Cl_2).
Lorenzo, M. *et al., Tetrahedron*, 2005, **61**, 9550-9554 (*isol, pmr, cmr, ms*)

8-Chloro-7-(dichloromethyl)-1-hydroxy-3-methyl-7-octen-4-one C-312



(*E*)-*form*

$C_{10}H_{15}Cl_3O_2$ 273.585

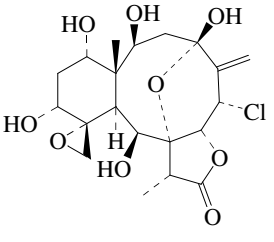
(*E*)-*form*

Ac: [188000-14-8]
$C_{12}H_{17}Cl_3O_3$ 315.623
Constit. of *Aplysia punctata*. Oil. $[\alpha]_D^{25}$ -3.7 (c, 0.19 in $CHCl_3$).

(*Z*)-*form*

Ac: [188000-15-9]
Constit. of *Aplysia punctata*.
Oil. $[\alpha]_D^{25}$ -5 (c, 1.3 in $CHCl_3$).
Ortega, M.J. *et al., J. Nat. Prod.*, 1997, **60**, 482-484 (*isol, pmr, cmr*)

6-Chloro-4,8:11,20-diepoxy-2,4,9,12,14-pentahydroxy-5(16)-briaren-18,7-olide C-313



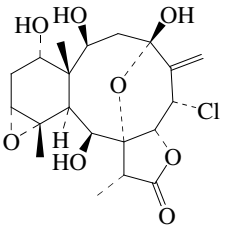
$C_{20}H_{27}ClO_9$ 446.881

(2β,4β,6α,7α,8α,9β,11α,12α,14α,17α)-*form*

2,9,12,14-Tetra-Ac: ***Juncin P***

[799804-60-7]
$C_{28}H_{35}ClO_{13}$ 615.029
Constit. of *Junceella juncea*. Powder. $[\alpha]_D$ -6.8 (c, 0.24 in $CHCl_3$).
Qi, S.-H. *et al., J. Nat. Prod.*, 2004, **67**, 1907-1910 (*isol, pmr, cmr*)

6-Chloro-4,8:11,12-diepoxy-2,4,9,14-tetrahydroxy-5(16)-briaren-18,7-olide C-314



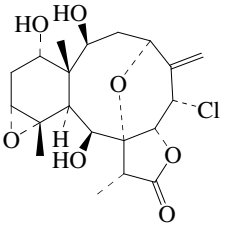
$C_{20}H_{27}ClO_8$ 430.881

(2β,4β*OH*,6α,7α,8α,9β,11α,12α,14α)-*form*

2,14-Di-Ac: ***4-Hydroxymilolide C***

[352273-97-3]
$C_{24}H_{31}ClO_{10}$ 514.956
Constit. of *Briareum stechei.*
$[\alpha]_D^{23}$ +8.4 (c, 0.47 in CH_2Cl_2).
Kwak, J.H. *et al., J. Nat. Prod.*, 2001, **64**, 754-760 (*isol, pmr, cmr*)

6-Chloro-4,8:11,12-diepoxy-2,9,14-trihydroxy-5(16)-briaren-18,7-olide C-315



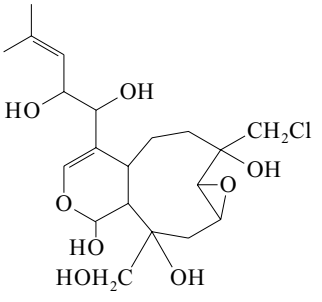
$C_{20}H_{27}ClO_7$ 414.882

(2β,4α,6α,7α,8α,9β,11α,12α,14α)-*form*

2,14-Di-Ac: ***Milolide C***

[352335-85-4]
$C_{24}H_{31}ClO_9$ 498.956
Constit. of *Briareum stechei.*
$[\alpha]_D^{23}$ -9.8 (c, 0.23 in MeOH).
Kwak, J.H. *et al., J. Nat. Prod.*, 2001, **64**, 754-760 (*isol, pmr, cmr*)

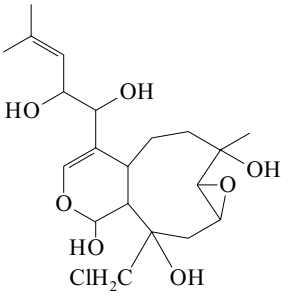
20-Chloro-7,8:17,18-diepoxy-10(17),13-xenicadiene-1,6,11,12,18,19-hexol C-316



$C_{20}H_{31}ClO_8$ 434.913

11,12,18,19-Tetra-Ac: ***19-Acetoxy-18-chloro-7,11-havannadiol***
$C_{28}H_{39}ClO_{12}$ 603.062
Constit. of *Xenia membranacea*. Amorph. $[\alpha]_D$ -17 (c, 0.3 in $CHCl_3$).
Almourabit, A. *et al., J. Nat. Prod.*, 1990, **53**, 894 (*isol, pmr, cmr*)

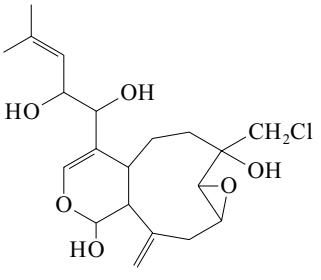
19-Chloro-7,8:17,18-diepoxy-10(17),13-xenicadiene-1,6,11,12,18-pentol C-317



$C_{20}H_{31}ClO_7$ 418.913

11,12,18-Tri-Ac: ***19-Chloro-7,11-havannadiol***
$C_{26}H_{37}ClO_{10}$ 545.025
Constit. of *Xenia membranacea*. Amorph. $[\alpha]_D$ -7 (c, 0.66 in $CHCl_3$).
Almourabit, A. *et al., J. Nat. Prod.*, 1990, **53**, 894 (*isol, pmr, cmr*)

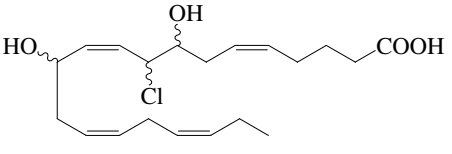
20-Chloro-7,8:17,19-diepoxy-1(19),10(17),13-xenicatriene-6,11,12,18-tetrol C-318



$C_{20}H_{29}ClO_6$ 400.898

11,12,18-Tri-Ac: ***11,19-Desoxy-7,18-havannachlorohydrin***
$C_{26}H_{35}ClO_9$ 527.01
Constit. of *Xenia membranacea*. Amorph. $[\alpha]_D$ +86 (c, 0.8 in $CHCl_3$).
Almourabit, A. *et al., J. Nat. Prod.*, 1990, **53**, 894 (*isol, pmr, cmr*)

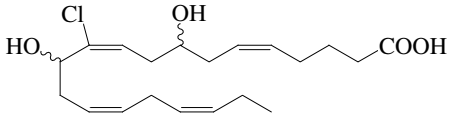
9-Chloro-8,12-dihydroxy-5,10,14,17-eicosatetraenoic acid C-319
[131917-10-7]



$C_{20}H_{31}ClO_4$ 370.915

(5Z,8ξ,9ξ,10Z,12ξ,14Z,17Z)-form
Isol. from *Balanus balanoides.*
Song, W.C. *et al., Biochim. Biophys. Acta*, 1990, **1047**, 239-246 (*isol*)

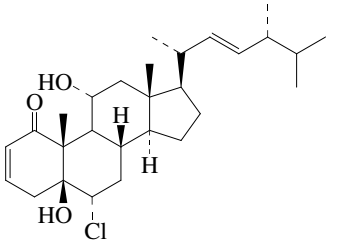
11-Chloro-8,12-dihydroxy-5,10,14,17-eicosatetraenoic acid C-320
[131917-11-8]



$C_{20}H_{31}ClO_4$ 370.915

(5Z,8ξ,9E,11ξ,14Z,17Z)-form
Isol. from *Balanus balanoides.*
Song, W.C. *et al., Biochim. Biophys. Acta*, 1990, **1047**, 239-246 (*isol*)

6-Chloro-5,11-dihydroxyergosta-2,22-dien-1-one C-321

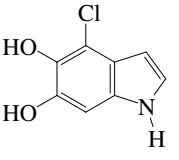


$C_{28}H_{43}ClO_3$ 463.099

(5β,6α,11α,22E,24R)-form
Yonarasterol G
[326794-16-5]
Constit. of *Clavularia viridis.*
Amorph. solid. $[\alpha]_D^{25}$ -33.6 (c, 0.14 in $CHCl_3$). λ_{max} 223 (log ϵ 3.83) (EtOH).

22,23-Dihydro: 6-Chloro-5,11-dihydroxyergost-2-en-1-one. ***Yonarasterol H***
[326794-17-6]
$C_{28}H_{45}ClO_3$ 465.114
Constit. of *Clavularia viridis.* Amorph. solid. $[\alpha]_D^{25}$ -16.3 (c, 0.19 in $CHCl_3$). λ_{max} 221 (log ϵ 3.79) (EtOH).
Iwashima, M. *et al., Steroids*, 2001, **66**, 25-32 (*isol, pmr, cmr*)

4-Chloro-5,6-dihydroxy-1*H*-indole C-322
*4-Chloro-1*H*-indole-5,6-diol*

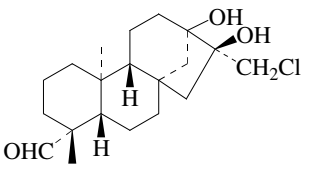


$C_8H_6ClNO_2$ 183.594

N-*Sulfonic acid: 4-Chloro-5,6-dihydroxy-1*H*-indole-1-sulfonic acid.* ***Ancorinolate C***
[473740-09-9]
$C_8H_6ClNO_5S$ 263.658
Alkaloid from the sponge *Ancorina* sp. Powder (as Na salt). λ_{max} 216 (log ϵ 4.14); 272 (log ϵ 3.78); 302 (log ϵ 3.64) (MeOH) (Na salt).

N,O^6-*Disulfo:* ***Ancorinolate A***
[473740-08-8]
$C_8H_6ClNO_8S_2$ 343.722
Alkaloid from the sponge *Ancorina* sp. Powder (as di-Na salt). λ_{max} 220 (log ϵ 4.31); 271 (log ϵ 3.86); 300 (log ϵ 3.56) (MeOH) (di-Na salt).
Meragelman, K.M. *et al., J.O.C.*, 2002, **67**, 6671-6677 (*Ancorinolates*)

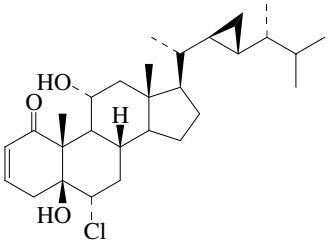
17-Chloro-13,16-dihydroxy-19-kauranal C-323



$C_{20}H_{31}ClO_3$ 354.916

(ent-16α OH)-form [765316-49-2]
Constit. of *Bruguiera gymnorrhiza*.
Amorph. solid. $[\alpha]_D^{20}$ -45 (c, 0.3 in $CHCl_3$).
Han, L. *et al., J. Nat. Prod.*, 2004, **67**, 1620-1623 (*isol, pmr, cmr*)

6-Chloro-5,11-dihydroxy-23-norgorgost-2-en-1-one C-324

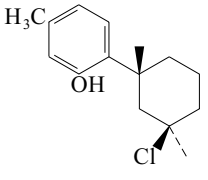


$C_{29}H_{45}ClO_3$ 477.125

(5β,6α,11α)-*form*
Yonarasterol I
[326794-18-7]
Constit. of *Clavularia viridis.*
Amorph. solid. $[\alpha]_D^{25}$ -14.5 (c, 0.11 in $CHCl_3$). λ_{max} 222 (log ϵ 3.86) (EtOH).
Iwashima, M. *et al., Steroids*, 2001, **66**, 25-32 (*isol, pmr, cmr*)

2-(3-Chloro-1,3-dimethylcyclohexyl)-5-methylphenol C-325

1-Chloro-3-(2-hydroxy-4-methylphenyl)-1,3-dimethylcyclohexane
[145382-77-0]

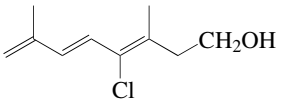


$C_{15}H_{21}ClO$ 252.783
Constit. of *Laurencia majuscula*. Yellow oil. $[\alpha]_D$ +14 (c, 1 in $CHCl_3$).
de Nys, R. *et al., Aust. J. Chem.*, 1992, **45**, 1611 (*isol, pmr, cmr*)

2-(4-Chloro-1,3-dimethylcyclohexyl)-5-methylphenol C-326

4-Chloro-1-(2-hydroxy-4-methylphenyl)-1,3-dimethylcyclohexane
[145382-78-1]
$C_{15}H_{21}ClO$ 252.783
Constit. of *Laurencia majuscula*. Brown oil. $[\alpha]_D$ +47 (c, 0.1 in $CHCl_3$).
de Nys, R. *et al., Aust. J. Chem.*, 1992, **45**, 1611 (*isol, pmr, cmr*)

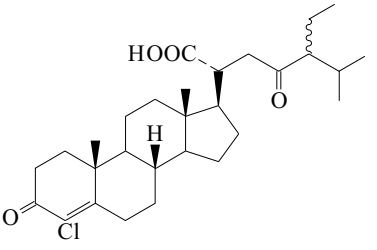
4-Chloro-3,7-dimethyl-3,5,7-octatrien-1-ol C-327



$C_{10}H_{15}ClO$ 186.681

(3*Z*,5*E*)-*form*
Ac: [187960-09-4]
$C_{12}H_{17}ClO_2$ 228.718
Constit. of *Aplysia punctata*. Oil.
Ortega, M.J. *et al., J. Nat. Prod.*, 1997, **60**, 482-484 (*isol, pmr, cmr*)

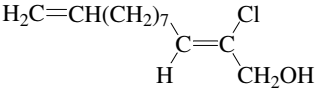
4-Chloro-3,23-dioxostigmast-4-en-21-oic acid C-328



$C_{29}H_{43}ClO_4$ 491.109

24ξ-*form*
Kiheisterone E
[149260-75-3]
Constit. of a *Strongylacidon* sp. λ_{max} 224 (ϵ 10000); 257 (ϵ 7940) (MeOH) (Derep). λ_{max} 258 (ϵ 10000) (MeOH) (Berdy).
Carney, J.R. *et al., J.O.C.*, 1993, **58**, 3460-3462 (*isol, pmr, cmr*)

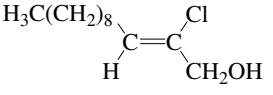
2-Chloro-2,11-dodecadien-1-ol C-329



$C_{12}H_{21}ClO$ 216.75

(*Z*)-*form*
Isol. from the red alga *Gracilaria verrucosa*.
Oil.
Shoeb, M. *et al., J. Nat. Prod.*, 2003, **66**, 1509-1511 (*isol, pmr, cmr*)

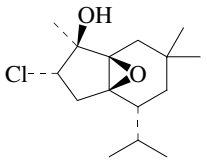
2-Chloro-2-dodecen-1-ol C-330



$C_{12}H_{23}ClO$ 218.766

(*Z*)-*form*
Isol. from the red alga *Gracilaria verrucosa*.
Oil.
Shoeb, M. *et al., J. Nat. Prod.*, 2003, **66**, 1509-1511 (*isol, pmr, cmr*)

8-Chloro-1,6-epoxy-9-brasilanol C-331



(1β,6β,8α,9β)-*form*

$C_{15}H_{25}ClO_2$ 272.814

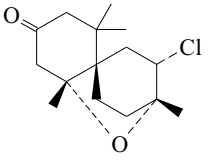
(1β,6β,8α,9β)-*form* [473925-58-5]
Constit. of *Laurencia obtusa*.
Oil. $[\alpha]_D$ +44.11 (c, 0.17 in $CHCl_3$). λ_{max} 203 (log ϵ 2.61) (hexane).

8-Dechloro, 8α-bromo: 8-Bromo-1,6-epoxy-9-brasilanol
[473925-60-9]
$C_{15}H_{25}BrO_2$ 317.265
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ +12 (c, 0.15 in $CHCl_3$). λ_{max} 207 (log ϵ 2.72) (hexane).

(1β,6β,8β,9α)-*form* [473925-59-6]
Oil. $[\alpha]_D$ -7.33 (c, 0.15 in $CHCl_3$). λ_{max} 202 (log ϵ 2.72) (hexane).
Iliopoulou, D. *et al., Org. Lett.*, 2002, **4**, 3263-3266 (*isol, pmr, cmr*)

4-Chloro-3,7-epoxy-9-chamigranone C-332

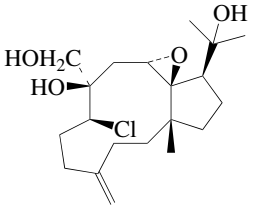
[108906-79-2]



$C_{15}H_{23}ClO_2$ 270.798
Constit. of *Laurencia obtusa*. Oil.

Brennan, M.R. *et al., Phytochemistry*, 1987, **26**, 1053

7-Chloro-10,11-epoxy-4(16)-dolabellene-8,17,18-triol C-333



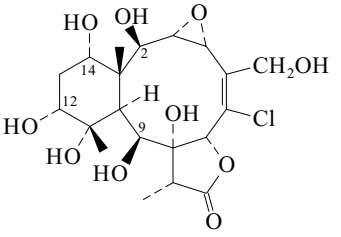
(1*R*,7*S*,8*R*,10*S*,11*S*,12*R*)-*form*

$C_{20}H_{33}ClO_4$ 372.931

(1*R*,7*S*,8*R*,10*S*,11*S*,12*R*)-*form*
Clavutriolin
[111233-44-4]
Isol. from the soft coral *Clavularia* sp.

(1*S*,7*S*,8*S*,10*S*,11*R*,12*S*)-*form*
Clavinflol B
[586387-99-7]
Isol. from *Clavularia inflata*.
Pale yellowish oil. $[\alpha]_D^{25}$ +8.9 (c, 0.36 in CH_2Cl_2).
Xia, Z. *et al., Jiegou Huaxue*, 1986, **5**, 263-267; *CA*, 1987, **107**, 233398d (*Clavutriolin, cryst struct*)
Shen, Y.C. *et al., J. Chin. Chem. Soc. (Taipei)*, 2003, **50**, 471-476 (*Clavinflol B*)

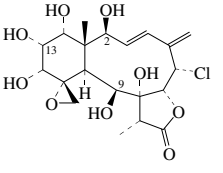
6-Chloro-3,4-epoxy-2,8,9,11,12,14,16-heptahydroxy-5-briaren-18,7-olide C-334



$C_{20}H_{29}ClO_{10}$ 464.896

2,9,12,14-Tetra-Ac: ***Briarein F***
$C_{28}H_{37}ClO_{14}$ 633.045
Constit. of *Briareum asbestinum*. Semi-solid. $[\alpha]_D^{25}$ -26.9 (c, 2 in $CHCl_3$).
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1996, **59**, 15 (*isol, pmr, cmr*)

6-Chloro-11,20-epoxy-2,8,9,12,13,14-hexahydroxy-3,5(16)-briaradien-18,7-olide C-335



(2β,3*E*,6α,7α,8α,9β,11α,12α,13α,14α,17α)-*form*

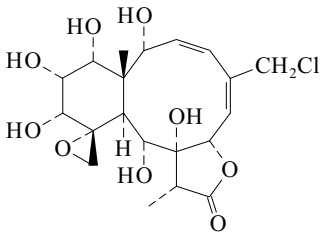
$C_{20}H_{27}ClO_9$ 446.881

(2β,3*E*,6α,7α,8α,9β,11α,12α,13α,14α,17α)-*form*
13-(3-Methylbutanoyl), 2,9,12,14-tetra-Ac: ***Juncin O***
[799804-59-4]
$C_{33}H_{43}ClO_{14}$ 699.147
Constit. of *Junceella junca*. Powder. $[\alpha]_D$ +36 (c, 1 in $CHCl_3$). λ_{max} 220 (MeOH).

(2β,3*Z*,6α,7α,8α,9β,11α,12α,13α,14α,17α)-*form*
2,9,13-Tri-Ac: ***Gemmacolide E***
[134915-02-9]
$C_{26}H_{33}ClO_{12}$ 572.992
Constit. of *Junceella gemmacea*. Oil. $[\alpha]_D$ +56 (c, 0.25 in $CHCl_3$).
2,9,13,14-Tetra-Ac: ***Gemmacolide D***
[134915-01-8]
$C_{28}H_{35}ClO_{13}$ 615.029
Constit. of *Junceella gemmacea*. Immunomodulator. Oil. $[\alpha]_D$ +88.3 (c, 0.66 in $CHCl_3$).
2,9,12,13,14-Penta-Ac: ***Juncin E***
[129602-22-8]
$C_{30}H_{37}ClO_{14}$ 657.067
Metab. of *Junceella juncea*. Insecticide. Oil. $[\alpha]_D^{25}$ -66 (c, 0.02 in $CHCl_3$).

Isaacs, S. *et al., J. Nat. Prod.*, 1990, **53**, 596 (*Juncin E*)
He, H. *et al., Tetrahedron*, 1991, **47**, 3271-3280 (*Gammacolides*)
Hamann, M.T. *et al., Heterocycles*, 1996, **42**, 325 (*Juncin E, cryst struct, abs config*)
Qi, S.H. *et al., J. Nat. Prod.*, 2004, **67**, 1907-1910 (*Juncin O*)

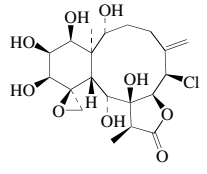
16-Chloro-11,20-epoxy-2,8,9,12,13,14-hexahydroxy-3,5-briaradien-18,7-olide C-336



$C_{20}H_{27}ClO_9$ 446.881

2,9,13,14-Tetra-Ac: ***Nuiinoalide B***
[173867-30-6]
$C_{28}H_{35}ClO_{13}$ 615.029
Constit. of an octocoral. Solid. $[\alpha]_D$ -9 (c, 0.52 in $CHCl_3$).
Hamann, M.T. *et al., Heterocycles*, 1996, **42**, 325 (*isol, pmr, cmr*)

6-Chloro-11,20-epoxy-2,8,9,12,13,14-hexahydroxy-5(16)-briaren-18,7-olide C-337



(1α,2α,6β,7β,8β,9α,10β,11β,13β,14β,17β)-*form*

$C_{20}H_{29}ClO_9$ 448.896

(1α,2α,6β,7β,8β,9α,10β,11β,12β,13β,14β,17β)-*form*

2,9,12,13,14-Penta-Ac: ***(+)-Gemmacolide A***
$C_{30}H_{39}ClO_{14}$ 659.082
Constit. of *Junceella juncea*. Cryst. (hexane/Me_2CO).
Mp 273-275°. $[\alpha]_D^{25}$ +2.4 (c,0.20 in $CHCl_3$).

13-(3-Methylbutanoyl), 2,9,12,14-tetra-Ac: ***(+)-Gemmacolide B***
$C_{33}H_{45}ClO_{14}$ 701.163
Constit. of *Junceella juncea*. Cryst. (hexane/$CHCl_3$).
Mp 298-300°. $[\alpha]_D^{25}$ +5.3 (c, 0.44 in $CHCl_3$). Error in struct. diag. in ref. Not clear whether this and its enantiomer (see below) are 2- or 3-methylbutanoyl.

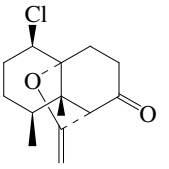
(1β,2β,6α,7α,8α,9β,10α,11α,12α,13α,14α,17α)-*form*

2,9,12,13,14-Penta-Ac: ***Gemmacolide A***
[134887-84-6]
$C_{30}H_{39}ClO_{14}$ 659.082
Constit. of the coelenterate *Junceella gemmacea*. Oil. $[\alpha]_D$ -2 (c, 0.2 in $CHCl_3$).

13-(3-Methylbutanoyl), 2,9,12,14-tetra-Ac: ***Gemmacolide B***
[134887-85-7]
$C_{33}H_{45}ClO_{14}$ 701.163
Constit. of *Junceella gemmacea*. Immunomodulator, shows insecticidal props. Oil. $[\alpha]_D$ -5.5 (c, 0.44 in $CHCl_3$).

12,13-Bis(2-methylbutanoyl), 2,9,14-tri-Ac: ***Juncin L***
[524741-53-5]
$C_{36}H_{51}ClO_{14}$ 743.243
Constit. of *Junceella juncea*. Cryst.
Mp 234-237°. $[\alpha]_D^{25}$ -7.4 (c, 0.5 in $CHCl_3$).
He, H. *et al., Tetrahedron*, 1991, **47**, 3271-3280 (*isol, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., J.C.S. Perkin 1*, 1997, 959-962 (*isol, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 2003, **66**, 507-510 (*Juncin L*)

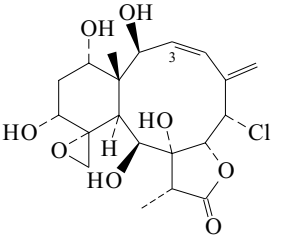
1-Chloro-10,11-epoxy-13-nor-11-nardosinen-7-one C-338



$C_{14}H_{19}ClO_2$ 254.756

(1β,10α)-*form*
Paralemnolin A
[870152-40-2]
Constit. of *Paralemnalia thyrsoides*.
Cryst.
Mp 96-98°. $[\alpha]_D^{25}$ -133 (c, 0.82 in $CHCl_3$).
Huang, H.-C. *et al., Tet. Lett.*, 2005, **46**, 7711-7714 (*Paralemnolin A, cryst struct, abs config*)

6-Chloro-11,20-epoxy-2,8,9,12,14-pentahydroxy-3,5(16)-briaradien-18,7-olide C-339



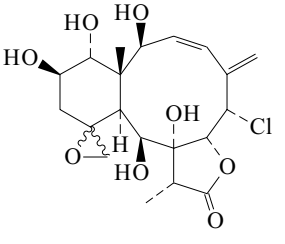
$C_{20}H_{27}ClO_8$ 430.881

2,9,12,14-Tetra-Ac: ***Juncin D***
[129602-21-7]
$C_{28}H_{35}ClO_{12}$ 599.03
Metab. of *Junceella juncea*. Oil. $[\alpha]_D^{25}$ -68 (c, 0.007 in $CHCl_3$).

O-*(3-Methylbutanoyl), tri-Ac:* ***Juncin C***
[129363-04-8]
$C_{31}H_{41}ClO_{12}$ 641.11
Metab. of *Junceella juncea*. Oil. $[\alpha]_D^{25}$ -79 (c, 0.02 in $CHCl_3$). Posn. of *O*-3-methylbutanoyl residue not detd.

3,4-Dihydro, O-*(3-methylbutanoyl), tri-Ac:* ***Juncin F***
[129363-06-0]
$C_{31}H_{43}ClO_{12}$ 643.126
Metab. of *Junceella juncea*. Oil. $[\alpha]_D^{25}$ -7 (c, 0.004 in $CHCl_3$). Posn. of 3-methylbutanoyl residue not detd.
Isaacs, S. *et al., J. Nat. Prod.*, 1990, **53**, 596 (*isol, pmr, cmr*)

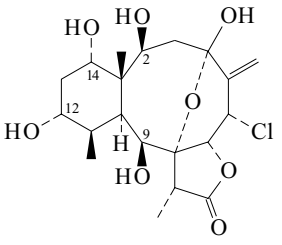
6-Chloro-11,20-epoxy-2,8,9,13,14-pentahydroxy-3,5(16)-briaradien-18,7-olide C-340



$C_{20}H_{27}ClO_8$ 430.881

2,9,13,14-Tetra-Ac: ***Junceellin B***
[111233-45-5]
$C_{28}H_{35}ClO_{12}$ 599.03
Constit. of *Junceella squamata*. Cryst.
Mp 228-230°. $[\alpha]_D^{25}$ -13.48 (c, 0.85 in $CHCl_3$).
Long, K. *et al., CA*, 1987, **107**, 215049m (*isol, pmr, cmr*)

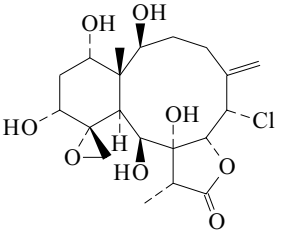
6-Chloro-4,8-epoxy-2,4,9,12,14-pentahydroxy-5(16)-briaren-18,7-olide C-341



$C_{20}H_{29}ClO_8$ 432.897

2,9,12,14-Tetra-Ac: ***Pteroidin***
[90042-99-2]
$C_{28}H_{37}ClO_{12}$ 601.046
Constit. of the sea pen *Pteroeides laboutei*. Cryst.
Mp 308-310°. $[\alpha]_D$ -10 (c, 0.58 in $CHCl_3$). Genus name often spelt Pteroides. λ_{max} 215 (EtOH) (Berdy).
12-Benzoyl, 2,9,14-tri-Ac: [90043-00-8]
$C_{33}H_{39}ClO_{12}$ 663.117
From *Pteroeides laboutei*. Ichthyotoxic. Cryst.
Mp 291-293°. $[\alpha]_D$ -4 (c, 0.54 in $CHCl_3$). λ_{max} 237 (MeOH) (Berdy).
Clastres, A. *et al., J. Nat. Prod.*, 1984, **47**, 155

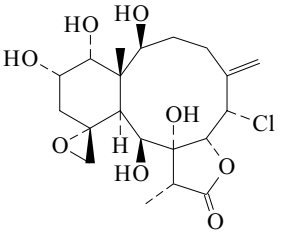
6-Chloro-11,20-epoxy-2,8,9,12,14-pentahydroxy-5(16)-briaren-18,7-olide C-342



$C_{20}H_{29}ClO_8$ 432.897

2,9,12,14-Tetra-Ac: ***Gemmacolide C***
[134887-86-8]
$C_{28}H_{37}ClO_{12}$ 601.046
Constit. of *Junceella gemmacea*. Oil. $[\alpha]_D$ +13.8 (c, 0.48 in $CHCl_3$).
14-(2-Methylbutanoyl), 2,9,12-tri-Ac: ***Juncin H***
[189513-66-4]
$C_{31}H_{43}ClO_{12}$ 643.126
Constit. of *Junceella juncea*. Cryst. (hexane/$CHCl_3$). $[\alpha]_D^{25}$ +9.8 (c, 0.83 in $CHCl_3$).
12-(3-Methylbutanoyl), 2-(2-methylpropanoyl), 9,14-di-Ac: ***Juncenolide F***
[853009-66-2]
$C_{33}H_{47}ClO_{12}$ 671.18
Constit. of *Junceella juncea*. Cryst. $[\alpha]_D$ +9.7 (c, 0.2 in CH_2Cl_2).
12,14-Bis(2-methylbutanoyl), 2,9-di-Ac: ***Juncin M***
[524741-54-6]
$C_{34}H_{49}ClO_{12}$ 685.207
Constit. of *Junceella juncea*. Amorph. powder. $[\alpha]_D^{25}$ +47.6 (c, 0.042 in $CHCl_3$).
He, H. *et al., Tetrahedron*, 1991, **47**, 3271-3280 (*Gemmacolide C*)
Anjaneyulu, A.S.R. *et al., J.C.S. Perkin 1*, 1997, 959-962 (*Juncin H*)
Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 2003, **66**, 507-510 (*Juncin M*)
Lin, Y.-C. *et al., Chem. Pharm. Bull.*, 2005, **53**, 128-130 (*Juncenolide F*)

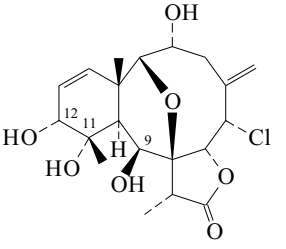
6-Chloro-11,20-epoxy-2,8,9,13,14-pentahydroxy-5(16)-briaren-18,7-olide C-343



$C_{20}H_{29}ClO_8$ 432.897

2,9,13,14-Tetra-Ac: ***Nuiinoalide A***
[173994-14-4]
$C_{28}H_{37}ClO_{12}$ 601.046
Constit. of an octocoral. Immunomodulatory agent. Solid.
$[\alpha]_D$ -15 (c, 1.2 in $CHCl_3$). λ_{max} 204 (ϵ 5545) (MeOH) (Berdy).
Hamann, M.T. *et al., Heterocycles*, 1996, **42**, 325 (*isol, pmr, cmr*)

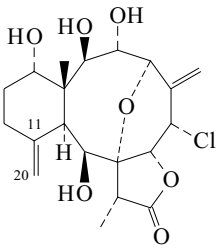
6-Chloro-2,8-epoxy-3,9,11,12-tetrahydroxy-5(16),13-briaradien-18,7-olide C-344



$C_{20}H_{27}ClO_7$ 414.882

9,11,12-Tri-Ac: ***Erythrolide G***
[132774-22-2]
$C_{26}H_{33}ClO_{10}$ 540.993
Constit. of *Erythropodium caribaeorum*. Gum.
12-Ketone, 9,11-di-Ac: ***Erythrolide E***
[132750-50-6]
$C_{24}H_{29}ClO_9$ 496.94
Isol. from *Erythropodium caribaeorum*. Powder (Me_2CO/hexane). Mp 128-129°. λ_{max} 215 (ϵ 8910) (MeOH) (Derep).
12-Ketone, 3,9,11-tri-Ac: [132750-62-0]
$C_{26}H_{31}ClO_{10}$ 538.978
Constit. of *Erythropodium caribaeorum*. Glass.
12-Ketone, 9-(hydroxyacetyl), 11-Ac: ***Erythrolide I***
[132750-52-8]
$C_{24}H_{29}ClO_{10}$ 512.94
Constit. of *Erythropodium caribaeorum*. Gum. λ_{max} 221 (ϵ 11700) (MeOH) (Derep).
12-Ketone, 9-(acetoxyacetyl), 11-Ac: ***Erythrolide F***
[132750-51-7]
$C_{26}H_{31}ClO_{11}$ 554.977
Constit. of *Erythropodium caribaeorum*. Powder (Me_2CO/hexane). Mp 118-119°. λ_{max} 218 (ϵ 5194) (MeOH) (Derep).
12-Ketone, 9-(acetoxyacetyl) 3,11-di-Ac: [132750-63-1]
$C_{28}H_{33}ClO_{12}$ 597.014
Constit. of *Erythropodium caribaeorum*. Powder.
Pordesimo, E.O. *et al., J.O.C.*, 1991, **56**, 2344 (*isol, pmr, cmr*)
Maharaj, D. *et al., J. Nat. Prod.*, 1999, **62**, 313-314 (*isol, pmr, cmr*)

6-Chloro-4,8-epoxy-2,3,9,14-tetrahydroxy-5(16),11(20)-briaradien-18,7-olide C-345



$C_{20}H_{27}ClO_7$ 414.882

9,14-Di-Ac: ***Junceellonoid D***
[868400-76-4]
$C_{24}H_{31}ClO_9$ 498.956
Constit. of *Junceella fragilis*. Powder. $[\alpha]_D$ -44.8 (c, 0.1 in MeOH/$CHCl_3$).

2,9,14-Tri-Ac: ***3-Deacetyljunceellin A***
[887332-06-1]
$C_{26}H_{33}ClO_{10}$ 540.993
Constit. of *Junceella fragilis*. Powder. $[\alpha]_D^{25}$ -5.9 (c, 0.44 in MeOH).

3,9,14-Tri-Ac: ***2-Deacetyljunceellin A***
[887332-07-2]
$C_{26}H_{33}ClO_{10}$ 540.993
Constit. of *Junceella fragilis*. Cryst. (CH_2Cl_2).
Mp 181-182°. $[\alpha]_D^{25}$ -17.4 (c, 0.63 in MeOH).

Tetra-Ac: ***Junceellin A***
[92508-09-3]
$C_{28}H_{35}ClO_{11}$ 583.031
Constit. of gorgonians *Junceella squamata* and *Junceella fragilis*.

11,20-Epoxide: 6-Chloro-4,8:11,12-diepoxy-2,3,9,14-tetrahydroxy-5(16)-briaren-18,7-olide
$C_{20}H_{27}ClO_8$ 430.881

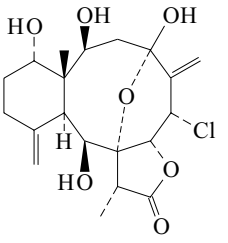
11α,20-Epoxide, 9,14-di-Ac: ***Junceellonoid C***
[868400-74-2]
$C_{24}H_{31}ClO_{10}$ 514.956
Constit. of *Junceella fragilis*. Powder. $[\alpha]_D$ -67.6 (c, 0.05 in Py).

11α,20-Epoxide, tetra-Ac: ***Praelolide***
[86425-67-4]
$C_{28}H_{35}ClO_{12}$ 599.03
Constit. of *Plexauroides praelonga*, *Gorgonella umbraculum*, *Junceella fragilis* and *Menella praelonga*.

17-Epimer, tetra-Ac: ***Junceellonoid E***
[868400-78-6]
$C_{28}H_{35}ClO_{11}$ 583.031
Constit. of *Junceella fragilis*. Powder. $[\alpha]_D$ -18 (c, 0.05 in $CHCl_3$).

Luo, Y. *et al., Bull. Chem. Soc. Jpn.*, 1983, 83-92; *CA*, **99**, 50572 (*Praelolide, isol, cryst struct*)
Yao, J. *et al., Zhongshan Daxue Xuebao Ziran Kexueban*, 1984, 83-87; *CA*, **101**, 211491 (*Junceellin A, cryst struct*)
Dai, J. *et al., Sci. Sin., Ser. B: (Engl. edn.)*, 1985, **28**, 1132-1142 (*Praelolide, isol, cryst struct*)
Shin, J. *et al., Tetrahedron*, 1989, **45**, 1633-1638 (*Praelolide, Junceellin A*)
Qi, S.-H. *et al., Helv. Chim. Acta*, 2005, **88**, 2349-2354 (*Junceellonoids C-E*)
Kubota, N.K. *et al., Bull. Chem. Soc. Jpn.*, 2006, **79**, 634-636 (*2,9,14-tri-Ac, 3,9,14-tri-Ac*)

6-Chloro-4,8-epoxy-2,4,9,14-tetrahydroxy-5(16),11(20)-briaradien-18,7-olide C-346



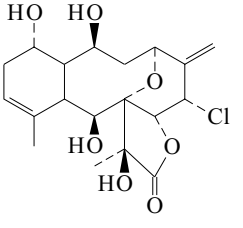
$C_{20}H_{27}ClO_7$ 414.882

2,9,14-Tri-Ac: ***Junceellolide A***
[121769-81-1]
$C_{26}H_{33}ClO_{10}$ 540.993
Constit. of gorgonian *Junceella fragilis*. Antiinflammatory agent.
Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 115-116°. $[\alpha]_D$ -7.9 (c, 0.6 in $CHCl_3$).

Enantiomer, 2,9,14-tri-Ac: ***(+)-Junceellolide A***
[221056-93-5]
$C_{26}H_{33}ClO_{10}$ 540.993
Constit. of *Junceella fragilis*. Powder. $[\alpha]_D^{22}$ +3.1 (c, 0.6 in CH_2Cl_2).

Shin, J. *et al., Tetrahedron*, 1989, **45**, 1633
Garcia, M. *et al., J. Nat. Prod.*, 1999, **62**, 257-260

6-Chloro-4,8-epoxy-2,9,14,17-tetrahydroxy-5(16),11-briaradien-18,7-olide C-347

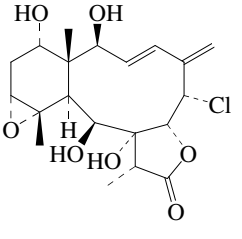


$C_{20}H_{27}ClO_7$ 414.882

2-Propanoyl, 14-Ac: 14-Acetoxy-6-chloro-4,8-epoxy-9,17-dihydroxy-2-propanoyloxy-5(16),11-briaradien-18,7-olide
[125028-90-2]
$C_{25}H_{33}ClO_9$ 512.983
Constit. of a *Briareum* sp. (PA1). Cryst.
Mp 260-262°.

Bowden, B.F. *et al., Aust. J. Chem.*, 1989, **42**, 1727 (*isol, pmr, cmr*)

6-Chloro-11,12-epoxy-2,8,9,14-tetrahydroxy-3,5(16)-briaradien-18,7-olide C-348



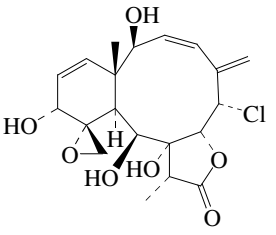
$C_{20}H_{27}ClO_7$ 414.882

(2β,3*E*,6α,8α,9β,11α,12α,17α)-*form*

2,9,14-Tri-Ac: [753001-76-2]
$C_{26}H_{33}ClO_{10}$ 540.993
Constit. of a *Pteroeides* sp. Solid. $[\alpha]_D^{26}$ +38 (c, 2.33 in $CHCl_3$).

Tanaka, C. *et al., J. Nat. Prod.*, 2004, **67**, 1368-1373 (*isol, pmr, cmr*)

6-Chloro-11,20-epoxy-2,8,9,12-tetrahydroxy-3,5(16),13-briaratrien-18,7-olide C-349

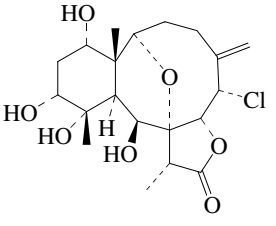


$C_{20}H_{25}ClO_7$ 412.866

(2β,3*Z*,6α,7α,8α,9β,11α,12α,17α)-*form*

2,9,12-Tri-Ac: [753001-72-8]
$C_{26}H_{31}ClO_{10}$ 538.978
Constit. of an *Ellisella* sp. Solid. $[\alpha]_D^{26}$ -59 (c, 0.106 in $CHCl_3$).
Tanaka, C. *et al., J. Nat. Prod.*, 2004, **67**, 1368-1373 (*isol, pmr, cmr*)

6-Chloro-2,8-epoxy-9,11,12,14-tetrahydroxy-5(16)-briaren-18,7-olide C-350



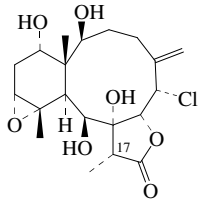
$C_{20}H_{29}ClO_7$ 416.898

(2α,6α,7α,8α,9β,11α,12α,14α)-*form*

9,14-Di-Ac: ***Erythrolide P***
[410096-46-7]
$C_{24}H_{33}ClO_9$ 500.972
Constit. of *Erythropodium caribaeorum*. Cryst. (Me_2CO/petrol). Mp 222-224°. $[\alpha]_D^{25}$ -16 (c, 0.25 in $CHCl_3$).

9,12,14-Tri-Ac: ***Erythrolide Q***
[410096-47-8]
$C_{26}H_{35}ClO_{10}$ 543.009
Constit. of *Erythropodium caribaeorum*. Gum. $[\alpha]_D^{25}$ -20 (c, 0.1 in $CHCl_3$).
Banjoo, D. *et al., J. Nat. Prod.*, 2002, **65**, 314-318 (*isol, pmr, cmr, cryst struct*)

6-Chloro-11,12-epoxy-2,8,9,14-tetrahydroxy-5(16)-briaren-18,7-olide C-351



(2β,6α,7α,8α,9β,11α,12α,14α17α)-*form*

$C_{20}H_{29}ClO_7$ 416.898

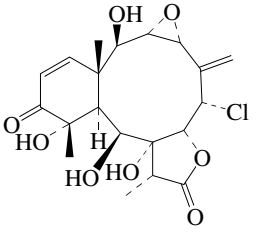
(2β,6α,7α,8α,9β,11α,12α,14α,17α)-*form*

2,9,14-Tri-Ac: ***Stylatulide***
[62950-37-2]
$C_{26}H_{35}ClO_{10}$ 543.009
Metab. of *Stylatula* spp. Cryst. (CH_2Cl_2/hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 179-181°. $[\alpha]_D$ +65.
▶ Toxic.

(2β,6α,7α,8α,9β,11α,12β,14α,17α)-*form*

2,9,14-Tri-Ac: ***17-Epistylatulide***
[74310-75-1]
$C_{26}H_{35}ClO_{10}$ 543.009
Constit. of a *Stylatula* sp. Cryst.
Mp 205-206°. $[\alpha]_D^{20}$ -18 (c, 0.3 in $CHCl_3$).
Wratten, S.J. *et al., J.A.C.S.*, 1977, **99**, 2824-2825 (*Stylatulide*)
Wratten, S.J. *et al., Tetrahedron*, 1979, **35**, 1907-1912 (*17-Epistylatulide*)

6-Chloro-3,4-epoxy-2,8,9,11-tetrahydroxy-12-oxo-5(16),13-briaradien-18,7-olide C-352

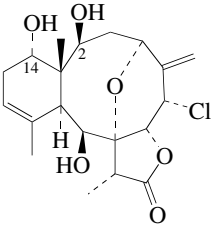


$C_{20}H_{25}ClO_8$ 428.865

(2β,3α,4α,6α,7α,8α,9β,11α,17α)-*form*

2,9-Di-Ac: ***Pachyclavulide D***
[877669-16-4]
$C_{24}H_{29}ClO_{10}$ 512.94
Constit. of *Pachyclavularia violacea*. Amorph. solid. $[\alpha]_D^{25}$ -30 (c, 0.04 in $CHCl_3$).
Iwasaki, J. *et al., J. Nat. Prod.*, 2006, **69**, 2-6

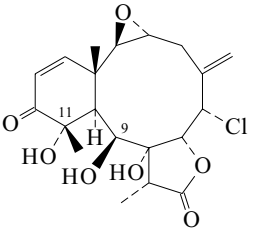
6-Chloro-4,8-epoxy-2,9,14-trihydroxy-5(16),11-briaradien-18,7-olide C-353



$C_{20}H_{27}ClO_6$ 398.882

2,14-Di-Ac: ***Excavatolide A***
[205581-09-5]
$C_{24}H_{31}ClO_8$ 482.957
Constit. of *Briareum excavatum*. Powder.
Mp >° 290. $[\alpha]_D^{28}$ +38 (c, 0.05 in Py).
Sheu, J.-H. *et al., J. Nat. Prod.*, 1998, **61**, 602-608 (*isol, pmr, cmr*)

6-Chloro-2,3-epoxy-8,9,11-trihydroxy-12-oxo-5(16),13-briaradien-18,7-olide C-354



$C_{20}H_{25}ClO_7$ 412.866

9,11-Di-Ac: ***Erythrolide C***
[132774-21-1]
$C_{24}H_{29}ClO_9$ 496.94
Constit. of *Erythropodium caribaeorum*. Powder (Me_2CO/hexane). Mp 125-129°. λ_{max} 215 (ϵ 8910) (MeOH) (Derep).

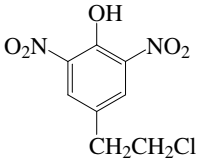
9-(Hydroxyacetyl), 11-Ac: ***Erythrolide U***
[627878-05-1]
$C_{24}H_{29}ClO_{10}$ 512.94
Constit. of *Erythropodium caribaeorum*. Glass. $[\alpha]_D^{25}$ -35.1. λ_{max} 216 (ϵ 6500) (MeOH).

9-(Acetoxyacetyl), 11-Ac: ***Erythrolide D***
[132750-48-2]
$C_{26}H_{31}ClO_{11}$ 554.977
Constit. of *Erythropodium caribaeorum*. Powder (Me_2CO/hexane). Mp 120-122°. λ_{max} 218 (ϵ 5194) (MeOH) (Derep).

Pordesimo, E.O. *et al., J.O.C.*, 1991, **56**, 2344 (*Erythrolides C-D*)
Taglialatela-Scafati, O. *et al., Eur. J. Org. Chem.*, 2003, 3515-3523 (*Erythrolide U*)

4-(2-Chloroethyl)-2,6-dinitrophenol C-355

2-(4-Hydroxy-3,5-dinitrophenyl)ethyl chloride

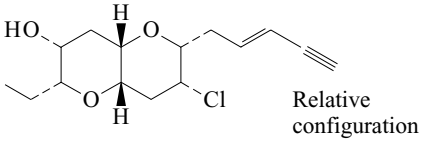


$C_8H_7ClN_2O_5$ 246.606
Isol. from the marine-derived *Flavobacterium* sp. T436.

Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, (*isol*)

7-Chloro-2-ethyloctahydro-6-(2-penten-4-ynyl)pyrano[3,2-*b*]pyran-3-ol, 9CI C-356

7-Chloro-6,10:9,13-diepoxy-12-hydroxy-3-pentadecen-1-yne
[148084-35-9]

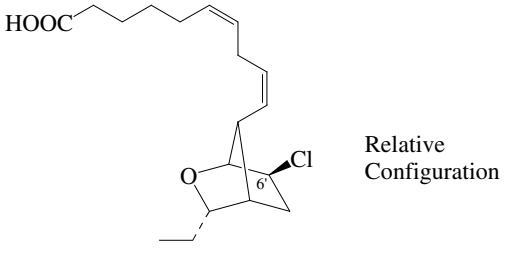


$C_{15}H_{21}ClO_3$ 284.782
Isol. from the red alga *Laurencia majuscula*. Oil. $[\alpha]_D^{22}$ -67.8 (c, 0.09 in $CHCl_3$).

Wright, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 394

10-(6-Chloro-3-ethyl-2-oxabicyclo[2.2.1]hept-7-yl)-6,9-decadienoic acid C-357

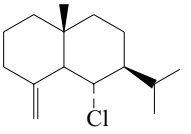
[625413-36-7]



$C_{18}H_{27}ClO_3$ 326.862
Oxylipin related to Cymathere ether B, C-1104. Isol. from the brown alga *Eisenia bicyclis*. Oil. $[\alpha]_D^{20}$ -12 (c, 0.02 in $CHCl_3$).

Dechloro, 6'S-hydroxy, (1→6')-lactone: [625413-35-6]
$C_{18}H_{26}O_3$ 290.402
Isol. from *Eisenia bicyclis*. Oil. $[\alpha]_D^{20}$ +74 (c, 0.06 in $CHCl_3$).
Kousaka, K. *et al., J. Nat. Prod.*, 2003, **66**, 1318-1323 (*isol, pmr, cmr*)

6-Chloro-4(15)-eudesmene C-358



$C_{15}H_{25}Cl$ 240.815

6α-form
Acanthene A
[149725-06-4]
Constit. of an *Acanthella* sp. and *Cadlina luteomarginata*.
Oil.

Burgoyne, D.L. *et al., Tetrahedron*, 1993, **49**, 4503-4510 (*isol, pmr, cmr*)

Chloroform C-359

Trichloromethane, 9CI. R20
[67-66-3]
$CHCl_3$
$CHCl_3$ 119.377
Manuf. by direct chlorination of Methane or Chloromethane, C-392 in the gas phase. Found in several natural sources incl. various plants and algae. Solvent, intermediate for manuf. of Chlorodifluoromethane, plastics intermediate. U.S. prodn. 266 530 t/a in 1989. Used in the detn. of phenols and as an extraction solv. Formerly used as anaesthetic. Topical remedy for Herpes simplex sores. Liq. Spar. sol. H_2O. d_4^{25} 1.48.
Mp -63.2°. Bp 61.3°. n_D^{20} 1.4467. Log P 1.95 (calc). Nonflammable. Slowly dec. in air and light forming $COCl_2$ (toxic) and other products. Forms hydrate with $18H_2O$, dec. at 1.6°. Forms azeotrope contg. 2.5% H_2O, Bp 56°.

▶ Vigorous reaction with Me_2CO and base, explosive reaction with some materials. Poss. human carcinogen. Skin, eye and respiratory tract irritant. Adverse systemic effects by inhalation can lead to loss of consciousness, cardiac respiratory failure and death. Hepatotoxic and nephrotoxic. Exp. carcinogen. Exp. reprod. and teratogenic effects. OES: long-term 2 ppm (Sk). Can autoxidise on storage to generate highly toxic phosgene. FS9100000

[865-49-6, 3170-80-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 83A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 122A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 116C (*ir*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 130; 1980, **8**, 92; 1986, **12**, 517; 1988, **13**, 9; 1990, **15**, 84 (*use*)
Dykes, M.H.M. *et al., Int. Anesthesiol. Clin.*, 1970, **8**, 357 (*rev, pharmacol*)
Legradi, L. *et al., Mikrochim. Acta*, 1972, 369 (*use*)
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Anderson, A. *et al., J. Chem. Phys.*, 1985, **82**, 99 (*Raman, conformn*)
Hahn, S. *et al., J. Solution Chem.*, 1985, **14**, 129 (*pmr*)
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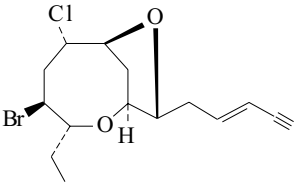
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*1996, **68**, 1 (*occur*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 578-579
Turk, E. *et al., Chem. Eng. News*, March 2, 1998, 6 (*haz, autoxidn*)
Stratmann, L. *et al., Chloroform the Quest for Oblivion*, Sutton Publishing, 2003, (*history*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0354

Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 303
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CHJ500

Chlorofucin C-360

[74683-12-8]



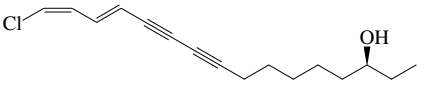
$C_{15}H_{20}BrClO_2$ 347.678

Abs. config. needs to be reassessed (1991). Constit. of *Laurencia pannosa* and *Laurencia snyderae*. Cryst. ($CHCl_3$).
Mp 86-88°. $[\alpha]_D^{20}$ +12 (c, 1.4 in $CHCl_3$).

(Z)-Isomer: ***(Z)-Chlorofucin***
$C_{15}H_{20}BrClO_2$ 347.679
Constit. of *Laurencia pannosa*. Oil. $[\alpha]_D^{24}$ -11.3 (c, 0.6 in $CHCl_3$). Possibly enantiomeric with parent.

Howard, B.M. *et al., Tetrahedron*, 1980, **36**, 1747-1751 (*cryst struct*)
Norte, M. *et al., Tetrahedron*, 1991, **47**, 9411
Suzuki, M. *et al., J. Nat. Prod.*, 2001, **64**, 597-602 (*isol, pmr, cmr*)

16-Chloro-13,15-hexadecadiene-9,11-diyn-3-ol, 9CI C-361



(3*S*,13*E*,15*Z*)-*form*

$C_{16}H_{21}ClO$ 264.794

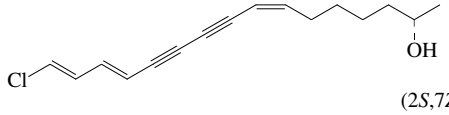
(3*S*,13*E*,15*Z*)-*form* [76480-36-9]
Defence chemical isol. from the nudibranch mollusc *Diaulula sandiegensis*. Also isol. from the sponge *Haliclona lunisimilis*.
$[\alpha]_D$ -14.9 (c, 1 in CH_2Cl_2). λ_{max} 229 (ε 17700); 238 (ε 39700); 296 (ε 37500); 316 (ε 39600) (pentane) (Derep).

Ac:
$C_{18}H_{23}ClO_2$ 306.831
Isol. from *Haliclona lunisimilis*. Pale yellow oil. $[\alpha]_D$ +13.6 (c, 1.3 in CH_2Cl_2). λ_{max} 225 (ε 21000); 240 (ε 24600); 300 (ε 38700); 319 (ε 40200) (CH_2Cl_2).

(3*S*,13*Z*,15*Z*)-*form*
Isol. from *Haliclona lunisimilis*.
Yellow oil. $[\alpha]_D$ -9.7 (c, 1.6 in CH_2Cl_2).

Walker, R.P. *et al., J.O.C.*, 1981, **46**, 1475-1478 (*isol, ir, pmr*)
De Jesus, R.P. *et al., J. Nat. Prod.*, 2003, **66**, 671-674 (*isol, cmr, abs config*)

16-Chloro-7,13,15-hexadecatriene-9,11-diyn-2-ol, 9CI C-362



(2*S*,7*Z*,13*E*,15*E*)-*form*

$C_{16}H_{19}ClO$ 262.778

(2*S*,7*Z*,13*E*,15*E*)-*form* [76480-32-5]
Isol. from the nudibranch *Diaulula sandiegensis*. λ_{max} 252 (ε 28250); 268 (ε 26800); 299 (ε 25600); 318 (ε 35800); 340 (ε 27400) (pentane).

(2*S*,7*Z*,13*E*,15*Z*)-*form* [76480-30-3]
Isol. from *Diaulula sandiegensis* and the sponge *Haliclona lunisimilis*.
$[\alpha]_D$ -6.8 (c, 1 in CH_2Cl_2). λ_{max} 254 (ε 21950); 269 (ε 20900); 300 (ε 20500); 320 (ε 29150); 342 (ε 22700) (pentane).

Ketone: 16-Chloro-7,13,15-hexadecatriene-9,11-diyn-2-one, 9CI
[76480-28-9]
$C_{16}H_{17}ClO$ 260.762
Isol. from *Diaulula sandiegensis*. λ_{max} 254 (ε 18900); 269 (ε 18700); 300 (ε 19500); 319 (ε 26800); 342 (ε 19500) (pentane).

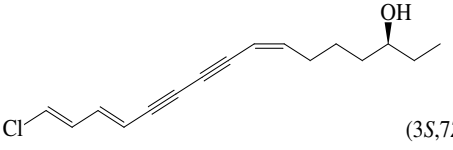
Ac:
$C_{18}H_{21}ClO_2$ 304.815
Isol. from *Haliclona lunisimilis*. Pale yellow oil. $[\alpha]_D$ +8.4 (c, 2.7 in CH_2Cl_2). λ_{max} 256 (ε 36600); 271 (ε 36300); 303 (ε 43200); 322 (ε 54300); 345 (ε 43400) (CH_2Cl_2).

(2*S*,7*Z*,13*Z*,15*Z*)-*form* [76480-31-4]
Isol. from *Diaulula sandiegensis* and the sponge *Haliclona lunisimilis*.
$[\alpha]_D$ -5.1 (c, 1 in CH_2Cl_2). λ_{max} 255 (ε 19250); 269 (ε 18700); 299 (ε 17500); 319 (ε 23500); 341 (ε 17200) (pentane).

Ketone: [76480-29-0]
$C_{16}H_{17}ClO$ 260.762
Isol. from *Diaulula sandiegensis*. λ_{max} 255 (ε 19250); 269 (ε 18700); 299 (ε 17500); 319 (ε 23500); 341 (ε 17200) (pentane).

Walker, R.P. *et al., J.O.C.*, 1981, **46**, 1475-1478 (*isol, ir, pmr*)
De Jesus, R.P. *et al., J. Nat. Prod.*, 2003, **66**, 671-674 (*isol, cmr*)

16-Chloro-7,13,15-hexadecatriene-9,11-diyn-3-ol, 9CI C-363



(3*S*,7*Z*,13*E*,15*E*)-*form*

$C_{16}H_{19}ClO$ 262.778

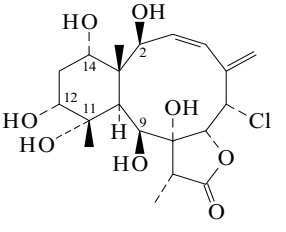
(3*S*,7*Z*,13*E*,15*E*)-*form* [76480-35-8]
Isol. from the nudibranch *Diaulula sandiegensis*. Chemical defence agent in nudibranches. λ_{max} 253 (ε 25100); 268 (ε 29250); 299 (ε 19850); 318 (ε 26300); 340 (ε 21300) (pentane).

(3*S*,7*Z*,13*E*,15*Z*)-*form* [76480-33-6]
Isol. from *Diaulula sandiegensis* and the sponge *Haliclona lunisimilis*.
$[\alpha]_D$ -13 (c, 1 in CH_2Cl_2). λ_{max} 254 (ε 20500); 269 (ε 21200); 300 (ε 25300); 319 (ε 31000); 342 (ε 20500) (pentane).

(3*S*,7*Z*,13*Z*,15*Z*)-*form* [76480-34-7]
Isol. from *Diaulula sandiegensis* and *Haliclona lunisimilis*.
$[\alpha]_D$ -18.1 (c, 1.1 in CH_2Cl_2). λ_{max} 254 (ε 22900); 269 (ε 22700); 300 (ε 21350); 319 (ε 29050); 341 (ε 21400) (pentane).

Walker, R.P. *et al., J.O.C.*, 1981, **46**, 1475-1478 (*isol, ir, pmr*)
De Jesus, R.P. *et al., J. Nat. Prod.*, 2003, **66**, 671-674 (*isol, cmr*)

6-Chloro-2,8,9,11,12,14-hexahydroxy-3,5(16)-briaradien-18,7-olide C-364



$C_{20}H_{29}ClO_8$ 432.897

2,9,11,12,14-Penta-Ac: ***Briarein A***. *Briarein*
[62681-06-5]
$C_{30}H_{39}ClO_{13}$ 643.083

Constit. of *Briareum asbestinum*. Cryst.
Mp 240-245°. $[\alpha]_D^{25}$ -58.2 (c, 2 in $CHCl_3$). λ_{max} 229 (ϵ 6600) (MeOH) (Derep).

12-Butanoyl, 2,9,14-tri-Ac: ***Briarein C***
[172854-59-0]
$C_{30}H_{41}ClO_{12}$ 629.099
Constit. of *Briareum asbestinum*. Cryst.
Mp 131.5-134°. $[\alpha]_D^{25}$ -9.5 (c, 2.4 in $CHCl_3$).

12-Butanoyl, 2,9,11,14-tetra-Ac: ***Briarein B***
[172854-58-9]
$C_{32}H_{43}ClO_{13}$ 671.137
Constit. of *Briareum asbestinum*. Cryst.
Mp 131.5-134°. $[\alpha]_D^{25}$ -9.5 (c, 2.4 in $CHCl_3$).

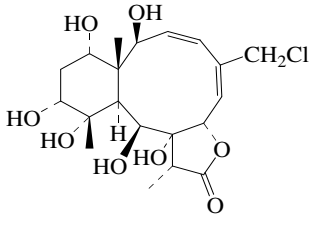
3α,4α-Epoxide, 2,9,12,14-tetra-Ac: ***Briarein E***
[172854-61-4]
$C_{28}H_{37}ClO_{13}$ 617.045
Constit. of *Briareum asbestinum*. Cryst.
Mp 160.2-161.8°. $[\alpha]_D^{26}$ +20.7 (c, 3.36 in $CHCl_3$).

3α,4α-Epoxide, 2,9,11,12,14-penta-Ac: ***Briarein D***
[172854-60-3]
$C_{30}H_{39}ClO_{14}$ 659.082
Constit. of *Briareum asbestinum*. Semi-solid. $[\alpha]_D^{25}$ -48 (c, 1.33 in $CHCl_3$).

3α,4α-Epoxide, 12-butanoyl, 2,9,11,14-tetra-Ac: ***Briarein G***
[172927-62-7]
$C_{32}H_{43}ClO_{14}$ 687.136
Constit. of *Briareum asbestinum*. Cryst.
Mp 238° dec. $[\alpha]_D^{25}$ -28 (c, 1.5 in $CHCl_3$).

Birks, J.E. *et al., Acta Cryst. B*, 1977, **33**, 704 (*cryst struct*)
Selover, S.J. *et al., J.O.C.*, 1981, **46**, 964 (*isol*)
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1996, **59**, 15 (*Briareins, isol, pmr, cmr, uv, ir*)

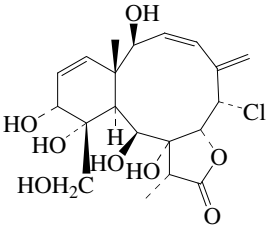
16-Chloro-2,8,9,11,12,12,14-hexahydroxy-3,5-briaradien-18,7-olide C-365



$C_{20}H_{29}ClO_8$ 432.897

(2β,5E,8α,9β,11α,12α,14α,17α)-form
12-Propanoyl, 2,9,14-tri-Ac: [753001-78-4]
$C_{29}H_{39}ClO_{12}$ 615.073
Constit. of a *Pteroeides* sp. Solid. $[\alpha]_D^{26}$ +12 (c, 0.35 in $CHCl_3$).
Tanaka, C. *et al., J. Nat. Prod.*, 2004, **67**, 1368-1373 (*isol, pmr, cmr*)

6-Chloro-2,8,9,11,12,20-hexahydroxy-3,5(16),13-briaratrien-18,7-olide C-366

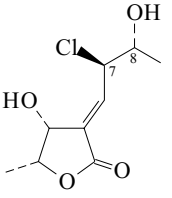


$C_{20}H_{27}ClO_8$ 430.881

(2β,3Z,6α,7α,8α,9β,11α,12α,17α)-form
2,9,12,20-Tetra-Ac: [753001-73-9]
$C_{28}H_{35}ClO_{12}$ 599.03
Constit. of an *Ellisella* sp. Solid. $[\alpha]_D^{26}$ -50 (c, 0.462 in $CHCl_3$).
Tanaka, C. *et al., J. Nat. Prod.*, 2004, **67**, 1368-1373 (*isol, pmr, cmr*)

3-(2-Chloro-3-hydroxybutenylidene)dihydro-4-hydroxy-5-methyl-2(3*H*)-furanone C-367

[182967-68-6]



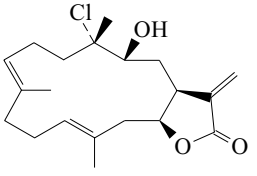
(7*R**,8*R**)–*form*

$C_9H_{13}ClO_4$ 220.652

(7R*,8R*)-form
Chlorocarolide A
Prod. by *Aspergillus ochraceus* obt. from the sponge *Jaspis* cf. *coriaceae.*
Yellow oil. $[\alpha]_D$ +78 (c, 2.5 in CH_2Cl_2).

(7S*,8S*)-form
Chlorocarolide B
Prod. by *Aspergillus ochraceus* obt. from *Jaspis* cf. *coriaceae.*
Yellow oil. $[\alpha]_D$ +29 (c, 2.2 in CH_2Cl_2).
Abrell, L.M. *et al., Tet. Lett.*, 1996, **37**, 2331-2334 (*isol, pmr, cmr*)

4-Chloro-3-hydroxy-7,11,15(17)-cembratrien-16,14-olide C-368

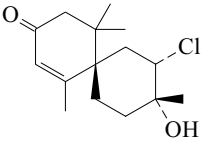


$C_{20}H_{29}ClO_3$ 352.9

(3S,4S,7E,11E,14S)-form [151694-00-7]
Constit. of *Eunicea mammosa.*
Cryst. $[\alpha]_D^{25}$ -22.36 (c, 0.76 in $CHCl_3$).
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 1101 (*isol, pmr, cmr, cryst struct*)

2-Chloro-3-hydroxy-7-chamigren-9-one C-369

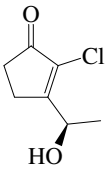
[108925-14-0]



$C_{15}H_{23}ClO_2$ 270.798
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ -46 (c, 0.22 in $CHCl_3$).
Brennan, M.R. *et al., Phytochemistry*, 1987, **26**, 1053

2-Chloro-3-(1-hydroxyethyl)-2-cyclopenten-1-one C-370

Trichodenone C



$C_7H_9ClO_2$ 160.6

(*R*)-*form* [203243-27-0]

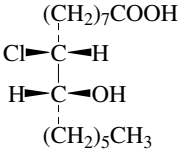
Prod. by a *Trichoderma harzianum* isol. from the sponge *Halichondria okadai*.

Oil. Sol. MeOH, $CHCl_3$, EtOAc, DMSO, hexane, Me_2CO; poorly sol. H_2O. $[\alpha]_D^{28}$ -10.8 (c, 1.1 in $CHCl_3$). λ_{max} 239 (log ϵ 3.89) (EtOH).

Amagata, T. *et al., J. Antibiot.*, 1998, **51**, 33-40 (*isol, uv, ir, cd, pmr, cmr*)
Usami, Y. *et al., Synlett*, 1999, 723-724 (*synth, abs config*)
Sakai, A. *et al., Tet. Lett.*, 2000, **41**, 6859-6863 (*synth*)

9-Chloro-10-hydroxyhexadecanoic acid C-371

[67101-32-0 (Me ester)]



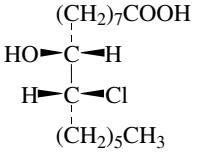
$C_{16}H_{31}ClO_3$ 306.872

(9*R,10*R**)-*form*** [64792-83-2]

Constit. of the jellyfish *Aurelia aurita*.

White, R.H. *et al., Biochemistry*, 1977, **16**, 4944-4948 (*isol*)

10-Chloro-9-hydroxyhexadecanoic acid C-372



$C_{16}H_{31}ClO_3$ 306.872

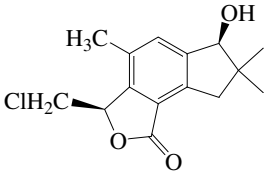
(9*R,10*R**)-*form*** [64792-84-3]

Constit. of the jellyfish *Aurelia aurita*.

[67101-33-1 (Me ester)]

White, R.H. *et al., Biochemistry*, 1977, **16**, 4944-4948 (*isol*)

4-Chloro-10-hydroxy-2,6,8-illudalatrien-15,5-olide C-373



$C_{15}H_{17}ClO_3$ 280.75

(5*R*,10*S*)-*form*

Alcyopterosin L

[288851-38-7]

Constit. of *Alcyonium paessleri*.

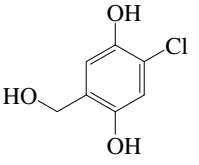
Oil. $[\alpha]_D^{25}$ -17.02 (c, 0.58 in $CHCl_3$). λ_{max} 224 (log ϵ 3.19); 240 (log ϵ 3.7); 298 (log ϵ 3.42) (CH_2Cl_2).

Palermo, J.A. *et al., J.O.C.*, 2000, **65**, 4482-4486 (*isol, pmr, cmr*)

2-Chloro-5-(hydroxymethyl)-1,4-benzenediol, 9CI C-374

4-Chloro-2,5-dihydroxybenzyl alcohol, 8CI. 4-Chloro-α,2,5-trihydroxytoluene. ***Amudol***

[31302-46-2]



$C_7H_7ClO_3$ 174.583

Metab. of *Penicillium martensii* and a marine *Aspergillus varians*. Antibiotic active against some gram-positive organisms. Sol. EtOAc, Et_2O; poorly sol. H_2O.

Mp 146-147°. λ_{max} 298 (ϵ 2344) (MeOH) (Berdy).

Kamal, A. *et al., Pak. J. Sci. Ind. Res.*, 1970, **13**, 236; 383; 1971, **14**, 59 (*synth*)
Sakamura, S. *et al., Agric. Biol. Chem.*, 1971, **35**, 105 (*synth*)
Séquin-Frey, M. *et al., Helv. Chim. Acta*, 1971, **54**, 851 (*synth*)
McCorkindale, N.J. *et al., Tetrahedron*, 1972, **28**, 1107 (*synth, nmr*)
Smetanina, O.F. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 243-244 (*marine isol*)

2-Chloro-6-(hydroxymethyl)-1,4-benzenediol, 9CI C-375

3-Chloro-2,5-dihydroxybenzyl alcohol, 8CI. 3-Chloro-α,2,5-trihydroxytoluene. ***Chlorogentisyl alcohol***

[32744-80-2]

$C_7H_7ClO_3$ 174.583

Prod. by *Penicillium canadense*, *Phyllosticta* spp. and a marine *Aspergillus varians*. Needles (EtOAc/petrol). Sol. Me_2CO, Et_2O, EtOAc; fairly sol. $CHCl_3$.

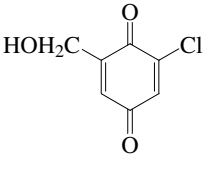
Mp 147-148° (140-141.5°). λ_{max} 220 (ϵ 4118); 297 (ϵ 2529) (MeOH) (Berdy). λ_{max} 294 (ϵ 3910); 314 (ϵ 7060); 320 (ϵ 8120); 408 (ϵ 4140); 433 (ϵ 4320) (EtOH) (Berdy). λ_{max} 262 (ϵ 3900) (EtOH-NaOH) (Berdy).

Sakamura, S. *et al., Agric. Biol. Chem.*, 1971, **35**, 105 (*synth*)
Séquin-Frey, M. *et al., Helv. Chim. Acta*, 1971, **54**, 851 (*synth*)
McCorkindale, N.J. *et al., Tetrahedron*, 1972, **28**, 1107 (*synth, nmr*)
Nabeta, K. *et al., Agric. Biol. Chem.*, 1975, **39**, 403; 409 (*isol*)
Smetanina, O.F. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 243-244 (*marine isol*)

2-Chloro-6-hydroxymethyl-1,4-benzoquinone C-376

2-Chloro-6-(hydroxymethyl)-2,5-cyclohexadiene-1,4-dione, 9CI. ***Chlorogentisylquinone****. Antibiotic FOM 8108. FOM 8108*

[333344-08-4]



$C_7H_5ClO_3$ 172.567

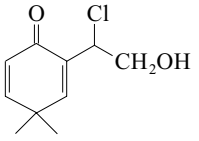
Prod. by a marine fungus *Agonomycetes* FOM-8108. Sphingomyelinase inhibitor. Brown needles. λ_{max} 258 (ϵ 37100); 325 (ϵ 1500) (MeOH).

Uchida, R. *et al., J. Antibiot.*, 2001, **54**, 882-889 (*synth*)
Japan. Pat., 2001, 103 990; *CA*, **134**, 279667b (*isol*)

2-Chloro-1-hydroxy-3(8),5-ochtodadien-4-one C-377

2-(1-Chloro-2-hydroxyethyl)-4,4-dimethyl-2,5-cyclohexadien-1-one, 9CI

[97457-28-8]



$C_{10}H_{13}ClO_2$ 200.664

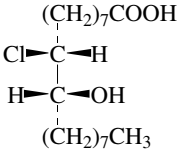
Constit. of red alga *Desmia hornemanni* (*Portieria hornemanni*). Pale-yellow oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{21}$ -87.2 (c, 1.29 in CH_2Cl_2). Unstable, spontaneously transformed into 4,5-dimethylbenzofuran. λ_{max} 237 (ϵ 8900) (EtOH) (Derep).

Higa, T. *et al., Tet. Lett.*, 1985, **26**, 2335-2336 (*isol*)
Kuniyoshi, M. *et al., J. Chin. Chem. Soc. (Taipei)*, 2003, **50**, 167-170 (*pmr, cmr*)

9-Chloro-10-hydroxyoctadecanoic acid C-378

[2632-61-3]

[13985-23-4 (*R**,*S**-form)]



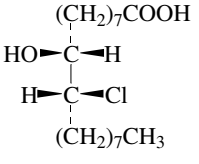
$C_{18}H_{35}ClO_3$ 334.925

(9*R,10*R**)-*form*** [13985-22-3]
Isol. from the jellyfish *Aurelia aurita*.
White, R.H. *et al., Biochemistry*, 1977, **16**, 4944-4948 (*isol*)

10-Chloro-9-hydroxyoctadecanoic acid C-379

[2632-62-4]

[13985-24-5 (*R**,*S**-form)]

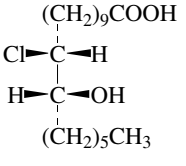


$C_{18}H_{35}ClO_3$ 334.925

(9*R,10*R**)-*form*** [13985-25-6]
Constit. of the jellyfish *Aurelia aurita*.
White, R.H. *et al., Biochemistry*, 1977, **16**, 4944-4948 (*isol*)

11-Chloro-12-hydroxyoctadecanoic acid C-380

[67101-36-4 (Me ester)]

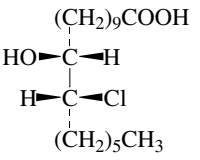


$C_{18}H_{35}ClO_3$ 334.925

(11*R,12*R**)-*form*** [64792-85-4]
Isol. from the jellyfish *Aurelia aurita*.
White, R.H. *et al., Biochemistry*, 1977, **16**, 4944-4948 (*isol*)

12-Chloro-11-hydroxyoctadecanoic acid C-381

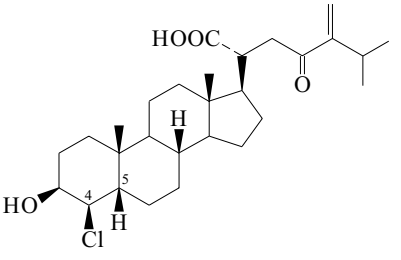
[67324-54-3 (Me ester)]



$C_{18}H_{35}ClO_3$ 334.925

(11*R,12*R**)-*form*** [64792-86-5]
Isol. from the jellyfish *Aurelia aurita*.
White, R.H. *et al., Biochemistry*, 1977, **16**, 4944-4948 (*isol*)

4-Chloro-3-hydroxy-23-oxoergost-24(28)-en-21-oic acid C-382

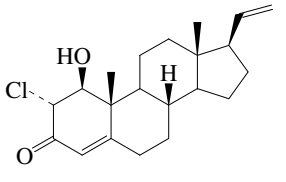


$C_{28}H_{43}ClO_4$ 479.098

(3β,4β,5β)-*form*
Kiheisterone D
[149260-74-2]
Constit. of a *Strongylacidon* sp.
$[\alpha]_D$ +46 (c, 0.57 in $CHCl_3$). λ_{max} 224 (ϵ 10000); 257 (ϵ 7940) (MeOH) (Derep). λ_{max} 220 (ϵ 12600) (MeOH) (Berdy).

4,5-Didehydro: 4-Chloro-3,23-dioxoergosta-4,24(28)-dien-21-oic acid. ***Kiheisterone C***
[149260-73-1]
$C_{28}H_{41}ClO_4$ 477.082
Constit. of a *Strongylacidon* sp.
$[\alpha]_D$ +71 (c, 0.55 in $CHCl_3$). λ_{max} 224 (ϵ 10000); 257 (ϵ 7940) (MeOH) (Derep). λ_{max} 224 (ϵ 10000); 257 (ϵ 8000) (MeOH) (Berdy).
Carney, J.R. *et al., J.O.C.*, 1993, **58**, 3460-3462 (*isol, pmr, cmr*)

2-Chloro-1-hydroxypregna-4,20-dien-3-one C-383



(1β,2α)-*form*

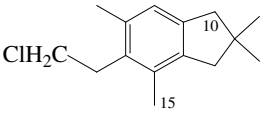
$C_{21}H_{29}ClO_2$ 348.912

(1β,2α)-*form* [690253-77-1]
Constit. of *Carijoa multiflora*. Oil. $[\alpha]_D^{25}$ +92 (c, 0.12 in $CHCl_3$).

(1β,2β)-*form* [690253-78-2]
Constit. of *Carijoa multiflora*. Oil. $[\alpha]_D^{25}$ -164 (c, 0.14 in $CHCl_3$).
Dorta, E. *et al., Tet. Lett.*, 2004, **45**, 915-918 (*isol, pmr, cmr*)

4-Chloro-2,6,8-illudalatriene C-384

Alcyopterosin A



$C_{15}H_{21}Cl$ 236.784
Constit. of *Alcyonium paessleri*. Oil. λ_{max} 232 (log ϵ 3.59); 258 (log ϵ 2.81); 272 (log ϵ 3.15); 282 (log ϵ 3.14) (CH_2Cl_2).

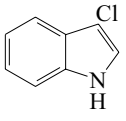
15-Hydroxy: 4-Chloro-2,6,8-illudalatrien-15-ol. ***Alcyopterosin D***
[288851-30-9]
$C_{15}H_{21}ClO$ 252.783
Constit. of *Alcyonium paessleri*. Cryst. (MeOH). Mp 107-108°. λ_{max} 214 (log ϵ 4.07); 232 (log ϵ 3.89); 286 (log ϵ 3.24) (CH_2Cl_2).

10S,15-Dihydroxy: 4-Chloro-2,6,8-illudalatriene-10,15-diol. ***Alcyopterosin K***
[288851-37-6]
$C_{15}H_{21}ClO_2$ 268.782
Constit. of *Alcyonium paessleri*. Cryst. (MeOH). Mp 108-110°. $[\alpha]_D^{25}$ +10 (c, 0.91 in $CHCl_3$). λ_{max} 234 (log ϵ 3.41); 278 (log ϵ 3.04); 286 (log ϵ 3.08) (CH_2Cl_2).

Palermo, J.A. *et al., J.O.C.*, 2000, **65**, 4482-4486 (*isol, pmr, cmr*)
Tanaka, R. *et al., J.A.C.S.*, 2002, **124**, 9682-9683 (*synth*)

3-Chloro-1*H*-indole, 9CI C-385

[16863-96-0]



C_8H_6ClN 151.595
Principal odorous component of the marine hemichordate *Ptychodera flava laysanica*.
Mp 95.5-96° dec.

N-*Benzoyl:*
$C_{15}H_{10}ClNO$ 255.703
Prisms (EtOH). Mp 97-99°.

Pappalardo, G. *et al., Gazz. Chim. Ital.*, 1958, **88**, 1147 (*synth, uv*)
Higa, T. *et al., Naturwissenschaften*, 1975, **62**, 395 (*isol*)

Chloroiodoacetic acid, 9CI C-386

[53715-09-6]
ClCHICOOH
$C_2H_2ClIO_2$ 220.394
Constit. of *Asparagopsis taxiformis*.

(+)-form
$[\alpha]_D$ +0.9 (H_2O).
NH_4 salt: $[\alpha]_D$ +23.5 (H_2O).

(±)-form
Leaflets. V. sol. H_2O, mod. sol. petrol. Mp 90°.

Phenyl ester:
$C_8H_6ClIO_2$ 296.491
Mp 110°.

Amide: Chloroiodoacetamide
[62872-35-9]
C_2H_3ClINO 219.409
Constit. of *Asparagopsis taxiformis*. Needles (H_2O or C_6H_6). Mp 140°.

Crompton, H. *et al., J.C.S.*, 1923, **123**, 576 (*synth*)
McMath, A.M. *et al., J.C.S.*, 1927, 538 (*synth, resoln*)
Seyferth, D. *et al., J. Organomet. Chem.*, 1974, **71**, 335 (*synth*)
Woolard, F.X. *et al., Tetrahedron*, 1976, **32**, 2843-2846 (*amide, isol*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617-620 (*isol*)

Chloroiodomethane C-387

[593-71-5]
$ClCH_2I$
CH_2ClI 176.384
Isol. from phytoplankton and various marine algae. Versatile organic synthon. Commercially available. Liq. Bp 108-109° (104-105°).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 71C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 105C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 102C (*ir*)
Miyano, S. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 2864 (*synth, pmr*)
Hahn, R.C. *et al., J.O.C.*, 1988, **53**, 1331 (*synth, bibl, use*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **2**, 1143-1146 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)

1-Chloro-3-iodo-2-propanol, 8CI C-388

[26484-95-7]
$ICH_2CH(OH)CH_2Cl$
C_3H_6ClIO 220.437
Isol. from the edible marine red alga *Asparagopsis taxiformis*.

(±)-form
Liq. d^{10} 2.06. Bp 226° Bp_9 110° $Bp_{0.2}$ 53-55°.

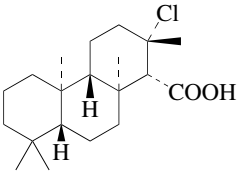
Ingold, C.K. *et al., J.C.S.*, 1931, 1666 (*synth*)
Woolard, F.X. *et al., Tetrahedron*, 1976, **32**, 2843-2846 (*isol, glc, ms*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Shargi, H. *et al., Tetrahedron*, 2003, **59**, 8509-8514 (*synth*)

1-Chloro-3-iodo-2-propanone, 9CI C-389

1-Chloro-3-iodoacetone
[62874-85-5]
$ClCH_2COCH_2I$
C_3H_4ClIO 218.421
Minor component of the red alga *Asparagopsis armata*. No phys. props. reported.

McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367 (*isol, ms*)
Fr. Pat., 1980, 2 436 127; *CA*, **94**, 15200e
Ger. Pat., 1987, 3 605 484; *CA*, **107**, 200926w

13-Chloro-15-isocopalanoic acid C-390



$C_{20}H_{33}ClO_2$ 340.932

(ent-13βCl)-form

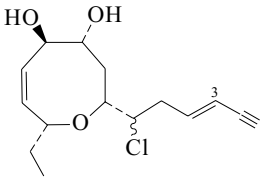
(3-Acetoxy-2-hydroxypropyl) ester: ***Verrucosin 7***
[188405-19-8]
$C_{25}H_{41}ClO_5$ 457.049
Constit. of *Doris verrucosa* and *Austrodoris kerguelenensis*. Protein kinase C activator. Morphogenetic hydra tentacle regeneration agent. Oil. $[\alpha]_D$ +19.1 (c, 0.35 in $CHCl_3$).

(2-Acetoxy-3-hydroxypropyl) ester: ***Verrucosin 9***
[188405-20-1]
$C_{25}H_{41}ClO_5$ 457.049
Constit. of *Doris verrucosa*. Protein kinase C activator. Morphogenetic hydra tentacle regeneration agent. Oil. $[\alpha]_D$ +25 (c, 0.04 in $CHCl_3$).

De Petrocellis, L. *et al., Experientia*, 1996, **52**, 874-877 (*isol*)
Gavagnin, M. *et al., Tetrahedron*, 1997, **53**, 1491-1504 (*isol, pmr, cmr*)

6-Chloro-3,11-lauthisadien-1-yne-9,10-diol C-391

10-Chloro-3,9-epoxy-4,12-pentadecadiene-14-yne-6,7-diol



$C_{15}H_{21}ClO_3$ 284.782

(3*E*)-*form*

Obt. from *Laurencia thyrsifera*. Oil.

(3*Z*)-*form*

Constit. of *Laurencia thyrsifera*. Oil.

Blunt, J.W. *et al., Aust. J. Chem.*, 1981, **34**, 2393

Chloromethane, 9CI C-392

Methyl chloride

[74-87-3]

H_3CCl

CH_3Cl 50.487

Manuf. by chlorination of methane or by liquid-phase hydrochlorination of methanol. A natural chloroalkane prod. by the marine and terrestrial biomass (estimated 5 m t a^{-1}). Probably the most abundant natural organohalogen. Accounts for ca. 25% of the chlorine in the atmosphere. Refrigerant. Methylating reagent used in manuf. of silicones and $PbMe_4$, low-temp. solv., extractant. Topical anaesthetic. Gas with ethereal odour. Mod. sol. H_2O.

Mp -97.7°. Bp -23.7°.

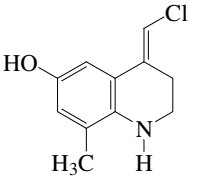
▶ Extremely flammable, fl. p. -50°, autoignition temp. 625/632°. Ignites or explodes on contact with BrF_3, BrF_5 and some metals. Effects of acute or chronic exposure often delayed. Mild exp. causes inebriation. Higher conc. produce a range of CNS effects plus gastrointestinal disturbances. Prolonged or repeated exposure to low conc. produces CNS effects which may persist for several months. Exp. reprod. and teratogenic effects. OES: long-term 50 ppm; short-term 100 ppm. PA6300000

[1111-89-3, 6806-86-6]

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 81C (*ir*)
Norris, J.F. *et al., J.A.C.S.*, 1924, **46**, 752 (*synth*)
Downie, I.M. *et al., Chem. Ind. (London)*, 1966, 900 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 674 (*use*)
Price, C.C. *et al., J.O.C.*, 1973, **38**, 615 (*pmr*)
Austin, G.T. *et al., Chem. Eng. (N.Y.)*, 1974, **81**, 87 (*rev*)
Miyajima, G. *et al., Org. Magn. Reson.*, 1974, **6**, 313 (*cmr*)
Hubrich, C. *et al., Ber. Bunsen-Ges. Phys. Chem.*, 1977, **81**, 437 (*uv*)
DeForest, E.M. *et al., Encycl. Chem. Process. Des.*, 1979, **8**, 214 (*rev*)
Wiberg, K.B. *et al., J.O.C.*, 1980, **45**, 4936 (*cmr*)
Colosimo, M. *et al., Org. Mass Spectrom.*, 1982, **17**, 286 (*ms*)
Anderson, A. *et al., J. Chem. Phys.*, 1985, **82**, 99 (*ir, Raman*)
IARC Monog., 1986, **41**, 161; *Suppl.* 7, 246; *Suppl.* 6, 389 (*rev, tox*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **5**, 1028 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1104
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **2**, 1146-1147 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1-423 (*rev, occur*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 3436
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 325
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0413
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 307, Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MIF765

4-Chloromethylene-1,2,3,4-tetrahydro-8-methyl-6-quinolinol C-393

4-Chloromethylene-1,2,3,4-tetrahydro-6-hydroxy-8-methylquinoline



$C_{11}H_{12}ClNO$ 209.675

(*E*)-*form*

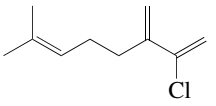
O-*(2,4-Di*-O-*methyl-β-D-xylopyranoside):* [501373-67-7]
$C_{18}H_{24}ClNO_5$ 369.844
Alkaloid from a Puerto Rican *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{22}$ -20.8 (c, 0.12 in $CHCl_3$). λ_{max} 212 (log ϵ 4.58); 241 (log ϵ 4.29); 269 (log ϵ 3.9) (MeOH).

Nogle, L.M. *et al., J. Nat. Prod.*, 2003, **66**, 217-220 (*isol, pmr, cmr, ms*)

2-Chloro-7-methyl-3-methylene-1,6-octadiene C-394

*2-Chloro-β-myrcene. 7-**Chloromyrcene***

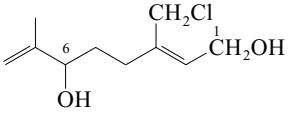
[55498-34-5]



$C_{10}H_{15}Cl$ 170.681
Constit. of *Chondrococcus* (*Desmia*) *hornemanni* (*Portieria hornemannii*) and *Chondrococcus japonicus*. Oil. λ_{max} 228 (ϵ 10250) (hexane).

Ichikawa, N. *et al., Chem. Lett.*, 1974, 1333-1336 (*isol, ms, pmr*)
Ichikawa, N. *et al., Proc. Jpn. Acad.*, 1975, **51**, 562 (*isol*)
Burreson, B.J. *et al., Tet. Lett.*, 1975, 2155-2158 (*isol*)

3-Chloromethyl-7-methyl-2,7-octadiene-1,6-diol C-395



$C_{10}H_{17}ClO_2$ 204.696

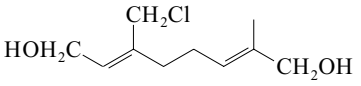
1-Me ether: 6-Chloromethyl-8-methoxy-2-methyl-1,6-octadien-3-ol, 9CI
[136980-53-5]
$C_{11}H_{19}ClO_2$ 218.723
Constit. of *Portieria hornemannii*. Oil. $[\alpha]_D^{25}$ -6.3 (c, 0.19 in $CHCl_3$).

6-Me ether: 3-Chloromethyl-6-methoxy-7-methyl-2,7-octadien-1-ol, 9CI
[136980-54-6]
$C_{11}H_{19}ClO_2$ 218.723
Constit. of *Portieria hornemannii*. Oil. $[\alpha]_D^{25}$ -18.3 (c, 0.12 in $CHCl_3$).

Di-Me ether: 6-Chloromethyl-3,8-dimethoxy-2-methyl-1,6-octadiene
[125538-05-8]
$C_{12}H_{21}ClO_2$ 232.749
Constit. of *Chondrococcus hornemanni*. Oil. $[\alpha]_D$ -23.9 (c, 0.004 in $CHCl_3$).

Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1983 (*Di-Me ether*)
Wright, A.D. *et al., Tetrahedron*, 1991, **47**, 5717 (*isol, pmr, cmr*)

6-Chloromethyl-2-methyl-2,6-octadiene-1,8-diol C-396



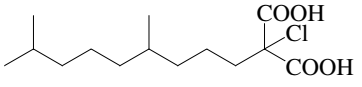
$C_{10}H_{17}ClO_2$ 204.696

(2E,6Z)-form

Di-Me ether: 6-Chloromethyl-1,8-dimethoxy-2-methyl-2,6-octadiene
[125538-06-9]
$C_{12}H_{21}ClO_2$ 232.749
Constit. of *Chondrococcus hornemanni*. Oil.
Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1983 (*isol, pmr, cmr*)

3-Chloro-1-nor-2,15-farnesanedioic acid C-397

2-Chloro-2-(4,8-dimethylnonyl)propanedioic acid

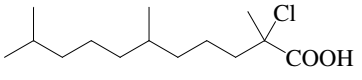


$C_{14}H_{25}ClO_4$ 292.802

Mono-Me ester: [158563-22-5]
$C_{15}H_{27}ClO_4$ 306.829
Isol. from the brown alga *Padina tetrastromatica*.
Parameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 1006-1008

3-Chloro-1-nor-2-farnesanoic acid C-398

2-Chloro-2,6,10-trimethylundecanoic acid
[158563-20-3]

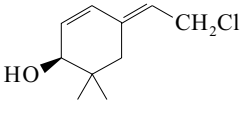


$C_{14}H_{27}ClO_2$ 262.819
Isol. from brown alga *Padina tetrastromatica*. Obt. as a mixt. with its bromo analogue.

Bromo analogue: ***3-Bromo-1-nor-2-farnesanoic acid***. *2-Bromo-2,6,10-trimethylundecanoic acid*
[158563-21-4]
$C_{14}H_{27}BrO_2$ 307.27
Isol. from *Padina tetrastromatica*.
Parameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 1006-1008

1-Chloro-2,4-ochtodadien-6-ol C-399

4-(2-Chloroethylidene)-6,6-dimethyl-2-cyclohexen-1-ol

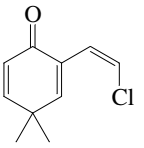


$C_{10}H_{15}ClO$ 186.681

(E)-form [73872-81-8]
Constit. of *Ochtodes crockeri*. Oil. $[\alpha]_D^{20}$ +5.7 (c, 1 in $CHCl_3$).
Paul, V.J. *et al., J.O.C.*, 1980, **45**, 3401 (*isol, struct*)
Zegarski, J. *et al., Tet. Lett.*, 1985, **26**, 1363 (*synth*)

1-Chloro-1,3(8),5-ochtodatrien-4-one C-400

2-(2-Chloroethenyl)-4,4-dimethyl-2,5-cyclohexadien-1-one

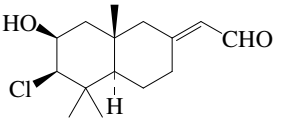


$C_{10}H_{11}ClO$ 182.649

(Z)-form [568597-57-9]
Constit. of *Portieria hornemanni*. Oil.

Bromo analogue: 2-(2-Bromoethenyl)-4,4-dimethyl-2,5-cyclohexadien-1-one. ***1-Bromo-1,3(8),5-ochtodatrien-4-one***
[568597-56-8]
$C_{10}H_{11}BrO$ 227.1
Isol. from *Portieria hornemanni*. Oil.
Kuniyoshi, M. *et al., J. Chin. Chem. Soc. (Taipei)*, 2003, **50**, 167-170 (*isol, pmr, cmr*)

[6-Chlorooctahydro-7-hydroxy-5,5,8*a*-trimethyl-2(1*H*)-naphthalenylidene]acetaldehyde C-401



(*E*)-*form*

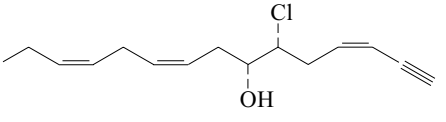
$C_{15}H_{23}ClO_2$ 270.798

(E)-form [321557-57-7]
Constit. of *Stylotella aurantium*. Oil. $[\alpha]_D^{25}$ +16 (c, 0.13 in $CHCl_3$). λ_{max} 235 (log ϵ 3.5); 285 (log ϵ 3.3) (MeOH).

(Z)-form [321557-58-8]
Constit. of *Stylotella aurantium*. Oil. $[\alpha]_D^{25}$ -28 (c, 0.13 in $CHCl_3$). λ_{max} 240 (log ϵ 3.9); 285 (log ϵ 3.1) (MeOH).
Musman, M. *et al., J. Nat. Prod.*, 2001, **64**, 111-113 (*isol, pmr, cmr*)

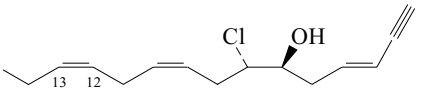
6-Chloro-3,9,12-pentadecatrien-1-yn-7-ol C-402

Prerogioloxepane



$C_{15}H_{21}ClO$ 252.783
Constit. of *Laurencia microcladia*. Oil.
Guella, G. *et al., Helv. Chim. Acta*, 1992, **75**, 303 (*isol, pmr, cmr*)

7-Chloro-3,9,12-pentadecatrien-1-yn-6-ol C-403



(3*E*,6*S*,7*S*,9*Z*,12*Z*)–*form*

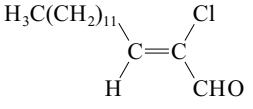
$C_{15}H_{21}ClO$ 252.783

(3E,6S,7S,9Z,12Z)-form [139026-38-3]
Constit. of *Laurencia pinnatifida*.
Ac: [139026-36-1]
$C_{17}H_{23}ClO_2$ 294.82
Constit. of *Laurencia pinnatifida*. Oil. $[\alpha]_D^{25}$ -12.9 (c, 0.35 in $CHCl_3$).

12,13-Dihydro: 7-Chloro-3,9-pentadecadien-1-yn-6-ol
[139026-41-8]
$C_{15}H_{23}ClO$ 254.799
Constit. of *Laurencia pinnatifida*. Oil. $[\alpha]_D^{25}$ +17 (c, 0.18 in $CHCl_3$).
12,13-Dihydro, Ac: [139026-43-0]
$C_{17}H_{25}ClO_2$ 296.836
Constit. of *Laurencia pinnatifida*. Oil. $[\alpha]_D^{25}$ -12.9 (c, 1.16 in $CHCl_3$).

(3*Z*,6*S*,7*S*,9*Z*,12*Z*)-*form* [139026-37-2]
Ac: [139026-35-0]
Constit. of *Laurencia pinnatifida*. Oil. $[\alpha]_D^{25}$ +18.5 (c, 0.85 in $CHCl_3$).
12,13-Dihydro: [139039-80-8]
Constit. of *Laurencia pinnatifida*. Oil. $[\alpha]_D^{25}$ -9.1 (c, 0.4 in $CHCl_3$).
12,13-Dihydro, Ac: [139026-42-9]
Constit. of *Laurencia pinnatifida*. Oil. $[\alpha]_D^{25}$ +39.7 (c, 0.47 in $CHCl_3$).
Norte, M. *et al., Tetrahedron*, 1991, **47**, 9411 (*isol, pmr, cmr*)

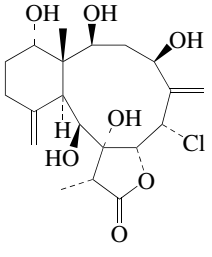
2-Chloro-2-pentadecenal C-404



$C_{15}H_{27}ClO$ 258.83

(*Z*)-*form* [155502-44-6]
Constit. of the red alga *Laurencia flexilis*. Oil.
de Nys, R. *et al., Phytochemistry*, 1993, **34**, 725 (*isol*)

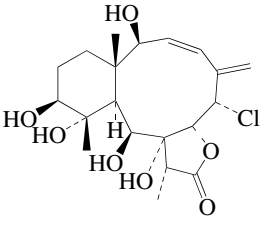
6-Chloro-2,4,8,9,14-pentahydroxy-5(16),11(20)-briaradien-18,7-olide C-405



$C_{20}H_{29}ClO_7$ 416.898

(2β,4β,6α,7α,8α,9β,14α,17α)-*form*
2,4,9,14-Tetra-Ac: ***Junceellonoid A***
[804557-37-7]
$C_{28}H_{37}ClO_{11}$ 585.046
Constit. of *Junceella fragilis*. Cryst.
Mp 167-169°. $[\alpha]_D^{20}$ +31.2 (c, 0.17 in $CHCl_3$).
Zhang, W. *et al., Helv. Chim. Acta*, 2004, **87**, 2341-2345 (*Junceellonoid A*)

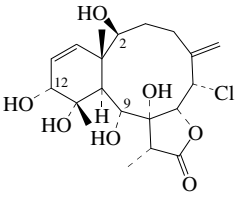
6-Chloro-2,8,9,11,12-pentahydroxy-3,5(16)-briaradien-18,7-olide C-406



$C_{20}H_{29}ClO_7$ 416.898

(2β,3*Z*,6α,7α,8α,9β,11α,12β,17α)-*form*
12-(2-Methylpropanoyl), 2-propanoyl, 9-Ac: ***Renillin A***
[851319-98-7]
$C_{29}H_{41}ClO_{10}$ 585.09
Constit. of *Renilla reniformis*. Amorph. powder. $[\alpha]_D^{25}$ -92 (c, 0.02 in $CHCl_3$).
Barsby, T. *et al., J. Nat. Prod.*, 2005, **68**, 511-516 (*Renillin A*)

6-Chloro-2,8,9,11,12-pentahydroxy-5(16),13-briaradien-18,7-olide C-407



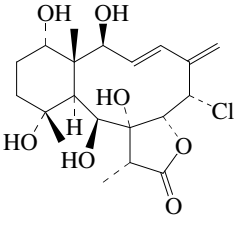
(2β,6α,7α,8α,9α,11α,12α)-*form*

$C_{20}H_{29}ClO_7$ 416.898

(2β,6α,7α,8α,9α,11α,12α)-*form*
2,9,12-Tri-Ac: ***Minabein 3***
[104993-09-1]
$C_{26}H_{35}ClO_{10}$ 543.009
Constit. of *Minabea*. Cryst. ($CHCl_3$).
Mp 241-243°.
12-Ketone, 2,9-di-Ac: ***Minabein 2***
[104993-08-0]
$C_{24}H_{31}ClO_9$ 498.956
Constit. of *Minabea* sp. Oil. λ_{max} 218 (ϵ 5810) (MeOH).

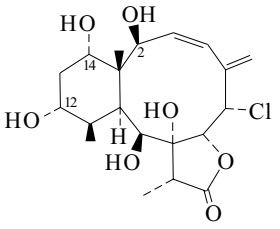
(2β,6α,7α,8α,9β,11α,12α)-*form*
13α,14α-Epoxide: 6-Chloro-13,14-epoxy-2,8,9,11,12-pentahydroxy-5(16)-briaren-18,7-olide
$C_{20}H_{29}ClO_8$ 432.897
13α,14α-Epoxide, 12-butanoyl, 2,9-di-Ac: [446823-30-9]
$C_{28}H_{39}ClO_{11}$ 587.062
Constit. of *Briareum asbestinum*. Solid. $[\alpha]_D^{26}$ -50.8 (c, 0.185 in $CHCl_3$).
13α,14α-Epoxide, 2,12-dibutanoyl, 9-Ac: [446823-29-6]
$C_{30}H_{43}ClO_{11}$ 615.116
Constit. of *Briareum asbestinum*. Solid. $[\alpha]_D^{24}$ -61.3 (c, 1.1 in $CHCl_3$).
Ksebati, M.B. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 835-851 (*Minabeins*)
González, N. *et al., J.O.C.*, 2002, **67**, 5117-5123 (*epoxide derivs*)

6-Chloro-2,8,9,11,14-pentahydroxy-3,5(16)-briaradien-18,7-olide C-408



$C_{20}H_{29}ClO_7$ 416.898
2,9,14-Tri-Ac: ***Umbraculolide D***
[288850-29-3]
$C_{26}H_{35}ClO_{10}$ 543.009
Constit. of *Gorgonella umbraculum*. Cryst. ($CHCl_3$).
Mp 210°. $[\alpha]_D^{25}$ +13 (c, 0.1 in $CHCl_3$).
Subrahmanyam, C. *et al., Tetrahedron*, 2000, **56**, 4585-4588 (*isol, pmr, cmr*)

6-Chloro-2,8,9,12,14-pentahydroxy-3,5(16)-briaradien-18,7-olide C-409

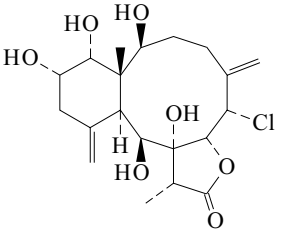


$C_{20}H_{29}ClO_7$ 416.898

14-Butanoyl, 2,9-di-Ac: ***Ptilosarcol***
[107716-26-7]
$C_{28}H_{39}ClO_{10}$ 571.063
Constit. of sea fern *Ptilosarcus gurneyi*. Shows insecticidal props. $[\alpha]_D^{26}$ -55.8 (c, 1.46 in CH_2Cl_2).

12-Ketone,14-butanoyl, 2,9-di-Ac: ***Ptilosarcone***
[64597-86-0]
$C_{28}H_{37}ClO_{10}$ 569.047
Constit. of *Ptilosarcus gurneyi*. Insecticidal. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{26}$ -76.7 (c, 0.64 in CH_2Cl_2). λ_{max} 230 (ϵ 6700) (MeOH) (Derep). λ_{max} 218 (ϵ 5100) (EtOH) (Berdy).
▶ LD_{50} (mus, ipr) 7.4 mg/kg.
Hendrickson, R.L. *et al., Tetrahedron*, 1986, **42**, 6565 (*isol*)
Williams, D.E. *et al., Can. J. Chem.*, 1987, **65**, 2244 (*deriv, struct*)

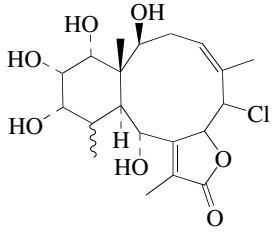
6-Chloro-2,8,9,13,14-pentahydroxy-5(16),11(20)-briaradien-18,7-olide C-410



$C_{20}H_{29}ClO_7$ 416.898

2,9,13,14-Tetra-Ac: ***Nuiinoalide C***
[173867-29-3]
$C_{28}H_{37}ClO_{11}$ 585.046
Constit. of an octocoral. Solid. $[\alpha]_D$ +29 (c, 0.4 in $CHCl_3$).
Hamann, M.T. *et al., Heterocycles*, 1996, **42**, 325 (*isol, pmr, cmr*)

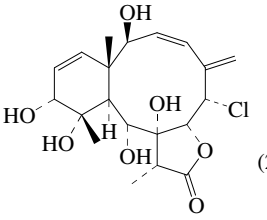
6-Chloro-2,9,12,13,14-pentahydroxy-4,8(17)-briaradien-18,7-olide C-411



$C_{20}H_{29}ClO_7$ 416.898

13-(3-Methylbutanoyl), 2,9,12,14-tetra-Ac: ***Juncin G***
[189513-64-2]
$C_{33}H_{45}ClO_{12}$ 669.164
Constit. of *Junceella juncea*. Oil. $[\alpha]_D^{25}$ +55.2 (c, 0.27 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., J.C.S. Perkin 1*, 1997, 959-962 (*isol, pmr*)

6-Chloro-2,8,9,11,12-pentahydroxy-3,5(16),13-briaratrien-18,7-olide C-412



(2β,3*Z*,6α,7α,8α,9α,11α,12α)-*form*

$C_{20}H_{27}ClO_7$ 414.882

(2β,3*Z*,6α,7α,8α,9α,11α,12α)-*form*

2,9-Di-Ac: ***Minabein 5***
[104993-11-5]
$C_{24}H_{31}ClO_9$ 498.956
Constit. of *Minabea* sp. Powder.
Mp 155-158°. λ_{max} 220 (ϵ 5000) (MeOH).

2,9,12-Tri-Ac: ***Minabein 4***
[104993-10-4]
$C_{26}H_{33}ClO_{10}$ 540.993
Constit. of *Minabea* sp. Powder.
Mp 227-230°. $[\alpha]_D$ -299 (c, 0.9 in $CHCl_3$). λ_{max} 222 (ϵ 4140) (MeOH).

12-Ketone, 2,9-di-Ac: ***Minabein 1***
[104993-07-9]
$C_{24}H_{29}ClO_9$ 496.94
Constit. of *Minabea* sp. Powder.
Mp 190-192°. $[\alpha]_D$ -48 (c, 1.5 in $CHCl_3$). λ_{max} 218 (ϵ 12060) (MeOH).

(2β,3*Z*,6α,7α,8α,9β,11α,12α)-*form*

2,9,12-Tri-Ac: ***Nuiinoalide D***
[173938-26-6]
$C_{26}H_{33}ClO_{10}$ 540.993
Constit. of an octocoral. Cryst. (MeOH).

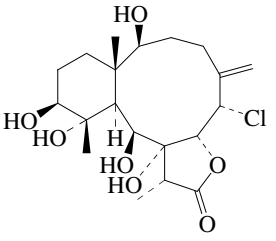
13α,14α-Epoxide: 6-Chloro-13,14-epoxy-2,8,9,11,12-pentahydroxy-3,5(16)-briaradien-18,7-olide
$C_{20}H_{27}ClO_8$ 430.881

13α,14α-Epoxide, 2-butanoyl, 9,12-di-Ac: ***11-Hydroxybrianthein Y***
[446881-29-4]
$C_{28}H_{37}ClO_{11}$ 585.046
Constit. of *Briareum asbestinum*. Solid. $[\alpha]_D^{27}$ -103.3 (c, 0.37 in $CHCl_3$).

13α,14α-Epoxide, 12-butanoyl, 2,9-di-Ac: ***11-Hydroxybrianthein U***
[446823-28-5]
$C_{28}H_{37}ClO_{11}$ 585.046
Constit. of *Briareum asbestinum*. Solid. $[\alpha]_D^{28}$ -128.6 (c, 0.55 in $CHCl_3$).

13α,14α-Epoxide, 2,12-dibutanoyl, 9-Ac: ***11-Hydroxybrianthein V***
[446823-26-3]
$C_{30}H_{41}ClO_{11}$ 613.1
Constit. of *Briareum asbestinum*. Cryst. $[\alpha]_D^{24}$ -124.4 (c, 1.16 in $CHCl_3$).
Ksebati, M.B. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 835-851 (*Nuiinoalide D*)
Hamann, M.T. *et al., Heterocycles*, 1996, **42**, 325 (*isol, pmr, cmr*)
González, N. *et al., J.O.C.*, 2002, **67**, 5117-5123 (*Hydroxybriantheins, isol, pmr, cmr, cryst struct*)
Lievens, S.C. *et al., J. Nat. Prod.*, 2004, **67**, 2130-2132 (*Minabein 4, cryst struct*)

6-Chloro-2,8,9,11,12-pentahydroxy-5(16)-briaren-18,7-olide C-413

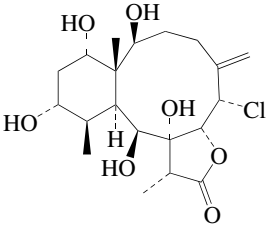


$C_{20}H_{31}ClO_7$ 418.913

(2β,6α,7α,8α,9β,11α,12β,17α)-*form*

12-(2-Methylpropanoyl), 2-propanoyl, 9-Ac: ***Renillin B***
[851319-99-8]
$C_{29}H_{43}ClO_{10}$ 587.105
Constit. of *Renilla reniformis*. Amorph. powder. $[\alpha]_D^{25}$ -52 (c, 0.015 in $CHCl_3$).
Barsby, T. *et al., J. Nat. Prod.*, 2005, **68**, 511-516 (*Renillin B*)

6-Chloro-2,8,9,12,14-pentahydroxy-5(16)-briaren-18,7-olide C-414

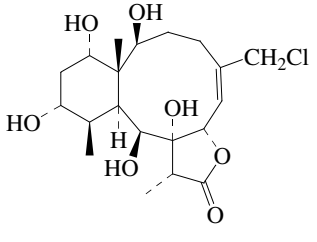


$C_{20}H_{31}ClO_7$ 418.913

(2β,6α,7α,8α,9β,12α,14α)-*form*

2,9,14-Tri-Ac: ***Briviolide C***
[868526-10-7]
$C_{26}H_{37}ClO_{10}$ 545.025
Constit. of a *Briareum* sp. Cryst. (MeOH).
Mp 171-172° dec. $[\alpha]_D$ -36 (c, 0.19 in MeOH).
Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 2083-2093 (*Briviolide C, cryst struct*)

16-Chloro-2,8,9,12,14-pentahydroxy-5-briaren-18,7-olide C-415



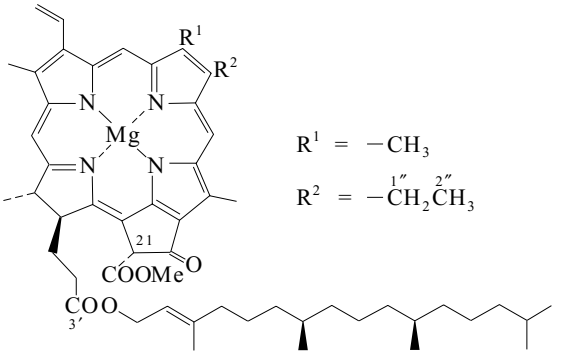
$C_{20}H_{31}ClO_7$ 418.913

(2β,5*E*,7α,8α,9β,12α,14α)-*form*

2,9,14-Tri-Ac: ***Briviolide B***
[868526-09-4]
$C_{26}H_{37}ClO_{10}$ 545.025
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ -32 (c, 0.34 in MeOH).
Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 2083-2093 (*Briviolide B*)

Chlorophyll a C-416

[3,7,11,15-Tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(2-)-N^{23},N^{24},N^{25},N^{26}]magnesium, 9CI
[479-61-8]



$C_{55}H_{72}MgN_4O_5$ 893.503
Green pigment of leaves of plants, occurring together with Chlorophyll b. Can be obt. readily in pure form from the blue-green alga *Anacystis nidulans*. Photosynthetic pigment. Dark green greasy powder (petrol) or leaflets. Sol. EtOAc, Et_2O; fairly sol. MeOH; poorly sol. hexane.
Mp 117-120°. $[\alpha]_D^{20}$ -262 (Me_2CO). Dilute acid removes Mg to form Phaeophytin a, P-297. Hydrol. by Chlorophyllase (or warm acid) → Phaeophorbide a, P-295. Acid catalysed methanolysis → see Phaeophorbide a P-295. Alkaline hydrol. → Chlorin e_6. Other esters e.g. geranylgeranyl are found in various microorganisms.
λ_{max} 409; 429; 498; 537; 577; 613; 660 (EtOH) (Berdy).

21-Epimer: ***Chlorophyll a′***
[22309-13-3]
$C_{55}H_{72}MgN_4O_5$ 893.503
Isol. from chlorophyll extracts.

3′-Free acid: ***Chlorophyllide a***
[14897-06-4]
$C_{35}H_{34}MgN_4O_5$ 614.982
Pigment from various spp. Intermed. in chlorophyll biosynth.

21-Hydroxy: ***13²-Hydroxychlorophyll a***
[71699-04-2]
$C_{55}H_{72}MgN_4O_6$ 909.502
Isol. from chlorophyll extracts. Artifact.

6-Chloro, 21-hydroxy: 20-Chloro-13²-hydroxychlorophyll a. ***Chlorophyll RCI***
[91488-37-8]
$C_{55}H_{71}ClMgN_4O_6$ 943.947
Isol. from chlorophyll extracts. Probable artifact.

1″,2″-Didehydro: 4-Vinyl-4-desethylchlorophyll a
$C_{55}H_{70}MgN_4O_5$ 891.487
Major chlorophyll from maize mutant.

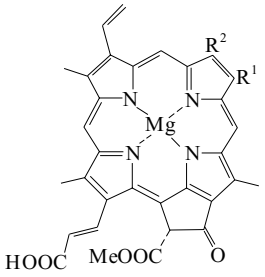
[1406-65-1, 117288-86-5, 118626-30-5]

Woodward, R.B. *et al., J.A.C.S.*, 1960, **82**, 3800 (*synth*)
Fleming, I. *et al., Nature (London)*, 1967, **216**, 151 (*abs config*)
Brockman, H. *et al., Annalen*, 1974, 1007
Chow, H.C. *et al., J.A.C.S.*, 1975, **97**, 7230 (*cryst struct*)
Chem. Biochem. Plant Pigm., (Ed. Goodwin, T.W.), Academic Press, London, 1976, (*book*)
Schoch, S. *et al., Z. Pflanzenphysiol.*, 1977, **83**, 427 (*isol*)
Gleixner, G. *et al., Experientia*, 1982, **38**, 303 (*purifn*)
Bazzaz, M.B. *et al., Tet. Lett.*, 1982, **23**, 1211 (*Divinylchlorophyll a*)
Lotjonen, S. *et al., Org. Magn. Reson.*, 1983, **21**, 757 (*cmr*)
Smith, K.M. *et al., Org. Magn. Reson.*, 1984, **22**, 779 (*pmr*)
Leeper, F.J. *et al., Nat. Prod. Rep.*, 1985, **2**, 19; 561; 1987, **4**, 441; 1989, **6**, 171 (*rev, biosynth*)
Fujiwara, M. *et al., J. Phys. Chem.*, 1986, **90**, 250; 5646 (*ir, Raman*)
Grotemeyer, J. *et al., J.A.C.S.*, 1986, **108**, 4233 (*ms*)
Tasumi, M. *et al., Adv. Spectrosc. (Chichester, U.K.)*, 1987, **14**, 407 (*rev, ir, Raman*)
Senge, M. *et al., FEBS Lett.*, 1988, **234**, 215 (*Chlorophyll RCI*)

Senge, M. *et al., Z. Naturforsch., C*, 1988, **43**, 515 (*13²-Hydroxychlorophyll a*)
Okazaki, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 3303 (*biosynth*)
Grese, R.P. *et al., J. Am. Soc. Mass Spectrom.*, 1990, **1**, 72 (*Chlorophyll RCI*)
Woodward, R.B. *et al., Tetrahedron*, 1990, **46**, 7599 (*synth, rev*)
Giacometti, G. *et al., Gazz. Chim. Ital.*, 1991, **121**, 457 (*pmr*)
Roth, L. *et al., Roth Collection of Natural Product Data*, VCH, Weinheim, 1995, (*bibl, spectra*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 581
Ruediger, W. *et al., Phytochemistry*, 1997, **46**, 1151-1167 (*rev, biosynth*)
Itoh, D. *et al., J. Nat. Prod.*, 2000, **63**, 1090-1093 (*biosynth*)

Chlorophyll c C-417

Chlorophyllide c



c_1, R^1 = CH=CH_2, R^2 = CH_3

c_2, R^1 = CH_2CH_3, R^2 = CH_3

c_3, R^1 = CH=CH_2, R^2 = COOMe

In spite of their name these are porphyrins, not dihydro derivs. (or chlorins). Widely distributed photosynthetic pigment in marine organisms, e.g. the diatom *Nitzschia closterium*. Cryst. (THF/petrol). λ_{max} 447; 578; 626 (Et_2O).

Chlorophyll c_1 [18901-56-9]

$C_{35}H_{28}MgN_4O_5$ 608.935

Chlorophyll c_2 [27736-03-4]

$C_{35}H_{30}MgN_4O_5$ 610.951

Chlorophyll c_3 [111308-93-1]

$C_{36}H_{28}MgN_4O_7$ 652.945

Isol. from Haptophyte *Emiliania huxleyi*.

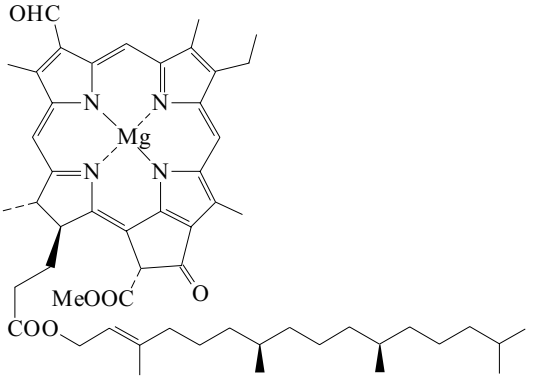
[1406-65-1]

Dougherty, R.C. *et al., J.A.C.S.*, 1970, **92**, 2826
Budzikiewicz, H. *et al., Tetrahedron*, 1971, **27**, 1447 (*isol, ir, pmr, ms, struct*)
Chem. Biochem. Plant Pigm., (Ed. Goodwin, T.W.), Academic Press, London, 1976, (*book*)
Clezy, P.S. *et al., Aust. J. Chem.*, 1978, **31**, 2491 (*synth*)
The Porphyrins, (Ed. Dolphin, D.), Academic Press, N.Y., 1978, (*book*)
Leeper, F.J. *et al., Nat. Prod. Rep.*, 1985, **2**, 19; 561; 1987, **4**, 441; 1989, **6**, 171 (*rev, biosynth*)
Tasumi, M. *et al., Adv. Spectrosc. (Chichester, U.K.)*, 1987, **14**, 407 (*rev, ir, Raman*)
Fookes, C.J.R. *et al., Chem. Comm.*, 1989, 1827 (*isol, pmr, struct, Chlorophyll c_3*)

Chlorophyll d C-418

[3,7,11,15-Tetramethyl-2-hexadecenyl-14-ethyl-9-formyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(2-)-N^{23},N^{24},N^{25},N^{26}]magnesium, 9CI

[519-63-1]



$C_{54}H_{70}MgN_4O_6$ 895.475

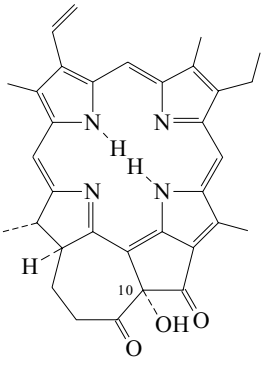
Photosynthetic pigment. Characteristic chlorophyll of red algae. Has been considered an artifact, but now thought to be a genuine nat. product. λ_{max} 445; 686 (Et_2O).

[1406-65-1]

Chem. Biochem. Plant Pigm., Goodwin, T.W., Ed., Academic Press, London, 1976, (*book*)
The Porphyrins, Dolphin, D., Ed., Academic Press, N.Y., 1978, (*book*)
Leeper, F.J. *et al., Nat. Prod. Rep.*, 1985, **2**, 19; 561; 1987, **4**, 441; 1989, **6**, 171 (*revs, biosynth*)

Chlorophyllone a C-419

[127266-93-7]



$C_{33}H_{32}N_4O_3$ 532.641

Isol. from *Ruditapes philippinarum*, *Crassostrea* sp. and *Patinopecten yessoensis*. Antioxidant. Dark green pigment. λ_{max} 408 (ϵ); 503 (ϵ); 534 (ϵ); 608 (ϵ); 665 (ϵ) (MeOH) (Derep).

10-Epimer: ***Epichlorophyllone a***

[134454-36-7]

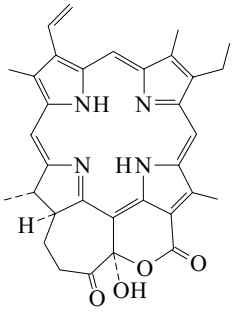
$C_{33}H_{32}N_4O_3$ 532.641

From *Ruditapes philippinarum* and *Patinopecten yessoensis*. Antioxidant.

Sakata, K. *et al., Tet. Lett.*, 1990, **31**, 1165-1168 (*isol, pmr, cmr, struct*)
Watanabe, N. *et al., J. Nat. Prod.*, 1993, **56**, 305 (*isol*)
Sakata, K. *et al., ACS Symp. Ser.*, 1994, **547**, 164 (*rev*)
Ma, L. *et al., J.O.C.*, 1996, **61**, 2501 (*synth, uv, pmr, cmr*)

Chlorophyllone lactone a C-420

[134381-11-6]

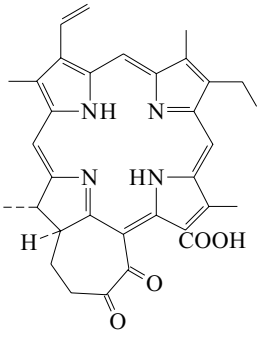


$C_{33}H_{32}N_4O_4$ 548.64

Isol. from *Ruditapes philippinarum* and various marine bivalves. Antioxidant. Dark green cryst. Mp >300°. λ_{max} 282; 400; 498; 529; 610; 667 (MeOH). λ_{max} 282; 400; 498; 529; 610; 667 (MeOH) (Berdy).

Watanabe, N. *et al., J. Nat. Prod.*, 1993, **56**, 305-317 (*isol, pmr, cmr, struct*)
Ma, L. *et al., J.O.C.*, 1996, **61**, 2501 (*synth, uv, pmr, cmr*)

Chlorophyllonic acid a C-421



Relative configuration

$C_{33}H_{32}N_4O_4$ 548.64

Me ester: [143070-43-3]
$C_{34}H_{34}N_4O_4$ 562.667

Isol. from the clam *Ruditapes philippinarum*, microalga *Fragillaria* sp., *Ruditapes phillipinarum* and *Patinopecten yessoensis*. Antioxidant. Brown plates ($CHCl_3$/MeOH).
Mp 219°. λ_{max} 278 (ϵ); 400 (ϵ); 504 (ϵ); 540 (ϵ); 610 (ϵ); 677 (ϵ) (MeOH) (Derep). λ_{max} 278; 400; 504; 540; 610; 677 (MeOH) (Berdy).

Yamamoto, K. *et al., Tet. Lett.*, 1992, **33**, 2587-2588 (*isol, struct*)
Watanabe, N. *et al., J. Nat. Prod.*, 1993, **56**, 305 (*isol*)
Ma, L. *et al., J.O.C.*, 1996, **61**, 2501 (*synth, pmr, cmr, uv*)

2-Chloro-2-propenoic acid, 9CI C-422

2-Chloroacrylic acid
[598-79-8]
$H_2C{=}CClCOOH$
$C_3H_3ClO_2$ 106.508

Occurs in *Asparagopsis taxiformis*. Cryst. (petrol). Sol. H_2O, EtOH, Et_2O.
Mp 65°. Bp 176-181° dec. Subl. The acid, esters and nitrile undergo free radical polym.

▶ LD_{50} (mus, ivn) 42 mg/kg. AS5952000

Me ester: Methyl 2-chloroacrylate
[80-63-7]
$C_4H_5ClO_2$ 120.535
Liq. V. sol. Et_2O. d^{20} 1.19. Bp 139° Bp_{51} 52°. n_D^{20} 1.4420. Q/e values for copolym., Q 2.43, e +0.35.

▶ Eye and skin irritant. LC_{50} (rat, ihl) 500 mg m^{-3} (2h exposure). AS6380000

Et ester: Ethyl 2-chloroacrylate
[687-46-7]
$C_5H_7ClO_2$ 134.562
Liq. V. sol. EtOH, Et_2O. d^{20} 1.14. Bp_{15} 44°. n_D^{20} 1.4384. Rate for radical polym., k_p = 1660 L mol^{-1} s^{-1}, $k_t = 3.33 \times 10^8$ L mol^{-1} s^{-1}.

▶ AS6340000

2,2,2-Trifluoroethyl ester: [74359-02-7]
$C_5H_4ClF_3O_2$ 188.533
Polymers are used in photoresists.

Ph ester: [46115-39-3]
$C_9H_7ClO_2$ 182.606
Bp_8 91-93°. n_D^{20} 1.5803.

Fluoride: [683-71-6]
C_3H_2ClFO 108.499
Liq. Bp 67-67.5°.

▶ LD_{50} (mus, ivn) 100 mg/kg.

Chloride: 2-Chloroacrylyl chloride
[21369-76-6]
$C_3H_2Cl_2O$ 124.954
Reactive dienophile. Liq. Bp_{79} 45-48° (lit. gives a pressure range).

▶ AT7400000

Amide: 2-Chloroacrylamide
[16490-68-9]
C_3H_4ClNO 105.523
Cryst. (C_6H_6). Mp 94°.

Nitrile: 2-Chloroacrylonitrile. 1-Chloro-1-cyanoethylene
[920-37-6]
C_3H_2ClN 87.508
Reactive dienophile. Liq. Bp 88°. n_D^{20} 1.4280.

▶ Highly toxic, flammable. AT5525000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 852A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1371B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 810B (*ir*)
Otto, R. *et al., Ber.*, 1885, **18**, 239 (*synth*)
McElvain, S.M. *et al., J.A.C.S.*, 1959, **81**, 2579 (*esters, synth*)
Lorette, N.B. *et al., J.O.C.*, 1961, **26**, 2324 (*nitrile*)
Losev, I.P. *et al., CA*, 1962, **56**, 1590c (*polym, esters*)
Pande, K.C. *et al., J.O.C.*, 1970, **35**, 1169 (*nitrile*)
Wesslen, B. *et al., Macromolecules*, 1971, **4**, 20 (*polym, Et ester*)
Yasnitskii, B.G. *et al., CA*, 1972, **76**, 85319c (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 77; 1975, **5**, 107 (*use*)
Tagieva, F.M. *et al., Azerb. Khim. Zh.*, 1977, 52; *CA*, **87**, 85329h (*polym, nitrile*)
Movsum-Zade, E.M. *et al., CA*, 1977, **86**, 4914z (*synth*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427 (*Q/e values, Me ester*)
Yamada, B. *et al., J. Macromol. Sci., Part A: Chem.*, 1983, **19**, 1023 (*polym, kinetics, Et ester*)
Lingnau, J. *et al., Macromolecules*, 1984, **17**, 941 (*polym, kinetics, Me ester*)
Babu, G.N. *et al., Macromolecules*, 1984, **17**, 2761 (*synth, polym, trifluoroethyl ester*)
Pathak, C.P. *et al., Macromolecules*, 1986, **19**, 1035 (*synth, polym, esters*)
Gajewski, J.J. *et al., J.A.C.S.*, 1989, **111**, 9078 (*Me ester, synth, pmr*)
Durig, J.R. *et al., J. Chem. Phys.*, 1990, **93**, 905 (*synth, fluoride, ir, Raman*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **2**, 1073-1074 (*nitrile, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CEE500; CEE750; MIF800

3-Chloro-2-propenoic acid, 9CI C-423

3-Chloroacrylic acid
[625-40-1]
$ClCH{=}CHCOOH$
$C_3H_3ClO_2$ 106.508

(Z)-form [1609-93-4]

Occurs in *Asparagopsis taxiformis*. Cotton defoliant and crop desiccant. Cryst. (HCl aq.). Sol. EtOH, Et_2O.
Mp 60.8-61.4°. $Bp_{17.5}$ 107°. pK_{a1} 3.45 (25°).

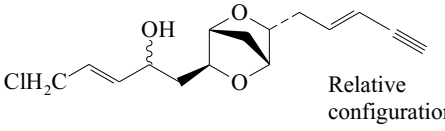
▶ Corrosive, lachrymator.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 516A; 516B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 805C; 806A (*nmr*)
Otto, R. *et al., Annalen*, 1887, **239**, 257 (*synth*)
Backer, H.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1935, **54**, 167

Marvel, C.S. *et al., J.A.C.S.*, 1940, **62**, 3497 (*synth*)
Herrett, R.A. *et al., Science (Washington, D.C.)*, 1963, **141**, 1192 (*use*)
McGreer, D.E. *et al., Can. J. Chem.*, 1973, **51**, 1239
Brailovskii, S.M. *et al., Zh. Org. Khim.*, 1977, **13**, 1158; *J. Org. Chem. USSR (Engl. Transl.)*, 1977, **13**, 1066 (*synth*)
Kozerski, L. *et al., Org. Magn. Reson.*, 1979, **12**, 365 (*cmr*)
Urdaneta, N.A. *et al., Synth. Commun.*, 2002, **32**, 3003-3009; 2004, **34**, 657-664 (*synth, pmr, ms*)

α-(3-Chloro-1-propenyl)-6-(2-penten-4-ynyl)-2,5-dioxabicyclo[2.2.1]heptane-3-ethanol, 9CI C-424

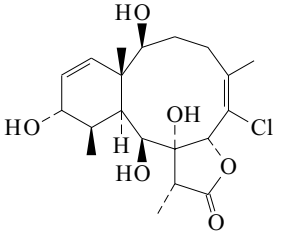
6,9:7,10-Diepoxy-1-chloro-2,12-pentadecadien-14-yn-4-ol
[148084-34-8]



$C_{15}H_{19}ClO_3$ 282.766
Isol. from the red alga *Laurencia majuscula*. Oil. $[\alpha]_D^{22}$ +79.9 (c, 0.31 in $CHCl_3$).

Wright, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 394 (*isol, pmr, cmr*)

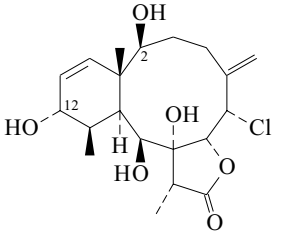
6-Chloro-2,8,9,12-tetrahydroxy-5,13-briaradien-18,7-olide C-425



$C_{20}H_{29}ClO_6$ 400.898

2,12-Di-Ac: ***Solenolide F***
[114094-33-6]
$C_{24}H_{33}ClO_8$ 484.973
Constit. of a *Solenopodium* sp. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ -45 (c, 1.52 in $CHCl_3$).
Groweiss, A. *et al., J.O.C.*, 1988, **53**, 2401

6-Chloro-2,8,9,12-tetrahydroxy-5(16),13-briaradien-18,7-olide C-426



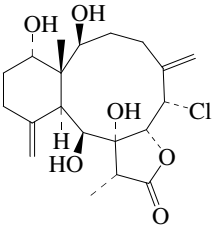
$C_{20}H_{29}ClO_6$ 400.898

13α,14α-Epoxide, 2,12-di-Ac: ***Solenolide B***
[114058-42-3]
$C_{24}H_{33}ClO_9$ 500.972
Constit. of a *Solenopodium* sp. Oil. $[\alpha]_D^{20}$ -5 (c, 1.02 in $CHCl_3$).

13α,14α-Epoxide, 12-hexanoyl, 2-Ac: ***Solenolide A***
[114094-31-4]
$C_{28}H_{41}ClO_9$ 557.079
Constit. of a *Solenopodium* sp. Shows antiviral and antiinflammatory props. Cryst. (Et_2O). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 132-133°. $[\alpha]_D^{20}$ -56 (c, 0.63 in $CHCl_3$).

12-Ketone, 2-Ac: ***Solenolide E***
[114058-44-5]
$C_{22}H_{29}ClO_7$ 440.92
Isol. from a *Solenopodium* sp. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ +11 (c, 0.5 in $CHCl_3$). λ_{max} 224 (ε 6900) (MeOH) (Derep).
Groweiss, A. *et al., J.O.C.*, 1988, **53**, 2401

6-Chloro-2,8,9,14-tetrahydroxy-5(16),11(20)-briaradien-18,7-olide C-427



$C_{20}H_{29}ClO_6$ 400.898

2,9,14-Tri-Ac: ***Umbraculolide C***
[288850-28-2]
$C_{26}H_{35}ClO_9$ 527.01
Constit. of *Gorgonella umbraculum*. Cryst. ($CHCl_3$).
Mp 184°. $[\alpha]_D^{25}$ -26 (c, 0.1 in $CHCl_3$).

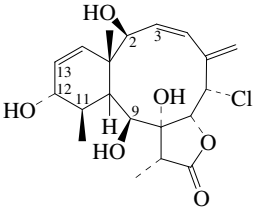
11,20-Epoxide: 6-Chloro-11,20-epoxy-2,8,9,14-tetrahydroxy-5(16)-briaren-18,7-olide
$C_{20}H_{29}ClO_7$ 416.898

11β,20-Epoxide, 2,9,14-tri-Ac: [753001-74-0]
$C_{26}H_{35}ClO_{10}$ 543.009
Constit. of an *Ellisella* sp. Solid. $[\alpha]_D^{26}$ -127 (c, 0.175 in $CHCl_3$).

11α,20-Epoxide, 2-(2-methylpropanoyl), 9,14-di-Ac: ***Juncenolide A***
[394248-11-4]
$C_{28}H_{39}ClO_{10}$ 571.063
Constit. of *Junceella juncea*. Cryst.
Mp 203-205°. $[\alpha]_D^{25}$ -25.5 (c, 0.05 in CH_2Cl_2).

Subrahmanyam, C. *et al., Tetrahedron*, 2000, **56**, 4585-4588 (*Umbraculolide C*)
Shen, Y.C. *et al., J. Nat. Prod.*, 2002, **65**, 54-56 (*Juncenolide A*)
Tanaka, C. *et al., J. Nat. Prod.*, 2004, **67**, 1368-1373 (*Ellisella constit*)

6-Chloro-2,8,9,12-tetrahydroxy-3,5(16),13-briaratrien-18,7-olide C-428



(2β,3*Z*,6α,7α,9β,12α)-*form*

$C_{20}H_{27}ClO_6$ 398.882

(2β,3*Z*,6α,7α,9β,12α)-*form*

2,9-Di-Ac: ***12-Ptilosarcenol***
[107745-47-1]
$C_{24}H_{31}ClO_8$ 482.957
Constit. of sea fern *Ptilosarcus gurneyi*. Shows insecticidal props.
$[\alpha]_D^{26}$ -62.9 (c, 0.56 in CH_2Cl_2).

2,9,12-Tri-Ac: [107716-28-9]
$C_{26}H_{33}ClO_9$ 524.994
Constit. of *Ptilosarcus gurneyi*.
$[\alpha]_D^{26}$ -82.4 (c, 0.40 in CH_2Cl_2).

12-Propanoyl, 2,9-di-Ac: [107716-27-8]
$C_{27}H_{35}ClO_9$ 539.021

Constit. of *Ptilosarcus gurneyi*.
$[\alpha]_D^{26}$ -117 (c, 0.90 in CH_2Cl_2). λ_{max} 218 (ϵ 5500) (EtOH) (Berdy).

13α,14α-Epoxide, 9,12-di-Ac: ***Brianthein X***
[87681-20-7]
$C_{24}H_{31}ClO_9$ 498.956
Constit. of *Briareum polyanthes*. Shows insecticidal props. Cryst. Mp 230-232° dec. λ_{max} 231 (ϵ 6900) (CH_2Cl_2) (Derep).

13α,14α-Epoxide, 2,9,12-tri-Ac: ***Brianthein Z***
[86105-70-6]
$C_{26}H_{33}ClO_{10}$ 540.993
From *Briareum polyanthes* and *Briareum asbestinum*. Cryst. Poorly sol. H_2O.
Mp 240-242° dec. λ_{max} 230 (ϵ 6700) (MeOH) (Derep).

13α,14α-Epoxide, 2-butanoyl, 9,12-di-Ac: ***Brianthein Y***
[87681-19-4]
$C_{28}H_{37}ClO_{10}$ 569.047
From *Briareum polyanthes* and *Briareum asbestinum*. CNS depressant. Cryst. Poorly sol. H_2O.
Mp 233-235° dec. λ_{max} 230 (ϵ 6700) (MeOH) (Derep). λ_{max} 229 (ϵ 6500) (CH_2Cl_2) (Berdy).

13α,14α-Epoxide, 2,12-dibutanoyl, 9-Ac: ***Brianthein V***
[117569-39-8]
$C_{30}H_{41}ClO_{10}$ 597.101
From *Briareum asbestinum*. Pale yellow needles. Poorly sol. H_2O.
Mp 222°. $[\alpha]_D^{20}$ -57 (c, 1.1 in $CHCl_3$).

3α,4α,13α:14α-Diepoxide, 9-Ac: ***Bis(deacyl)solenolide D***
$C_{22}H_{29}ClO_9$ 472.918
Isol. from marine sponge *Psammaplysilla purpurea*. Inhibitor of biofilm formation and biofouling. Glass. $[\alpha]_D^{20}$ -14.5 (c, 0.51 in MeOH).

3α,4α:13α,14α-Diepoxide, 12-butanoyl, 9-Ac: ***Milolide D***
[352335-87-6]
$C_{26}H_{35}ClO_{10}$ 543.009
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ -45 (c, 0.43 in CH_2Cl_2).

3α,4α:13α,14α-Diepoxide,12-hexanoyl, 2,9-di-Ac: ***Milolide E***
[352335-90-1]
$C_{30}H_{41}ClO_{11}$ 613.1
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ -53.6 (c, 0.084 in CH_2Cl_2).

12-Ketone, 2,9-di-Ac: ***Ptilosarcenone***
[64597-87-1]
$C_{24}H_{29}ClO_8$ 480.941
Constit. of *Ptilosarcus gurneyi* and *Tochuina tetraquetra*. Insecticide. Cryst.
Mp 153-155°. $[\alpha]_D^{26}$ -72.4 (c, 1.01 in CH_2Cl_2). λ_{max} 220 (ϵ 9000) (MeOH) (Derep). λ_{max} 224 (ϵ 12600) (EtOH) (Berdy).

12-Ketone, 2-butanoyl, 9-Ac: [111621-37-5]
$C_{26}H_{33}ClO_8$ 508.995
Constit. of *Tochuina tetraquetra*. Oil. $[\alpha]_D^{25}$ -49.2 (c, 0.41 in CH_2Cl_2).

(2β,3*Z*,6α,7α,9β,12β)-*form*

13α,14α-Epoxide, 9,12-di-Ac: ***Briaexcavatolide H***
[256388-09-7]
$C_{24}H_{31}ClO_9$ 498.956
Constit. of *Briareum excavatum*. Powder.
Mp 201-203°. $[\alpha]_D^{25}$ -254 (c, 0.1 in $CHCl_3$). λ_{max} 228 (log ϵ 5426) ($CHCl_3$).

13α,14α-Epoxide, 2,9,12-tri-Ac: ***Briaexcavatolide I***
[256388-10-0]
Constit. of *Briareum excavatum*.
Powder.
Mp 224-226°. $[\alpha]_D^{25}$ -53 (c, 0.1 in $CHCl_3$). λ_{max} 226 (ϵ 5568) ($CHCl_3$).

3α,4α:13α,14α-Diepoxide, 9-Ac: ***Briaexcavatolide G***
[256388-08-6]
$C_{22}H_{29}ClO_9$ 472.918
Constit. of *Briareum excavatum*. Powder.
Mp 233-235°. $[\alpha]_D^{25}$ -18 (c, 0.2 in MeOH).

3α,4α:13α,14α-Diepoxide, 2,9-di-Ac: ***Solenolide C***
[114094-32-5]
$C_{24}H_{31}ClO_{10}$ 514.956
Isol. from a *Solenopodium* sp. and *Briareum stechei*. Amorph. solid.
Mp 196-198° dec. $[\alpha]_D^{20}$ -25 (c, 0.76 in MeOH). Struct. revised in 1992.

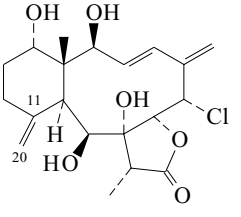
3α,4α:13α,14α-Diepoxide, 9,12-di-Ac: ***Brianolide***
[131400-39-0]
$C_{24}H_{31}ClO_{10}$ 514.956
Constit. of a *Briareum* sp. Antiinflammatory. Plates (MeOH aq.).
Mp 225-226°. $[\alpha]_D^{23}$ -15 (c, 0.1 in MeOH).

3α,4α:13α,14α-Diepoxide, 2,9,12-tri-Ac: ***Solenolide D***. *Briaexcavatolide E*
[114058-43-4]
$C_{26}H_{33}ClO_{11}$ 556.993
Isol. from a *Solenopodium* sp. and *Briareum excavatum*. Amorph. solid or powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 171-173° Mp 183-185°. $[\alpha]_D^{20}$ -16 (c, 0.89 in $CHCl_3$). $[\alpha]_D^{26}$ -27 (c, 0.1 in MeOH).

3α,4α:13α,14α-Diepoxide, 12-butanoyl, 9-Ac: ***Briaexcavatolide F***
[256388-07-5]
$C_{26}H_{35}ClO_{10}$ 543.009
Constit. of *Briareum excavatum*. Powder.
Mp 184-186°. $[\alpha]_D^{25}$ -21 (c, 0.1 in MeOH).

Wratten, S.J. *et al., Tet. Lett.*, 1977, 1559-1562 (*Ptilosarcenone*)
Grode, S.H. *et al., J.O.C.*, 1983, **48**, 5203-5207 (*Briantheins*)
Hendrickson, R.L. *et al., Tetrahedron*, 1986, **42**, 6565-6570 (*Ptilosarcus gurneyi constits*)
Williams, D.E. *et al., Can. J. Chem.*, 1987, **65**, 2244-2247 (*Ptilosarcenone*)
Coval, S.J. *et al., J. Nat. Prod.*, 1988, **51**, 981-984 (*Brianthein V, cryst struct*)
Groweiss, A. *et al., J.O.C.*, 1988, **53**, 2401-2406 (*Solenolides*)
Kobayashi, J. *et al., Experientia*, 1991, **47**, 501-502 (*Brianolide, cryst struct*)
Cheng, J.F. *et al., Tet. Lett.*, 1992, **33**, 101-104 (*Solenolides, struct*)
Yamada, A. *et al., Bull. Chem. Soc. Jpn.*, 1997, **70**, 3061-3069 (*Bisdeacylsolenoide D*)
Sheu, J.H. *et al., J. Nat. Prod.*, 1998, **61**, 602-608 (*Brianolide, pmr, cmr*)
Sheu, J.H. *et al., Tetrahedron*, 1999, **55**, 14555-14564 (*Briaexcavatolides*)
Kwak, J.H. *et al., J. Nat. Prod.*, 2001, **64**, 754-760 (*Milolides*)

6-Chloro-2,8,9,14-tetrahydroxy-3,5(16),11(20)-briaratrien-18,7-olide C-429



(2β,3*E*,6α,7α,8α,9β,14α)–*form*

$C_{20}H_{27}ClO_6$ 398.882

(2β,3*E*,6α,7α,8α,9β,14α)-*form*

2,9,14-Tri-Ac: ***Junceellolide B***
[121798-80-9]
$C_{26}H_{33}ClO_9$ 524.994
Constit. of *Junceella fragilis*. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 95-96°. $[\alpha]_D$ +9.4 (c, 1.3 in $CHCl_3$). Unusual 3*E*-config. λ_{max} 230 (ϵ 7000) (MeOH) (Berdy).

11α,20-Epoxide, 2,9,14-tri-Ac: ***Junceellolide C***
[121769-82-2]
$C_{26}H_{33}ClO_{10}$ 540.993
Constit. of *Junceella fragilis*. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 120-125°. $[\alpha]_D$ +36.1 (c, 1.2 in $CHCl_3$). λ_{max} 230 (ϵ 7100) (MeOH) (Berdy).

11,20-Epoxide: 6-Chloro-11,20-epoxy-2,8,9,14-tetrahydroxy-3,5(16)-briaradien-18,7-olide

(2β,3*Z*,6α,7α,8α,9β,14α)-*form*

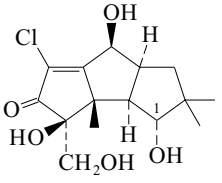
2,9,14-Tri-Ac: ***Juncin B***
[129622-89-5]
$C_{26}H_{33}ClO_9$ 524.994
Metab. of *Junceella juncea*. Oil. $[\alpha]_D^{25}$ -55 (c, 0.003 in $CHCl_3$).

11α,20-Epoxide, 2,9,14-tri-Ac: ***Juncin A***
[129705-40-4]
$C_{26}H_{33}ClO_{10}$ 540.993
Metab. of *Junceella juncea*. Oil. $[\alpha]_D^{25}$ -79 (c, 0.02 in $CHCl_3$).

11β,20-Epoxide, 2,9,14-tri-Ac: [753001-75-1]
$C_{26}H_{33}ClO_{10}$ 540.993
Constit. of an *Ellisella* sp. Solid. $[\alpha]_D^{26}$ -127 (c, 0.175 in $CHCl_3$).

Shin, J. *et al., Tetrahedron*, 1989, **45**, 1633 (*Junceellolides B,C*)
Isaacs, S. *et al., J. Nat. Prod.*, 1990, **53**, 596 (*Juncins A,B*)
Tanaka, C. *et al., J. Nat. Prod.*, 2004, **67**, 1368-1373 (*Ellisella constit*)

6-Chloro-1,4,8,15-tetrahydroxy-6-hirsuten-5-one C-430



$C_{15}H_{21}ClO_5$ 316.781

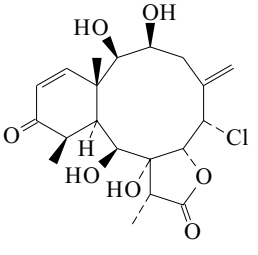
(1α,4β,8β)-*form*

1-(2-Hydroxyoctanoyl): ***Chloriolin B***
[158402-64-3]
$C_{23}H_{35}ClO_7$ 458.978
Metab. of a fungus separated from a *Jaspis* marine sponge. Solid. $[\alpha]_D$ +31.5 (c, 0.005 in MeOH).

1-Octanoyl: ***Chloriolin C***
[158402-65-4]
$C_{23}H_{35}ClO_6$ 442.979
Metab. of a fungus separated from a *Jaspis* marine sponge. Solid. $[\alpha]_D$ +27.5 (c, 0.002 in MeOH).

Cheng, X.-C. *et al., J.O.C.*, 1994, **59**, 6344 (*isol, pmr, cmr*)

6-Chloro-2,3,8,9-tetrahydroxy-12-oxo-5(16),13-briaradien-18,7-olide C-431



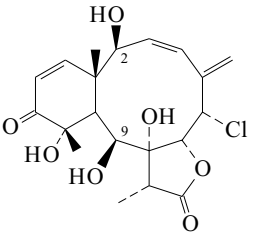
$C_{20}H_{27}ClO_7$ 414.882

2-Propanoyl, 3,9-di-Ac: [125009-88-3]
$C_{27}H_{35}ClO_{10}$ 555.02
Constit. of a *Briareum* sp. (PA1). Cryst.
Mp 264-266°. $[\alpha]_D$ +50 (c, 0.1 in $CHCl_3$).

13α,14α-Epoxide, 12β-alcohol, 3,9-di-Ac: ***Briaexcavatolide J***
[256388-11-1]
$C_{24}H_{33}ClO_{10}$ 516.971
Constit. of *Briareum excavatum*. Powder.
Mp 183-185°. $[\alpha]_D^{25}$ -26 (c, 0.1 in $CHCl_3$).

Bowden, B.F. *et al., Aust. J. Chem.*, 1989, **42**, 1727 (*2-propanoyl-di-Ac*)
Sheu, J.-H. *et al., Tetrahedron*, 1999, **55**, 14555-14564 (*Briaexcavatolide J*)

6-Chloro-2,8,9,11-tetrahydroxy-12-oxo-3,5(16),13-briaratrien-18,7-olide C-432

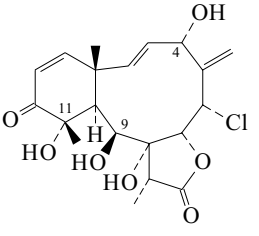


$C_{20}H_{25}ClO_7$ 412.866

2,9-Di-Ac: ***11-Hydroxyptilosarcenone***
[107796-07-6]
$C_{24}H_{29}ClO_9$ 496.94
Isol. from sea fern *Ptilosarcus gurneyi*.
$[\alpha]_D^{26}$ -62.5 (c, 0.74 in CH_2Cl_2).

Hendrickson, R.L. *et al., Tetrahedron*, 1986, **42**, 6565

6-Chloro-4,8,9,11-tetrahydroxy-12-oxo-2,5(16),13-briaratrien-18,7-olide C-433



$C_{20}H_{25}ClO_7$ 412.866

9,11-Di-Ac: ***Erythrolide R***
[627878-02-8]
$C_{24}H_{29}ClO_9$ 496.94
Constit. of *Erythropodium caribaeorum*. Oil. $[\alpha]_D^{25}$ +15.4. λ_{max} 216 (ϵ 7500) (MeOH).

4,9,11-Tri-Ac: ***Erythrolide B***
[89999-15-5]
$C_{26}H_{31}ClO_{10}$ 538.978
Constit. of *Erythropodium caribaeorum*. Foam. λ_{max} 218 (ϵ 5194) (MeOH) (Derep).

2α,3α-Epoxide: 6-Chloro-2,3-epoxy-4,8,9,11-tetrahydroxy-12-oxo-5(16),13-briaratrien-18,7-olide
$C_{20}H_{25}ClO_8$ 428.865

2α,3α-Epoxide, 4,9,11-tri-Ac: ***Erythrolide T***
[627878-04-0]
$C_{26}H_{31}ClO_{11}$ 554.977
Constit. of *Erythropodium caribaeorum*. Glass. $[\alpha]_D^{25}$ +25.7. λ_{max} 214 (ϵ 8965) (MeOH).

Look, S.A. *et al., J.A.C.S.*, 1984, **106**, 5026 (*isol*)
Pordesimo, E.O. *et al., J.O.C.*, 1991, **56**, 2344 (*isol, pmr, cmr*)
Dookran, R. *et al., J. Nat. Prod.*, 1993, **56**, 1051 (*pmr, cmr*)
Taglialatela-Scafati, O. *et al., Eur. J. Org. Chem.*, 2003, 3515-3523 (*Erythrolides R,T*)

1-Chloro-1-tridecene-6,8-diol C-434

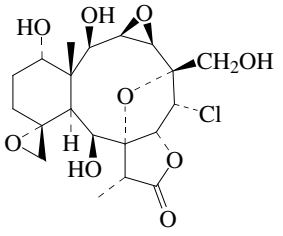
[69616-84-8]
$H_3C(CH_2)_4CH(OH)CH_2CH(OH)(CH_2)_3CH{=}CHCl$
$C_{13}H_{25}ClO_2$ 248.792

(1*E*,6*R*,8*R*)-*form*

Constit. of the marine cyanophytes *Schizothrix calcicola* and *Oscillatoria nigroviridis*.
Cryst. (pentane).

Mp 55.7-58°. $[\alpha]_D^{27}$ -12.2 (c, 3.3 in $CHCl_3$). Probable abs. config.
Mynderse, J.S. *et al., Phytochemistry*, 1978, **17**, 1325-1326 (*isol*)

6-Chloro-3,4:5,8:11,20-triepoxy-2,9,14,16-tetrahydroxy-18,7-briaranolide C-435



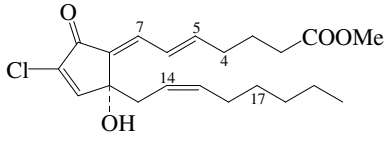
$C_{20}H_{27}ClO_9$ 446.881

(2β,3β,4β,5*S*,6α,7α,8*R*,9β,11α,14α)-*form*

2,9,14-Tri-Ac: ***Juncenolide G***
[853009-67-3]
$C_{26}H_{33}ClO_{12}$ 572.992
Constit. of *Junceella juncea*. Cryst. $[\alpha]_D$ +6.5 (c, 0.2 in CH_2Cl_2).
Lin, Y.-C. *et al., Chem. Pharm. Bull.*, 2005, **53**, 128-130 (*Juncenolide G*)

Chlorovulones C-436

10-Chloro-12-hydroxy-9-oxoprosta-5,7,10,14-tetraenoic acid methyl ester



(5*E*,7*E*,14*Z*)-*form*

$C_{21}H_{29}ClO_4$ 380.91

(5*E*,7*E*,14*Z*)-*form*

Chlorovulone II
[100295-80-5]
Constit. of *Clavularia viridis*. Antitumour agent. $[\alpha]_D$ +22.7 (c, 0.75 in $CHCl_3$). λ_{max} 237 (ε 11000); 313 (ε 11000) (EtOH) (Derep). λ_{max} 237 (ε 10000); 312 (ε 10100) (EtOH) (Berdy).

Ac: ***12*-O-*Acetylchlorovulone II***
[105394-15-8]
$C_{23}H_{31}ClO_5$ 422.948
Constit. of *Clavularia viridis*. Oil. λ_{max} 233 (ε 11000); 307 (ε 12000) (MeOH).

*10*R,*11*S*-Epoxide:* ***10,11-Epoxychlorovulone II***
[628294-22-4]
$C_{21}H_{29}ClO_5$ 396.91
Constit. of *Clavularia viridis*. Oil. $[\alpha]_D^{25}$ -21.5 (c, 0.02 in $CHCl_3$). λ_{max} 298 (ε 18000) (MeOH).

Bromo analogue: ***Bromovulone II***
$C_{21}H_{29}BrO_4$ 425.362
Isol. from *Clavularia viridis*. Pale yellow oil. $[\alpha]_D^{25}$ +23 (c, 0.25 in CH_2Cl_2).

Bromo analogue, Ac: ***12*-O-*Acetylbromovulone II***
[628294-15-5]
$C_{23}H_{31}BrO_5$ 467.399
Constit. of *Clavularia viridis*. Oil. λ_{max} 230 (ε 11000); 308 (ε 11000) (MeOH).

*Bromo analgoue, 10*R,*11*S*-epoxide:* ***10,11-Epoxybromovulone II***
[628294-20-2]
$C_{21}H_{29}BrO_5$ 441.361
Constit. of *Clavularia viridis*. Oil. $[\alpha]_D^{25}$ -57.3 (c, 0.01 in $CHCl_3$). λ_{max} 298 (ε 12000) (MeOH).

Iodo analogue: ***Iodovulone II***
[629626-33-1]
$C_{21}H_{29}IO_4$ 472.362
Constit. of *Clavularia viridis*. Oil. $[\alpha]_D^{25}$ +23.7 (c, 0.07 in $CHCl_3$). $[\alpha]_D^{25}$ +44.6 (c, 0.9 in CH_2Cl_2). λ_{max} 241 (ε 16000); 311 (ε 14000) (MeOH).

Iodo analogue, Ac: ***12*-O-*Acetyliodovulone II***
[628294-13-3]
$C_{23}H_{31}IO_5$ 514.399
Constit. of *Clavularia viridis*. Oil. λ_{max} 238 (ε 14000); 307 (ε 13000) (MeOH).

*Iodo analogue, 10*R,*11*S*-epoxide: 10,11-Epoxyiodovulone II*
[628294-18-8]
Constit. of *Clavularia viridis*.
Oil. $[\alpha]_D^{25}$ -20.3 (c, 0.05 in $CHCl_3$). λ_{max} 300 (ε 21000) (MeOH).

(5*E*,7*Z*,14*Z*)-*form*

Chlorovulone III
[100295-79-2]
Constit. of *Clavularia viridis*.
$[\alpha]_D$ +27.3 (c, 0.033 in $CHCl_3$). λ_{max} 237 (ε 11000); 313 (ε 11000) (EtOH) (Derep). λ_{max} 238 (ε 13200); 315 (ε 11900) (EtOH) (Berdy).

Ac: ***12*-O-*Acetylchlorovulone III***
[628294-17-7]
$C_{23}H_{31}ClO_5$ 422.948
Constit. of *Clavularia viridis*. Oil. λ_{max} 231 (ε 9800); 309 (ε 8500) (MeOH).

Bromo analogue: ***Bromovulone III***
$C_{21}H_{29}BrO_4$ 425.362
Isol. from *Clavularia viridis*. Cytotoxic. Pale yellow oil. $[\alpha]_D^{25}$ +39 (c, 0.38 in CH_2Cl_2).

Bromo analogue, Ac: ***12*-O-*Acetylbromovulone III***
[628294-16-6]
$C_{23}H_{31}BrO_5$ 467.399
Constit. of *Clavularia viridis*. Oil. λ_{max} 219 (ε 8600); 237 (sh) (ε 7400); 312 (ε 6700) (MeOH).

*Bromo analogue, 4*R*-hydroxy, 17,18-didehydro(*Z*-):* ***17,18-Didehydro-4*R*-hydroxybromovulone III***
$C_{21}H_{27}BrO_5$ 439.345
Isol. from the yellow coral *Dendronephthya* sp. Oil. $[\alpha]_D^{22}$ -18.5 (c, 0.14 in MeOH).

*Bromo analogue, 4*R*-hydroxy, 17,18-didehydro(*Z*-), 4-*O*-β-D-glucopyranoside:*
$C_{27}H_{37}BrO_{10}$ 601.487
Isol. from the yellow coral *Dendronephthya* sp. Powder. $[\alpha]_D^{23}$ -118 (c, 0.12 in MeOH).

*Bromo analogue, 4*S*-hydroxy, 17,18-didehydro(*Z*-):* ***17,18-Didehydro-4*S*-hydroxybromovulone III***
$C_{21}H_{27}BrO_5$ 439.345
Isol. from the red coral *Dendronephthya* sp. Oil. $[\alpha]_D^{22}$ -17.5 (c, 0.15 in MeOH). λ_{max} 248 (log ε 4.08); 313 (log ε 4.01) (EtOH).

*Bromo analogue, 4*S*-hydroxy, 17,18-didehydro(*Z*-), 4-*O*-α-D-glucopyranoside:*
$C_{27}H_{37}BrO_{10}$ 601.487
Isol. from the red coral *Dendronephthya* sp. Powder. $[\alpha]_D^{23}$ +112 (c, 0.11 in MeOH).

Iodo analogue: ***Iodovulone III***
[629626-49-9]
$C_{21}H_{29}IO_4$ 472.362
Constit. of *Clavularia viridis*. Oil. $[\alpha]_D^{25}$ +25 (c, 0.02 in $CHCl_3$). $[\alpha]_D^{25}$ +8.6 (c, 0.27 in CH_2Cl_2). λ_{max} 239 (ε 14000); 317 (ε 11000) (MeOH).

Iodo analogue, Ac: ***12*-O-*Acetyliodovulone III***
[628294-14-4]
$C_{23}H_{31}IO_5$ 514.399
Constit. of *Clavularia viridis*. Oil. λ_{max} 225 (ε 15000); 245 (ε 8600) (MeOH).

(5*Z*,7*E*,14*Z*)-*form*

Chlorovulone I
[100295-81-6]
Constit. of the stolonifer *Clavularia viridis*. Antitumour agent. Oil. $[\alpha]_D$ -1.2 (c, 0.17 in $CHCl_2$). λ_{max} 243 (ε 14600); 315 (ε 15100) (MeOH) (Derep).

Ac: ***12*-O-*Acetylchlorovulone I***
[119341-87-6]
$C_{23}H_{31}ClO_5$ 422.948
Constit. of *Clavularia viridis*. Oil. λ_{max} 236 (ϵ 11000); 309 (ϵ 13000) (MeOH).

*10*R,*11*S-*Epoxide:* ***10,11-Epoxychlorovulone I***
[112163-50-5]
$C_{21}H_{29}ClO_5$ 396.91
Constit. of *Clavularia viridis*. Oil. $[\alpha]_D$ -24.1 (c, 0.4 in $CHCl_3$). λ_{max} 300 (ϵ 4300) (EtOH) (Berdy).

Bromo analogue: ***Bromovulone I***
[105343-04-2]
$C_{21}H_{29}BrO_4$ 425.362
Prostanoid isol. from Japanese marine stolonifer *Clavularia viridis*. Antitumour agent, antiproliferative agent. Oil. λ_{max} 247 (ϵ 12000); 312 (ϵ 12000) (MeOH) (Derep).

*Bromo analogue, 10*R,*11*S-*epoxide:* ***10,11-Epoxybromovulone I***
[628294-21-3]
$C_{21}H_{29}BrO_5$ 441.361
Constit. of *Clavularia viridis*. Oil. $[\alpha]_D^{25}$ -18.5 (c, 0.01 in $CHCl_3$). λ_{max} 299 (ϵ 9700) (MeOH).

Iodo analogue: ***Iodovulone I***
[105343-03-1]
$C_{21}H_{29}IO_4$ 472.362
Isol. from *Clavularia viridis*. Antitumour agent, antiproliferative. Oil. λ_{max} 240 (ϵ 22000); 313 (ϵ 19500) (MeOH) (Derep).

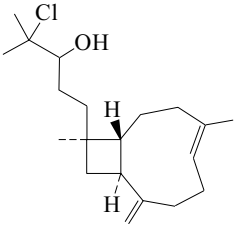
*Iodo analogue, 10*R,*11*S-*epoxide:* ***10,11-Epoxyiodovulone I***
[628294-19-9]
$C_{21}H_{29}IO_5$ 488.362
Constit. of *Clavularia viridis*. Oil. $[\alpha]_D^{25}$ -97.3 (c, 0.04 in $CHCl_3$). λ_{max} 300 (ϵ 17000) (MeOH).

(5*Z*,7*Z*,14*Z*)-*form*
Chlorovulone IV
[100201-69-2]
Constit. of *Clavularia viridis*.
No phys. props. reported.

Iodo analogue: ***Iodovulone IV***
[383414-97-9]
$C_{21}H_{29}IO_4$ 472.362
Constit. of *Clavularia viridis*. Oil. λ_{max} 237 (ϵ 5400); 312 (ϵ 6300) (MeOH).

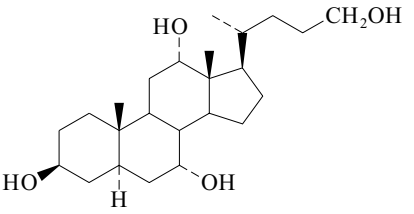
Iguchi, K. *et al., Tet. Lett.*, 1985, **26**, 5787-5790 (*isol, struct*)
Iguchi, K. *et al., Chem. Comm.*, 1986, 981-982 (*Bromovulone I, Iodovulone I*)
Nagaoka, H. *et al., Tet. Lett.*, 1986, **27**, 223-226 (*abs config, synth*)
Iguchi, K. *et al., Chem. Pharm. Bull.*, 1987, **35**, 4375-4376 (*Epoxychlorovulone I*)
Ciufolini, M.A. *et al., J.O.C.*, 1998, **63**, 1668-1675 (*synth*)
Rezanka, T. *et al., Eur. J. Org. Chem.*, 2003, 309-316 (*Didehydro-4-hydroxy bromovulones III*)
Watanabe, K. *et al., J. Nat. Prod.*, 2003, **66**, 1434-1440 (*Iodovulones, cd, pmr, cmr*)
Shen, Y.-C. *et al., J. Nat. Prod.*, 2004, **67**, 542-546 (*Bromovulones II, III, Iodovulones II, III*)

15-Chloro-4,8(19)-xeniaphylladien-14-ol C-437



$C_{20}H_{33}ClO$ 324.933
Constit. of *Nephthea chabrolii*. Oil. $[\alpha]_D$ -15 (c, 0.36 in $CHCl_3$).
Ahond, A. *et al., Aust. J. Chem.*, 1981, **34**, 2657

Cholane-3,7,12,24-tetrol C-438



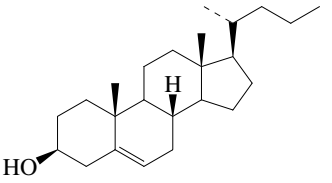
$C_{24}H_{42}O_4$ 394.593

(3α,5α,7α,12α)-*form*
Petromyzonol
[28979-29-5]
Bile substance produced by the larval form of the lamprey *Petromyzon marinus*.
Cryst.
Mp 229-231°. $[\alpha]_D^{23}$ +29.5 (c, 1.5 in EtOH).

3-Ketone: 7,12,24-Trihydroxycholan-3-one. 3-Ketopetromyzonol
$C_{24}H_{40}O_4$ 392.578

3-Ketone, 24-sulfate: ***3-Ketopetromyzonol sulfate***
[435327-06-3]
$C_{24}H_{40}O_7S$ 472.642
Pheromone of sea lamprey (*Petromyzon marinus*).
Zhu, X. *et al., Can. J. Chem.*, 1987, **65**, 2447 (*synth, bibl*)
Yun, S.-S. *et al., Steroids*, 2003, **68**, 297-304 (*3-Ketopetromyzonol sulfate*)

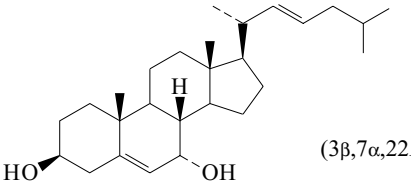
Chol-5-en-3-ol C-439



$C_{24}H_{40}O$ 344.579

3β-*form* [5255-15-2]
Isol. from sponge *Damiriana hawaiiana*.
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476

Cholesta-5,22-diene-3,7-diol C-440



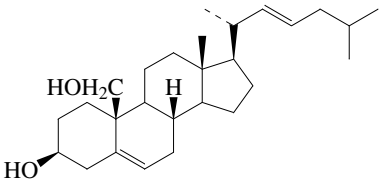
(3β,7α,22*E*)–*form*

$C_{27}H_{44}O_2$ 400.643

(3β,7α,22*E*)-*form* [145075-03-2]
Constit. of *Cliona copiosa*.

(3β,7β,22*E*)-*form* [145075-02-1]
Constit. of *Cliona copiosa*.
Notaro, G. *et al., J. Nat. Prod.*, 1992, **55**, 1588 (*isol, pmr, ms*)

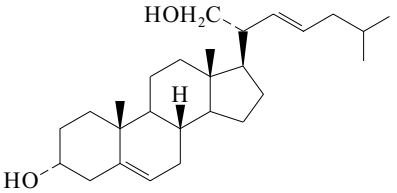
Cholesta-5,22-diene-3,19-diol C-441



$C_{27}H_{44}O_2$ 400.643

(3β,22*E*)-*form*
Acanthovagasteroid A
[815586-45-9]
Constit. of *Acanthogorgia vagae.*
Cryst.
Mp 157-159°. $[\alpha]_D^{20}$ -21.1 (c, 0.36 in $CHCl_3$).
Zhang, W. *et al., J. Nat. Prod.*, 2004, **67**, 2083-2085 (*isol, pmr, cmr*)

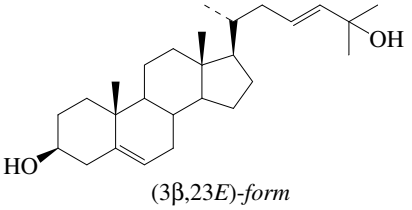
Cholesta-5,22-diene-3,21-diol C-442



$C_{27}H_{44}O_2$ 400.643

(3α,20*R*,22*E*)-*form*
Disulfate: [100942-74-3]
$C_{27}H_{44}O_8S_2$ 560.772
Isol. from *Ophioderma longicaudum* and *Euretaster insignis.*
Riccio, R. *et al., Tetrahedron*, 1985, **41**, 6041-6046 (*isol*)

Cholesta-5,23-diene-3,25-diol C-443



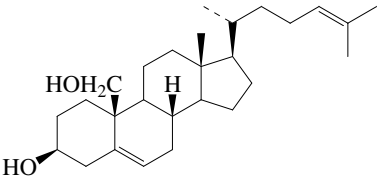
(3β,23*E*)-*form*

$C_{27}H_{44}O_2$ 400.643

(3β,23*E*)-*form*
trans-*Liagosterol*
[57800-59-6]
Minor constit. of red algae *Liagora distenta* and *Scinaia furcellata.*
25-Hydroperoxide: ***25-Hydroperoxycholesta-5,23-dien-3β-ol***
[174796-78-2]
$C_{27}H_{44}O_3$ 416.643
Constit. of *Galaxaura marginata*. Powder. Mp 148-151°. $[\alpha]_D^{20}$ -41 (c, 0.05 in $CHCl_3$).

(3β,23*Z*)-*form*
cis-*Liagosterol*
[57800-58-5]
Constit. of red algae *Liagora distenta* and *Scinaia furcellata.*
Cryst. (EtOH) (as mono-Ac). Mp 114-119° (as mono-Ac).
$[\alpha]_D$ -39.4 (c, 0.2 in $CHCl_3$) (as mono-Ac).
Fattorusso, E. *et al., Phytochemistry*, 1975, **14**, 1579-1582 (*Liagosterols*)
Sheu, J.-H. *et al., J. Nat. Prod.*, 1996, **59**, 23-26 (*hydroperoxide*)

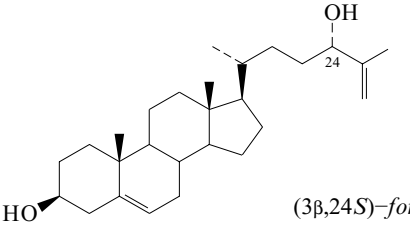
Cholesta-5,24-diene-3,19-diol C-444



$C_{27}H_{44}O_2$ 400.643

3β-*form*
Acanthovagasteroid B
[815586-47-1]
Constit. of *Acanthogorgia vagae.*
Amorph. powder. $[\alpha]_D^{20}$ -47.6 (c, 0.08 in $CHCl_3$).
19-Carboxylic acid: 3-Hydroxycholesta-5,24-dien-19-oic acid
$C_{27}H_{42}O_3$ 414.627
*19-Carboxylic acid, 3-*O*-sulfate:*
$C_{27}H_{42}O_6S$ 494.691
Constit. of *Toxadocia zumi*. Amorph. powder.
24,25-Dihydro, 19-carboxylic acid: 3-Hydroxycholest-5-en-19-oic acid
$C_{27}H_{44}O_3$ 416.643
*24,25-Dihydro, 19-carboxylic acid, 3-*O*-sulfate:*
$C_{27}H_{44}O_6S$ 496.707
Constit. of *Toxadocia zumi.*
Nakatsu, T. *et al., Experientia*, 1983, **39**, 759-761 (*carboxylic acid 3-sulfates*)
Zhang, W. *et al., J. Nat. Prod.*, 2004, **67**, 2083-2085 (*Acanthovagasteroid B*)

Cholesta-5,25-diene-3,24-diol C-445



(3β,24*S*)–*form*

$C_{27}H_{44}O_2$ 400.643

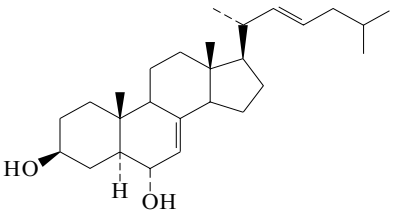
(3β,24*S*)-*form* [61947-94-2]
Isol. from the brown alga *Rhodymenia palmata*, the red algae *Asparagopsis armata, Rissoella verruculosa* and the tetraspora *Falkenbergia rufolanosa*. Cryst. (Me_2CO). Mp 192-195°.

(3β,24ξ)-*form*
Constit. of *Galaxaura marginata* (Galaxauraceae).
Powder. Mp 193-195°. $[\alpha]_D^{26}$ -37 (c, 0.05 in $CHCl_3$).
24-Hydroperoxide: ***24-Hydroperoxycholesta-5,25-dien-3-ol***
$C_{27}H_{44}O_3$ 416.643
Constit. of *Galaxaura marginata*. Powder. $[\alpha]_D^{24}$ -38 (c, 0.2 in $CHCl_3$).

[88156-15-4, 88156-16-5]

Morisaki, M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 3214
Nagano, H. *et al., J. Chem. Res., Miniprint*, 1977, 2522 (*synth*)
Combaut, G. *et al., J. Nat. Prod.*, 1979, **42**, 150 (*isol*)
Francisco, C. *et al., Steroids*, 1979, **34**, 163 (*synth*)
Koizumi, N. *et al., J.C.S. Perkin 1*, 1983, 1401 (*synth*)
Kabore, S.A. *et al., Phytochemistry*, 1983, **22**, 1239 (*isol*)
Sheu, J.-H. *et al., J. Nat. Prod.*, 1996, **59**, 23 (*hydroperoxide*)

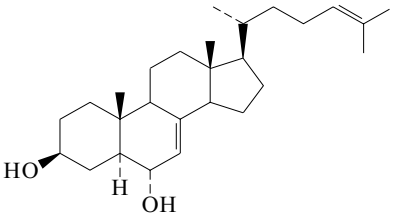
Cholesta-7,22-diene-3,6-diol C-446



$C_{27}H_{44}O_2$ 400.643

(3β,5α,6α,22*E*)-*form*
Constit. of *Spongionella gracilis*. Cryst. (MeOH/petrol). Mp 172-174°.
Madaio, A. *et al., J. Nat. Prod.*, 1989, **52**, 952 (*isol, pmr*)

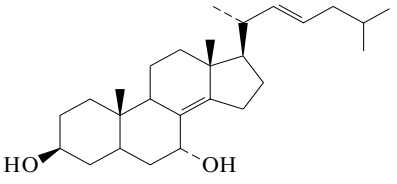
Cholesta-7,24-diene-3,6-diol, 9CI C-447



$C_{27}H_{44}O_2$ 400.643

(3β,5α,6α)-*form* [106534-43-4]
Constit. of *Spongionella gracilis*.
Piccialli, V. *et al., J. Nat. Prod.*, 1986, **49**, 779

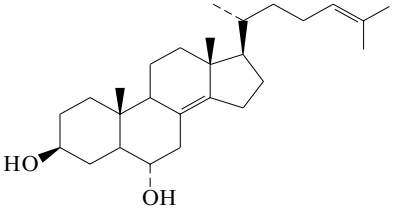
Cholesta-8(14),22-diene-3,7-diol C-448



$C_{27}H_{44}O_2$ 400.643

(3β,5α,7α,22*E*)-*form* [141859-97-4]
Constit. of *Pellina semitubulosa*.
Notaro, G. *et al., J. Nat. Prod.*, 1992, **55**, 773 (*isol, pmr*)

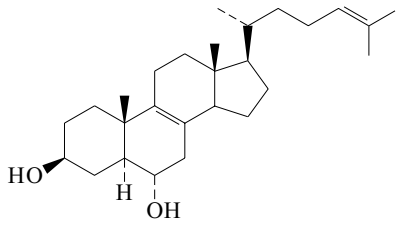
Cholesta-8(14),24-diene-3,6-diol C-449



$C_{27}H_{44}O_2$ 400.643

(3β,7α)-*form* [147395-09-3]
Constit. of a *Dysidea* sponge from the South China Sea. Cryst. Mp 184-185°. $[\alpha]_D^{35}$ +16.7 (c, 0.036 in MeOH).
Zhang, Y.L. *et al., Chin. Chem. Lett.*, 1992, **3**, 981 (*isol, pmr, cmr*)
Zhang, Y.L. *et al., Chin. J. Chem.*, 1993, **11**, 560 (*isol, pmr, cmr*)

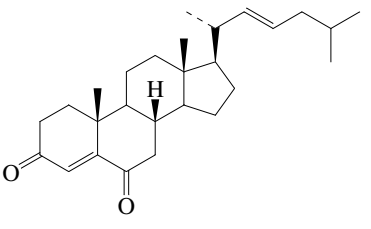
Cholesta-8,24-diene-3,6-diol C-450



$C_{27}H_{44}O_2$ 400.643

(3β,5α,6α)-*form*
3-O-*[β-D-Galactopyranosyl-(1→2)-β-D-glucopyranoside], 6-sulfate:* ***Laeviuscoloside A***
[129393-24-4]
$C_{39}H_{64}O_{15}S$ 804.992
Constit. of *Henricia laeviuscola*. $[\alpha]_D$ +9.3.
D'Auria, M.V. *et al., Gazz. Chim. Ital.*, 1990, **120**, 155-163 (*isol, pmr, cmr*)

Cholesta-4,22-diene-3,6-dione C-451



$C_{27}H_{40}O_2$ 396.612

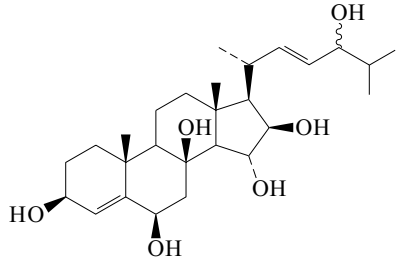
(22*E*)-*form* [888041-26-7]
Constit. of *Dendrophyllia cornigera*. Oil. $[\alpha]_D^{25}$ -25 (c, 0.1 in CH_2Cl_2). λ_{max} 205 (log ϵ 2.14); 250 (log ϵ 2.38) (CH_2Cl_2).
Kontiza, I. *et al., Steroids*, 2006, **71**, 177-181

Cholesta-7,22-diene-2,3,5,6,9,11,19-heptol C-452

$C_{27}H_{44}O_7$ 480.64

(2α,3β,5α,6β,11α)-*form* [114395-64-1]
Isol. from *Dysidea etheria*.
Cryst. Mp 260° dec. $[\alpha]_D^{25}$ -28.6 (c, 0.7 in EtOH).
11,19-Di-Ac: 11α,19-Diacetoxycholesta-7,22-diene-2α,3β,5α,6β,9α-pentol
[114395-63-0]
$C_{31}H_{48}O_9$ 564.715
Isol. from *Dysidea etheria*. Cryst. Mp 150°. $[\alpha]_D^{25}$ -53.3 (c, 2.3 in EtOH).
West, R.R. *et al., J.O.C.*, 1988, **53**, 2782

Cholesta-4,22-diene-3,6,8,15,16,24-hexol C-453

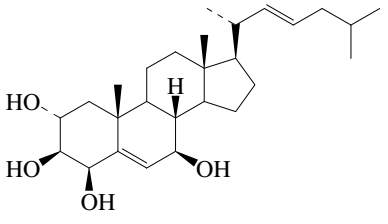


$C_{27}H_{44}O_6$ 464.641

(3β,6β,8β,15α,16β,22*E*,24ξ)-*form*

3-O-*β*-D-*Xylopyranoside, 15-sulfate:* ***Aphelasteroside B***
[142013-85-2]
$C_{32}H_{52}O_{13}S$ 676.821
Constit. of *Aphelasterias japonica*. $[\alpha]_D$ -16.8 (c, 1 in MeOH).
Finamore, E. *et al., J. Nat. Prod.*, 1992, **55**, 767-772 (*isol, pmr, cmr*)

Cholesta-5,22-diene-2,3,4,7-tetrol C-454

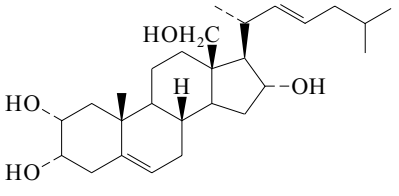


$C_{27}H_{44}O_4$ 432.642

(2α,3β,4β,7β,22*E*)-*form*

4-O-*[β*-D-*Galactopyranosyl-(1→2)-β*-D-*xylopyranoside]:* ***Wondosterol B***
[252023-83-9]
$C_{38}H_{62}O_{13}$ 726.9
Constit. of an association of sponges *Jaspis* sp. and *Poecillastra* sp.
Amorph. solid. $[\alpha]_D^{23}$ +46.2 (c, 0.5 in MeOH).
Ryu, G. *et al., Tetrahedron*, 1999, **55**, 13171-13178 (*isol, pmr, cmr*)

Cholesta-5,22-diene-2,3,16,18-tetrol C-455

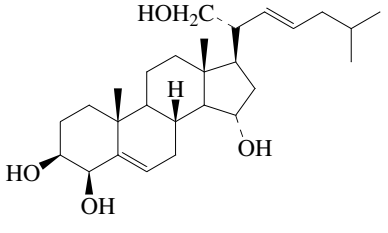


$C_{27}H_{44}O_4$ 432.642

(2α,3α,16α,22*E*)-*form*

2,16,18-Tri-Ac:
$C_{33}H_{50}O_7$ 558.754
Constit. of *Eudendrium glomeratum*. Cryst. (MeOH).
Mp 194-196°. $[\alpha]_D^{26}$ +57 (c, 0.04 in $CHCl_3$).
Fattorusso, E. *et al., J. Nat. Prod.*, 1985, **48**, 784

Cholesta-5,22-diene-3,4,15,21-tetrol C-456



$C_{27}H_{44}O_4$ 432.642

(3β,4β,15α,22*E*)-*form*

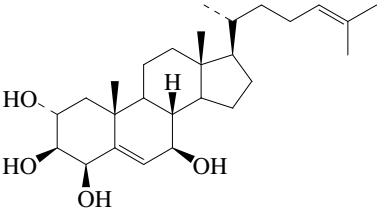
3-O-*[β*-D-*Galactopyranosyl-(1→2)-α*-L-*arabinopyranosyl-(1→3)-[β*-D-*galactopyranosyl-(1→4)]-β*-D-*glucopyranoside]:* ***Mycaloside C***
[593280-52-5]
$C_{50}H_{82}O_{23}$ 1051.184
Constit. of *Mycale laxissima*. Solid.
Mp 226-229°. $[\alpha]_D^{25}$ -28.2 (c, 0.6 in MeOH).

22,23-Dihydro, 15-ketone: 3,4,21-Trihydroxycholest-5-en-15-one
$C_{27}H_{44}O_4$ 432.642

22,23-Dihydro, 15-ketone, 3-O-*[β*-D-*galactopyranosyl-(1→2)-α*-L-*arabinopyranosyl-(1→3)-[β*-D-*galactopyranosyl-(1→4)]-β*-D-*glucopyranoside]:* ***Mycaloside G***
[593280-56-9]
$C_{50}H_{82}O_{23}$ 1051.184
Constit. of *Mycale laxissima*. Solid.
Mp 210-214°. $[\alpha]_D^{25}$ -27.2 (c, 0.68 in MeOH).

22,23-Dihydro, 15-ketone, 3-O-*[β*-D-*galactopyranosyl-(1→2)-α*-L-*arabinopyranosyl-(1→3)-[β*-D-*galactopyranosyl-(1→4)]-6*-O-*acetyl-β*-D-*glucopyranoside]:* ***Mycaloside F***
[593280-55-8]
$C_{52}H_{84}O_{24}$ 1093.221
Constit. of *Mycale laxissima*. Solid.
Mp 213-216°. $[\alpha]_D^{25}$ -38 (c, 0.38 in MeOH).
Antonov, A.S. *et al., J. Nat. Prod.*, 2003, **66**, 1082-1088 (*isol, pmr, cmr*)

Cholesta-5,24-diene-2,3,4,7-tetrol C-457

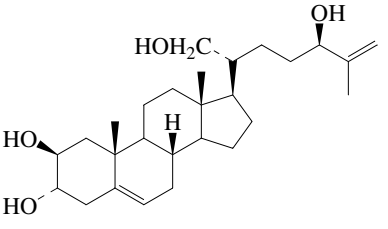


$C_{27}H_{44}O_4$ 432.642

(2α,3β,4β,7β)-*form*

4-O-*[β*-D-*Galactopyranosyl-(1→2)-β*-D-*xylopyranoside]:* ***Wondosterol C***
[252023-85-1]
$C_{38}H_{62}O_{13}$ 726.9
Constit. of an association of sponges *Jaspis* sp. and *Poecillastra* sp.
Amorph. solid. $[\alpha]_D^{23}$ +62.7 (c, 0.8 in MeOH).
Ryu, G. *et al., Tetrahedron*, 1999, **55**, 13171-13178 (*isol, pmr, cmr*)

Cholesta-5,25-diene-2,3,21,24-tetrol C-458



(2β,3α,24*R*)-*form*

$C_{27}H_{44}O_4$ 432.642

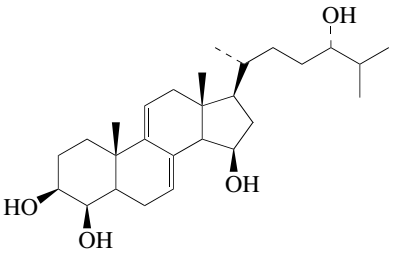
(2β,3α,24*R*)-*form*

3,21-Disulfate: [161470-25-3]
$C_{27}H_{44}O_{10}S_2$ 592.771
Constit. of *Ophiopholis aculeata*.

(2β,3α,24*S*)-*form*

3,21-Disulfate: [161470-26-4]
$C_{27}H_{44}O_{10}S_2$ 592.771
Constit. of *Ophiopholis aculeata*.
Fedarov, S.N. *et al., J. Nat. Prod.*, 1994, **57**, 1631-1637 (*isol, pmr, cmr*)

Cholesta-7,9(11)-diene-3,4,15,24-tetrol C-459

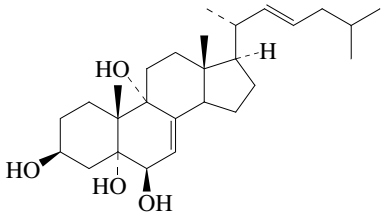


$C_{27}H_{44}O_4$ 432.642

(3β,4β,5α,15β,24*S*)-*form*

*3-(2-*O*-Methyl-β-D-xylopyranoside):* ***Moniloside B***
[147391-80-8]
$C_{33}H_{54}O_8$ 578.785
Constit. of *Fromia monilis.*
$[\alpha]_D$ -24.2 (MeOH). λ_{max} 235; 242; 250 (MeOH).
Casapullo, A. *et al., J. Nat. Prod.*, 1993, **56**, 105-115 (*isol, pmr, cmr*)

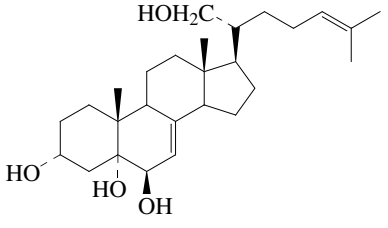
Cholesta-7,22-diene-3,5,6,9-tetrol, 9CI C-460



$C_{27}H_{44}O_4$ 432.642

(3β,5α,6β,9α,22*E*)-*form* [133056-65-2]
Constit. of *Spongia officinalis.*
Cryst. (MeOH aq.).
Mp 220-222°. $[\alpha]_D^{25}$ -16.6 (c, 0.06 in MeOH).
Migliuolo, A. *et al., J. Nat. Prod.*, 1990, **53**, 1414 (*isol, pmr, cmr*)

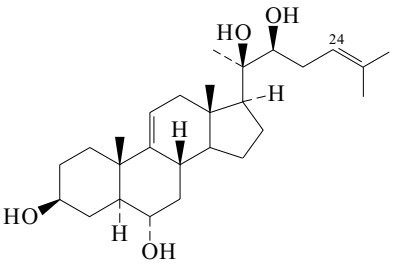
Cholesta-7,24-diene-3,5,6,21-tetrol C-461



$C_{27}H_{44}O_4$ 432.642

(3α,5α,6β)-*form* [614748-63-9]
Constit. of *Trimusculus peruvianus.*
Oil. $[\alpha]_D^{25}$ +53 (c, 0.58 in $CHCl_3$).
Diaz-Marrero, A.R. *et al., ARKIVOC*, 2003, **x**, 107-117 (*isol, pmr, cmr, ms*)

Cholesta-9(11),24-diene-3,6,20,22-tetrol C-462



$C_{27}H_{44}O_4$ 432.642

(3β,5α,6α,20*R*,22*S*)-*form*

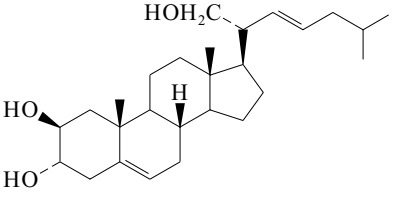
*6-*O*-[β-D-Fucopyranosyl-(1→2)-β-D-quinovopyranosyl-(1→4)[β-D-quinovopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-β-D-quinovopyranoside], 3-sulfate:* ***Protoreasteroside***
[96751-81-4]
$C_{56}H_{92}O_{27}S$ 1229.393
Isol. from the starfish *Protoreaster nodosus* and from *Pentaceraster alveolatus.*
$[\alpha]_D$ +3.8 (c, 1 in MeOH). Registry number refers to Na salt.

*6-*O*-[β-D-Fucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→4)-[β-D-quinovopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-β-D-quinovopyranoside], 3-sulfate:* ***Reticulatoside A***
[161996-24-3]
$C_{55}H_{90}O_{27}S$ 1215.366
Constit. of *Oreaster reticulatus.*
$[\alpha]_D$ -7.9.

24,25-Dihydro: Cholest-9(11)-ene-3,6,20,22-tetrol
$C_{27}H_{46}O_4$ 434.658

*24,25-Dihydro, 6-*O*-[β-D-fucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→4)-[β-D-quinovopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-β-D-quinovopyranoside], 3-sulfate:* ***Reticulatoside B***
[161996-25-4]
$C_{55}H_{92}O_{27}S$ 1217.382
Constit. of *Oreaster reticulatus.*
$[\alpha]_D$ -6.6.
Riccio, R. *et al., J. Nat. Prod.*, 1985, **48**, 266-272 (*Protoreasteroside*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1995, **58**, 10-26 (*Reticulatosides*)

Cholesta-5,22-diene-2,3,21-triol C-463

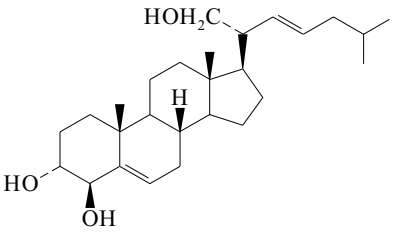


$C_{27}H_{44}O_3$ 416.643

(2β,3α,22*E*)-*form*

3,21-Disulfate: [162830-25-3]
$C_{27}H_{44}O_9S_2$ 576.771
Constit. of *Ophiura texturata* and *Ophionotus victoriae.*
$[\alpha]_D$ -7.4.
D'Auria, M.V. *et al., J. Nat. Prod.*, 1995, **58**, 189-196 (*isol, pmr*)

Cholesta-5,22-diene-3,4,21-triol C-464

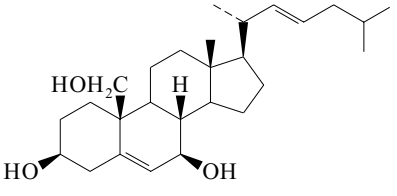


$C_{27}H_{44}O_3$ 416.643

(3α,4β,22*E*)-*form*

3,21-Disulfate: [161470-23-1]
$C_{27}H_{44}O_9S_2$ 576.771
Constit. of *Ophiopholis aculeata*, *Ophiotrix fragilis* and *Ophiura texturata*.
$[\alpha]_D$ -6.36.
Tri-Ac:
Amorph. $[\alpha]_D^{20}$ -125 (c, 0.2 in EtOH).
Fedorov, S.N. *et al., J. Nat. Prod.*, 1994, **57**, 1631-1637 (*Ophiopholis aculeata constit*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1995, **58**, 189-196 (*3,21-disulfate, isol, pmr*)

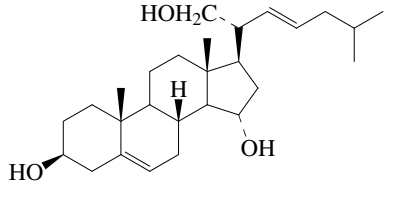
Cholesta-5,22-diene-3,7,19-triol C-465



$C_{27}H_{44}O_3$ 416.643

(3β,7β,22*E*)-*form* [139765-39-2]
Constit. of *Antipathes subpinnata*.
Cryst.
Mp 150-152°.
Aiello, A. *et al., J. Nat. Prod.*, 1992, **55**, 321 (*isol, pmr, cmr*)

Cholesta-5,22-diene-3,15,21-triol C-466

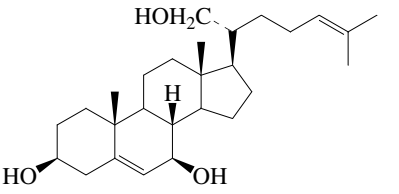


$C_{27}H_{44}O_3$ 416.643

(3β,15α,22*E*)-*form*

3-O-*[β-D-Galactopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→4)]-β-D-glucopyranoside]:* ***Mycaloside E***
[593280-54-7]
$C_{50}H_{82}O_{22}$ 1035.185
Constit. of *Mycale laxissima*. Solid.
Mp 221-225°. $[\alpha]_D^{25}$ -25.5 (c, 0.45 in MeOH).
Antonov, A.S. *et al., J. Nat. Prod.*, 2003, **66**, 1082-1088 (*isol, pmr, cmr*)

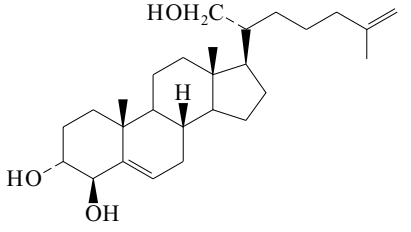
Cholesta-5,24-diene-3,7,21-triol C-467



$C_{27}H_{44}O_3$ 416.643

(3β,7β)-*form* [614748-62-8]
Constit. of *Trimusculus peruvianus.*
Oil. $[\alpha]_D^{25}$ -20 (c, 0.25 in $CHCl_3$).
Díaz-Marrero, A.R. *et al., ARKIVOC*, 2003, **x**, 107-117 (*isol, pmr, cmr*)

Cholesta-5,25-diene-3,4,21-triol C-468

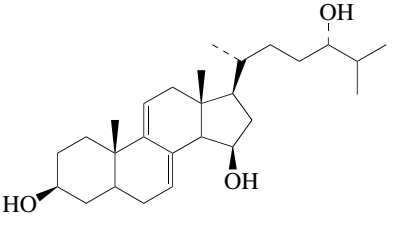


$C_{27}H_{44}O_3$ 416.643

(3α,4β)-*form*

3,21-Disulfate: [161470-22-0]
$C_{27}H_{44}O_9S_2$ 576.771
Constit. of *Ophiopholis aculeata*. Amorph. solid. $[\alpha]_D^{20}$ -40 (c, 0.1 in H_2O).
Tri-Ac:
Amorph. $[\alpha]_D^{20}$ -103 (c, 0.2 in EtOH).
Fedarov, S.N. *et al., J. Nat. Prod.*, 1994, **57**, 1631-1637 (*3,21-disulfate, isol, pmr, cmr*)

Cholesta-7,9(11)-diene-3,15,24-triol C-469

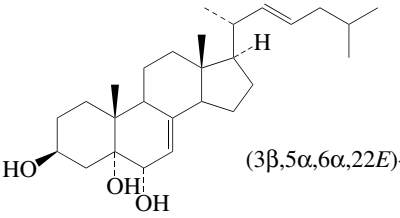


$C_{27}H_{44}O_3$ 416.643

(3β,5α,15β,24*S*)-*form*

3-(2-O-*Methyl-β-D-xylopyranoside):* ***Moniloside A***
[147362-15-0]
$C_{33}H_{54}O_7$ 562.785
Constit. of *Fromia monilis.*
$[\alpha]_D$ -30.2 (MeOH). λ_{max} 235 (ε 12300); 242; 250 (MeOH) (Berdy).
Casapullo, A. *et al., J. Nat. Prod.*, 1993, **56**, 105-115 (*isol, pmr, cmr*)

Cholesta-7,22-diene-3,5,6-triol, 9CI C-470



(3β,5α,6α,22*E*)-*form*

$C_{27}H_{44}O_3$ 416.643

(3β,5α,6α,22*E*)-*form*
Homaxisterol D₁
[877373-36-9]
Constit. of a *Homaxinella* sp.
Amorph. solid.

(3β,5α,6β,22*E*)-*form* [100667-74-1]
Constit. of *Patinopecten yessoensis*, *Heliometra glacialis maxima*, *Spongionella gracilis* and *Myriapora truncata*.
$[\alpha]_D$ -25 (MeOH).

6-Me ether: ***6-Methoxycholesta-7,22-diene-3,5-diol***
$C_{28}H_{46}O_3$ 430.67
Isol. from demosponge *Spongia agaricina*.
$[\alpha]_D$ -159 (c, 0.02 in $CHCl_3$).

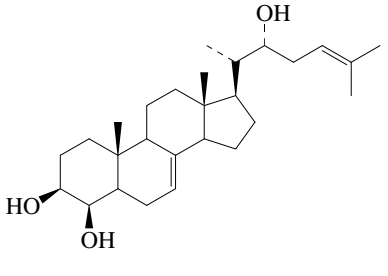
6-Butyl ether: ***Homaxisterol A₁***
[849906-44-1]
$C_{31}H_{52}O_3$ 472.75
Constit. of a *Homaxinella* sp. Oil.

22,23-Dihydro: ***Cholest-7-ene-3,5,6-triol, 9CI***
[15361-40-7]
$C_{27}H_{46}O_3$ 418.659
Constit. of *Patinopecten yessoensis* and *Aplysia juliana*.
$[\alpha]_D$ -20.8 (MeOH).

22,23-Dihydro, 6-Me ether: ***6-Methoxycholest-7-ene-3,5-diol***
[117585-48-5]
$C_{28}H_{48}O_3$ 432.685
Constit. of *Aplysia juliana*. Also from demosponge *Spongia agaricina*.
$[\alpha]_D$ -55.6 (c, 0.19 in $CHCl_3$). $[\alpha]_D$ -159 (c, 0.02 in $CHCl_3$).

Cafieri, F. *et al., J. Nat. Prod.*, 1985, **48**, 944-947 (*isol, pmr*)
Aiello, A. *et al., J. Nat. Prod.*, 1988, **51**, 999-1002 (*Spongia isolates*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1988, **51**, 1098-1103 (*isol, pmr*)
Yamaguchi, Y. *et al., Chem. Lett.*, 1992, 1713-1714 (*22,23-dihydro 6-Me ether*)
Shubina, L.K. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **119**, 505-511 (*Heliometra constit*)
Mansoor, T.A. *et al., J. Nat. Prod.*, 2005, **68**, 331-336; 2006, **69**, 131-134 (*Homaxisterols*)

Cholesta-7,24-diene-3,4,22-triol C-471

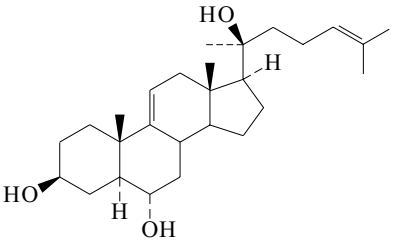


$C_{27}H_{44}O_3$ 416.643

(3β,4β,5α,22*R*)-*form* [671781-86-5]
Constit. of *Aglaia rubiginosa*.
Cryst.
Mp 235-237°. $[\alpha]_D^{24}$ -29.3 (c, 1 in MeOH). λ_{max} 220 (log ϵ 3.17) (MeOH).

Rivero-Cruz, J.F. *et al., J. Nat. Prod.*, 2004, **67**, 343-347 (*isol, pmr, cmr*)

Cholesta-9(11),24-diene-3,6,20-triol C-472



$C_{27}H_{44}O_3$ 416.643

(3β,5α,6α,20*S*)-*form*
3-O-*Sulfate:* [101129-06-0]
$C_{27}H_{44}O_6S$ 496.707
Isol. from the starfish *Asterias amurensis* (as Na salt).

6-O-*[6-Deoxy-4*-O-*sulfo-β-D-glucopyranoside], 3-sulfate:* ***Latespinoside A***
[178200-90-3]
$C_{33}H_{54}O_{13}S_2$ 722.914
Constit. of *Astropecten latespinosus*. Amorph. powder.
Mp 205-207°. $[\alpha]_D$ +20.8 (c, 0.33 in MeOH).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate:* ***Cosmasteroside A***
[158243-22-2]
$C_{55}H_{90}O_{26}S$ 1199.366
Constit. of *Cosmasterias lurida*.

6-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Ruberoside E***
[685561-53-9]
$C_{56}H_{92}O_{26}S$ 1213.393
Constit. of *Asterias rubens*.

6-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate:* ***Astersaponin 4****. Ovarian asterosaponin 4. Asterosaponin 4. Co-Aris III*
[101222-70-2]
$C_{56}H_{92}O_{27}S$ 1229.393
Constit. of *Asterias amurensis*. Cryst. or powder.
Mp 207-209° (189-201°). $[\alpha]_D^{22}$ -1.5. $[\alpha]_D$ +3.7 (MeOH).

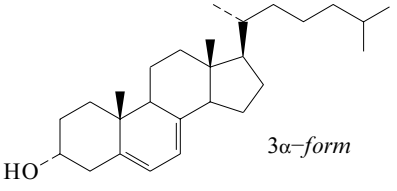
6-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-[β-D-galactopyranosyl-(1→3)-6-deoxy-β-D-galactopyranosyl-(1→2)-6-deoxy-β-D-galactopyranosyl-(1→4)]-α-L-arabinopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Forbeside D***
[136803-86-6]
$C_{62}H_{102}O_{31}S$ 1375.535
Isol. from *Asterias forbesi*. Powder (as Na salt).
Mp 213° dec. (Na salt). $[\alpha]_D$ -4.7 (c, 0.6 in H_2O).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Solasteroside A***
[143016-88-0]
$C_{56}H_{92}O_{26}S$ 1213.393
Constit. of *Solaster borealis*.
$[\alpha]_D$ +1.1 (MeOH).

6-O-*[β-D-Galactopyranosyl-(1→3)-β-D-fucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Asteriidoside C***
[214976-56-4]
$C_{62}H_{102}O_{31}S$ 1375.535
Constit. of a starfish (Asteriidae).
$[\alpha]_D$ +10.7 (c, 1 in MeOH).

6-O-*[β-D-Galactopyranosyl-(1→3)-β-D-arabinopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Asteriidoside E***
[214976-59-7]
$C_{61}H_{100}O_{31}S$ 1361.508
Constit. of a starfish (Asteriidae).
$[\alpha]_D$ +8.5 (c, 1 in MeOH).
Okano, K. *et al., Agric. Biol. Chem.*, 1985, **49**, 2823-2826 (*Asterosaponin 4*)
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1829-1832 (*Co-Aris III*)
Riccio, R. *et al., J.C.S. Perkin 1*, 1988, 1337-1347 (*Asterosaponin 4, sulfate*)
Findlay, J.A. *et al., Can. J. Chem.*, 1991, **69**, 1134-1140 (*Forbeside D*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1992, **55**, 866-877 (*Solasteroside A*)
Roccatagliata, A.J. *et al., J. Nat. Prod.*, 1994, **57**, 747-754 (*Cosmasteroside A*)
Higuchi, R. *et al., Annalen*, 1996, 837-840 (*Latespinoside A*)
De Marino, S. *et al., J. Nat. Prod.*, 1998, **61**, 1319-1327 (*Asteriidosides*)
Sandvoss, M. *et al., Magn. Reson. Chem.*, 2003, **41**, 949-954 (*Ruberoside E*)

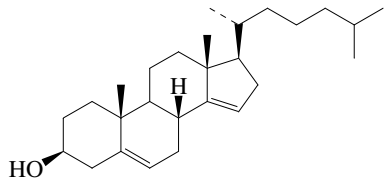
Cholesta-5,7-dien-3-ol C-473



$C_{27}H_{44}O$ 384.644

3β-*form*
7-Dehydrocholesterol. *Provitamin D_3*
[434-16-2]
Occurs in man and higher animals as Vitamin D precursor. Constit. of sponges, tunicates, molluscs and fish. Isol. from the horned snail *Buccinum undatum* and pigskin. Irradiation with uv light prod. previtamin D_3.
Plates (MeOH aq./Et_2O).
Mp 150-151° (anhyd.). $[\alpha]_D^{20}$ -113.6 ($CHCl_3$). Oxid. in air.
▶ FZ5650000
Bernstein, S. *et al., J.O.C.*, 1949, **14**, 433 (*synth, 3β-form*)
Yablonskaya, E.V. *et al., Khim. Prir. Soedin.*, 1973, **9**, 739; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 708 (*synth, 3β-form*)
Iida, T. *et al., Steroids*, 1977, **29**, 453 (*pmr, 3β-form*)
Kirk, D.N. *et al., J.C.S. Perkin 2*, 1990, 1567 (*pmr*)

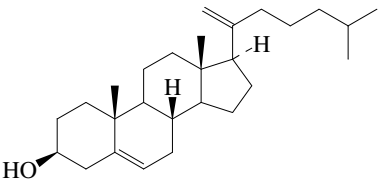
Cholesta-5,14-dien-3-ol C-474



$C_{27}H_{44}O$ 384.644

3β-*form* [82507-26-4]
Constit. of *Aiptasia pulchella*.
Withers, N.W. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1982, **79**, 3764-3768 (*isol, pmr*)

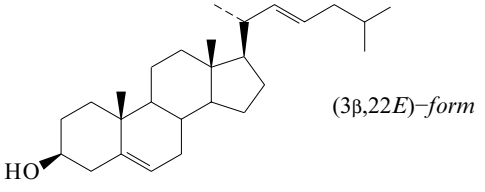
Cholesta-5,20-dien-3-ol, 9CI C-475



$C_{27}H_{44}O$ 384.644

3β-*form*
20-Dehydrocholesterol
[41083-90-3]
Constit. of *Mandevilla pentlandiana* and a *Zoanthus* sp.
Mp 111-112°.
Ac: [33168-77-3]
$C_{29}H_{46}O_2$ 426.681
Cryst. (MeOH). Mp 101-102°. $[\alpha]_D$ -48 ($CHCl_3$).
Sheikh, Y.M. *et al., J.O.C.*, 1973, **38**, 3545 (*synth, pmr, ms*)
Byon, C.Y. *et al., J.O.C.*, 1977, **42**, 3619 (*synth*)
Cabrera, G. *et al., Phytochemistry*, 1991, **30**, 1239 (*isol, pmr, cmr*)
Babu, U.V. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 627 (*isol, pmr, cmr*)

Cholesta-5,22-dien-3-ol, 9CI C-476



$C_{27}H_{44}O$ 384.644

(3β,22*E*)-*form*
22E-Dehydrocholesterol
[34347-28-9]
Constit. of a dinoflagellate symbiont of *Zoanthus sociatus*, *Bathyplotes natans*, *Pseudostichopus trachus*, *Synapta maculata*, *Trochostoma orientale* and many other marine organisms incl. *Bathyplotes natans*, *Pseudostichopus trachus*, *Trochostoma orientale*, *Henricia sanguinolenta*, *Marthasterias glacialis*, *Porania pulvillus*, *Placopecten magellanicus* and *Tridacna gigas.*
Cryst. (EtOH).
Mp 133.5-134°. $[\alpha]_D^{23}$ -60 (c, 1 in $CHCl_3$).
3-O-*Sulfate:* [80677-76-5]
[151890-95-8 (Na salt)]
$C_{27}H_{44}O_4S$ 464.708
Constit. of *Euretaster insignis*, *Cucumaria japonica*, *Asterias rubens*, *Gymnocrinus richeri* and *Eupentacta fraudatrix*.
3-O-*β-D-Xylopyranoside:* [151890-80-1]
$C_{32}H_{52}O_5$ 516.76
Constit. of *Eupentacta fraudatrix*.
Formyl: [848123-82-0]
$C_{28}H_{44}O_2$ 412.654
Constit. of a *Dendronephthya* sp. Amorph. powder. $[\alpha]_D^{25}$ -22.5 (c, 0.13 in $CHCl_3$).
Ac: [26033-11-4]
Cryst. (Et_2O/MeOH). Mp 128-129°. $[\alpha]_D^{23}$ -63.2 (c, 1.15 in $CHCl_3$).
Me ether: 3-Methoxycholesta-5,22-diene
[86851-20-9]
$C_{28}H_{46}O$ 398.671
Constit. of *Jereicopsis graphidiophora*.

(3β,22*Z*)-*form*

22Z-Dehydrocholesterol

[26033-10-3]

Constit. of the scallop *Placopecten magellanicus* and the red alga *Hypnea japonica*.

Cryst. (MeOH).

Mp 134-136°. $[\alpha]_D$ -58.5 ($CHCl_3$).

Ac: [25819-79-8]

Cryst. (Et_2O/MeOH). Mp 117-119°. $[\alpha]_D^{23}$ -68 (c, 1 in $CHCl_3$).

(3β,20*S*,22*E*)-*form*

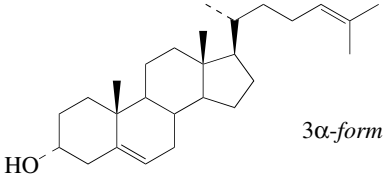
Mp 154-155°. $[\alpha]_D^{28.5}$ -63.1 (c, 1.01 in $CHCl_3$).

Ac: Mp 107-108°. $[\alpha]_D^{29}$ -66.6 (c, 1.01 in $CHCl_3$).

[566-89-2]

Bergmann, W. *et al., J.O.C.*, 1958, **23**, 1245-1247 (*3β,22E-form, synth*)
Tsuda, K. *et al., J.A.C.S.*, 1960, **82**, 1442-1443 (*3β,22Z-form, isol*)
Tsuda, K. *et al., Chem. Pharm. Bull.*, 1961, **9**, 529-532 (*3β,20S,22E-form*)
Tamura, T. *et al., Can. J. Biochem.*, 1964, **42**, 1331-1337 (*isol*)
Hutchins, R.F.N. *et al., Steroids*, 1970, **15**, 113-130 (*synth, pmr*)
Idler, D.R. *et al., Comp. Biochem. Physiol., A: Comp. Physiol.*, 1971, **38**, 581 (*isol, Placopecten*)
Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*isol*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195-200 (*pmr*)
Wright, J.L.C. *et al., Can. J. Chem.*, 1978, **56**, 1898-1903 (*cmr*)
Kokke, W.C.M.C. *et al., Tet. Lett.*, 1979, 3601-3604 (*isol, ir, nmr, ms*)
Goodfellow, R.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **76**, 575-578 (*sulfate, occur*)
D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1984, 2277-2282 (*sulfate*)
Bratrakov, S.G. *et al., Khim. Prir. Soedin.*, 1984, 470-477; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 444-450 (*sulfate*)
De Riccardis, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **100**, 647-651 (*sulfate, occur*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*3-Methoxycholestadiene*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*3β,22E-form, occur*)
Volkman, J.K. *et al., Phytochemistry*, 1999, **52**, 659-668 (*occur, dinoflagellates*)
Li, G. *et al., Steroids*, 2005, **70**, 13-18 (*formyl*)

Cholesta-5,24-dien-3-ol, 9CI C-477



$C_{27}H_{44}O$ 384.644

3α-*form* [67392-80-7]

Cryst. (MeOH). Mp 137-139°. $[\alpha]_D^{28}$ -43.5 ($CHCl_3$).

Ac: [67383-62-4]

$C_{29}H_{46}O_2$ 426.681

Cryst. (MeOH). Mp 112-115°. $[\alpha]_D^{28}$ -47.5 ($CHCl_3$).

3β-*form*

Desmosterol

[313-04-2]

Constit. of the seeds of *Funtumia latifolia*, chick embryos and rat skin. Found in red algae *Rhodymenia palmata* and *Halosaccion ramentaceum* and other marine organisms, e.g. *Patinopecten yessoensis.*

Cryst. (Me_2CO/MeOH).

Mp 121.5-122.5°. $[\alpha]_D^{20}$ -38.2 (c, 1.143 in $CHCl_3$).

Ac: [2665-04-5]

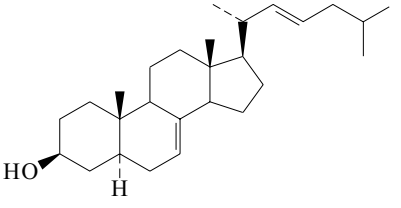
Cryst. (MeOH/Me_2CO). Mp 99°. $[\alpha]_D^{28}$ -44.8 ($CHCl_3$).

(3β,20*S*)-*form* [59532-46-6]

Cryst. (MeOH). Mp 125-127°.

Idler, D.R. *et al., Steroids*, 1968, **11**, 465 (*3β-form, isol*)
Charles, G. *et al., C. R. Hebd. Seances Acad. Sci.*, 1969, **268**, 2105 (*isol*)
Ener, M.A. *et al., J. Biol. Chem.*, 1973, **248**, 6697 (*ms, 3β-form*)
Dasgupta, S.K. *et al., J.O.C.*, 1974, **39**, 1658 (*synth, pmr, 3β-form*)
Chen, S.-M.L. *et al., J.A.C.S.*, 1975, **97**, 5297 (*biosynth*)
Kobayashi, M. *et al., Steroids*, 1975, **26**, 605 (*isol, Patinopecten*)
Takeshita, T. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1928 (*synth*)
Bu'lock, J.D. *et al., Phytochemistry*, 1976, **15**, 1249 (*biosynth*)
Burstein, S. *et al., Steroids*, 1976, **27**, 361 (*synth, ir, pmr, 3β,20S-form*)
Ochi, K. *et al., Steroids*, 1977, **30**, 795 (*synth, pmr*)
Koreeda, M. *et al., J.O.C.*, 1980, **45**, 1172; 1174 (*synth, 3β-form*)
Takano, S. *et al., Chem. Comm.*, 1983, 760 (*synth*)
Kircher, H.W. *et al., J.O.C.*, 1987, **52**, 2586 (*synth, 3β-form*)
Ikuina, Y. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1755 (*synth*)
Giner, J.L. *et al., Phytochemistry*, 1992, **31**, 3865 (*biosynth*)
Corey, E.J. *et al., Tet. Lett.*, 1998, **39**, 9351-9354 (*synth*)
Spencer, T.A. *et al., J.O.C.*, 2000, **65**, 1919-1923 (*synth*)
Westover, E.J. *et al., Steroids*, 2003, **68**, 159-166 (*synth*)

Cholesta-7,22-dien-3-ol, 9CI C-478



$C_{27}H_{44}O$ 384.644

(3β,5α,22*E*)-*form* [50364-21-1]

Constit. of *Asterias amurensis, Axinella cannabina, Crambe crambe, Haliclona flavescens* , *Astropecten indicus*, *Parathyona* sp., *Cucumaria* sp., *Eupentacta fraudatrix*, *Bathyplotes natans*, *Holothuria nobilis*, *Holothuria scabra* and many other marine spp.

Needles (MeOH).

Mp 129-130.5°. $[\alpha]_D^{25}$ -13.3 (c, 1.085 in $CHCl_3$).

3-O-*Sulfate:* [88341-74-6]

[152005-18-0]

$C_{27}H_{44}O_4S$ 464.708

Constit. of *Eupentacta fraudatrix*, *Gymnocrinus richeri*, *Asterias rubens* and *Euretaster insignis.*

3-O-*β*-D-*Xylopyranoside:* [74185-10-7]

$C_{32}H_{52}O_5$ 516.76

Constit. of *Eupentacta fraudatrix*.

Ac: [28636-25-1]

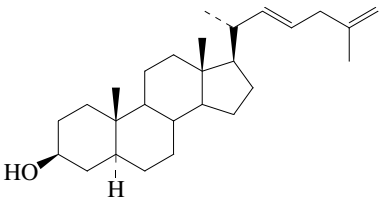
$C_{29}H_{46}O_2$ 426.681

Plates (MeOH). Mp 140-142.5°. $[\alpha]_D^{25}$ -14.9 (c, 1.051 in $CHCl_3$).

[20780-37-4, 40600-59-7, 51446-63-0]

Sakai, K. *et al., Chem. Pharm. Bull.*, 1963, **11**, 529-530 (*synth*)
Kobayashi, M. *et al., Tetrahedron*, 1973, **29**, 1193-1196 (*isol, ir, ms*)
Zielinski, J. *et al., Steroids*, 1982, **39**, 675-680 (*Eupentacta fraudatrix constits*)
Kalinovskaya, N.I. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **74**, 597-601; **76**, 167-171 (*isol*)
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol*)
D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1984, 2277-2282 (*sulfate*)
Moseichuk, A.V. *et al., Khim. Prir. Soedin.*, 1984, **20**, 621-623; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 585 (*ms*)
Veares, M.P. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1988, **90**, 25-28 (*sulfate*)
De Riccardis, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **100**, 647-651 (*sulfate*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*occur*)

Cholesta-22,25-dien-3-ol C-479

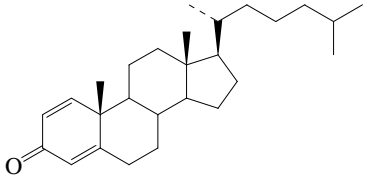


$C_{27}H_{44}O$ 384.644

(3β,5α,22*E*)-*form* [241166-24-5]
Present in sponge *Fasciospongia cavernosa*.
De Rosa, S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1999, **123**, 235-239

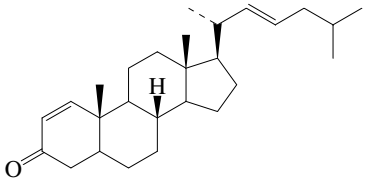
Cholesta-1,4-dien-3-one, 9CI C-480

[566-91-6]



$C_{27}H_{42}O$ 382.628
Isol. from crinoid *Gymnocrinus richeri*. Cryst. (MeOH). Mp 112°. $[\alpha]_D$ +31 ($CHCl_3$). λ_{max} 243 (ϵ 12000) (EtOH).
Wilds, A.L. *et al., J.A.C.S.*, 1946, **68**, 1712-1715 (*synth*)
Barton, D.H.R. *et al., J.C.S. Perkin 1*, 1980, 2209-2212 (*synth*)
Fürst, A. *et al., Helv. Chim. Acta*, 1981, **64**, 1870-1892 (*synth*)
Barton, D.H.R. *et al., J.C.S. Perkin 1*, 1982, 1947-1952 (*synth*)
De Riccardis, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **100**, 647-651 (*isol*)

Cholesta-1,22-dien-3-one C-481

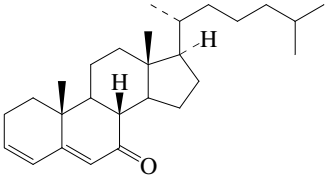


$C_{27}H_{42}O$ 382.628

(22*E*)-*form*
Dendronesterone A
[771534-36-2]
Constit. of *Dendronephthya gigantea*.
Solid. $[\alpha]_D^{25}$ +16 (c, 0.3 in $CHCl_3$). λ_{max} 226 (log ϵ 3.6) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 2004, **67**, 1650-1653 (*isol, pmr, cmr*)

Cholesta-3,5-dien-7-one, 9CI C-482

[567-72-6]



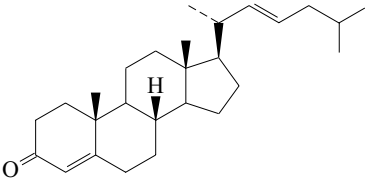
$C_{27}H_{42}O$ 382.628
Isol. from sponge *Damiriana hawaiiana*, poss. as artifact. Cryst. (EtOH). Mp 116°. $[\alpha]_D^{20}$ -30 (c, 1.1 in $CHCl_3$).

2,4-Dinitrophenylhydrazone:
Orange needles ($CHCl_3$/MeOH). Mp 225-226°. $[\alpha]_D$ -380 (c, 0.382 in $CHCl_3$).

Oxime: [19588-37-5]
$C_{27}H_{43}NO$ 397.643
Plates (MeOH). Mp 178-180°.

Reich, H.J. *et al., J.A.C.S.*, 1969, **91**, 7445 (*cmr*)
Smith, L.L. *et al., Steroids*, 1973, **22**, 627 (*synth, uv, ir*)
Lin, Y.Y. *et al., Biomed. Mass Spectrom.*, 1978, **5**, 604 (*ms*)
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476 (*isol*)
Shafiullah, *et al., J.C.S. Perkin 1*, 1979, 2727 (*synth, ir, pmr*)
Kohout, L. *et al., Coll. Czech. Chem. Comm.*, 1981, **46**, 1828; 1986, **51**, 429 (*synth, ir, pmr*)

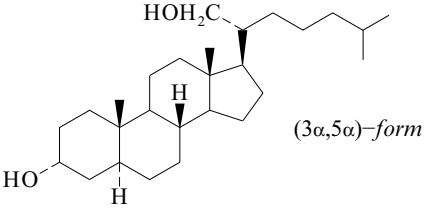
Cholesta-4,22-dien-3-one C-483



$C_{27}H_{42}O$ 382.628

(22*E*)-*form* [55688-43-2]
Constit. of the sponges *Esperiopsis edwardii* and *Stelletta clarella*.
Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*isol, ms*)
Japan. Pat., 1977, 77 116 456; *CA*, **88**, 136852 (*synth*)
Seldes, A.M. *et al., Tetrahedron*, 1988, **44**, 1359-1362 (*isol*)

Cholestane-3,21-diol, 9CI C-484



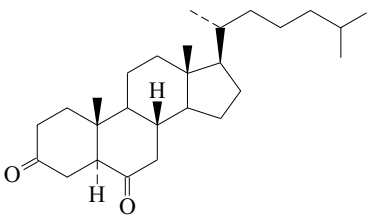
$C_{27}H_{48}O_2$ 404.675

(3α,5α)-*form*
Disulfate: [100942-72-1]
$C_{27}H_{48}O_8S_2$ 564.803
Constit. of *Ophiopholis aculeata, Ophiopholis sarsi*, *Heliometra glacialis maxima*, *Asteronyx loveni* and *Stegophiura brachiactis*.
Cryst. (MeOH). Mp 176-178°. $[\alpha]_D^{20}$ -11 (c, 0.1 in EtOH).

(3β,5α)-*form* [95062-37-6]
Disulfate: [95062-39-8]
Constit. of the starfish *Euretaster insignis*.
D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1984, 2277-2282 (*3β,5α, disulfate*)
Riccio, R. *et al., Tetrahedron*, 1985, **41**, 6041-6046 (*disulfate, isol, pmr, cmr*)
Fedarov, S.N. *et al., J. Nat. Prod.*, 1994, **57**, 1631-1637 (*Ophiopholis aculeata constit, isol*)

Cholestane-3,6-dione C-485

[13492-22-3]



$C_{27}H_{44}O_2$ 400.643

5α-*form* [2243-09-6]
Isol. from the red alga *Acanthophora spicifera*. Cryst. (MeOH). Mp 172-173°. $[\alpha]_D^{25}$ +4 (c, 1.6 in $CHCl_3$). Genus name given as Acantophora.

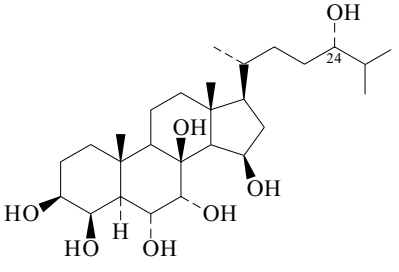
Dioxime:
$C_{27}H_{46}N_2O_2$ 430.673
Mp 208-210°.

3-(Di-Me acetal): 3,3-Dimethoxycholestan-6-one
$C_{29}H_{50}O_3$ 446.712
Mp 74.5-75.5°. $[\alpha]_D$ -1 (c, 1 in $CHCl_3$).

5β-*form* [22799-16-2]
Cryst. (MeOH). Mp 178-180°. $[\alpha]_D$ -72 ($CHCl_3$).

Barton, D.H.R. *et al., J.C.S.*, 1948, 783 (*synth*)
Fieser, L. *et al., Steroids*, Reinhold, New York, 1959, 44 (*synth*)
Nussim, M. *et al., J.O.C.*, 1964, **29**, 1120 (*synth*)
Snatzke, G. *et al., Tetrahedron*, 1964, **20**, 1243 (*cd*)
Blaszczak, L.C. *et al., J.O.C.*, 1974, **39**, 258 (*synth*)
Dave, V. *et al., Can. J. Chem.*, 1980, **58**, 2666 (*cmr*)
D'Auria, M. *et al., Synthesis*, 1980, 245 (*synth*)
Wahidulla, S. *et al., Phytochemistry*, 1987, **26**, 2864 (*isol*)
Pande, P.P. *et al., Synth. Commun.*, 1998, **28**, 4193-4200 (*synth, ir, pmr*)

Cholestane-3,4,6,7,8,15,24-heptol C-486



$C_{27}H_{48}O_7$ 484.672

(3β,4β,5α,6α,7α,8β,15β,24*S*)-*form*

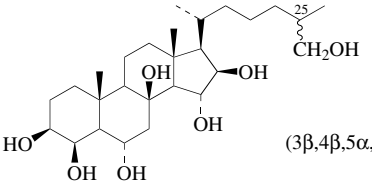
6-Sulfate: [854215-33-1]
$C_{27}H_{48}O_{10}S$ 564.736
Constit. of *Hippasteria phygiana*. Amorph. solid. $[\alpha]_D^{20}$ +14.1 (c, 0.25 in EtOH).

*24-*O*-[3-*O*-Methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside], 6-sulfate:* ***Phrygioside A***
[854516-42-0]
$C_{38}H_{66}O_{18}S$ 842.995
Constit. of *Hippasteria phygiana*. Cryst. (MeOH).
Mp 129-131°. $[\alpha]_D^{20}$ -10.9 (c, 0.33 in EtOH).

*24-*O*-[6-Deoxy-2,4-di-*O*-methyl-β-D-glucopyranosyl-(1→2)-6-deoxy-5-*O*-sulfo-β-D-galactofuranoside]:* ***Imbricatoside A***
[128855-06-1]
$C_{41}H_{72}O_{18}S$ 885.075
Constit. of *Dermasterias imbricata*.

Bruno, I. *et al., J. Nat. Prod.*, 1990, **53**, 366-374 (*Imbricatoside A*)
Levina, E.V. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2004, **53**, 2634-2638 (*Phrygioside A*)

Cholestane-3,4,6,8,15,16,26-heptol C-487



(3β,4β,5α,6α,8β,15α,16β,25ξ)-*form*

$C_{27}H_{48}O_7$ 484.672

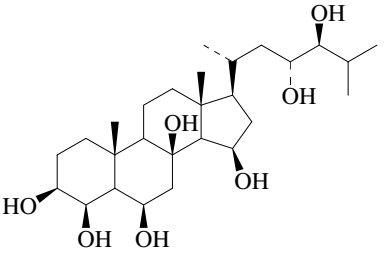
(3β,4β,5α,6α,15α,16β,25ξ)-*form* [93368-88-8]
Constit. of *Protoreaster nodosus*. Cryst. (MeOH). Mp 241-243°. $[\alpha]_D$ +28.4 (c, 1 in MeOH).

(3β,4β,5α,6α,15β,16β,25*S*)-*form* [102130-12-1]
Constit. of *Halityle regularis*.

*26-*O*-β-D-Xylopyranoside:* ***Coscinasteroside E***
[105377-94-4]
$C_{32}H_{56}O_{11}$ 616.788
Constit. of *Coscinasterias tenuispina*. $[\alpha]_D$ -11.8 (MeOH).

Minale, L. *et al., J. Nat. Prod.*, 1984, **47**, 790-795 (*Protoreaster constit*)
Riccio, R. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 869-893 (*Coscinasteroside E*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1986, **49**, 67-78 (*Halityle constit*)

Cholestane-3,4,6,8,15,23,24-heptol C-488

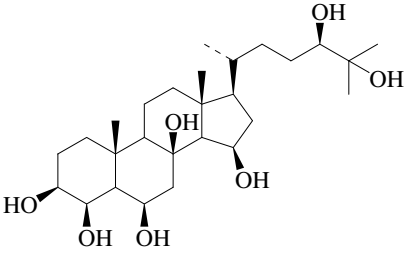


$C_{27}H_{48}O_7$ 484.672

(3β,4β,5α,6β,8β,15β,23*R*,24*S*)-*form* [876620-21-2]
Constit. of *Henricia leviuscula*.
Amorph. powder. $[\alpha]_D$ -5 (c, 0.18 in MeOH).

Ivanchina, N.V. *et al., J. Nat. Prod.*, 2006, **69**, 224-228 (*Henricia leviuscula constit*)

Cholestane-3,4,6,8,15,24,25-heptol C-489

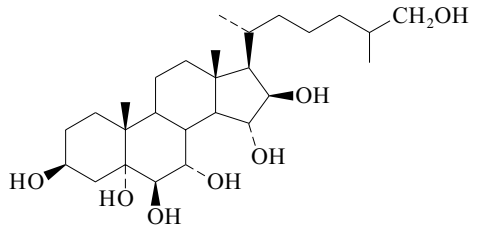


$C_{27}H_{48}O_7$ 484.672

(3β,4β,5α,6β,8β,15β,24*R*)-*form* [876620-22-3]
Constit. of *Henricia leviuscula*.
Amorph. powder. $[\alpha]_D$ -2.4 (c, 0.3 in MeOH).

Ivanchina, N.V. *et al., J. Nat. Prod.*, 2006, **69**, 224-228

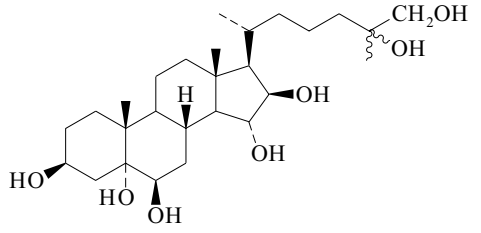
Cholestane-3,5,6,7,15,16,26-heptol C-490



$C_{27}H_{48}O_7$ 484.672

(3β,5α,6β,7α,15α,16β)-*form* [93368-85-5]
Constit. of *Luidia maculata*. Cryst. (MeOH). Mp 243-246°. $[\alpha]_D$ -4.7 (c, 0.5 in MeOH).
Minale, L. *et al., J. Nat. Prod.*, 1984, **47**, 784-789 (*isol, pmr, cmr*)

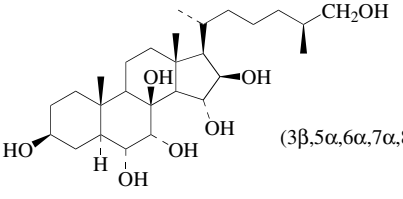
Cholestane-3,5,6,15,16,25,26-heptol C-491



$C_{27}H_{48}O_7$ 484.672

(3β,5α,6β,15α,16β,25ξ)-*form* [162442-05-9]
Constit. of *Ctenodiscus crispatus*. Cryst. Mp 241-242°. $[\alpha]_D$ +19 (c, 0.5 in MeOH).
Kicha, A.A. *et al., Izv. Akad. Nauk, Ser. Khim.*, 1994, **43**, 1821; *Russ. Chem. Bull. (Engl. Transl.)*, 1994, **43**, 1726 (*isol, pmr, cmr*)

Cholestane-3,6,7,8,15,16,26-heptol C-492



(3β,5α,6α,7α,8β,15α,16β,25*S*)-*form*

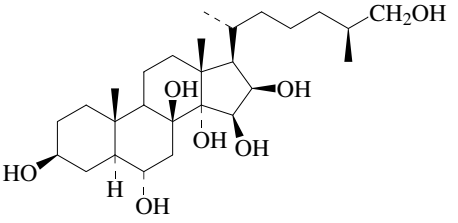
$C_{27}H_{48}O_7$ 484.672

(3β,5α,6α,7α,8β,15α,16β,25*S*)-*form* [100101-16-4]
Constit. of *Protoreaster nodosus* and *Patiria pectinifera*. Cryst. (MeOH). Mp 255-258°. $[\alpha]_D$ +33.8 (c, 1 in MeOH).
3-O-*(2*-O-*Methyl-β-D-xylopyranoside):* [100007-39-4]
$C_{33}H_{58}O_{11}$ 630.815
Constit. of *Poraster superbus*. $[\alpha]_D$ +3.4 (MeOH).

(3β,5α,6α,7α,8β,15β,16β,25*S*)-*form* [124649-08-7]
Constit. of *Pycnopodia helianthoides* and *Solaster borealis*. $[\alpha]_D$ +16.

(3β,5α,6β,7α,8β,15α,16β,25*S*)-*form* [129893-34-1]
Constit. of a *Rosaster* sp. $[\alpha]_D$ +5.5 (c, 1 in MeOH).
Riccio, R. *et al., Tetrahedron*, 1982, **38**, 3615-3622 (*Protoreaster nodosus constit*)
Riccio, R. *et al., Gazz. Chim. Ital.*, 1985, **115**, 505-509 (*Poreaster superbus saponin*)
Bruno, I. *et al., J. Nat. Prod.*, 1989, **52**, 1022-1026 (*Pycnopodia helianthoides constit*)
Bruno, I. *et al., Gazz. Chim. Ital.*, 1990, **120**, 449-451 (*Rosaster constit*)

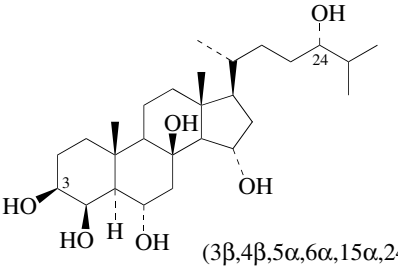
Cholestane-3,6,8,14,15,16,26-heptol C-493



$C_{27}H_{48}O_7$ 484.672

(3β,5α,6α,15β,16β,25*S*)-*form* [128855-09-4]
Constit. of *Dermasterias imbricata*. $[\alpha]_D$ +41 (c, 0.5 in MeOH).
Bruno, I. *et al., J. Nat. Prod.*, 1990, **53**, 366-374 (*isol, pmr, cmr*)

Cholestane-3,4,6,8,15,24-hexol C-494



(3β,4β,5α,6α,15α,24*S*)-*form*

$C_{27}H_{48}O_6$ 468.673

(3β,4β,5α,6α,15α,24*S*)-*form*
24-O-*α-L-Arabinofuranoside:* ***Attenuatoside C***
[86425-59-4]
$C_{32}H_{56}O_{10}$ 600.788
Constit. of *Hacelia attenuata*.
$[\alpha]_D$ +4.7 (MeOH).
24-O-*(3*-O-*Methyl-β-D-xylopyranoside):* ***Borealoside D***
[143016-87-9]
$C_{33}H_{58}O_{10}$ 614.815
Constit. of *Solaster borealis*.
$[\alpha]_D$ +15.5 (MeOH).
24-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside], 6*-O-*sulfate:* ***Validoside A***
$C_{39}H_{68}O_{17}S$ 841.022
Isol. from starfish *Odontaster validus*.
$[\alpha]_D^{20}$ -13.3 (c, 2.5 in MeOH) (as Na salt).
15-Ketone: 3,4,6,8,24-Pentahydroxycholestan-15-one. ***Certonardosterol Q2***
[781646-77-3]
$C_{27}H_{46}O_6$ 466.657
Constit. of *Certonardoa semiregularis*. Cryst. $[\alpha]_D^{21}$ +60 (c, 0.07 in MeOH).

(3β,4β,5α,6α,15β,24*S*)-*form* [99481-54-6]
Constit. of echinoderms *Gomophia watsoni* and *Nardoa tuberculata*. Toxic to brine shrimp. $[\alpha]_D$ +7.2 (c, 0.4 in MeOH).
24-O-*α-L-Arabinofuranoside:* ***Attenuatoside BII***
[86425-60-7]
$C_{32}H_{56}O_{10}$ 600.788
Constit. of *Hacelia attenuata*.
$[\alpha]_D$ -9 (MeOH).
24-O-*β-D-Xylopyranoside, 3*-O-*sulfate:* ***Glacialoside B***
[117585-46-3]
$C_{32}H_{56}O_{13}S$ 680.853
Isol. from the starfish *Marthasterias glacialis* (as Na salt). Sol. MeOH, butanol; fairly sol. H_2O. $[\alpha]_D$ +2 (c, 0.1 in MeOH).

24-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→5)-α-L-arabinofuranoside]:* ***Attenuatoside B1***
[86425-61-8]
$C_{38}H_{66}O_{14}$ 746.931
Constit. of *Crossaster papposus* and *Hacelia attenuata*. Cryst.
Mp 295-298°. $[\alpha]_D$ -24.6 (c, 1.2 in MeOH).

24-O-*[4*-O-*Methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside]:* ***Culcitoside C5***
[138169-01-4]
$C_{38}H_{66}O_{14}$ 746.931
Constit. of *Culcita novaeguineae.*
$[\alpha]_D$ -22.4 (MeOH).

24-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside]:* ***Culcitoside C1****. Halityloside D*
[102130-11-0]
$C_{39}H_{68}O_{14}$ 760.958
Isol. from the starfishes *Culcita novaeguineae* and *Linckia guildingi* and from *Halityle regularis.*
Mp 245-248°. $[\alpha]_D$ -35.8 (c, 0.6 in MeOH).

24-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→5)-α-L-arabinofuranoside]:* ***Crossasteroside P4***
[168433-98-5]
$C_{39}H_{68}O_{14}$ 760.958
Constit. of *Crossaster papposus.* Amorph. $[\alpha]_D$ -40.6 (c, 0.7 in MeOH).

24-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→2)-β-D-xylofuranoside]:* ***Certonardoside K***
[620604-19-5]
$C_{39}H_{68}O_{14}$ 760.958
Constit. of *Certonardoa semiregularis.* Cryst. $[\alpha]_D^{21}$ -24.2 (c, 0.12 in MeOH).

24-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→2)-β-D-xylofuranoside], 6*-O-*sulfate:* ***Certonardoside F***
[476437-82-8]
$C_{39}H_{68}O_{17}S$ 841.022
Constit. of *Certonardoa semiregularis.* Cryst.

(3β,4β,5α,6β,15α,24*S*)-*form*

3-O-*(2*-O-*Methyl-β-D-xylopyranoside), 24*-O-*α-L-arabinofuranoside:* ***Granulatoside A***
[100665-53-0]
$C_{38}H_{66}O_{14}$ 746.931
Constit. of *Choriaster granulatus* and *Thromidia catalai.*
$[\alpha]_D$ -16 (MeOH).

3-O-*(2,3-Di*-O-*methyl-β-D-xylopyranoside):* ***Tumidoside B***
[877175-41-2]
$C_{34}H_{60}O_{10}$ 628.842
Constit. of *Henricia tumida.*
$[\alpha]_D^{20}$ -7 (c, 0.1 in MeOH).

3-O-*(2,4-Di*-O-*methyl-β-D-xylopyranoside):* ***Forbeside I****. Laeviuscoloside I. Henricioside H1*
[129369-40-0]
$C_{34}H_{60}O_{10}$ 628.842
Isol. from the starfish *Asterias forbesi* and *Henricia laeviuscola.*
Powder.
Mp 214° dec. $[\alpha]_D$ -8 (c, 0.6 in H_2O). $[\alpha]_D$ -4.9 (c, 0.93 in MeOH).

3-O-*(2,4-Di*-O-*methyl-β-D-xylopyranoside), 24*-O-*α-L-arabinofuranoside:* ***Forbeside J****. Laeviuscoloside G. Levisculoside G*
[129369-39-7]
[168570-44-3]
$C_{39}H_{68}O_{14}$ 760.958
Isol. from *Asterias forbesi*, *Henricia derjugini* and *Henricia laeviuscola*. Powder.
Mp 250° dec Mp 221-223°. $[\alpha]_D$ -17.4 (c, 1 in H_2O). $[\alpha]_{Hg}$ -27.6 (c, 2 in MeOH).

3-O-*(2,3,4-Tri*-O-*methyl-β-D-xylopyranoside):* ***Sanguinoside B***
[714952-37-1]
$C_{35}H_{62}O_{10}$ 642.869
Constit. of *Henricia sanguinolenta* and *Henricia leviuscula leviuscula*.

(3β,4β,5α,6β,15β,24*S*)-*form* [168294-60-8]
Constit. of a *Henricia* sp.
Cryst.
Mp 274-275°. $[\alpha]_D$ -1.9 (c, 0.8 in MeOH).

3-O-*(2*-O-*Methyl-β-D-xylopyranoside):* ***Moniloside D***
[147362-17-2]
$C_{33}H_{58}O_{10}$ 614.815
Constit. of echinoderm *Fromia monilis.*
$[\alpha]_D$ -18.4 (MeOH).

24-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside]:* ***Gomophioside A***
[99481-51-3]
$C_{39}H_{68}O_{14}$ 760.958
Constit. of *Gomophia watsoni.*

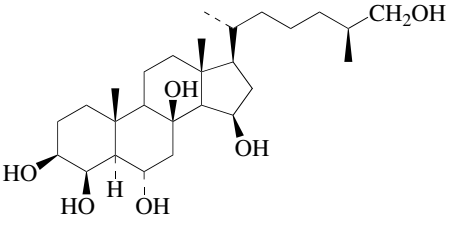
(3β,4β,5α,6β,15α,24ξ)-*form*

24-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→3)-α-L-arabinofuranoside]:* ***Echinasteroside B2***
[109521-79-1]
$C_{38}H_{66}O_{14}$ 746.931
Constit. of *Echinaster sepositus.* Cryst.
Mp 262-265°. $[\alpha]_D^{20}$ -24.22 (c, 2.2 in EtOH).

15-Ac, 24-O-*[2*-O-*methyl-β-D-xylopyranosyl-(1→3)-α-L-arabinofuranoside]:* ***Echinasteroside B1***
[109521-80-4]
$C_{40}H_{68}O_{15}$ 788.968
Constit. of *Echinaster sepositus.* Cryst.
Mp 266-269°. $[\alpha]_D^{20}$ -12.36 (c, 0.6 in EtOH).

Minale, L. *et al., Experientia*, 1983, **39**, 567-569; 569-571 (*Halityloside D, Attenuatosides*)
Riccio, R. *et al., Gazz. Chim. Ital.*, 1985, **115**, 405-409; 1990, **120**, 155-163 (*Attenuatosides*)
Pizza, C. *et al., Gazz. Chim. Ital.*, 1985, **115**, 585-589 (*Granulatoside A*)
Kicha, A.A. *et al., Khim. Prir. Soedin.*, 1985, **21**, 801-804; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 760-766 (*Culcitoside C1*)
Levina, E.V. *et al., Khim. Prir. Soedin.*, 1987, **23**, 246-249; *Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 206-208 (*Echinasterosides*)
Riccio, R. *et al., J. Nat. Prod.*, 1988, **51**, 989-992 (*Glacialoside B*)
Findlay, J.A. *et al., J. Nat. Prod.*, 1991, **54**, 428-435 (*Forbesides*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1991, **54**, 1254-1264; 1992, **55**, 866-877 (*Culcitoside C5, Borealoside D*)
Vázquez, M.J. *et al., Annalen*, 1993, 1257-1262 (*Validoside A*)
Kicha, A.A. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 547-548 (*Levisculoside G*)
Casapullo, A. *et al., J. Nat. Prod.*, 1993, **56**, 105-115 (*Moniloside D*)
Kicha, A.A. *et al., Khim. Prir. Soedin.*, 1993, **29**, 249-253; 257-260; 257-260; *Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 206-210; 213-216 (*Henricioside H1, Crossasteroside P4, Attenuatoside B1*)
Wang, W. *et al., J. Nat. Prod.*, 2002, **65**, 1649-1656; 2004, **67**, 1654-1660 (*Certonardoside F, Certonardosterol Q2*)
Wang, W. *et al., Chem. Pharm. Bull.*, 2003, **51**, 435-439 (*Certonardoside K*)
Kalinovskii, A.I. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2004, **30**, 191-195; *CA*, **141**, 85820v (*Sanguinoside B*)
Levina, E.V. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2005, **31**, 467-474 (*Tumidoside B*)

Cholestane-3,4,6,8,15,26-hexol C-495



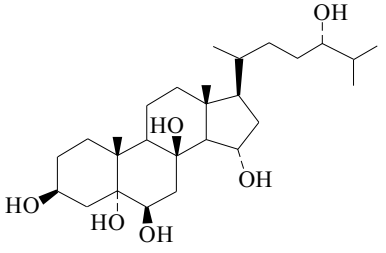
$C_{27}H_{48}O_6$ 468.673

(3β,4β,5α,6α,8β,15β,25*S*)-*form*
Certonardosterol A3
[781646-85-3]
Iso. from *Certonardoa semiregularis.*
Cryst.

26-O-*β-D-Xylopyranoside:* ***Coscinasteroside F***
[105377-93-3]

$C_{32}H_{56}O_{10}$ 600.788
Constit. of *Coscinasterias tenuispina*.
$[\alpha]_D$ -8.8 (MeOH).
Riccio, R. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 869-893 (*Coscinasteroside F*)
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 1654-1660 (*Certonadosterol A_3*)

Cholestane-3,5,6,8,15,24-hexol C-496

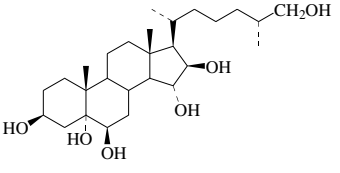


$C_{27}H_{48}O_6$ 468.673

(3β,5α,6β,15α,24*S*)-*form*
*24-[2-*O*-Methyl-β-D-xylopyranosyl-(1→2)-L-arabinofuranoside]:* ***Nodososide***†
[83210-62-2]
$C_{38}H_{66}O_{14}$ 746.931
Constit. of the starfish *Protoreaster nodosus*. Noncryst. Sol. MeOH, butanol. $[\alpha]_D$ -21.3.
*3-*O*-(2-*O*-Methyl-β-D-xylopyranoside), 24-*O*-α-L-arabinofuranoside:* ***Isonodososide***
[97671-45-9]
$C_{38}H_{66}O_{14}$ 746.931
Isol. from starfish *Acanthaster planci*.
$[\alpha]_D$ -15 (MeOH).

(3β,5α,6α,15α,24*S*)-*form*
*24-*O*-[2-*O*-Methyl-β-D-xylopyranosyl-(1→2)-arabinofuranoside]:* ***6-Epinodososide***
[106534-48-9]
$C_{38}H_{66}O_{14}$ 746.931
Constit. of *Pentaceraster alveolatus*.
Riccio, R. *et al., Tet. Lett.*, 1982, **23**, 2899-2902 (*Nodososide, isol, pmr, cmr*)
D'Auria, M.V. *et al., Gazz. Chim. Ital.*, 1984, **114**, 469-470 (*Nodososide, isol, abs config*)
Pizza, C. *et al., J. Chem. Res., Synop.*, 1985, 76-77; *J. Chem. Res., Miniprint*, 1985, 969-986 (*Isonodososide*)
Zollo, F. *et al., J. Nat. Prod.*, 1986, **49**, 919-921 (*6-epimer*)

Cholestane-3,5,6,15,16,26-hexol C-497



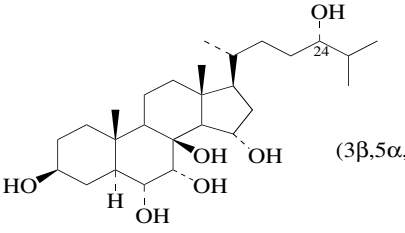
(3β,5α,6β,15α,16β,25*R*)-*form*

$C_{27}H_{48}O_6$ 468.673

(3β,5α,6β,15α,16β,25*R*)-*form* [149341-83-3]
Constit. of *Tremaster novaecaledoniae*. $[\alpha]_D$ +17.2 (MeOH).
15-Sulfate: [149231-00-5]
$C_{27}H_{48}O_9S$ 548.737
Isol. from *Tremaster novaecaledoniae*. $[\alpha]_D$ +21.5 (MeOH) (as Na salt). Isol. as Na salt to which CAS no. refers.

(3β,5α,6β,15α,16β,25*S*)-*form* [130856-16-5]
Constit. of *Luidia maculata*, *Luidia clathrata*, *Myxoderma platyacanthum* and *Styracaster caroli*. Oil. $[\alpha]_D$ +12.1 (c, 0.5 in MeOH).
15-Sulfate: [129725-35-5]
Constit. of *Myxoderma platyacanthum* and a *Rosaster* sp.
$[\alpha]_D$ +12.8 (c, 1 in MeOH) (as Na salt).
16-Sulfate: [165815-77-0]
$C_{27}H_{48}O_9S$ 548.737
Constit. of *Luidia clathrata*. $[\alpha]_D$ +16.
26-Sulfate: [165815-78-1]
$C_{27}H_{48}O_9S$ 548.737
Constit. of *Luidia clathrata*.
3-Sulfate: [178496-78-1]
$C_{27}H_{48}O_9S$ 548.737
Constit. of *Luidia quinaria*. Amorph. $[\alpha]_D$ +38 (c, 1.2 in MeOH).
[93368-83-3]
Minale, L. *et al., J. Nat. Prod.*, 1984, **47**, 784-789 (*Luidia maculata constits*)
Bruno, I. *et al., Gazz. Chim. Ital.*, 1990, **120**, 449-451 (*15-sulfate*)
Finamore, E. *et al., J.O.C.*, 1991, **56**, 1146-1153 (*Myxoderma platyacanthum constits*)
De Riccardis, F. *et al., Gazz. Chim. Ital.*, 1993, **123**, 79-86 (*25R-isomer*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1994, **57**, 1361-1373; 1995, **58**, 653-671 (*sulfates, isol, pmr, cmr*)
Andriyashchenko, P.V. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1996, **45**, 473-476; *Russ. Chem. Bull. (Engl. Transl.)*, 1996, **45**, 455-458 (*3-sulfate*)

Cholestane-3,6,7,8,15,24-hexol C-498



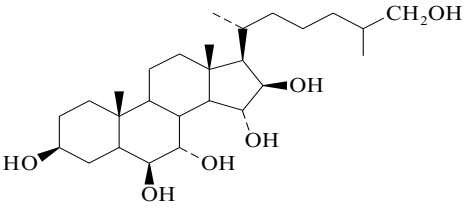
(3β,5α,6α,7α,15α,24*S*)-form

$C_{27}H_{48}O_6$ 468.673

(3β,5α,6α,7α,15α,24*S*)-*form*
*24-*O*-[4-*O*-Methyl-β-D-xylopyranosyl-(1→2)-3-*O*-methyl-β-D-xylopyranoside]:* ***Crossasteroside A***
[101767-68-4]
$C_{39}H_{68}O_{14}$ 760.958
Constit. of starfish *Crossaster papposus*. Muscle contraction inhibitor. Sol. MeOH; poorly sol. $CHCl_3$. $[\alpha]_D$ -19.5 (c, 1.6 in MeOH).
*24-*O*-[β-D-Xylopyranosyl-(1→2)-3-*O*-methyl-β-D-xylopyranoside]:* ***Crossasteroside D***
[111036-42-1]
$C_{38}H_{66}O_{14}$ 746.931
Constit. of *Crossaster papposus*. Sol. MeOH; poorly sol. $CHCl_3$. $[\alpha]_D$ -9.2 (MeOH).

(3β,5α,6α,7α,15β,24*S*)-*form*
*24-*O*-[6-Deoxy-2,4-di-*O*-methyl-β-D-glucopyranosyl-(1→2)-6-deoxy-5-*O*-sulfo-β-D-galactofuranoside]:* ***Imbricatoside B***
[128855-05-0]
$C_{41}H_{72}O_{17}S$ 869.076
Constit. of *Dermasterias imbricata*. $[\alpha]_D$ +2 (c, 0.5 in MeOH).
Andersson, L. *et al., J. Chem. Res., Synop.*, 1985, 366; 1987, 246 (*Crossasterosides*)
Bruno, I. *et al., J. Nat. Prod.*, 1990, **53**, 366-375 (*Imbricatoside B*)

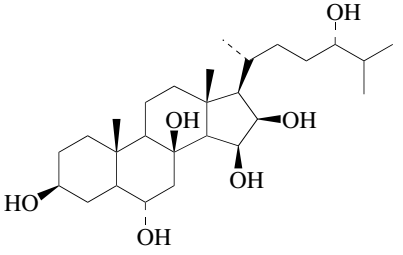
Cholestane-3,6,7,15,16,26-hexol C-499



$C_{27}H_{48}O_6$ 468.673

(3β,5α,6β,7α,15α,16β)-*form* [93368-84-4]
Constit. of *Luidia maculata*. Cryst. (MeOH). Mp 238-241°. $[\alpha]_D$ +3.8 (c, 0.5 in MeOH).
Minale, L. *et al., J. Nat. Prod.*, 1984, **47**, 784

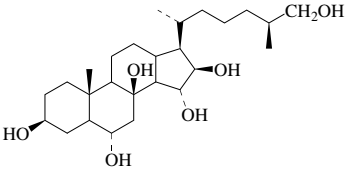
Cholestane-3,6,8,15,16,24-hexol C-500



$C_{27}H_{48}O_6$ 468.673

(3β,5α,6α,8β,15β,16β,24*S*)-*form*
24-O-*(3*-O-*Methyl-5*-O-*sulfo-β-*D-*xylofuranoside):* ***Indicoside C***
[113557-93-0]
$C_{33}H_{58}O_{13}S$ 694.879
Constit. of *Astropecten indicus*. $[\alpha]_D$ -3.8 (c, 0.5 in MeOH).
Riccio, R. *et al., Gazz. Chim. Ital.*, 1987, **117**, 755-757 (*isol, pmr, cmr*)

Cholestane-3,6,8,15,16,26-hexol C-501



(3β,5α,6α,15α,16β,25*S*)-*form*

$C_{27}H_{48}O_6$ 468.673

(3β,5α,6α,15α,16β,25*S*)-*form* [94799-81-2]
Constit. of starfish *Protoreaster nodosus*, *Oreaster reticulatus* and *Astropecten scoparius*. Cryst. (MeOH). Mp 285-287°. $[\alpha]_D$ +13.8 (c, 1.5 in MeOH).
3-O-*(2*-O-*Methyl-β-*D-*xylopyranoside):* [100007-38-3]
$C_{33}H_{58}O_{10}$ 614.815
Constit. of *Poraster superbus*.
$[\alpha]_D$ +10.4 (MeOH).

(3β,5α,6α,15β,16β,25*S*)-*form* [102208-08-2]
Constit. of *Crossaster papposus*, *Lysastrosoma anthosticta*, *Halityle regularis* and *Pycnopodia helianthoides*. Cryst. (MeOH). Mp 261-263°. $[\alpha]_D^{20}$ +37.8 (c, 2.5 in EtOH). $[\alpha]_D$ 0 (MeOH).
26-O-*β-*D-*Xylopyranoside:* ***Lysastroside A***
[454234-69-6]
$C_{32}H_{56}O_{10}$ 600.788
Constit. of *Lysastrosoma anthosticta*. Amorph. solid. $[\alpha]_D^{20}$ +5.6 (c, 1.2 in EtOH).

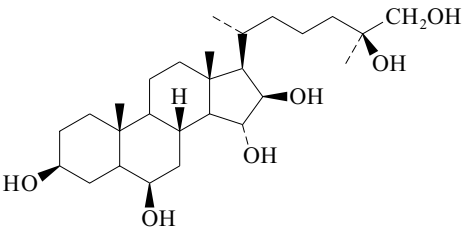
(3β,5α,6α,15β,16β,25ξ)-*form*
Isol. from starfish *Crossaster papposus*. Mp 262-264°. $[\alpha]_{Hg}$ +35.4 (c, 0.3 in MeOH).

(3β,5α,6β,15α,16β,25*R*)-*form* [112137-71-0]
Isol. from starfish of Echinasteridae family.

(3β,5α,6β,15α,16β,25*S*)-*form* [181229-17-4]
Isol. from starfish *Sphaerodiscus placenta*.

(3β,5α,6β,15α,16β,25ξ)-*form* [123750-23-2]
Isol. from starfish *Hacelia attenuata* and *Crossaster papposus*.
Minale, L. *et al., Tet. Lett.*, 1982, **23**, 1841-1844 (*Hacelia attenuata constit*)
Riccio, R. *et al., Tetrahedron*, 1982, **38**, 3615-3622 (*isol, struct*)
Riccio, R. *et al., Gazz. Chim. Ital.*, 1985, **115**, 505-509 (*methylxyloside*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1986, **49**, 67-78 (*Halityle regularis constit*)
Zollo, F. *et al., J. Nat. Prod.*, 1987, **50**, 794-799 (*Sphaerodiscus placenta constit*)
Kicha, A.A. *et al., Khim. Prir. Soedin.*, 1989, 432-433; 1990, 218-221; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 175-177 (*Crossaster papposus constits*)
Iorizzi, M. *et al., Tetrahedron*, 1996, **52**, 10997-11012 (*Echinasteridae constit*)
Levina, E.V. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2002, **51**, 535-539 (*Lysastroside A*)

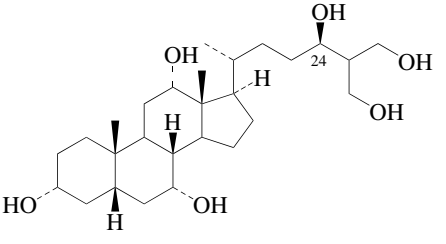
Cholestane-3,6,15,16,25,26-hexol C-502



$C_{27}H_{48}O_6$ 468.673

(3β,5α,6β,15α,16β,25*S*)-*form* [181034-92-4]
Constit. of an Antarctic starfish (Echinasteridae).
$[\alpha]_D$ +5 (MeOH).
Iorizzi, M. *et al., Tetrahedron*, 1996, **52**, 10997-11012 (*isol, pmr, cmr*)

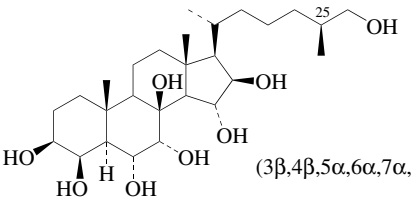
Cholestane-3,7,12,24,26,27-hexol C-503



$C_{27}H_{48}O_6$ 468.673

(3α,5β,7α,12α,24*R*)-*form*
Scymnol
[6785-34-8]
Isol. from bile of sharks and rays *Scymnus borealis*, *Rhizoprionodon acutus*, *Lamna ditropsis*, *Raja erinacea*. Liver protectant, antiseborrhoeic, respiratory stimulant. Cryst. (EtOAc). Sol. H_2O, MeOH.
Mp 187°. $[\alpha]_D$ +38.2 (EtOH). Forms a hydrate, Mp 120° (115°) from MeOH aq.
*26-Sulfate(25*S-*):* [30424-32-9]
[119068-78-9 (Na salt), 119068-79-0 (K salt), 140851-10-1 (26-Sulfate (25*R*-)-)]
$C_{27}H_{48}O_9S$ 548.737
Constit. of *Lamna ditropis*, *Rhizoprionodon acutus* and *Raja erinacea*. Amorph. powder (as Na salt). $[\alpha]_D^{25}$ +33.8 (c, 0.5 in MeOH). $[\alpha]_D^{25}$ +21.75 (c, 0.5 in MeOH).
Bridgewater, R.J. *et al., Biochem. J.*, 1962, **82**, 285-290 (*Scymnol, synth, bibl*)
Ishida, H. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4408-4413; 1992, **40**, 864-868 (*sulfates*)
Karlaganis, G. *et al., J. Lipid Res.*, 1989, **30**, 317-322 (*Raja erinacea constit*)
Amiet, R.G. *et al., Aust. J. Chem.*, 1993, **46**, 1347-1354 (*synth, pmr, cmr*)
Ishida, H. *et al., Chem. Pharm. Bull.*, 1994, **42**, 2514-2517 (*Rhizoprionodon acutus constit*)
Ishida, H. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1289-1292 (*cmr*)
Adhikari, R. *et al., Aust. J. Chem.*, 2005, **58**, 34-38 (*synth*)

Cholestane-3,4,6,7,8,15,16,26-octol C-504



(3β,4β,5α,6α,7α,15α,16β,25*S*)-*form*

$C_{27}H_{48}O_8$ 500.671

(3β,4β,5α,6α,7α,15α,16β,25*S*)-*form* [100019-24-7]
[86424-19-3]
Constit. of starfish *Protoreaster nodosus*, *Pentaceraster alveolatus*, *Oreaster reticulatus* and *Asterina pectinifera*.
Cryst. (MeOH).
Mp 263-266°. $[\alpha]_D$ +10 (c, 1 in MeOH).

6-O-*Sulfate:* [100101-34-6]
$C_{27}H_{48}O_{11}S$ 580.736
Constit. of *Oreaster reticulatus* and *Asterina pectinifera*.

(3β,4β,5α,6α,7α,15β,16β,25*S*)-*form* [128298-63-5]
Constit. of *Asterina pectinifera* and *Astropecten scoparius.*
Cryst.
Mp 270-274°. $[\alpha]_D^{25}$ +26.4 (c, 1 in MeOH).

(3β,4β,5α,6α,7α,15β,16β,25ξ)-*form*

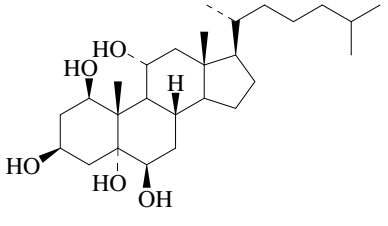
15,16-Isopropylidene: [852709-55-8]
$C_{30}H_{52}O_8$ 540.736
Constit. of *Asterina pectinifera*. Amorph. powder.
Mp 140-145°. $[\alpha]_D^{18}$ +8.5 (c, 1.06 in MeOH).

(3β,4β,5α,6β,7α,8β,15α,16β,25*S*)-*form* [129893-35-2]
Constit. of a *Rosaster* sp. and *Pycnopodia helianthus.*
$[\alpha]_D$ +9 (c, 1 in MeOH).

(3β,4β,5α,6β,7α,8β,15β,16β,25*S*)-*form* [142797-28-2]
Constit. of *Solaster borealis.*

Riccio, R. *et al., Tetrahedron*, 1982, **38**, 3615-3622 (*Protoreaster nodosus constit, cmr*)
Segura de Correa, R. *et al., J. Nat. Prod.*, 1985, **48**, 751-755 (*Oreaster reticulatus constits*)
Higuchi, R. *et al., Annalen*, 1988, 1185-1189 (*Asterina pectinifera constits*)
Bruno, I. *et al., J. Nat. Prod.*, 1989, **52**, 1022-1026 (*Pycnopodia helianthus constit*)
Bruno, I. *et al., Gazz. Chim. Ital.*, 1990, **120**, 449-451 (*Rosaster constit, isol, pmr, cmr*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1992, **55**, 866-877 (*Solaster borealis constit*)
Zhang, L.-X. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 25-29 (*isopropylidene*)

Cholestane-1,3,5,6,11-pentol C-505



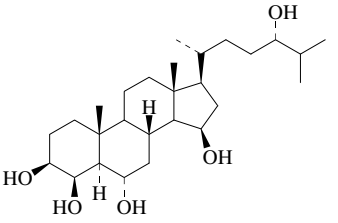
$C_{27}H_{48}O_5$ 452.673

(1β,3β,5α,6β,11α)-*form* [253195-37-8]
Constit. of *Sinularia dissecta.*

1,3,6,11-Tetra-Ac: [253195-41-4]
Cryst. Mp 218-220°. $[\alpha]_D^{25}$ -19.9 (c, 0.45 in $CHCl_3$).

Ramesh, P. *et al., Steroids*, 1999, **64**, 785-789 (*isol, pmr, cmr*)

Cholestane-3,4,6,15,24-pentol C-506



(3β,4β,5α,6α,15β,24*S*)-*form*

$C_{27}H_{48}O_5$ 452.673

(3β,4β,5α,6α,15β,24*S*)-*form* [777940-73-5]
Amorph. powder.

24-O-*β*-D-*Xylofuranoside:* ***Certonardoside H₄***
[781646-90-0]
$C_{32}H_{56}O_9$ 584.789
Constit. of *Certonardoa semiregularis.* Cryst. $[\alpha]_D^{21}$ -27.1 (c, 0.12 in MeOH).

24-O-*[2*-O-*Methyl-β*-D-*xylopyranosyl-(1→2)-β*-D-*xylofuranoside]:* ***Certonardoside H₃***
[781646-89-7]
$C_{38}H_{66}O_{13}$ 730.932
Constit. of *Certonardoa semiregularis.* Cryst. $[\alpha]_D^{21}$ -12.5 (c, 0.14 in MeOH).

24-O-*[2,4-Di*-O-*methyl-β*-D-*xylopyranosyl-(1→2)-β*-D-*xylofuranoside]:* ***Certonardoside H***
[476437-86-2]
$C_{39}H_{68}O_{13}$ 744.958
Constit. of *Certonardoa semiregularis.* Cryst.

24-O-*[2,4-Di*-O-*methyl-β*-D-*xylopyranosyl-(1→2)-β*-D-*xylofuranoside], 6*-O-*sulfate:* ***Certonardoside G***
[476437-84-0]
$C_{39}H_{68}O_{16}S$ 825.023
Constit. of *Certonardoa semiregularis.* Cryst.

(3β,4β,5α,6β,15α,24*S*)-*form*

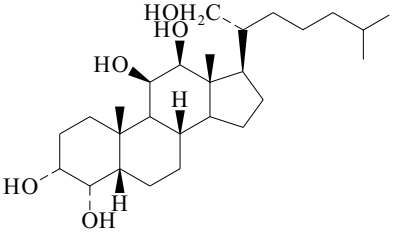
3-O-*[2,4-Di*-O-*methyl-β*-D-*xylopyranoside], 24*-O-*α*-L-*arabinofuranoside:* ***Laeviuscoloside F***
[129369-38-6]
$C_{39}H_{68}O_{13}$ 744.958
Constit. of *Henricia laeviuscola*. $[\alpha]_D$ -0.8.

(3β,4β,5α,6β,15β,24*S*)-*form*

3-(*2*-O-*Methyl-β*-D-*xylopyranoside):* ***Moniloside C***
[147362-16-1]
$C_{33}H_{58}O_9$ 598.816
Constit. of *Fromia monilis.*

D'Auria, M.V. *et al., Gazz. Chim. Ital.*, 1990, **120**, 155-163 (*Laeviuscoloside F*)
Casapullo, A. *et al., J. Nat. Prod.*, 1993, **56**, 105-115 (*Moniloside C*)
Wang, W. *et al., J. Nat. Prod.*, 2002, **65**, 1649-1656; 2004, **67**, 1654-1660 (*Certonardosides*)

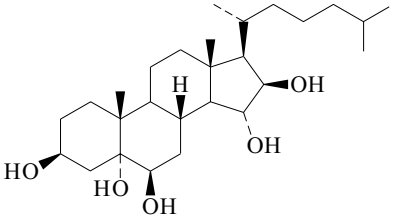
Cholestane-3,4,11,12,21-pentol C-507



$C_{27}H_{48}O_5$ 452.673

(3α,4α,5β,11β,12β,20*R*)-*form*
Cryst. (MeOH/hexane). Mp 125-128°.
3,21-Disulfate: [100942-71-0]
$C_{27}H_{48}O_{11}S_2$ 612.802
Constit. of ophiuroids *Ophioderma longicaudum*, *Ophiocoma echinata*, *Ophiocoma scolopendrina*, *Ophiocoma wendti*, *Ophionereis reticulata* and *Ophiozona impressa*. Mod. cytotoxic agent. Cryst. (MeOH/$CHCl_3$). Mp 192-195°. $[\alpha]_D$ +10.8 (c, 0.9 in MeOH).
Riccio, R. *et al., Tetrahedron*, 1985, **41**, 6041-6046 (*3,21-disulfate, isol*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1995, **58**, 189-196 (*3,21-disulfate, occur*)

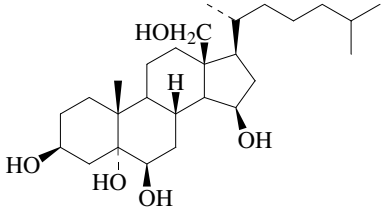
Cholestane-3,5,6,15,16-pentol C-508



$C_{27}H_{48}O_5$ 452.673

(3β,5α,6β,15α,16β)-*form*
16-Sulfate: [165815-76-9]
$C_{27}H_{48}O_8S$ 532.737
Constit. of *Luidia clathrata*. $[\alpha]_D$ +14.5.
Iorizzi, M. *et al., J. Nat. Prod.*, 1995, **58**, 653-671 (*isol, pmr, cmr*)

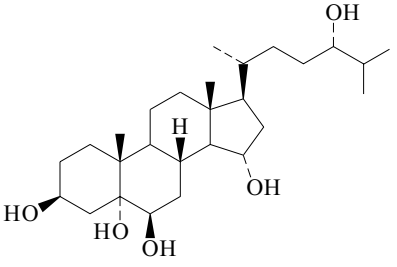
Cholestane-3,5,6,15,18-pentol C-509



$C_{27}H_{48}O_5$ 452.673

(3β,5α,6β,15β)-*form*
18-Ac: ***Dendronesterol B***
[265121-06-0]
$C_{29}H_{50}O_6$ 494.71
Constit. of *Dendronephthya gigantea*. Amorph. solid. $[\alpha]_D^{25}$ +1 (c, 0.9 in MeOH).
Yoshikawa, K. *et al., J. Nat. Prod.*, 2000, **63**, 670-672 (*isol, pmr, cmr*)

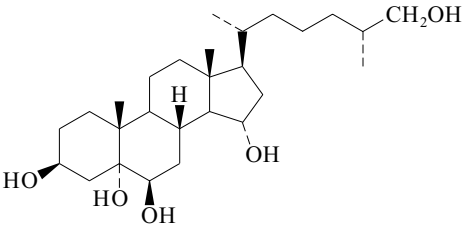
Cholestane-3,5,6,15,24-pentol C-510



$C_{27}H_{48}O_5$ 452.673

(3β,5α,6β,15α,24*S*)-*form*
15-O-*Sulfate:* [165815-84-9]
$C_{27}H_{48}O_8S$ 532.737
Constit. of *Luidia clathrata*. Antifeedant. Antibarnacle agent. $[\alpha]_D$ +24.6.
24-O-*Sulfate:* [876620-24-5]
$C_{27}H_{48}O_8S$ 532.737
Constit. of *Henricia leviuscula*. Amorph. powder. $[\alpha]_D$ +34 (c, 0.1 in MeOH).
24-O-*β*-D-*Xylopyranoside:* ***Rathbunioside R₂***
[350689-92-8]
$C_{32}H_{56}O_9$ 584.789
Constit. of *Asterias rathbuni*. Amorph. powder. $[\alpha]_D$ +13.1 (c, 0.45 in MeOH).
Iorizzi, M. *et al., J. Nat. Prod.*, 1995, **58**, 653-671 (*15-sulfate*)
Ivanchina, N.V. *et al., J. Nat. Prod.*, 2001, **64**, 945-947 (*Rathbunioside R_2*)
Ivanchina, N.V. *et al., J. Nat. Prod.*, 2006, **69**, 224-228 (*24-sulfate*)

Cholestane-3,5,6,15,26-pentol C-511

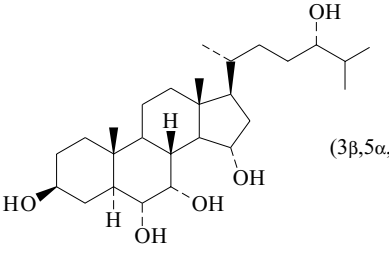


$C_{27}H_{48}O_5$ 452.673

(3β,5α,6β,15α,25*R*)-*form* [160538-71-6]
Constit. of *Styracaster caroli* and *Luidia ludwigi*.
$[\alpha]_D$ +21.4 (MeOH).

(3β,5α,6β,15α,25*S*)-*form* [130799-36-9]
Constit. of *Myxoderma platyacanthum*.
$[\alpha]_D$ +13 (MeOH).
15-Sulfate: [174322-61-3]
[130799-35-8 (Na salt)]
$C_{27}H_{48}O_8S$ 532.737
Constit. of *Luidia ludwigi*, *Myxoderma platyacanthum* and *Luidia quinaria*.
26-Sulfate: [173740-55-1]
$C_{27}H_{48}O_8S$ 532.737
Constit. of *Luidia ludwigi*.
$[\alpha]_D^{25}$ +64 (c, 0.1 in MeOH).
26-β-D-Xylopyranoside, 15-sulfate:
[130829-31-1 (Na salt)]
$C_{32}H_{56}O_{12}S$ 664.853
Constit. of *Myxoderma platyacanthum*.
Finamore, E. *et al., J.O.C.*, 1991, **56**, 1146-1153 (*Myxoderma platyacanthum constits*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1994, **57**, 1361-1373 (*isol, pmr, cmr*)
Roccatagliata, A.J. *et al., J. Nat. Prod.*, 1995, **58**, 1941-1944 (*26-sulfate*)

Cholestane-3,6,7,15,24-pentol C-512



(3β,5α,6α,7α,15α,24*S*)–*form*

$C_{27}H_{48}O_5$ 452.673

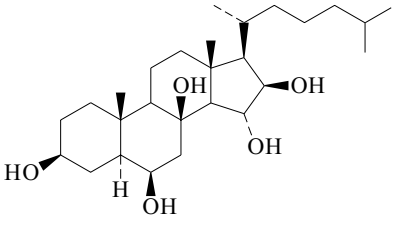
(3β,5α,6α,7α,15α,24*S*)-*form*

24-O-*β*-D-Xylopyranoside, 15-sulfate: ***Amurensoside B***
[115178-53-5]
$C_{32}H_{56}O_{12}S$ 664.853
Constit. of *Asterias amurensis.*
$[\alpha]_D$ +12.5 (MeOH).

(3β,5α,6α,7α,15β,24*S*)-*form*

24-O-*β*-D-Xylopyranoside: ***Amurensoside D***
[115193-15-2]
$C_{32}H_{56}O_9$ 584.789
Constit. of *Asterias amurensis.*
$[\alpha]_D$ -4.5 (MeOH).
Riccio, R. *et al., J.C.S. Perkin 1*, 1988, 1337-1347 (*isol, pmr, cmr*)

Cholestane-3,6,8,15,16-pentol C-513

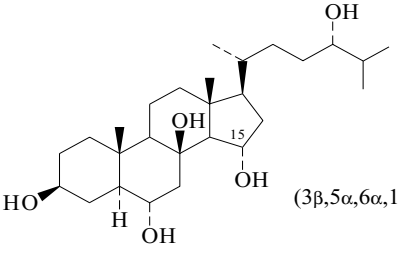


$C_{27}H_{48}O_5$ 452.673

(3β,5α,6β,8β,15α,16β)-*form*

3-O-*[2,4-Di*-O-*methyl-β*-D-*xylopyranoside], 15-sulfate:* ***Laeviuscoloside B***
[129389-94-2]
$C_{34}H_{60}O_{12}S$ 692.907
Constit. of *Henricia laeviuscola.*
$[\alpha]_D$ +1.5.
D'Auria, M.V. *et al., Gazz. Chim. Ital.*, 1990, **120**, 155-163 (*isol, pmr, cmr*)

Cholestane-3,6,8,15,24-pentol, 9CI C-514



(3β,5α,6α,15α,24*S*)–*form*

$C_{27}H_{48}O_5$ 452.673

(3β,5α,6α,15α,24*S*)-*form* [117121-29-6]
Occurs in starfish *Asterina pectinifera.*
Needles (MeOH aq.).
Mp 236-239°. $[\alpha]_D$ +53 (c, 1.02 in MeOH).

6-Sulfate: [161996-23-2]
$C_{27}H_{48}O_8S$ 532.737
Constit. of *Oreaster reticulatus.*

24-Sulfate: [142013-86-3]
$C_{27}H_{48}O_8S$ 532.737
Constit. of *Aphelasterias japonica.*
$[\alpha]_D$ +23.5 (c, 0.5 in MeOH). CAS no. refers to Na salt.

24-O-*α*-L-*Arabinofuranoside, 6-sulfate:* ***Oreasteroside I***
[161996-30-1]
$C_{32}H_{56}O_{12}S$ 664.853
Constit. of *Oreaster reticulatus.*
$[\alpha]_D$ +10.

24-O-*(3*-O-*Sulfo-α*-L-*arabinofuranoside):* [99957-31-0]
$C_{32}H_{56}O_{12}S$ 664.853
Isol. from seastars *Oreaster reticulatus* and *Patiria miniata.*

24-O-*(3*-O-*Methyl-α*-L-*arabinofuranoside):* ***Oreasteroside A***
[100019-25-8]
$C_{33}H_{58}O_9$ 598.816
Constit. of *Oreaster reticulatus.*
$[\alpha]_D$ +20.

24-O-*(3*-O-*Methyl-α*-L-*arabinofuranoside), 6-sulfate:* ***Oreasteroside H***
[161996-29-8]
$C_{33}H_{58}O_{12}S$ 678.88
Constit. of *Oreaster reticulatus.*
$[\alpha]_D$ +5.

24-(3-O-*Methyl-5*-O-*sulfo-α*-L-*arabinofuranoside):* ***Asterosaponin P_1***
[80764-19-8]
$C_{33}H_{58}O_{12}S$ 678.88
Constit. of starfish *Patiria pectinifera* and *Oreaster reticulatus.* Cryst.
Mp 191-192°. $[\alpha]_D$ +3 (c, 0.6 in MeOH).

24-O-*(3*-O-*Sulfo-β*-D-*xylopyranoside):* ***Helianthoside***†
[151113-62-1]
$C_{32}H_{56}O_{12}S$ 664.853
Constit. of *Heliaster helianthus.* Cryst.
Mp 210-212°. $[\alpha]_D^{20}$ -15.3 (c, 1.7 in MeOH).

24-O-*(3*-O-*Methyl-β*-D-*xylopyranoside):* ***Borealoside C***
[143016-86-8]
$C_{33}H_{58}O_9$ 598.816
Constit. of *Solaster borealis.*
$[\alpha]_D$ +6.7 (MeOH).

24-O-*(3*-O-*Methyl-4*-O-*sulfo-β*-D-*xylopyranoside):* ***Phrygioside B***
[868860-82-6]
$C_{33}H_{58}O_{12}S$ 678.88
Constit. of *Hippasteria phrygiana.* Amorph. solid. $[\alpha]_D$ -6.9 (c, 0.2 in MeOH).

24-O-*[β*-D-*Xylopyranosyl-(1→2)-3*-O-*sulfo-α*-L-*arabinofuranoside]:* ***Miniatoside B***
[128269-47-6]
$C_{37}H_{64}O_{16}S$ 796.969
Constit. of *Patiria miniata.*
$[\alpha]_D$ -12.3 (MeOH).

24-O-*[β*-D-*Xylopyranosyl-(1→2)-5*-O-*sulfo-α*-L-*arabinofuranoside]:* ***Borealoside B***
[143049-28-9]
$C_{37}H_{64}O_{16}S$ 796.969
Constit. of *Solaster borealis.*
$[\alpha]_D$ +1.4 (MeOH).

24-O-*[2*-O-*Methyl-β*-D-*xylopyranosyl-(1→2)-5*-O-*sulfo-α*-L-*arabinofuranoside]:* ***Borealoside A***
[143016-85-7]
$C_{38}H_{66}O_{16}S$ 810.996
Constit. of *Solaster borealis.*
$[\alpha]_D$ 0 (MeOH).

24-O-*[β*-D-*Xylopyranosyl-(1→2)-3*-O-*methyl-α*-L-*arabinofuranoside]:* ***Oreasteroside B***
[162000-92-2]
$C_{38}H_{66}O_{13}$ 730.932
Constit. of *Oreaster reticulatus.*
$[\alpha]_D$ -15.

24-O-*[4*-O-*Methyl-β*-D-*xylopyranosyl-(1→2)-α*-L-*arabinofuranoside]:* ***Crossasteroside C***
[111036-41-0]
$C_{38}H_{66}O_{13}$ 730.932
Constit. of *Crossaster papposus.* Sol. MeOH; poorly sol. $CHCl_3$.
$[\alpha]_D$ -8 (MeOH).

24-O-*[2*-O-*Methyl-β*-D-*xylopyranosyl-(1→2)-α*-L-*arabinofuranoside]:* ***Oreasteroside C***
[162063-18-5]
$C_{38}H_{66}O_{13}$ 730.932
Constit. of *Oreaster reticulatus.*
$[\alpha]_D$ -7.5.

24-O-*[2*-O-*Methyl-β*-D-*xylopyranosyl-(1→2)-3*-O-*methyl-α*-L-*arabinofuranoside]:* ***Oreasteroside D***
[161996-26-5]
$C_{39}H_{68}O_{13}$ 744.958

Constit. of *Oreaster reticulatus*.
$[\alpha]_D$ -15.3.

24-O-*[4*-O-*Methyl-β-D-xylopyranosyl-(1→2)-3*-O-*methyl-β-D-xylopyranoside]:* ***Crossasteroside B***
[111036-40-9]
$C_{39}H_{68}O_{13}$ 744.958
Constit. of *Crossaster papposus*. Muscle contraction inhibitor. Sol. MeOH; poorly sol. $CHCl_3$. $[\alpha]_D$ -5 (MeOH).

15-Ketone: 3,6,8,24-Tetrahydroxycholestan-15-one. ***Certonardosterol Q_3***
[781646-78-4]
$C_{27}H_{46}O_5$ 450.657
Constit. of *Certonardoa semiregularis*. Cryst.

(3β,5α,6α,15β,24*S*)-*form* [99481-53-5]
Constit. of *Certonardoa semiregularis* and *Gomophia watsoni*.
$[\alpha]_D$ +12 (c, 0.3 in MeOH).

3-O-*β-D-Xylopyranoside, 24-sulfate:* ***Glacialoside A***
[117585-52-1]
$C_{32}H_{56}O_{12}S$ 664.853
Isol. from the starfish *Marthasterias glacialis* (as Na salt). Sol. MeOH, butanol; fairly sol. H_2O. $[\alpha]_D$ +3 (c, 0.7 in MeOH).

3-O-*β-D-Xylopyranoside, 24*-O-*β-D-glucopyranoside:* ***Distolasteroside D_3***. *Asterosaponin D_3*
[109521-78-0]
$C_{38}H_{66}O_{14}$ 746.931
Constit. of *Distolasterias nipon*. Cryst.
Mp 295-298°. $[\alpha]_D^{20}$ -13.1 (c, 0.15 in MeOH).

3-O-*β-D-Xylopyranoside, 24*-O-*(6*-O-*sulfo-β-D-glucopyranoside):* ***Distolasteroside D_4***
[154099-02-2]
$C_{38}H_{66}O_{17}S$ 826.995
Constit. of *Distolasterias nipon*.

24-O-*α-L-Arabinofuranoside:* ***Attenuatoside AII***
[88191-35-9]
$C_{32}H_{56}O_9$ 584.789
Constit. of *Hacelia attenuata*. Amorph. $[\alpha]_D$ -15.7 (MeOH).

24-O-*[3*-O-*Methyl-2*-O-*sulfo-β-D-xylopyranoside]:* ***Validoside B***
$C_{33}H_{58}O_{12}S$ 678.88
Isol. from starfish *Odontaster validus*.
$[\alpha]_D^{20}$ +2.3 (c, 6.0 in MeOH) (as Na salt).

24-O-*(5*-O-*Sulfo-α-L-arabinofuranoside):* ***Scoparioside A***
[131466-95-0]
$C_{32}H_{56}O_{12}S$ 664.853
Constit. of the starfish *Astropecten scoparius*. Isol. as Na salt.

24-O-*(4*-O-*Sulfo-β-D-xylopyranoside):* ***Luridoside A***
[151078-92-1]
$C_{32}H_{56}O_{12}S$ 664.853
Isol. from the starfish *Cosmasterias lurida*.
$[\alpha]_D^{25}$ +3.7 (c, 0.4 in MeOH) (as Na salt). CAS no. refers to Na salt.

24-O-*(5*-O-*Sulfo-β-D-xylofuranoside):* ***Scoparioside B***
[131466-96-1]
$C_{32}H_{56}O_{12}S$ 664.853
Constit. of *Astropecten scoparius*. Isol. as Na salt.

24-O-*β-Xylopyranoside:* ***Pycnopodioside A***
[124609-38-7]
$C_{32}H_{56}O_9$ 584.789
Isol. from the starfish *Pycnopodia helianthoides*.
$[\alpha]_D$ +2.

24-O-*β-D-Xylopyranoside, 3-sulfate:* ***Pycnopodioside B***
[124596-51-6]
$C_{32}H_{56}O_{12}S$ 664.853
Isol. from *Pycnopodia helianthoides*.
$[\alpha]_D$ +1.8.

3,24-Di-O-*β-D-xylopyranoside:* ***Distolasteroside D_1***. *Asterosaponin D_1*
[109527-67-5]
$C_{37}H_{64}O_{13}$ 716.905
Constit. of *Distolasterias nipon*. Cryst.
Mp 285-288°. $[\alpha]_D^{20}$ -17.9 (c, 0.24 in MeOH).

24-O-*(3*-O-*Methyl-4*-O-*sulfo-β-D-xylopyranoside):* ***Scoparioside C***
[131501-27-4]
$C_{33}H_{58}O_{12}S$ 678.88
Constit. of *Astropecten scoparius*. Isol. as Na salt.

24-O-*(3*-O-*Methyl-5-sulfato-β-D-xylofuranoside):* ***Indicoside B***†
[113626-21-4]
$C_{33}H_{58}O_{12}S$ 678.88
Constit. of starfish *Astropecten indicus*. Amorph. $[\alpha]_D$ -3 (MeOH).

24-O-*β-D-Glucopyranoside, 6-sulfate:* ***Pycnopodioside C***
[124596-52-7]
$C_{33}H_{58}O_{13}S$ 694.879
Isol. from *Pycnopodia helianthoides*.
$[\alpha]_D$ +4.2.

24-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside]:* ***Attenuatoside AI***
[86425-62-9]
$C_{38}H_{66}O_{13}$ 730.932
Constit. of *Hacelia attenuata*. Amorph. $[\alpha]_D$ -20.6 (MeOH).

24-O-*[β-D-Xylopyranosyl-(1→2)-3*-O-*methyl-α-L-arabinofuranoside]:* ***Oreasteroside E***
[161996-27-6]
$C_{38}H_{66}O_{13}$ 730.932
Constit. of *Oreaster reticulatus*.
$[\alpha]_D$ -16.6.

24-O-*[4*-O-*Methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside]:* ***Culcitoside C_4***
[138192-12-8]
$C_{38}H_{66}O_{13}$ 730.932
Constit. of *Culcita novaeguineae*.
$[\alpha]_D$ -20.3 (MeOH).

24-O-*[2,3-Di*-O-*methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside]:* ***Mediasteroside M_4***
[221290-78-4]
$C_{39}H_{68}O_{13}$ 744.958
Constit. of *Mediaster murrayi*. Amorph. powder. $[\alpha]_D$ -10.4 (c, 0.2 in MeOH).

24-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside]:* ***Halityloside E***
[102040-10-8]
$C_{39}H_{68}O_{13}$ 744.958
Constit. of *Halityle regularis*.
$[\alpha]_D$ -20 (MeOH).

24-O-*[β-D-Xylopyranosyl-(1→5)-α-L-arabinofuranoside]:* ***Mediasteroside M_2***
[221290-65-9]
$C_{37}H_{64}O_{13}$ 716.905
Constit. of *Mediaster murrayi*. Amorph. powder. $[\alpha]_D$ -15.8 (c, 1.2 in MeOH).

24-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→5)-α-L-arabinofuranoside]:* ***Mediasteroside M_1***
[221290-53-5]
$C_{38}H_{66}O_{13}$ 730.932
Constit. of *Mediaster murrayi*. Amorph. powder. $[\alpha]_D$ -36 (c, 0.3 in MeOH).

24-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→5)-α-L-arabinofuranoside]:* ***Mediasteroside M_3***
[221290-77-3]
$C_{39}H_{68}O_{13}$ 744.958
Constit. of *Mediaster murrayi*. Amorph. powder. $[\alpha]_D$ -22.5 (c, 0.4 in MeOH).

(3β,5α,6β,15α,24*S*)-*form* [877035-06-8]
Constit. of *Henricia tumida*.
$[\alpha]_D^{20}$ +4 (c, 0.1 in MeOH).

3-O-*β-D-Xylopyranoside, 24-sulfate:* ***Pisasteroside B***
[123154-34-7]
$C_{32}H_{56}O_{12}S$ 664.853
Isol. from the starfish *Pisaster giganteus* (as Na salt).
$[\alpha]_D^{25}$ +6 (c, 1 in MeOH).

24-O-*β-D-Xylopyranoside, 3-sulfate:* ***Aphelasteroside A***
[142013-84-1]
$C_{32}H_{56}O_{12}S$ 664.853

Constit. of *Aphelasterias japonica*.
$[\alpha]_D$ -6 (c, 0.5 in MeOH).

24-O-*β*-D-*Xylopyranoside, 6-sulfate:* ***Coscinasteroside B***
[105404-84-0]
$C_{32}H_{56}O_{12}S$ 664.853
Constit. of *Coscinasterias tenuispina*.
$[\alpha]_D$ +7.2 (MeOH). CAS no. refers to Na salt.

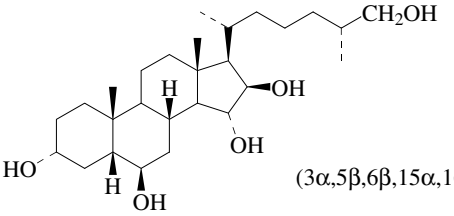
3-O-*(2*-O-*Methyl-β*-D-*xylopyranoside), 24*-O-*α*-L-*arabinofuranoside:* ***5-Deoxyisonodososide***
[97671-46-0]
$C_{38}H_{66}O_{13}$ 730.932
Constit. of *Acanthaster planci* and *Choriaster granulatus*.
$[\alpha]_D$ -13 (MeOH).

(3β,5α,6β,15β,24*S*)-*form*

24-O-*[2,4-Di*-O-*methyl-β*-D-*xylopyranosyl-(1→2)-α*-L-*arabinofuranoside]:* ***Halityloside F***
[102060-00-4]
$C_{39}H_{68}O_{13}$ 744.958
Constit. of *Halityle regularis*, *Culcita nova-guineae* and *Nardoa tuberculata*. Toxic to brine shrimp. Sol. MeOH. $[\alpha]_D$ -14.1 (MeOH).

Minale, L. *et al., Experientia*, 1983, **39**, 567-569 (*Attenuatoside AI*)
Minale, L. *et al., J. Nat. Prod.*, 1983, **46**, 736-741 (*Attenuatoside AII*)
Kicha, A.A. *et al., Tet. Lett.*, 1983, **24**, 3893-3896 (*Asterosaponin P_1*)
Riccio, R. *et al., Gazz. Chim. Ital.*, 1985, **115**, 405-409 (*synth, ms, pmr, cmr*)
Pizza, C. *et al., Gazz. Chim. Ital.*, 1985, **115**, 585-589 (*5-Deoxyisonodososide*)
Segura de Correa, R. *et al., J. Nat. Prod.*, 1985, **48**, 751-755 (*3-sulfoarabinoside*)
Riccio, R. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 869-893 (*Coscinasteroside B*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1986, **49**, 67-78 (*Halitylosides*)
Riccio, R.L. *et al., Gazz. Chim. Ital.*, 1987, **117**, 755-757 (*Indicoside B*)
Andersson, L. *et al., J. Chem. Res., Synop.*, 1987, 246; *J. Chem. Res., Miniprint*, 1987, 2085-2096 (*Crossasterosides*)
Kapustina, I.I. *et al., Khim. Prir. Soedin.*, 1987, **23**, 250-255; *Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 209-213 (*Asterosaponins, Distolasterosides*)
Higuchi, R. *et al., Annalen*, 1988, 1185-1189 (*Asterina pectinifera constit*)
Riccio, R. *et al., J. Nat. Prod.*, 1988, **51**, 989-992 (*Glacialoside A*)
Zollo, F. *et al., J. Nat. Prod.*, 1989, **52**, 693-700 (*Pisasteroside B*)
Bruno, I. *et al., J. Nat. Prod.*, 1989, **52**, 1022-1026 (*Pycnopodiosides*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1990, **53**, 94-101 (*Miniatoside B*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1990, **53**, 1225-1233; 1991, **54**, 1254-1264; 1992, **55**, 866-877; 1993, **56**, 1786-1798; 1995, **58**, 10-26 (*Scopariosides, Oreasterosides, Borealosides, Distolasteroside D_4, Culcitoside C4*)
Cho, Y. *et al., Annalen*, 1992, 79-81 (*Asterosaponin P1, cryst struct*)
Finamore, E. *et al., J. Nat. Prod.*, 1992, **55**, 767-772 (*Aphelasteroside A*)
Vázquez, M.J. *et al., Annalen*, 1993, 1257-1262 (*Validoside B*)
Vazquez, M J. *et al., Can. J. Chem.*, 1993, **71**, 1147-1151 (*Helianthoside*)
Maier, M.S. *et al., J. Nat. Prod.*, 1993, **56**, 939-942 (*Luridoside A*)
Kicha, A.A. *et al., J. Nat. Prod.*, 1999, **62**, 279-282 (*Mediasterosides*)
Wang, W. *et al., J. Nat. Prod.*, 2003, **66**, 384-391; 2004, **67**, 1654-1660 (*3β,5α,6α,15β,24S-form, Certonardosterol Q_3*)
Levina, E.V. *et al., J. Nat. Prod.*, 2005, **68**, 1541-1544 (*Phrygioside B*)
Levina, E.V. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2005, **31**, 467-474 (*Henricia tumida constit*)

Cholestane-3,6,15,16,26-pentol C-515



(3α,5β,6β,15α,16β,25*R*)-*form*

$C_{27}H_{48}O_5$ 452.673

(3α,5β,6β,15α,16β,25*R*)-*form*
Isol. from starfish *Tremaster novocaledoniae*.
$[\alpha]_D$ +32.1 (MeOH).

(3β,5α,6α,15β,16β,25ξ)-*form* [192325-49-8]
Constit. of *Ceramaster patagonicus*.
$[\alpha]_D$ +13.8 (c, 1.4 in MeOH).

(3β,5α,6β,15α,16β,25*R*)-*form* [181034-91-3]
[192325-52-3]
Constit. of an Antarctic starfish. $[\alpha]_D$ +1 (MeOH).

*22,23-Didehydro(*E-*):* ***Cholest-22-ene-3,6,15,16,26-pentol***
[181034-90-2]
$C_{27}H_{46}O_5$ 450.657
Constit. of an Antarctic starfish.
$[\alpha]_D$ -0.83 (MeOH).

(3β,5α,6β,15α,16β,25*S*)-*form* [82485-96-9]
Constit. of *Hacelia attenuata* and an Antarctic starfish (Echinasteridae). Cryst. Mp 197-199°. $[\alpha]_D$ 0.

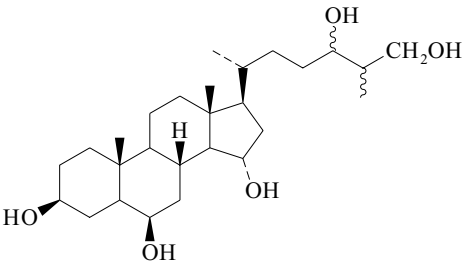
*22,23-Didehydro(*E-*):* [181034-89-9]
Constit. of an Antarctic starfish. $[\alpha]_D$ +8 (MeOH).

(3β,5α,15α,16β,25ξ)-*form*

6-Ketone: ***3,15,16,26-Tetrahydroxycholestan-6-one***
[181034-93-5]
$C_{27}H_{46}O_5$ 450.657
Constit. of an Antarctic starfish. $[\alpha]_D$ -6.6 (MeOH).

Minale, L. *et al., Tet. Lett.*, 1982, **23**, 1841-1844 (*Hacelia attenuata constits*)
Zollo, F. *et al., J. Nat. Prod.*, 1987, **50**, 794-799 (*synth*)
De Riccardis, F. *et al., Gazz. Chim. Ital.*, 1993, **123**, 79-86 (*3α,5β,6β,15α,16β,25R-form*)
Iorizzi, M. *et al., Tetrahedron*, 1996, **52**, 10997-11012 (*Antarctic starfish constits*)
Kicha, A.A. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1997, **46**, 186-191 (*Ceramaster patagonicus constit*)
Izzo, I. *et al., J.O.C.*, 1998, **63**, 4438-4443 (*synth*)

Cholestane-3,6,15,24,26-pentol C-516



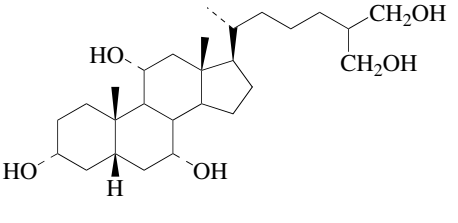
$C_{27}H_{48}O_5$ 452.673

(3β,5α,6β,15α,24ξ,25ξ)-*form*

24-O-*β*-D-*Xylopyranoside:* ***Solasteroside S_1***
[161897-71-8]
$C_{32}H_{56}O_9$ 584.789
Constit. of *Solaster dawsoni*. Amorph.solid. $[\alpha]_D$ +5.7 (c, 0.7 in MeOH).

Kicha, A.A. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1993, **42**, 943-949 (*isol, pmr, cmr*)

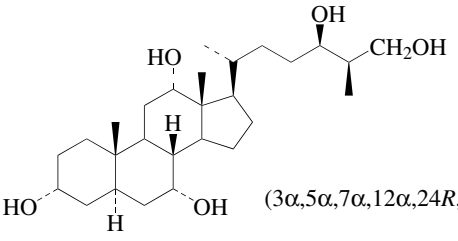
Cholestane-3,7,11,26,27-pentol C-517



$C_{27}H_{48}O_5$ 452.673

(3α,5β,7α,11α)-*form*
Molanol
*26-Sulfate (25*R-*):* [203739-15-5]
$C_{27}H_{48}O_8S$ 532.737
Constit. of bile of sunfish *Mola mola*. Amorph. powder. $[\alpha]_D^{25}$ +11 (c, 1 in MeOH).
*26-Sulfate (25*S-*):* [203739-16-6]
$C_{27}H_{48}O_8S$ 532.737
Constit. of bile of sunfish *Mola mola*. Amorph. powder. $[\alpha]_D^{25}$ +17.6 (c, 1 in MeOH).
Ishida, H. *et al., Chem. Pharm. Bull.*, 1998, **46**, 12-16 (*isol, pmr, cmr*)

Cholestane-3,7,12,24,26-pentol C-518



(3α,5α,7α,12α,24*R*,25*R*)-*form*

$C_{27}H_{48}O_5$ 452.673
Abs. config. of side chain detd. in 1994.

(3α,5α,7α,12α,24*R*,25*R*)-*form*
5α-Chimerol
[27857-11-0]
Isol. from fish *Catostomus commersoni*. Mp 234-235°. $[\alpha]_D^{24}$ +33.5 (c, 1.1 in EtOH).
26-Sulfate: [53990-54-8]
[60696-58-4]
$C_{27}H_{48}O_8S$ 532.737
Constit. of the bile of *Catostomus commersoni* and *Ctenopharyngodon idella*.

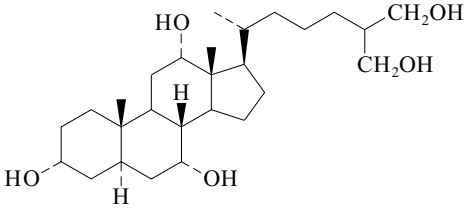
(3α,5β,7α,12α,24*R*,25*R*)-*form*
Chimerol. *Chimaerol*
[1256-87-7]
Constit. of the bile of *Chimaera monstrosa* and humans. Also isol. from bile of sharks *Lamna ditropis* and *Rhizoprionodon acutus*. Cryst. (EtOH aq.). Mp 180-182°. $[\alpha]_D$ +41.5 (c, 1.2 in EtOH).
26-Sulfate: [162600-38-6]
Constit. of the bile of *Chimaera monstrosa*, *Lamna ditropis*, *Rhizoprionodon acutus*, *Dasyatis akajei*, *Acipenser guldenstaedti*, *Acipenser stellatus* and *Huso fuso*. Amorph. powder. $[\alpha]_D^{25}$ +23.9 (c, 0.5 in MeOH).

[47698-94-2]

Bridgwater, R.J. *et al., Biochem. J.*, 1963, **87**, 28-31 (*Chimerol sulfate*)
Haslewood, G.A.D. *et al., Bile Salt Metab.*, 1969, 151 (*rev*)
Anderson, I.G. *et al., Biochem. J.*, 1970, **116**, 581-587 (*5α-Chimerol*)
Kurokis, S. *et al., J. Lipid Res.*, 1985, **26**, 230-240 (*5β-form, isol*)
Ishida, H. *et al., Chem. Pharm. Bull.*, 1994, **42**, 2514-2517 (*Chimerol sulfate, isol, abs config*)

Cholestane-3,7,12,26,27-pentol, 9CI C-519

Cyprinol



$C_{27}H_{48}O_5$ 452.673

(3α,5α,7α,12α)-*form*
5α-Cyprinol
[2952-70-7]
Constit. of bile salts of *Cyprinia* fish, *Latimeria chalumnae* (coelacanth), bullfrog, and *Megalobactrachus japonicus* (giant salamander). Mp 242°. $[\alpha]_D^{23}$ +29 (c, 1.7 in EtOH).
*26-*O*-Sulfate:* ***Carp toxin***
[53939-18-7]
$C_{27}H_{48}O_8S$ 532.737
Isol. from carp bile (*Cyprinus carpio*). Toxin.

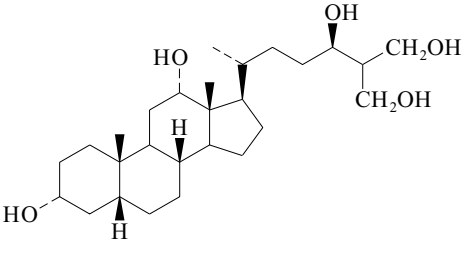
(3α,5β,7α,12α)-*form*
5β-Cyprinol
[2486-18-2]
Constit. of bile salts of *Rana nigromaculata* (frog); of eel, humans, and *Latimeria chalumnae*. Cryst. (MeOH/EtOAc).
Mp 173-174°.
*26-*O*-Sulfate(25*R-*):* [203739-17-7]
$C_{27}H_{48}O_8S$ 532.737
Constit. of bile of sunfish *Mola mola*. Amorph. powder. $[\alpha]_D^{25}$ +39.6 (c,1 in MeOH).
*26-*O*-Sulfate(25*S-*):* [203739-18-8]
$C_{27}H_{48}O_8S$ 532.737
Constit. of bile of sunfish *Mola mola*. Amorph. powder. $[\alpha]_D^{25}$ +21.2 (c,1 in MeOH).

(3β,5α,7α,12α)-*form*
Latimerol
[2860-99-3]
Constit. of bile salts of coelacanth, *Latimeria chalumnae*. Cryst. (Me_2CO).
Mp 235-236°. $[\alpha]_D^{23}$ +33 (c, 1.1 in EtOH).

[53939-19-8, 63307-55-1]

Hoshita, T. *et al., J. Biochem. (Tokyo)*, 1963, **53**, 291-294; **54**, 369-374 (*synth, ir, 3α,5β,7α,12α-form, 3α,5α,7α,12α-form*)
Anderson, I.G. *et al., Biochem. J.*, 1964, **93**, 34-39 (*ir, 3β,5α,7α,12α-form*)
Kazuno, T. *et al., J. Biochem. (Tokyo)*, 1965, **58**, 243-247 (*isol, 3α,5β,7α,12α-form*)
Cross, A.D. *et al., Steroids*, 1965, **5**, 655-662 (*pmr*)
Amimoto, K. *et al., J. Biochem. (Tokyo)*, 1966, **59**, 340-343 (*isol, 3α,5α,7α,12α-form*)
Haslewood, G.A.D. *et al., Biochem. J.*, 1968, **108**, 263-268 (*synth, 3α,5β,7α,12α-form*)
Noma, Y. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2686-2691 (*isol, 3α,5α,7α,12α-form*)
Kuwabara, M. *et al., J. Lipid Res.*, 1984, **25**, 361-368 (*isol, ms, 3α,5β,7α,12α-form*)
Asakawa, M. *et al., Toxicon*, 1990, **28**, 1063-1069 (*Carp toxin*)
Ishida, H. *et al., Chem. Pharm. Bull.*, 1998, **46**, 12-16 (*Cyprinol sulfates*)

Cholestane-3,12,24,26,27-pentol C-520



$C_{27}H_{48}O_5$ 452.673

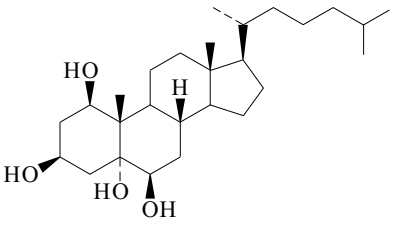
(3α,5β,12α,24*R*)-*form*
7-Deoxyscymnol
[180048-10-6]
Constit. of megamouth shark bile *Megachasma pelagios*. Plates.
Mp 192.5-194°. $[\alpha]_D^{25}$ +54.6 (c, 0.7 in MeOH).
26-Sulfate: [180048-09-3]
$C_{27}H_{48}O_8S$ 532.737

Constit. of megamouth shark bile *Megachasma pelagios*. Amorph. powder.

[180048-08-2]

Ishida, H. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1289-1292 (*isol, pmr, cmr*)

Cholestane-1,3,5,6-tetrol C-521

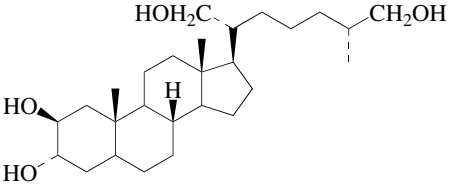


$C_{27}H_{48}O_4$ 436.674

(1β,3β,5α,6β)-*form* [72534-12-4]
Isol. from *Sarcophyton glaucum*, *Lobophytum* sp. and the gorgonian *Echinomuraceae splendens*.
Cryst. (Me_2CO/hexane).
Mp 261-264°. $[\alpha]_D$ -6 (c, 1.15 in MeOH).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1848 (*isol, synth*)
Raju, B.L. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 1033-1037 (*isol*)
Parameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 2002, **41**, 1093-1096 (*isol, pmr, cmr*)

Cholestane-2,3,21,26-tetrol C-522



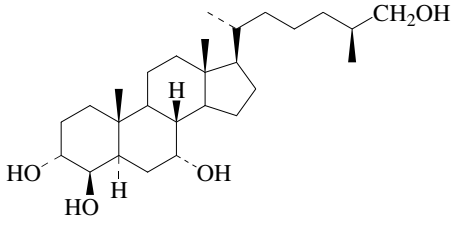
$C_{27}H_{48}O_4$ 436.674

(2β,3α,20*R*,25*R*)-*form*
3,21-Disulfate: [214129-63-2]
$C_{27}H_{48}O_{10}S_2$ 596.802
Constit. of *Pteraster tesselatus*.

Levina, E.V. *et al., J. Nat. Prod.*, 1998, **61**, 1423-1426 (*isol, pmr, cmr*)

Cholestane-3,4,7,26-tetrol C-523

[501345-91-1]

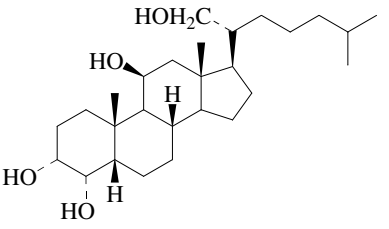


$C_{27}H_{48}O_4$ 436.674

(3α,4β,7α,24*S*)-*form*
3,26-Disulfate: ***SAAF***
[612086-13-2]
Isol. from ascidian *Ciona intestinalis*. Sperm-activating and attracting factor. Solid.

Oishi, T. *et al., Tetrahedron*, 2004, **60**, 6971-6980 (*isol, pmr, synth, abs config*)

Cholestane-3,4,11,21-tetrol C-524

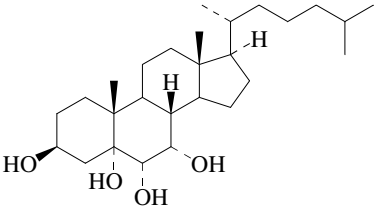


$C_{27}H_{48}O_4$ 436.674

(3α,4α,5β,11β)-*form* [109152-37-6]
$[\alpha]_D$ +46.4.
3,21-Disulfate: [109152-31-0]
[143503-22-4 (di-Na salt)]
$C_{27}H_{48}O_{10}S_2$ 596.802
Major polar steroid component of ophiuroids *Ophiocoma dentata*, *Ophioderma longicaudum*, *Ophiarthrum elegans*, *Ophioplocus januarii*, *Ophiarachna incrassata*, *Ophiocoma scolopendrina*, *Ophionereis reticulata*, *Ophiozona impressa*, *Ophiocoma wendti* and *Ophiocoma echinata*. Protein-tyrosine kinase inhibitor. Amorph. powder. $[\alpha]_D$ +41.3 (MeOH) (as di-Na salt).
11-Ketone, 3,21-disulfate: [109152-34-3]
$C_{27}H_{46}O_{10}S_2$ 594.786
Isol. from *Ophiarthrum elegans*. $[\alpha]_D$ +25.

D'Auria, M.V. *et al., J.O.C.*, 1987, **52**, 3947-3952; 1989, **54**, 234-239 (*3,21-disulfate, isol, synth*)
D'Auria, M.V. *et al., Nat. Prod. Lett.*, 1993, **3**, 197-201 (*3,21-disulfate*)
Fu, X. *et al., J. Nat. Prod.*, 1994, **57**, 1591-1594 (*3,21-disulfate, isol, pmr, cmr*)
Roccatagliata, A.J. *et al., J. Nat. Prod.*, 1996, **59**, 887-889 (*3,21-disulfate, isol, pmr, cmr*)

Cholestane-3,5,6,7-tetrol C-525



(3β,5α,6α,7α)-*form*

$C_{27}H_{48}O_4$ 436.674

(3β,5α,6α,7α)-*form*
3,6,7-Tri-Ac: [123122-20-3]
$C_{33}H_{54}O_7$ 562.785
Needles (hexane). Mp 221.5-222.5°. $[\alpha]_D^{22}$ +16.9 (c, 1.01 in $CHCl_3$).

(3β,5α,6α,7β)-*form*
3,6,7-Tri-Ac: [123039-11-2]
Cryst. (hexane). Mp 190.6-191.2°. $[\alpha]_D^{22}$ +7.9 (c, 3.05 in $CHCl_3$).

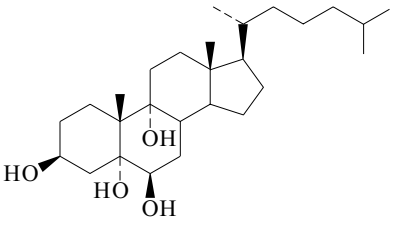
(3β,5α,6β,7α)-*form*
3,7-Di-Ac: [123039-14-5]
$C_{31}H_{52}O_6$ 520.748
Cryst. (hexane). Mp 226.5-228.5°. $[\alpha]_D^{22}$ +23.3 (c, 1.79 in $CHCl_3$).
3,6,7-Tri-Ac: [62107-21-5]
$C_{33}H_{54}O_7$ 562.785
Oil.

(3β,5α,6β,7β)-*form* [62073-86-3]
Constit. of *Plexaurella grisea*.
3,7-Di-Ac: [123039-13-4]
Fine needles (MeOH aq.). Mp 210-211°. $[\alpha]_D^{21}$ +23.3 (c, 1.79 in $CHCl_3$).

3,6,7-Tri-Ac: [62107-22-6]
Oil.

Kawato, M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 3109-3113 (*synth*)
Warren, J. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 147 (*synth, pmr, ir*)
Rueda, A. *et al., Steroids*, 2001, **66**, 897-904 (*isol*)

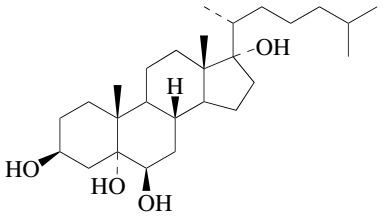
Cholestane-3,5,6,9-tetrol C-526



$C_{27}H_{48}O_4$ 436.674

(3β,5α,6β)-*form* [61235-71-0]
Constit. of the gorgonian *Pseudopterogorgia elisabethae.*
Schmitz, F.J. *et al., Steroids*, 1976, **28**, 211

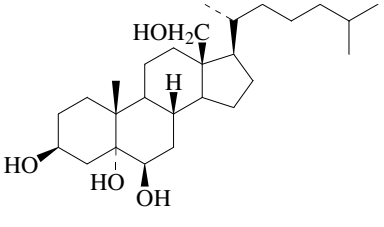
Cholestane-3,5,6,17-tetrol C-527



$C_{27}H_{48}O_4$ 436.674

(3β,5α,6β,17α)-*form*
6-Ac: ***Punicin***
[211118-98-8]
$C_{29}H_{50}O_5$ 478.711
Constit. of *Lophogorgia punicea*. Amorph. solid.
Mp 132-134°. $[\alpha]_D^{25}$ -31 (c, 1 in $CHCl_3$). λ_{max} 249 (3.17) ($CHCl_3$).
Epitanio, R. de A. *et al., J. Braz. Chem. Soc.*, 1998, **9**, 187-192; *CA*, **129**, 159281w (*isol, pmr, cmr*)

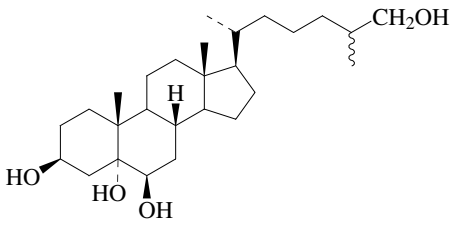
Cholestane-3,5,6,18-tetrol C-528



$C_{27}H_{48}O_4$ 436.674

(3β,5α,6β)-*form*
18-Ac: ***Dendronesterol A***
[265121-05-9]
$C_{29}H_{50}O_5$ 478.711
Constit. of *Dendronephthya gigantea*. Amorph. solid. $[\alpha]_D^{25}$ +3.42 (c, 1 in MeOH).
Yoshikawa, K. *et al., J. Nat. Prod.*, 2000, **63**, 670-672 (*isol, pmr, cmr*)

Cholestane-3,5,6,26-tetrol C-529



$C_{27}H_{48}O_4$ 436.674

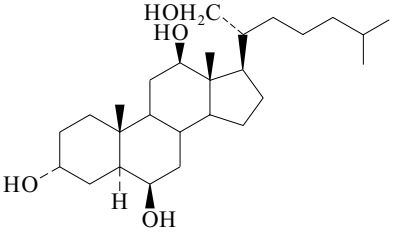
(3β,5α,6β,25ξ)-*form* [172303-95-6]
Constit. of *Telesto riisei*. Cryst. Mp 212-214°. $[\alpha]_D^{25}$ -70 (c, 0.02 in MeOH).

26-Ac: [172303-94-5]
$C_{29}H_{50}O_5$ 478.711
Constit. of *Telesto riisei*. Cryst. Mp 200-202°. $[\alpha]_D^{25}$ +3.52 (c, 0.34 in MeOH).

*26-Ac, 3-*O*-(3-*O*-acetyl-β-D-arabinopyranoside):* ***Riisein A***
[297764-84-2]
$C_{36}H_{60}O_{10}$ 652.864
Constit. of *Telesto riisei* (*Carijoa riisei*). Powder.
Mp 187-189°. $[\alpha]_D^{25}$ -61 (c, 0.1 in $CHCl_3$).

*26-Ac, 3-*O*-(4-*O*-acetyl-β-D-arabinopyranoside):* ***Riisein B***
[297764-85-3]
$C_{36}H_{60}O_{10}$ 652.864
Constit. of *Telesto riisei* (*Carijoa riisei*). Powder.
Mp 188-191°. $[\alpha]_D^{25}$ -85 (c, 0.1 in $CHCl_3$).
Liyanage, G.K. *et al., J. Nat. Prod.*, 1996, **59**, 148-151 (*isol, pmr, cmr*)
Maia, L.F. *et al., J. Nat. Prod.*, 2000, **63**, 1427-1430 (*Riiseins*)

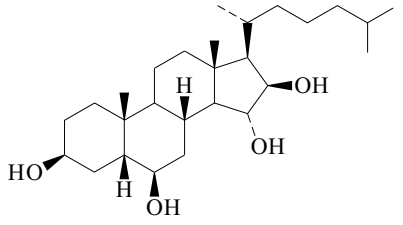
Cholestane-3,6,12,21-tetrol C-530



$C_{27}H_{48}O_4$ 436.674

(3α,5α,6β,12β)-*form*
*12-*O*-β-D-Xylopyranoside, 3-sulfate, Na salt:* ***Longicaudoside A***
[99494-32-3]
$C_{32}H_{55}NaO_{11}S$ 670.836
Constit. of *Ophioderma longicaudum.*
*12-*O*-β-D-Glucopyranoside, 3-sulfate, Na salt:* ***Longicaudoside B***
[99458-04-5]
$C_{33}H_{57}NaO_{12}S$ 700.862
From *Ophioderma longicaudum*. $[\alpha]_D$ +3.8 (c, 1.0 in MeOH).
Riccio, R. *et al., J.O.C.*, 1986, **51**, 533-536

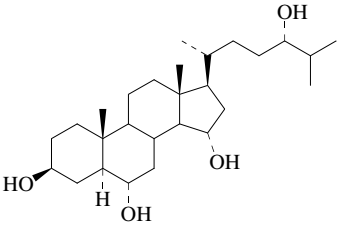
Cholestane-3,6,15,16-tetrol C-531



$C_{27}H_{48}O_4$ 436.674

(3β,5β,6β,15α,16β)-*form*
Constit. of *Luidia clathrata*. $[\alpha]_D$ +28.
Iorizzi, M. *et al., J. Nat. Prod.*, 1995, **58**, 653-671 (*isol, pmr, cmr*)

Cholestane-3,6,15,24-tetrol C-532



(3β,5α,6α,15α,24*S*)-*form*

$C_{27}H_{48}O_4$ 436.674

(3β,5α,6α,15α,24*S*)-*form* [53190-88-8]
Aglycone from the saponins of *Asterias amurensis.*
Cryst. (Me_2CO). Mp 197-199°. $[\alpha]_D^{21}$ +45.7 (c, 0.5 in MeOH).
3-O-*(2*-O-*Methyl-β-D-xylopyranoside), 24*-O-*α-L-arabinofuranoside:* ***Granulatoside B***
[100665-54-1]
$C_{38}H_{66}O_{12}$ 714.932
Constit. of *Choriaster granulatus.* $[\alpha]_D$ -12 (MeOH).
24-O-*β-D-Xylopyranoside, 15*-O-*sulfate:* ***Amurensoside A***
[115178-52-4]
$C_{32}H_{56}O_{11}S$ 648.854
Constit. of *Asterias amurensis.* $[\alpha]_D$ +16.7 (MeOH).
Tetra-Ac: [53190-89-9]
Mp 137-138.5°. $[\alpha]_D^{21}$ +66.2 (c, 1 in $CHCl_3$).

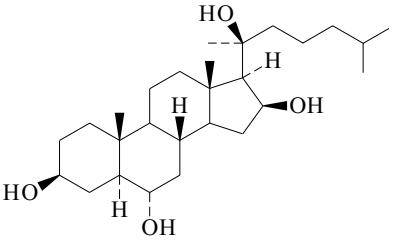
(3β,5α,6α,15β,24*S*)-*form*
Certonardosterol F
[517900-54-8]
Constit. of *Certonardoa semiregularis.* Cryst.
24-O-*β-D-Xylofuranoside:* ***Certonardoside N***
[620604-41-3]
$C_{32}H_{56}O_8$ 568.79
Constit. of *Certonardoa semiregularis.* Cryst.
24-O-*β-D-Xylopyranoside:* ***Rathbunioside R1***
[350689-78-0]
$C_{32}H_{56}O_8$ 568.79
Constit. of *Asterias rathbuni*. Amorph. powder. $[\alpha]_D$ -0.2 (c, 1.6 in MeOH).
24-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→2)-β-D-xylofuranoside]:* ***Certonardoside L***
[620604-22-0]
$C_{39}H_{68}O_{12}$ 728.959
Constit. of *Certonardoa semiregularis.* Cryst.

(3β,5α,6β,15α,24*S*)-*form* [877035-07-9]
Constit. of *Henricia tumida.* $[\alpha]_D^{20}$ -6.4 (c, 0.1 in MeOH).

(3β,5α,6β,15β,24*S*)-*form*
Constit. of starfish *Henricia sanguinolenta*. Cryst. (MeOH).
Mp 235.5-237°. $[\alpha]_D^{20}$ -4.5 (c, 0.36 in EtOH).

(3β,5α,6β,24*S*)-*form*
15-Ketone: ***3,6,24-Trihydroxycholestan-15-one***
$C_{27}H_{46}O_4$ 434.658
Constit. of starfish *Henricia sanguinolenta*. Cryst. (MeOH).
Mp 93-94.5°. $[\alpha]_D^{20}$ +9.1 (c, 0.6 in EtOH).
Kamiya, Y. *et al., Tet. Lett.*, 1974, 655
Pizza, C. *et al., Gazz. Chim. Ital.*, 1985, **115**, 585 (*Granulatoside B*)
Riccio, R. *et al., J.C.S. Perkin 1*, 1988, 1337-1347 (*Amurensoside A*)
Ivanchina, N.V. *et al., J. Nat. Prod.*, 2001, **64**, 945-947 (*Rathbunioside R_1*)
Levina, E.V. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2002, **51**, 2295-2298; 2003, **52**, 1623-1628 (*Henricia sanguinolenta constits*)
Wang, W. *et al., Chem. Pharm. Bull.*, 2003, **51**, 435-439 (*Certonardosides L,N*)
Wang, W. *et al., J. Nat. Prod.*, 2003, **66**, 384-391 (*Certonardosterol F*)
Levina, E.V. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2005, **31**, 467-474 (*Henricia tumida constit*)

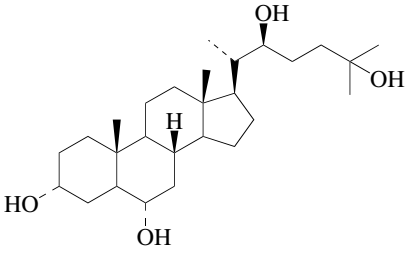
Cholestane-3,6,16,20-tetrol C-533



$C_{27}H_{48}O_4$ 436.674

(3β,5α,6α,16β)-*form*
3-O-*β-D-Glucuronopyranoside, 6-sulfate:* ***Downeyoside L***
[174324-06-2]
$C_{33}H_{56}O_{13}S$ 692.864
Constit. of *Henricia downeyae.*
$[\alpha]_D$ -11.5.
Palagiano, E. *et al., J. Nat. Prod.*, 1996, **59**, 348-354 (*isol, pmr, cmr*)

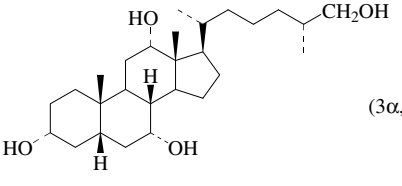
Cholestane-3,6,22,25-tetrol C-534



$C_{27}H_{48}O_4$ 436.674

(3α,5α,6α,22S)-*form*
3,6-Di-Ac: [201800-62-6]
$C_{31}H_{52}O_6$ 520.748
Constit. of *Gersemia fruticosa*. Apoptosis inducer. Oil. $[\alpha]_D$ +37.3 (c, 0.67 in MeOH).
koljak, R. *et al., Tetrahedron*, 1998, **54**, 179-186 (*isol, pmr, cmr*)

Cholestane-3,7,12,26-tetrol C-535



(3α,5β,7α,12α,25*R*)-*form*

$C_{27}H_{48}O_4$ 436.674

(3α,5β,7α,12α,25*R*)-*form* [27857-14-3]
Intermed. in the biosynth. of cholic acid from cholesterol.
Cryst. (EtOAc).
Mp 200-202°. $[\alpha]_D$ +36.5 (c, 1.14 in EtOH).

26-Aldehyde: 3,7,12-Trihydroxycholestan-26-al
[78148-66-0]
[3836-01-9 (general no. for aldehyde)]
$C_{27}H_{46}O_4$ 434.658
Intermed. in biosynth. of cholic acid from cholesterol. Noncryst.

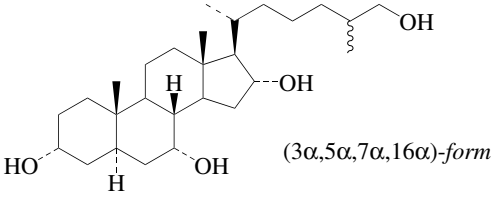
(3α,5β,7α,12α,25*S*)-*form* [134002-65-6]
Cryst. (EtOAc). Mp 154-155° (138-140°). $[\alpha]_D$ +9.2 (c, 1.01 in EtOH).

(3α,5α,7α,12α,25ξ)-*form*
27-Deoxy-5α-cyprinol
[862-52-2]
Isol. from lungfish, carp and coelacanth *Latimeria chalumnae*.
Mp 232°. $[\alpha]_D$ +39.

(3α,5β,7α,12α,25ξ)-*form*
27-Deoxy-5β-cyprinol
[862-53-3]
Isol. from frogs and toads. Also from manatee *Trichechus manatus*.
Cryst. (EtOAc/diisopropyl ether).
Mp 268-269°.

Okuda, A. *et al., Acta Chem. Scand.*, 1965, **19**, 2160-2165 (*sldehyde, synth*)
Anderson, I.G. *et al., Biochem. J.*, 1970, **116**, 581-587 (*synth*)
Anderson, I.G. *et al., Biochem. J.*, 1974, **141**, 485-494 (*27-Deoxy-5α-cyprinol, isol*)
Amos, B. *et al., Biochem. J.*, 1977, **161**, 201-204 (*27-Deoxy-5β-cyprinol, isol*)
Dayal, B. *et al., Steroids*, 1981, **37**, 205-211 (*synth*)
Okuda, A. *et al., J. Biol. Chem.*, 1983, **258**, 2899-2905 (*aldehyde, biochem*)
Wang, M.Y. *et al., CA*, 1986, **104**, 48109 (*isol*)
Karoki, S. *et al., J. Lipid Res.*, 1988, **29**, 509-522 (*27-Deoxy-5β-cyprinol*)
Batta, A.K. *et al., J. Chromatogr.*, 1991, **184**, 184-188 (*hplc*)
Holmberg-Betsholz, I. *et al., J. Biol. Chem.*, 1993, **268**, 11079-11085 (*biochem*)
Kurosawa, T. *et al., Steroids*, 1995, **60**, 439-444 (*synth*)
Une, M. *et al., J. Chromatogr., B: Biomed. Appl.*, 1996, **682**, 157-161 (*hplc*)

Cholestane-3,7,16,26-tetrol C-536



(3α,5α,7α,16α)-*form*

$C_{27}H_{48}O_4$ 436.674

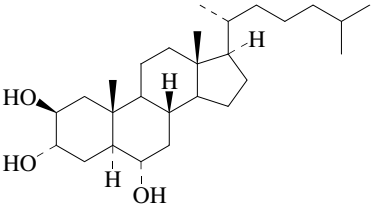
(3α,5α,7α,16α)-*form*
3-Epimyxinol
[68907-97-1]
Constit. of hagfish bile.
Cryst. (EtOAc).
Mp 178°.

(3β,5α,7α,16α)-*form*
Myxinol
[16812-98-9]
Bile alcohol from gall bladder of the hagfish *Heptatetrus burgeri*.
Cryst. (EtOAc aq.).
Mp 206°. $[\alpha]_D$ -15 (c, 1.2 in EtOH).

3,26-Disulfate: ***Myxinol disulfate***
[881182-67-8]
$C_{27}H_{48}O_{10}S_2$ 596.802
Constit. of the bile of *Myxine glutinosa* and *Eptatretus stoutii*.
Cryst. (MeOH).
Mp 195° dec.

Haslewood, G.A.D. *et al., Biochem. J.*, 1966, **100**, 233-237 (*Myxinol 3,26-disulfate*)
Cross, A.D. *et al., Biochem. J.*, 1966, **100**, 238-240 (*pmr*)
Anderson, I.G. *et al., Biochem. J.*, 1967, **104**, 1061-1063 (*struct*)
Une, M. *et al., Tet. Lett.*, 1978, 2527-2530 (*3-Epimyxinol*)

Cholestane-2,3,6-triol C-537



(2β,3α,5α,6α)-*form*

$C_{27}H_{48}O_3$ 420.674

(2β,3α,5α,6α)-*form*
Tri-O-*sulfate:* ***Halistanol sulfate C***
[143049-14-3]
$C_{27}H_{48}O_{12}S_3$ 660.867
Constit. of *Pseudaxinyssa digitata* and an *Epipolasis* sp. Thrombin inhibitor. $[\alpha]_D^{21}$ +27.5 (c, 1 in MeOH).

(2β,3β,5α,6β)-*form* [16126-42-4]
Leaflets (MeOH). Mp 213-219°. $[\alpha]_D^{26}$ +23 (c, 0.98 in dioxan).

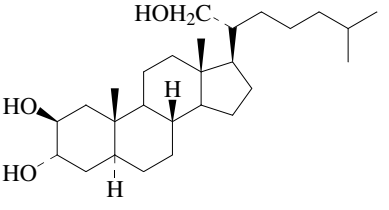
2,3-Di-Ac: [26753-94-6]
$C_{31}H_{52}O_5$ 504.749
Cryst. (MeOH). Mp 165-167.5°. $[\alpha]_D^{20}$ +17 (c, 2.4 in $CHCl_3$).

2,3-isopropylidene: [16126-38-8]
$C_{30}H_{52}O_3$ 460.739
Needles (Me_2CO). Mp 217-222°. $[\alpha]_D$ +37 (c, 1.09 in dioxan).

[117829-52-4, 117829-53-5]

Mori, H. *et al., Chem. Pharm. Bull.*, 1967, **15**, 466-473 (*synth*)
Cerny, V. *et al., Coll. Czech. Chem. Comm.*, 1970, **35**, 1235-1254 (*2,3-di-Ac*)
Kanazawa, S. *et al., Tetrahedron*, 1992, **48**, 5467-5472 (*Epipolasis constit*)
Bifulco, G. *et al., J. Nat. Prod.*, 1994, **57**, 164-167 (*trisulfate, isol*)

Cholestane-2,3,21-triol C-538



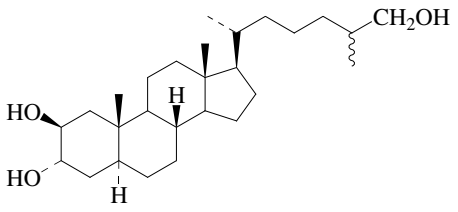
$C_{27}H_{48}O_3$ 420.674

(2β,3α,5α)-*form*
3,21-Di-O-*sulfate:* [497946-03-9]
$C_{27}H_{48}O_9S_2$ 580.803
Constit. of *Pteraster pulvillus* and *Littorina kurila*. Amorph. powder. $[\alpha]_D$ +14 (c, 0.05 in MeOH).

Ivanchina, N.V. *et al., J. Nat. Prod.*, 2003, **66**, 298-301 (*isol, pmr, cmr*)
Kusaykin, M.I. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2006, **32**, 63-70 (*isol, Littorina*)

Cholestane-2,3,26-triol C-539

[109152-39-8]

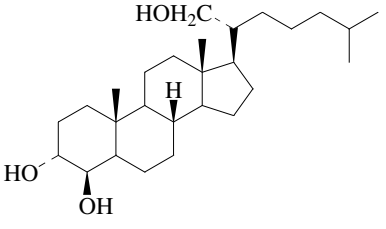


$C_{27}H_{48}O_3$ 420.674

(2β,3α,5α,25ξ)-*form*

Trisulfate: [109152-35-4]
$C_{27}H_{48}O_{12}S_3$ 660.867
Constit. of brittle star *Ophiarachna incrassata*. Protein-tyrosine kinase inhibitor. Amorph. powder.
D'Auria, M.V. *et al., J.O.C.*, 1987, **52**, 3947-3952 (*synth*)
Fu, X. *et al., J. Nat. Prod.*, 1994, **57**, 1591-1594 (*isol*)

Cholestane-3,4,21-triol C-540



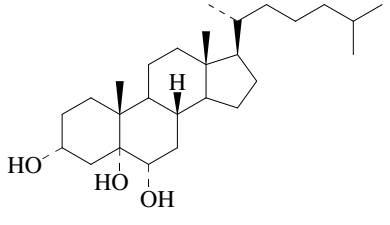
$C_{27}H_{48}O_3$ 420.674

(3α,4β,5α)-*form*

3,21-Di-O-*sulfate:* [292833-55-7]
$C_{27}H_{48}O_9S_2$ 580.803
Constit. of *Gorgonocephalus chilensis* and *Pteraster pulvillus.* $[\alpha]_D$ +6.5 (c, 1.1 in MeOH).
Maier, M.S. *et al., Molecules*, 2000, **5**, 348-349; *CA*, **133**, 235391g (*isol, pmr, cmr*)
Ivanchina, N.V. *et al., J. Nat. Prod.*, 2003, **66**, 298-301 (*isol, pmr, cmr*)

Cholestane-3,5,6-triol C-541

[115510-05-9]



(3α,5α,6α)-*form*

$C_{27}H_{48}O_3$ 420.674

(3α,5α,6α)-*form*
Cryst. (AcOH). Mp 168-172°. $[\alpha]_D$ +13 (c, 1.5 in $CHCl_3$). No CAS no. to 13CI.

(3α,5α,6β)-*form* [2701-11-3]
Solid. Mp 205-206°. $[\alpha]_D^{30}$ -4 (dioxan).
3,6-Di-Ac:
$C_{31}H_{52}O_5$ 504.749
Cryst. (MeOH). Mp 62°. $[\alpha]_D^{25}$ -44 ($CHCl_3$).

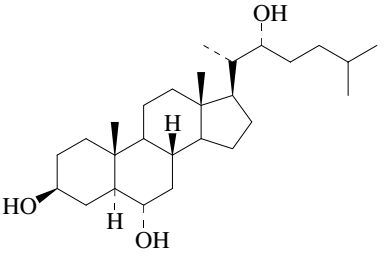
(3β,5α,6α)-*form* [35089-25-9]
Constit. of human atherosclerotic plaques.
Cryst. (Me_2CO).
Mp 240-241° (236-238°). $[\alpha]_D$ +21 ($CHCl_3$).
3,6-Di-Ac: [7199-72-6]
Cryst. (MeOH). Mp 186-188°.

(3β,5α,6β)-*form* [1253-84-5]
Constit. of coelenterate *Pteroeides esperi*. Trace constit. of sponge *Damiriana hawaiiana*. Angiotic and cytophatic agent. Cryst.
Mp 237-240° (226-228°). $[\alpha]_D$ +50 (MeOH).
6-Ac: ***Guggulsterol V***
[6120-71-4]
$C_{29}H_{50}O_4$ 462.712
Constit. of *Commiphora mukul*. Cryst.
Mp 148°.
3,6-Di-Ac: [1260-68-0]
Cryst. (MeOH). Mp 167-169°.

(3β,5β,6α)-*form* [24222-78-4]
No phys. props. reported.

(3β,5β,6β)-*form* [79254-30-1]
Cryst. (MeOH). Mp 127-128°. $[\alpha]_D^{20}$ +22 (c, 1.0 in $CHCl_3$).
3,6-Di-Ac:
Cryst. (MeOH). Mp 165-167°. $[\alpha]_D$ +16 ($CHCl_3$).
Fudge, A.J. *et al., J.C.S.*, 1954, 958-964 (*3α,5α,6α-form, synth*)
Bowers, A. *et al., J.A.C.S.*, 1959, **81**, 5233-5242 (*3β,5α,6α-form, synth*)
Snatzke, G. *et al., Annalen*, 1964, **676**, 188-202 (*3β,5β,6β-form, synth*)
Mousseron-Canet, M. *et al., Bull. Soc. Chim. Fr.*, 1966, 3853-3858 (*3α,5α,6β-form, synth*)
Purushothaman, K.K. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 802-804 (*3β,5α,6β-form, Guggulsterol V*)
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476 (*occur, sponge*)
Valisolalao, J. *et al., Tetrahedron*, 1983, **39**, 2779-2785 (*3β,5α,6β-form, synth*)
Nashed, N.T. *et al., Arch. Biochem. Biophys.*, 1985, **241**, 149-162 (*3β,5β,6β-form, 3β,5β,6α-form, synth*)
Datta, P.K. *et al., J. Nat. Prod.*, 1990, **53**, 1347-1348 (*3β,5α,6β-form, isol*)
Breuer, O. *et al., Biochim. Biophys. Acta*, 1996, **1302**, 145-152 (*3β,5α,6α-form, isol*)
Zhao, K. *et al., Synth. Commun.*, 2001, **31**, 2619-2624 (*3α,5α,6β-form, synth, pmr*)

Cholestane-3,6,22-triol C-542

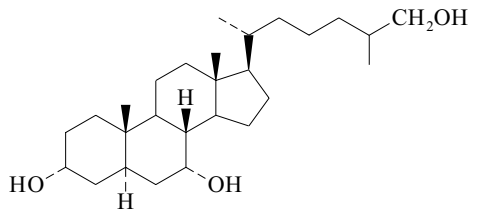


$C_{27}H_{48}O_3$ 420.674

(3β,5α,6α,22*R*)-*form*

3,6-Disulfate: [149230-99-9]
$C_{27}H_{48}O_9S_2$ 580.803
Isol. from the starfish *Tremaster novaecaledoniae.* $[\alpha]_D$ +36.4 (MeOH).
22-Ac, 3,6-disulfate: [149261-52-9]
$C_{29}H_{50}O_{10}S_2$ 622.84
Isol. from *Tremaster novaecaledoniae.* $[\alpha]_D$ +21.2 (MeOH) (as di-Na salt).
De Riccardis, F. *et al., Gazz. Chim. Ital.*, 1993, **123**, 79-86 (*isol, pmr, cmr*)

Cholestane-3,7,26-triol C-543



$C_{27}H_{48}O_3$ 420.674

(3α,5α,7α,25ξ)-*form* [56194-10-6]
Constit. of bile of the hagfish *Heptatetrus burgeri*.
Mp 187-188°.

(3α,5β,7α,25*R*)-*form* [66807-58-7]
Cryst. (MeOH). Mp 155-157°. $[\alpha]_D^{25}$ +15.9 (MeOH).

(3α,5β,7α,25*S*)-*form* [66807-59-8]
Cryst. (MeOH/Me_2CO). Mp 138-140°. $[\alpha]_D^{25}$ +8.8 (MeOH).

(3α,5β,7α,25ξ)-*form* [15313-69-6]
Isol. from human bile.

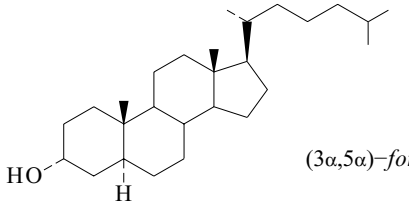
(3β,5α,7α,25*R*)-*form* [43204-14-4]
Needles (Me_2CO). Mp 206-207°. $[\alpha]_D^{23}$ +12.6 ($CHCl_3$).

(3β,5α,7α,25ξ)-*form*
16-Deoxymyxinol
[23455-17-6]
Isol. from the hagfish *Heptatetrus burgeri* and *Myxine glutinosa*.
7-Ac:
Cryst. (Me_2CO). Mp 144-146°.
3,7-Di-Ac:
Cryst. (Me_2CO). Mp 134-136°.
Tri-Ac:
Cryst. (Me_2CO or MeOH). Mp 109-110°.

(3β,5α,7β,25*R*)-*form* [43204-24-6]
Fine needles (Me_2CO). Mp 201°. $[\alpha]_D^{23}$ +62 ($CHCl_3$).
Noll, B.W. *et al., J. Lipid Res.*, 1973, **14**, 391-399 (*3β,5α,7α,25R-form, synth*)
Mui, M.M. *et al., Steroids*, 1974, **24**, 239-250 (*3β,5α,7α,25*R-*form, synth*)
Shefer, S. *et al., J. Biol. Chem.*, 1978, **253**, 6386 (*biosynth*)
Dayal, B. *et al., J. Lipid Res.*, 1978, **19**, 191-196 (*3α,5β,7α,25*R/S-*form*)
Une, M. *et al., Tet. Lett.*, 1978, 2527-2530 (*Heptatetrus burgeri constits*)
Batta, A.K. *et al., J. Lipid Res.*, 1980, **21**, 130-135 (*cmr*)
Kuroki, S. *et al., J. Lipid Res.*, 1985, **26**, 230-240 (*isol, 3α,5β,7α-form*)

Cholestan-3-ol C-544

[27409-41-2]



(3α,5α)–*form*

$C_{27}H_{48}O$ 388.676

(3α,5α)-*form*
Epicholestanol. *Epidihydrocholesterin*. *Dihydrin*. *Presteron*
[516-95-0] Agent for alveolar blennorrhea. Needles (EtOH). Mp 185-186°. $[\alpha]_D^{20}$ +34 ($CHCl_3$).
▶ Exp. reprod. and teratogenic effects (large dose). FZ6328000
3-O-*Sulfate:* [107585-01-3]
[56816-66-1 (Na salt)]
$C_{27}H_{48}O_4S$ 468.74
Mp 136-137° (as Na salt). $[\alpha]_D^{29}$ +15 (EtOH) (Na salt).
Ac: [1107-59-1]
$C_{29}H_{50}O_2$ 430.713
Cryst. (MeOH). Mp 96°. $[\alpha]_D$ +30 ($CHCl_3$).

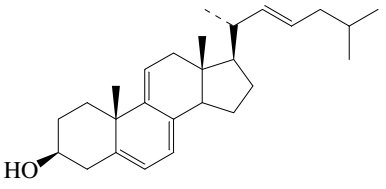
(3α,5β)-*form*
Epicoprostanol. *Epicoprosterol*
[516-92-7]
Found in ambergris and faecal material. Minor sterol from *Petrosia ficiformis*, prob. as an endobacterial metab.
Mp 107-108°. $[\alpha]_D$ +31 ($CHCl_3$).

(3β,5α)-*form*
Cholestanol. *Zymostanol*
[80-97-7]
[17608-41-2]
Occurs in human faeces, gallstones and eggs. Also found in adrenal tissue. Found in various marine organisms; sponges such as *Hymeniacidon perleve*, ascidians *Halocynthia papillosa*, *Microcosmus sulcatus* and *Microcosmus savignyi*, clam *Patinopecten yessoensis*, sea cucumbers such as *Cladolabes bifurcatus*, *Eupentacta fraudatrix*, *Bathyplotes natans*, *Holothuria nobilis*, *Holothuria scabra* , *Pseudostichopus trachus*, *Synapta maculata* and *Trochostoma orientale*. Leaflets (EtOH). Mp 142-143°. $[\alpha]_D^{22}$ +27.4 ($CHCl_3$).
3-O-*Sulfate:* [1491-96-9]
[72205-15-3 (K salt), 107584-99-6]
Occurs in marine organisms such as *Asterias rubens*, *Marthasterias glacialis*, *Porania pulvillus*, *Henricia sanguinolenta*, *Eupentacta fraudatrix* and many others.
Mp 174-175.5° (as Na salt). $[\alpha]_D^{29}$ +16.6 (EtOH) (Na salt).
3-O-*β*-*D*-*Xylopyranoside:* [72016-33-2]
$C_{32}H_{56}O_5$ 520.791
Constit. of *Eupentacta fraudatrix*.
Ac: [1255-88-5]
Prisms (MeOH/EtOAc). Mp 110-111°. $[\alpha]_D^{20}$ +11.5 ($CHCl_3$).
Me ether: 3-Methoxycholestane
[1981-90-4]
$C_{28}H_{50}O$ 402.702
Constit. of the sponge *Jereicopsis graphidiophora*. Mp 86-87°.

(3β,5β)-*form*
Coprostanol. *Coprosterol*. *Stercorin*
[360-68-9]
[17608-41-2]
Major sterol from faeces. Constit. of *Halocynthia papillosa*, *Petrosia ficiformis*, *Microcosmus savignyi* and *Styela plicata*. Used to monitor disposal of human excretion.
Mp 96-100°. $[\alpha]_D$ +26 ($CHCl_3$).
Ac: [4947-63-1]
Mp 89°.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1047D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 566C; 567A (*nmr*)
Ruzicka, L. *et al., Helv. Chim. Acta*, 1934, **17**, 1407-1416 (*Epicoprostanol, Coprostanol, synth*)
Barnett, J. *et al., J.C.S.*, 1940, 1390-1393 (*synth*)
Heath-Brown, B. *et al., J.C.S.*, 1940, 1482-1489 (*Zymostanol, synth*)
Org. Synth., Coll. Vol., 2, 1943, 191-193 (*Cholestanol, synth*)
Bergmann, W. *et al., J.O.C.*, 1945, **10**, 580-586 (*Cholestanol, synth*)
Lederer, E. *et al., Helv. Chim. Acta*, 1946, **29**, 1354-1365 (*occur*)
Lieberman, S. *et al., J.A.C.S.*, 1948, **70**, 1427-1432 (*Cholestanol and Epicholestanol sulfates, synth*)
Shoppee, C.W. *et al., J.C.S.*, 1950, 687-689 (*Epicoprostanol, Cholestanol, synth*)
Douglas, G.H. *et al., J.C.S.*, 1959, 1720-1723 (*Epicoprostanol, synth*)
Meittinen, T.A. *et al., Acta Chem. Scand.*, 1967, **21**, 286-290 (*Cholestanol, occur*)
Michnowicz, J. *et al., Org. Mass Spectrom.*, 1972, **6**, 765-783 (*ms*)
Erdman, T.R. *et al., Tetrahedron*, 1972, **28**, 5163-5173 (*3β,5α-form, isol*)
Ishige, M. *et al., Can. J. Chem.*, 1973, **51**, 3923-3926 (*Epicoprostanol, synth*)
Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*Cholestanol, isol, sponges, ms*)
Kobayashi, M. *et al., Steroids*, 1975, **26**, 605 (*isol, Patinopecten*)
Eggert, H. *et al., J.O.C.*, 1976, **41**, 71-78 (*cmr*)
Iida, T. *et al., J. Lipid Res.*, 1979, **20**, 279-284 (*pmr*)
Goodfellow, R.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **76**, 575-578 (*3β-sulfate, occur*)

Valente, C. *et al., J.O.C.*, 1984, **49**, 44-51 (*Epicholestanol, synth, bibl*)
Zollo, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **85**, 559-560 (*Cholestanol, Coprostanol, occur*)
Seidel, S.B. *et al., Steroids*, 1986, **47**, 49-62 (*Coprostanol, Epicoprostanol, isol, sponge*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*Me ether*)
Kanie, K. *et al., Bull. Chem. Soc. Jpn.*, 2000, **73**, 1875-1892 (*Me ether*)
Nakajima, N. *et al., Phytochemistry*, 2002, **60**, 275-279 (*biosynth*)
Lewis, R.J.*et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EBA100

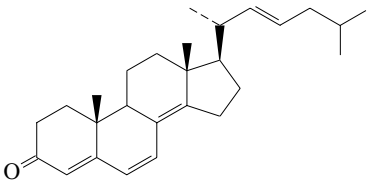
Cholesta-5,7,9(11),22-tetraen-3-ol C-545



$C_{27}H_{40}O$ 380.612

(3β,22*E*)-*form* [85733-70-6]
Constit. of the sponge *Axinella cannabina*.
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol, pmr, ms*)

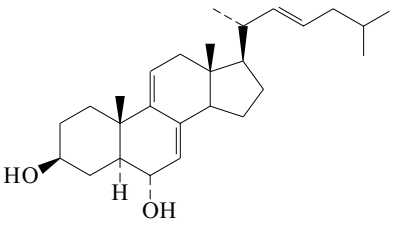
Cholesta-4,6,8(14),22-tetraen-3-one C-546



$C_{27}H_{38}O$ 378.597

(22*E*)-*form* [126149-90-4]
Constit. of *Dysidea herbacea* and *Dictyonella incisa*.
Oil. $[\alpha]_D^{25}$ +705 ($CHCl_3$).
Ciminiello, P. *et al., J. Nat. Prod.*, 1989, **52**, 1331 (*isol, pmr, cmr*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 72 (*isol, pmr*)

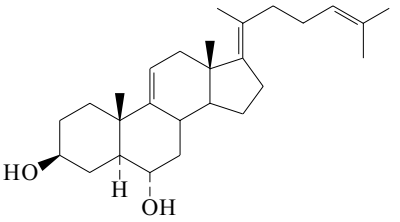
Cholesta-7,9(11),22-triene-3,6-diol C-547



$C_{27}H_{42}O_2$ 398.628

(3β,5α,6α,22*E*)-*form* [124596-60-7]
Constit. of *Spongionella gracilis*. Cryst. (MeOH/petrol). Mp 184-186°.
Madaio, A. *et al., J. Nat. Prod.*, 1989, **52**, 952-961 (*isol, pmr, ms*)

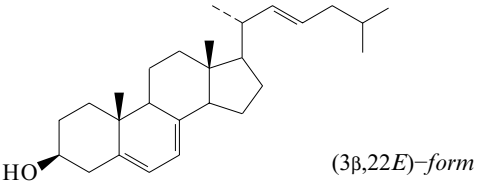
Cholesta-9(11),17(20),24-triene-3,6-diol C-548



$C_{27}H_{42}O_2$ 398.628

(3β,5α,6α)-*form* [37926-43-5]
Obt. by partial hydrolysis of saponin of the starfish *Asterias vulgaris* and *Acanthaster planci*. Needles (Me_2CO aq.). Mp 141-142°. $[\alpha]_D^{21}$ +43.2 ($CHCl_3$).
[89064-34-6, 89064-35-7]
Sheikh, Y.M. *et al., Tet. Lett.*, 1972, 3721-3724 (*synth, ir, pmr, ms*)
Findlay, J.A. *et al., J. Nat. Prod.*, 1983, **46**, 876-880 (*isol*)

Cholesta-5,7,22-trien-3-ol, 9CI C-549



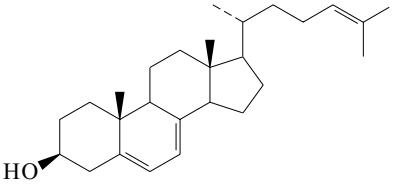
(3β,22*E*)–*form*

$C_{27}H_{42}O$ 382.628
Constit. of sponge, *Axinella cannabina* and other sponges.

(3β,22*E*)-*form* [22643-62-5]
Constit. of *Axinella cannabina* and other sponges. Also isol. from *Porphyridium cruentum*. Cryst. (MeOH). Mp 118-123°. $[\alpha]_D^{24}$ -118 (c, 1.2 in $CHCl_3$).
Ac: [22643-91-0]
$C_{29}H_{44}O_2$ 424.665
Cryst. (MeOH). Mp 144°. $[\alpha]_D^{24}$ -78 (c, 1.0 in $CHCl_3$).

(3β,22*Z*)-*form* [67920-53-0]
Cryst. (EtOH). Mp 148-151°. $[\alpha]_D^{24}$ -132 (c, 0.9 in $CHCl_3$).
Ac: [67920-54-1]
Mp 116-117°.
[19633-95-5, 26339-29-7]
Mallory, F.B. *et al., Tet. Lett.*, 1968, 6103 (*synth, uv, 3β,22E-form*)
Ahmad, M.S. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 936 (*synth*)
Garry, A.B. *et al., J.C.S. Perkin 1*, 1977, 809 (*synth*)
Bogoslovskii, N.A. *et al., Zh. Obshch. Khim.*, 1978, **48**, 908 (*synth, uv*)
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147 (*isol, pmr, 3β,22E-form*)
Sicinski, R.R. *et al., Bioorg. Chem.*, 1987, **15**, 152 (*synth, uv, pmr, ms*)

Cholesta-5,7,24-trien-3-ol, 9CI C-550



$C_{27}H_{42}O$ 382.628

3β-*form*

7,8-Didehydrodesmosterol

[1715-86-2]

Constit. of pig tissues. Isol. from various yeasts, e.g. *Saccharomyces cerevisiae* and *Candida guilliermondi* Isol. from sponges *Dysidea avara* and *Ircinia pipetta*. Needles (MeOH). Mp 104-107°. $[\alpha]_D$ -122 (c, 0.77 in $CHCl_3$).

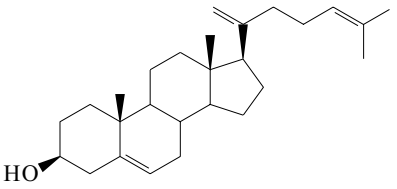
Ac: [17137-77-8]

$C_{29}H_{44}O_2$ 424.665

Cryst. (MeOH). Mp 78-81°.

Scallen, T.J. *et al., J. Lipid Res.*, 1968, **10**, 121-127 (*isol, synth*)
Barton, D.H. *et al., J.C.S. Perkin 1*, 1974, 1326-1333 (*isol*)
Moreau, J.P. *et al., J.O.C.*, 1974, **39**, 2018 (*synth, ir, pmr, ms*)
Yang, S.S. *et al., Steroids*, 1980, **35**, 329-334 (*synth, uv, ir, pmr, ms*)
Schönauer, K. *et al., Annalen*, 1983, 1031 (*synth, uv, pmr, ms*)
Andreev, A.V. *et al., Khim. Prir. Soedin.*, 1986, **22**, 196; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 182 (*isol*)
Sica, D. *et al., Comp. Biochem. Physiol.*, 1987, **88**, 293-296 (*isol, sponges*)

Cholesta-5,20,24-trien-3-ol, 9CI C-551



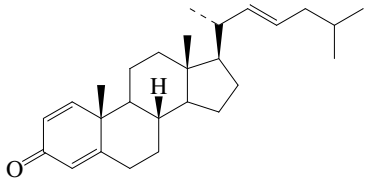
$C_{27}H_{42}O$ 382.628

3β-*form* [41083-97-0]

Constit. of roots of *Mandevilla pentlandiana* and the marine algae *Bryopteris pennata* and *Scinaia fascicularis*. Needles (MeOH aq.). Mp 88-91°. $[\alpha]_D^{21}$ -55.7 (c, 0.35 in $CHCl_3$).

Sheikh, Y.M. *et al., J.O.C.*, 1973, **38**, 3545-3553 (*synth, ms*)
Hayee-Memon, A. *et al., Pak. J. Pharm. Sci.*, 1991, **4**, 27-34 (*Scinaia fascicularis constit*)
Cabrera, G. *et al., Phytochemistry*, 1991, **30**, 1239-1243 (*Mandevilla pentlandiana constit*)
Siddiqui, S. *et al., Pak. J. Pharm. Sci.*, 1994, **7**, 73-82 (*Bryopsis pennata constit*)

Cholesta-1,4,22-trien-3-one C-552



$C_{27}H_{40}O$ 380.612

(22*E*)-*form*

Dendronesterone C

[771534-38-4]

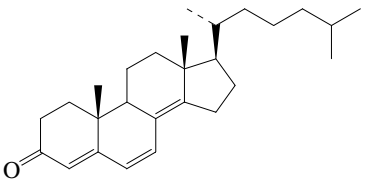
Constit. of *Dendronephthya gigantea*.

Solid. $[\alpha]_D^{25}$ +26 (c, 0.6 in $CHCl_3$). λ_{max} 245 (log ϵ 4.1) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2004, **67**, 1650-1653 (*isol, pmr, cmr*)

Cholesta-4,6,8(14)-trien-3-one C-553

[58028-23-2]

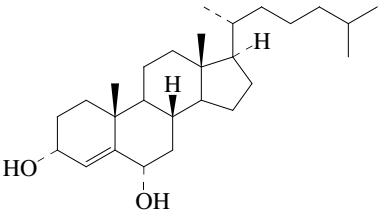


$C_{27}H_{40}O$ 380.612

Constit. of the sponge *Dysidea herbacea*. Prisms (hexane). Mp 61-63°. $[\alpha]_D^{20}$ +647 (c, 1.23 in $CHCl_3$).

Emke, A. *et al., J.C.S. Perkin 1*, 1977, 820-822 (*synth*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 72-74 (*isol, pmr, cmr*)
Boehme, R.M. *et al., Steroids*, 1994, **59**, 265-269 (*synth*)

Cholest-4-ene-3,6-diol, 9CI C-554



(3α,6α)-*form*

$C_{27}H_{46}O_2$ 402.659

(3α,6α)-*form* [65082-85-1]

Cryst. (Et_2O). Mp 189-191°. $[\alpha]_D^{20}$ +70 (c, 1.2 in $CHCl_3$).

Di-Ac:

$C_{31}H_{50}O_4$ 486.734

Prisms (MeOH). Mp 108-109°. $[\alpha]_D$ +158 (c, 1.03 in $CHCl_3$).

(3α,6β)-*form* [66175-88-0]

Constit. of red alga *Acanthophora spicifera*.

Cryst.

Mp 248°.

Di-Ac: [2572-52-3]

Cryst. (MeOH aq.). Mp 102-102.5°. $[\alpha]_D$ +136 (c, 0.55 in $CHCl_3$).

(3β,6α)-*form* [15013-60-2]

Needles (MeOH). Mp 184-186°.

3-Ac: [65082-82-8]

$C_{29}H_{48}O_3$ 444.696

Amorph. $[\alpha]_D^{20}$ +7 (c, 1.3 in $CHCl_3$).

Di-Ac:

Cryst. (pentane). Mp 166-167°. $[\alpha]_D$ +26 (c, 1.0 in $CHCl_3$).

3-Me ether: 3-Methoxycholest-4-en-6-ol

[85198-21-6]

$C_{28}H_{48}O_2$ 416.686

Cryst. (Et_2O/hexane). Mp 123-124°. $[\alpha]_D$ +0.3 (EtOH).

Di-Me ether: 3,6-Dimethoxycholest-4-ene

[14211-20-2]

$C_{29}H_{50}O_2$ 430.713

Cryst. (MeOH). Mp 106°. $[\alpha]_D$ +11 (c, 0.32 in MeOH).

(3β,6β)-*form* [570-88-7]

Needles (petrol). Mp 257-258°. $[\alpha]_D^{20}$ +9 (c, 0.6 in $CHCl_3$).

3-Ac: [50391-72-5]

Mp 119°. $[\alpha]_D$ -20 (c, 1.00 in $CHCl_3$).

Di-Ac: [2572-51-2]

Cryst. (MeOH). Mp 133-133.5°. $[\alpha]_D$ -13.5 (c, 2.07 in $CHCl_3$).

3-Me ether: [2701-10-2]

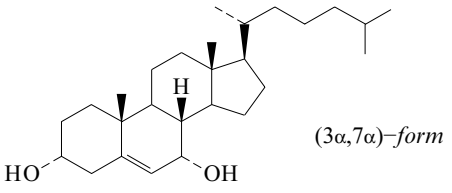
Cryst. (MeOH). Mp 145-147°. $[\alpha]_D$ +21 (c, 0.44 in $CHCl_3$).

6-Me ether: 6-Methoxycholest-4-en-3-ol
[13327-77-0]
$C_{28}H_{48}O_2$ 416.686
Cryst. (MeOH). Mp 104-105° and 141-142° (double Mp). $[\alpha]_D$ +36.

Di-Me ether: [13327-79-2]
Needles (MeOH). Mp 138-139°. $[\alpha]_D$ +40 (c, 0.77 in $CHCl_3$).

Rosenheim, O. *et al., J.C.S.*, 1943, 135; 1947, 377
Pelc, B. *et al., Coll. Czech. Chem. Comm.*, 1952, **22**, 1457
Snatzke, G. *et al., Annalen*, 1964, **676**, 188 (*synth, 3β,6β-form*)
Collins, D.G. *et al., Aust. J. Chem.*, 1964, **17**, 677 (*synth, 3β,6β-form*)
Julia, S. *et al., Bull. Soc. Chim. Fr.*, 1966, 2277 (*synth, 3β,6α-form*)
Kulig, M.J. *et al., J.O.C.*, 1973, **38**, 3639 (*synth, ir*)
Kasal, A. *et al., Coll. Czech. Chem. Comm.*, 1974, **39**, 603 (*synth, 3β,6β-form*)
Kočovský, P. *et al., Coll. Czech. Chem. Comm.*, 1977, **42**, 2415 (*synth, pmr*)
Schwartz, A. *et al., J.C.S. Perkin 1*, 1977, 2470 (*synth, 3α,6β-form*)
Aringer, L. *et al., Biomed. Mass Spectrom.*, 1981, **8**, 183 (*ms*)
Fischli, A. *et al., Helv. Chim. Acta*, 1982, **65**, 2697 (*synth, ir, pmr, ms, 3α,6α-form*)
Holland, H.L. *et al., Can. J. Chem.*, 1983, **61**, 2165 (*synth, cmr*)
Wahidulla, S. *et al., Phytochemistry*, 1998, **48**, 1203-1206 (*isol, pmr, cmr*)
Zhao, K. *et al., Synth. Commun.*, 2001, **31**, 2619-2624 (*3α,6α-form, 3α,6β-form, synth, pmr, cmr*)

Cholest-5-ene-3,7-diol, 9CI C-555



(3α,7α)–*form*

$C_{27}H_{46}O_2$ 402.659

(3α,7α)-*form* [75686-38-3]
Cryst. (MeOH). Mp 174°. $[\alpha]_D$ +9 ($CHCl_3$).

Di-Ac: [98620-80-5]
$C_{31}H_{50}O_4$ 486.734
$[\alpha]_D$ +9 ($CHCl_3$).

(3α,7β)-*form* [75686-39-4]
Needles (MeOH). Mp 172-176°. $[\alpha]_D$ +38 ($CHCl_3$). $[\alpha]_D^{20}$ -2 (c, 2.8 in $CHCl_3$).

3-Ac: [98674-04-5]
$C_{29}H_{48}O_3$ 444.696
$[\alpha]_D^{20}$ +10 (c, 2.6 in $CHCl_3$).

Di-Ac: [98620-79-2]
$[\alpha]_D^{20}$ +24 (c, 2.8 in $CHCl_3$).

(3β,7α)-*form*
7α-Hydroxycholesterol
[566-26-7]
Constit. of *Cliona copiosa*.
Cryst. (MeOH).
Mp 188-189°. $[\alpha]_D$ -91 (c, 0.9 in $CHCl_3$).

3-Ac: [19317-90-9]
Mp 139-140°.

Di-Ac: [17974-76-4]
Cryst. (Me_2CO). Mp 122-123°. $[\alpha]_D$ -175 (c, 0.16 in $CHCl_3$).

3-Me ether: 3-Methoxycholest-5-en-7-ol
$C_{28}H_{48}O_2$ 416.686
Cryst. (Et_2O). Mp 158-160°. $[\alpha]_D$ -126 (c, 1.2 in $CHCl_3$).

(3β,7β)-*form*
7β-Hydroxycholesterol
[566-27-8]
Constit. of *Cliona copiosa*. Found in the thymus glands of humans, sheep, cattle and trout. Proliferation inhibitor. Cryst. (Me_2CO). Mp 172-176° Mp 180-181° (double Mp). $[\alpha]_D$ +3.3 ($CHCl_3$).

3-Ac: [17974-77-5]
Cryst. (Et_2O). Mp 108-112°. $[\alpha]_D$ -12 (c, 1.2 in $CHCl_3$).

7-Ac: [17974-78-6]
$C_{29}H_{48}O_3$ 444.696
Cryst. (MeOH aq.). Mp 131-132°. $[\alpha]_D$ +76 (c, 0.9 in $CHCl_3$).

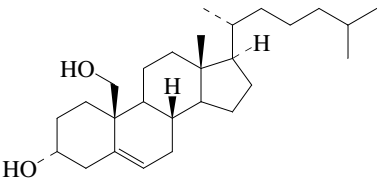
Di-Ac: [18099-24-6]
Cryst. (MeOH). Mp 108-112°. $[\alpha]_D$ +55 (c, 1.7 in $CHCl_3$).

5β,6β-Epoxide: ***5,6-Epoxycholestane-3,7-diol***
[62073-79-4]
$C_{27}H_{46}O_3$ 418.659
Constit. of *Plexaurella grisea*.

[16840-37-2]

Wintersteiner, O. *et al., J.A.C.S.*, 1942, **64**, 2453 (*synth*)
Nickon, A. *et al., J.A.C.S.*, 1965, **87**, 3921 (*synth*)
Shoppee, C.W. *et al., J.C.S.(C)*, 1968, 981 (*synth, ir*)
Teng, J.I. *et al., J.O.C.*, 1973, **38**, 119 (*synth, ir, pmr, ms*)
Cunningham, I.M. *et al., J.C.S. Perkin 1*, 1974, 2458 (*synth, ir, pmr*)
Kawata, M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 3109-3113 (*epoxide, synth*)
Smith, L.L. *et al., J.A.C.S.*, 1978, **100**, 6206 (*synth*)
Lin, Y.Y. *et al., Lipids*, 1980, **15**, 756 (*ms*)
Cosme, F.G. *et al., J.C.S. Perkin 1*, 1983, 2325
Stary, I. *et al., Coll. Czech. Chem. Comm.*, 1985, **50**, 1227 (*synth, pmr, 3α,7β-form*)
Akihisa, T. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 680 (*synth, pmr*)
Notaro, G. *et al., J. Nat. Prod.*, 1992, **55**, 1588 (*isol, pmr, ms*)
Reisch, J. *et al., Pharmazie*, 1994, **49**, 75 (*isol*)
Rueda, A. *et al., Steroids*, 2001, **66**, 897-904 (*epoxide, isol*)

Cholest-5-ene-3,19-diol, 9CI C-556



(3α)-*form*

$C_{27}H_{46}O_2$ 402.659

3α-*form* [14908-15-7]
Mp 163-164°. $[\alpha]_D^{27}$ -75 (c, 0.60 in $CHCl_3$).

3-Ac: [15077-32-4]
$C_{29}H_{48}O_3$ 444.696
Cryst. (MeOH aq.). Mp 98-99°. $[\alpha]_D^{27}$ -8 (c, 1.22 in $CHCl_3$).

Di-Ac: [14908-16-8]
$C_{31}H_{50}O_4$ 486.734
Cryst. (MeOH). Mp 76-77° (68.5°). $[\alpha]_D^{27}$ -81 (c, 0.87 in $CHCl_3$).

3β-*form*
19-Hydroxycholesterol
[561-63-7]
Cryst. (CH_2Cl_2/MeOH). Mp 162-164° (153-155°). $[\alpha]_D$ -27 (c, 0.960 in $CHCl_3$).

3-(4-O-Acetyl-β-D-arabinopyranoside): [848392-51-8]
$C_{34}H_{56}O_7$ 576.812
Constit. of *Junceella juncea*. Powder.

3-Ac: [750-59-4]
Cryst. (Me_2CO). Mp 120-121°. $[\alpha]_D$ -32 (c, 1.045 in $CHCl_3$).

19-Ac: [73532-71-5]
$C_{29}H_{48}O_3$ 444.696
Cryst. (Me_2CO). Mp 103.5-104.5°.

Di-Ac: [21072-68-4]
Mp 69-70°. $[\alpha]_D^{20}$ -71 (EtOH).

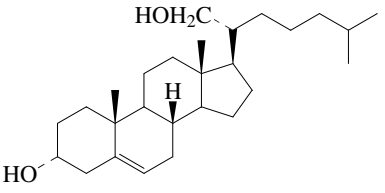
3-Me ether: 3-Methoxycholest-5-en-19-ol
[21072-63-9]
$C_{28}H_{48}O_2$ 416.686
Cryst. (Me_2CO). Mp 171-172°.

19-Me ether: 19-Methoxycholest-5-en-3-ol
[1106-13-4]
Cryst. (Me_2CO). Mp 144-146°. $[\alpha]_D^{20}$ -40 (c, 1.9 in $CHCl_3$).

Kalvoda, J. *et al., Helv. Chim. Acta*, 1963, **46**, 1361 (*synth, ir, 3β-form*)
Moriarty, R.M. *et al., Tetrahedron*, 1965, **21**, 547 (*synth, 3β-form*)

Tanabe, K. *et al., Chem. Pharm. Bull.*, 1967, **15**, 15 (*synth, 3β-form*)
Watanabe, Y. *et al., J.O.C.*, 1968, **33**, 468 (*synth, ir, 3α-form*)
Kirkien-Konasiewicz, A.M. *et al., Org. Mass Spectrom.*, 1968, **1**, 567 (*ms, 3β-form*)
Lin, Y.Y. *et al., Lipids*, 1980, **15**, 756 (*ms, 3β-form*)
Fajkoš, J. *et al., Coll. Czech. Chem. Comm.*, 1982, **47**, 144 (*synth, 3α-form*)
Qi, S.-H. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1476-1478 (*isol, pmr, cmr*)

Cholest-5-ene-3,21-diol, 9CI C-557



(3α,20*R*)-*form*

$C_{27}H_{46}O_2$ 402.659

3α-*form*

Disulfate: [292833-54-6]
$C_{27}H_{46}O_8S_2$ 562.788
Constit. of *Ophiopholis aculeata*, *Ophiarachna incrassata*, *Gorgonocephalus chilensis*, *Ophioderma longicaudum*, *Ophiolepis superba*, *Ophionotus victoriae*, *Ophiothrix fragilis*, *Ophiura sarsi*, *Ophiura texturata*, *Ophiozona impressa* and *Stegophiura brachiactis*. Protein-tyrosine kinase inhibitor. Cryst. (MeOH).
Mp 176-178°. $[\alpha]_D^{20}$ -11 (c, 0.1 in EtOH).

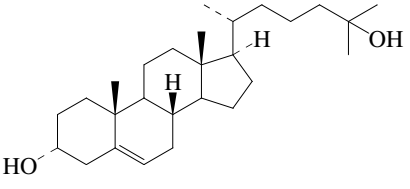
3β-*form*

21-Hydroxycholesterol
[63216-21-7]
Constit. of *Euretaster insignis*. Cryst. (Et_2O). Mp 157-161°.

(3β,20*S*)-*form* [63268-03-1]
Mp 147-149°.

Byon, C.Y. *et al., J.O.C.*, 1977, **42**, 3619 (*synth, pmr*)
Wicha, J. *et al., J.C.S. Perkin 1*, 1978, 1282 (*synth, ir, pmr*)
Lin, Y.Y. *et al., Lipids*, 1980, **15**, 756 (*ms*)
D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1984, 2277-2282 (*Euretaster, isol*)
Riccio, R. *et al., Tetrahedron*, 1985, **41**, 6041-6046 (*disulfate, isol*)
D'Auria, M.V. *et al., J.O.C.*, 1989, **54**, 234-239 (*isol, pmr, cmr*)
Fu, X. *et al., J. Nat. Prod.*, 1994, **57**, 1591-1594 (*disulfate*)
Fedarov, S.N. *et al., J. Nat. Prod.*, 1994, **57**, 1631-1637 (*disulfate, isol, cmr*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1995, **58**, 189-196 (*disulfate, occur*)
Shubina, L.K. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **119**, 505-511 (*occur, rev*)
Maeir, M.S. *et al., Molecules*, 2000, **5**, 348-349; *CA*, **133**, 235391g (*disulfate*)

Cholest-5-ene-3,25-diol, 9CI C-558



3α-*form*

$C_{27}H_{46}O_2$ 402.659
Isol. from sponge *Damiriana hawaiiana*.

3α-*form*

Cryst. (MeOH). Mp 156-157°. $[\alpha]_D^{28}$ -41.5 ($CHCl_3$).

3-Ac: [67371-50-0]
$C_{29}H_{48}O_3$ 444.696
Oil.

3β-*form*

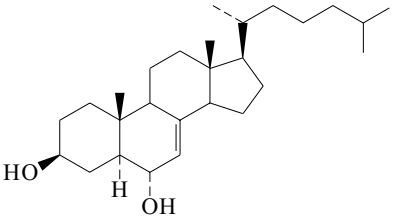
25-Hydroxycholesterol
[2140-46-7]
Needles (MeOH). Mp 179-181°. $[\alpha]_D^{25}$ -39 (c, 1.05 in $CHCl_3$).

3-Ac: [10525-22-1]
Cryst. (Me_2CO). Mp 139-140°. $[\alpha]_D^{25}$ -41.4 (c, 1.05 in $CHCl_3$).

Di-Ac: [59975-17-6]
$C_{31}H_{50}O_4$ 486.734
Plates (MeOH). Mp 119-120°.

Campbell, J.A. *et al., Steroids*, 1969, **13**, 567 (*synth, pmr, 3β-form*)
van Lier, J.E. *et al., J.O.C.*, 1970, **35**, 3627 (*synth, ir, pmr, 3β-form*)
Narwid, T.A. *et al., Helv. Chim. Acta*, 1974, **57**, 771 (*synth, ir, pmr*)
Ochi, K. *et al., Steroids*, 1977, **30**, 795 (*synth, pmr, ms, 3α-form*)
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1479 (*isol, Damiriana hawaiiana constit*)
Wicha, J. *et al., J.C.S. Perkin 1*, 1978, 1282 (*synth, ir, pmr, ms 3β-form*)
Ochi, K. *et al., Chem. Pharm. Bull.*, 1979, **27**, 252 (*synth, 3β-form*)

Cholest-7-ene-3,6-diol, 9CI C-559



$C_{27}H_{46}O_2$ 402.659

(3β,5α,6α)-*form* [2259-91-8]
Constit. of *Spongionella gracilis*. Cryst. (MeOH). Mp 194-195°. $[\alpha]_D$ +47 (c, 1 in $CHCl_3$).

Di-Me ether: 3β,6α-Dimethoxy-5α-cholest-7-ene
$C_{29}H_{50}O_2$ 430.713
Cryst. (MeOH). Mp 70-71°.

3-Ac: [17181-88-3]
$C_{29}H_{48}O_3$ 444.696
Needles (MeOH). Mp 156-157° (143-145°).

6-Ac: [53296-84-7]
$C_{29}H_{48}O_3$ 444.696
Needles (Et_2O). Mp 122-123°.

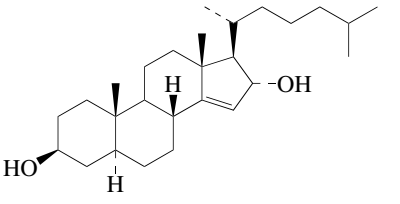
Di-Ac: [53296-83-6]
$C_{31}H_{50}O_4$ 486.734
Plates (MeOH). Mp 116-119°.

(3β,5α,6β)-*form* [2259-90-7]
Cryst. (MeOH). Mp 214-215°. $[\alpha]_D$ -34 (MeOH).

Di-Ac: [76026-11-4]
Mp 138-141°. $[\alpha]_D$ -79 (c, 1 in $CHCl_3$).

Aberhart, D.J. *et al., Phytochemistry*, 1973, **12**, 1065 (*synth, ir, pmr, ms, 3β,5α,6α-form*)
Galbraith, M.N. *et al., Aust. J. Chem.*, 1974, **27**, 1087 (*synth, 3β,5α,6α-form*)
Kulig, M.J. *et al., J.O.C.*, 1974, **39**, 3398 (*synth*)
de Simone, F. *et al., J.C.S. Perkin 1*, 1981, 1855 (*synth, pmr, cmr, ms*)
Piccialli, V. *et al., J. Nat. Prod.*, 1988, **49**, 779 (*isol*)

Cholest-14-ene-3,16-diol C-560

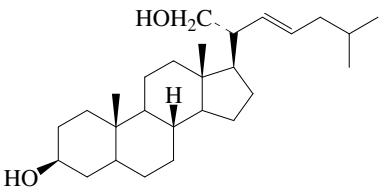


$C_{27}H_{46}O_2$ 402.659

(3β,5α,16α)-*form* [139953-32-5]
Constit. of *Topsentia aurantiaca*.

Ciminiello, P. *et al., Steroids*, 1992, **57**, 62-66 (*isol, pmr, cmr*)

Cholest-22-ene-3,21-diol C-561



$C_{27}H_{46}O_2$ 402.659

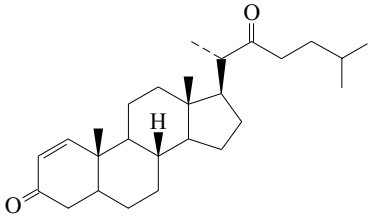
(3β,5α,22E)-form [95062-38-7]
Constit. of *Euretaster insignis.*

Disulfate: [95062-40-1]
$C_{27}H_{46}O_8S_2$ 562.788
Constit. of *Euretaster insignis.*

D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1984, 2277-2282 (*isol, pmr, ms*)

Cholest-1-ene-3,22-dione C-562

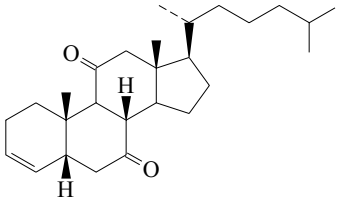
[161776-76-7]
[813436-42-9]



$C_{27}H_{42}O_2$ 398.628
Constit. of *Alcyonium gracillimum*, *Lemnalia cervicorni* and a *Scleronephthya* sp. Solid.
Mp 55-57°. $[\alpha]_D$ +22.4 (c, 0.5 in $CHCl_3$).

Seo, Y. *et al., Tetrahedron*, 1995, **51**, 2497-2506 (*Alcyonium gracillimum constit*)
Duh, C.-Y. *et al., J. Nat. Prod.*, 2004, **67**, 1650-1653 (*Lemnalia cervicorni constit*)
Yan, X.-H. *et al., Youji Huaxue*, 2004, **24**, 1233-1238; *CA*, **142**, 71702 (*isol, pmr*)

Cholest-3-ene-7,11-dione C-563

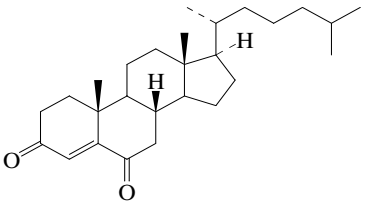


$C_{27}H_{42}O_2$ 398.628

5β-form
Hypneadione
[126394-74-9]
Constit. of *Hypnea musciformis.*
Cryst. $[\alpha]_D$ -20.5 (c, 5.03 in $CHCl_3$). λ_{max} 213 ($CHCl_3$).
Babu, J.M. *et al., Phytochemistry*, 1989, **28**, 3237-3239 (*isol, pmr, cmr*)

Cholest-4-ene-3,6-dione, 9CI C-564

[984-84-9]



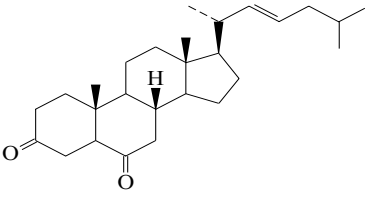
$C_{27}H_{42}O_2$ 398.628
Can be prepared semisynthetically from cholesterol by incubating with a spp. of Mycobacterium. Isol. from the sponges *Cinachyra tarentina* and *Geodia cydonium*. Cryst. (MeOH).
Mp 132-134° (122-123°). $[\alpha]_D^{22}$ -41 ($CHCl_3$).

3-Oxime (E-): ***Astralienone A***
[63635-43-8]
[67814500 E-f-or-m]
$C_{27}H_{43}NO_2$ 413.642
Constit. of *Cinachyrella australiensis.* Cryst. (C_6H_6/petrol).
Mp 221-223° Mp 137-138°. λ_{max} 279 ($CDCl_3$).

6-Oxime (E-): ***6-Hydroximinocholest-4-en-3-one***
[188968-44-7]
$C_{27}H_{43}NO_2$ 413.642
Constit. of a *Cinachyrella* sponge.
$[\alpha]_D$ +136. λ_{max} 271 (no solvent reported).

Org. Synth., Coll. Vol., 4, 1963, 189
Jones, J.G.L. *et al., J.C.S.(C)*, 1968, 2698 (*synth, uv, ir, pmr*)
Boswell, G.A. *et al., J.O.C.*, 1968, **33**, 3699 (*synth, uv, ir*)
Kulig, M.J. *et al., J.O.C.*, 1973, **38**, 3639 (*synth, uv, ir*)
Ishige, M. *et al., Can. J. Chem.*, 1976, **54**, 2581 (*synth*)
Oka, K. *et al., J.O.C.*, 1978, **43**, 3790-3791 (*oximes, synth*)
Holland, H.L. *et al., Tet. Lett.*, 1981, **22**, 5127 (*synth*)
D'Auria, M. *et al., Synthesis*, 1985, 988 (*synth*)
Tischler, M. *et al., Can. J. Chem.*, 1988, **66**, 1173 (*synth, ir, pmr, cmr*)
Migliuolo, A. *et al., J. Nat. Prod.*, 1990, **53**, 1262-1266; 1991, **54**, 371 (*isol, pmr, cmr, ms*)
Aiello, A. *et al., J. Nat. Prod.*, 1991, **54**, 281 (*isol, pmr, cmr*)
Hector, M. *et al., Synth. Commun.*, 1996, **26**, 1075 (*synth, uv, pmr*)
Rodriguez, J. *et al., Tet. Lett.*, 1997, **38**, 1833-1836 (*6-oxime*)
Xiao, D.-J. *et al., Youji Huaxue*, 2005, **25**, 1606-1609 (*3-oxime*)

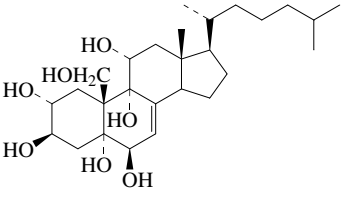
Cholest-22-ene-3,6-dione C-565



$C_{27}H_{42}O_2$ 398.628

22E-form [166038-28-4]
Constit. of *Hypnea musciformis.* Cryst.
Gosavi, K. *et al., Chem. Lett.*, 1995, 519 (*cryst struct*)

Cholest-7-ene-2,3,5,6,9,11,19-heptol C-566



(2α,3β,5α,6β,11α)-*form*

$C_{27}H_{46}O_7$ 482.656

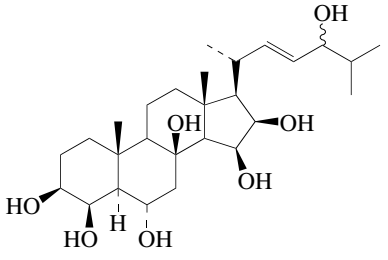
(2α,3β,5α,6β,11α)-*form* [114395-62-9]
Isol. from *Dysidea etheria*. Cryst. Mp 240-260° dec. $[\alpha]_D^{25}$ -24.2 (c, 1.2 in EtOH).

11-Ac: [114395-67-4]
$C_{29}H_{48}O_8$ 524.693
Isol. from *Dysidea etheria*. Cryst. Mp 211-220°. $[\alpha]_D^{25}$ -40.9 (c, 1.1 in EtOH).

11,19-Di-Ac: [114395-61-8]
$C_{31}H_{50}O_9$ 566.731
Isol. from *Dysidea etheria*. Cryst. Mp 164°. $[\alpha]_D^{25}$ -51.1 (c, 3.7 in EtOH).

(2β,3α,5β,6α,11α)-*form* [120711-48-0]
Isol. from sponge *Dysidea etheria*. Mp 230-250° dec. $[\alpha]_D^{25}$ +23.1 (c, 0.78 in EtOH).
West, R.R. *et al., J.O.C.*, 1988, **53**, 2782-2787; 1989, **54**, 3234-3236

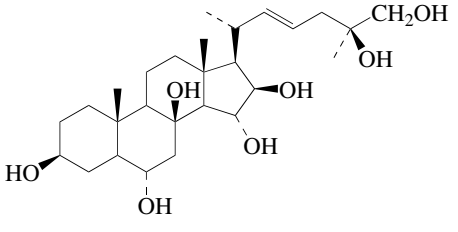
Cholest-22-ene-3,4,6,8,15,16,24-heptol C-567



$C_{27}H_{46}O_7$ 482.656

(3β,4β,5α,6α,15β,16β,22*E*,24ξ)-*form*
3-Sulfate: [105404-80-6]
$C_{27}H_{46}O_{10}S$ 562.72
Constit. of *Coscinasterias tenuispina*. Isol. as Na salt to which CAS number refers.
Riccio, R. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 869-893 (*isol, pmr, cmr, ms*)

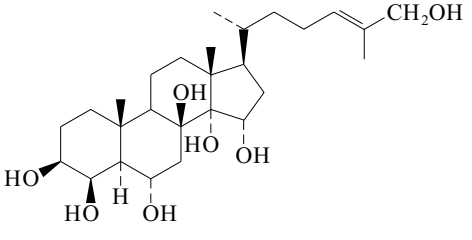
Cholest-22-ene-3,6,8,15,16,25,26-heptol C-568



$C_{27}H_{46}O_7$ 482.656

(3β,5α,6α,8β,15α,16β,22*E*,25*S*)-*form* [181034-97-9]
Constit. of an Antarctic starfish (Echinasteridae). $[\alpha]_D$ +4 (MeOH).
Iorizzi, M. *et al., Tetrahedron*, 1996, **52**, 10997-11012 (*isol, pmr, cmr*)

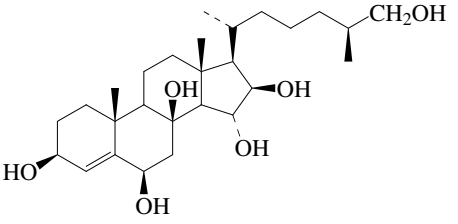
Cholest-24-ene-3,4,6,8,14,15,26-heptol, 9CI C-569



$C_{27}H_{46}O_7$ 482.656

(3β,4β,5α,6α,15α,24*E*)-*form* [102988-69-2]
15-Sulfate: [103021-33-6]
$C_{27}H_{46}O_{10}S$ 562.72
Constit. of *Archaster typicus*.
15-Sulfate, Na salt: $[\alpha]_D$ +43.6 (c, 1 in MeOH).
Riccio, R. *et al., J.C.S. Perkin 1*, 1986, 665-670 (*15-sulfate*)

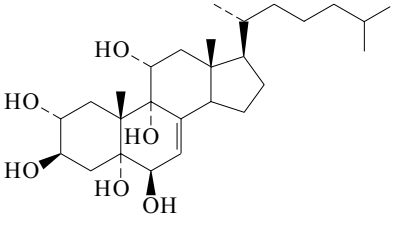
Cholest-4-ene-3,6,8,15,16,26-hexol C-570



$C_{27}H_{46}O_6$ 466.657

(3β,6β,15α,16β,25*S*)-*form*
3-O-*(2*-O-*Methyl-β-D-xylopyranoside)*: ***Echinasteroside C***
[156398-63-9]
$C_{33}H_{56}O_{10}$ 612.799
Isol. from *Echinaster brasiliensis*. $[\alpha]_D$ -16.6.
Iorizzi, M. *et al., J. Nat. Prod.*, 1993, **56**, 2149-2162

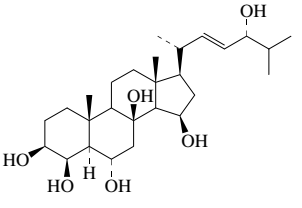
Cholest-7-ene-2,3,5,6,9,11-hexol C-571



$C_{27}H_{46}O_6$ 466.657

(2α,3β,5α,6β,9α,11α)-*form* [142780-47-0]
Constit. of *Dysidea fragilis*.
11-Ac: [142780-48-1]
$C_{29}H_{48}O_7$ 508.694
Constit. of *Dysidea fragilis*.
Milkova, T.S. *et al., J. Nat. Prod.*, 1992, **55**, 974 (*isol, pmr, cmr*)

Cholest-22-ene-3,4,6,8,15,24-hexol C-572



(3β,4β,5α,6α,8β,15β,22*E*,24*R*)-*form*

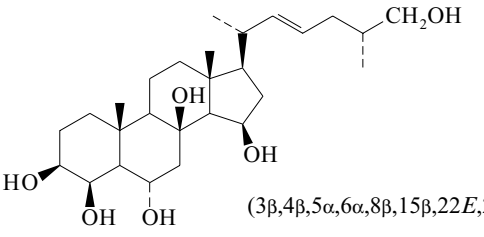
$C_{27}H_{46}O_6$ 466.657

(3β,4β,5α,6α,8β,15β,22*E*,24*R*)-*form* [181034-98-0]
Constit. of an Antarctic starfish (Echinasteridae) and *Acodontaster conspicuus*. $[\alpha]_D$ -10 (MeOH). $[\alpha]_D$ +4.2 (c, 1 in MeOH).
24-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside]*: ***22-Dehydrohalityloside D***
[112058-08-9]
$C_{39}H_{66}O_{14}$ 758.942
Constit. of *Sphaerodiscus placenta*.

(3β,4β,5α,6β,8β,15α,22*E*,24*R*)-*form*

3-O-*[2,4-Di*-O-*methyl-β-D-xylopyranoside]:* ***Laeviuscoloside H***
[129393-26-6]
$C_{34}H_{58}O_{10}$ 626.826
Constit. of *Henricia laeviuscola*.
Zollo, F. *et al., J. Nat. Prod.*, 1987, **50**, 794-799 (*22-Dehydrohalityloside D*)
D'Auria, M.V. *et al., Gazz. Chim. Ital.*, 1990, **120**, 155-163 (*Laeviuscoloside H*)
Iorizzi, M. *et al., Tetrahedron*, 1996, **52**, 10997-11012 (*Antarctic starfish constit*)
De Marino, S. *et al., J. Nat. Prod.*, 1997, **60**, 959-966 (*Acodontaster conspicuus constit*)

Cholest-22-ene-3,4,6,8,15,26-hexol C-573



(3β,4β,5α,6α,8β,15β,22*E*,25*R*)–*form*

$C_{27}H_{46}O_6$ 466.657

(3β,4β,5α,6α,8β,15β,22*E*,25*R*)-*form*

26-O-*α-L-Arabinofuranoside:* ***Antarcticoside H***
[181034-78-6]
$C_{32}H_{54}O_{10}$ 598.773
Constit. of an Antarctic starfish. $[\alpha]_D$ -28 (MeOH).

26-O-*(3*-O-*Methyl-β-D-xylopyranoside):* ***Antarcticoside E***
[181034-75-3]
$C_{33}H_{56}O_{10}$ 612.799
Constit. of an Antarctic starfish (Echinasteridae). $[\alpha]_D$ -8.6 (MeOH).

26-O-*β-D-Galactofuranoside:* ***Antarcticoside I***
[181034-79-7]
$C_{33}H_{56}O_{11}$ 628.799
Constit. of an Antarctic starfish. $[\alpha]_D$ -26.1 (MeOH).

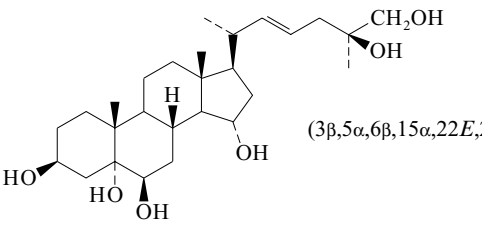
26-O-*[β-D-Xylopyranosyl-(1→2)-α-L-arabinofuranoside]:* ***Antarcticoside G***
[181034-77-5]
$C_{37}H_{62}O_{14}$ 730.888
Constit. of an Antarctic starfish. $[\alpha]_D$ -21.8 (MeOH).

(3β,4β,5α,6α,8β,15β,22*E*,25*S*)-*form*

26-O-*(3*-O-*Methyl-β-D-xylopyranoside):* ***Antarcticoside D***
[181034-26-4]
$C_{33}H_{56}O_{10}$ 612.799
Constit. of an Antarctic starfish. $[\alpha]_D$ -12 (MeOH).

26-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside]:* ***Antarcticoside F***
[181034-76-4]
$C_{39}H_{66}O_{14}$ 758.942
Constit. of an Antarctic starfish. $[\alpha]_D$ -26 (MeOH).
Iorizzi, M. *et al., Tetrahedron*, 1996, **52**, 10997-11012 (*isol, pmr, cmr*)

Cholest-22-ene-3,5,6,15,25,26-hexol C-574



(3β,5α,6β,15α,22*E*,25*S*)–*form*

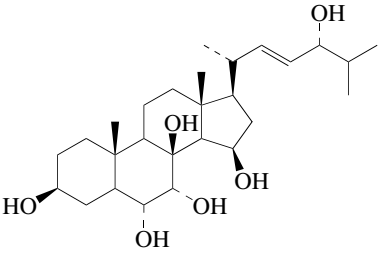
$C_{27}H_{46}O_6$ 466.657

(3β,5α,6β,15α,22*E*,25*S*)-*form* [160538-69-2]

26-Sulfate: [160538-77-2]
$C_{27}H_{46}O_9S$ 546.721
Constit. of *Styracaster caroli*.
$[\alpha]_D$ +5.2 (MeOH).

(3β,5α,6β,15β,22*E*,25*S*)-*form*
Constit. of *Styracaster caroli*.
$[\alpha]_D$ -14.6 (MeOH).
Iorizzi, M. *et al., J. Nat. Prod.*, 1994, **57**, 1361 (*isol, pmr, cmr*)

Cholest-22-ene-3,6,7,8,15,24-hexol C-575

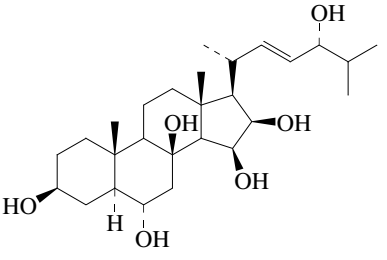


$C_{27}H_{46}O_6$ 466.657

(3β,5α,6α,7α,8β,15β,22*E*,24*R*)-*form*

3,24-Di-O-*β-D-xylopyranoside, 15-sulfate:* ***Asteriidoside I***
[214976-64-4]
$C_{37}H_{62}O_{17}S$ 810.953
Constit. of a starfish (Asteriidae).
$[\alpha]_D$ -8.8 (c, 1 in MeOH).
De Marino, S. *et al., J. Nat. Prod.*, 1998, **61**, 1319-1327 (*isol, pmr, cmr*)

Cholest-22-ene-3,6,8,15,16,24-hexol C-576

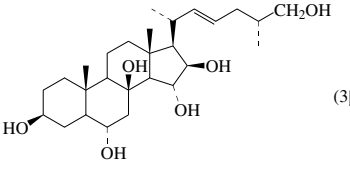


$C_{27}H_{46}O_6$ 466.657

(3β,5α,6α,15β,16β,22*E*,24*R*)-*form*

24-O-*β-D-Xylopyranoside, 3-sulfate:* ***Distolasteroside D5***
[154073-57-1]
$C_{32}H_{54}O_{13}S$ 678.837
Constit. of *Distolasterias nipon*.
Iorizzi, M. *et al., J. Nat. Prod.*, 1993, **56**, 1786-1798 (*Distolasteroside D5*)

Cholest-22-ene-3,6,8,15,16,26-hexol C-577



(3β,5α,6α,15α,16β,22*E*,25*R*)-*form*

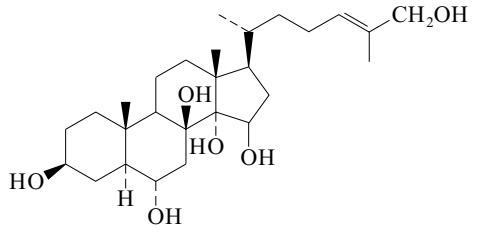
$C_{27}H_{46}O_6$ 466.657

(3β,5α,6α,15α,16β,22*E*,25*R*)-*form* [181034-96-8]
Constit. of an Antarctic starfish (Echinasteridae).
$[\alpha]_D$ +12 (MeOH).

(3β,5α,6α,15α,16β,22*E*,25*S*)-*form* [181034-95-7]
Constit. of an Antarctic starfish (Echinasteridae).
$[\alpha]_D$ +16 (MeOH).

(3β,5α,6α,15β,16β,22*E*,25*S*)-*form*
Constit. of *Dermasterias imbricata*.
3,26-Di-O-*β*-D-*xylopyranoside:* ***Asteriidoside F***
[214976-61-1]
$C_{37}H_{62}O_{14}$ 730.888
Constit. of a starfish (Asteriidae).
$[\alpha]_D$ -8.3 (c, 1 in MeOH).
Bruno, I. *et al., J. Nat. Prod.*, 1990, **53**, 366-374 (*Dermasterias constit*)
Iorizzi, M. *et al., Tetrahedron*, 1996, **52**, 10997-11012 (*Echinasteridae constits*)
De Marino, S. *et al., J. Nat. Prod.*, 1998, **61**, 1319-1327 (*Asteriidoside F*)

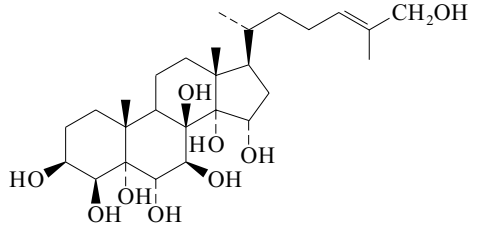
Cholest-24-ene-3,6,8,14,15,26-hexol, 9CI C-578



$C_{27}H_{46}O_6$ 466.657

(3β,5α,6α,24*E*)-*form* [102988-68-1]
15-Sulfate: [103021-32-5]
$C_{27}H_{46}O_9S$ 546.721
Constit. of *Archaster typicus*.
15-Sulfate, Na salt: $[\alpha]_D$ +54.5 (c, 1 in MeOH).
Riccio, R. *et al., J.C.S. Perkin 1*, 1986, 665-670

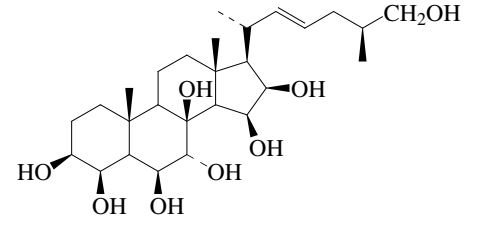
Cholest-24-ene-3,4,5,6,7,8,14,15,26-nonol C-579



$C_{27}H_{46}O_9$ 514.655

(3β,4β,5α,6α,7β,15α,24*E*)-*form*
6-Sulfate: [102988-67-0]
$C_{27}H_{46}O_{12}S$ 594.719
Constit. of *Archaster typicus*.
6-Sulfate, Na salt: $[\alpha]_D$ +47.4 (c, 0.5 in MeOH).
Riccio, R. *et al., J.C.S. Perkin 1*, 1986, 665-670 (*6-sulfate*)

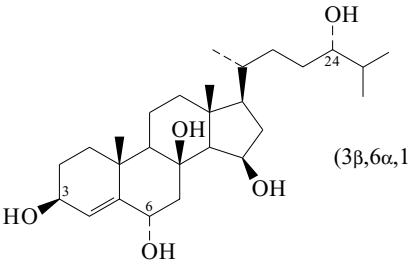
Cholest-22-ene-3,4,6,7,8,15,16,26-octol C-580



$C_{27}H_{46}O_8$ 498.656

(3β,4β,5α,6β,7α,15β,16β,22*E*,25*S*)-*form* [142780-31-2]
Constit. of *Solaster borealis*.
Iorizzi, M. *et al., J. Nat. Prod.*, 1992, **55**, 866-877 (*isol, pmr*)

Cholest-4-ene-3,6,8,15,24-pentol C-581



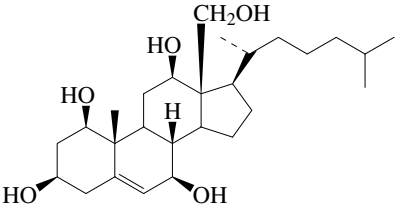
(3β,6α,15β,24*S*)–*form*

$C_{27}H_{46}O_5$ 450.657

(3β,6α,15β,24*S*)-*form*
3-O-*β*-D-*Xylopyranoside, 24-sulfate:* ***Pisasteroside E***
[131985-13-2]
$C_{32}H_{54}O_{12}S$ 662.837
Isol. from the starfish *Pisaster giganteus* (as Na salt).
$[\alpha]_D$ 0 (MeOH).

(3β,6β,15α,24*S*)-*form*
3-O-*β*-D-*Xylopyranoside, 24-sulfate:* ***Pisasteroside D***
[131985-42-7]
$C_{32}H_{54}O_{12}S$ 662.837
Isol. from *Pisaster giganteus* (as Na salt). $[\alpha]_D$ 0 (MeOH).
Zollo, F. *et al., J. Nat. Prod.*, 1990, **53**, 1000

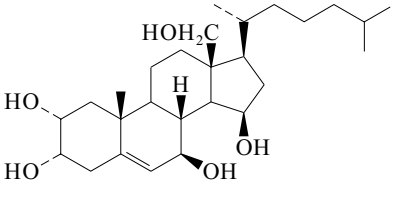
Cholest-5-ene-1,3,7,12,18-pentol C-582



$C_{27}H_{46}O_5$ 450.657

(1β,3β,7β,12β)-*form*
1,7,12,18-Tetra-Ac: [174476-01-8]
$C_{35}H_{54}O_9$ 618.806
Isol. from gastropods *Trimusculus conica* and *Trimusculus reticulatus*.
Manker, D.C. *et al., J. Chem. Ecol.*, 1996, **22**, 23-35

Cholest-5-ene-2,3,7,15,18-pentol C-583

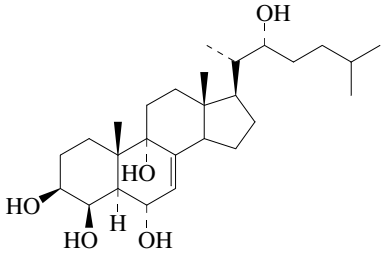


$C_{27}H_{46}O_5$ 450.657

(2α,3α,7β,15β)-*form*
2,7,15,18-Tetra-Ac: [96964-91-9]
$C_{35}H_{54}O_9$ 618.806
Constit. of *Eudendrium glomeratum*. Cryst. (MeOH).

Mp 139-141°. $[\alpha]_D^{26}$ +96 (c, 0.03 in $CHCl_3$).
Fattorusso, E. *et al., J.O.C.*, 1985, **50**, 2868-2870

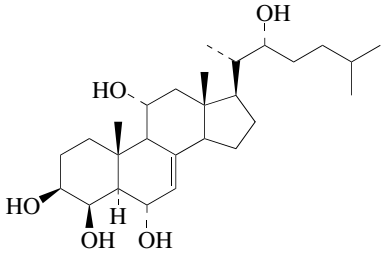
Cholest-7-ene-3,4,6,9,22-pentol C-584



$C_{27}H_{46}O_5$ 450.657

(3β,4β,5α,6α,9α,22*R*)-*form*
3,4,6-Tri-Ac: ***Agosterol E***
[603113-59-3]
$C_{33}H_{52}O_8$ 576.769
Constit. of *Acanthodendrilla* sp. $[\alpha]_D^{25}$ +21.8 (c, 0.73 in $CHCl_3$).
Tsukamoto, S. *et al., J. Nat. Prod.*, 2003, **66**, 1181-1185 (*isol, pmr, cmr*)

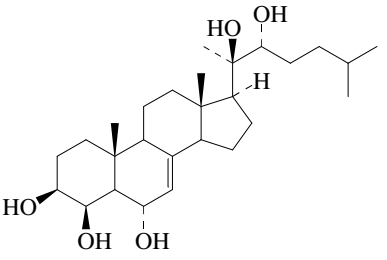
Cholest-7-ene-3,4,6,11,22-pentol C-585



$C_{27}H_{46}O_5$ 450.657

(3β,4β,5α,6α,11α,22*R*)-*form*
3,4-Di-Ac: ***Agosterol B***
[236094-26-1]
$C_{31}H_{50}O_7$ 534.732
Constit. of a *Spongia* sp. $[\alpha]_D$ -5.5 (c, 0.1 in $CHCl_3$).
4,6-Di-Ac: ***Agosterol F***
[255830-16-1]
$C_{31}H_{50}O_7$ 534.732
Constit. of *Acanthodendrilla* sp. $[\alpha]_D$ +43 (c, 0.712 in $CHCl_3$).
3,4,6-Tri-Ac: ***Agosterol A***
[213549-32-7]
$C_{33}H_{52}O_8$ 576.769
Constit. of a *Spongia* sp. Multidrug resistance modulator.
Amorph. solid. $[\alpha]_D$ +27.3 (c, 0.1 in MeOH).
4,6,11-Tri-Ac: ***Agosterol G***
[603113-63-9]
$C_{33}H_{52}O_8$ 576.769
Constit. of *Acanthodendrilla* sp. $[\alpha]_D^{25}$ +41 (c, 0.108 in $CHCl_3$).
Aoki, S. *et al., Tet. Lett.*, 1998, **39**, 6303-6306 (*isol, pmr, cmr*)
Aoki, S. *et al., CA*, 1999, **131**, 142192m (*isol, activity*)
Aoki, S. *et al., Tetrahedron*, 1999, **55**, 13965-13972 (*isol, pmr, cmr, activity*)
Murakami, N. *et al., Chem. Eur. J.*, 2001, **7**, 2663-2670 (*synth*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 2003, **66**, 1181-1185 (*Agosterols F,G*)

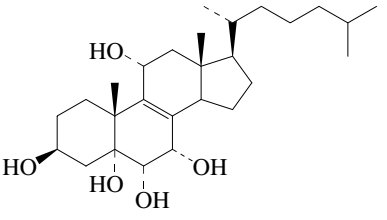
Cholest-7-ene-3,4,6,20,22-pentol C-586



$C_{27}H_{46}O_5$ 450.657

(3β,4β,5α,6α,20*R*,22*R*)-*form*
4,6-Di-Ac: ***Agosterol C₂***
[603113-61-7]
$C_{31}H_{50}O_7$ 534.732
Constit. of *Acanthodendrilla* sp.
$[\alpha]_D^{24}$ +41.2 (c, 1.56 in $CHCl_3$).
3,4,6-Tri-Ac: ***Agosterol D₂***
[236094-28-3]
$C_{33}H_{52}O_8$ 576.769
Constit. of a *Spongia* sp.
$[\alpha]_D$ +28 (c, 0.2 in $CHCl_3$).
Aoki, S. *et al., Tetrahedron*, 1999, **55**, 13965-13972 (*isol, pmr, cmr*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 2003, **66**, 1181-1185 (*isol, pmr, cmr*)

Cholest-8-ene-3,5,6,7,11-pentol C-587



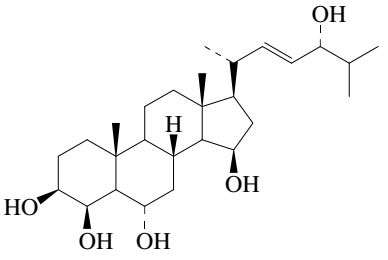
(3β,5α,6α,7α,11α)-form

$C_{27}H_{46}O_5$ 450.657

(3β,5α,6α,7α,11α)-*form*
6,7-Di-Ac: [268735-55-3]
$C_{31}H_{50}O_7$ 534.732
Constit. of a *Dysidea* sp. Powder. $[\alpha]_D^{24}$ +74 (c, 0.68 in $CHCl_3$).
λ_{max} 231 (log ϵ 1.13); 250 (log ϵ 0.3) (CH_2Cl_2).
3,6,7-Tri-Ac: [268735-56-4]
$C_{33}H_{52}O_8$ 576.769
Constit. of a *Dysidea* sp. Powder. $[\alpha]_D^{24}$ +21 (c, 0.03 in $CHCl_3$).
λ_{max} 231 (log ϵ 2.27); 244 (log ϵ 1.7) (CH_2Cl_2).

(3β,5α,6β,7α)-*form*
11-Ketone: 3,5,6,7-Tetrahydroxycholest-8-en-11-one. ***Incrustasterol A***
[163318-77-2]
Constit. of *Dysidea incrustans* and *Dysidea fragilis.*
$[\alpha]_D$ +42.7 (c, 1 in MeOH).
7,11-Diketone: 3,5,6-Trihydroxycholest-8-ene-7,11-dione. ***Incrustasterol B***
[163318-78-3]
$C_{27}H_{42}O_5$ 446.626
Constit. of *Dysidea incrustans.*
$[\alpha]_D$ +10.6 (c, 1 in MeOH). λ_{max} 276 (ϵ 12000) (MeOH) (Berdy).
Aiello, A. *et al., Steroids*, 1995, **60**, 666 (*isol, pmr, cmr*)
Casapullo, A. *et al., Tet. Lett.*, 1995, **36**, 2669-2672 (*isol, pmr, cmr*)
Izzo, I. *et al., Tet. Lett.*, 1996, **37**, 4775-4776 (*synth*)
Leone, P. de A. *et al., J. Nat. Prod.*, 2000, **63**, 694-697 (*isol, pmr, cmr*)

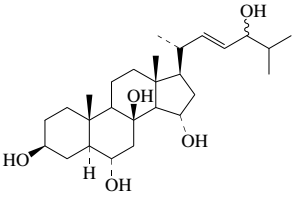
Cholest-22-ene-3,4,6,15,24-pentol C-588



$C_{27}H_{46}O_5$ 450.657

(3β,4β,5α,6α,15β,22*E*,24*R*)-*form*
Amorph. powder.
24-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→2)-β-D-xylofuranoside]:* ***Certonardoside M***
[620604-30-0]
$C_{39}H_{66}O_{13}$ 742.943
Constit. of *Certonardoa semiregularis*. Cryst.
Wang, W. *et al., Chem. Pharm. Bull.*, 2003, **51**, 435-439 (*isol, pmr, cmr*)

Cholest-22-ene-3,6,8,15,24-pentol C-589



(3β,5α,6α,8β,15α,22*E*,24ξ)-*form*

$C_{27}H_{46}O_5$ 450.657

(3β,5α,6α,8β,15α,22*E*,24ξ)-*form* [192325-50-1]
Constit. of *Ceramaster patagonicus*.
$[\alpha]_D$ 0 (c, 0.2 in MeOH).

(3β,5α,6α,8β,15β,22*E*,24*R*)-*form* [129829-90-9]
Constit. of an Antarctic starfish (Echinasteridae) and *Acodontaster conspicuus*.
$[\alpha]_D$ +12.3 (MeOH). $[\alpha]_D$ +8.7 (c, 1 in MeOH).
24-O-*β-D-Xylopyranoside, 3*-O-*sulfate:* ***Minutoside A***
[863919-17-9]
$C_{32}H_{54}O_{12}S$ 662.837
Constit. of *Anasterias minuta*. Amorph. powder. $[\alpha]_D^{20}$ -14.7 (c, 0.32 in MeOH).
3,24-Di-O-*β-D-xylopyranoside, 15-sulfate:* ***Asteriidoside H***
[214976-63-3]
$C_{37}H_{62}O_{16}S$ 794.953
Constit. of a starfish (Asteriidae).
$[\alpha]_D$ -8.3 (C, 1 in MeOH).

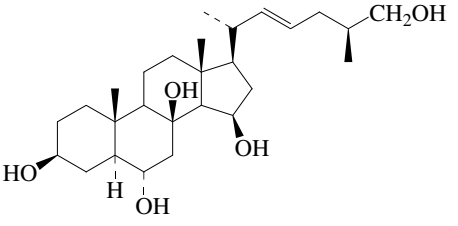
(3β,5α,6α,8β,15β,22*E*,24*S*)-*form*
24-O-*(4*-O-*Sulfo-β-D-xylopyranoside):* ***Luridoside B***
[151041-64-4]
$C_{32}H_{54}O_{12}S$ 662.837
Isol. from the starfish *Cosmasterias lurida*.
$[\alpha]_D^{25}$ +1.5 (c, 0.3 in MeOH) (as Na salt). CAS no. refers to Na salt.

(3β,5α,6α,8β,15β,22*E*,24ξ)-*form*
24-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Ceramasteroside C₅***
[192325-57-8]
$C_{38}H_{64}O_{13}$ 728.916
Constit. of *Ceramaster patagonicus*.
24-[2,4-Di-O-*methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinopyranoside]:* ***Poranoside A***. *22-Dehydrohalityloside E*
[112058-01-2]
$C_{39}H_{66}O_{13}$ 742.943
Constit. of *Porania pulvillus* and *Sphaerodiscus placenta*.
$[\alpha]_D^{22}$ -9 (c, 0.1 in MeOH).

(3β,5α,6β,8β,15α,22*E*,24*S*)-*form*
24-O-*β-D-Xylopyranoside, 15-sulfate:* ***Scoparioside D***
[131466-97-2]
$C_{32}H_{54}O_{12}S$ 662.837
Constit. of the starfish *Astropecten scoparius* and *Coscinasterias tenuispina*. Isol. as Na salt.
3,24-Di-O-*β-D-xylopyranoside:* ***Asterosaponin D₂***. *Distolasteroside D₂*
[109527-66-4]
$C_{37}H_{62}O_{13}$ 714.889
Constit. of *Distolasterias nipon*. Cryst.
Mp 281-284°. $[\alpha]_D^{20}$ -10.8 (c, 0.27 in MeOH).

(3β,5α,6β,8β,15α,22*E*,24ξ)-*form*
15-Sulfate: [105404-86-2]
$C_{27}H_{46}O_8S$ 530.722
Constit. of *Coscinasterias tenuispina*.
$[\alpha]_D$ +10 (MeOH) (as Na salt). CAS no. refers to Na salt.
Riccio, R. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 869-893 (*Luridoside B*)
Zollo, F. *et al., J. Nat. Prod.*, 1987, **50**, 794-799 (*Poranoside A*)
Andersson, L. *et al., J. Nat. Prod.*, 1987, **50**, 944-947 (*Poranoside A*)
Kapustina, I.I. *et al., Khim. Prir. Soedin.*, 1987, **23**, 250; *Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 209 (*Asterosaponin D₂, Distolasteroside D₂*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1990, **53**, 1225-1233 (*Scoparioside D*)
Maier, M.S. *et al., J. Nat. Prod.*, 1993, **56**, 939-942 (*Luridoside B*)
Iorizzi, M. *et al., Tetrahedron*, 1996, **52**, 10997-11012 (*Antarctic starfish constit*)
De Marino, S. *et al., J. Nat. Prod.*, 1997, **60**, 959-966 (*isol, pmr, cmr*)
Kicha, A.A. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1997, **46**, 186-191 (*Ceramasteroside C₅, isol, pmr, cmr*)
De Marino, S. *et al., J. Nat. Prod.*, 1998, **61**, 1319-1327 (*Asteriidoside H*)
Chludil, H.D. *et al., J. Nat. Prod.*, 2005, **68**, 1279-1283 (*Minutoside A*)

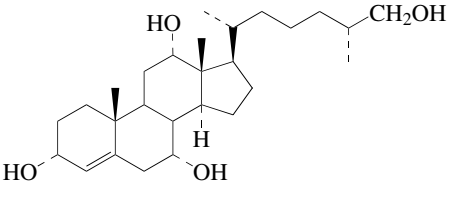
Cholest-22-ene-3,6,8,15,26-pentol C-590



$C_{27}H_{46}O_5$ 450.657

(3β,5α,6α,15β,22*E*,25*S*)-*form* [128855-07-2]
Constit. of *Dermasterias imbricata*.
$[\alpha]_D$ +7.1 (c, 0.5 in MeOH).
Bruno, I. *et al., J. Nat. Prod.*, 1990, **53**, 366-374 (*isol, pmr, cmr*)

Cholest-4-ene-3,7,12,26-tetrol C-591



$C_{27}H_{46}O_4$ 434.658
Mosesins incorrectly named in CA.

(3α,7α,12α,25*R*)-*form*
7-O-*(6*-O-*Acetyl-β-D-galactopyranoside), 26-Ac:* ***Mosesin 1***
[101691-11-6]
$C_{37}H_{60}O_{11}$ 680.874

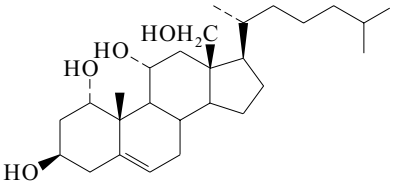
Isol. from the Moses sole (*Paradachirus marmoratus*). Shark repellent.

*4,5-Dihydro, 7-*O*-β-D-galactopyranoside, 26-Ac:* ***Mosesin 4***
[101691-14-9]
$C_{35}H_{60}O_{10}$ 640.853
Isol. from *Paradachirus marmoratus*. Shark repellent.

*4,5-Dihydro, 7-*O*-(6-*O*-acetyl-β-D-galactopyranoside), 26-Ac:* ***Mosesin 3***
[101691-13-8]
$C_{37}H_{62}O_{11}$ 682.89
Isol. from *Paradachirus marmoratus*. Shark repellent.

Tachibana, K. *et al., Toxicon*, 1988, **26**, 839-853 (*isol*)

Cholest-5-ene-1,3,11,18-tetrol C-592



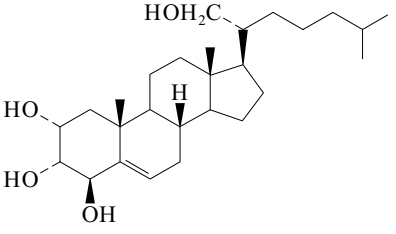
$C_{27}H_{46}O_4$ 434.658

(1α,3β,11α)-*form*

18-Ac: [97190-35-7]
$C_{29}H_{48}O_5$ 476.695
Isol. from *Sinularia dissecta*.

Jagodzinska, B.M. *et al., J.O.C.*, 1985, **50**, 2988

Cholest-5-ene-2,3,4,21-tetrol C-593



$C_{27}H_{46}O_4$ 434.658

(2α,3α,4β)-*form*

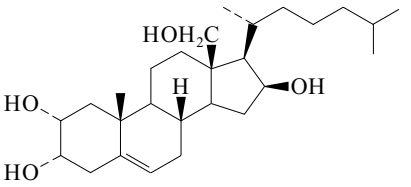
3,21-Disulfate: [155544-31-3]
$C_{27}H_{46}O_{10}S_2$ 594.786
Constit. of *Ophioderma longicaudum*. Highly cytotoxic.

24,25-Didehydro: Cholesta-5,24-diene-2,3,4,21-tetrol
$C_{27}H_{44}O_4$ 432.642

24,25-Didehydro, 3,21-disulfate: [202649-94-3]
$C_{27}H_{44}O_{10}S_2$ 592.771
Constit. of *Astrotoma agassizii*. Powder. $[\alpha]_D^{25}$ +1.4 (c, 0.14 in MeOH).

D'Auria, M.V. *et al., Nat. Prod. Lett.*, 1993, **3**, 197-201 (*3,21-disulfate, isol, pmr, cmr*)
Shubina, L.K. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **119**, 505-511 (*3,21-disulfate, occur, rev*)
Roccatagliata, A.J. *et al., J. Nat. Prod.*, 1998, **61**, 370-376 (*24,25-didehydro 3,21-disulfate*)

Cholest-5-ene-2,3,16,18-tetrol, 9CI C-594



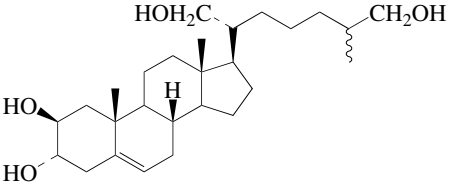
$C_{27}H_{46}O_4$ 434.658

(2α,3α,16β)-*form*

2,16,18-Tri-Ac: 2α,16β,18-Triacetoxycholest-5-en-3α-ol
[110042-28-9]
$C_{33}H_{52}O_7$ 560.77
Constit. of *Eudendrium glomeratum*. Amorph. powder. $[\alpha]_D^{20}$ +17.2 (c, 0.03 in $CHCl_3$).

Aiello, A. *et al., J. Nat. Prod.*, 1987, **50**, 191

Cholest-5-ene-2,3,21,26-tetrol C-595



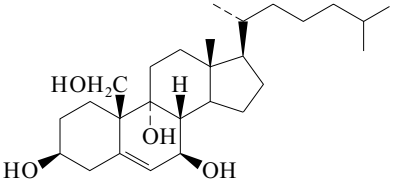
$C_{27}H_{46}O_4$ 434.658

(2β,3α,20*R*,25ξ)-*form*

2,21-Disulfate: [214129-62-1]
$C_{27}H_{46}O_{10}S_2$ 594.786
Constit. of *Pteraster tesselatus*. Cryst. (MeOH aq.).
Mp 187-189°. $[\alpha]_D^{20}$ -17 (c, 17.2 in MeOH).

Levina, E.V. *et al., J. Nat. Prod.*, 1998, **61**, 1423-1426 (*isol, pmr, cmr*)

Cholest-5-ene-3,7,9,19-tetrol C-596

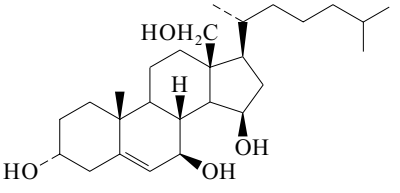


$C_{27}H_{46}O_4$ 434.658

(3β,7β,9α)-*form* [139765-40-5]
Constit. of *Antipathes subpinnata*. Cryst. Mp 165-167°.

Aiello, A. *et al., J. Nat. Prod.*, 1992, **55**, 321 (*isol, pmr, cmr*)

Cholest-5-ene-3,7,15,18-tetrol, 9CI C-597

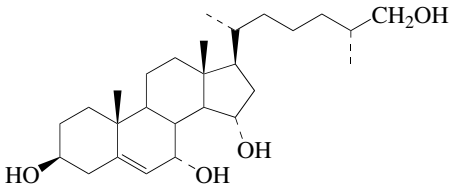


$C_{27}H_{46}O_4$ 434.658

(3α,7β,15β)-*form*

7,15,18-Tri-Ac: [110025-80-4]
$C_{33}H_{52}O_7$ 560.77
Constit. of *Eudendrium glomeratum*. $[\alpha]_D^{20}$ +23 (c, 0.03 in $CHCl_3$).
Aiello, A. *et al., J. Nat. Prod.*, 1987, **50**, 191

Cholest-5-ene-3,7,15,26-tetrol C-598

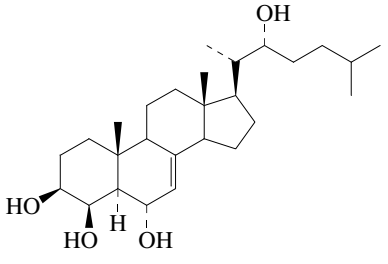


$C_{27}H_{46}O_4$ 434.658

(3β,7α,15α,25*R*)-*form*

7-O-β-D-Galactopyranoside, 26-Ac: ***Mosesin 2***
[101691-12-7]
$C_{35}H_{58}O_{10}$ 638.837
Isol. from the Moses sole (*Paradachirus marmoratus*). Shark repellent. Incorrectly named in CA.
Tachibana, K. *et al., Toxicon*, 1988, **26**, 839-853 (*isol*)

Cholest-7-ene-3,4,6,22-tetrol C-599

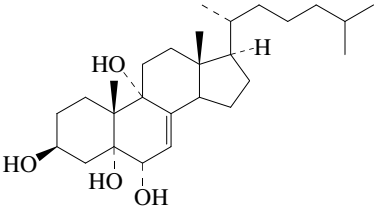


$C_{27}H_{46}O_4$ 434.658

(3β,4β,5α,6α,22*R*)-*form*

4,6-Di-Ac: ***Agosterol C***
[236094-27-2]
$C_{31}H_{50}O_6$ 518.732
Constit. of a *Spongia* sp. $[\alpha]_D$ +49.5 (c, 0.7 in $CHCl_3$).
Aoki, S. *et al., Tetrahedron*, 1999, **55**, 13965-13972 (*isol, pmr, cmr*)

Cholest-7-ene-3,5,6,9-tetrol, 9CI C-600



(3β,5α,6α,9α)-*form*

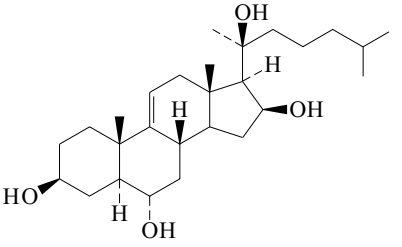
$C_{27}H_{46}O_4$ 434.658

(3β,5α,6α,9α)-*form*

6-Sulfate:
$C_{27}H_{46}O_7S$ 514.722
Constit. of *Dysidea fragilis* from the Venice lagoon.

(3β,5α,6β,9α)-*form* [133056-64-1]
Constit. of *Spongia officinalis*. Cryst. (MeOH aq.). Mp 218-220°. $[\alpha]_D^{25}$ -33.3 (c, 0.06 in MeOH).
Migliuolo, A. *et al., J. Nat. Prod.*, 1990, **53**, 1414 (*isol, pmr, cmr*)
Aiello, A. *et al., Steroids*, 1995, **60**, 666 (*isol, pmr, cmr*)

Cholest-9(11)-ene-3,6,16,20-tetrol C-601

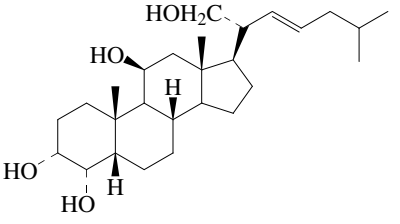


$C_{27}H_{46}O_4$ 434.658

(3β,5α,6α,16β)-*form*

3-O-β-D-Glucuronopyranoside, 6-sulfate: ***Downeyoside K***
[174324-05-1]
$C_{33}H_{54}O_{13}S$ 690.848
Constit. of *Henricia downeyae*. $[\alpha]_D$ -12.
Palagiano, E. *et al., J. Nat. Prod.*, 1996, **59**, 348-354 (*isol, pmr, cmr*)

Cholest-22-ene-3,4,11,21-tetrol C-602

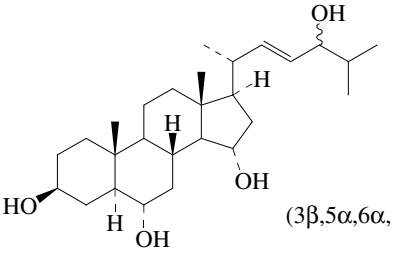


$C_{27}H_{46}O_4$ 434.658

(3α,4α,5β,11β,22*E*)-*form*

3,21-Disulfate: [109152-33-2]
$C_{27}H_{46}O_{10}S_2$ 594.786
Constit. of *Ophioplocus januarii*. $[\alpha]_D$ -24.5.
D'Auria, M.V. *et al., J.O.C.*, 1987, **52**, 3947-3952 (*isol, pmr*)
Roccatagliata, A.J. *et al., J. Nat. Prod.*, 1996, **59**, 887-889 (*isol*)

Cholest-22-ene-3,6,15,24-tetrol C-603



(3β,5α,6α,15α,22*E*,24ξ)-*form*

$C_{27}H_{46}O_4$ 434.658

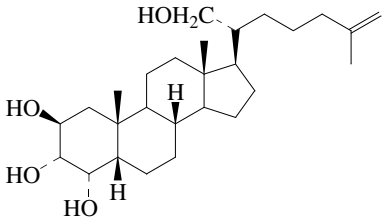
(3β,5α,6α,15α,22*E*,24ξ)-*form*

24-O-(4-Sulfo-β-D-xylopyranoside): ***Amurensoside C***
[115178-54-6]
$C_{32}H_{54}O_{11}S$ 646.838
Constit. of *Asterias amurensis*. $[\alpha]_D$ +6.8.

(3β,5α,6α,15β,22*E*,24*R*)-*form*
Certonardosterol G
[517900-55-9]
Constit. of *Certonardoa semiregularis*. Cryst.

Riccio, R. *et al., J.C.S. Perkin 1*, 1988, 1337-1347 (*Amurensoside C*)
Wang, W. *et al., J. Nat. Prod.*, 2003, **66**, 384-391 (*Certonardosterol G*)

Cholest-25-ene-2,3,4,21-tetrol C-604

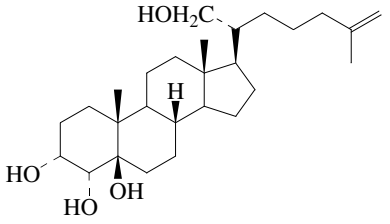


$C_{27}H_{46}O_4$ 434.658

(2β,3α,4α,5β)-*form* [116407-26-2]
[116407-22-8]

3,21-Disulfate: [116407-21-7]
$C_{27}H_{46}O_{10}S_2$ 594.786
Isol. from the Pacific ophiuroid *Ophiolepis superba*.
$[\alpha]_D$ +9 (MeOH) (as di-Na salt).
D'Auria, M.V. *et al., J.O.C.*, 1989, **54**, 234-239 (*isol, pmr, cmr, synth*)

Cholest-25-ene-3,4,5,21-tetrol C-605

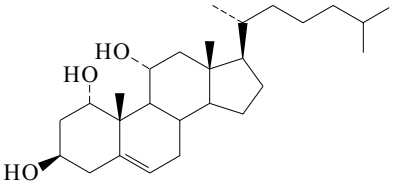


$C_{27}H_{46}O_4$ 434.658

(3α,4α,5β)-*form* [116407-24-0]
Glass.

3,21-Disulfate: [116407-20-6]
$C_{27}H_{46}O_{10}S_2$ 594.786
Isol. from the Pacific ophiuroid *Ophiolepis superba*.
$[\alpha]_D$ +9.1 (MeOH) (as di-Na salt).
D'Auria, M.V. *et al., J.O.C.*, 1989, **54**, 234-239 (*isol, pmr, cmr, synth*)

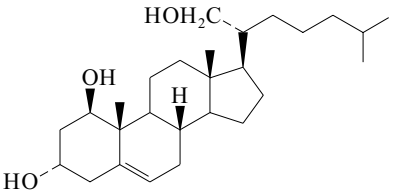
Cholest-5-ene-1,3,11-triol C-606



$C_{27}H_{46}O_3$ 418.659

(1α,3β,11α)-*form*
1α,11α-Dihydroxycholesterol
[95513-60-3]
Constit. of *Sinularia dissecta*.
Jagodzinska, B.M. *et al., J.O.C.*, 1985, **50**, 1435

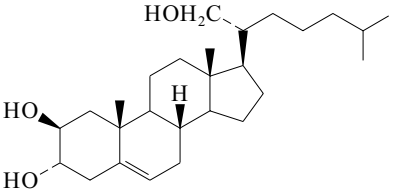
Cholest-5-ene-1,3,21-triol C-607



$C_{27}H_{46}O_3$ 418.659

(1β,3α)-*form*
3,21-Disulfate: [160522-15-6]
$C_{27}H_{46}O_9S_2$ 578.787
Constit. of brittle star *Ophiarachna incrassata*. Protein-tyrosine kinase inhibitor. Amorph. solid. $[\alpha]_D$ +16.7 (c, 0.62 in MeOH aq.).
Fu, X. *et al., J. Nat. Prod.*, 1994, **57**, 1591-1594 (*isol, pmr, cmr*)

Cholest-5-ene-2,3,21-triol C-608



$C_{27}H_{46}O_3$ 418.659

(2β,3α)-*form* [132310-92-0]
Cryst. Mp 158-160°. $[\alpha]_D^{20}$ -15.6 (c, 2.1 in $CHCl_3$).

2,21-Disulfate: [155521-20-3]
[169832-00-2]
$C_{27}H_{46}O_9S_2$ 578.787
Constit. of *Ophioderma longicaudum*, *Aphiophiura ponderosa*, *Asteronyx loveni*, *Astrotoma agassizii* and *Pteraster tessellatus.*
Amorph. solid. $[\alpha]_D^{20}$ +2 (c, 4.8 in MeOH).

3,21-Disulfate: [162830-24-2]
[292833-53-5]
$C_{27}H_{46}O_9S_2$ 578.787
Constit. of *Ophiothrix fragilis*, *Gorgonocephalus chilensis*, *Ophiura texturata*, *Gorgonocephalus caryi*, *Ophiura leptoctenia*, *Ophionotus victoriae* and *Pteraster tessellatus.*
$[\alpha]_D$ +8.7. Genus name given as *Ophiotrix* in ref.

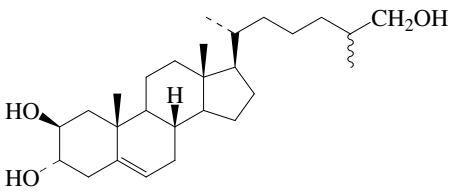
Tri-O-*sulfate:* [132310-91-9]
$C_{27}H_{46}O_{12}S_3$ 658.851
Constit. of *Ophiura leptoctenia*. Cryst. (MeOH) (as tri-Na salt). Mp 151-153°. $[\alpha]_D^{20}$ +4.1 (c, 1.0 in MeOH).

24,25-Didehydro: Cholesta-5,24-diene-2,3,21-triol
$C_{27}H_{44}O_3$ 416.643

24,25-Didehydro, 2,21-disulfate: [202649-91-0]
$C_{27}H_{44}O_9S_2$ 576.771
Constit. of *Astrotoma agassizii*. Powder. $[\alpha]_D^{25}$ -13 (c, 0.92 in MeOH).

Levina, E.V. *et al., Khim. Prir. Soedin.*, 1990, 483-487; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 408-411 (*trisulfate*)
D'Auria, M.V. *et al., Nat. Prod. Lett.*, 1993, **3**, 197-201 (*2,21-disulfate*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1995, **58**, 189-196 (*3,21-disulfate, isol, pmr, cmr*)
Levina, E.V. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1996, **114**, 49-52 (*2,21-disulfate, isol, pmr, cmr*)
Shubina, L.K. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **119**, 505-511 (*3,21-disulfate*)
Roccatagliata, A.J. *et al., J. Nat. Prod.*, 1998, **61**, 370-374 (*24,25-didehydro 2,21-disulfate, isol, pmr, cmr*)
Maier, M.S. *et al., Molecules*, 2000, **5**, 348-349; *CA*, **133**, 235391g (*disulfates*)

Cholest-5-ene-2,3,26-triol C-609

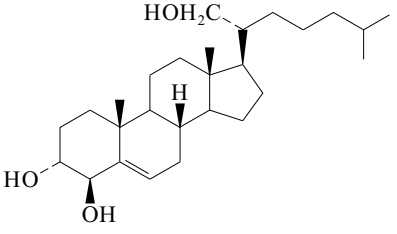


$C_{27}H_{46}O_3$ 418.659

(2β,3α,25ξ)-*form*

Trisulfate: [109152-36-5]
$C_{27}H_{46}O_{12}S_3$ 658.851
Constit. of *Ophiarachna incrassata*.
D'Auria, M.V. *et al., J.O.C.*, 1987, **52**, 3947-3942 (*trisulfate, isol, pmr, cmr*)
Fu, X. *et al., J. Nat. Prod.*, 1994, **57**, 1591-1594 (*trisulfate, isol*)

Cholest-5-ene-3,4,21-triol C-610



$C_{27}H_{46}O_3$ 418.659

(3α,4β)-*form* [117675-16-8]
Mp 103-105°. $[\alpha]_D^{20}$ -15 (c, 6.1 in $CHCl_3$).

3-O-*Sulfate:*
[117675-13-5 (Na salt)]
$C_{27}H_{46}O_6S$ 498.723
Constit. of *Ophiura sarsi* and *Ophiura leptoctenia*. Cryst. (as Na salt). Mp 120-122° (Na salt). $[\alpha]_D^{20}$ -12.37 (c, 10.15 in MeOH) (Na salt).

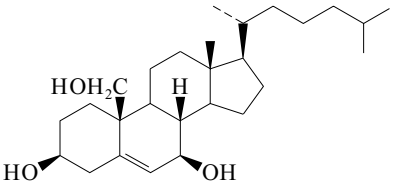
21-Sulfate: [760939-35-3]
[454203-05-5]
$C_{27}H_{46}O_6S$ 498.723
Isol. from *Diplopteraster multipes*.

3,21-Disulfate: [155521-21-4]
[132310-90-8]
$C_{27}H_{46}O_9S_2$ 578.787
Constit. of *Ophiopholis aculeata*, *Pteraster pulvillus*, *Ophiothrix fragilis*, *Ophiura texturata*, *Ophionotus victoriae* and *Ophiura sarsi*. Cryst. (MeOH). Mp 190-191°. $[\alpha]_D^{20}$ -17 (c, 0.1 in MeOH). Genus name given as *Ophiotrix* in ref.

Tri-Ac:
Cryst. (MeOH). Mp 82-83°. $[\alpha]_D^{20}$ -29 (c, 0.1 in $CHCl_3$).

Levina, E.V. *et al., Khim. Prir. Soedin.*, 1988, 375-379; 1990, 483-487; *Chem. Nat. Compd. (Engl. Transl.)*, 1988, **24**, 316-320; 1990, **26**, 408-411 (*3-sulfate*)
Fedorov, S.N. *et al., J. Nat. Prod.*, 1994, **57**, 1631-1637 (*3,21-disulfate, isol, pmr, cmr*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1995, **58**, 189-196 (*3,21-disulfate, isol, pmr, cmr*)
Maier, M.S. *et al., Molecules*, 2000, **5**, 348-349; *CA*, **133**, 235391g (*3,21-disulfate*)
Levina, E.V. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2002, **28**, 189-193 (*21-sulfate*)
Ivanchina, N.V. *et al., J. Nat. Prod.*, 2003, **66**, 298-301 (*3,21-disulfate*)

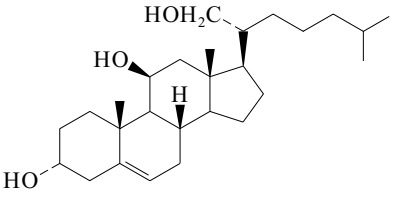
Cholest-5-ene-3,7,19-triol C-611



$C_{27}H_{46}O_3$ 418.659

(3β,7β)-*form* [139765-38-1]
Constit. of *Antipathes subpinnata*. Cryst. Mp 154-156°.
Aiello, A. *et al., J. Nat. Prod.*, 1992, **55**, 321 (*isol, pmr, cmr*)

Cholest-5-ene-3,11,21-triol C-612

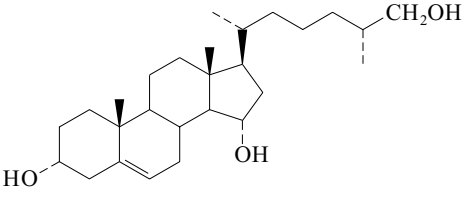


$C_{27}H_{46}O_3$ 418.659

(3α,11β)-*form*

3,21-Disulfate: [162830-26-4]
$C_{27}H_{46}O_9S_2$ 578.787
Constit. of *Ophionereis reticulata*. $[\alpha]_D$ -7.6.
D'Auria, M.V. *et al., J. Nat. Prod.*, 1995, **58**, 189-196 (*isol, pmr, cmr*)

Cholest-5-ene-3,15,26-triol C-613



$C_{27}H_{46}O_3$ 418.659

(3α,15α,25*R*)-*form*

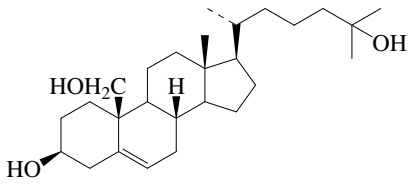
15-O-*[2-(Acetylamino)-2-deoxy-β-D-glucopyranosyl], 26-Ac:* ***Pavoninin 3***
[94425-99-7]
$C_{37}H_{61}NO_9$ 663.89
Ichthyotoxic, haemolytic and shark-repelling factor of the sole *Pardachirus pavoninus*. $[\alpha]_D^{29}$ +15 (c, 0.7 in EtOH).

15-O-*[2-(Acetylamino)-2-deoxy-β-D-glucopyranosyl], 26-Ac, 5α,6-dihydro:* ***Pavoninin 4***
[94359-66-7]
$C_{37}H_{63}NO_9$ 665.906
Ichthyotoxic, haemolytic and shark-repelling factor of *Pardachirus pavoninus*. $[\alpha]_D^{30}$ +36 (c, 0.8 in EtOH).

15-O-*[2-(Acetylamino)-2-deoxy-β-D-glucopyranosyl], 26-Ac, 3-epimer:* ***Pavoninin 5***
[94480-49-6]
$C_{37}H_{61}NO_9$ 663.89
Ichthyotoxic, haemolytic and shark-repelling factor of *Pardachirus pavoninus*. $[\alpha]_D^{29}$ +21 (c, 0.7 in EtOH).

Tachibana, K. *et al., Tetrahedron*, 1985, **41**, 1027-1037 (*Pavoninins*)
Williams, J.R. *et al., J.O.C.*, 2005, **70**, 10732-10736 (*Pavoninin 4, synth*)
Gong, H. *et al., Org. Lett.*, 2006, **8**, 2253-2255 (*synth*)

Cholest-5-ene-3,19,25-triol C-614



$C_{27}H_{46}O_3$ 418.659

3β-*form*

3-O-*β-D-Arabinopyranoside:* ***Junceelloside D***
[850145-13-0]
$C_{32}H_{54}O_7$ 550.774
Constit. of *Junceella juncea*. Powder. $[\alpha]_D^{20}$ -113.6 (c, 0.59 in Py).

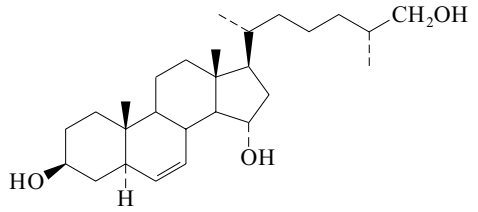
3-O-*(3*-O-*Acetyl-β-D-arabinopyranoside):* ***Junceelloside B***
[850145-10-7]
$C_{34}H_{56}O_8$ 592.812
Constit. of *Junceella juncea*. Powder. $[\alpha]_D^{20}$ -113.9 (c, 0.64 in Py).

3-O-*(4*-O-*Acetyl-β-D-arabinopyranoside):* ***Junceelloside A***
[850145-08-3]
$C_{34}H_{56}O_8$ 592.812
Constit. of *Junceella juncea*. Powder. $[\alpha]_D^{20}$ -114.5 (c, 0.85 in Py).

25-Ac, 3-O-*β-D-arabinopyranoside:* ***Junceelloside C***
[850145-12-9]
$C_{34}H_{56}O_8$ 592.812
Constit. of *Junceella juncea*. Powder. $[\alpha]_D^{20}$ -114 (c, 0.55 in Py).

Qi, S. *et al., Magn. Reson. Chem.*, 2005, **43**, 266-268 (*Junceellosides*)

Cholest-6-ene-3,15,26-triol C-615



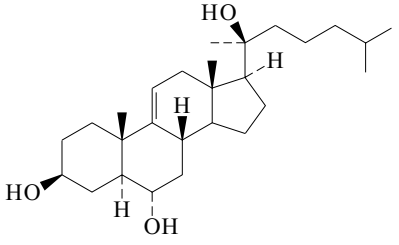
$C_{27}H_{46}O_3$ 418.659

(3β,5α,15α,25*R*)-*form*

15-O-*[2-(Acetylamino)-2-deoxy-β-D-glucopyranosyl], 26-Ac:* ***Pavoninin 6***
[94359-65-6]
$C_{37}H_{61}NO_9$ 663.89
Ichthyotoxic, haemolytic and shark-repelling factor of sole *Pardachirus pavoninus*. $[\alpha]_D^{30}$ -25 (c, 2.4 in EtOH).

Tachibana, K. *et al., Tetrahedron*, 1985, **41**, 1027-1037

Cholest-9(11)-ene-3,6,20-triol C-616



$C_{27}H_{46}O_3$ 418.659

(3β,5α,6α,20*S*)-*form*

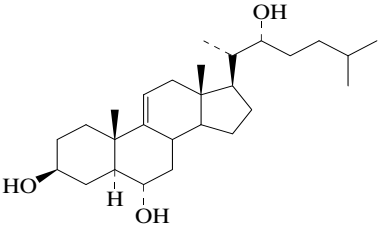
6-O-*(4*-O-*Sulfo-6-deoxy-β-D-glucopyranoside), 3*-O-*sulfate:* ***Latespinoside B***
[178200-91-4]
$C_{33}H_{56}O_{13}S_2$ 724.93
Constit. of *Astropecten latespinosus*. Amorph. powder.
Mp 200-201°. $[\alpha]_D$ +19.7 (c, 0.79 in MeOH).

6-O-*[β-D-Galactopyranosyl-(1→3)-β-D-fucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate:* ***Ruberoside A***
[270249-47-3]
$C_{62}H_{104}O_{31}S$ 1377.551
Constit. of *Asterias rubens*.

6-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* [270088-57-8]
$C_{56}H_{94}O_{26}S$ 1215.409
Constit. of *Asterias rubens*.

Higuchi, R. *et al., Annalen*, 1996, 837-840 (*Latespinoside B*)
Sandvoss, M. *et al., Eur. J. Org. Chem.*, 2000, 1253-1262 (*Asterias rubens constits*)

Cholest-9(11)-ene-3,6,22-triol C-617



$C_{27}H_{46}O_3$ 418.659

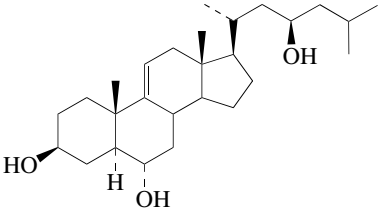
(3β,5α,6α,22*R*)-*form*

3,6-Di-O-*sulfate:* [149253-61-2]
$C_{27}H_{46}O_9S_2$ 578.787
Isol. from the starfish *Tremaster novaecaledoniae*. $[\alpha]_D$ +25 (MeOH) (as di-Na salt).

22-Ac, 3,6-di-O-*sulfate:* [149230-98-8]
$C_{29}H_{48}O_{10}S_2$ 620.824
Isol. from *Tremaster novaecaledoniae*.
$[\alpha]_D$ +27.2 (MeOH) (as di-Na salt).

De Riccardis, F. *et al., Gazz. Chim. Ital.*, 1993, **123**, 79-86 (*isol, pmr, cmr*)

Cholest-9(11)-ene-3,6,23-triol C-618



(3β,5α,6α,23*R*)-*form*

$C_{27}H_{46}O_3$ 418.659

(3β,5α,6α,23*R*)-*form*

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate:* ***Nipoglycoside D***
[154073-60-6]
$C_{57}H_{96}O_{27}S$ 1245.435
Constit. of *Distolasterias nipon*.
$[\alpha]_D$ +3.6 (MeOH).

(3β,5α,6α,23*S*)-*form*

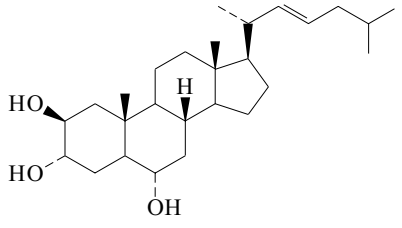
3,6-Disulfate: [142013-87-4]
$C_{27}H_{46}O_9S_2$ 578.787
Constit. of *Aphelasterias japonica*.
$[\alpha]_D$ +24.2 (c, 1 in MeOH).

(3β,5α,6α,23ξ)-*form* [38965-34-3]
Constit. of the starfish *Marthasterias glacialis*, also present as Asterosaponins A and B in starfish *Asterias amurensis.*
Needles (EtOAc).
Mp 240-243°. $[\alpha]_D^{25}$ +41.5 (c, 0.26 in EtOH). See note on Asterosaponins under 3,6-Dihydroxycholesta-9(11),24-dien-23-one, D-626.

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-*xylo-*hexopyranosid-4-uloside-4′-hydrate], 3*-O-*sulfate:* ***Ruberoside B***
[270249-48-4]
$C_{57}H_{96}O_{27}S$ 1245.435
Constit. of *Asterias rubens.*

Ikegami, S. *et al., Tet. Lett.*, 1972, 3725-3728 (*3β,5α,6α,23ξ-form, isol*)
Finamore, E. *et al., J. Nat. Prod.*, 1992, **55**, 767-772 (*disulfate*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1993, **56**, 1786-1798 (*Nipoglycoside D*)
Sandvoss, M. *et al., Eur. J. Org. Chem.*, 2000, 1253-1262 (*Ruberoside B*)

Cholest-22-ene-2,3,6-triol C-619



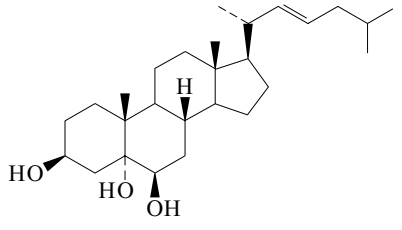
$C_{27}H_{46}O_3$ 418.659

(2β,3α,5α,6α,22*E*)-*form*

Trisulfate: [163815-32-5]
$C_{27}H_{46}O_{12}S_3$ 658.851
Constit. of *Trachyopsis halichondroides* and *Cymbastela coralliophila*.

Makarieva, T.N. *et al., Steroids*, 1995, **60**, 316-320 (*isol, pmr, ms*)

Cholest-22-ene-3,5,6-triol C-620

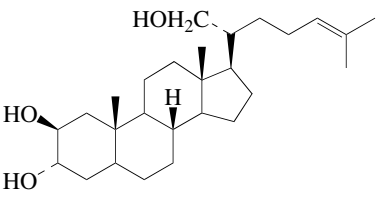


$C_{27}H_{46}O_3$ 418.659

(3β,5α,6β,22*E*)-*form*
Constit. of *Cliona copiosa*.

Notaro, G. *et al., J. Nat. Prod.*, 1991, **54**, 1570 (*isol, pmr*)

Cholest-24-ene-2,3,21-triol C-621



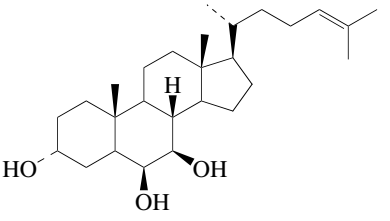
$C_{27}H_{46}O_3$ 418.659

(2β,3α,5α)-*form*

3,21-Disulfate: [202649-92-1]
$C_{27}H_{46}O_9S_2$ 578.787
Constit. of *Astrotoma agassizii*. Powder. $[\alpha]_D^{25}$ +20.4 (c, 0.25 in MeOH).

Roccatagliata, A.J. *et al., J. Nat. Prod.*, 1998, **61**, 370-376 (*isol, pmr, cmr*)

Cholest-24-ene-3,6,7-triol C-622

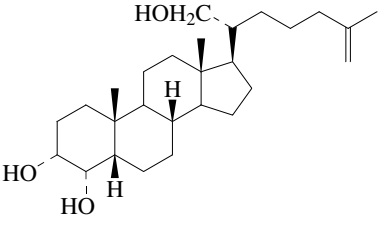


$C_{27}H_{46}O_3$ 418.659

(3α,5α,6β,7β)-*form* [201800-59-1]
Constit. of *Gersemia fruticosa*. Apoptosis inducer. Amorph. powder. $[\alpha]_D$ +47.4 (c, 2.1 in MeOH).

Koljak, R. *et al., Tetrahedron*, 1998, **54**, 179-186 (*isol, pmr, cmr*)

Cholest-25-ene-3,4,21-triol C-623



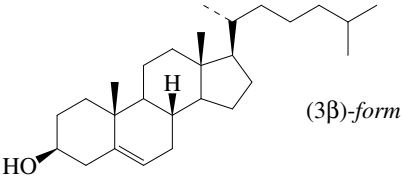
$C_{27}H_{46}O_3$ 418.659

(3α,4α,5β)-*form*

3,21-Disulfate: [116407-16-0]
$C_{27}H_{46}O_9S_2$ 578.787
Isol. from the Pacific ophiuroid *Ophiolepis superba*.
$[\alpha]_D$ +9.1 (MeOH) (as di-Na salt).

D'Auria, M.V. *et al., J.O.C.*, 1989, **54**, 234-239 (*isol, pmr, cmr, struct*)

Cholest-5-en-3-ol C-624



$C_{27}H_{46}O$ 386.66

▶ FZ8400000

3β-*form*
Cholesterol, BAN, USAN. *Cholesterin*. *NSC 8798*
[57-88-5]
Characteristic sterol of higher animals. Constit., either free or as esters, of fish liver oils, egg yolk, bile, bran, gallstones, and many marine organisms such as *Cladolabes bifurcalus*, *Cucumaria* sp., *Eupentacta fraudatrix*, *Bathyplotes natans*, *Holothuria nobilis*, *Holothuria scabra*, *Pseudostichopus trachus*, *Synapta maculata*. Constit. of scent material of cotton-top tamarin monkey (*Saguinus oedipus*). Present in *Bugula neritina* and marine algal lipids. Pharmaceutical aid (emulsifying agent). Emollient. Pearly leaflets (EtOH aq.). Mp 148.5° (anhyd.). $[\alpha]_D$ -31.12 (Et_2O).
▶ Exp. reprod. and teratogenic effects (very large doses).

3-O-*Sulfate: Cholesteryl sulfate*
[1256-86-6]
[2864-50-8 (Na salt)]
$C_{27}H_{46}O_4S$ 466.724
Occurs in eggs of the sea urchin *Anthocidaris crassispina*, the starfish *Euretaster insignis*, *Asterias rubens*, brittle star *Macrophiotrix longipeda*, sea urchin *Strongylocentrotus intermedius*, sea lily *Himerometra robustipinna*, *Echinus esculentus*, *Echinocardium cordatum*, *Antedon bifida*, *Ophiocomina nigra*, *Eupentacta fraudatrix* and many other marine organisms. Mp 170-173° (as Na salt). $[\alpha]_D$ -20.8 (MeOH).

3-O-*β-D-Xylopyranoside:* [104720-15-2]
$C_{32}H_{54}O_5$ 518.776
Constit. of *Eupentacta fraudatrix*.

Formyl: Cholesteryl formate
[4351-55-7]
$C_{28}H_{46}O_2$ 414.67
Constit. of the soft coral *Dendronephthya* sp. and red alga *Grateloupia turuturu*. Cryst. (Me_2CO). Mp 96°.

Tetracosanoyl: Cholesteryl tetracosanoate
[73024-96-1]
$C_{51}H_{92}O_2$ 737.287
Isol. from skin surface lipids of *Equus* ssp. and from the sponge *Tedania annhelans*.

Hexacosanoyl: Cholesteryl hexacosanoate
[87080-57-7]
$C_{53}H_{96}O_2$ 765.34
Isol. from skin surface lipids of *Equus* spp. and from the sponge *Tedania annhelans*.

Ethoxyacetyl: ***Chethoxyrol***
[55560-77-5]
$C_{31}H_{52}O_3$ 472.75
Constit. of *Hilsa ilisha*. Plates (EtOAc/MeOH). Mp 82-83°. $[\alpha]_D^{20}$ -53.8 ($CHCl_3$).

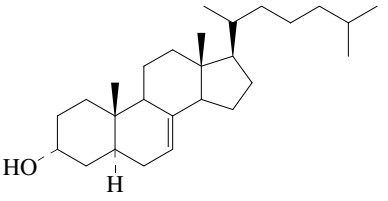
Me ether: 3-Methoxycholest-5-ene. O-*Methylcholesterol*. *Cholesterol methyl ether*. *NSC 95435*
[1174-92-1]
$C_{28}H_{48}O$ 400.687
Constit. of the sponge *Jereicopsis graphidiophora*. Cryst. (EtOH). Mp 84.5°. $[\alpha]_D^{20}$ -45.8 ($CHCl_3$).

(3β,20*S*)-*form*
20-Epicholesterol
[34026-89-6]
Constit. of *Macoma balthica*.
Cryst. (MeOH/Me_2CO). Mp 152-153°. $[\alpha]_D^{20}$ -54.2 (c, 0.52 in $CHCl_3$).

[1256-86-6, 16134-40-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1048B; 1058C; 1059A; 1059B; 1059C; 1059D; 1060A; 1060D; 1064D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 568A; 596C; 597B; 597C; 598A; 598B; 598C; 599A; 599C; 608B (*nmr*)
Page, I.H. *et al., Biochem. Z.*, 1930, **220**, 304-326 (*fatty acid esters*)
Bladon, P. *et al., J.C.S.*, 1952, 2737-2744 (*uv, 3β-form*)
Johnson, D.R. *et al., J.A.C.S.*, 1953, **75**, 52-55 (*ir, 3β-form*)
Cook, R.P. *et al., Cholesterol (Chem., Biochem. Pathol.)*, Academic Press, N.Y., 1958, (*rev*)
Mahadevan, V. *et al., J. Lipid Res.*, 1962, **3**, 106-110 (*fatty esters*)
Johnson, W.S. *et al., Tetrahedron, Suppl.*, No. 8, 1966, 541-601 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 141 (*use*)
Mulheirn, L.J. *et al., Chem. Soc. Rev.*, 1972, **1**, 259-291 (*biosynth, rev, 3β-form*)
Yoshizawa, T. *et al., CA*, 1974, **82**, 83282k (*3β-form, sulfate, isol*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195-200 (*pmr*)
Bu'lock, J.D. *et al., Phytochemistry*, 1976, **15**, 1249-1251 (*biosynth*)
Hudec, J. *et al., Tetrahedron*, 1976, **32**, 2475-2506 (*cd*)
Partridge, L.G. *et al., J.O.C.*, 1977, **42**, 2799-2805 (*ms*)
Berman, E. *et al., J.O.C.*, 1977, **42**, 3325-3330 (*cmr*)
Piacenza, L.P.L. *et al., J.O.C.*, 1977, **42**, 3778-3379 (*synth*)
Shieh, H.S. *et al., Nature (London)*, 1977, **267**, 287-289 (*cryst struct*)
Joseph-Nathan, P. *et al., J.A.C.S.*, 1979, **101**, 1289-1291 (*3β-form, cmr*)
Sawzik, P. *et al., Liq. Cryst., Proc. Int. Conf.*, Pittsburgh, USA, 1979, 171 (*esters*)
Nakahara, M. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 2499-2501 (*esters*)
Tanabe, M. *et al., J.A.C.S.*, 1980, **102**, 862-863 (*3β,20S-form, synth, pmr*)
Fedarov, S.N. *et al., CA*, 1981, **97**, 69582 (*3β-sulfate, occur*)
Meiboom, S. *et al., Phys. Rev. A: Gen. Phys.*, 1981, **24**, 468-475 (*esters, props*)
Sucrow, W. *et al., Annalen*, 1982, 1897-1906 (*synth, ms*)
Schneider, H.J. *et al., J.O.C.*, 1982, **47**, 4216-4221 (*cmr*)
Ohmori, M. *et al., Tet. Lett.*, 1982, **23**, 4709-4712 (*synth*)
Goto, R. *et al., Chem. Pharm. Bull.*, 1983, **31**, 3528-3533 (*3β,20S-form, synth*)
Goodfellow, R.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **76**, 575-578 (*3β-form, 3β-sulfate, occur*)
Schmuff, N.R. *et al., J.O.C.*, 1983, **48**, 1404-1412 (*3β,20S-form, synth, pmr*)
D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1984, 2277-2282 (*3β-sulfate*)
Seo, S. *et al., J.C.S. Perkin 1*, 1986, 411-414 (*3β-form, pmr*)
Haider, S.I. *et al., J. Nat. Prod.*, 1987, **50**, 261-262 (*Chethoxyrol*)
Ramachandran, R. *et al., J. Magn. Reson.*, 1988, **79**, 357-362 (*cmr*)
Jarzębski, A. *et al., Steroids*, 1990, **55**, 256-258 (*20S-form, isol*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Fernandez, I. *et al., Synlett*, 1993, 489-490 (*formyl*)
Nagano, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 944-946 (*biosynth*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*3β-form, occur*)
Li, G. *et al., Steroids*, 2005, **70**, 13-18 (*formyl*)

Cholest-7-en-3-ol, 9CI C-625



(3α,5α)-*form*

$C_{27}H_{46}O$ 386.66

(3α,5α)-*form* [24039-00-7]
Cryst. (hexane/Et_2O). Mp 175-176°. $[\alpha]_D$ +1 (c, 0.68 in $CHCl_3$).

(3β,5α)-*form*
Lathosterol. *γ-Cholesterol*
[80-99-9]
Isol. from *Ambrosia elatior*, *Asterias rubens*, *Asterias pectinifera*, *Cucumaria* sp., *Eupentacta fraudatrix*, *Bathyplotes natans*, *Holothuria nobilis*, *Holothuria scabra*, *Trochostoma orientale*, *Marthasterias glacialis*, *Henricia sanguinolenta* and *Psolus fabricii*. Intermed. in biosyth. of steroids in the echinoderms. Shows antimutagenic activity. Needles (Me_2CO).
Mp 125-127°. $[\alpha]_D^{23}$ +4.8 (c, 0.90 in $CHCl_3$).
▶ FZ7000000

3-O-*Sulfate:* [80685-30-9]
[151891-06-4]
$C_{27}H_{46}O_4S$ 466.724
Constit. of *Parathyona* sp., *Asterias rubens*, *Psolus fabricii*, *Henricia downeyae*, *Marthasterias glacialis*, *Henricia sanguinolenta*, *Eupentacta fraudatrix* and *Cucumaria lactea*.

3-O-*β-D-Xylopyranoside:* [74185-03-8]
$C_{32}H_{54}O_5$ 518.776
Constit. of *Eupentacta fraudatrix*.

Ac: [2465-00-1]
$C_{29}H_{48}O_2$ 428.697
Cryst. (MeOH). Mp 119-121°. $[\alpha]_D^{21}$ +2.5 (c, 0.84 in $CHCl_3$).

(3β,5α,14β)-*form* [59531-50-9]
Mp 90°. $[\alpha]_D^{21}$ -6.21 (c, 1 in $CHCl_3$).

Ac: [59531-52-1]
Oil.

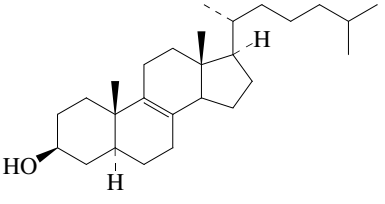
(3β,5β)-*form* [16826-36-1]
Cryst. (Me_2CO aq.). Mp 105-106°. $[\alpha]_D^{22}$ +49 ($CHCl_3$).

Ac: [16826-37-2]
Cryst. (Et_2O/MeOH). Mp 90-91°. $[\alpha]_D$ +48 ($CHCl_3$).

[6036-58-4]

Evans, D.E. *et al., J.C.S.*, 1956, 4821-4824 (*synth*)
Cohen, C.F. *et al., Steroids*, 1967, **9**, 591-600 (*synth, 3β,5β-form*)
Sucrow, W. *et al., Chem. Ber.*, 1969, **102**, 2629-2635 (*synth, pmr, ms, 3β,5α-form*)
Ener, M.A. *et al., J. Biol. Chem.*, 1973, **248**, 6697-6700 (*ir, ms, 3β,5α-form*)
Breslow, R. *et al., J.A.C.S.*, 1973, **95**, 3251-3262 (*synth, pmr, 3α,5α-form*)
Anastasia, M. *et al., J.C.S. Perkin 1*, 1976, 378-380 (*synth, ir, 3β,5α,14β-form*)
Hudec, J. *et al., Tetrahedron*, 1976, **32**, 2475-2506 (*cd*)
Tsuda, M. *et al., J.O.C.*, 1979, **44**, 1282-1289; 1290-1293 (*cmr, 3β,5α-form*)
Ishige, M. *et al., Can. J. Chem.*, 1980, **58**, 1061-1068 (*synth, ir, pmr, 3α,5α-form*)
Galbraith, M.N. *et al., Aust. J. Chem.*, 1981, **34**, 2607-2618 (*synth, ir, pmr, 3β,5β-form*)
Smetanina, O.F. *et al., Khim. Prir. Soedin.*, 1981, 585-588; *Chem. Nat. Compd. (Engl. Transl.)*, 1981, **17**, 422-424 (*3β,5α-form, sulfate*)
Ohmoto, T. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2780-2786 (*isol, synth, ir, pmr, cmr, 3β,5α-form*)
Goodfellow, R.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **76**, 575-578 (*3β,5α-form, occur, sulfate*)
Goad, L.J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **84**, 189-196 (*3β,5α-form, sulfate*)
Cordiero, M.L. *et al., Tet. Lett.*, 1988, **29**, 2159-2162 (*biosynth*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*xyloside*)
Devarenne, T.P. *et al., Phytochemistry*, 1995, **40**, 1125-1131 (*biosynth*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*3β,5α-form, occur*)
Han, Y.H. *et al., Biol. Pharm. Bull.*, 2000, **23**, 1247-1249 (*isol, activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, CMD000

Cholest-8-en-3-ol C-626



(3β,5α)-*form*

$C_{27}H_{46}O$ 386.66

(3β,5α)-*form*
Zymostenol
[566-97-2]
Constit. of *Axinella cannabina* and *Chattonella antiqua*.
Cryst. (MeOH).
Mp 128-129°. $[\alpha]_D^{23}$ +51.6 (c, 1.26 in $CHCl_3$).

Ac: [5258-86-6]
$C_{29}H_{48}O_2$ 428.697
Plates (EtOAc/MeOH). Mp 123.5-125°. $[\alpha]_D^{25}$ +52 (c, 1.80 in $CHCl_3$).

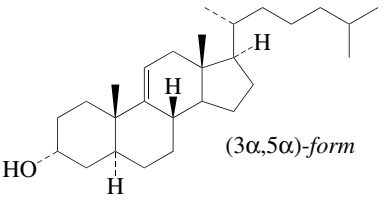
(3β,5α,14β)-*form* [73465-16-4]
Oil.

Ac: [73465-17-5]
Liq. $[\alpha]_D^{22}$ +92 ($CHCl_3$).

[7199-91-9, 17137-74-5]

Ellis, B. *et al., J.C.S.*, 1951, 2402 (*synth, ir, 3β,5α-form*)
Bladon, P. *et al., J.C.S.*, 1952, 2737 (*uv, 3β,5α-form*)
Tsuda, K. *et al., J.A.C.S.*, 1954, **76**, 2933 (*synth, 3β,5α-form*)
Tsuda, M. *et al., J.O.C.*, 1979, **44**, 1290 (*cmr, 3β,5α-form*)
Anastasia, M. *et al., J.O.C.*, 1980, **45**, 2528 (*synth, 3β,5α,14β-form*)
Anastasia, M. *et al., J.O.C.*, 1981, **46**, 3421 (*synth, 3β,5α-form*)
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*Axinella, isol*)
Groenneberg, T.O. *et al., Chem. Scr.*, 1984, **24**, 100-103 (*Castor fiber, isol*)
Nichols, P.D. *et al., Phytochemistry*, 1987, **26**, 2537-2541 (*Chattonella, isol*)
Dolle, R.E. *et al., Chem. Comm.*, 1988, 19 (*synth, 3β,5α-form*)
Wilson, W.K. *et al., J. Lipid Res.*, 1996, **37**, 1529-1555 (*pmr, cmr*)

Cholest-9(11)-en-3-ol, 9CI C-627



(3α,5α)-*form*

$C_{27}H_{46}O$ 386.66

(3α,5α)-*form* [37772-32-0]
Cryst. (EtOH). Mp 164-167° (155-157°). $[\alpha]_D$ +26 ($CHCl_3$).

Ac: [37772-03-5]
$C_{29}H_{48}O_2$ 428.697
Mp 80.5-82°.

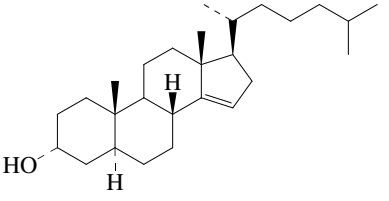
(3β,5α)-*form* [23820-76-0]
Constit. of *Cladolabes bifurcatus*, *Cucumaria* sp., *Eupentacta fraudatrix*, *Holothuria nobilis*, *Holothuria scabra* and *Synapta maculata*.
Cryst. (MeOH).
Mp 134-135°. $[\alpha]_D^{25}$ +25 (c, 0.13 in $CHCl_3$).

3-O-β-D-Xylopyranoside: [151890-78-7]
$C_{32}H_{54}O_5$ 518.776
Constit. of *Eupentacta fraudatrix*.

Ac: [64548-09-0]
Needles (MeOH). Mp 105-108°. $[\alpha]_D^{25}$ +24 (c, 0.17 in $CHCl_3$).

Edward, J.T. *et al., J.O.C.*, 1970, **35**, 1426-1430 (*synth, ir, 3β,5α-form*)
Schneider, J.J. *et al., Tetrahedron*, 1972, **28**, 2717 (*synth, 3β,5α-form*)
Breslow, R. *et al., J.A.C.S.*, 1973, **95**, 3251-3262; 1977, **99**, 905-911 (*synth, pmr, ir, bibl*)
Morisaki, M. *et al., Chem. Pharm. Bull.*, 1984, **32**, 865-871 (*synth, pmr, ms, 3β,5α-form*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*xyloside*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*3β,5α-form, occur*)
Ponomarenko, L.P. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2001, **128**, 53-62 (*3β,5α-form, occur*)

Cholest-14-en-3-ol C-628



(3α,5α)-*form*

$C_{27}H_{46}O$ 386.66

(3α,5α)-*form* [35479-88-0]
Cryst. (MeCN). Mp 128-129°. $[\alpha]_D$ +27 ($CHCl_3$). Forms 1:1 solvate with solvent alcohol.

(3α,5β)-*form* [59462-96-3]
Mp 172.5-173°.

(3β,5α)-*form* [20780-35-2]
Constit. of zooxanthellae isol. from *Aiptasia pulchella*.
Cryst. (MeOH). Mp 129-130°. $[\alpha]_D^{20}$ +30.5 (c, 1 in $CHCl_3$).

Benzoyl: [6673-66-1]
Cryst. (Me_2CO). Mp 167-168°. $[\alpha]_D$ +32 ($CHCl_3$).

Ac: [40446-06-8]

$C_{29}H_{48}O_2$ 428.697
Needles (MeOH). Mp 91-92°. $[\alpha]_D$ +22.8 (c, 1.6 in $CHCl_3$).

(3β,5β)-*form* [16826-41-8]
Needles (Me_2CO/MeCN). Mp 115°. $[\alpha]_D$ +27 (c, 1 in $CHCl_3$).

Benzoyl: [16826-40-7]
Cryst. (Me_2CO/MeOH). Mp 88-90°. $[\alpha]_D$ +47 (c, 1 in $CHCl_3$).

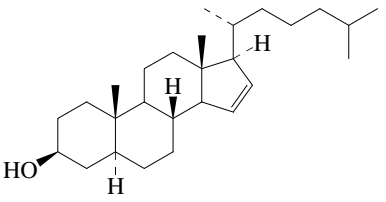
(3β,5α,17α)-*form* [56193-34-1]

Benzoyl: [66808-37-5]
Cryst. (MeOH). Mp 67-70°. $[\alpha]_D^{21}$ +61.1 ($CHCl_3$).

Cragg, G.M.L. *et al., J.C.S.(C)*, 1966, 1266 (*synth, 3β,5α-form*)
Cohen, C.F. *et al., Steroids*, 1967, **9**, 591 (*synth, 3β,5β-form*)
Breslow, R. *et al., J.A.C.S.*, 1970, **92**, 732; 1973, **95**, 3251 (*synth, ir, pmr, 3α,5α-form*)
Caspi, E. *et al., J.O.C.*, 1975, **40**, 2005 (*pmr, cmr, 3β,5α,17α-form*)
Corcoran, R.J. *et al., Tet. Lett.*, 1976, 317 (*synth*)
Anastasia, M. *et al., J.O.C.*, 1978, **43**, 3505 (*synth*)
Schroepfer, G.J. *et al., Chem. Phys. Lipids*, 1981, **29**, 201 (*synth, 3β,5β-form*)
Withers, N.W. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1982, **79**, 3764-3768 (*isol*)

Cholest-15-en-3-ol, 9CI C-629

[83681-83-8]

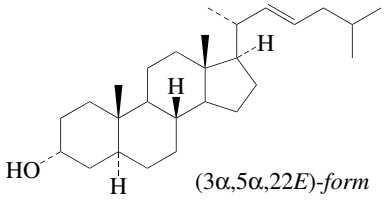


$C_{27}H_{46}O$ 386.66

(3β,5α)-*form*
Constit. of *Topsentia aurantiaca*.

Eggersdorfer, M.L. *et al., J.O.C.*, 1982, **47**, 5304 (*synth, ms*)
Ciminiello, P. *et al., Steroids*, 1992, **57**, 62 (*isol, pmr, cmr*)

Cholest-22-en-3-ol, 9CI C-630



(3α,5α,22*E*)-*form*

$C_{27}H_{46}O$ 386.66

(3α,5α,22*E*)-*form* [115305-06-1]
Constit. of sponge *Esperiopsis edwardii*.

(3β,5α,22*E*)-*form* [58560-38-6]
Constit. of scallop *Patinopecten yessoensis*; sponges *Esperiopsis edwardii* or *Axinella cannabina*; also found in jellyfish.
Mp 121°. $[\alpha]_D$ +12 (c, 0.4 in$CHCl_3$).

3-O-*Sulfate:* [151891-01-9]
$C_{27}H_{46}O_4S$ 466.724
Constit. of *Eupentacta fraudatrix*.

3-O-*β-D-Xylopyranoside:* [74185-09-4]
$C_{32}H_{54}O_5$ 518.776
Constit. of *Eupentacta fraudatrix*.

Ac: [39832-68-3]
Mp 105-106.5°. $[\alpha]_D$ 0 ($CHCl_3$).

(3β,5α,22*Z*)-*form* [60325-48-6]

Ac: [62787-96-6]
Mp 104-105.5°.

(3β,5α,22ξ)-*form*
Constit. of *Hymeniacidon perleve*. Cryst. (MeOH). Mp 117-117.5°.

Ac:
Cryst. (MeOH). Mp 104-108°.

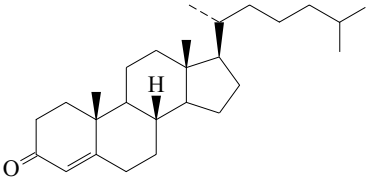
(3β,5β,22*E*)-*form*
Isol. from sponge *Petrosia ficiformis*, prob. as an endobacterial metab.

[39832-30-9]

Erdman, T.R. *et al., Tetrahedron*, 1972, **28**, 5163 (*isol, 3β,5α-form*)
Kobayashi, M. *et al., Steroids*, 1975, **26**, 605 (*isol, ms, 3β,5α,22E-form*)
Tam Ha, T.B. *et al., Steroids*, 1982, **40**, 433 (*isol, ms, 3β,5β,22E-form*)
Seidel, S.B. *et al., Steroids*, 1986, **47**, 49-62 (*3β,5β,22E-form*)
Seldes, A.M. *et al., Tetrahedron*, 1988, **44**, 1359 (*isol, pmr, ms*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)

Cholest-4-en-3-one, 9CI C-631

[601-57-0]



$C_{27}H_{44}O$ 384.644
Isol. from the sponges *Cinachyra tarentina*, *Damiriana hawaiiana* and *Stelletta clarella* and from the roots and resin of *Dracaena cinnabari*. Cryst. (Me_2CO/MeOH).
Mp 80-81.5°. $[\alpha]_D^{22}$ +87 (c, 0.1 in $CHCl_3$).

▶ FZ7700000

E-*Oxime:* [66538-08-7]
$C_{27}H_{45}NO$ 399.659
Mp 65° Mp 152° (double Mp).

Z-Oxime: [66514-00-9]
$C_{27}H_{45}NO$ 399.659
Mp 152-153°.

E-*2,4-Dinitrophenylhydrazone:* [13914-34-6]
Cryst. (C_6H_6/MeOH). Mp 239-240°.

Z-2,4-Dinitrophenylhydrazone: [13914-35-7]
Cryst. (C_6H_6/MeOH). Mp 199-201°.

10α-*form* [23820-66-8]
Oil.

2,4-Dinitrophenylhydrazone: [23820-67-9]
Red cryst. Mp 185-185.5°.

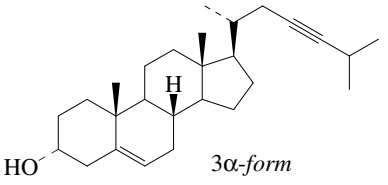
(±)-*form* [14615-14-6]
Mp 113-115° Mp 120-121° (double Mp).

[22033-87-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1052C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 578B (*nmr*)
Oppenauer, R.V. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1937, **56**, 137-144 (*synth*)
Horvath, J. *et al., Nature (London)*, 1947, **160**, 639 (*synth*)
Oppenauer, R.V. *et al., Org. Synth., Coll. Vol., 3*, 1955, 207-209 (*synth*)
Parsons, J. *et al., Anal. Chem.*, 1956, **28**, 1514-1518 (*cryst struct*)
Henbest, H.B. *et al., J.C.S.*, 1957, 997-1000 (*ir*)
Labhart, H. *et al., Helv. Chim. Acta*, 1959, **42**, 2219-2227 (*uv*)
Org. Synth., Coll. Vol., 4, 1963, 192-195; 195-201 (*synth*)
Keana, J.F.W. *et al., Steroids*, 1964, **4**, 457-462 (*synth, uv, (±)-form*)
Haner, B. *et al., Acta Cryst.*, 1966, **20**, 930 (*cryst struct*)
Johnson, W.S. *et al., Tetrahedron*, Suppl. No. 8, 1966, 541-601 (*synth, uv, (±)-form*)
Edward, J.T. *et al., J.O.C.*, 1970, **35**, 1426-1430 (*synth, ir, 10α-form*)
Westphal, D. *et al., Annalen*, 1975, 2038-2052 (*synth, ir, pmr*)
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 14701-1476 (*isol, Damiriana*)
Brown, F.J. *et al., J.A.C.S.*, 1980, **102**, 807-817 (*ms*)
Kirk, D.N. *et al., J.C.S. Perkin 1*, 1980, 2591-2596 (*synth*)
Manley, R.P. *et al., J.O.C.*, 1980, **45**, 4385-4387 (*synth*)
Rizvi, S.Q.A. *et al., J.O.C.*, 1981, **46**, 1127-1132 (*cmr*)

Lee, K.M. *et al., Nouv. J. Chim.*, 1986, **10**, 675 (*synth*)
Lin, H.-J. *et al., Synth. Commun.*, 1986, **16**, 1357-1361 (*synth*)
Iida, T. *et al., Magn. Reson. Chem.*, 1987, **25**, 558-560 (*cmr*)
Masooud, M. *et al., Phytochemistry*, 1995, **38**, 795-796 (*isol, Dracaena*)

Cholest-5-en-23-yn-3-ol C-632



$C_{27}H_{42}O$ 382.628

3α-form

5β,6-Dihydro: [123158-90-7]
Minor sterol of *Calyx nicaeensis*, prob. as endobacterial metab.

3β-*form* [63015-91-8]
Constit. of *Calyx nicaeensis*.
Needles (MeOH).
Mp 119-120°. $[\alpha]_D$ -38.8 ($CHCl_3$).

Ac: [63015-90-7]
Mp 118-121°. $[\alpha]_D$ -38.4 (c, 4 in $CHCl_3$).

5β,6-Dihydro: Cholest-23-yn-3-ol. Coprost-23-yn-3-ol
[124660-17-9]
$C_{27}H_{44}O$ 384.644
Minor sterol in sponge *Calyx nicaeensis*, prob. as an endobacterial metab.

Steiner, E. *et al., Helv. Chim. Acta*, 1977, **60**, 475-481 (*isol, synth*)
Ha, T.B.T. *et al., Steroids*, 1989, **53**, 487-489 (*dihydro*)
Atta-ur-Rahman, *et al., Phytochemistry*, 1999, **52**, 495-499 (*isol, ir, pmr, ms*)

Choline C-633

2-Hydroxy-N,N,N-*trimethylethanaminium(1+), 9CI. (2-Hydroxyethyl)trimethylammonium. Amanitin*†. *Arachine. Araquine. Bilineurine. Sincalin. Sinkalin*
[62-49-7]
$Me_3N^{\oplus}CH_2CH_2OH$
$C_5H_{14}NO^{\oplus}$ 104.172
Occurs free and combined in many animal and vegetable prods., e.g. bile, brain, yolk of egg, hops, belladonna, strophanthus, and the seeds, leaves and stems of many other plants. Constit. of Lecithin.
Acetylcholine precursor. Present free and as esters in the hypobranchial glands of molluscs. Lipotropic agent. Nutritional supplement.

▶ FZ9625000

Sulfate (inner salt): N,N,N-*Trimethyl-2-(sulfooxy)ethanaminium hydroxide inner salt, 9CI. Cholinesulfuric acid*
[4858-96-2]
$C_5H_{13}NO_4S$ 183.228
Present in *Penicillium* spp., *Aspergillus sydowi, Porphyra umbilicalis, Ptilota pectinata* and *Dermatiscum thunbergii*. Cryst.
Mp 300° dec.

O-*(3-Methyl-2-butenoyl):* ***Senecioylcholine****. β,β-Dimethylacrylylcholine*
[20284-79-1]
$C_{10}H_{20}NO_2^{\oplus}$ 186.274
Alkaloid from the hypobranchial body of the marine snail *Thais floridana*. Also isol. in salt form from the gastropod *Mancinella keineri*. Sol. H_2O.
Mp 160° (as iodide).

O-*(2-Pentadecenoyl):* [116613-92-4]
$C_{20}H_{40}NO_2^{\oplus}$ 326.542
Constit. of toxic skin secretions of the trunkfish *Anoplocapros lenticularis*. *E*- and *Z*-isomers detected. Poss. artifact derived from homologue of Pahutoxin, P-47. Genus name incorr. given as Anoplacapros.

O-*(2-Hexadecenoyl):*
$C_{21}H_{42}NO_2^{\oplus}$ 340.568
Constit. of the toxic skin secretions of the trunkfish *Anoplocapros lenticularis*, *Aracana aurita*, *Aracana ornata*, *Lactoria fornasini*, *Ostracion cubicus*, *Rhinesomas reipublicae*, *Strophiurichthys inermis* and *Strophiurichthys robustus*. *E*- and *Z*-isomers detected. Poss. artifact.

O-*(2-Heptadecenoyl):*
$C_{22}H_{44}NO_2^{\oplus}$ 354.595
Constit. of the toxic skin secretions of the trunkfish *Anoplocapros lenticularis*, *Aracana ornata*, *Lactoria fornasini*, *Ostracion cubicus* and *Strophiurichthys robustus*. *E*- and *Z*-isomers detected. Poss. artifact.

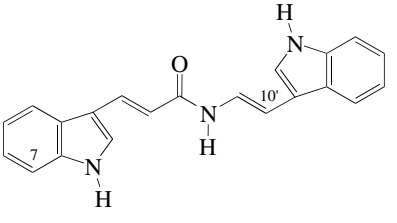
O-*(2-Octadecenoyl):*
$C_{23}H_{46}NO_2^{\oplus}$ 368.622
Constit. of toxic skin secretions of the trunkfish *Anoplocapros lenticularis* and *Aracana ornata*. *E*- and *Z*-isomers detected. Poss. artifact.

[87-67-2, 23038-04-2, 55357-38-5, 64681-08-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 395D; **2**, 292B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 616C; 859C (*nmr*)
Renshaw, R.R. *et al., J.A.C.S.*, 1910, **32**, 128 (*synth*)
Fourneau, E. *et al., Bull. Soc. Chim. Fr.*, 1914, **15**, 548 (*esters, synth*)
Tammelin, L.E. *et al., Acta Chem. Scand.*, 1956, **10**, 145-146 (*esters, synth*)
Whitaker, V.P. *et al., Biochem. J.*, 1959, **71**, 32-34 (*3-methyl-2-butenoyl*)
Harper, S.H. *et al., Chem. Ind. (London)*, 1966, 419 (*sulfate*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 142 (*use*)
Byrn, S.R. *et al., J.O.C.*, 1976, **41**, 2283 (*conformn, ir, cryst struct*)
Baker, J.T. *et al., Tet. Lett.*, 1976, 1233-1234 (*Choline, Senecioylcholine, occur, molluscs*)
Zeisel, S.H. *et al., Annu. Rev. Nutr.*, 1981, **1**, 195 (*rev*)
Goldberg, A.S. *et al., Toxicon*, 1988, **26**, 651-663 (*alkenoyl derivs, occur*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 199 (*rev*)
Frydenvang, K. *et al., Acta Cryst. C*, 1992, **48**, 1343; 1994, **50**, 617 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1037; 1317

Chondriamide A C-634

*3-(1*H-*Indol-3-yl)*-N-*[2-(1*H-*indol-3-yl)ethenyl]-2-propenamide, 9CI*
[142677-09-6]



$C_{21}H_{17}N_3O$ 327.385
Alkaloid from the red alga *Chondria* sp. Cytotoxic. Shows antiviral activity. Anthelmintic agent. Yellow cryst. (MeOH aq.).
Mp 193-194°. λ_{max} 208 (ε 27700); 226 (ε 31200); 278 (ε 12900); 364 (ε 26500) (MeOH) (Derep).

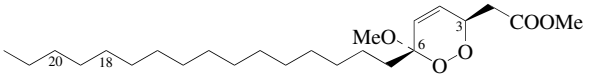
(10'Z)-Isomer: ***Chondriamide C***
[218774-24-4]
$C_{21}H_{17}N_3O$ 327.385
Alkaloid from *Chondria atropurpurea*. Anthelmintic agent. Yellow powder.
Mp 230.5-232°. λ_{max} 208 (log ε 4.43); 275 (log ε 3.7); 358 (log ε 4.33) (MeOH).

7-Hydroxy: ***Chondriamide B***
[142677-10-9]
$C_{21}H_{17}N_3O_2$ 343.384
From *Chondria* sp. Cytotoxic. Shows mild antifungal activity. Yellow cryst. (MeOH aq.).
Mp 208-209°. λ_{max} 208 (ε 27700); 226 (ε 31200); 278 (ε 12900); 364 (ε 26500) (MeOH) (Derep). λ_{max} 206 (ε 26154); 222 (ε 25134); 274 (ε 10923); 368 (ε 21846) (MeOH) (Berdy).

Palermo, J.A. *et al., Tet. Lett.*, 1992, **33**, 3097-3100 (*isol, uv, ir, pmr, cmr, ms, struct, Chondriamide B*)
Davyt, D. *et al., J. Nat. Prod.*, 1998, **61**, 1560-1563 (*Chondriamide C, isol, pmr, cmr*)
Wang, X. *et al., J.O.C.*, 2001, **66**, 8215-8221 (*synth*)

Chondrillin C-635

Methyl 6-hexadecyl-3,6-dihydro-6-methoxy-1,2-dioxin-3-acetate, 9CI



(3*R*,6*S*)-*form*

$C_{24}H_{44}O_5$ 412.609

Abs. configs. revised in 1997.

(3*R*,6*S*)-*form*

(+)-trans-*form*

[61656-50-6]

Constit. of *Chondrilla* spp.

Pale yellow oil which forms a waxy solid.

Mp 30°. $[\alpha]_D^{20}$ +144.

20,21-Didehydro: ***20*E-*Chondrillene***

[131985-18-7]

$C_{24}H_{42}O_5$ 410.593

Constit. of *Plakortis lita*. Oil.

18,19,20,21-Tetradehydro: ***18*E,*20*E-*Chondrillidiene***

[131985-19-8]

$C_{24}H_{40}O_5$ 408.577

Constit. of *Plakortis lita*. Light yellow oil.

(3*S*,6*S*)-*form*

(+)-cis-*form*. ***Plakorin***. 6-epi-*Chondrillin*

[124264-01-3]

Constit. of *Plakortis* spp. Antitumour agent. Solid.

Mp 42.5-43.5°. $[\alpha]_D^{30}$ +30.5 (c, 1.09 in $CHCl_3$). $[\alpha]_D^{27}$ +44.3 (c, 0.2 in $CHCl_3$).

20,21-Didehydro: ***3*-epi-*20*E-*Chondrillene***

[132074-83-0]

$C_{24}H_{42}O_5$ 410.593

Constit. of *Plakortis lita*. Solid.

Mp 34-35°. $[\alpha]_D$ +22.5 (c, 0.16 in $CHCl_3$).

18,19,20,21-Tetradehydro: ***3*-epi-*18*E,*20*E-*Chondrillidiene***

[132076-73-4]

$C_{24}H_{40}O_5$ 408.577

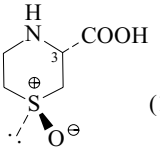
Constit. of *Plakortis lita*. Solid.

Mp 28-29°. $[\alpha]_D$ +21.1 (c, 0.39 in $CHCl_3$).

Wells, R.J. *et al., Tet. Lett.*, 1976, 2637 (*isol*)
Murayama, T. *et al., Experientia*, 1989, **45**, 898 (*Plakorin*)
De Guzman, F.S. *et al., J. Nat. Prod.*, 1990, **53**, 926 (*isol, pmr, cmr*)
Snider, B.B. *et al., J.A.C.S.*, 1992, **114**, 1790 (*synth*)
Dussault, P.H. *et al., J.A.C.S.*, 1997, **119**, 3824-3825 (*synth, abs config*)
Dussault, P.H. *et al., J.O.C.*, 1999, **64**, 1789-1797 (*synth*)

Chondrine C-636

*3-Thiomorpholinecarboxylic acid 1-oxide, 9CI. Tetrahydro-2*H*-1,4-thiazine-3-carboxylic acid 1-oxide. Yunaine. Apocycloalliin*



(1*S*,3*R*)–*form*

$C_5H_9NO_3S$ 163.197

(1*S*,3*R*)-*form* [23652-74-6]

Constit. of red alga *Chondria crassicaulis*, green alga *Enteromorpha linza* and brown algae *Undaria pinnatifida* and *Zonaria sinclairii*.

Mp 252° dec. (sealed tube). $[\alpha]_D^{26}$ +19 (c, 1.0 in H_2O).

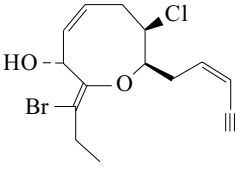
(1*S*,3*S*)-*form*

$[\alpha]_D^{25}$ -55.1 (H_2O).

Tominaga, F. *et al., J. Biochem. (Tokyo)*, 1963, **54**, 222 (*isol*)
Carson, J.F. *et al., J.O.C.*, 1964, **29**, 2203 (*synth*)
Däbritz, E. *et al., Chem. Ber.*, 1965, **98**, 781 (*synth*)
Madgwick, J.C. *et al., Arch. Biochem. Biophys.*, 1970, **141**, 766 (*isol*)
Carson, J.F. *et al., J.O.C.*, 1970, **35**, 1594 (*synth, pmr*)
Fowden, L. *et al., J.C.S.(C)*, 1971, 833 (*uv, cd*)
Palmer, K.J. *et al., Acta Cryst. B*, 1972, **28**, 2789 (*cryst struct*)
Shiraiwa, T. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 341-347 (*synth*)

Chondriol C-637

[41744-44-9]



$C_{15}H_{18}BrClO_2$ 345.663

Revised struct. Constit. of *Chondria oppositiclada*. Shows antibiotic activity. Oil. Sol. MeOH, hexane. λ_{max} 221 (ϵ 98000) (MeOH) (Berdy).

Ac:

$C_{17}H_{20}BrClO_3$ 387.7

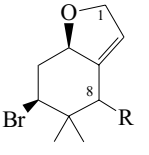
Cryst. Mp 53-54.5°. $[\alpha]_D$ +54.9 (MeOH).

Fenical, W. *et al., Tet. Lett.*, 1974, 1507

Chondrocole A C-638

*6-Bromo-4-chloro-2,4,5,6,7,7*a*-hexahydro-5,5-dimethylbenzofuran, 9CI. 6-Bromo-8-chloro-1,4-epoxy-2-ochtodene*

[57461-72-0]



R = α–Cl

$C_{10}H_{14}BrClO$ 265.577

Constit. of *Chondrococcus hornemanni*. Oil. $[\alpha]_D$ -16 (c, 6.2 in $CHCl_3$).

8-Epimer: ***Chondrocole B***

[57496-04-5]

$C_{10}H_{14}BrClO$ 265.577

Constit. of *Chondrococcus hornemanni*. Oil.

1-Oxo: ***Chondrocolactone***. *6-Bromo-4-chloro-5,6,7,7*a*-tetrahydro-5,5-dimethyl-2(4*H*)-benzofuranone, 9CI. 6-Bromo-8-chloro-1,4-epoxy-2-ochtoden-1-one*

[68612-44-2]

$C_{10}H_{12}BrClO_2$ 279.56

Constit. of *Chondrococcus hornemanni*. Cryst. (CH_2Cl_2/hexane). Mp 107-108°. $[\alpha]_D^{24}$ -48 (c, 0.6 in CH_2Cl_2).

Burreson, B.J. *et al., Tet. Lett.*, 1975, 2155 (*isol*)
Woolard, F.X. *et al., Tet. Lett.*, 1978, 2367 (*cmr, struct*)

Chondrocole C C-639

*4,6-Dibromo-2,4,5,6,7,7*a*-hexahydro-5,5-dimethylbenzofuran, 9CI. 6,8-Dibromo-1,4-epoxy-2-ochtodene*

[58086-77-4]

As Chondrocole A, C-638 with R = β-Br

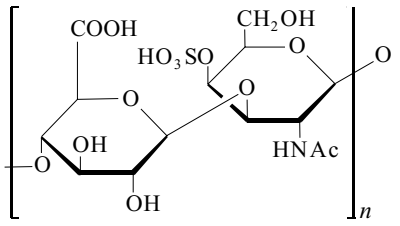
$C_{10}H_{14}Br_2O$ 310.028

Constit. of *Chondrococcus hornemanni*.

Burreson, B.J. *et al., Chem. Lett.*, 1975, 1111

Chondroitin sulfate C-640

Chondroitinsulfuric acid



$C_{14}H_{21}NO_{14}S$ 459.384

Mucopolysaccharides containing D-Glucuronic acid and sulfated *N*-Acetyl-D-galactosamine. MW = 20,000-50,000. Polymeric. Minimum formula given. Type A (illus.) is the 4-sulfate and type C is the 6-sulfate. A 4,6-di-*O*-sulfated variant is also known. Main source human cartilage and aorta (type A), heart valves, shark cartilage (type C). Component of the heparinoid danaparoid. Used in the treatment of ischaemic heart disease, osteoporosis and hyperlipidaemias. Also used as an adjunct to ocular surgery. Shows antiviral activity against tobacco mosaic virus. $[\alpha]_D$ -25 (H_2O) (type A).

▶ Exp. teratogen.

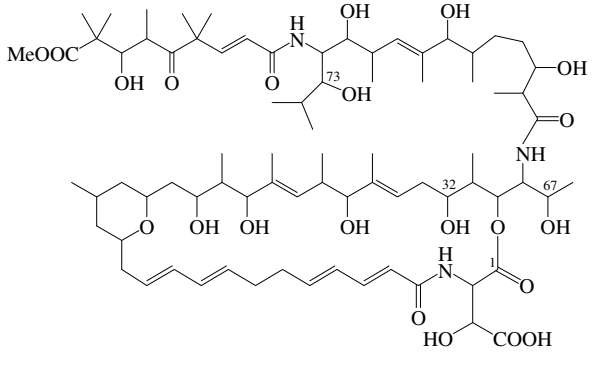
Na salt: ***Chondroitin sulfate sodium, JAN***
[9082-07-9]
[12678-07-8 (6-sulfate, Na salt), 39455-18-0 (4-sulfate, Na salt)]
$[\alpha]_D^{20}$ -12 (H_2O) (type C).

[24967-93-9 (4-sulfate), 25322-46-7 (6-sulfate)]

Jeanloz, R.W. *et al., Methods Carbohydr. Chem.*, 1972, **5**, 110 (*prep*)
Brewer, C.F. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1975, **72**, 3421 (*cmr*)
Hamer, G. *et al., Carbohydr. Res.*, 1976, **49**, 37 (*pmr*)
Lindahl, U. *et al., Annu. Rev. Biochem.*, 1978, **47**, 385
Carr, S.A. *et al., J. Carbohydr. Chem.*, 1984, **3**, 381-401 (*ms*)
Probst, L.E. *et al., J. Cataract. Refract. Surgery*, 1994, **20**, 145 (*use*)
Sano, Y. *et al., Carbohydr. Polym.*, 1997, **33**, 125-129 (*activity*)
Yeung, B.K.S. *et al., J. Carbohydr. Chem.*, 2002, **21**, 799-865 (*rev, synth*)
Martindale, The Extra Pharmacopoeia, 33rd edn., Pharmaceutical Press, 2002, 1594

Chondropsin B C-641

[301847-25-6]



$C_{79}H_{129}N_3O_{22}$ 1472.895
Isol. from the sponge *Chondropsis* sp. Antitumour agent. Powder. $[\alpha]_D^{27}$ +30.6 (c, 0.36 in MeOH). λ_{max} 227 (ϵ 14790); 260 (ϵ 13120) (MeOH).

*32-*O*-(3-Carboxy-3-hydroxypropanoyl):* ***Chondropsin A***
[301847-23-4]
$C_{83}H_{133}N_3O_{26}$ 1588.968
Isol. from sponges *Chondropsis* sp. and *Psammoclemma* sp. Antitumour agent. Powder. $[\alpha]_D^{27}$ +7.1 (c, 0.28 in MeOH). λ_{max} 229 (ϵ 15370); 259 (ϵ 16230) (MeOH).

*73-Deoxy, 32-*O*-(3-carboxy-3-hydroxypropanoyl):* ***73-Deoxychondropsin A***
[336820-20-3]
$C_{83}H_{133}N_3O_{25}$ 1572.969
Isol. from the sponges *Ircinia* sp. and *Psammoclemma* sp. Cytotoxic agent. Powder. $[\alpha]_D$ +2 (c, 0.3 in MeOH). λ_{max} 216 (log ϵ 4.62); 226 (log ϵ 4.61); 261 (log ϵ 4.56) (MeOH).

*73-Deoxy, de(methoxycarbonyl), 32-*O*-(3-carboxy-3-hydroxypropanoyl):* ***Chondropsin C***
[336820-22-5]
$C_{81}H_{131}N_3O_{23}$ 1514.932
Isol. from an *Ircinia* sp. sponge. Cytotoxic agent. Powder. $[\alpha]_D$ +2.7 (c, 0.3 in MeOH). λ_{max} 222 (log ϵ 4.66); 228 (log ϵ 4.64); 261 (log ϵ 4.58) (MeOH).

*(1→67)-Lactone isomer, 32-*O*-(3-carboxy-3-hydroxypropanoyl):* ***Chondropsin D***
[374564-50-8]
$C_{83}H_{133}N_3O_{26}$ 1588.968
Isol. from a *Chondropsis* sp. Gum. $[\alpha]_D^{27}$ -5 (c, 0.06 in MeOH). λ_{max} 225 (log ϵ 4.18); 262 (log ϵ 4.01) (MeOH).

Cantrell, C.L. *et al., J.A.C.S.*, 2000, **122**, 8825-8829 (*Chondropsins A,B*)
Rashid, M.A. *et al., J. Nat. Prod.*, 2001, **64**, 1341-1344 (*Chondropsin D*)
Rashid, M.A. *et al., Tet. Lett.*, 2001, **42**, 1623-1626 (*73-Deoxychondropsin A, Chondropsin C*)
Chevallier, C. *et al., Nat. Prod. Res.*, 2004, **18**, 479-484 (*Psammoclemma isolates*)

Chondrosione C-642

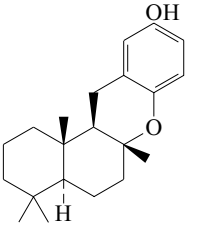
[62111-85-7]
[62111-86-8]

$C_{21}H_{28}O_3$ 328.45

Struct. not fully determined. A tetracyclic triolefinic β-diketone also contg. an epoxide grouping. Isol. from a sponge *Chondrosia* sp. Shows antimicrobial props. Golden noncryst. solid. There are no compds. on the DNP database of known struct. fitting these structural requirements and MF (2005).

Ravi, B.N. *et al., CA*, 1974, **86**, 145824

Chromazonarol C-643



(+)–*form*

$C_{21}H_{30}O_2$ 314.467
λ_{max} 210 (ϵ 16200); 300 (ϵ 3100) (MeOH) (Derep).

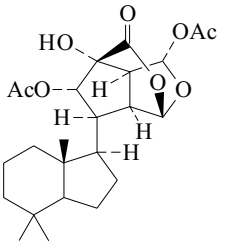
(+)-form
ent-*Chromazonarol*
[57457-77-9]
Constit. of *Dysidea pallescens.*
Ac:
Cryst. (petrol). Mp 118-121°. $[\alpha]_D^{25}$ +39 (c, 1 in $CHCl_3$).

(-)-form [57291-88-0]
Constit. of *Dictyopteris undulata.* Antifeedant. Ichthyotoxin. Gum. $[\alpha]_D^{25}$ -50 (c, 1 in $CHCl_3$). λ_{max} 219; 228; 298 (MeOH) (Berdy).
Ac:
Cryst. (petrol). Mp 116-118°. $[\alpha]_D^{25}$ -34 (c, 1.3 in $CHCl_3$).

Fenical, W. *et al., Experientia*, 1975, **31**, 1004
Cimino, G. *et al., Experientia*, 1975, **31**, 1117
Ishibashi, H. *et al., J.A.C.S.*, 2004, **126**, 11122-11123 (*synth*)

Chromodorolide A C-644

[119878-93-2]

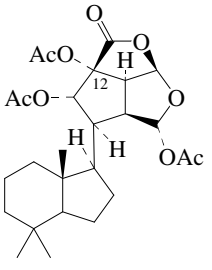


$C_{24}H_{34}O_8$ 450.528
Constit. of *Chromodoris cavae* and an Australian marine sponge. Cytotoxic agent. Cryst. (MeOH).
Mp 133-134°. $[\alpha]_D$ -74 (c, 0.1 in CH_2Cl_2).

Dumdei, E.J. *et al., J.A.C.S.*, 1989, **111**, 2712-2713 (*isol, pmr, cmr, cryst struct*)
Morris, S.A. *et al., Can. J. Chem.*, 1991, **69**, 768-771 (*isol, pmr, cmr*)
Rungprom, W. *et al., Mar. Drugs*, 2004, **2**, 101-107 (*isol*)

Chromodorolide B C-645

[135446-84-3]



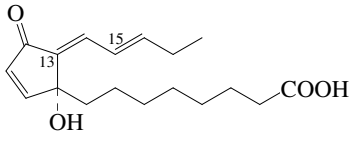
$C_{26}H_{36}O_9$ 492.565
Constit. of *Chromodoris cavae* and an Australian marine sponge. Cytotoxic and antimicrobial agent. Oil. $[\alpha]_D$ -95 (c, 0.1 in CH_2Cl_2).

O^{12}-*De-Ac:* ***Chromodorolide C***
[850087-95-5]
$C_{24}H_{34}O_8$ 450.528
Constit. of an Australian aplysinid marine sponge. Oil. $[\alpha]_D$ -78 (c, 0.1 in CH_2Cl_2).

Morris, S.A. *et al., Can. J. Chem.*, 1991, **69**, 768-771 (*Chromodorolide B*)
Rungprom, W. *et al., Mar. Drugs*, 2004, **2**, 101-107 (*Chromodorolide C*)

Chromomoric acid D C-646

1-Hydroxy-4-oxo-5-(2-pentenylidene)-2-cyclopentene-1-octanoic acid. 9-Hydroxy-12-oxo-10,13,15-phytotrienoic acid



(13*E*,15*E*)-*form*

$C_{18}H_{26}O_4$ 306.401
Biogenetic numbering shown.

(13*E*,15*E*)-*form*
Chromomoric acid D II
[81905-31-9]
Constit. of *Chromolaena morii*.

(13*E*,15*Z*)-*form*
Chromomoric acid D I
[81905-30-8]
Constit. of *Chromolaena morii*.

(13*Z*,15*E*)-*form*
Chromomoric acid D III
[81905-32-0]
Constit. of *Chromolaena morii*.

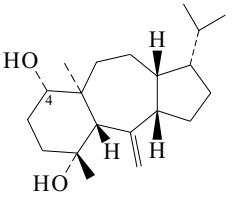
11-Bromo, Me ester: ***11-Bromochromomoric acid D III Me ester***
$C_{19}H_{27}BrO_4$ 399.324
Isol. from the coral *Dendrophyllia* sp.
$[\alpha]_D^{22}$ -14.2 (c, 0.13 in MeOH). λ_{max} 246 (log ϵ 4.28); 312 (log ϵ 4.03) (MeOH).

(13*Z*,15*Z*)-*form*
Chromomoric acid D IV
Constit. of *Chromolaena morii*.

Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 125-127 (*isol*)
Liu, Z.-Y. *et al., Tetrahedron*, 1998, **54**, 12561-12570 (*synth, struct*)
Rezanka, T. *et al., Eur. J. Org. Chem.*, 2003, 309-316 (*11-Bromochromomoric acid D III*)

13(20)-Chromophycene-1,4-diol C-647

Chromophycadiol



$C_{20}H_{34}O_2$ 306.487
New carbon skeleton formally related to dolastane by a methyl migration.

4-Ac: ***Chromophycadiol monoacetate***
$C_{22}H_{36}O_3$ 348.525
Constit. of a *Dictyota* sp. Cryst.
Mp 137-139°. $[\alpha]_D$ +26.5 (c, 0.65 in $CHCl_3$).

Clardy, J. *et al., Chem. Comm.*, 1987, 767 (*isol, cryst struct*)

Chrysolaminarin C-648

Leucosin, 9CI. Chrysolaminaran
[9013-94-9]
Polysaccharide. Consists mainly of β(1→3)-linked glucosyl residues with some branching. Closely similar to Laminarin, L-21 from the related brown algae, but has a lower proportion (sometimes close to zero) of terminal mannitol residues and a shorter mean chain length. Isol. from diatoms and related algae. Reserve carbohydrate. Cryst.

Beattie, A. *et al., Biochem. J.*, 1961, **79**, 531 (*isol, struct*)
Archibald, A.R. *et al., Biochem. J.*, 1963, **88**, 444 (*isol, struct*)
McConville, M. *et al., Carbohydr. Res.*, 1986, **153**, 330 (*isol, struct*)

Chrysophsins C-649

Peptides containing 20-25 amino acid residues. Isol. from gills of the sea bream *Chrysophrys major*. Antimicrobial agents.

Chrysophsin 1

$C_{136}H_{212}N_{46}O_{25}$ 2891.464

Chrysophsin 2

$C_{136}H_{212}N_{48}O_{25}$ 2919.477

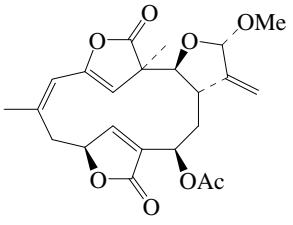
Chrysophsin 3

$C_{74}H_{122}N_{18}O_{19}$ 1567.887

Iijima, N. *et al., Eur. J. Biochem.*, 2003, **270**, 675-686 (*isol, struct*)

Ciereszkolide C-650

[795288-97-0]



$C_{23}H_{26}O_8$ 430.454

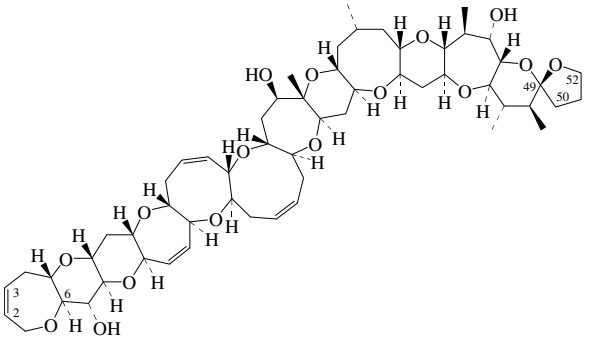
Constit. of *Pseudopterogorgia kallos*. Cryst. $[\alpha]_D^{20}$ +13.7 (c, 0.7 in $CHCl_3$). λ_{max} 203 (ϵ 21900); 238 (ϵ 8900) (MeOH).

Marrero, J. *et al., Eur. J. Org. Chem.*, 2004, 3909-3912 (*isol, pmr, cmr, cryst struct*)

Ciguatoxin 3C (Pacific) C-651

P-CTX 3C. CTX 3C

[148471-85-6]



$C_{57}H_{82}O_{16}$ 1023.265

Similar to Ciguatoxin (Pacific), C-652. Isol. from the dinoflagellate *Gambierdiscus toxicus*.

▶ Highly toxic, LD_{50} (mus, ipr) 0.0013 mg/kg.

51β-Hydroxy: ***51-Hydroxyciguatoxin 3C****. 51-HydroxyCTX 3C*

[263336-59-0]

$C_{57}H_{82}O_{17}$ 1039.265

Isol. from *Gymnothorax javanicus*.

2,3-Dihydro, 2-hydroxy: ***2,3-Dihydro-2-hydroxyciguatoxin 3C***

[287732-78-9]

$C_{57}H_{84}O_{17}$ 1041.28

Isol. from fish.

2,3-Dihydro, 3-hydroxy: 2,3-Dihydro-3-hydroxyciguatoxin 3C, 9CI

[263336-60-3]

$C_{57}H_{84}O_{17}$ 1041.28

Isol. from fish.

2,3-Dihydro, 2β,3α-dihydroxy: ***2,3-Dihydro-2,3-dihydroxyciguatoxin 3C****. Ciguatoxin 2A1. CTX 2A1*

[185220-06-8]

[263336-62-5]

$C_{57}H_{84}O_{18}$ 1057.28

Isol. from the moray eel *Gymnothorax javanicus*.

2,3-Dihydro, 2,3,51-trihydroxy: ***2,3-Dihydro-2,3,51-trihydroxyciguatoxin 3C***

[263336-63-6]

$C_{57}H_{84}O_{19}$ 1073.279

Isol. from fish.

2,3-Dihydro, 2-oxo, 51-hydroxy: ***2,3-Dihydro-51-hydroxy-2-oxociguatoxin 3C, 9CI***

[287732-77-8]

$C_{57}H_{82}O_{18}$ 1055.264

Isol. from fish.

2,3-Dihydro, 3-oxo, 51-hydroxy: ***2,3-Dihydro-51-hydroxy-3-oxociguatoxin 3C, 9CI***

[263336-61-4]

$C_{57}H_{82}O_{18}$ 1055.264

Isol. from fish.

49,52-Deepoxy, 49,52-dihydroxy: **M-*Secociguatoxin 3C*.** *49,52-Deepoxy-49,52-dihydroxyciguatoxin 3C, 9CI*

[287411-98-7]

$C_{57}H_{84}O_{17}$ 1041.28

Isol. from *Gambierdiscus toxicus*. M-Ring-opened form, i.e. 52-hydroxy-52-(3-hydroxypropyl).

1,6-Deepoxy, 1,6,51-trihydroxy, 2,3-dihydro: **A-*Seco-2,3-dihydro-51-hydroxyciguatoxin 3C***

[263336-64-7]

$C_{57}H_{86}O_{18}$ 1059.296

Isol. from fish. *A*-Ring-opened form, i.e. 6-hydroxy-5-(4-hydroxybutyl).

49,52-Deepoxy, 49-methoxy, 52-hydroxy: 49,52-Deepoxy-52-hydroxy-49-methoxyciguatoxin 3C, 9CI. **M-*Seco*-4-O-*methylciguatoxin 3C***

[287411-99-8]

$C_{58}H_{86}O_{17}$ 1055.307

Isol. from *Gambierdiscus toxicus*.

49,52-Deepoxy, 2,3-dihydro, 49-methoxy, 2,52-dihydroxy: **M-*Seco-2,3-dihydro-2-hydroxy-49-O-methylciguatoxin 3C***

[374624-43-8]

$C_{58}H_{88}O_{18}$ 1073.322

Isol. from fish.

49-Epimer: ***49-Epiciguatoxin 3C****. P-CTX 3B*

[263336-58-9]

$C_{57}H_{82}O_{16}$ 1023.265

Isol. from *Gambierdiscus toxicus*.

Satake, M. *et al., Tet. Lett.*, 1993, **34**, 1975; 1998, **39**, 1197-1198 (*isol, derivs, pmr, cmr*)

Yasumoto, T. *et al., CA*, 2000, **133**, 39329d (*derivs, isol*)

Food Sci. Technol., Seafood and Freshwater Toxins, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*revs*)

Yasumoto, T. *et al., J.A.C.S.*, 2000, **122**, 4988-4989 (*ms, occur*)

Inoue, M. *et al., Acc. Chem. Res.*, 2004, **37**, 954-960 (*rev, synth*)

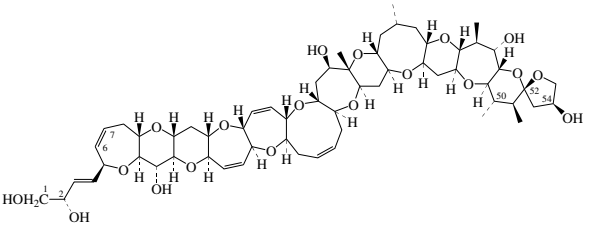
Inoue, M. *et al., J.A.C.S.*, 2006, **128**, 9352-9354 (*51-HydroxyCTX 3C, synth*)

Nicholson, G.M. *et al., Mar. Drugs*, 2006, **4**, 82-118 (*rev, activity*)

Ciguatoxin (Pacific) C-652

Pacific Ciguatoxin 1. P-CTX 1

[11050-21-8]



$C_{60}H_{86}O_{19}$ 1111.328

Earliest known of this group of toxins; sometimes simply known as Ciguatoxin or CTX. Isol. from the moray eel (*Gymnothorax javanicus*) and other fish and shellfish esp. coral reef spp. Present in the dinoflagellate *Gambierdiscus toxicus*. Causes ciguatera food poisoning. *G. toxicus* is the primary cause.

▶ GD0760000

7-Oxo, 6,7-dihydro: ***7-Oxociguatoxin***

[263336-55-6]

$C_{60}H_{86}O_{20}$ 1127.327

Isol. from fish.

3ξ-Hydroxy, 7-oxo, 3,4,6,7-tetrahydro: ***3,4-Dihydro-3-hydroxy-7-oxociguatoxin****. 3-Hydroxy-7-oxociguatoxin*

[263336-57-8]

$C_{60}H_{88}O_{21}$ 1145.343

Isol. from fish.

4ξ-Hydroxy, 7-oxo, 3,4,6,7-tetrahydro: ***3,4-Dihydro-4-hydroxy-7-oxociguatoxin***. *4-Hydroxy-7-oxociguatoxin*
[287732-85-8]
$C_{60}H_{88}O_{21}$ 1145.343
Isol. from fish.

7ξ-Hydroxy, 6,7-dihydro: ***6,7-Dihydro-7-hydroxyciguatoxin***. *7-Hydroxyciguatoxin*
[263336-56-7]
$C_{60}H_{88}O_{20}$ 1129.343
Isol. from fish.

54-Deoxy: ***54-Deoxyciguatoxin***. *Pacific Ciguatoxin 3. P-CTX 3*
[139341-09-6]
$C_{60}H_{86}O_{18}$ 1095.329
Isol. from *Lycodontis javanicus*, the moray eel (*Gymnothorax javanicus*). λ_{max} 215 (MeOH) (Berdy).

54-Deoxy, 50-hydroxy: ***54-Deoxy-50-hydroxyciguatoxin, 9CI***
[263336-54-5]
$C_{60}H_{86}O_{19}$ 1111.328
Isol. from fish.

1,2,54-Trideoxy, 1,2-didehydro: ***Gambiertoxin 4B***. *GT 4B. Pacific Ciguatoxin 4B. P-CTX 4B. Ciguatoxin 4B*
[123676-76-6]
$C_{60}H_{84}O_{16}$ 1061.314
Isol. from *Gambierdiscus toxicus*. Neurotoxin. Cardiotoxin. Ichthyotoxin. λ_{max} 223 (ϵ 22000) (MeCN) (Berdy).

1,2,54-Trideoxy, 52,55-dihydroxy, 52,55-deepoxy, 1,2-didehydro: **M-*Secociguatoxin 4A***
[287412-00-4]
$C_{60}H_{86}O_{17}$ 1079.329
Isol. from *Gambierdiscus toxicus*.

52-Epimer: ***52-Epiciguatoxin***
[189013-49-8]
$C_{60}H_{86}O_{19}$ 1111.328
Isol. from fish.

52-Epimer, 54-deoxy: ***Pacific Ciguatoxin 2***. *P-CTX 2*
[142185-85-1]
$C_{60}H_{86}O_{18}$ 1095.329
Isol. from *Lycodontis javanicus*. Cardiotoxin. λ_{max} 215 (MeOH) (Berdy).

▶ GD0760100

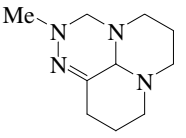
52-Epimer, 1,2,54-trideoxy, 1,2-didehydro: ***Pacific Ciguatoxin 4A***. *P-CTX 4A. Ciguatoxin 4A*
[66231-73-0]
$C_{60}H_{84}O_{16}$ 1061.314
Isol. from *Gambierdiscus toxicus* and *Scarus gibbus*. Amorph. solid. A toxin isol. from various parrotfish (*Scarus* sp.) and named Scaritoxin or SG 1 probably corresponds to a mixture of CTX 4A and 4B. λ_{max} 226 (MeOH).

54-Epimer: ***54-Epiciguatoxin***
[287732-40-5]
$C_{60}H_{86}O_{19}$ 1111.328
Isol. from fish.

52,54-Diepimer: ***52,54-Diepiciguatoxin***
[287732-42-7]
$C_{60}H_{86}O_{19}$ 1111.328
Isol. from fish.

Scheuer, P.J. *et al., Bioact. Mol.*, 1989, **10**, 265 (*occur*)
Murata, M. *et al., J.A.C.S.*, 1990, **112**, 4380 (*pmr, struct*)
Lewis, R.J. *et al., Toxicon*, 1991, **29**, 1115 (*isol, derivs*)
Murata, M. *et al., Tet. Lett.*, 1992, **33**, 525 (*cmr, struct*)
Satake, M. *et al., Biosci., Biotechnol., Biochem.*, 1997, **60**, 2103-2105 (*Ciguatoxin 4A*)
Satake, M. *et al., J.A.C.S.*, 1997, **119**, 11325-11326 (*abs config*)
Oguri, H. *et al., Tetrahedron*, 1997, **53**, 3057-3072 (*abs config*)
Food Sci. Technol., Seafood and Freshwater Toxins, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*revs*)
Yasumoto, T. *et al., J.A.C.S.*, 2000, **122**, 4988-4989 (*ms, occur*)
Inoue, M. *et al., J.A.C.S.*, 2006, **128**, 9352-9354 (*synth*)
Nicholson, G.M. *et al., Mar. Drugs*, 2006, **4**, 82-118 (*rev, activity*)

Cinachyramine C-653

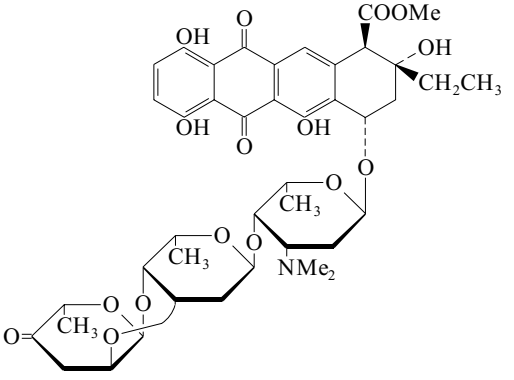


$C_{10}H_{18}N_4$ 194.279
Constit. of *Cinachyrella* sp. Oil (as TFA salt).

Shimogawa, H. *et al., Tet. Lett.*, 2006, **47**, 1409-1411 (*isol, cd, pmr, cmr*)

Cinerubin B C-654

Ryemycin B_1. 1-Hydroxyaclacinomycin B. MA 144B_2. Antibiotic MA 144B_2. Ciclamycin 1. Aclacinomycin B_2
[35906-51-5]



$C_{42}H_{51}NO_{16}$ 825.862
Anthracycline antibiotic. Isol. from *Streptomyces antibioticus, Streptomyces griseorubiginosus, Streptomyces galilaeus*, *Streptomyces niveorubes* and marine *Streptomyces* sp. B8904. Active against gram-positive bacteria, viruses and tumours. Orange-red cryst.
Mp 168-178° Mp 240-243° dec. λ_{max} 233 (ϵ 46800); 257 (ϵ 24600); 289 (ϵ 9090); 460 (ϵ 11100); 491 (ϵ 13800); 510 (ϵ 10700); 525 (ϵ 9330) (MeOH aq. with base) (Derep). λ_{max} 240 (ϵ 22800); 258 (ϵ 22000); 290 (ϵ 8860); 297 (ϵ 8820); 487 (ϵ 13500); 496 (ϵ 14500); 516 (ϵ 11000); 592 (ϵ 9400) (MeOH aq./NaOH) (Derep). λ_{max} 234 (ϵ 43000); 257 (ϵ 20000); 290 (ϵ 8000); 410 (sh); 465 (sh); 481 (ϵ 11300); 491 (ϵ 12500); 510 (ϵ 10600); 523 (ϵ 7470) (95% MeOH/pH 7) (Derep).

▶ QI9277700

N-*De-Me:* ***Cinerubin M***
$C_{41}H_{49}NO_{16}$ 811.835
Prod. by the marine *Streptomyces* sp. B8904. Red powder.

1-Epimer: ***10-Epicinerubin B***. *Antibiotic 80334C*
[104758-18-1]
$C_{42}H_{51}NO_{16}$ 825.862
Prod. by *Actinosporangium xiangfaensis*. Cytotoxic agent. Red powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -20 ($CHCl_3$). λ_{max} 233 (E1%/1cm 456); 257 (E1%/1cm 245); 293 (E1%/1cm 106); 492 (E1%/1cm 155); 512 (E1%/1cm 131); 527 (E1%/1cm 118); 581 (MeOH) (Berdy). λ_{max} 239 (E1%/1cm 449); 294 (E1%/1cm 98); 566 (E1%/1cm 197); 601 (E1%/1cm 96) (MeOH/NaOH) (Berdy).

5^C-Epimer: ***Spartanamicin A***. *Ciclamycin 2. 80334B. Antibiotic 80334B*
[104759-19-5]
$C_{42}H_{51}NO_{16}$ 825.862
Prod. by a *Micromonospora* sp. *Actinosporangium xianfanensis*, *Streptomyces capoamus* and *Streptomyces galilaeus*. Antifungal agent. Orange powder.
Mp 174-176°.

[134910-03-5, 134910-04-6]

Ettlinger, L. *et al., Chem. Ber.*, 1959, **92**, 1867 (*isol, uv, ir*)

Richle, W. *et al., Helv. Chim. Acta*, 1972, **55**, 467 (*cryst struct, pmr*)
David, L. *et al., J. Antibiot.*, 1980, **33**, 49 (*isol*)
Oki, T. *et al., J. Antibiot.*, 1980, **33**, 49 (*isol*)
David, L. *et al., Tetrahedron*, 1982, **38**, 1631 (*ms*)
Yoshimoto, A. *et al., J. Antibiot.*, 1992, **45**, 1005 (*Betaclamycin B*)
Nair, M.G. *et al., J. Antibiot.*, 1992, **45**, 1738 (*Spartanamicin A*)
Phipps, R.K. *et al., ARKIVOC*, 2004, **x**, 94-100 (*marine, isol*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TAH650

Cionin C-655

[126985-56-6]

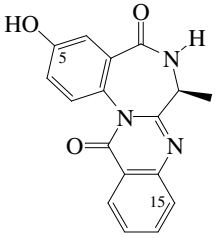
H-Asn-Tyr(SO_3H)-Tyr(SO_3H)-Gly-Trp-Met-Asp-Phe-NH_2

Isol. from the neural ganglion of the protochordate *Ciona intestinalis*.

Johnsen, A.H. *et al., J. Biol. Chem.*, 1990, **265**, 3054 (*isol, struct*)

Circumdatin C C-656

[223130-61-8]



$C_{17}H_{13}N_3O_3$ 307.308

Prod. by a terrestrial strain of *Aspergillus ochraceus*. Solid. $[\alpha]_D^{22}$ -75 (c, 0.16 in MeOH). λ_{max} 229 (log ϵ 4.31); 272 (log ϵ 3.85); 312 (log ϵ 3.5) (MeOH).

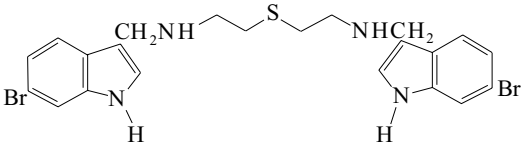
Deoxy: ***Circumdatin F***
[232922-23-5]
$C_{17}H_{13}N_3O_2$ 291.309
Prod. by a terrestrial strain of *Aspergillus ochraceus*. Solid. $[\alpha]_D$ -18.9 (c, 0.1 in MeOH).

Deoxy, 15-hydroxy: ***Circumdatin G***
[326597-48-2]
$C_{17}H_{13}N_3O_3$ 307.308
Prod. by a marine strain of *Aspergillus ochraceus*. Powder. $[\alpha]_D$ -21.7 (c, 0.2 in MeOH). λ_{max} 215 (log ϵ 2.58); 235 (log ϵ 2.64); 276 (log ϵ 1.96); 278 (log ϵ 2.17); 327 (log ϵ 1.98) (MeOH).

Rahbaek, L. *et al., J. Nat. Prod.*, 1999, **62**, 904-905 (*Circumdatin F*)
Rahbaek, L. *et al., J.O.C.*, 1999, **64**, 1689-1692 (*Circumdatin C*)
Dai, J.-R. *et al., J. Nat. Prod.*, 2001, **64**, 125-126 (*Circumdatin G*)
Witt, A. *et al., J.O.C.*, 2001, **66**, 2784-2788 (*synth*)
Snider, B. *et al., Tetrahedron*, 2001, **57**, 3301-3307 (*Circumdatin F, synth*)
Liu, J.-F. *et al., J.O.C.*, 2005, **70**, 10488-10493 (*Circumdatin F, synth*)

Citorellamine C-657

[99102-23-5]



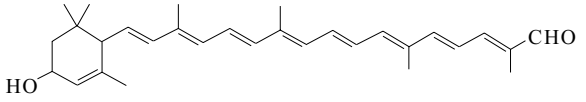
$C_{22}H_{24}Br_2N_4S$ 536.332

Initially considered to be a C_{11} monomer. Alkaloid from the tunicate *Polycitorella mariae*. Exhibits cytotoxicity and potent antimicrobial activity. Needles (MeOH).
Mp 210° dec. λ_{max} 225 (ϵ 18000); 285 (ϵ 3000); 291 (ϵ 2800) (MeOH) (Derep).

Roll, D.M. *et al., Tet. Lett.*, 1985, **26**, 4303-4306 (*uv, ir, pmr, cmr, ms*)
Moriarty, R.M. *et al., Tet. Lett.*, 1987, **28**, 749-752 (*pmr, cmr, ms, struct, synth*)

α-Citraurin C-658

3-Hydroxy-8′-apo-ϵ-caroten-8′-al



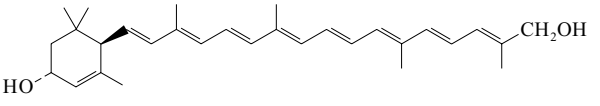
$C_{30}H_{40}O_2$ 432.645

Constit. of avocado (*Persea americana*). Also isol. from the sea hare *Aplysia kurodai*. Cryst. (MeOH).
Mp 153°. $[\alpha]_D^{18}$ +372 (C_6H_6).

Karrer, P. *et al., Helv. Chim. Acta*, 1938, **21**, 445 (*synth*)
Gross, J. *et al., Phytochemistry*, 1973, **12**, 2259-2263 (*Persea, isol*)
Yamashita, E. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1990, **96**, 465-470 (*Aplysia, isol*)

α-Citraurinol C-659

8′-Apo-ϵ-carotene-3,8′-diol
[130196-31-5]



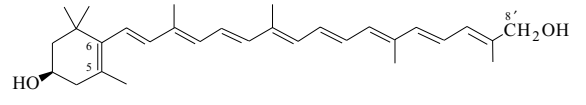
$C_{30}H_{42}O_2$ 434.661

Constit. of *Aplysia kurodai*.

Yamashita, E. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1990, **96**, 465 (*isol, pmr*)

β-Citraurol C-660

8′-Apo-β-carotene-3,8′-diol. β-Citraurinol
[57593-78-9]



$C_{30}H_{42}O_2$ 434.661

Constit. of citrus hybrid peel. Isol. from the sea hare *Aplysia kurodai*.

Di-Ac:
Cryst. (petrol/MeOH). Mp 92°.

8′-Aldehyde: 3-Hydroxy-8′-apo-β-caroten-8′-al. ***β-Citraurin***
[650-69-1]
$C_{30}H_{40}O_2$ 432.645
Constit. of orange peel. Isol. from *Aplysia kurodai*. Cryst. (EtOH or Et_2O/petrol).
Mp 146-147°.

*8′-Aldehyde, 5*R*,6*S*-epoxide: 5,6-Epoxy-3-hydroxy-8′-apo-β-caroten-8′-al.* ***β-Citraurin epoxide****. Apo-8′-violaxanthal*
[71869-83-5]
$C_{30}H_{40}O_3$ 448.644
Isol. from orange peel. Cryst. (C_6H_6/petrol). Unnatural (5*S*,6*R*)-diastereoisomer also prepd. (Mp 158°). λ_{max} 424; 448; 477 (hexane).

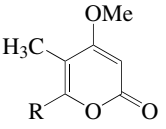
8′-Deoxy: 8′-Apo-β-caroten-3-ol. ***β-Citraurinene***
[58947-97-0]
$C_{30}H_{42}O$ 418.661
Constit. of citrus peel. Orange cryst. (CH_2Cl_2/petrol).
Mp 141°.

[75715-17-2, 75715-18-3]

Leuenberger, U. *et al., J.O.C.*, 1976, **41**, 891-892 (*β-Citraurol*)
Leuenberger, U. *et al., Phytochemistry*, 1976, **15**, 227-229 (*β-Citraurinene*)
Pfander, H. *et al., Pure Appl. Chem.*, 1979, **51**, 565-580 (*synth*)

Pfander, H. *et al., Helv. Chim. Acta*, 1980, **63**, 716-727; 1377-1382 (*abs config, synth, biosynth*)
Molnár, P. *et al., Phytochemistry*, 1980, **19**, 633-637 (*β-Citraurin epoxide*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 483; 484 (*bibl*)
Yamashita, E. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1990, **96**, 465-470 (*Aplysia, isol*)
Deli, J. *et al., Helv. Chim. Acta*, 1998, **81**, 1815-1820 (*β-Citraurin, pmr, cmr*)
Lóránd, T. *et al., Helv. Chim. Acta*, 2002, **85**, 1691-1697 (*ir*)

Citreopyrones C-661



Citreopyrone A R = -CH=CHCH=CHCHO(*E,E-*)
" B R = -CH=CHCHO(*E-*)
" C R = -CHO
" D R = -CH=CHCH=CHCH=CHCOCH$_3$(*all E-*)
" E R = -CH=CHCH=CHCOCH$_3$(*E,E-*)
" F R = -CH=CHCOCH$_3$(*E-*)

Prod. by *Penicillium citreo-viride* and *Penicillium pedemontanum*.

Citreopyrone A
*5-(4-Methoxy-5-methyl-2-oxo-2*H*-pyran-6-yl)-2,4-pentadienal, 9CI. 4-Methoxy-5-methyl-6-(5-oxo-1,3-pentadienyl)-2*H*-pyran-2-one*
[102103-72-0]
$C_{12}H_{12}O_4$ 220.224
Yellow powder. Mp 187-190° (synthetic).

*ω-Carboxylic acid: 5-(4-Methoxy-5-methyl-2-oxo-2*H*-pyran-6-yl)-2,4-pentadienoic acid.* ***Herbarin A***
[433285-41-7]
$C_{12}H_{12}O_5$ 236.224
Prod. by *Cladosporium herbarum* isol. from the sponge *Aplysina aerophoba*.

Citreopyrone B
*4-Methoxy-5-methyl-6-(3-oxo-1-propenyl)-2*H*-pyran-2-one, 9CI. Secocitreoviridin. Secocitreoviridinol*
[79498-33-2]
$C_{10}H_{10}O_4$ 194.187
Yellow powder. Mp 207° dec.

*ω-Carboxylic acid: 3-(4-Methoxy-5-methyl-2-oxo-2*H*-pyran-6-yl)-2-propenoic acid.* ***Herbarin B***
[433285-42-8]
$C_{10}H_{10}O_5$ 210.186
Prod. by *Cladosporium herbarum* isol. from the sponge *Aplysina aerophoba*.

Citreopyrone C
*4-Methoxy-5-methyl-2-oxo-2*H*-pyran-6-carboxaldehyde, 9CI. 6-Formyl-4-methoxy-5-methyl-2*H*-pyran-2-one*
[66616-90-8]
$C_8H_8O_4$ 168.149
Yellowish powder. Mp 134-136° (synthetic).

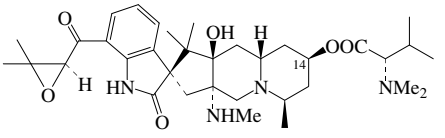
Citreopyrone D
*4-Methoxy-5-methyl-6-(7-oxo-1,3,5-octatrienyl)-2*H*-pyran-2-one, 9CI*
[186354-05-2]
$C_{15}H_{16}O_4$ 260.289
Yellow powder.

Citreopyrone E
*4-Methoxy-5-methyl-6-(5-oxo-1,3-hexadienyl)-2*H*-pyran-2-one, 9CI*
[186354-06-3]
$C_{13}H_{14}O_4$ 234.251
Yellow powder.

Citreopyrone F
*4-Methoxy-5-methyl-6-(3-oxo-1-butenyl)-2*H*-pyran-2-one, 9CI*
[186354-07-4]
$C_{11}H_{12}O_4$ 208.213
Yellowish powder.

Niwa, M. *et al., Chem. Lett.*, 1981, 1285-1288 (*isol, Secocitreoviridin*)
Suzuki, E. *et al., J. Chem. Res., Synop.*, 1982, 224-225 (*synth, Citreopyrone B*)
Patel, P. *et al., J.C.S. Perkin 1*, 1991, 1941-1945 (*synth, Citreopyrones A,C*)
Whang, K. *et al., J.O.C.*, 1991, **56**, 7174-7177 (*synth, Citreopyrones*)
Kosemura, S. *et al., Chem. Lett.*, 1997, 33-34 (*isol, ir, pmr, cmr*)
Jadulco, R. *et al., J. Nat. Prod.*, 2002, **65**, 730-733 (*Herbarins*)

Citrinadin A C-662



Absolute Configuration

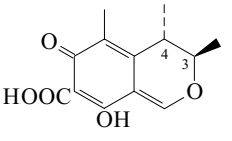
$C_{35}H_{52}N_4O_6$ 624.819
Prod. by *Penicillium citrinum* (strain N-059) isol. from the alga *Actinotrichia fragilis*. Cytotoxic. Oil. $[\alpha]_D^{19}$ -17 (c, 0.4 in MeOH). λ_{max} 224 (ϵ 9000); 230 (sh); 249 (ϵ 9600); 265 (sh); 335 (ϵ 3100) (MeOH).

14-De(acyloxy): ***Citrinadin B***
$C_{28}H_{39}N_3O_4$ 481.634
Prod. by *Penicillium citrinum* (strain N-059). Pale yellow solid. $[\alpha]_D^{20}$ +8 (c, 1 in MeOH). λ_{max} 203 (ϵ 12500); 223 (ϵ 7600); 248 (ϵ 9800); 333 (ϵ 3100) (MeOH).

Tsuda, M. *et al., Org. Lett.*, 2004, **6**, 3087-3089 (*isol, pmr, cmr*)
Mugishima, T. *et al., J.O.C.*, 2005, **70**, 9430-9435 (*abs config*)

Citrinin C-663

*4,6-Dihydro-8-hydroxy-3,4,5-trimethyl-6-oxo-3*H*-2-benzopyran-7-carboxylic acid, 9CI. Meleamycin. Antimycin*†*. Monascidin A*
[518-75-2]



$C_{13}H_{14}O_5$ 250.251
Isol. from *Penicillium citrinum*, *Guanomyces polythrix*, *Aspergillus terreus*, *Monascus* spp. and other microorganisms. Phytotoxic agent. Lemon-yellow needles (EtOH or MeOH).
Mp 178-179° dec. $[\alpha]_D^{18}$ -37.4 (EtOH). Log P 0.68 (calc). Strong acid. λ_{max} 250 (ϵ 9250); 331 (ϵ 10500) (MeOH) (Derep).
▶ Severe skin irritant. LD_{50} (mus, orl) 112 mg/kg. Exp. reprod. and teratogenic effects. Exp. hepatotoxic and nephrotoxic effects. DJ2275000

Me ester:
Prisms (C_6H_6 or Me_2CO). Mp 138°. $[\alpha]_D^{18}$ +217.1 (c, 0.38 in Me_2CO). $[\alpha]_D^{20}$ +96.9 ($CHCl_3$).

Phenylhydrazide: Mp 207° dec.

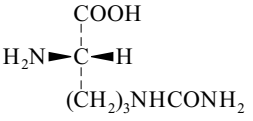
[112245-94-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 544B (*ir*)
Wyllie, J. *et al., CA*, 1946, **40**, 2190 (*isol*)
Sprenger, R.D. *et al., J.O.C.*, 1946, **11**, 189 (*struct*)
Warren, H.H. *et al., J.A.C.S.*, 1949, **71**, 3422 (*synth*)
Johnson, D.H. *et al., J.C.S.*, 1950, 2971 (*synth*)
Rodig, O.R. *et al., Chem. Comm.*, 1971, 1553 (*cryst struct*)
Saito, M. *et al., Microb. Toxins*, Academic Press, N.Y., 1971, **6**, 299 (*rev*)
Barber, J.A. *et al., J.C.S. Perkin 1*, 1981, 2577; 1986, 2101; 1987, 2743 (*biosynth, synth, struct, pmr, cmr*)
Colombo, L. *et al., J.C.S. Perkin 1*, 1981, 2594 (*biosynth*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2220 (*uv, ir, pmr, ms, cd*)
Sankawa, U. *et al., Tetrahedron*, 1983, **39**, 3583 (*biosynth*)
Destro, R. *et al., J.A.C.S.*, 1984, **106**, 7269 (*cryst struct, tautom*)
IARC Monog., 1986, **40**, 67; Suppl. 7, 60 (*rev, tox*)

Regan, A.C. *et al., Chem. Comm.*, 1987, 520 (*synth*)
Roedel, T. *et al., Annalen*, 1995, 885 (*synth, ir, pmr, cmr*)
Blanc, P.J. *et al., Int. J. Food Microbiol.*, 1995, **27**, 201 (*Monascidin A*)
Poupko, R. *et al., J. Phys. Chem. A*, 1997, **101**, 5097-5102 (*cmr, tautom*)
Močias, M. *et al., J. Nat. Prod.*, 2000, **63**, 757-761 (*activity*)
Clark, B. *et al., Org. Biomol. Chem.*, 2006, **4**, 1520-1528 (*isol, uv, ms, props*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 824
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CMS775

Citrulline C-664

N^5-*(Aminocarbonyl)ornithine, 9CI.* N^5-*Carbamoylornithine, 8CI.* *2-Amino-5-ureidovaleric acid. 5-Ureidoornithine. Stimol*



$C_6H_{13}N_3O_3$ 175.187
Log P -4.59 (calc).

(S)-form

L-form
[372-75-8]
Occurs in the juice of watermelon *Citrullus vulgaris*, the green alga *Enteromorpha intestinalis* and the red alga *Grateloupia filicina*. Widely distributed in the Cucurbitaceae and various other plants incl. algae and fungi. Diuretic agent. Used as arginine substitute in the treatment of inborn errors of urea synthesis, carbamyl phosphate synthetase and ornithine transcarbamylase deficiency. Prisms (MeOH aq.).
Mp 222°. $[\alpha]_D^{25}$ +22 (c, 2 in 1*M* HCl). pK_{a1} 2.43; pK_{a2} 9.41 (25°, 0.1*M* NaCl). Pharmacol. active enantiomer.

Hydrochloride: $[\alpha]_D^{22}$ +17.9 (c, 2 in H_2O). Dec. at 185°.

Cu salt:
Blue prisms. Mp 257-258°.

2-N-*Benzoyl, Me ester:*
$C_{14}H_{19}N_3O_4$ 293.322
Dec. at 120°.

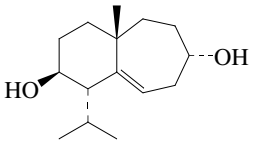
2-N-*Benzoyl, amide:*
$C_{13}H_{18}N_4O_3$ 278.31
Dec. at 140°.

[627-77-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 784B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1279C (*nmr*)
Biochem. Prep., 1953, **3**, 100-103; 104-107 (*synth*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1964, **18**, 2412-2414 (*ord*)
Dunnill, P.M. *et al., Phytochemistry*, 1965, **4**, 933-944 (*occur*)
Ashida, T. *et al., Acta Cryst. B*, 1972, **28**, 1367-1374 (*cryst struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 2391 (*occur*)
Msall, M. *et al., N. Engl. J. Med.*, 1984, **310**, 1500 (*pharmacol*)
Wakamiya, T. *et al., Tetrahedron*, 1984, **40**, 235-240 (*isol, bibl*)
Toffoli, P. *et al., Acta Cryst. C*, 1987, **43**, 945-947 (*cryst struct*)
Drauz, K. *et al., Angew. Chem., Int. Ed.*, 1991, **30**, 712-714 (*synth*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1337

Cladidiol C-665

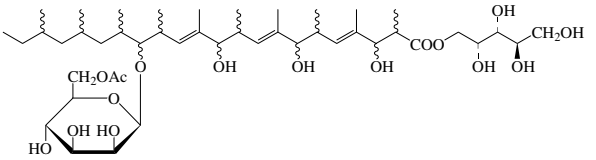
[701211-90-7]



$C_{15}H_{26}O_2$ 238.369
Constit. of a *Cladiella* sp. Oil. $[\alpha]_D^{20}$ +112 (c, 0.64 in $CHCl_3$). λ_{max} 203 (MeOH).

Ata, A. *et al., Helv. Chim. Acta*, 2004, **87**, 592-597 (*isol, pmr, cmr*)

Cladionol A C-666

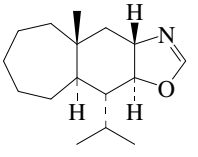


$C_{45}H_{80}O_{16}$ 877.117
Related to Roselipin 1A, R-76. Prod. by the marine-derived fungus *Gliocladium* sp. (strain L049). Cytotoxic. Amorph. solid. $[\alpha]_D^{25}$ +36 (c, 0.2 in MeOH).

Kasai, Y. *et al., J. Nat. Prod.*, 2005, **68**, 777-779 (*isol, pmr, cmr*)

Cladioxazole C-667

[602297-42-7]



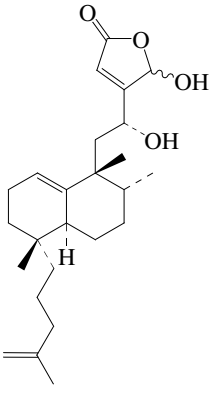
Relative Configuration

$C_{16}H_{27}NO$ 249.395
Alkaloid from the soft coral *Cladiella* sp. Oil.

Ata, A. *et al., Tet. Lett.*, 2003, **44**, 6951-6953 (*isol, pmr, cmr*)

Cladocoran B C-668

[204650-79-3]



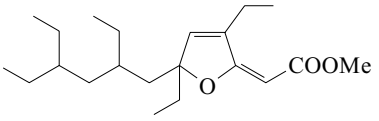
$C_{25}H_{38}O_4$ 402.573
Constit. of *Cladocora cespitosa*. Pale yellow oil. $[\alpha]_D^{20}$ -59.9 (c, 0.6 in $CHCl_3$). Related to Dysidiolide, D-1284. Stereochem. revised in 2003. λ_{max} 224 (ϵ 8700) (EtOH).

18-Ac: ***Cladocoran A***
[204650-78-2]
$C_{27}H_{40}O_5$ 444.61
Constit. of *Cladocora cespitosa*. Pale yellow oil. $[\alpha]_D^{20}$ -25.8 (c, 0.4 in $CHCl_3$). Stereochem. revised in 2003. λ_{max} 224 (ϵ 8400) (EtOH).

Fontana, A. *et al., J.O.C.*, 1998, **63**, 2845-2849 (*isol, pmr, cmr*)
Miyaoka, H. *et al., J.O.C.*, 2003, **68**, 3476-3479 (*synth, struct*)
Marcos, I.S. *et al., J.O.C.*, 2003, **68**, 7496-7504 (*synth*)

Cladocrocin A C-669

[148031-30-5]

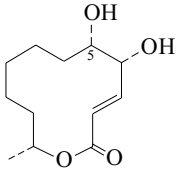


$C_{21}H_{36}O_3$ 336.514
Isol. from the sponge *Cladocroce incurvata*.
$[\alpha]_D$ +50.9.

D'Auria, M.V. *et al., J. Nat. Prod.*, 1993, **56**, 418 (*isol, pmr, cmr*)

Cladospolide A C-670

5,6-Dihydroxy-12-methyloxacyclododec-3-en-2-one, 9CI. 4,5,11-Trihydroxy-2-dodecenoic acid 1,11-lactone. 4,5-Dihydroxy-2-dodecen-11-olide
[77663-54-8]



(E)–form

$C_{12}H_{20}O_4$ 228.288

Macrolide-type antibiotic. Currently undergoing stereochemical studies (2006). Prod. by *Cladosporium fulvum* and *Cladosporium cladosporioides*. Phytotoxin. Needles (C_6H_6). Sol. EtOAc; poorly sol. H_2O.
Mp 92-93°. $[\alpha]_D^{18}$ -30 (c, 0.4 in MeOH). λ_{max} 217 (ϵ 10650) (MeOH) (Berdy).

4-Ketone: ***Cladospolide D***
$C_{12}H_{18}O_4$ 226.272
Prod. by *Cladosporium* sp. FT-0012. Antifungal agent. Oil. $[\alpha]_D^{28}$ +56 (c, 0.1 in MeOH). λ_{max} 204 (ϵ 22400) (MeOH).

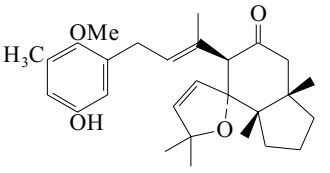
4,11-Diepimer: ***Cladospolide C***
[171866-20-9]
$C_{12}H_{20}O_4$ 228.288
Prod. by *Cladosporium tenuissimum*. Sol. MeOH.
Mp 90-91°. $[\alpha]_D^{22}$ +59.7 (c, 0.4 in MeOH). λ_{max} 214 (ϵ 2512) (MeOH) (Berdy).

(Z)-Isomer, 4,11-diepimer: ***Cladospolide B***
[96443-55-9]
Prod. by *Cladosporium cladosporioides*, *Cladosporium tenuissimum* and an unidentified marine fungus.
Powder. Sol. C_6H_6, EtOH; poorly sol. H_2O.
Mp 109-110°. $[\alpha]_D^{22}$ +45 (c, 0.4 in MeOH). λ_{max} 212 (ϵ 9170) (MeOH) (Derep). λ_{max} 211 (ϵ 5730) (MeOH) (Berdy).

Hirota, A. *et al., Agric. Biol. Chem.*, 1981, **45**, 799-800; 1985, **49**, 731-735; 903-904 (*isol, struct, props*)
Mori, K. *et al., Annalen*, 1987, 863 (*synth*)
Maemoto, S. *et al., Chem. Lett.*, 1987, 109 (*synth, bibl*)
Fujii, Y. *et al., Phytochemistry*, 1995, **40**, 1443-1446 (*isol, pmr, cmr*)
Smith, C.J. *et al., J. Nat. Prod.*, 2000, **63**, 142-145 (*marine fungal metab*)
Zhang, H. *et al., J. Antibiot.*, 2001, **54**, 635-641 (*Cladospolide D*)
Banwell, M.G. *et al., Org. Biomol. Chem.*, 2004, **2**, 2050-2060; 2005, **3**, 1081-1088 (*synth*)
Pandey, S.K. *et al., Tet. Lett.*, 2005, **46**, 6625-6627 (*Cladospolide B, synth*)
Sharma, G.V.M. *et al., Tet. Lett.*, 2006, **47**, 6531-6535; 6537-6540 (*synth, abs config*)

Claraenone C-671

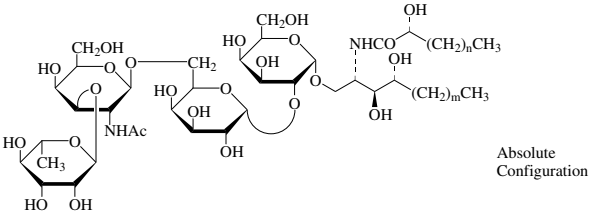
[149864-72-2]



$C_{28}H_{38}O_4$ 438.606
Constit. of a *Cystoseira* sp.
$[\alpha]_D^{25}$ -35.8 (c, 0.52 in $CHCl_3$). λ_{max} 201 (ϵ); 281 (ϵ) (MeOH assumed, not reported) (Derep).

Norte, M. *et al., Tet. Lett.*, 1993, **34**, 3485 (*isol, pmr, cmr*)

Clarhamnoside C-672



Isol. as a mixt. of homologues where n = 18-22 (major component n = 20) and m = 11-15 with some branched components (major component m = 14). Isol. from the marine sponge *Agelas clathrodes*. Solid. $[\alpha]_D^{25}$ +25 (c, 0.2 in MeOH).

Costantino, V. *et al., J.O.C.*, 2004, **69**, 1174-1179

Clathculine A C-673

$H_2C{=}CHCH_2CH_2CH{=}CHC{\equiv}C(CH_2)_9NMeCH_2CH_2NHMe$
$C_{21}H_{38}N_2$ 318.545

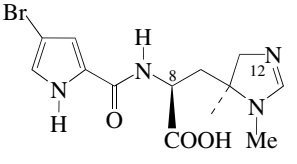
(Z)-form [300811-99-8]
Isol. from the sponge *Clathrina* aff. *reticulum*. Isol. as a mixt. with Clathculine B. λ_{max} 234 (ϵ 6300); 246 (ϵ 7600); 285 (ϵ 2800) (EtOH).

16,17-Dihydro: ***Clathculine B***
[300812-19-5]
$C_{21}H_{40}N_2$ 320.56
Isol. from *Clathrina* aff. *reticulum*.

Rudi, A. *et al., J. Nat. Prod.*, 2000, **63**, 1434-1436 (*isol, pmr, cmr, uv*)

Clathramide A C-674

[182888-51-3]



$C_{13}H_{17}BrN_4O_3$ 357.206

Neutral form shown. Exists as zwitterion with +ve charge distributed onto the two imidazole N's. Alkaloid from the Caribbean sponge *Agelas clathrodes*. Exhibits moderate antifungal activity. Amorph. solid. $[\alpha]_D^{25}$ -5 (c, 0.001 in MeOH). λ_{max} 208 (ϵ 14900); 230 (ϵ 13000); 265 (ϵ 10900) (MeCN).

8-Epimer: ***Clathramide B***
[183072-78-8]
$C_{13}H_{17}BrN_4O_3$ 357.206
From *Agelas clathrodes*. Exhibits moderate antifungal actiivity.

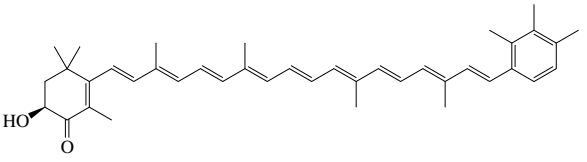
Amorph. solid. $[\alpha]_D^{25}$ +11 (c, 0.001 in MeOH). λ_{max} 208; 230 (ϵ 13000); 265 (ϵ 10900) (MeCN).

N-*De-Me:* ***Clathramide C***
[200264-71-7]
$C_{12}H_{15}BrN_4O_3$ 343.18
Alkaloid from *Agelas dispar*. Amorph. solid. $[\alpha]_D^{25}$ -6 (c, 0.001 in MeOH). λ_{max} 208 (ϵ 14900); 230 (ϵ 13000); 265 (ϵ 10900) (MeCN).

N-*De-Me, 8-epimer:* ***Clathramide D***
[200264-72-8]
$C_{12}H_{15}BrN_4O_3$ 343.18
Alkaloid from *Agelas dispar*. Serotonin receptor antagonist. λ_{max} 208 (ϵ 14900); 230 (ϵ 13000); 265 (ϵ 10900) (MeCN) (Berdy).

Cafieri, F. *et al., Tetrahedron*, 1996, **52**, 13713-13720 (*isol, uv, ir, pmr, cmr, struct*)
Cafieri, F. *et al., J. Nat. Prod.*, 1998, **61**, 122-125 (*isol, uv, ir, pmr, cmr, ms*)

Clathriaxanthin C-675



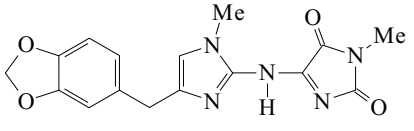
$C_{40}H_{50}O_2$ 562.834

(*S*)-*form* [60476-08-6]
Constit. of *Clathria frondifera* and *Tedania digitata*.

Tanaka, Y. *et al., Nippon Suisan Gakkaishi*, 1976, **42**, 801-805 (*isol*)
Tanaka, Y. *et al., Fish. Sci.*, 2001, **67**, 378-379 (*isol, abs config*)

Clathridine A C-676

[122759-55-1]



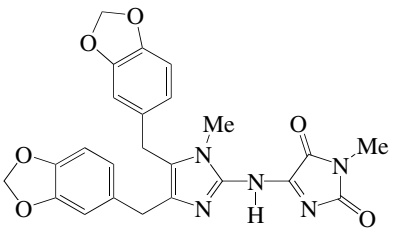
$C_{16}H_{15}N_5O_4$ 341.326
Metab. from the marine sponge *Clathrina clathrus* and the nudibranch *Notodoris gardineri*. Cryst. ($CHCl_3$). Fairly sol. MeOH; poorly sol. butanol, hexane.
Mp 260-262° dec. λ_{max} 285 (ϵ 5400); 371 (ϵ 14700) (MeOH) (Derep). λ_{max} 284; 359 (MeOH/NaOH) (Berdy).

Zn complex: ***Clathridine Zn***
[122780-90-9]
$C_{32}H_{28}N_{10}O_8Zn$ 746.025
Metab. of *Clathrina clathrus* and a *Leucetta* sp. Yellow microcryst. ($Et_2O/CHCl_3$). Fairly sol. MeOH; poorly sol. butanol, hexane.
Mp 158-160°. λ_{max} 285 (ϵ 9500); 361 (ϵ 22700); 372 (ϵ 22500); 399 (sh) (ϵ 13300) (MeOH) (Derep).

Ciminiello, P. *et al., Tetrahedron*, 1989, **45**, 3873-3878 (*isol, uv, ir, pmr, cmr, ms, struct*)
Ciminiello, P. *et al., Tetrahedron*, 1990, **46**, 4387-4392 (*Zn-Clathridine, cryst struct*)
Alvi, K.A. *et al., Tetrahedron*, 1993, **49**, 329-336 (*isol*)
Ohta, S. *et al., Tet. Lett.*, 2000, **41**, 4623-4627 (*synth*)

Clathridine B C-677

[146556-28-7]

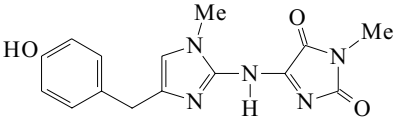


$C_{24}H_{21}N_5O_6$ 475.46
Metab. from the nudibranch *Notodoris gardineri*. Yellow oil. λ_{max} 285; 377 (MeOH).

Alvi, K.A. *et al., Tetrahedron*, 1993, **49**, 329 (*isol, uv, pmr, cmr, ms, struct*)

Clathridine C C-678

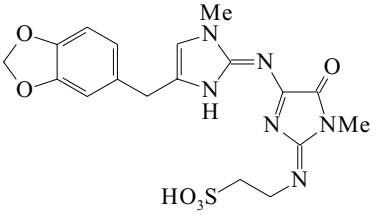
[152273-86-4]



$C_{15}H_{15}N_5O_3$ 313.315
Alkaloid from the sponge *Leucetta* sp. Weakly cytotoxic. Yellow plates (DMSO).
Mp 255-257°. Related to Clathridine A, C-676.

Carroll, A.R. *et al., Aust. J. Chem.*, 1993, **46**, 1229 (*isol, uv, ir, pmr, cmr, ms, struct*)

Clathridine-9-*N*-(2-sulfoethyl)imine C-679

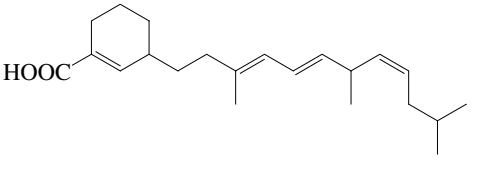


$C_{18}H_{20}N_6O_6S$ 448.459
Alkaloid from the marine sponge *Leucetta microraphis*. Yellow needles.
Mp 275-277° dec. λ_{max} 232 (ϵ 9530); 278 (ϵ 8610); 382 (ϵ 13700) (MeOH) (Derep).

He, H.-Y. *et al., J.O.C.*, 1992, **57**, 2176-2178 (*isol, uv, ir, pmr, cmr, cryst struct*)

Clathrin A C-680

3-(3,7,11-Trimethyl-3,5,8-dodecatrienyl)-1-cyclohexene-1-carboxylic acid
[282522-35-4]

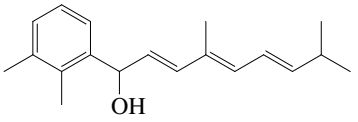


$C_{22}H_{34}O_2$ 330.509
Constit. of a *Clathria* sp. Yellow oil. $[\alpha]_D$ +34.3 (c, 0.5 in $CHCl_3$). λ_{max} 236 (log ϵ 4.1); 275 (log ϵ 4.6) (EtOH).

Capon, R.J. *et al., J. Nat. Prod.*, 2000, **63**, 821-824 (*isol, pmr, cmr*)

Clathrin B C-681

α-(3,7-Dimethyl-1,3,5-octatrienyl)-2,3-dimethylbenzenemethanol, 9CI. 1-(2,3-Dihydroxyphenyl)-4,8-dimethyl-2,4,6-nonatrien-1-ol
[282522-36-5]



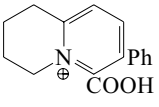
$C_{19}H_{26}O$ 270.414
Constit. of a *Clathria* sp. Yellow oil. $[\alpha]_D$ -25.4 (c, 1 in $CHCl_3$). λ_{max} 267 (log ϵ 4); 285 (log ϵ 4.8); 327 (log ϵ 3.6) (EtOH).

Ketone: 1-(2,3-Dimethylphenyl)-4,8-dimethyl-2,4,6-nonatrien-1-one. ***Clathrin C***
[282522-37-6]
$C_{19}H_{24}O$ 268.398
Constit. of a *Clathria* sp. Yellow oil. λ_{max} 285 (log ϵ 4); 295 (log ϵ 4); 307 (log ϵ 4.1) (EtOH).

Capon, R.J. *et al., J. Nat. Prod.*, 2000, **63**, 821-824 (*isol, pmr, cmr*)

Clathryimine A C-682

6-Carboxy-1,2,3,4-tetrahydro-7-phenylquinolizinium inner salt, 9CI
[175669-25-7]



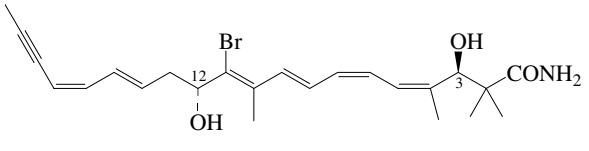
$C_{16}H_{16}NO_2^{\oplus}$ 254.308
Exists as zwitterion (COO^-). Alkaloid from the Indo-Pacific sponge *Clathria basilana*. Viscous amber oil. Readily decarboxylates to Clathyrimine B. λ_{max} 241 (ϵ 5500); 291 (ϵ 4500) (MeOH).

Decarboxy: 1,2,3,4-Tetrahydro-1-phenylquinolizinium, 9CI. Clathryimine B
[175669-26-8]
$C_{15}H_{16}N^{\oplus}$ 210.298
Viscous brown oil. Counterion not specified.

Sperry, S. *et al., Tet. Lett.*, 1996, **37**, 2389-2390 (*isol, uv, ir, pmr, cmr, struct*)
Daab, J.C. *et al., Monatsh. Chem.*, 2003, **134**, 573-583 (*Clathryimine B, synth*)

Clathrynamide A C-683

11-Bromo-3,12-dihydroxy-2,2,4,10-tetramethyl-4,6,8,10,14,16-eicosahexaen-18-ynamide
[160638-12-0]



Absolute Configuration

$C_{24}H_{32}BrNO_3$ 462.426
Isol. from the marine sponges *Clathria* sp. and *Psammoclemma* sp. Antifungal agent. Pale yellow oil. $[\alpha]_D^{23}$ +149 (c, 0.022 in MeOH). λ_{max} 247 (ϵ 19500); 309 (ϵ 29500); 321 (ϵ 38000); 336 (ϵ 28800) (MeOH).

N-*(4-Hydroxy-1-methylpentyl):* ***Clathrynamide B***
[152273-73-9]
$C_{30}H_{44}BrNO_4$ 562.586
Isol. from a *Clathria* sp. Gum. $[\alpha]_D^{25}$ +76 (c, 0.0033 in MeOH). λ_{max} 267 (ϵ 17400); 307 (ϵ 23400); 321 (ϵ 30200); 337 (ϵ 23400) (no solvent reported).

N-*(1-Methyl-4-oxopentyl):* ***Clathrynamide C***
[152273-74-0]
$C_{30}H_{42}BrNO_4$ 560.57
Isol. from a *Clathria* sp. Gum. λ_{max} 268 (ϵ 25700); 307 (ϵ 36300); 321 (ϵ 38000); 337 (ϵ 29500) (no solvent reported).

Debromo: ***Debromoclathrynamide A***
[602306-79-6]
$C_{24}H_{33}NO_3$ 383.53
Isol. from a *Psammoclemma* sp. Pale yellow oil. $[\alpha]_D^{23}$ +159 (c, 0.02 in MeOH). λ_{max} 263 (sh) (log ϵ 4.4); 272 (log ϵ 4.42); 283 (log ϵ 4.36); 297 (log ϵ 4.53); 310 (log ϵ 4.64); 324 (log ϵ 4.54) (MeOH).

*6*E*-Isomer:* ***(6E)-Clathyrnamide A***
[603129-66-4]
$C_{24}H_{32}BrNO_3$ 462.426
Isol. from a *Psammoclemma* sp. Pale yellow oil. $[\alpha]_D^{23}$ -58 (c, 0.02 in MeOH). λ_{max} 268 (log ϵ 3.84); 294 (sh) (log ϵ 3.83); 308 (log ϵ 4.09); 322 (log ϵ 4.24); 338 (log ϵ 4.16) (MeOH).

*(4*E*,6*E*)-Isomer, debromo:* ***(4E,6E)-Debromoclathrynamide A***
[602302-49-8]
$C_{24}H_{33}NO_3$ 383.53
Isol. from a *Psammoclemma* sp. Pale yellow oil. $[\alpha]_D^{24}$ -80 (c, 0.004 in MeOH). λ_{max} 272 (log ϵ 4.02); 284 (log ϵ 3.99); 298 (log ϵ 4.11); 312 (log ϵ 4.22); 327 (log ϵ 4.15) (MeOH).

Ohta, S. *et al., Tet. Lett.*, 1993, **34**, 5935-5938 (*isol*)
Ojika, M. *et al., Biosci., Biotechnol., Biochem.*, 2003, **67**, 1568-1573 (*abs config, Psammoclemma constits*)

Clavanins C-684

Val-Phe-Gln-Phe-Leu-Gly-Lys-Ile-Ile-His-His-Val-Gly-Asn-Phe-Val-His-Gly-Phe-Ser-His-Val-Phe-NH_2

A family of peptides comprising 23 amino acid residues; struct. of Clavanin A shown. Isol. from *Styela clava*. Show antimicrobial props.

Clavanin A [192879-22-4]
$C_{131}H_{185}N_{35}O_{26}$ 2666.121

Clavanin B [207289-94-9]
$C_{131}H_{185}N_{37}O_{26}$ 2694.135

Clavanin C [207289-95-0]
$C_{133}H_{190}N_{34}O_{26}$ 2681.176

Clavanin D [207289-97-2]
$C_{131}H_{191}N_{35}O_{26}$ 2672.169

Clavanin E [193337-05-2]
$C_{130}H_{193}N_{35}O_{25}$ 2646.174

Zhao, G. *et al., FEBS Lett.*, 1997, **410**, 490-492 (*isol*)
Pat. Coop. Treaty (WIPO), 1998, 98 20 028; *CA*, **128**, 319289q (*isol*)
Lehrer, R.I. *et al., Adv. Exp. Med. Biol.*, 2001, **484**, 71-76 (*rev*)

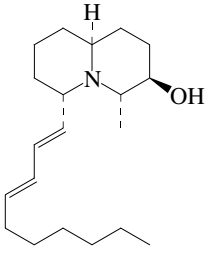
Clavaspirin C-685

$C_{119}H_{187}N_{35}O_{24}$ 2492.006
Peptide containing 23 amino acid residues; *C*-amidated. Isol. from the tunicate *Styela clava*. Shows antibacterial and haemolytic activity.

Lee, I.H. *et al., J. Pept. Res.*, 2001, **58**, 445-456 (*isol*)

Clavepictine B C-686

*6-(1,3-Decadienyl)octahydro-4-methyl-2*H*-quinolizin-3-ol, 9CI*
[132621-84-2]



Absolute Configuration

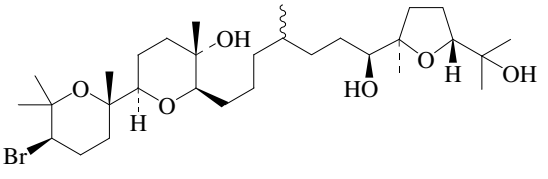
$C_{20}H_{35}NO$ 305.503
Alkaloid from the tunicate *Clavelina picta*. Cytotoxic agent. Cryst. Mp 70-72°. $[\alpha]_D$ +27.1 (c, 0.03 in CH_2Cl_2). λ_{max} 230 (ϵ 18000) (EtOH) (Derep).

O-*Ac:* ***Clavepictine A***
[132621-83-1]
$C_{22}H_{37}NO_2$ 347.54
Alkaloid from *Clavelina picta*. Cytotoxic agent. Oil. $[\alpha]_D$ -75.6 (c, 0.7 in CH_2Cl_2). λ_{max} 230 (ϵ 19000) (EtOH) (Derep).

Raub, M.F. *et al., J.A.C.S.*, 1991, **113**, 3178-3180 (*isol, struct*)
Toyooka, N. *et al., J.O.C.*, 1996, **61**, 4882-4883 (*synth*)
Ha, J.D. *et al., J.O.C.*, 1997, **62**, 4550-4551 (*synth*)
Ha, J.D. *et al., J.A.C.S.*, 1999, **121**, 10012-10020 (*synth*)
Toyooka, N. *et al., Tetrahedron*, 1999, **55**, 15209-15224 (*synth, abs config*)
Xu, S. *et al., Org. Lett.*, 2006, **8**, 3179-3182 (*synth*)

Clavidol C-687

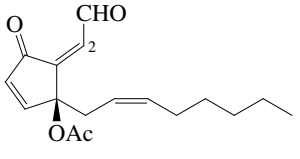
[477867-56-4]



$C_{30}H_{55}BrO_6$ 591.665
Constit. of *Laurencia viridis*. Amorph. solid. $[\alpha]_D^{25}$ +1.1 (c, 0.18 in $CHCl_3$).

Souto, M.L. *et al., Tetrahedron*, 2002, **58**, 8119-8125 (*isol, pmr, cmr*)

Clavirin I C-688



Absolute Configuration

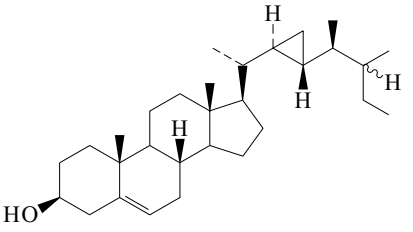
$C_{17}H_{22}O_4$ 290.358
Isol. from *Clavularia viridis*. Oil. $[\alpha]_D^{25}$ -17.1 (c, 0.48 in $CHCl_3$).

*2*E*-Isomer:* ***Clavirin II***
$C_{17}H_{22}O_4$ 290.358
Isol. from *Clavularia viridis*. Oil. $[\alpha]_D^{25}$ -33.7 (c, 0.43 in $CHCl_3$).

Iwashima, M. *et al., Tet. Lett.*, 1999, **40**, 6455-6459 (*isol, synth*)

Clavisterol A C-689

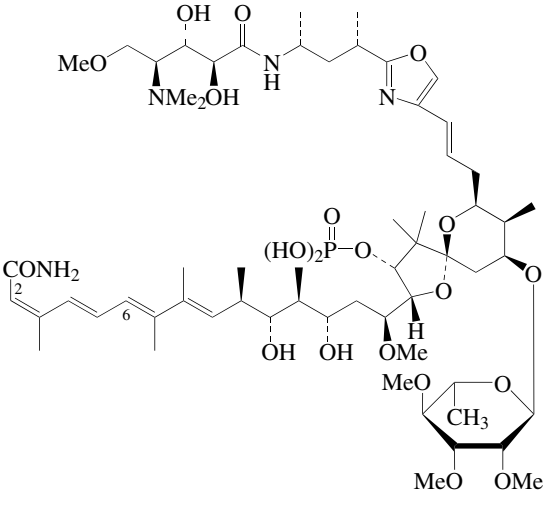
25-Ethyl-23,27-dinorgorgost-5-en-3-ol, 9CI. 26-Methyl-23-norgorgost-5-en-3-ol
[135729-45-2]



$C_{30}H_{50}O$ 426.724
Constit. of *Clavularia viridis*. Needles (Me_2CO/petrol). Mp 158-160°. $[\alpha]_D^{20}$ -2.5 (c, 0.233 in $CHCl_3$).

Su, J. *et al., CA*, 1991, **115**, 110910x (*isol, pmr*)

Clavosine A C-690



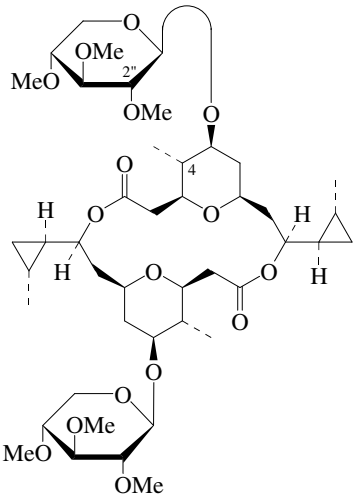
$C_{60}H_{101}N_4O_{20}P$ 1229.447
Isol. from the sponge *Myriastra clavosa*. Cytotoxic agent and inhibitor of protein phosphatases. Powder. $[\alpha]_D$ -5 (c, 0.36 in CH_2Cl_2). λ_{max} 228 (ϵ 20920); 332 (ϵ 23270) (MeOH).

*(2*E*)-Isomer:* ***Clavosine B***
$C_{60}H_{101}N_4O_{20}P$ 1229.447
Isol. from *Myriastra clavosa*. Cytotoxic agent and inhibitor of protein phosphatases. Powder. $[\alpha]_D$ -3.2 (c, 0.62 in CH_2Cl_2). λ_{max} 228 (ϵ 18570); 328 (ϵ 23000) (MeOH).

*(2*E*,6*Z*)-Isomer:* ***Clavosine C***
$C_{60}H_{101}N_4O_{20}P$ 1229.447
Isol. from *Myriastra clavosa*. Cytotoxic agent and inhibitor of protein phosphatases. Powder. $[\alpha]_D$ -31.7 (c, 0.12 in CH_2Cl_2). λ_{max} 228 (ϵ 20300); 318 (ϵ 19960) (MeOH).

Fu, X. *et al., J.O.C.*, 1998, **63**, 7957-7963

Clavosolide A C-691



$C_{44}H_{72}O_{16}$ 857.043

Stereochem. revised in 2006. Isol. from the sponge *Myriastra clavosa*. Sl. greenish viscous oil. $[\alpha]_D$ -48.5 (c, 1 in $CHCl_3$).

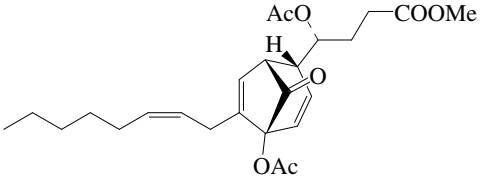
2″-O-De-Me: ***Clavosolide B***
$C_{43}H_{70}O_{16}$ 843.016
Isol. from *Myriastra clavosa*. Sl. greenish viscous oil. $[\alpha]_D$ -41 (c, 0.5 in $CHCl_3$).

4″-O-De-Me: ***Clavosolide C***
$C_{43}H_{70}O_{16}$ 843.016
Isol. from *Myriastra clavosa*. Solid. $[\alpha]_D$ -20 (c, 0.04 in MeOH).

4-Demethyl: ***Clavosolide D***
$C_{43}H_{70}O_{16}$ 843.016
Isol. from *Myriastra clavosa*. Oil.

Rao, M.R. *et al., J. Nat. Prod.*, 2002, **65**, 386-388 (*isol, pmr, cmr*)
Erickson, K.L. *et al., J. Nat. Prod.*, 2002, **65**, 1303-1306 (*isol, pmr, cmr*)
Son, J.B. *et al., Org. Lett.*, 2006, **8**, 661-664; 3411 (*synth*)
Smith, A.B. *et al., Org. Lett.*, 2006, **8**, 3315-3318 (*synth, stereochem*)
Chakraborty, T.K. *et al., Tet. Lett.*, 2006, **47**, 7435-7438 (*synth*)

Clavubicyclone C-692

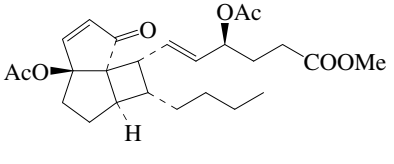


$C_{25}H_{34}O_7$ 446.539
Isol. from *Clavularia viridis*. Prostanoid-related oxylipin. Oil. $[\alpha]_D^{25}$ -59.4 (c, 0.53 in $CHCl_3$). λ_{max} 203 (ϵ 7600) (EtOH).

Iwashima, M. *et al., J.O.C.*, 2002, **67**, 2977-2981 (*isol, pmr, cmr*)
Ito, H. *et al., Org. Lett.*, 2006, **8**, 4883-4885 (*synth*)

Clavucyclin C-693

[270568-13-3]



Absolute Configuration

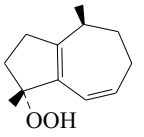
$C_{25}H_{34}O_7$ 446.539

Isol. from *Clavularia viridis*. Cytotoxic. $[\alpha]_D$ +9.7 ($CHCl_3$).

Iwashima, M. *et al., CA*, 2000, **133**, 4530k (*isol*)

Clavukerin C C-694

1,2,3,4,5,6-Hexahydro-1,4-dimethyl-1-azulenyl hydroperoxide, 9CI
1,2,3,4,5,6-Hexahydroxy-1-hydroperoxy-1,4-dimethylazulene
[91283-76-0]

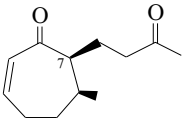


$C_{12}H_{18}O_2$ 194.273
Constit. of the soft coral *Clavularia koellikeri*. Unstable oil. $[\alpha]_D^{20}$ -61 ($CHCl_3$). λ_{max} 247 (sh) (ϵ 8300); 255 (ϵ 8500) (MeOH) (Derep).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1667

Clavularin A C-695

6-Methyl-7-(3-oxobutyl)-2-cyclohepten-1-one, 9CI
[86582-92-5]



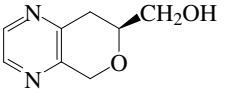
$C_{12}H_{18}O_2$ 194.273
Constit. of *Clavularia koellikeri*. Cytotoxic. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. λ_{max} 221 (ϵ 9800) (hexane) (Derep). λ_{max} 271 (ϵ 9700) (hexane) (Berdy).

7-Epimer: ***Clavularin B***
[86746-90-9]
$C_{12}H_{18}O_2$ 194.273
Constit. of *Clavularia koellikeri*. Cytotoxic. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. λ_{max} 221 (ϵ 9800) (hexane) (Derep). λ_{max} 227 (ϵ 9200) (cyclohexane) (Berdy).

Endo, M. *et al., Chem. Comm.*, 1983, 322-323; 980 (*isol, pmr, struct*)
Urech, R. *et al., Aust. J. Chem.*, 1986, **39**, 433 (*synth*)
Still, I.W.J. *et al., Tet. Lett.*, 1987, **28**, 2489 (*synth*)
Kim, S.K. *et al., J.O.C.*, 1991, **56**, 6829 (*synth*)
Tamura, R. *et al., J.O.C.*, 1993, **58**, 4471 (*synth*)
Weinmann, H. *et al., Synthesis*, 1995, 1097 (*synth, ir, pmr, cmr, ms*)
Hiroya, K. *et al., Synlett*, 1999, 529-532 (*synth*)

Clavulazine C-696

*7,8-Dihydro-5*H*-pyrano[3,4-*b*]pyrazine-7-methanol, 9CI*
[220525-28-0]

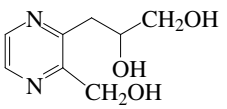


$C_8H_{10}N_2O_2$ 166.179

(S)-form
Alkaloid from the soft coral *Clavularia viridis*.
Needles (EtOAc/hexane).
Mp 101-102°. $[\alpha]_D$ -99.4 (c, 0.17 in $CHCl_3$). λ_{max} 272 (log ϵ 3.89); 277 (log ϵ 3.89); 310 (log ϵ 3.06) (EtOH).

Watanabe, K. *et al., Heterocycles*, 1998, **49**, 269-274 (*isol, pmr, cmr*)
Shen, Y.-C. *et al., J. Chin. Chem. Soc. (Taipei)*, 2004, **51**, 1421-1424 (*isol, pmr, cmr, ms*)
Kumar, S.P. *et al., Tet. Lett.*, 2006, **47**, 7149-7151 (*synth*)

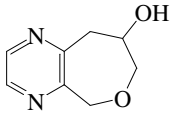
Clavulazol A C-697



$C_8H_{12}N_2O_3$ 184.194
Alkaloid from the soft coral *Clavularia viridis*. Amorph. solid. $[\alpha]_D^{25}$ -22.8 (c, 1 in MeOH). λ_{max} 277 (log ϵ 3.89); 311 (log ϵ 3.01) (no solvent reported).

Shen, Y.-C. *et al., J. Chin. Chem. Soc. (Taipei)*, 2004, **51**, 1421-1424 (*isol, pmr, cmr, ms*)

Clavulazol B C-698



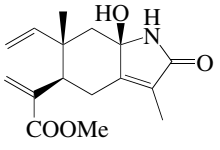
$C_8H_{10}N_2O_2$ 166.179

(-)-*form*
Alkaloid from the soft coral *Clavularia viridis*.
Amorph. solid. $[\alpha]_D^{25}$ -58.9 (c, 1 in MeOH). λ_{max} 272 (log ϵ 3.88); 278 (log ϵ 3.86); 309 (log ϵ 3.29) (no solvent reported).

Shen, Y.-C. *et al., J. Chin. Chem. Soc. (Taipei)*, 2004, **51**, 1421-1424 (*isol, pmr, cmr, ms*)

Clavulinin C-699

[185559-59-5]

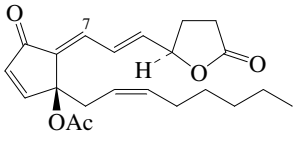


$C_{16}H_{21}NO_4$ 291.346
Constit. of *Clavularia inflata*. Needles.
Mp 190-191°.

Su, J. *et al., Chin. Sci. Bull.*, 1996, **41**, 1877-1880; *CA*, **126**, 87252a (*isol, pmr, cmr*)

Clavulolactone II C-700

12-(Acetyloxy)-4-hydroxy-9-oxo-5,7,10,14-prostatetraen-1-oic acid γ-lactone, 9CI
[166547-17-7]



Absolute Configuration

$C_{22}H_{28}O_5$ 372.46
Isol. from the soft coral *Clavularia viridis*. Oil. $[\alpha]_D^{25}$ -25.6 (c, 0.3 in $CHCl_3$).

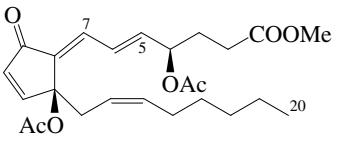
5Z-Isomer: ***Clavulolactone I***
$C_{22}H_{28}O_5$ 372.46
Isol. from *Clavularia viridis*. Oil. $[\alpha]_D$ -7.8 (c, 0.26 in $CHCl_3$). λ_{max} 231 (log ϵ 4.14); 292 (log ϵ 4.2) (EtOH).

7Z-Isomer: ***Clavulolactone III***
[166939-90-8]
$C_{22}H_{28}O_5$ 372.46
Isol. from *Clavularia viridis*. Oil. $[\alpha]_D^{25}$ -7.3 (c, 0.2 in $CHCl_3$).

Iguchi, K. *et al., J. Nat. Prod.*, 1995, **58**, 790 (*isol, uv, ir, cmr, pmr*)
Iwashima, M. *et al., J. Nat. Prod.*, 1999, **62**, 352-354 (*Clavulolactone I*)

Clavulones C-701

Methyl 4,12-bis(acetyloxy)-9-oxo-5,7,10,14-prostatetraen-1-oate, 9CI. Claviridenones



(5*E*,7*E*)-*form*

$C_{25}H_{34}O_7$ 446.539
Antiinflammatory agents.

(5*E*,7*E*)-*form*
Clavulone II. *Claviridenone C*
[85700-43-2]
Constit. of *Clavularia viridis*.
Yellowish oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +10.9 ($CHCl_3$). λ_{max} 230 (ϵ 12000); 292 (ϵ 14000) (EtOH) (Derep). λ_{max} 230 (ϵ 11700); 293 (ϵ 15000) (MeOH) (Berdy).

20-Acetoxy: ***20-Acetoxyclavulone II***
[88216-92-6]
$C_{27}H_{36}O_9$ 504.576
Constit. of *Clavularia viridis*. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +3.7 (c, 0.54 in $CHCl_3$). λ_{max} 230 (ϵ 14200); 292 (ϵ 18700) (MeOH) (Berdy).

4-Epimer: ***4-Epiclavulone II***
[243470-37-3]
$C_{25}H_{34}O_7$ 446.539
Constit. of *Clavularia viridis*. Oil. $[\alpha]_D^{25}$ -18.7 (c, 0.3 in $CHCl_3$). λ_{max} 228 (log ϵ 4.28); 291 (log ϵ 4.27) (EtOH).

(5*E*,7*Z*)-*form*
Clavulone III. *Claviridenone B*
[85700-44-3]
Constit. of *Clavularia viridis*.
Yellowish oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +45.5 ($CHCl_3$). λ_{max} 230 (ϵ 12000); 292 (ϵ 14000) (EtOH) (Derep). λ_{max} 230 (ϵ 13300); 293 (ϵ 13100) (MeOH) (Berdy).

20-Acetoxy: ***20-Acetoxyclavulone III***
[88216-93-7]
$C_{27}H_{36}O_9$ 504.576
Constit. of *Clavularia viridis*. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +26.4 (c, 0.86 in $CHCl_3$). λ_{max} 230 (ϵ 12400); 295 (ϵ 12100) (MeOH) (Berdy).

4-Epimer: ***4-Epiclavulone III***
[243470-38-4]
$C_{25}H_{34}O_7$ 446.539
Constit. of *Clavularia viridis*. Oil. $[\alpha]_D^{25}$ -10 (c, 0.06 in $CHCl_3$). λ_{max} 229 (log ϵ 4.23); 295 (log ϵ 4.14) (EtOH).

(5*Z*,7*E*)-*form*
Clavulone I. *Claviridenone D*
[85700-42-1]
Constit. of *Clavularia viridis*.
Yellowish oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -28.9 ($CHCl_3$). λ_{max} 230 (ϵ 12000); 292 (ϵ 14000) (EtOH) (Derep). λ_{max} 230 (ϵ 13600); 292 (ϵ 17300) (MeOH) (Berdy).

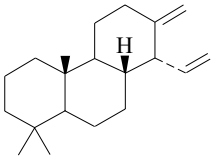
20-Acetoxy: 20-Acetoxyclavulone I
[88216-91-5]
$C_{27}H_{36}O_9$ 504.576
Constit. of *Clavularia viridis*. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ -31.1 (c, 0.09 in $CHCl_3$). λ_{max} 230 (ϵ 10900); 288 (ϵ 13700) (EtOH) (Berdy).

17,18-Didehydro(Z-): ***17,18-Dehydroclavulone I***. *17,18-Dehydroclaviridenone D. 17,18-Didehydroclavulone I*
[221194-77-0]
$C_{25}H_{32}O_7$ 444.524
Isol. from *Clavularia viridis*. Oil. $[\alpha]_D^{25}$ -27.1 (c, 0.31 in $CHCl_3$). λ_{max} 228 (log ϵ 3.98); 293 (log ϵ 4.01) (EtOH).

(5*Z*,7*Z*)-*form*
Clavulone IV. *Claviridenone A*
[85611-86-5]
Constit. of *Clavularia viridis*.
Yellowish oil. Sol. H_2O; poorly sol. H_2O. $[\alpha]_D$ -82.2 ($CHCl_3$). λ_{max} 230 (ϵ 12000); 292 (ϵ 14000) (EtOH) (Derep). λ_{max} 230 (ϵ 11700); 293 (ϵ 15000) (MeOH) (Berdy).
Kikuchi, H. *et al., Tet. Lett.*, 1982, **23**, 5171-5174; 1983, **24**, 1549-1552 (*Clavulones I-III, isol, struct, abs config*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1440-1443 (*Claviridenones*)
Iguchi, K. *et al., Tet. Lett.*, 1983, **24**, 4433-4434 (*Acetoxyclavulones*)
Corey, E.J. *et al., J.A.C.S.*, 1984, **106**, 3384 (*Clavulone I, synth*)
Nagaoka, H. *et al., Tet. Lett.*, 1984, **25**, 3621-3624 (*Clavulone II, synth*)
Hashimoto, S. *et al., Tet. Lett.*, 1985, **26**, 2679-2682 (*Clavulones I, II, synth*)
Shibasaki, M. *et al., Tet. Lett.*, 1985, **26**, 3841-3844 (*Clavulone I, synth*)
Kitagawa, I. *et al., Tetrahedron*, 1985, **41**, 995-1005 (*Claviridenones A-D, struct*)
Takemoto, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1106-1111 (*Clavulone III, synth*)
Klunder, A.J.H. *et al., Tet. Lett.*, 1991, **32**, 3131-3132 (*Clavulone I, synth*)
Iwashima, M. *et al., Chem. Pharm. Bull.*, 1999, **47**, 884-886 (*4-Epiclavulones*)
Iwashima, M. *et al., J. Nat. Prod.*, 1999, **62**, 352-354 (*Dehydroclavulone I*)

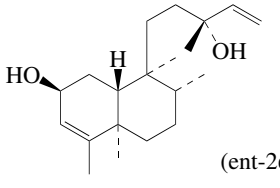
13(17),15-Cleistanthadiene C-702

[97605-24-8]



$C_{20}H_{32}$ 272.473
Constit. of *Amphibolis antartica*. Oil. $[\alpha]_D$ +42 (c, 8 in $CHCl_3$).
Dunlop, R.W. *et al., Phytochemistry*, 1985, **24**, 977-979

3,14-Clerodadiene-2,13-diol C-703



(ent-2α,13*S*)-*form*

$C_{20}H_{34}O_2$ 306.487

(*ent*-2α,13*S*)-*form*
2β-Hydroxykolavelool
[221466-42-8]
Constit. of *Aristolochia chamissonis*.
Amorph. solid. $[\alpha]_D^{25}$ -38.5 (c, 0.09 in $CHCl_3$).
2-Hydroperoxide: 2-Hydroperoxy-3,14-clerodadien-13-ol. ***2β-Hydroperoxykolavelool***
[221465-53-8]
$C_{20}H_{34}O_3$ 322.487
Amorph. solid. $[\alpha]_D^{25}$ -20 (c, 0.1 in $CHCl_3$).
2-Ketone: ***13-Epi-2-oxokolavelool***
[221466-41-7]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Aristolochia chamissonis*. Amorph. solid (hexane).
Mp 158-159°. $[\alpha]_D^{25}$ -25 (c, 0.1 in $CHCl_3$).

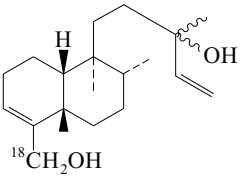
(*ent*-2β,13*R*)-*form*
Roseostachenol
[159440-60-5]
Isol. from *Stachys rosea*.
Cryst. (EtOH).
Mp 127°. $[\alpha]_D$ +16.8 (c, 0.178 in $CHCl_3$). C-13 config. determined in 1999.
2-Ketone: 13-Hydroxy-3,14-clerodadien-2-one. ***Roseostachenone***. *Nakamurol B*
[144606-88-2]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Stachys rosea* and *Agelas nakamurai*. Cryst. (EtOH). Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O.
Mp 121°. $[\alpha]_D^{20}$ -7.9 (c, 0.54 in $CHCl_3$). $[\alpha]_D^{25}$ -12.8 (c, 0.8 in $CHCl_3$). λ_{max} 235 (ϵ 8511) (MeOH) (Berdy).

(*ent*-2β,13*S*)-*form*
2α-Hydroxykolavelool. *13-Epiroseostachenol*
[221466-43-9]
Constit. of *Aristolochia chamissonis*.
Amorph. solid. $[\alpha]_D^{25}$ +10 (c, 0.1 in $CHCl_3$).

(*ent*-5α,13ξ)-*form*
2-Ketone: ***Nakamurol C***
$C_{20}H_{32}O_2$ 304.472
Constit. of *Agelas nakamurai*. Oil. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{25}$ -8 (c, 0.4 in $CHCl_3$). λ_{max} 246 (ϵ 6456) (MeOH) (Berdy).

(5α,8α,13*S*)-*form*
2-Ketone: Constit. of *Guarea trichilioides*.
Oil. $[\alpha]_D^{25}$ -8 (c, 0.4 in $CHCl_3$).
Fazio, C. *et al., Phytochemistry*, 1992, **31**, 3147; 1994, **37**, 501 (*isol, pmr, cmr*)
Shoji, N. *et al., J. Nat. Prod.*, 1996, **59**, 448-450 (*Nakamurols*)
Farlan, M. *et al., Phytochemistry*, 1996, **41**, 1159 (*isol, pmr, cmr*)
Bomm, M.D. *et al., Phytochemistry*, 1999, **50**, 455-461 (*Aristolochia chamissonis constits, cryst struct*)

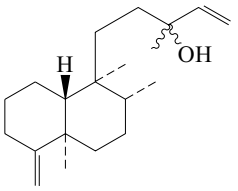
3,14-Clerodadiene-13,18-diol C-704



$C_{20}H_{34}O_2$ 306.487

(*ent*-5α,13ξ)-*form*
Sagittariol
[56497-92-8]
Constit. of *Sagittaria sagittifolia* (arrowhead).
Cryst. (C_6H_6/hexane).
Mp 109°. $[\alpha]_D$ +41 ($CHCl_3$).
18-(2-Pyrrolecarbonyl): ***Nakamurol D***
[174756-41-3]
$C_{25}H_{37}NO_3$ 399.572
Constit. of *Agelas nakamurai*. Pale yellow oil. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{25}$ -8.5 (c, 1.2 in $CHCl_3$).
13-Epimer: ***Deacetylrigidusol***
[329689-18-1]
$C_{20}H_{34}O_2$ 306.487
Constit. of *Haplopappus rigidus*. Gum. $[\alpha]_D^{24}$ -21.1 (c, 1.21 in $CHCl_3$).
13-Epimer, 18-Ac: ***Rigidusol***
[329688-58-6]
$C_{22}H_{36}O_3$ 348.525
Constit. of *Haplopappus rigidus*. Gum. $[\alpha]_D^{24}$ -31.8 (c, 0.11 in $CHCl_3$).
Sharma, S.C. *et al., Phytochemistry*, 1975, **14**, 1055; 1984, **23**, 1194 (*Sagittariol*)
Shoji, N. *et al., J. Nat. Prod.*, 1996, **59**, 448-450 (*Nakamurol D*)
Morales, G. *et al., Phytochemistry*, 2000, **55**, 863-866 (*Rigidusol, Deacetylrigidusol*)

4(18),14-Clerodadien-13-ol C-705



$C_{20}H_{34}O$ 290.488

(*ent*-13ξ)-*form*

Chelodane

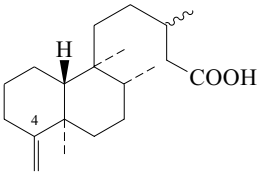
[145458-08-8]

Constit. of *Chelonaplysilla erecta*.

Oil.

Rudi, A. *et al., J. Nat. Prod.*, 1992, **55**, 1408 (*isol, pmr, cmr*)

4(18)-Cleroden-15-oic acid C-706



$C_{20}H_{34}O_2$ 306.487

(*ent*-13ξ)-*form* [120552-38-7]

Constit. of *Ageratina ixiocladon*.

Et ester: [672953-29-6]

$C_{22}H_{38}O_2$ 334.541

Constit. of *Clausena dunniana*.

(1-Acetoxy-3-hydroxy-2-propyl) ester: [588701-37-5]

$C_{25}H_{42}O_5$ 422.604

Constit. of *Austrodoris kerguelenensis*.

*(3-Hydroxy-1-tigloyloxy-2-propyl) ester (*S-*):* ***Archidorin***

[153415-51-1]

$C_{28}H_{46}O_5$ 462.668

Constit. of *Archidoris tuberculata*. Ichthyotoxic agent. Amorph. powder. Sol. MeOH. $[\alpha]_D^{25}$ +12.1 (c, 0.3 in $CHCl_3$). λ_{max} 210 (ϵ 12300) (MeOH) (Berdy).

*(3-Hydroxy-2*S*-tigloyloxypropyl) ester:* ***Isoarchidorin***

[154030-51-0]

$C_{28}H_{46}O_5$ 462.668

Constit. of *Archidoris pseudoargus*.

4α,18-Epoxide: **ent-*4β,18-Epoxy-15-clerodanoic acid***

[120552-40-1]

$C_{20}H_{34}O_3$ 322.487

Constit. of *Ageratina ixiocladon*.

4β,18-Epoxide: **ent-*4α,18-Epoxy-15-clerodanoic acid***

[120662-28-4]

$C_{20}H_{34}O_3$ 322.487

Constit. of *Ageratina ixiocladon*.

Tanayo-Castillo, G. *et al., Phytochemistry*, 1989, **28**, 139

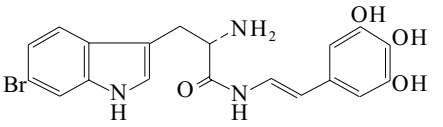
Cimino, G. *et al., J. Nat. Prod.*, 1993, **56**, 1642-1646 (*Archidorin*)

Soriente, A. *et al., Nat. Prod. Lett.*, 1993, **3**, 31-35 (*Isoarchidorin*)

He, H.-P. *et al., Helv. Chim. Acta*, 2003, **86**, 3187-3193 (*isol, pmr, cmr*)

Gavagnin, M. *et al., Tetrahedron*, 2003, **59**, 5579-5583 (*Austrodoris kerguelenensis constit*)

Clionamide C-707



$C_{19}H_{18}BrN_3O_4$ 432.273

(*S*)-*form* [68835-91-6]

Major metab. from the sponge *Cliona celata*. Chelate forming. Unstable yellow powder. $[\alpha]_D$ +32.1 (c, 2.12 in MeOH). λ_{max} 227 (ϵ 31000); 291 (ϵ 11000); 296 (ϵ 12000); 311 (sh) (ϵ 9400) (MeOH) (Derep).

Tetra-Ac: ***Tetraacetylclionamide***

[68857-44-3]

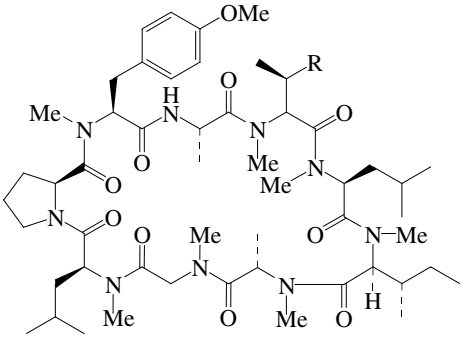
$C_{27}H_{26}BrN_3O_8$ 600.422

Isol. from *Cliona celata*. Cryst. (THF/diisopropyl ether). Mp 209-211°. $[\alpha]_D$ +45 (c, 0.7 in Me_2CO).

Andersen, R.J. *et al., Can. J. Chem.*, 1979, **57**, 2325 (*isol, uv, ir, pmr, cmr, ms, struct*)

Stonard, R.J. *et al., J.O.C.*, 1980, **45**, 3687 (*isol, deriv*)

Clonostachysin A C-708



R = CH_3

$C_{53}H_{87}N_9O_{10}$ 1010.325

Prod. by marine-derived fungus *Clonostachys rogersoniana* HJK9. Active against the dinoflagellate *Prorocentrum micans*. Powder. $[\alpha]_D^{25}$ -97 (c, 0.06 in MeOH). λ_{max} 282 (ϵ 820) (MeOH).

Adachi, K. *et al., J. Antibiot.*, 2005, **58**, 145-150 (*isol, pmr, cmr, ms*)

Clonostachysin B C-709

As Clonostachysin A, C-708 with

R = $-CH_2CH_3$

$C_{54}H_{89}N_9O_{10}$ 1024.351

Prod. by marine-derived fungus *Clonostachys rogersoniana* HJK9. Active against the dinoflagellate *Prorocentrum micans*. Powder. $[\alpha]_D^{25}$ -87 (c, 0.03 in MeOH). λ_{max} 282 (ϵ 1000) (MeOH).

Adachi, K. *et al., J. Antibiot.*, 2005, **58**, 145-150 (*isol, pmr, cmr, ms*)

Clupeine C-710

[9007-31-2]

H-Ala-Arg-Arg-Arg-Arg-Ser-Arg-Arg-Ala-Ser-Arg-Pro-Val-Arg-Arg-Arg-Arg-Pro-Arg-Arg-Val-Ser-Arg-Arg-Arg-Arg-Ala-Arg-Arg-Arg-Arg-OH

Peptide. Consists of 3 main molecular species, YI, YII and Z. Struct. of Z shown. Isol. from sperm nuclei of Pacific herring (*Clupea pallasii*). Protamine. Sol. H_2O.

[11061-43-1, 12291-22-4, 39368-62-2]

Iwai, K. *et al., J. Biochem. (Tokyo)*, 1971, **69**, 493 (*struct, Z*)

Suzuki, K. *et al., J. Biochem. (Tokyo)*, 1972, **72**, 1419; 1433 (*struct, YI, YII*)

Clytin C-711

Phialidin

[149372-06-5]

Peptide containing 189 amino acid residues with 3 $Ca^{2\oplus}$-binding sites. Isol. from the hydroid *Clytia gregarium* (formerly *Phialidium gregarium*). $Ca^{2\oplus}$-activated photoprotein.

Inouye, S. *et al., FEBS Lett.*, 1993, **315**, 343-346

CMP-*N*-acetylneuraminate monooxygenase C-712

E.C. 1.14.18.2. CMP-N-*acetylneuraminate, ferrocytochrome-*b_5*:oxygen oxidoreductase (*N-*acetyl-hydroxylating)*. N-*Acetylneuraminate hydroxylase. E.C. 1.14.13.35 (transferred)*

[116036-67-0]

Oxidoreductase enzyme. Abundant in most mammals but not present in humans; also isol. from *Asterias rubens*. Catalyses the reaction of CMP-*N*-acetylneuraminate with O_2 and ferrocytochrome b_5 to give CMP-*N*-glycolylneuraminate, H_2O and ferricytochrome b_5.

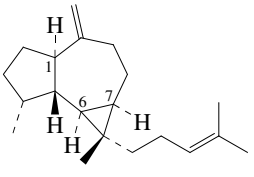
Schauer, R. *et al., Methods Enzymol.*, 1978, **50**, 374-386 (*pig submandibular glands*)
Kozutsumi, Y. *et al., J. Biochem. (Tokyo)*, 1990, **109**, 704-706 (*mouse liver*)
Schlenza, W. *et al., Glycobiology*, 1994, **4**, 675-683 (*pig submandibular glands*)
Schneckenburger, P. *et al., Glycoconjugate J.*, 1994, **11**, 194-203 (*mouse liver*)
Gollub, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2003, **134**, 89-101 (*Asterias rubens*)

CNC 2 C-713

Complex mixt. of galactocerebroside homologues. Isol. from the starfish *Culcita novaeguineae*. Amorph. powder. $[\alpha]_D$ +2.1 (c, 1 in Py).

Inagaki, M. *et al., Chem. Pharm. Bull.*, 2006, **54**, 260-261 (*isol, cmr*)

10(14),17-Cneorubadiene C-714



(1α,4α,5β,6α,7α)-*form*

$C_{20}H_{32}$ 272.473

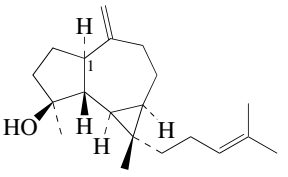
(1α,4α,5β,6α,7α)-*form*
Cneorubin W₂
[77346-64-6]
Constit. of *Cneorum tricoccon*.
Oil. $Bp_{0.05}$ 42°.

(1β,4α,5β,6α,7α)-*form*
Cneorubin W₁
[77399-43-0]
Constit. of *Cneorum tricoccon*.
Oil. $Bp_{0.05}$ 42°.

(1β,4α,5β,6α,7β)-*form*
Emmottene
[169221-35-6]
Constit. of *Briareum polyanthes*.
Oil. Unusual *trans*-bicyclo[5.1.0]octane ring system.

Trautmann, D. *et al., Chem. Ber.*, 1980, **113**, 3848 (*Cneorubins*)
Cronan, J.M. *et al., J.O.C.*, 1995, **60**, 6864-6865 (*Emmottene*)

10(14),17-Cneorubadien-4-ol C-715



$C_{20}H_{32}O$ 288.472

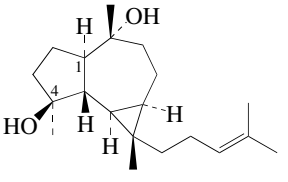
(1α,4β,5β)-*form* [193411-73-3]
Constit. of a *Sinularia* coral.
Oil. $[\alpha]_D^{25}$ -25.9 (c, 1.5 in $CHCl_3$).

10α,14-Epoxide: ***10,14-Epoxy-17-cneoruben-4-ol***
[193411-76-6]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Sinularia* coral. Oil. $[\alpha]_D^{25}$ -42.5 (c, 1 in $CHCl_3$).

(1β,4β,5β)-*form*
Cneorubin X
[77346-63-5]
Isol. from *Cneorum tricoccon*.
Oil. $Bp_{0.05}$ 65°. $[\alpha]_D^{20}$ -26 (c, 0.8 in Me_2CO).

Trautmann, D. *et al., Chem. Ber.*, 1980, **113**, 3848 (*Cneorubin X*)
Anjaneyulu, A.S.R. *et al., Tetrahedron*, 1997, **53**, 9301-9312 (*Sinularia constits*)

17-Cneorubene-4,10-diol C-716



$C_{20}H_{34}O_2$ 306.487

(1α,4β,5β,10α)-*form*
10-Me ether: 10-Methoxy-17-cneoruben-4-ol
[193411-75-5]
$C_{21}H_{36}O_2$ 320.514
Constit. of *Sinularia* coral. Oil. $[\alpha]_D^{25}$ -23.7 (c, 0.7 in $CHCl_3$).

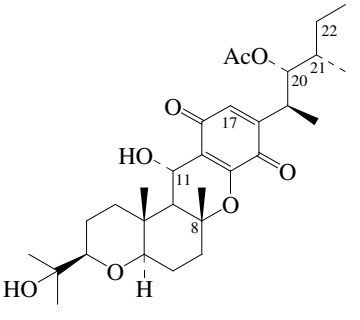
(1β,4α,5β,10α)-*form* [193411-74-4]
Constit. of a *Sinularia* coral.
Oil. $[\alpha]_D^{25}$ -19.6 (c, 0.7 in $CHCl_3$).

Anjaneyulu, A.S.R. *et al., Tetrahedron*, 1997, **53**, 9301-9312 (*isol, pmr, cmr*)

Cochlioquinone A C-717

Luteoleersin

[32450-25-2]



$C_{30}H_{44}O_8$ 532.673

CAS numbering shown. Prod. by *Bipolaris cynodontis* and *Cochliobolus miyabeanus*. NADH-ubiquinone reductase inhibitor. Inhibitor of diacylglycerol kinase. Phytotoxin; inhibitor of root growth. Nematocide. Cryst. (hexane).
Mp 130-132°. λ_{max} 245 (ϵ 3300); 280 (ϵ 11000); 398 (ϵ 900) (MeOH) (Derep). λ_{max} 270 (ϵ 22000); 399 (ϵ 2400) (MeOH) (Berdy).

21,22-Didehydro(Z-): ***Stemphone A***
[54854-92-1]
$C_{30}H_{42}O_8$ 530.657
Prod. by *Bipolaris cynodontis*, *Cochliobolus miyabeanus*, *Stemphylium sarcinaeforme*, *Stemphylium sarcinae* and *Drechslera sacchari*. NADH-ubiquinone reductase inhibitor. Inhibitor of diacylglycerol kinase. Phytotoxin. Active against *Sarcina lutea* and phytopathogenic fungi. Yellow needles (hexane). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O, bases, acids.
Mp 161°. $[\alpha]_D^{29}$ +146 (c, 1 in EtOH). λ_{max} 245 (ϵ 3300); 280 (ϵ 11000); 398 (ϵ 900) (MeOH) (Derep). λ_{max} 267 (ϵ 9890); 390 (ϵ 1030) (MeOH) (Berdy).

11-Deoxy, 20-ketone, O*-de-Ac:* ***Cochlioquinone B***
[32450-26-3]
$C_{28}H_{40}O_6$ 472.62
Prod. by *Bipolaris cynodontis*, *Cochliobolus miyabeanus* and *Drechslera dematioidea*. NADH-ubiquinone reductase inhibitor. Phytotoxic agent, inhibitor of root growth. Yellow cryst. (Et_2O).
Mp 168-169°. $[\alpha]_D^{22}$ +111.5 (c, 0.1 in EtOH). λ_{max} 401 (MeOH) (Derep). λ_{max} 260 (ϵ 22000); 395 (ϵ 2100) (EtOH) (Berdy).

17-Methoxy: ***17-Methoxycochlioquinone A***
$C_{31}H_{46}O_9$ 562.699
Prod. by *Bipolaris brizae*. Antagonist of the human chemokine receptor CCR5. Yellow oil. $[\alpha]_D^{25}$ +141 (c, 0.2 in $CHCl_3$). λ_{max} 283 (log ϵ 4.04); 386 (log ϵ 3.52) (MeOH).

Hydroquinone, 11-ketone: ***Isocochlioquinone A***
[156759-06-7]
$C_{30}H_{44}O_8$ 532.673
Prod. by *Bipolaris bicolor* and the marine-derived *Drechslera dematioidea*. Phytotoxin. Yellow cryst. + $\frac{1}{2}H_2O$ (hexane).
Mp 166-168°. $[\alpha]_D^{22}$ +148 (c, 0.21 in EtOH). λ_{max} 214 (log ϵ 4.16); 283 (log ϵ 3.97); 338 (log ϵ 3.59) (EtOH). λ_{max} 243 (ϵ 12000); 283 (ϵ 24000); 383 (ϵ 6500) (EtOH).

Hydroquinone, 11-deoxy, 20-ketone, O*-de-Ac:* ***Isocochlioquinone C***
$C_{28}H_{42}O_6$ 474.636
Prod. by *Bipolaris cynodontis* and the marine-derived *Drechslera dematioidea*. Yellow solid. $[\alpha]_D^{20}$ +155.5 (c, 0.2 in EtOH). $[\alpha]_D$ +287.4 (c, 0.27 in MeOH). λ_{max} 211 (log ϵ 4.06); 238 (sh) (log ϵ 3.71); 281 (log ϵ 3.84); 290 (sh) (log ϵ 3.78); 382 (log ϵ 3.39) (EtOH). λ_{max} 250 (ϵ 8600); 302 (ϵ 5500) (MeOH).

8-Epimer: ***Epicochlioquinone A***
[147384-57-4]
$C_{30}H_{44}O_8$ 532.673
Prod. by *Stachybotrys bisbyi* SANK17777. Acyl CoA-cholesterol transferase inhibitor. Yellow cryst. (hexane/Me_2CO).
Mp 158-161°. $[\alpha]_D$ +43.4 (c, 1.2 in EtOH). λ_{max} 270 (ϵ 10500); 386 (ϵ 1120) (MeOH) (Berdy).

8-Epimer, 11-Me ether: ***11-O-Methylepicochlioquinone A***
$C_{31}H_{46}O_8$ 546.7
Prod. by *Stachybotrys chartarum*. Antagonist of human chemokine receptor CCR5. Yellow solid. $[\alpha]_D^{25}$ +38 (c, 0.12 in $CHCl_3$). λ_{max} 270 (log ϵ 4.04); 385 (log ϵ 3.52) (MeOH).

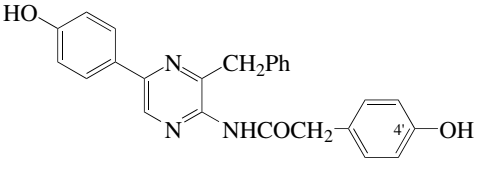
8-Epimer, 11-deoxy, 20-ketone, O*-de-Ac:* ***Epicochlioquinone B***
[157183-69-2]
$C_{28}H_{40}O_6$ 472.62
Prod. by *Neobulgaria pura* A4588. Platelet aggregation inhibitor. Yellow needles. Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. H_2O.
Mp 161-162°. Shows small positive opt. rotation. λ_{max} 260 (ϵ 10530) (MeOH).

8-Epimer, hydroquinone, 11-deoxy, 20-ketone, O*-de-Ac:* ***Epidihydrocochlioquinone B***
[157078-26-7]
$C_{28}H_{42}O_6$ 474.636
Prod. by *Neobulgaria pura* A4588. Off-white solid. Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. H_2O. Shows small positive opt. rotation. λ_{max} 294 (ϵ 7153) (MeOH).

Scott, P.M. *et al., Can. J. Microbiol.*, 1968, **14**, 1015 (*isol, Stemphone*)
Huber, C. *et al., Acta Cryst. B*, 1975, **31**, 108 (*cryst struct, Stemphone*)
Canonica, L. *et al., Gazz. Chim. Ital.*, 1976, **106**, 147 (*isol, struct*)
Canonica, L. *et al., Chem. Comm.*, 1978, 679 (*biosynth*)
Schaeffer, J.M. *et al., J. Antibiot.*, 1990, **43**, 1179 (*props*)
Miyagawa, H. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1143-1145 (*Stemphone, Isocochlioquinone A*)
Ogawara, H. *et al., J. Antibiot.*, 1994, **47**, 499; 1995, **48**, 1076 (*Stemphone, isol, props*)
Lorenzen, K. *et al., Z. Naturforsch., C*, 1994, **49**, 312-320 (*Epicochlioquinone B*)
Fujioka, T. *et al., J. Antibiot.*, 1996, **49**, 409 (*Epicochlioquinone A*)
Lim, C.-M. *et al., J. Pestic. Sci. (Int. Ed.)*, 1996, **21**, 213-217; 1998, **23**, 281-288 (*activity*)
Osterhage, C. *et al., J. Nat. Prod.*, 2002, **65**, 306-313 (*Cochlioquinone B, Isocochlioquinones A,C*)
Yoganathan, K. *et al., J. Antibiot.*, 2004, **57**, 59-63 (*17-Methoxycochlioquinone A, 11-O-Methylepicochlioquinone A*)

Coelenteramide C-718

[50611-86-4]



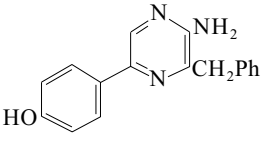
$C_{25}H_{21}N_3O_3$ 411.459
The light-emitter in *Aequorea, Cavernularia obesa* and other bioluminescent coelenterates. Blue fluorescent compd.

4′-Deoxy: Renilla *Oxyluciferin*
[50909-85-8]
[145022-31-7]
$C_{25}H_{21}N_3O_2$ 395.46
Chemiluminescent agent from *Renilla reniformis*.

Hori, K. *et al., Biochemistry*, 1973, **12**, 4463; 1975, **14**, 2371-2376 (Renilla *Oxyluciferin*)
Shimomura, O. *et al., Chem. Lett.*, 1975, 247 (*isol*)
Shimomura, O. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1975, **72**, 1546 (*isol*)

Coelenteramine C-719

4-[(5-Amino-6-phenylmethyl)pyrazinyl]phenol, 9CI. 2-Amino-3-benzyl-5-(4-hydroxyphenyl)pyrazine
[37156-84-6]



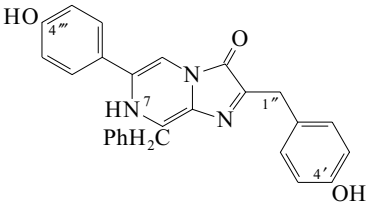
$C_{17}H_{15}N_3O$ 277.325
Isol. from jellyfish *Aequorea*. Luminescent agent. Yellow needles. Mp 217-219°.

2-Ac:
Yellow needles. Mp 199-200°.

Shimonura, O. *et al., Biochemistry*, 1972, **11**, 1602
Kishi, Y. *et al., Tet. Lett.*, 1972, 2747 (*synth*)
Hori, K. *et al., Chem. Comm.*, 1973, 492

Coelenterazine C-720

6-(4-Hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]-8-(phenylmethyl)imidazo[1,2-a]pyrazin-3(7H)-one, 9CI. Oplophorus *Luciferin*. Watasenia *Preluciferin*
[55779-48-1]



$C_{26}H_{21}N_3O_3$ 423.47
Bioluminescence factor isol. from various marine sources incl. *Aequorea victoria*. Yellow cryst.
Mp 176-181° dec.

4′,4‴-Di-O-sulfate: **Watasenia *Luciferin***
[61369-27-5]
$C_{26}H_{21}N_3O_9S_2$ 583.599
Isol. from *Watasenia scintillans*.

4′-Deoxy: 6-(4-Hydroxyphenyl)-2,8-bis(phenylmethyl)imidazo[1,2-a]pyrazin-3(7H)-one, 9CI. **Renilla *Luciferin***
[50909-86-9]
$C_{26}H_{21}N_3O_2$ 407.471
Isol. from *Renilla reniformis* and other marine animals. Bioluminescence factor.

1″,7-Didehydro: ***Dehydrocoelenterazine***. Watasenia *Dehydropreluciferin*
[62541-09-7]
$C_{26}H_{19}N_3O_3$ 421.454
Isol. from the liver of *Watasenia scintillans*. Bioluminescence factor. Dark red cryst. (Et_2O). Dec. at *ca*. 250°.

Inoue, S. *et al., Tet. Lett.*, 1976, **34**, 2971 (*Watasenia Luciferin*)
Inoue, S. *et al., Chem. Lett.*, 1977, 259 (*Dehydrocoelenterazine*)
Inoue, S. *et al., Tet. Lett.*, 1977, 2685 (*Coelenterazine*)
Inoue, S. *et al., Chem. Lett.*, 1980, 299 (*synth*)
Shimomura, O. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, 65; 435 (*occur*)
Teranishi, K. *et al., Bull. Chem. Soc. Jpn.*, 1990, **63**, 3132 (*synth, conformn*)
Kakoi, H. *et al., Phytochemistry*, 1998, **48**, 1669-1672 (*synth*)
Adamczyk, M. *et al., Org. Prep. Proced. Int.*, 2001, **33**, 477-485 (*synth, ir, pmr*)
Wu, C. *et al., Tetrahedron*, 2001, **57**, 9575-9583 (*biosynth, bibl*)

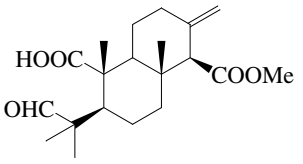
Coelenterolysin C-721

[160307-18-6]
Polypeptide; struct. unknown. Isol. from the coelenteric fluid of the sea anemone *Phymactis clematis*. Haemolytic agent. Toxin.

Meinardi, E. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1994, **109**, 153-161 (*isol, activity*)
Meinardi, E. *et al., Biochem. Biophys. Res. Commun.*, 1995, **216**, 348-354 (*props*)

Coeloic acid C-722

[883725-48-2]

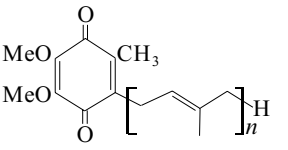


$C_{20}H_{30}O_5$ 350.454
Constit. of *Coelocarteria* cfr. *singaporensis*. Amorph. solid.

Fattorusso, E. *et al., Tet. Lett.*, 2006, **47**, 2197-2200 (*Coeloic acid*)

Coenzyme Q C-723

Mitoquinone. Ubiquinone



A group of related substances having n = 1-12; the main naturally occurring homologues have n = 6-10. Subscript number (≡ Ubiquinone no.) indicates n. For lowest homologue, see 2,3-Dihydroxy-5-methyl-1,4-benzoquinone. In redox bioequilibrium with the reduced forms (hydroquinones), the CAS nos. for some of which are given in this entry. Occur in animal and microorganism mitochondria. Isol. from many sources, some of which are specifically indicated below. Participate in cellular electron transport.

Coenzyme Q_1
Ubiquinone 1
[727-81-1]
$C_{14}H_{18}O_4$ 250.294
Red oil.

Coenzyme Q_2
Ubiquinone 2
[606-06-4]
[5677-55-4, 75426-27-6]
$C_{19}H_{26}O_4$ 318.412
Red oil.

Coenzyme Q_3
Ubiquinone 3
[1173-76-8]
$C_{24}H_{34}O_4$ 386.53
Red oil.

Coenzyme Q_4
Ubiquinone 4
[4370-62-1]
$C_{29}H_{42}O_4$ 454.648
Isol. from various bacteria and yeasts. Red oil.

6′,7′R,10′,11′R,14′,15′-Hexahydro: Hexahydrocoenzyme Q_4. ***Phytylubiquinone***. *H_6CoQ_4*
[362-45-8]
$C_{29}H_{48}O_4$ 460.696
Isol. from *Torula* spp. and various bacteria. Radioprotectant. Oil.
$Bp_{0.01}$ 155-160°.

Coenzyme Q_5
Ubiquinone 5
[4370-61-0]
$C_{34}H_{50}O_4$ 522.767
Isol. from an *Escherichia coli* strain.

Coenzyme Q_6
Ubiquinone 6. *Ubiquinone 30*
[1065-31-2]
$C_{39}H_{58}O_4$ 590.885
Isol. from bakers' yeast (*Saccharomyces cerevisiae*) and *Torula spp.*
Orange-yellow cryst. (EtOH) or red oil.
Mp 19-20° (16°).

Coenzyme Q_7
Ubiquinone 7. *Ubiquinone 35*
[303-95-7]
$C_{44}H_{66}O_4$ 659.003
Isol. from *Torula utilis* and *Candida utilis*. Orange-red cryst. (petrol).
Mp 31-32°.

▶GU5310000

Coenzyme Q_8

Ubiquinone 8. Ubiquinone 40

[2394-68-5]

$C_{49}H_{74}O_4$ 727.121

Prod. by *Azotobacter vinelandii* and *Pseudomonas alkanolytica*. Immunomodulator. Antifouling agent. Orange plates (petrol). Mp 37-38°. λ_{max} 275; 405 (MeOH) (Berdy).

Coenzyme Q_9

Ubiquinone 9. Ubiquinone 45

[303-97-9]

$C_{54}H_{82}O_4$ 795.239

Isol. from *Penicillium chrysogenum, Torula utilis* and *Pseudomonas alkanolytica*. Also isol. from the marine *Nocardia* sp. KMM 3749. Orange cryst. (EtOH).

Mp 45.2°.

▶DK4786000

34′,35′-Dihydro: ***Dihydroubiquinone 9***. *Dihydroubiquinone 45*

[142628-59-9]

$C_{54}H_{84}O_4$ 797.255

Isol. from *Aureobasidium pullulans*.

Coenzyme Q_{10}

Ubiquinone 10. Ubiquinone 50. Ubidecarenone, BAN, INN. NSC 140865. Many other names

[303-98-0]

$C_{59}H_{90}O_4$ 863.358

Isol. from beef heart and other mammalian sources in which it is the principal representative of its class. Cardiovascular agent, used to treat congestive heart failure. Used in the treatment of Huntington's disease. Orange cryst. (MeOH or EtOH) at low temp.

Mp 49.9°. Log P 20.24 (uncertain value) (calc).

▶Exp. reprod. and teratogenic effects. DK3900000

38′,39′-Dihydro: ***Coenzyme Q_{10} (H-10)***. *CoQ_x. Ubiquinol 50*

[992-78-9]

$C_{59}H_{92}O_4$ 865.373

Prod. by a strain of *Penicillium stipitatum*, by *Gliocladium roseum* and *Gibberella fujikuroi*. Orange-yellow cryst. (EtOH).

Mp 29°.

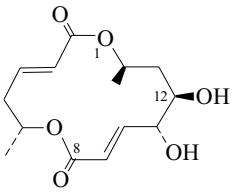
[606-06-4, 727-81-1, 1173-76-8, 4370-62-1, 24663-35-2, 24663-36-3, 75763-46-1]

Gloor, U. *et al., Helv. Chim. Acta*, 1958, **41**, 2357; 1960, **43**, 1745 (*synth*)
Lester, R.L. *et al., J.A.C.S.*, 1958, **80**, 4751 (*isol*)
Shunk, C.H. *et al., J.A.C.S.*, 1958, **80**, 4753 (*Coenzymes Q_1, Q_2, Q_3*)
Crane, F.L. *et al., Biochim. Biophys. Acta*, 1959, **32**, 73 (*isol*)
Gale, P.H. *et al., Biochem. Biophys. Res. Commun.*, 1963, **12**, 414 (*Coenzyme Q_{10} (H-10)*)
Gale, P.H. *et al., Biochemistry*, 1963, **2**, 196 (*Coenzyme Q_{10} (H-10)*)
Mahler, H.R. *et al., Biochemistry*, 1964, **3**, 893-895 (*Coenzyme Q_6, isol*)
Morimoto, H. *et al., Biochem. Z.*, 1965, **343**, 329 (*ir, ms, pmr*)
Lavate, W.V. *et al., J. Biol. Chem.*, 1965, **240**, 524 (*Coenzyme Q_{10} (H-10)*)
Friis, P. *et al., J.A.C.S.*, 1966, **88**, 4754 (*biosynth*)
Weinstock, L.M. *et al., J. Chem. Eng. Data*, 1967, **12**, 155 (*hexahydrocoenzyme Q_4*)
Muraca, R.F. *et al., J.A.C.S.*, 1967, **89**, 1505 (*ms*)
Morimoto, H. *et al., Annalen*, 1969, **729**, 158 (*ir, pmr, uv, ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, nos. 4256-4260 (*occur, bibl*)
The Vitamins, (Sebrell, W.H. *et al*, Ed.), Academic Press, 1972, 355 (*rev*)
Inoue, S. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 3098-3101 (*synth, ir, pmr, uv*)
Hegedus, L.S. *et al., J.A.C.S.*, 1976, **98**, 3901
Biomed. Clin. Aspects Coenzyme Q, Elsevier, N.Y., 1977, **1-3**, (*books*)
Terao, S. *et al., J.C.S. Perkin 1*, 1978, 1101 (*cmr, pmr*)
Terao, S. *et al., J.O.C.*, 1979, **44**, 868 (*synth*)
Naruta, Y. *et al., J.O.C.*, 1980, **45**, 4097 (*synth*)
Boicelli, C.A. *et al., Membr. Biochem.*, 1981, **4**, 105 (*pmr, cmr, config*)
Fujita, Y. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 1325(*synth*)
Cascone, A. *et al., Boll. Chim. Farm.*, 1984, **123**, 555 (*pharmacol, Ubidecarenone*)
Masaki, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3959 (*synth*)
Kalén, A. *et al., Acta Chem. Scand., Ser. B*, 1987, **41**, 70 (*biosynth*)
Konishi, K. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1531 (*biochem, bibl*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 8345 (*synonyms*)
Eren, D. *et al., J.A.C.S.*, 1988, **110**, 4356 (*synth*)
Greenberg, S.M. *et al., Med. Clin. North Am.*, 1988, **72**, 243 (*rev, pharmacol*)
Morimoto, H. *et al., Naturwissenschaften*, 1989, **76**, 200-205 (*synth*)
Rüttimann, A. *et al., Helv. Chim. Acta*, 1990, **73**, 790 (*synth, bibl*)
Takizawa, K. *et al., FEMS Microbiol. Lett.*, 1992, **92**, 129 (*Dihydroubiquinone 9*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1425
Merz, A. *et al., Synthesis*, 1993, 797 (*Coenzyme Q_2*)
Lipshutz, B.H. *et al., J.A.C.S.*, 1996, **118**, 5512 (*synth*)
Duvold, T. *et al., Tet. Lett.*, 1997, **38**, 6181-6184 (*biosynth*)
Boullais, C. *et al., Tetrahedron*, 1997, **53**, 2505 (*synth, Ubiquinone-3*)
Org. Synth., Coll. Vol., 9, 1998, 741-744 (*Coenzyme Q_1, synth, ir, pmr*)
Giner, J.-L. *et al., Tet. Lett.*, 1998, **39**, 8021-8022 (*biosynth*)
Lipshutz, B.H. *et al., J.A.C.S.*, 1999, **121**, 11664-11673 (*synth*)
Tran, M.T. *et al., Pharmacotherapy (Carlisle, Mass.)*, 2001, **21**, 797-806 (*Coenzyme Q_{10}, rev*)
Ferrante, R.J. *et al., J. Neurosci.*, 2002, **22**, 1592-1599 (*Coenzyme Q_{10}, pharmacol*)
Lipshutz, B.H. *et al., J.A.C.S.*, 2002, **124**, 14282-14283 (*Coenzyme Q_{10}, synth*)
Kuznetsova, T.A. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2002, **51**, 1951-1953 (*Coenzyme Q_9, isol*)
Lu, L. *et al., Synth. Commun.*, 2004, **34**, 4049-4053 (*Coenzyme Q_1, synth*)
Yu, X.-J. *et al., Helv. Chim. Acta*, 2005, **88**, 2575-2581 (*Coenzyme Q_{10}, synth*)
Lipshutz, B.H. *et al., Org. Lett.*, 2005, **7**, 4095-4097 (*Coenzyme Q_1, synth*)
Dai, H.-F. *et al., Helv. Chim. Acta*, 2006, **89**, 1317-1321 (*synth*)
ewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, UAH000

Colletodiol C-724

11,12-Dihydroxy-6,14-dimethyl-1,7-dioxacyclotetradeca-3,9-diene-2,8-dione, 9CI. DG 4

[21142-67-6]



$C_{14}H_{20}O_6$ 284.308

Numbering systems vary. Constit. of *Colletotrichum capsici* and *Chaetomium funicola* and the marine-derived *Varicosporina ramulosa*. Immunosuppressive agent. Cryst. (Me_2CO/petrol). Sol. MeOH, EtOAc, bases, $CHCl_3$; poorly sol. H_2O. Mp 163-164°. $[\alpha]_D$ +36 (c, 1 in $CHCl_3$). Biol. inactive. λ_{max} 212 (ϵ 19000) (EtOH) (Derep). λ_{max} 206 (MeOH). λ_{max} 210 (ϵ 20300) (MeOH) (Berdy).

Di-Ac:

Rods. Mp 130-131°.

Dibenzoyl:

Prisms (EtOAc/petrol). Mp 103-105°.

11-Ketone: 12-Hydroxy-6,14-dimethyl-1,7-dioxacyclotetradeca-3,9-diene-2,8,11-trione, 9CI. ***Colletoketol****. Grahamimycin A*

[50376-39-1]

[76023-57-9]

$C_{14}H_{18}O_6$ 282.293

Metab. of *Chaetomium capsici*, *Cytospora* sp. ATCC 20502 and the marine-derived *Varicosporina ramulosa*. Prisms (Me_2CO/petrol). Sol. MeOH, EtOAc, bases, $CHCl_3$; poorly sol. H_2O. Mp 147.5-150° dec. (142-143°). $[\alpha]_D^{25}$ -34.2 (c, 0.05 in $CHCl_3$) (-24). Struct. of Grahamimycin A revised and shown to be identical with Colletoketol.

9,10-Dihydro: ***9,10-Dihydrocolletodiol***

$C_{14}H_{22}O_6$ 286.324

Prod. by the marine-derived *Varicosporina ramulosa*. Cryst. Mp 146-147°. $[\alpha]_D^{20}$ -5 (c, 0.42 in $CHCl_3$).

9,10-Dihydro, 11,12-diketone: ***Grahamimycin A1***

[74838-13-4]

$C_{14}H_{18}O_6$ 282.293

Isol. from *Cytospora* sp. ATCC 20502 and the marine-derived *Varicosporina ramulosa*. Antibiotic, weakly active against gram-positive and -negative bacteria and blue-green algae. Yellow rhomboids. Sol. MeOH, hexane; poorly sol. H_2O.
Mp 91-92°. $[\alpha]_D^{22}$ -14.7 (c, 0.76 in $CHCl_3$). λ_{max} 426 (ϵ 16) (EtOH) (Berdy).

11-Deoxy: ***Colletol***
[50376-40-4]
$C_{14}H_{20}O_5$ 268.309
From *Chaetomium capsici*. Needles (EtOAc/petrol).
Mp 101-104°. $[\alpha]_D$ -38.4 (c, 0.95 in $CHCl_3$).

12-Deoxy: ***Colletallol***
[50376-41-5]
$C_{14}H_{20}O_5$ 268.309
From *Chaetomium capsici*. Oil.

11-Epimer, 12-deoxy, 5-oxo: ***Acremonol***. *4-Ketoclonostachydiol*
$C_{14}H_{18}O_6$ 282.293
Prod. by an *Acremonium*-like fungus and a marine-derived *Gliocladium* sp. Cytotoxic. Solid.
Mp 83-84°. $[\alpha]_D^{25}$ +40 (c, 0.3 in MeOH).

11-Epimer, 12-deoxy, 5β-hydroxy: ***Clonostachydiol***
[147317-35-9]
$C_{14}H_{20}O_6$ 284.308
Prod. by *Clonostachys cylindrospora* and a marine-derived *Gliocladium* sp. Anthelmintic. Cryst.
Mp 164°. $[\alpha]_D^{20}$ +103 (c, 1 in MeOH). λ_{max} 212 (ϵ 19000) (EtOH) (Derep).

11-Epimer, 12-deoxy, 5α-hydroxy, 3,4-dihydro: ***Acremodiol***
$C_{14}H_{22}O_6$ 286.324
Prod. by an *Acremonium*-like fungus. Solid.
Mp 110-112°. $[\alpha]_D^{25}$ +98 (c, 0.3 in MeOH).

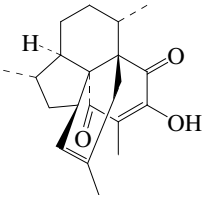
12-Epimer: ***Epicolletodiol***. *DG-3*
[184529-64-4]
$C_{14}H_{20}O_6$ 284.308
Prod. by *Diplogelasinospora grovesii*. Immunosuppressive agent.
Pale yellow oil. $[\alpha]_D^{24}$ -19.1 (c, 0.13 in $CHCl_3$). λ_{max} 210 (log ϵ 3.87) (MeOH).

11,12-Diepimer, 9,10-dihydro: ***9,10-Dihydro-11,12-diepicolletodiol***
$C_{14}H_{22}O_6$ 286.324
Prod. by the marine-derived *Varicosporina ramulosa*. Solid.
Mp 152-154°. $[\alpha]_D^{20}$ -48 (c, 0.3 in $CHCl_3$).

MacMillan, J. *et al., J.C.S. Perkin 1*, 1973, 1487 (*isol*)
Ronald, R.C. *et al., Tet. Lett.*, 1980, **21**, 681 (*Grahamimycin A1, isol, struct*)
U.S. Pat., 1980, 4 220 718; *CA*, **94**, 28879 (*Grahamimycin A*)
Gurusuddaiah, S. *et al., Antimicrob. Agents Chemother.*, 1981, **19**, 153-165 (*isol, Grahamimycins*)
Amstutz, R. *et al., Helv. Chim. Acta*, 1981, **64**, 1796 (*cryst struct*)
Seidel, W. *et al., Tet. Lett.*, 1982, **23**, 159 (*Grahamimycin A1, synth*)
Ghiringelli, D. *et al., Tet. Lett.*, 1983, **24**, 287 (*synth, Grahamimycin A1*)
Tsutsui, H. *et al., Tet. Lett.*, 1984, **25**, 2159; 2163 (*synth*)
Simpson, T.J. *et al., Chem. Comm.*, 1985, 1822 (*biosynth, nmr*)
Hillis, L.R. *et al., J.O.C.*, 1985, **50**, 470 (*synth*)
Wakamatsu, T. *et al., Tet. Lett.*, 1985, **26**, 1989 (*Colletallol*)
Schnurrenberger, P. *et al., Annalen*, 1987, 733 (*synth, bibl*)
Keck, G.E. *et al., J.O.C.*, 1989, **54**, 896; 1991, **56**, 6606 (*synth, Colletol*)
Dommerholt, F.J. *et al., Tet. Lett.*, 1991, **32**, 1495 (*Colletallol*)
Ohta, K. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 523 (*synth, Grahamimycin A1*)
Grabley, S. *et al., J. Antibiot.*, 1993, **46**, 343 (*Clonostachydiol*)
Rao, A.V.R. *et al., Tet. Lett.*, 1995, **36**, 139; 143 (*Clonostachydiol*)
Sharma, G.V.M. *et al., Tet. Lett.*, 1995, **36**, 4117 (*synth, Colletol*)
Amigoni, S.J. *et al., J.O.C.*, 1997, **62**, 6374-6378 (*Colletallol, synth*)
Fujimoto, H. *et al., Chem. Pharm. Bull.*, 1998, **46**, 423-429 (*isol, pmr, cmr, Epicolletodiol, activity*)
Höller, U. *et al., Acta Cryst. C*, 1999, **55**, 1310-1313 (*Colletoketol, cryst struct*)
Höller, U. *et al., Eur. J. Org. Chem.*, 1999, 2949-2955 (*Varicosporina colletodiols*)
Solladie, G. *et al., Eur. J. Org. Chem.*, 2000, 357-364 (*synth, Colletodiol, Colletol*)
Kobayashi, Y. *et al., J.O.C.*, 2000, **65**, 221-7224 (*Colletoketol, synth*)
Berg, A. *et al., J. Antibiot.*, 2002, **55**, 660-662 (*Acremonol, Acremodiol*)
Hunter, T.J. *et al., Org. Lett.*, 2002, **4**, 4447-4450 (*synth*)
Lang, G. *et al., J. Nat. Prod.*, 2006, **69**, 621-624 (*Gliocladium, isol*)
BouzBouz, S. *et al., Tet. Lett.*, 2006, **47**, 901-904 (*Colletol, synth*)

Colombiasin A C-725

[260547-32-8]

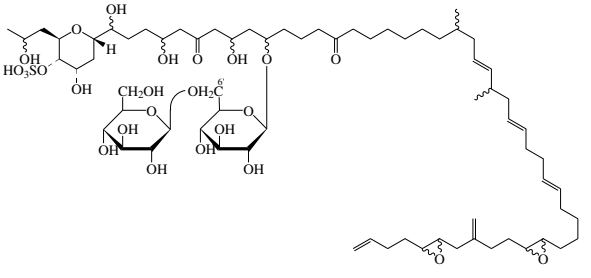


$C_{20}H_{26}O_3$ 314.424
Constit. of *Pseudopterogorgia elisabethae*. Yellow oil. $[\alpha]_D^{25}$ -55.3 (c, 0.9 in $CHCl_3$). λ_{max} 209 (ϵ 6600) (MeOH).

Rodriguez, A.D. *et al., Org. Lett.*, 2000, **2**, 507-510 (*isol, pmr, cmr*)
Nicolaou, K.C. *et al., Angew. Chem., Int. Ed.*, 2001, **40**, 2482-2486 (*synth*)
Kim, A.I. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 1267-1270 (*synth*)
Nicolaou, K.C. *et al., Classics in Total Synthesis II: More Targets, Strategies, Methods*, Wiley-VCH, 2003, 423 (*rev, synth*)
Boezio, A.A. *et al., Angew. Chem., Int. Ed.*, 2004, **44**, 6046-6050 (*synth*)
Harrowven, D.C. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 1221-1222 (*synth*)
Pihko, A.J. *et al., Tetrahedron*, 2005, **61**, 8769-8807 (*synth, rev*)

Colopsinol A C-726

[222415-27-2]



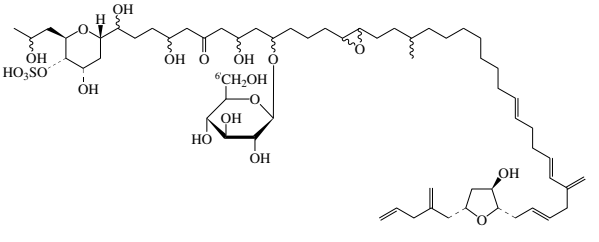
$C_{71}H_{120}O_{25}S$ 1405.78
Isol. from an *Amphidinium* sp. Amorph. solid (as Na salt). $[\alpha]_D^{20}$ -11 (c, 0.35 in MeOH) (Na salt). CAS no. refers to Na salt.

6′-O-Deglucosyl: ***Colopsinol E***
$C_{65}H_{110}O_{20}S$ 1243.638
Isol. from an *Amphidinium* sp. Amorph. solid (as Na salt).

Kobayashi, J. *et al., J.O.C.*, 1999, **64**, 1478-1482 (*Colopsinol A*)
Kubota, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1447-1451 (*Colopsinol E*)

Colopsinol C C-727

[259867-67-9]

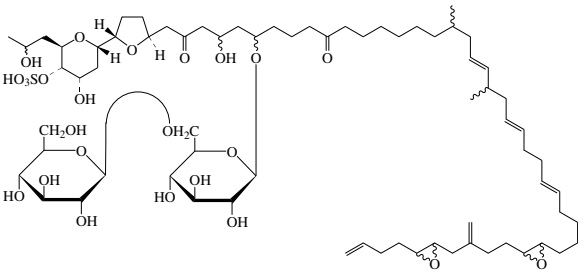


$C_{62}H_{104}O_{20}S$ 1201.558
Isol. from an *Amphidinium* sp. Amorph. solid (as Na salt). λ_{max} 232 (ϵ 10000) (MeOH).

6′-O-β-D-Glucopyranosyl: ***Colopsinol B***
[259867-57-7]
$C_{68}H_{114}O_{25}S$ 1363.7
Isol. from an *Amphidinium* sp. Amorph. solid (as Na salt). λ_{max} 232 (ϵ 13000) (MeOH).

Kubota, T. *et al., J.C.S. Perkin 1*, 1999, 3483-3487

Colopsinol D C-728

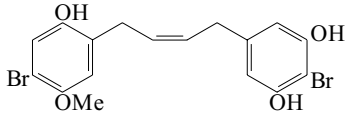


$C_{71}H_{118}O_{24}S$ 1387.765
Isol. from an *Amphidinium* sp. Amorph. solid (as Na salt).

Kubota, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1447-1451

Colpol C-729

2-Bromo-5-[4-(4-bromo-2-hydroxy-5-methoxyphenyl)-2-butenyl]-1,3-benzenediol, 9CI. 1-(4-Bromo-3,5-dihydroxyphenyl)-4-(4-bromo-2-hydroxy-5-methoxyphenyl)-2-butene
[151013-34-2]

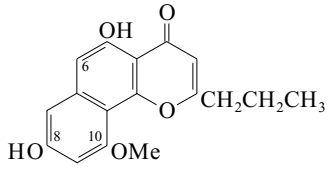


$C_{17}H_{16}Br_2O_4$ 444.119
Constit. of the alga *Colpomenia sinuosa*. Cytotoxic. λ_{max} 216 (ϵ 4200); 298 (ϵ 800) (MeOH).

Green, D. *et al., J. Nat. Prod.*, 1993, **56**, 1201 (*isol, pmr, uv, ir, cmr*)

Comaparvin C-730

*5,8-Dihydroxy-10-methoxy-2-propyl-4*H*-naphtho[1,2-*b*]pyran-4-one, 9CI*
[34434-17-8]



$C_{17}H_{16}O_5$ 300.31
Pigment from the crinoid *Comanthus parvicirrus*. Yellow needles. Mp 232-233°.

*8-*O*-Sulfate:* [33646-77-4]
$C_{17}H_{16}O_8S$ 380.375
Isol. from *Comanthus parvicirrus timorensis.*

O*-De-Me,* O^8*-Me:* ***5,10-Dihydroxy-8-methoxy-2-propyl-4*H*-naptho[1,2-*b*]pyran-4-one, 9CI***
[111397-58-1]
$C_{17}H_{16}O_5$ 300.31
Constit. of *Comanthus parvicirrus timorensis*. Yellow needles (MeOH).
Mp 184-186° dec.

*6-Methoxy: 5,8-Dihydroxy-6,10-dimethoxy-2-propyl-4*H*-naphtho[1,2-*b*]pyran-4-one, 9CI.* ***6-Methoxycomaparvin***
[111397-48-9]
$C_{18}H_{18}O_6$ 330.337
Pigment from *Comanthus parvicirrus*. Bright yellow needles. Mp 200-201.5° dec. (chars from 195°).

*6-Methoxy, 8-*O*-sulfate:* [33646-78-5]
$C_{18}H_{18}O_9S$ 410.401
Isol. from *Comanthus parvicirrus timorensis.*

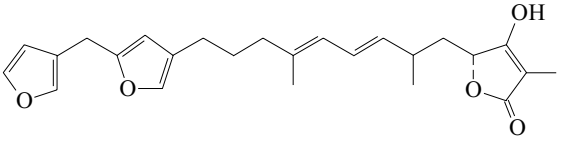
6-Methoxy, O^5*-Me: 8-Hydroxy-5,6,10-trimethoxy-2-propyl-4*H*-naphtho[1,2-*b*]pyran-4-one, 9CI.* ***6-Methoxycomaparvin 5-methyl ether***
[111397-49-0]
$C_{19}H_{20}O_6$ 344.363
Constit. of *Comanthus parvicirrus timorensis*. Yellow needles (Me_2CO).
Mp 221-222° dec.

6-Methoxy, O^5*-Me, 8-*O*-sulfate:* [33646-79-6]
$C_{19}H_{20}O_9S$ 424.428
Constit. of *Comanthus parvicirrus timorensis.*

6-Methoxy, di-Me ether: [60658-78-8]
Needles (cyclohexane). Mp 93-94°.

Smith, I.R. *et al., Aust. J. Chem.*, 1971, **24**, 1487-1499 (*sulfates, isol, struct*)
Rideout, J.A. *et al., Aust. J. Chem.*, 1976, **29**, 1087-1098 (*synth*)
Sakuma, Y. *et al., Aust. J. Chem.*, 1987, **40**, 1613-1616 (*6-Methoxycomaparvin, 6-methoxy 5-Me ether*)

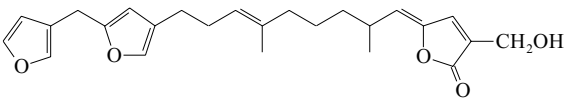
Cometin A C-731



$C_{25}H_{30}O_5$ 410.509
Constit. of a *Spongia* sp. Pale-yellow oil. $[\alpha]_D^{20}$ -11.5 (c, 0.5 in $CHCl_3$).

Urban, S. *et al., Aust. J. Chem.*, 1992, **45**, 1255 (*isol, pmr, cmr*)

Cometin B C-732



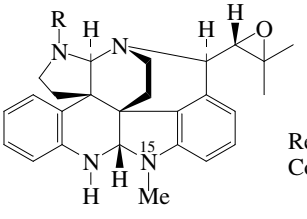
$C_{25}H_{30}O_5$ 410.509
Constit. of a *Spongia* sp. Pale-yellow oil. $[\alpha]_D^{20}$ -48.2 (c, 0.37 in $CHCl_3$).

Deoxy: ***Cometin C***
$C_{25}H_{30}O_4$ 394.51
Constit. of a *Spongia* sp. Pale-yellow oil. $[\alpha]_D^{20}$ -57.8 (c, 0.39 in $CHCl_3$).

Urban, S. *et al., Aust. J. Chem.*, 1992, **45**, 1255 (*isol, pmr, cmr*)

Communesin A C-733

[148439-45-6]



Relative Configuration

R = $COCH_3$

$C_{28}H_{32}N_4O_2$ 456.586
Communesin alkaloids have been isol. from *Penicillium* spp. by two different groups of workers simultaneously, and various Communesin names have been given to different but closely similar compds. See also under Communesin B, C-734. Metab. from the mycelium of a strain of *Penicillium* sp. isol. from the marine alga *Enteromorpha intestinalis*. Also prod. by the terrestrial *Penicillium expansum* Link MK-57. Cytotoxic and insecticidal agent. Amorph. powder.

Mp 194-196° Mp >300°. $[\alpha]_D^{20}$ -174 (c, 1.34 in $CHCl_3$). λ_{max} 208 (ϵ 53700); 247 (ϵ 12300); 268 (ϵ 11500); 290 (sh) (ϵ 3980); 315 (ϵ 2880) (EtOH) (Derep).

N-*De-Me:* ***Communesin E***†. *Communesin D*†
[727416-58-2]
$C_{27}H_{30}N_4O_2$ 442.56
Prod. by *Penicillium expansum* Link MK-57. Insecticidal agent. Amorph. powder.
Mp 250° dec. $[\alpha]_D^{20}$ -156 (c, 0.11 in $CHCl_3$). λ_{max} 243 (ϵ 9700) (MeOH).

21,22-Deepoxy, 21,22-didehydro: ***Communesin F***. *Communesin E*†
[727416-60-6]
$C_{28}H_{32}N_4O$ 440.587
Prod. by *Penicillium expansum* Link MK-57. Insecticidal agent. Amorph. powder.
Mp 144-147°. $[\alpha]_D^{20}$ -264 (c, 0.34 in $CHCl_3$). λ_{max} 268 (ϵ 10900) (MeOH).

Numata, A. *et al., Tet. Lett.*, 1993, **34**, 2355-2358 (*isol, ir, pmr, cmr*)
Hayashi, H. *et al., Biosci., Biotechnol., Biochem.*, 2004, **68**, 753-756 (*isol, pmr, cmr, ms*)
Wigley, L.J. *et al., Phytochemistry*, 2006, **67**, 561-569 (*biosynth*)
May, J.A. *et al., Tetrahedron*, 2006, **62**, 5262-5271 (*biosynth, struct*)

Communesin B C-734

Nomofungin
[148439-46-7]
As Communesin A, C-733 with
R = $H_2C{=}CHCH{=}CHCH_2CO–$
$C_{32}H_{36}N_4O_2$ 508.662
Struct. of Nomofungin revised in 2003. See comment under Communesin A, C-733. Metab. from the mycelium of a strain of *Penicillium* sp. isol. from the marine alga *Enteromorpha intestinalis* and from the terrestrial *Penicillium expansum* Link MK-57. Isol. from an unidentified fungus from the bark of *Ficus microcarpa* (Nomofungin). Cytotoxic, mycotoxin and insecticide. Amorph. powder.
Mp 165-170° (152-154°). $[\alpha]_D^{20}$ -74.9 (c, 1.5 in $CHCl_3$). $[\alpha]_D^{22}$ +8.7 (c, 0.2 in $CHCl_3$). λ_{max} 208 (ϵ 45700); 250 (sh) (ϵ 32400); 266 (ϵ 38900); 315 (ϵ 3090) (EtOH) (Derep).

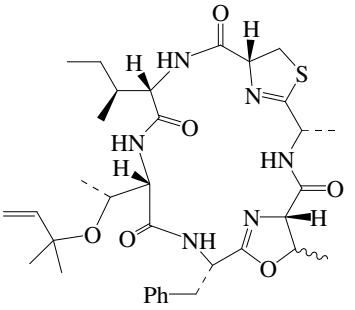
N-*De-Me:* ***Communesin C***†
[648413-35-8]
$C_{31}H_{34}N_4O_2$ 494.635
Prod. by a *Penicillium* sp. isol. from the marine sponge *Axinella verrucosa*.
$[\alpha]_D$ -30 (c, 0.04 in MeOH). λ_{max} 206; 271 (MeOH).

N-*De-Me,* N^{15}*-formyl:* ***Communesin D***†. *Communesin C*†
[648413-36-9]
$C_{32}H_{34}N_4O_3$ 522.646
Prod. by a *Penicillium* sp. isol. from *Axinella verrucosa* and by the terrestrial *Penicillium expansum* Link MK-57. Amorph. powder.
Mp 190-195°. $[\alpha]_D$ +23.3 (c, 0.04 in MeOH). $[\alpha]_D^{20}$ +150 (c, 0.14 in $CHCl_3$). λ_{max} 206; 267 (MeOH).

Numata, A. *et al., Tet. Lett.*, 1993, **34**, 2355-2358 (*isol, pmr, cmr, struct*)
Ratnayake, A.S. *et al., J.O.C.*, 2001, **66**, 8717-8721; 2003, **68**, 1640 (*Nomofungin*)
May, J.A. *et al., Tet. Lett.*, 2003, **44**, 1203-1205 (*struct*)
Hayashi, H. *et al., Biosci., Biotechnol., Biochem.*, 2004, **68**, 753-756 (*isol, pmr, cmr, ms*)
Jadulco, R. *et al., J. Nat. Prod.*, 2004, **67**, 78-81 (*isol, pmr, cmr, ms*)
Wigley, L.J. *et al., Phytochemistry*, 2006, **67**, 561-569 (*biosynth*)
May, J.A. *et al., Tetrahedron*, 2006, **62**, 5262-5271 (*biosynth, struct*)

Comoramide A C-735

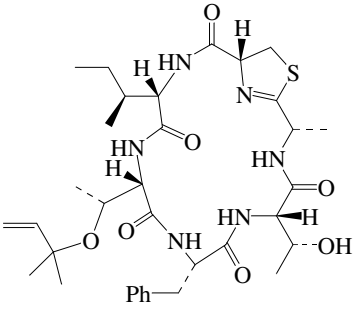
[217449-19-9]



$C_{34}H_{48}N_6O_6S$ 668.856
Cyclic peptide alkaloid. Isol. from *Didemnum molle*. Cytotoxic agent. Amorph. powder. $[\alpha]_D$ +0.5 (c, 0.17 in MeOH).
Rudi, A. *et al., Tetrahedron*, 1998, **54**, 13203-13210 (*isol, pmr, cmr, ms*)

Comoramide B C-736

[217449-22-4]



$C_{34}H_{50}N_6O_7S$ 686.871
Cyclic peptide alkaloid. Isol. from *Didemnum molle*. Cytotoxic agent. Amorph. powder. $[\alpha]_D$ -100 (c, 0.05 in MeOH).
Rudi, A. *et al., Tetrahedron*, 1998, **54**, 13203-13210 (*isol, pmr, cmr, ms*)

Conantokin L C-737

[202994-87-4]
Gly-Glu-Glu-Glu-Val-Ala-Lys-Met-Ala-Ala-Glu-Leu-Ala-Arg-Glu-Asp-Ala-Val-Asn-NH_2
$C_{87}H_{139}N_{25}O_{40}S$ 2207.265
Peptide with 4-carboxyglutamate residues at positions 3, 4, 11 and 15. Isol. from venom of *Conus lynceus*.
Jimenez, E.C. *et al., Epilepsy Res.*, 2002, **51**, 73-80 (*isol*)
Layer, R.J. *et al., Curr. Med. Chem.*, 2004, **11**, 3073-3084 (*rev*)

Conantokin R C-738

[202925-60-8]
Gly-Glu-Glu-Glu-Val-Ala-Lys-Met-Ala-Ala-Glu-Leu-Ala-Arg-Glu-Asn-Ile-Ala-Lys-Gly-Cys-Lys-Val-Asn-Cys-Tyr-Pro
$C_{127}H_{201}N_{35}O_{49}S_3$ 3098.388
Peptide containing 4-carboxyglutamate residues at positions 3, 4, 11 and 15. Isol. from venom of *Conus radiatus*.
White, H.S. *et al., J. Pharmacol. Exp. Ther.*, 2000, **292**, 425-432 (*isol*)

Conantokin T C-739

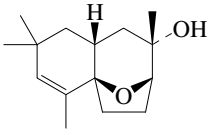
GEXXYQKMLXNLRXAEVKKNA amide
[127476-26-0]
H-Gly-Glu-Gla-Gla-Tyr-Gln-Lys-Met-Leu-Gla-Asn-Leu-Arg-Gla-Ala-Glu-Val-Lys-Lys-Asn-Ala-NH_2

Peptide; contains 4 residues of the modified amino acid, γ-carboxyglutamate (Gla) (=X). Isol. from the venom of the fish-hunting cone snail, *Conus tulipa*. Induces sleep-like symptoms in young mice.

Haack, J.A. *et al., J. Biol. Chem.*, 1990, **265**, 6025-6029 (*isol*)
Skjaerbaek, N. *et al., J. Biol. Chem.*, 1997, **272**, 2291-2299 (*pmr, cd, soln struct*)

Confertol C-740

[593261-04-2]

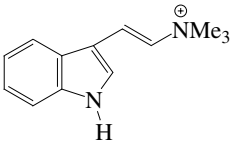


$C_{15}H_{24}O_2$ 236.353
Constit. of *Sinularia conferta*.
$[\alpha]_D^{20}$ +119 (c, 0.1 in MeOH).

Su, J.-Y. *et al., Huaxue Xuebao*, 2003, **61**, 1097-1100 (*isol, pmr, cmr*)

Conicamine C-741

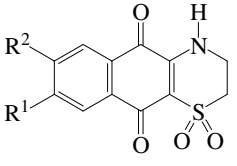
*2-(1*H*-Indol-3-yl)*-N,N,N-*trimethylethenaminium*
[648437-96-1]



$C_{13}H_{17}N_2^{\oplus}$ 201.291
Alkaloid from the tunicate *Aplidium conicum*. Histamine antagonist. Counterion not specified.

Aiello, A. *et al., Bioorg. Med. Chem. Lett.*, 2003, **13**, 4481-4483 (*isol, pmr, cmr*)

Conicaquinone A C-742



$R^1 = -CH_2CH_2CH{=}C(CH_3)_2$, $R^2 = H$

$C_{18}H_{19}NO_4S$ 345.418
Alkaloid from the ascidian *Aplidium conicum*. Cytotoxic. λ_{max} 261 (ε 16600); 298 (ε 7400) (MeOH).

Aiello, A. *et al., Eur. J. Org. Chem.*, 2003, 898-900 (*isol, pmr, cmr*)

Conicaquinone B C-743

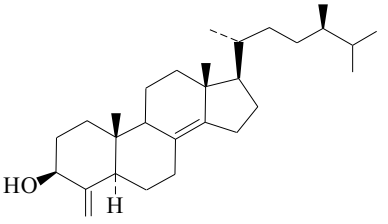
As Conicaquinone A, C-742 with
$R^1 = H$, $R^2 = -CH_2CH_2CH{=}C(CH_3)_2$

$C_{18}H_{19}NO_4S$ 345.418
Isol. from the ascidian *Aplidium conicum*. Cytotoxic. λ_{max} 263 (ε 14700); 300 (ε 8050) (MeOH).

Aiello, A. *et al., Eur. J. Org. Chem.*, 2003, 898-900 (*isol, pmr, cmr*)

Conicasterol C-744

24-Methyl-4-methylenecholest-8(14)-en-3-ol. 4-Methyleneergost-8(14)-en-3-ol
[76758-18-4]



$C_{29}H_{48}O$ 412.698
Constit. of *Theonella conica*. Cryst.
Mp 142-143°. $[\alpha]_D^{25}$ +97 ($CHCl_3$).

3-Ketone: 24-Methyl-4-methylenecholest-8(14)-en-3-one. 4-Methyleneergost-8(14)-en-3-one. ***Conicasterone***
[76758-20-8]
$C_{29}H_{46}O$ 410.682
Constit. of *Theonella swinhoei*. Cryst. (MeCN).
Mp 91-93°. $[\alpha]_D^{26}$ +42.1 (c, 1.25 in $CHCl_3$).

7α-Hydroxy: 24-Methyl-4-methylenecholest-8(14)-ene-3,7-diol. 4-Methyleneergost-8(14)-ene-3,7-diol. ***7-Hydroxyconicasterol***
[169565-77-9]
$C_{29}H_{48}O_2$ 428.697
Isol. from *Theonella swinhoei*. Cryst. (MeOH).
Mp 160-161°. $[\alpha]_D^{20}$ +9.4 (c, 0.16 in $CHCl_3$). Incorr. stereochem. given in CA.

15α-Hydroxy: 24-Methyl-4-methylenecholest-8(14)-ene-3,15-diol. 4-Methyleneergost-8(14)-ene-3,15-diol. ***15-Hydroxyconicasterol***
$C_{29}H_{48}O_2$ 428.697
Isol. from *Theonella swinhoei*. Incorr. stereochem. given in CA.

7α,15α-Dihydroxy: 24-Methyl-4-methylenecholest-8(14)-ene-3,7,15-triol. 4-Methyleneergost-8(14)-ene-3,7,15-triol. ***7,15-Dihydroxyconicasterol***
$C_{29}H_{48}O_3$ 444.696
Isol. from *Theonella swinhoei*. Incorr. stereochem. given in CA. Also isol. as 15-monoacyl deriv.

7α-Methoxy: 7-Methoxy-24-methyl-4-methylenecholest-8(14)-en-3-ol. 7-Methoxy-4-methyleneergost-8(14)-en-3-ol. ***7-Methoxyconicasterol***
[169565-78-0]
$C_{30}H_{50}O_2$ 442.724
Isol. from *Theonella swinhoei*. Cryst. (MeOH).
Mp 160.5-161°. Incorr. stereochem. given in CA.

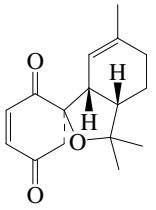
15α-Methoxy, 7α-hydroxy: 15-Methoxy-24-methyl-4-methylenecholest-8(14)-ene-3,7-diol. 15-Methoxy-4-methyleneergost-8(14)-ene-3,7-diol. ***7α-Hydroxy-15α-methoxyconicasterol***
$C_{30}H_{50}O_3$ 458.723
Isol. from *Theonella swinhoei*.
$[\alpha]_D^{20}$ +27 (c, 0.23 in $CHCl_3$). Incorr. stereochem. given in CA.

15β-Methoxy, 7α-hydroxy: ***7α-Hydroxy-15β-methoxyconicasterol***
$C_{30}H_{50}O_3$ 458.723
Isol. from *Theonella swinhoei*.
$[\alpha]_D^{20}$ +34.1 (c, 0.13 in $CHCl_3$). Incorr. stereochem. given in CA.

Kho, E. *et al., J.O.C.*, 1981, **46**, 1836
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1773 (*Conicasterone*)
Inouye, Y. *et al., Chem. Lett.*, 1994, 419 (*isol, cmr, cryst struct*)
Sugo, Y. *et al., Steroids*, 1995, **60**, 738-742 (*Theonella swinhoei constits*)

Conidione C-745

[459174-30-2]

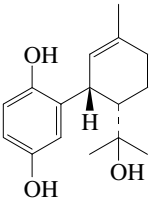


$C_{16}H_{20}O_3$ 260.332
Constit. of *Aplidium conicum*. Orange oil. $[\alpha]_D^{27}$ +0.5 (c, 0.2 in $CHCl_3$). λ_{max} 206 (ϵ 12338); 222 (ϵ 11844); 293 (ϵ 8961) (MeOH).

Garrido, L. *et al., J. Nat. Prod.*, 2002, **65**, 1328-1331 (*isol, pmr, cmr*)

Conitriol C-746

[459174-33-5]



$C_{16}H_{22}O_3$ 262.348
Constit. of *Aplidium conicum*. Oil. $[\alpha]_D^{27}$ +1 (c, 0.26 in $CHCl_3$). λ_{max} 212 (ϵ 11589); 295 (ϵ 4406) (MeOH).

Garrido, L. *et al., J. Nat. Prod.*, 2002, **65**, 1328-1331 (*isol, pmr, cmr*)

Conkunitzin S1 C-747

Conk-S1

Peptide containing 60 amino acid residues. Isol. from venom of the cone snail *Conus striatus*. Neurotoxin which interacts with voltage-gated K channels.

Bayrhuber, M. *et al., J. Biol. Chem.*, 2005, **280**, 23766-23770 (*isol*)

Conophysin R C-748

[461055-59-4]
[451532-36-8]

Peptide containing 84 amino acid residues including 14 cysteines; member of the neurophysin family. Isol. from the venom of the cone snail *Conus radiatus*. Neuropeptide.

Lirazan, M. *et al., Toxicon*, 2002, **40**, 901-908; 2003, **41**, 257 (*isol, struct*)

Conopressin G C-749

Lys-conopressin G
[111317-91-0]
H-Cys-Phe-Ile-Arg-Asn-Cys-Pro-Lys-Gly-NH_2
$C_{44}H_{71}N_{15}O_{10}S_2$ 1034.271

Neuropeptide. A homologue of oxytocin. Struct. of reduced form shown. Isol. from venom of the marine snails *Conus geographus* and *Conus imperialis*; also from the CNS of the leech *Erpobdella octoculata*.

Cruz, L.J. *et al., J. Biol. Chem.*, 1987, **262**, 15821 (*isol, struct*)
Kruszynski, M. *et al., Experientia*, 1990, **46**, 771 (*synth*)
Salzet, M. *et al., Eur. J. Biochem.*, 1993, **217**, 897-903 (*isol, leech*)
Nielsen, D.B. *et al., Toxicon*, 1994, **32**, 845-848 (*isol*)

Conopressin S C-750

[111317-90-9]
H-Cys-Ile-Ile-Arg-Asn-Cys-Pro-Arg-Gly-NH_2
$C_{41}H_{73}N_{17}O_{10}S_2$ 1028.268

Neuropeptide. A homologue of oxytocin. Struct. of reduced form shown. Isol. from venom of the marine snail *Conus striatus*.

Cruz, L.J. *et al., J. Biol. Chem.*, 1987, **262**, 15821-15824 (*isol, struct*)
Kruszynski, M. *et al., Experientia*, 1990, **46**, 771-773 (*synth*)

Conorfamide Sr 1 C-751

[409327-39-5]
H-Gly-Pro-Met-Gly-Trp-Val-Pro-Val-Phe-Tyr-Arg-Phe-NH_2
$C_{73}H_{99}N_{17}O_{13}S$ 1454.757
Isol. from the venom of the mollusc, *Conus spurius*. Neuropeptide.

Maillo, M. *et al., Toxicon*, 2002, **40**, 401-407 (*isol, struct*)

δ-Conotoxin Am 2766 C-752

Cys-Lys-Gln-Ala-Gly-Glu-Ser-Cys-Asp-Ile-Phe-Ser-Gln-Asn-Cys-Cys-Val-Gly-Thr-Cys-Ala-Phe-Ile-Cys-Ile-Glu-NH_2
$C_{113}H_{173}N_{31}O_{38}S_6$ 2766.191
Isol. from venom of the snail *Conus amadis*. Sodium channel modulator.

Sudarslal, S. *et al., FEBS Lett.*, 2003, **553**, 209-212 (*isol*)

α-Conotoxin Au I C-753

Gly-Cys-Cys-Ser-Tyr-Pro-Pro-Cys-Phe-Ala-Thr-Asn-Ser-Asp-Tyr-Cys-NH_2

Peptides of the conotoxin A-superfamily. Struct. of α-Conotoxin Au IA shown. Isol. from venom of *Conus aulicus*. Blockers of mammalian nicotinic acetylcholine receptors.

α-Conotoxin Au IA [216299-20-6]
$C_{72}H_{96}N_{18}O_{24}S_4$ 1725.921

α-Conotoxin Au IB [216299-21-7]
$C_{65}H_{89}N_{17}O_{21}S_4$ 1572.783

α-Conotoxin Au IC [223416-43-1]
$C_{70}H_{94}N_{18}O_{22}S_4$ 1667.884

Luo, S. *et al., J. Neurosci.*, 1998, **18**, 8571-8579 (*isol*)

Conotoxin au5a C-754

[287387-00-2]
Phe-Cys-Cys-Pro-Phe-Ile-Arg-Tyr-Cys-Cys-Trp
$C_{67}H_{85}N_{15}O_{13}S_4$ 1436.765
Peptide of the conotoxin T-superfamily. Isol. from the venom of *Conus aulicus*. Causes dorsal fin drooping in fish.

5-Valine analogue: Conotoxin au5b
[287386-99-6]
$C_{63}H_{85}N_{15}O_{13}S_4$ 1388.721
Isol. from *Conus aulicus*. Causes dorsal fin drooping in fish.

Walker, C.S. *et al., J. Biol. Chem.*, 1999, **274**, 30664-30771 (*isol*)

Conotoxin Be I C-755

Cys-Cys-Lys-Gln-Ser-Cys-Thr-Thr-Cys-Met-Pro-Cys-Cys-Trp

Two peptides of the conotoxin M-superfamily. Struct. of Conotoxin Be IA shown. Isol. from venom of *Conus betulinus*.

Conotoxin Be IA [259257-22-2]
$C_{61}H_{91}N_{17}O_{19}S_7$ 1590.954

Conotoxin Be IB [259257-23-3]
$C_{68}H_{94}N_{18}O_{18}S_6$ 1643.996

Chen, J.S. *et al., J. Nat. Toxins*, 1999, **8**, 341-349 (*isol*)

Conotoxin Be II C-756

Arg-Cys-Ala-His-Gly-Thr-Tyr-Tyr-Ser-Asn-Asp-Ser-Gln-Gln-Cys-Leu-Leu-Asn-Cys-Cys-Trp-Trp-Gly-Gly-Gly-Asp-His-Cys-Cys-Arg

Struct. of Conotoxin Be IIA shown. Isol. from venom of *Conus betulinus*.

Conotoxin Be IIA [259257-24-4]
$C_{141}H_{196}N_{46}O_{44}S_6$ 3431.777

Conotoxin Be IIB [259257-25-5]
$C_{102}H_{150}N_{30}O_{42}S_6$ 2660.879
Peptide containing a 4-hydroxyproline residue at position 13.
Chen, J.S. *et al., J. Nat. Toxins*, 1999, **8**, 341-349 (*isol*)

κ-Conotoxin Bt X C-757

Cys-Arg-Ala-Glu-Gly-Thr-Tyr-Cys-Glu-Asn-Asp-Ser-Gln-Cys-Cys-Leu-Asn-Glu-Cys-Cys-Trp-Gly-Gly-Cys-Gly-His-Pro-Cys-Arg-His-Pro-NH_2
$C_{137}H_{192}N_{46}O_{52}S_8$ 3571.829
Peptide containing 4-carboxyglutamate residues at positions 4, 9 and 18 and a 4-hydroxyproline residue at position 27. Isol. from venom of *Conus betulinus*. Modulator of potassium channels.
Fan, C.X. *et al., J. Biol. Chem.*, 2003, **278**, 12624-12633 (*isol*)

α-Conotoxin Bu IA C-758

Gly-Cys-Cys-Ser-Thr-Pro-Pro-Cys-Ala-Val-Leu-Tyr-Cys-NH_2
$C_{54}H_{82}N_{14}O_{16}S_4$ 1311.59
Isol. from the venom of *Conus bullatus*.
Zam, L.A. *et al., J. Biol. Chem.*, 2005, **280**, 80-87 (*isol*)

ω-Conotoxin C VI C-759

Cys-Lys-Ser-Thr-Gly-Ala-Ser-Cys-Arg-Arg-Thr-Ser-Tyr-Asp-Cys-Cys-Thr-Gly-Ser-Cys-Arg-Ser-Gly-Arg-Cys-NH_2

Four peptides of the conotoxin O-superfamily. Struct. of ω-Conotoxin C VIA shown. Isol. from venom of *Conus catus*. Calcium channel blockers. For ω-Conotoxin C VID see ω-Conotoxin CVID, C-763.

ω-Conotoxin C VIA [325164-06-5]
$C_{97}H_{161}N_{39}O_{36}S_6$ 2641.975

ω-Conotoxin C VIB [325164-09-8]
$C_{102}H_{173}N_{41}O_{32}S_7$ 2710.206

ω-Conotoxin C VIC [325164-11-2]
$C_{107}H_{180}N_{38}O_{35}S_7$ 2783.295
Lewis, R.J. *et al., J. Biol. Chem.*, 2000, **275**, 35335-35344 (*isol*)

Conotoxin Cc Tx C-760

Excitotoxin CcTx
Peptide containing 4-hydroxyproline residues at positions 2, 17 and 22; X is a glycosylated serine or threonine residue. Isol. from venom of *Conus consors*. Causes contraction and extension of the caudal and dorsal fins in fish.
Le Gall, F. *et al., Eur. J. Neurosci.*, 1999, **11**, 3134-3142 (*isol*)

α-Conotoxin Cn I C-761

Gly-Arg-Cys-Cys-His-Pro-Ala-Cys-Gly-Lys-Tyr-Tyr-Ser-Cys-NH_2

Two peptides of the conotoxin A-superfamily. Struct. of α-Conotoxin Cn IA shown. Isol. from venom of *Conus consors*. Blockers of nicotinic acetylcholine receptors.

α-Conotoxin Cn IA [228404-43-1]
$C_{63}H_{91}N_{21}O_{17}S_4$ 1542.806

α-Conotoxin Cn IB [228404-45-3]
$C_{55}H_{76}N_{16}O_{15}S_4$ 1329.568
Favreau, P. *et al., Biochemistry*, 1999, **38**, 6317-6326

ω-Conotoxin Cn VIIA C-762

[388078-56-6]
Cys-Lys-Gly-Lys-Gly-Ala-Pro-Cys-Thr-Arg-Leu-Met-Tyr-Asp-Cys-Cys-His-Gly-Ser-Cys-Ser-Ser-Ser-Lys-Gly-Arg-Cys-NH_2
$C_{110}H_{179}N_{39}O_{35}S_7$ 2832.326
Peptide of the conotoxin O-superfamily with a 4-hydroxyproline residue at position 7. Isol. from venom of *Conus consors*. Blocker of N-type calcium channels.
Favreau, P. *et al., Biochemistry*, 2001, **40**, 14567-14575 (*isol*)

ω-Conotoxin CVID C-763

AM 336
Cys-Lys-Ser-Lys-Gly-Ala-Lys-Cys-Ser-Lys-Leu-Met-Tyr-Asp-Cys-Cys-Ser-Gly-Ser-Cys-Ser-Gly-Thr-Val-Gly-Arg-Cys-NH_2
Peptide containing 27 amino acid residues. Isol. from the venom of the piscivorous cone snail *Conus catus*. N-type calcium channel blocker. ω-Conotoxins (CVIA-C) also isol.
Lewis, R.J. *et al., J. Biol. Chem.*, 2000, **275**, 35335-35344; 2003, **278**, 4057-4062 (*isol, struct, activity*)
Scott, D.A. *et al., Eur. J. Pharmacol.*, 2002, **451**, 279-286 (*pharmacol*)
Smith, M.T. *et al., Pain*, 2002, **96**, 119-127 (*pharmacol*)

Conotoxin de7a C-764

Ala-Cys-Lys-Pro-Lys-Asn-Asn-Leu-Cys-Ala-Ile-Thr-Glu-Met-Ala-Glu-Cys-Cys-Ser-Gly-Phe-Cys-Leu-Ile-Tyr-Arg-Cys-Ser-NH_2
$C_{129}H_{202}N_{36}O_{43}S_7$ 3169.692
Peptide containing 4-carboxyglutamate residues at positions 13 and 16 and a 4-hydroxyproline residue at position 4. Isol. from venom of *Conus delesserti*.
Aguilar, M.B. *et al., Peptides (N.Y.)*, 2005, **26**, 23-27 (*isol*)

α-Conotoxin E I C-765

[170663-33-9]
Arg-Asp-Pro-Cys-Cys-Tyr-His-Pro-Thr-Cys-Asn-Met-Ser-Asn-Pro-Gln-Ile-Cys-NH_2
$C_{83}H_{125}N_{27}O_{27}S_5$ 2093.395
Peptide of the conotoxin A-superfamily, containing a 4-hydroxyproline residue at position 3. Isol. from the venom of *Conus ermineus*. Blocker of nicotinic acetylcholine receptors.
Martinez, J.S. *et al., Biochemistry*, 1995, **34**, 14519-14526 (*isol*)

α-Conotoxin E IV C-766

Gly-Cys-Cys-Gly-Pro-Tyr-Pro-Asn-Ala-Ala-Cys-His-Pro-Cys-Gly-Cys-Lys-Val-Gly-Arg-Pro-Pro-Tyr-Cys-Asp-Arg-Pro-Ser-Gly-Gly-NH_2

Two peptides of the conotoxin A-superfamily. Struct. of α-Conotoxin E IVA shown. Isol. from venom of *Conus ermineus*. Inhibitors of nicotinic acetylcholine receptors.

α-Conotoxin E IVA [197502-64-0]
$C_{124}H_{183}N_{41}O_{41}S_6$ 3096.456
Contains 4-hydroxyproline residues at positions 7, 13, 21, 22 and 27.

α-Conotoxin E IVB [197502-65-1]
$C_{123}H_{183}N_{41}O_{42}S_6$ 3100.444
Contains 4-hydroxyproline residues at positions 7, 13, 21, 22 and 27.
Jacobsen, R. *et al., J. Biol. Chem.*, 1997, **272**, 22531-22537 (*isol*)
Chi, S.W. *et al., J. Biol. Chem.*, 2003, **278**, 42208-42213 (*soln struct*)

δ-Conotoxin E VIA C-767

[651716-03-9]
Asp-Asp-Cys-Ile-Lys-Pro-Tyr-Gly-Phe-Cys-Ser-Leu-Pro-Ile-Leu-Lys-Asn-Gly-Leu-Cys-Cys-Ser-Gly-Ala-Cys-Val-Gly-Val-Cys-Ala-Asp-Leu-NH_2
$C_{140}H_{220}N_{36}O_{43}S_6$ 3287.889
Peptide of the conotoxin O-superfamily containing a 4-hydroxyproline residue at position 6. Isol. from venom of *Conus ermineus*. Inhibitor of sodium channel inactivation.

Barbier, J. *et al., J. Biol. Chem.*, 2004, **279**, 4680-4685 (*isol*)
Volpon, L. *et al., J. Biol. Chem.*, 2004, **279**, 21356-21366 (*soln struct*)

α-Conotoxin Ep I C-768

[211050-66-7]

Gly-Cys-Cys-Ser-Asp-Pro-Arg-Cys-Asn-Met-Asn-Asn-Pro-Asp-Tyr-Cys-NH_2

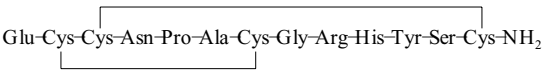
$C_{67}H_{99}N_{23}O_{28}S_6$ 1867.052

Peptide of the conotoxin A-superfamily with a sulfotyrosine residue at position 15. Isol. from venom of *Conus episcopatus*. Blocker of nicotinic acetylcholine receptors.

Loughnan, M. *et al., J. Biol. Chem.*, 1998, **273**, 15667-15674 (*isol*)

α-Conotoxin G I C-769

[76862-65-2]



$C_{55}H_{80}N_{20}O_{18}S_4$ 1437.624

Peptide neurotoxin from sea snail *Conus geographus*. Neurotoxin. Paralytic toxin, blocks nicotinic cholinoceptors. Sol. H_2O.

α-Conotoxin G IA [78301-21-0]

$C_{63}H_{95}N_{23}O_{20}S_4$ 1622.85

α-Conotoxin G IB

$C_{63}H_{95}N_{23}O_{20}S_4$ 1622.85

α-Conotoxin G IC

$C_{61}H_{92}N_{24}O_{20}S_4$ 1609.811

α-Conotoxin G ID

$C_{84}H_{132}N_{30}O_{31}S_4$ 2186.413

Contains a 4-carboxyglutamate residue at position 4 and a 4-hydroxyproline residue at position 16.

Gray, W.R. *et al., J. Biol. Chem.*, 1981, **256**, 4734-4740 (*isol, biochem*)
Gray, W.R. *et al., Biochemistry*, 1984, **23**, 2796-2802 (*synth, struct*)
Atherton, E. *et al., J.C.S. Perkin 1*, 1985, 2065-2074 (*synth*)
Guddat, L.W. *et al., Biochemistry*, 1996, **35**, 11329-11335 (*cryst struct*)
Maslennikov, I.V. *et al., Eur. J. Biochem.*, 1998, **254**, 238-247 (*soln struct*)
Gehrmann, J. *et al., J. Mol. Biol.*, 1998, **278**, 401-405 (*pmr, struct*)
McIntosh, J.M. *et al., J. Biol. Chem.*, 2002, **277**, 33610-33615 (*α-Conotoxin G IC, isol*)
Nicke, A. *et al., J. Biol. Chem.*, 2003, **278**, 3137-3144 (*α-Conotoxin G ID, isol*)
Chi, S.W. *et al., Biochem. J.*, 2004, **380**, 347-352 (*α-Conotoxin G IC, soln struct*)

Conotoxin G V, 9CI C-770

Conantokin G

[93438-65-4]

H-Gly-Glu-Gla-Gla-Leu-Gln-Gla-Asp-Glu-Gla-Leu-Ile-Arg-Gla-Lys-Ser-Asn-NH_2

$C_{88}H_{136}N_{24}O_{46}$ 2266.176

Peptide; contains 5 residues of the modified amino acid, γ-carboxyglutamate (Gla). Isol. from the venom of a fish-hunting cone snail (*Conus geographus*). Neurotoxin. Selective NMDA antagonist. Induces a sleep-like state in young mice when injected intracerebrally. Induces hyperactivity in adult mice.

McIntosh, J.M. *et al., J. Biol. Chem.*, 1984, **259**, 14343-14346 (*isol, struct*)
Rivier, J. *et al., Biochemistry*, 1987, **26**, 8508-8512 (*synth*)
Mena, E.E. *et al., Neurosci. Lett.*, 1990, **118**, 241-244 (*pharmacol*)
Skjaerbaek, N. *et al., J. Biol. Chem.*, 1997, **272**, 2291-2299 (*pmr, cd, soln struct*)

α-Conotoxin G II C-771

[78277-78-8]

Glu-Cys-Cys-His-Pro-Ala-Cys-Gly-Lys-His-Phe-Ser-Cys-NH_2

$C_{57}H_{81}N_{19}O_{16}S_4$ 1416.649

Peptide of the conotoxin A-superfamily. Isol. from venom of *Conus geographus*. Inhibitor of nicotinic acetylcholine receptors.

Gray, W.R. *et al., J. Biol. Chem.*, 1981, **256**, 4734-4740 (*isol*)

μ-Conotoxin G IIIA C-772

Geographutoxin I

[129129-65-3]

H-Arg-Asp-Cys-Cys-Thr-*trans*-Hyp-*trans*-Hyp-Lys-Lys-Cys-Lys-Asp-Arg-Gln-Cys-Lys-*trans*-Hyp-Gln-Arg-Cys-Cys-Ala-NH_2

$C_{100}H_{170}N_{38}O_{32}S_6$ 2609.074

Reduced form shown. Toxin isol. from *Conus geographus*. Voltage-dependent sodium channel blocker in muscle. Sol. H_2O.

▶ Paralytic poison.

[86394-16-3]

Nakamura, H. *et al., Experientia*, 1983, **39**, 590-591 (*isol*)
Sato, S. *et al., FEBS Lett.*, 1983, **155**, 277-280 (*struct*)
Cruz, J.L. *et al., J. Biol. Chem.*, 1985, **260**, 9280-9288 (*isol*)
Hatanaka, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 236-238 (*synth*)
Hidaka, Y. *et al., FEBS Lett.*, 1990, **264**, 29-32 (*struct*)
Lancelin, J.M. *et al., Biochemistry*, 1991, **30**, 6908-6916 (*struct*)

μ-Conotoxin G IIIB C-773

Geographutoxin II

[140678-12-2]

H-Arg-Asp-Cys-Thr-Hyp-Hyp-Arg-Lys-Cys-Lys-Asp-Arg-Cys-Lys-Hyp-Met-Lys-Cys-Cys-Ala-NH_2

$C_{92}H_{160}N_{34}O_{28}S_6$ 2382.883

Struct. of reduced form shown. Isol. from the venom of the marine snail *Conus geographus*. Toxin. Skeletal muscle Na channel specific blocking agent.

▶ Paralytic poison.

[86414-29-1]

Sato, S. *et al., FEBS Lett.*, 1983, **155**, 277-280 (*isol, struct*)
Cruz, J.L. *et al., J. Biol. Chem.*, 1985, **260**, 9280-9285 (*isol*)
Sato, S. *et al., Pept. Chem.*, 1989, 97 (*synth*)
Kubo, S. *et al., Pept. Chem.*, 1989, 257 (*synth*)
Kubo, S. *et al., Pept. Res.*, 1993, **6**, 66-72 (*synth*)
Hill, J.M. *et al., Biochemistry*, 1996, **35**, 8824-8835 (*struct, pmr*)

μ-Conotoxin G IIIC C-774

[98183-99-4]

Arg-Asp-Cys-Cys-Thr-Pro-Pro-Lys-Lys-Cys-Lys-Asp-Arg-Arg-Cys-Lys-Pro-Leu-Lys-Cys-Cys-Ala-NH_2

$C_{102}H_{177}N_{37}O_{30}S_6$ 2594.146

Peptide of the conotoxin M-superfamily containing 4-hydroxyproline residues at positions 6, 7 and 17. Isol. from venom of *Conus geographus*. Na channel blocker.

Cruz, L.J. *et al., J. Biol. Chem.*, 1985, **260**, 9280-9288 (*isol*)

ω-Conotoxin G VIA C-775

[106375-28-4]

Cys-Lys-Ser-Pro-Gly-Ser-Ser-Cys-Ser-Pro-Thr-Ser-Tyr-Asn-Cys-Cys-Arg-Ser-Cys-Asn-Pro-Tyr-Thr-Lys-Arg-Cys-Tyr-NH_2

$C_{120}H_{182}N_{38}O_{43}S_6$ 3037.383

Struct. consists of a single polypeptide chain containing 27 amino acids and 3 disulfide bridges, with 4-hydroxyproline residues at positions 4, 10 and 21. Isol. from venom of *Conus geographus*. Neurotoxin. Selective blocker of neuronal N-type Ca^{2+} channels. Pharmacological tool. Two analogues, ω-Conotoxins G VI B and G VI C, also isol.

[92078-76-7]

Olivera, B.M. *et al., Biochemistry*, 1984, **23**, 5087-5090 (*isol, struct*)
Nishuichi, Y. *et al., Pept. Chem.*, 1985, **23**, 77 (*synth*)
Olivera, B.M. *et al., Science (Washington, D.C.)*, 1985, **230**, 1338-1343 (*analogues*)
Rivier, J. *et al., J. Biol. Chem.*, 1987, **262**, 1194-1198 (*synth, pharmacol*)
McCleskey, E.W. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1987, **84**, 4327-4331 (*pharmacol*)
Gray, W.R. *et al., Annu. Rev. Biochem.*, 1988, **57**, 665-700 (*rev*)
Sevilla, P. *et al., Biochem. Biophys. Res. Commun.*, 1993, **192**, 1238-1244 (*pmr*)
Skalicky, J.J. *et al., Protein Sci.*, 1993, **2**, 1591-1603 (*conformn*)

ω-Conotoxin G VIIA C-776

Cys-Lys-Ser-Pro-Gly-Thr-Pro-Cys-Ser-Arg-Gly-Met-Arg-Asp-Cys-Cys-Thr-Ser-Cys-Leu-Leu-Tyr-Ser-Asn-Lys-Cys-Arg-Arg-Tyr

$C_{131}H_{212}N_{44}O_{43}S_7$ 3315.847

Peptide of the conotoxin O-superfamily containing 4-hydroxyproline residues at positions 4 and 7. Isol. from venom of *Conus geographus*. Ca channel blocker.

21-Serine analogue:
$C_{128}H_{206}N_{44}O_{44}S_7$ 3289.766
Isol. from venom of *Conus geographus*.

Olivera, B.M. *et al., Science (Washington, D.C.)*, 1985, **230**, 1338-1343 (*isol*)

σ-Conotoxin G VIIIA C-777

[212834-24-7]

Gly-Cys-Thr-Arg-Thr-Cys-Gly-Gly-Pro-Lys-Cys-Thr-Gly-Thr-Cys-Thr-Cys-Thr-Asn-Ser-Ser-Lys-Cys-Gly-Cys-Arg-Tyr-Asn-Val-His-Pro-Ser-Gly-Trp-Gly-Cys-Gly-Cys-Ala-Cys-Ser-NH_2

$C_{158}H_{242}BrN_{55}O_{55}S_{10}$ 4192.549

Peptide of the conotoxin S-superfamily containing a 4-hydroxyproline residue at position 9 and a 6-bromotryptophan residue at position 34. Isol. from venom of *Conus geographus*.

England, I.J. *et al., Science (Washington, D.C.)*, 1998, **281**, 575-578 (*isol*)

Conotoxin Gla-Mr II C-778

Ser-Cys-Asp-Ser-Glx-Phe-Ser-Ser-Glx-Phe-Cys-Glx-Gln-Phe-Glx-Glx-Arg-Ile-Cys-Ser-Cys-Ser-Thr-His-Val-Cys-Cys-His-Leu-Ser-Ser-Ser-Lys-Arg-Asp-Gln-Cys-Met-Thr-Trp-Asn-Arg-Cys-Leu-Ser-Ala-Gln-Thr-Gly-Asn

Peptide containing 50 amino acid residues incl. 5 γ-carboxyglutamic acid residues and 8 cysteine residues. Isol. from venom of *Conus marmoreus*.

Hansson, K. *et al., Biochem. Biophys. Res. Commun.*, 2004, **319**, 1081-1087 (*isol*)

Conotoxin Gla-Mr III C-779

Phe-Cys-Cys-Arg-Thr-Gln-Glu-Val-Cys-Cys-Glu-Ala-Ile-Lys-Asn-NH_2

$C_{72}H_{112}N_{22}O_{26}S_4$ 1830.073

Peptide; a member of the conotoxin T-superfamily containing 4-hydroxyglutamate residues at positions 7 and 11. Isol. from venom of *Conus marmoreus*.

Hansson, K. *et al., Biochem. Biophys. Res. Commun.*, 2004, **319**, 1081-1087 (*isol*)

Conotoxin Gla-Mr IV C-780

Cys-Cys-Ile-Thr-Phe-Glu-Ser-Cys-Cys-Glu-Phe-Asp-Leu

$C_{65}H_{89}N_{13}O_{26}S_4$ 1596.754

Peptide; a member of the conotoxin T-superfamily containing 4-carboxyglutamate residues at positions 6 and 10. Isol. from venom of *Conus marmoreus*.

Hansson, K. *et al., Biochem. Biophys. Res. Commun.*, 2004, **319**, 1081-1087 (*isol*)

Conotoxin Gla(1)-Tx VI C-781

[265109-49-7]

Gly-Met-Trp-Gly-Glu-Cys-Lys-Asp-Gly-Leu-Thr-Thr-Cys-Leu-Ala-Pro-Ser-Glu-Cys-Cys-Ser-Glu-Asp-Cys-Glu-Gly-Ser-Cys-Thr-Met-Trp

$C_{137}H_{194}Br_2N_{34}O_{59}S_8$ 3677.568

Peptide of the conotoxin O-superfamily, containing 6-bromotryptophan residues at positions 3 and 31, 4-carboxyglutamate residues at positions 5, 18, 22 and 25, and a 4-hydroxyproline residue at position 16. Isol. from venom of *Conus textile*.

Kalume, D.E. *et al., J. Mass Spectrom.*, 2000, **35**, 145-156 (*synth, ms*)

Conotoxin Gm 9.1 C-782

Conotoxin Gm 9a
[268545-83-1]

Ser-Cys-Asn-Asn-Ser-Cys-Gln-Ser-His-Ser-Asp-Cys-Ala-Ser-His-Cys-Ile-Cys-Thr-Phe-Arg-Gly-Cys-Gly-Ala-Val-Asn-NH_2

$C_{106}H_{161}N_{39}O_{39}S_6$ 2798.072

Peptide of the conotoxin P-superfamily. Isol. from venom of *Conus gloriamaris*.

Lirazan, M.B. *et al., Biochemistry*, 2000, **39**, 1583-1588 (*isol*)
Miles, R.A. *et al., J. Biol. Chem.*, 2002, **277**, 43033-43040 (*synth, struct*)

δ-Conotoxin Gm VIA C-783

[157897-79-5]

Val-Lys-Pro-Cys-Arg-Lys-Glu-Gly-Gln-Leu-Cys-Asp-Phe-Ile-Phe-Gln-Asn-Cys-Cys-Arg-Gly-Trp-Asn-Cys-Val-Leu-Phe-Cys-Val

$C_{145}H_{222}N_{42}O_{38}S_6$ 3354.003

Peptide of the conotoxin O-superfamily. Isol. from venom of *Conus gloriamaris*. Inhibits the inactivation of voltage-sensitive sodium channels.

Shon, K.J. *et al., Biochemistry*, 1994, **33**, 11420-11425 (*isol*)

Conotoxin GS C-784

[115757-31-8]

Ala-Cys-Ser-Gly-Arg-Gly-Ser-Arg-Cys-Pro-Pro-Gln-Cys-Cys-Met-Gly-Leu-Arg-Cys-Gly-Arg-Gly-Asn-Pro-Gln-Lys-Cys-Ile-Gly-Ala-His-Glu-Asp-Val

$C_{139}H_{226}N_{52}O_{48}S_7$ 3618.096

Peptide of the conotoxin S-superfamily, with 5-hydroxyproline residues at positions 10 and 11 and a 4-carboxyglutamic acid residue at position 32. Isol. from the venom of *Conus geographus*. Sodium channel inhibitor.

Yanagawa, Y. *et al., Biochemistry*, 1988, **27**, 6256-6262 (*isol*)
Hill, J.M. *et al., Structure (London)*, 1997, **5**, 571-583 (*soln struct*)

α-Conotoxin Im I C-785

[156467-85-5]

Gly-Cys-Cys-Ser-Asp-Pro-Arg-Cys-Ala-Trp-Arg-Cys-NH_2

$C_{52}H_{78}N_{20}O_{15}S_4$ 1351.577

Peptide of the conotoxin A-superfamily. Isol. from venom of *Conus imperialis*. Inhibitor of nicotinic acetylcholine receptors.

McIntosh, J.M. *et al., J. Biol. Chem.*, 1994, **269**, 16733-16739 (*isol*)
Maslennikov, I.V. *et al., FEBS Lett.*, 1999, **444**, 275-280 (*pmr*)
Gehrmann, J. *et al., J. Med. Chem.*, 1999, **42**, 2364-2372 (*soln struct*)

α-Conotoxin Im II C-786

[528818-52-2]

Ala-Cys-Cys-Ser-Asp-Arg-Arg-Cys-Arg-Trp-Arg-Cys-NH_2

$C_{57}H_{92}N_{26}O_{15}S_4$ 1509.783

Peptide of the conotoxin A-superfamily. Isol. from venom of *Conus imperialis*. Inhibitor of nicotinic acetylcholine receptors.

Ellison, M. *et al., J. Biol. Chem.*, 2003, **278**, 757-764 (*isol, synth*)

Conotoxin KK 0 C-787

King Kong peptide. Conus textile neovicarius *Toxin IA*. *Conotoxin TxIA*
[117144-21-5]

H-Trp-Cys-Lys-Gln-Ser-Gly-Glu-Met-Cys-Asn-^{11}Leu-Leu-Asp-Gln-Asn-Cys-Cys-Asp-Gly-Tyr-Cys-Ile-Val-^{24}Leu-Val-Cys-Thr-OH

$C_{125}H_{191}N_{33}O_{41}S_7$ 3036.542

Reduced form shown. Neurotoxin isol. from the venom of the snail *Conus textile*. Molluscan neuronal ion channel blocker. Exhibits strong paralytic activity to molluscs, but not to vertebrates.

11-L-Valine-24-L-phenylalanine analogue: Conus textile neovicarius *Toxin IB*. *Conotoxin TxIB*
[138659-48-0]
$C_{125}H_{187}N_{33}O_{41}S_7$ 3032.511
Isol. from the venom of the snail *Conus textile neovicarius*.

[117069-04-2, 128194-63-8]

Hillyard, D.R. *et al., Biochemistry*, 1989, **28**, 358-361 (*isol*)
Fainzilber, M. *et al., Eur. J. Biochem.*, 1991, **202**, 589-595 (*isol*)
Spira, M.E. *et al., Isr. J. Med. Sci.*, 1993, **29**, 530-543 (*pharmacol, rev*)
Lev-Ram, V. *et al., Brain Res.*, 1994, **640**, 48-55 (*pharmacol*)

α-Conotoxin M I C-788

Conotoxin M I

[83481-45-2]

H-Gly-Arg-Cys-Cys-His-Pro-Ala-Cys-Gly-Lys-Asn-Tyr-Ser-Cys-NH_2

$C_{58}H_{92}N_{21}O_{17}S_4$ 1483.759

Struct. of reduced form shown. Isol. from the venom of the marine snail *Conus magus*. Neurotoxin. Acts at acetylcholine receptors at vertebrate neuromuscular junctions.

[88217-10-1]

McIntosh, M. *et al., Arch. Biochem. Biophys.*, 1982, **218**, 329-334 (*isol, struct*)
Gray, W.R. *et al., J. Biol. Chem.*, 1983, **258**, 12247-12251 (*synth, struct*)
Gouda, H. *et al., Biochim. Biophys. Acta*, 1997, **1343**, 327-334 (*soln struct*)
Gouda, H. *et al., Chem. Pharm. Bull.*, 2001, **49**, 249-252 (*pmr, struct*)

α-Conotoxin M II C-789

[175735-93-0]

Gly-Cys-Cys-Ser-Asn-Pro-Val-Cys-His-Leu-Glu-His-Ser-Asn-Leu-Cys-NH_2

$C_{67}H_{103}N_{23}O_{22}S_4$ 1710.956

Peptide of the conotoxin A-superfamily. Isol. from venom of *Conus magus*. Inhibitor of nicotinic acetylcholine receptors.

Cartier, G.E. *et al., J. Biol. Chem.*, 1996, **271**, 7522-7528 (*isol*)
Shon, K.J. *et al., Biochemistry*, 1997, **36**, 15693-15700 (*soln struct*)
Hill, J.M. *et al., Biochemistry*, 1998, **37**, 15621-15630 (*soln struct*)

ω-Conotoxin M VIIA C-790

ω-Conotoxin M VIIA (reduced) cyclic (1→16), (8→20), (15→25)tris(disulfide). ***Ziconotide, INN, USAN.*** *Prialt. SNX III. CI 1009*

[107452-89-1]

$C_{102}H_{172}N_{36}O_{32}S_7$ 2639.165

Peptide containing 24 amino acid residues. Isol. from venom of the cone snail *Conus magus*. Selective blocker of neuronal N-type Ca^{2+}-channels. Neuroprotective agent. Non-opioid analgesic. Used in the treatment of severe chronic pain. Approved by FDA (2004) for management of severe chronic pain

Olivera, B.M. *et al., Biochemistry*, 1987, **26**, 2086-2090 (*isol, synth, activity*)
Bowersox, S.S. *et al., J. Cardiovasc. Pharmacol.*, 1992, **20**, 756-764 (*pharmacol*)
Stoehr, S.J. *et al., Neurosci. Lett.*, 1993, **161**, 113-116 (*activity*)
Simmonds, R.G. *et al., Int. J. Pept. Protein Res.*, 1994, **43**, 363-366 (*synth*)
Kohno, T. *et al., Biochemistry*, 1995, **34**, 10256-10265 (*soln struct*)
Basus, V.J. *et al., FEBS Lett.*, 1995, **370**, 163-169 (*soln struct*)
Bowersox, S. *et al., Drugs of the Future*, 1998, **23**, 152-160 (*rev, pharmacol*)
Jain, K.K. *et al., Expert Opin. Invest. Drugs*, 2000, **9**, 2403-2410 (*rev*)
Azimi-Zonooz, A. *et al., Brain Res.*, 2001, **907**, 61-70 (*pharmacol*)
Wermeling, D. *et al., J. Clin. Pharmacol.*, 2003, **43**, 624-636 (*pharmacokinet*)
Miljanich, G.P. *et al., Curr. Med. Chem.*, 2004, **11**, 3029-3040 (*pharmacol*)
Staats, P.S. *et al., J. Am. Med. Assoc.*, 2004, **291**, 63-70 (*clin trial*)

ω-Conotoxin M VIIB C-791

[107452-90-4]

Cys-Lys-Gly-Lys-Gly-Ala-Ser-Cys-His-Arg-Thr-Ser-Tyr-Asp-Cys-Cys-Thr-Gly-Ser-Cys-Asn-Arg-Gly-Lys-Cys-NH_2

$C_{99}H_{160}N_{38}O_{34}S_6$ 2618.983

Peptide of the conotoxin O-superfamily. Isol. from venom of *Conus magus*. Calcium channel blocker.

Olivera, B.M. *et al., Biochemistry*, 1987, **26**, 2086-2090 (*isol*)

ω-Conotoxin M VIIC C-792

[147794-23-8]

[168831-68-3]

Cys-Lys-Gly-Lys-Gly-Ala-Pro-Cys-Arg-Lys-Thr-Met-Tyr-Asp-Cys-Cys-Ser-Gly-Ser-Cys-Gly-Arg-Arg-Gly-Lys-Cys-NH_2

$C_{106}H_{178}N_{40}O_{33}S_7$ 2765.282

Peptide of the conotoxin O-superfamily with a 4-hydroxyproline residue at position 7. Isol. from venom of *Conus magus*. Calcium channel blocker.

Hillyard, D.R. *et al., Neuron*, 1992, **9**, 69-77 (*isol*)
Farr-Jones, S. *et al., J. Mol. Biol.*, 1995, **248**, 106-124 (*soln struct*)

ω-Conotoxin M VIID C-793

[153887-08-2]

Cys-Gln-Gly-Arg-Gly-Ala-Ser-Cys-Arg-Lys-Thr-Met-Tyr-Asn-Cys-Cys-Ser-Gly-Ser-Cys-Asn-Arg-Gly-Arg-Cys-NH_2

$C_{99}H_{164}N_{42}O_{33}S_7$ 2695.108

Peptide of the conotoxin O-superfamily. Isol. from venom of *Conus magus*. Calcium channel blocker.

Monje, V.D. *et al., Neuropharmacology*, 1993, **32**, 1141-1149 (*isol*)
Civera, C. *et al., Biochem. Biophys. Res. Commun.*, 1999, **254**, 32-35 (*soln struct*)

λ-Conotoxin Mr X C-794

[328057-48-3]

Gly-Ile-Cys-Cys-Gly-Val-Ser-Phe-Cys-Tyr-Pro-Cys

$C_{53}H_{74}N_{12}O_{16}S_4$ 1263.502

Peptide with 2 disulfide bridges (Cys^3 - Cys^{12}, Cys^4 - Cys^9) and a 4-hydroxyproline residue at position 11. Isol. from venom of *Conus marmoreus*.

Balaji, R.A. *et al., J. Biol. Chem.*, 2000, **275**, 39516-39522 (*isol*)

Conotoxin mr 3 C-795

Gly-Cys-Cys-Gly-Ser-Phe-Ala-Cys-Arg-Phe-Gly-Cys-Val-Pro-Cys-Cys-Val

Peptides of the M-conotoxin superfamily. Structure of Conotoxin mr 3a shown. Isol. from *Conus marmoreus*.

Conotoxin mr 3a

$C_{69}H_{100}N_{20}O_{20}S_6$ 1722.067

Induces seizures in mice. Contains a 4-hydroxyproline residue at position 14.

Conotoxin mr 3b

$C_{87}H_{127}N_{27}O_{24}S_6$ 2127.523

Contains a 4-hydroxyproline residue at position 16.

McDougal, O.M. *et al., Biochemistry*, 2004, **43**, 425-429 (*isol, struct*)
Corpuz, G.P. *et al., Biochemistry*, 2005, **44**, 8176-8178 (*isol*)

χ-Conotoxin Mr IB C-796

Val-Gly-Val-Cys-Cys-Gly-Tyr-Lys-Leu-Cys-His-Pro-Cys

$C_{58}H_{88}N_{16}O_{16}S_4$ 1393.695

Peptide with a 4-hydroxyproline residue at position 12. Isol. from the venom of *Conus marmoreus*.

Sharpe, I.A. *et al., Nat. Neurosci.*, 2001, **4**, 902-907 (*isol*)

λ-Conotoxin Mr VI C-797

Val-Cys-Cys-Gly-Tyr-Lys-Leu-Cys-His-Pro-Cys

Struct. of λ-Conotoxin Mr VIA shown. Isol. from venom of *Conus marmoreus*. Inhibit the neuronal noradrenaline transporter.

λ-Conotoxin Mr VIA [328057-47-2]

$C_{51}H_{76}N_{14}O_{14}S_4$ 1237.511

Peptide with 2 disulfide bridges (Cys^2 - Cys^{11}, Cys^3 - Cys^8) and a 4-hydroxyproline residue at position 10.

λ-Conotoxin Mr VIB

χ-Conotoxin Mr IA

[316350-62-6]

$C_{57}H_{85}N_{17}O_{17}S_4$ 1408.666

Peptide with 2 disulfide bridges (Cys^4 - Cys^{13}, Cys^5 - Cys^{10}) and a 4-hydroxyproline residue at position 12.

McIntosh, J.M. *et al., J. Biol. Chem.*, 2000, **275**, 32391-32397 (*isol*)
Balaji, R.A. *et al., J. Biol. Chem.*, 2000, **275**, 39516-39522 (*isol*)
Sharpe, I.A. *et al., Nat. Neurosci.*, 2001, **4**, 902-907 (*Mr VIB, isol*)

Conotoxin Mr VIA C-798

μ-O-Conotoxin MR VIA

H-Ala-Cys-Arg-Lys-Lys-Trp-Glu-Tyr-Cys-Ile-Val-Pro-Ile-Ile-Gly-Phe-Ile-Tyr-Cys-Cys-Pro-Gly-Leu-Ile-Cys-Gly-Pro-Phe-Val-Cys-Val-OH

$C_{163}H_{243}N_{37}O_{36}S_6$ 3489.335

Isol. from the venom of *Conus marmoreus*. Sodium channel blocking agent.

Fainzilber, M. *et al., Biochemistry*, 1995, **34**, 5364-5371 (*isol, struct*)
McIntosh, J.M. *et al., J. Biol. Chem.*, 1995, **270**, 16796-16802 (*synth*)
Daly, N.J. *et al., J. Biol. Chem.*, 2004, **279**, 25774-25782 (*pmr, struct*)

Conotoxin Mr VIB C-799

μ-O-Conotoxin MR VIB

H-Ala-Cys-Ser-Lys-Lys-Trp-Glu-Tyr-Cys-Ile-Val-Pro-Ile-Leu-Gly-Phe-Val-Tyr-Cys-Cys-Pro-Gly-Leu-Ile-Cys-Gly-Pro-Phe-Val-Cys-Val-OH

$C_{159}H_{234}N_{34}O_{37}S_6$ 3406.199

Isol. from the venom of *Conus marmoreus*. Sodium channel-blocking agent.

Fainzilber, M. *et al., Biochemistry*, 1995, **34**, 5364-5371 (*isol, struct*)

Conotoxin mr3a C-800

Gly-Cys-Cys-Gly-Ser-Phe-Ala-Cys-Arg-Phe-Gly-Cys-Val-Pro-Cys-Cys-Val

$C_{69}H_{100}N_{20}O_{20}S_6$ 1722.067

Peptide containing a 4-hydroxyproline residue at position 14. Isol. from venom of *Conus marmoreus*. Induces rolling seizures in mice.

McDougal, O.M. *et al., Biochemistry*, 2004, **43**, 425-429 (*isol, struct*)

δ-Conotoxin Ng VIA C-801

[161812-03-9]

Ser-Lys-Cys-Phe-Ser-Pro-Gly-Thr-Phe-Cys-Gly-Ile-Lys-Pro-Gly-Leu-Cys-Cys-Ser-Val-Arg-Cys-Phe-Ser-Leu-Phe-Cys-Ile-Ser-Phe-Glu

$C_{150}H_{222}N_{36}O_{42}S_6$ 3394.016

Peptide of the conotoxin O-superfamily containing 4-hydroxyproline residues at positions 6 and 14. Isol. from venom of *Conus nigropunctatus*. Inhibits the inactivation of voltage-sensitive sodium channels.

Fainzilber, M. *et al., J. Biol. Chem.*, 1995, **270**, 1123-1129 (*isol*)

α-Conotoxin P IA C-802

[669050-68-4]

Arg-Asp-Pro-Cys-Cys-Ser-Asn-Pro-Val-Cys-Thr-Val-His-Asn-Pro-Gln-Ile-Cys-NH_2

$C_{79}H_{125}N_{27}O_{25}S_4$ 1981.286

Isol. from venom of *Conus purpurascens*.

Dowell, C. *et al., J. Neurosci.*, 2003, **23**, 8445-8452 (*isol*)

ψ-Conotoxin P III C-803

His-Pro-Pro-Cys-Cys-Leu-Tyr-Gly-Lys-Cys-Arg-Arg-Tyr-Pro-Gly-Cys-Ser-Ser-Ala-Ser-Cys-Cys-Gln-Arg-NH_2

Peptides of the conotoxin M-superfamily. Struct. of ψ-Conotoxin P IIIE shown. Isol. from venom of *Conus purpurascens*. Inhibitors of nicotinic acetylcholine receptors.

ψ-Conotoxin P IIIE [191718-73-7]

$C_{108}H_{166}N_{38}O_{33}S_6$ 2717.13

Contains 4-hydroxyproline residues at positions 2, 3 and 14.

ψ-Conotoxin P IIIF [451530-21-5]

$C_{111}H_{165}N_{33}O_{32}S_6$ 2666.122

Contains 4-hydroxyproline residues at positions 2, 3, 12 and 14.

Shon, K.J. *et al., Biochemistry*, 1997, **36**, 9581-9587 (*P IIIE, isol*)
Mitchell, S.S. *et al., Biochemistry*, 1998, **37**, 1215-1220 (*P IIIE, soln struct*)
Van Wagoner, R.M. *et al., Biochemistry*, 2003, **42**, 6353-6362 (*P IIIF, isol, struct*)

μ-Conotoxin P IIIA C-804

[184840-20-8]

5-OxoPro-Arg-Leu-Cys-Cys-Gly-Phe-Pro-Lys-Ser-Cys-Arg-Ser-Arg-Gln-Cys-Lys-Pro-His-Arg-Cys-Cys

$C_{103}H_{165}N_{39}O_{29}S_6$ 2606.076

Peptide of the conotoxin M-superfamily containing 4-hydroxyproline residues at positions 8 and 18. Isol. from *Conus purpurascens*. Sodium channel blocker.

Shon, K.J. *et al., J. Neurosci.*, 1998, **18**, 4473-4481 (*isol*)
Nielsen, K.J. *et al., J. Biol. Chem.*, 2002, **277**, 27247-27255 (*soln struct*)

α-Conotoxin P IVA C-805

[162381-43-3]

Gly-Cys-Cys-Gly-Ser-Tyr-Pro-Asn-Ala-Ala-Cys-His-Pro-Cys-Ser-Cys-Lys-Asp-Arg-Pro-Ser-Tyr-Cys-Gly-Gln-NH_2

$C_{103}H_{150}N_{34}O_{37}S_6$ 2648.92

Peptide of the conotoxin A-superfamily containing 4-hydroxyproline residues at positions 7, 13 and 20. Isol. from venom of *Conus purpurascens*. Inhibitor of nicotinic acetylcholine receptors.

13-Proline analogue: [162381-44-4]
$C_{103}H_{150}N_{34}O_{36}S_6$ 2632.92

Isol. from venom of *Conus purpurascens*. Contains 4-hydroxyproline residues at positions 7 and 20.

7-Proline, 13-proline analogue: [162381-41-1]
$C_{103}H_{150}N_{34}O_{35}S_6$ 2616.921

Isol. from venom of *Conus purpurascens*. Contains a 4-hydroxyproline residue at position 20.

Hopkins, C. *et al., J. Biol. Chem.*, 1995, **270**, 22361-22367 (*isol*)
Han, K.H. *et al., Biochemistry*, 1997, **36**, 1669-1677 (*pmr*)

δ-Conotoxin P VIA C-806

Lockjaw peptide

Glu-Ala-Cys-Tyr-Ala-Pro-Gly-Thr-Phe-Cys-Gly-Ile-Lys-Pro-Gly-Leu-Cys-Cys-Ser-Glu-Phe-Cys-Leu-Pro-Gly-Val-Cys-Phe-Gly-NH_2

$C_{131}H_{189}N_{31}O_{38}S_6$ 2998.515

Peptide of the conotoxin O-superfamily containing 4-hydroxyproline residues at positions 6 and 15. Isol. from venom of *Conus purpurascens*. Inhibits the inactivation of voltage-sensitive sodium channels.

Shon, K.J. *et al., Biochemistry*, 1995, **34**, 4913-4918 (*isol*)

κ-Conotoxin P VIIA C-807

Fin-popping peptide

[196605-79-5]

Cys-Arg-Ile-Pro-Asn-Gln-Lys-Cys-Phe-Gln-His-Leu-Asp-Asp-Cys-Cys-Ser-Arg-Lys-Cys-Asn-Arg-Phe-Asn-Lys-Cys-Val

$C_{133}H_{210}N_{46}O_{39}S_6$ 3269.803

Peptide of the conotoxin O-superfamily containing a 4-hydroxyproline residue at position 4. Isol. from venom of *Conus purpurascens*. Potassium channel inhibitor.

Scanlon, M.J. *et al., Structure (London)*, 1997, **5**, 1585-1597 (*soln struct*)
Savarin, P. *et al., Biochemistry*, 1998, **37**, 5407-5416 (*soln struct*)
Shon, K.J. *et al., J. Biol. Chem.*, 1998, **273**, 33-38 (*isol*)

Conotoxin p5a C-808

Gly-Cys-Cys-Pro-Lys-Gln-Met-Arg-Cys-Cys-Thr-Leu-NH_2

$C_{51}H_{88}N_{18}O_{14}S_5$ 1337.698

Peptide of the conotoxin T-superfamily. Isol. from venom of *Conus purpurascens*.

Walker, C.S. *et al., J. Biol. Chem.*, 1999, **274**, 30664-30671 (*isol*)

α-Conotoxin Pn I C-809

Gly-Cys-Cys-Ser-Leu-Pro-Pro-Cys-Ala-Ala-Asn-Asn-Pro-Asp-Tyr-Cys-NH_2

Peptides of the conotoxin A-superfamily with sulfated tyrosine residues. Struct. of α-Conotoxin Pn IA shown. Isol. from *Conus pennaceus*. Inhibitors of nicotinic acetylcholine receptors.

α-Conotoxin Pn IA [157961-36-9]

α-Conotoxin Pn IB [157998-82-8]

Fainzilber, M. *et al., Biochemistry*, 1994, **33**, 9523-9529; 1995, **34**, 8649-8656 (*isol, struct*)
Hu, S.H. *et al., Structure (London)*, 1996, **4**, 417-423 (*Pn IA, cryst struct*)
Hu, S.H. *et al., Biochemistry*, 1997, **36**, 11323-11330 (*Pn IB, cryst struct*)
Wolfender, J.L. *et al., J. Mass Spectrom.*, 1999, **34**, 447-454 (*ms*)

μ-Conotoxin Pn IV C-810

Cys-Cys-Lys-Tyr-Gly-Trp-Thr-Cys-Leu-Leu-Gly-Cys-Ser-Pro-Cys-Gly-Cys

Peptides of the conotoxin M-superfamily. Struct. of μ-Conotoxin Pn IVA shown. Isol. from venom of *Conus pennaceus*. Sodium channel blockers.

μ-Conotoxin Pn IVA [168074-61-1]

$C_{74}H_{107}N_{19}O_{21}S_6$ 1791.17

μ-Conotoxin Pn IVB [168074-62-2]

$C_{79}H_{106}N_{20}O_{21}S_6$ 1864.224

Fainzilber, M. *et al., Biochemistry*, 1995, **34**, 8649-8656 (*isol*)

ω-Conotoxin Pn VI C-811

Gly-Cys-Leu-Glu-Val-Asp-Tyr-Phe-Cys-Gly-Ile-Pro-Phe-Ala-Asn-Asn-Gly-Leu-Cys-Cys-Ser-Gly-Asn-Cys-Val-Phe-Val-Cys-Thr-Pro-Gln-NH_2

Peptides of the conotoxin O-superfamily. Struct. of ω-Conotoxin Pn VIA shown. Isol. from venom of *Conus pennaceus*. Calcium channel blockers.

ω-Conotoxin Pn VIA [183614-14-4]

$C_{141}H_{204}N_{36}O_{42}S_6$ 3267.775

ω-Conotoxin Pn VIB [183614-15-5]

$C_{137}H_{189}N_{33}O_{41}S_7$ 3178.659

Kits, K.S. *et al., J. Neurochem.*, 1996, **67**, 2155-2163 (*isol*)

γ-Conotoxin Pn VIIA C-812

[201615-12-5]

Asp-Cys-Thr-Ser-Trp-Phe-Gly-Arg-Cys-Thr-Val-Asn-Ser-Glu-Cys-Cys-Ser-Asn-Ser-Cys-Asp-Gln-Thr-Tyr-Cys-Glu-Leu-Tyr-Ala-Phe-Pro-Ser

$C_{152}H_{209}N_{39}O_{59}S_6$ 3718.945

Peptide of the conotoxin O-superfamily containing 4-carboxyglutamate residues at positions 14 and 26 and a 4-hydroxyproline residue at position 31. Isol. from venom of *Conus pennaceus*.

Fainzilber, M. *et al., Biochemistry*, 1998, **37**, 1470-1477 (*isol*)

Conotoxin r 11 C-813

Peptides with a D-amino acid at the third position from the *C*-terminus; members of the I-conotoxin superfamily. Isol. from *Conus radiatus* venom.

Conotoxin r 11a Contains 46 amino acid residues including a D-Phe residue.

Conotoxin r 11b Contains 46 amino acid residues including a D-Phe residue.

Conotoxin r 11c Contains 45 amino acid residues including a D-Leu residue.

Buczek, O. *et al., FEBS J.*, 2005, **272**, 4178-4188 (*r 11b, r 11c*)
Buczek, O. *et al., J. Biol. Chem.*, 2005, **280**, 4247-4253 (*r 11a*)

Conotoxin rg11a C-814

Cys-Gln-Ala-Tyr-Gly-Glu-Ser-Cys-Ser-Ala-Val-Val-Arg-Cys-Cys-Asp-Pro-Asn-Ala-Val-Cys-Cys-Gln-Tyr-Pro-Glu-Asp-Ala-Val-Cys-Val-Thr-Arg-Gly-Tyr-Cys-Arg-Pro-Pro-Ala-Thr-Val-Leu-Thr

$C_{194}H_{298}N_{56}O_{64}S_8$ 4695.353

Peptide, member of the conotoxin I-superfamily. Isol. from venom of *Conus regius*.

Vianna Braga, M.C. *et al., Toxicon*, 2005, **45**, 113-122 (*isol*)

α-Conotoxin S I C-815

Conotoxin S I

[115797-06-3]

H-Ile-Cys-Cys-Asn-Pro-Ala-Cys-Gly-Pro-Lys-Tyr-Ser-Cys-NH_2

$C_{55}H_{84}N_{16}O_{16}S_4$ 1353.63

Struct. of reduced form shown. Isol. from *Conus striatus*. Toxin. Nicotinic acetylcholine receptor antagonist.

▶ α-Conotoxins are potent paralytic toxins by ipr or other forms of parenteral administration.

Gray, W.R. *et al., Annu. Rev. Biochem.*, 1988, **57**, 665-700 (*rev*)
Zafaralla, G.C. *et al., Biochemistry*, 1988, **27**, 7102-7105 (*isol, struct, synth*)
Munson, M.C. *et al., J.A.C.S.*, 1993, **115**, 10203-10210 (*synth*)
Hann, R.M. *et al., Biochemistry*, 1994, **33**, 14058-14063 (*pharmacol*)
Hargittai, B. *et al., J. Pept. Res.*, 1999, **54**, 468-479 (*synth*)
Benie, A.J. *et al., FEBS Lett.*, 2000, **476**, 287-295 (*soln struct*)

α-Conotoxin S IA C-816

[135190-31-7]

Tyr-Cys-Cys-His-Pro-Ala-Cys-Gly-Lys-Asn-Phe-Asp-Cys-NH_2

$C_{60}H_{82}N_{18}O_{17}S_4$ 1455.682

Peptide of the conotoxin A-superfamily. Isol. from venom of *Conus striatus*. Inhibits nicotinic acetylcholine receptors.

Myers, R.A. *et al., Biochemistry*, 1991, **30**, 9370-9377 (*isol, synth*)

α-Conotoxin S II C-817

[143294-31-9]

Gly-Cys-Cys-Cys-Asn-Pro-Ala-Cys-Gly-Pro-Asn-Tyr-Gly-Cys-Gly-Thr-Ser-Cys-Ser

$C_{66}H_{95}N_{21}O_{26}S_6$ 1790.998

Peptide of the conotoxin A-superfamily. Isol. from venom of *Conus striatus*. Inhibits nicotinic acetylcholine receptors.

Ramilo, C.A. *et al., Biochemistry*, 1992, **31**, 9919-9926 (*isol*)

κ-Conotoxin S IVA C-818

5-OxoPro-Lys-Ser-Leu-Val-Pro-Ser-Val-Ile-Thr-Thr-Cys-Cys-Gly-Tyr-Asp-Pro-Gly-Thr-Met-Cys-Pro-Pro-Cys-Arg-Cys-Thr-Asn-Ser-Cys-NH_2

Peptide of the conotoxin A-superfamily containing 4-hydroxyproline residues at positions 17, 22 and 23 and a glycosylated serine residue at position 7. Isol. from venom of *Conus striatus*. Inhibitor of voltage-sensitive K channels.

Craig, A.G. *et al., Biochemistry*, 1998, **37**, 16019-16035 (*isol*)

ω-Conotoxin S VIA C-819

Cys-Arg-Ser-Ser-Gly-Ser-Pro-Cys-Gly-Val-Thr-Ser-Ile-Cys-Cys-Gly-Arg-Cys-Tyr-Arg-Gly-Lys-Cys-Thr-NH_2

$C_{95}H_{157}N_{35}O_{32}S_6$ 2493.897

Peptide of the conotoxin O-superfamily with a 4-hydroxyproline residue at position 7. Isol. from venom of *Conus striatus*. Calcium channel blocker.

3-Proline analogue:
$C_{95}H_{157}N_{35}O_{31}S_6$ 2477.897
Present in venom of *Conus striatus*.

3-Proline, 19-serine analogue:
$C_{95}H_{155}N_{35}O_{31}S_6$ 2475.881
Present in venom of *Conus striatus*.

Ramilo, C.A. *et al., Biochemistry*, 1992, **31**, 9919-9926 (*isol*)
Lu, B.S. *et al., Peptides (N.Y.)*, 1999, **20**, 1139-1144 (*derivs*)

ω-Conotoxin S VIB C-820

[150433-82-2]

Cys-Lys-Leu-Lys-Gly-Gln-Ser-Cys-Arg-Lys-Thr-Ser-Tyr-Asp-Cys-Cys-Ser-Gly-Ser-Cys-Gly-Arg-Ser-Gly-Lys-Cys-NH_2

$C_{105}H_{176}N_{38}O_{36}S_6$ 2739.174

Peptide of the conotoxin O-superfamily. Isol. from venom of *Conus striatus*. Calcium channel blocker.

Ramilo, C.A. *et al., Biochemistry*, 1992, **31**, 9919-9926 (*isol*)
Nielsen, K.J. *et al., J. Mol. Biol.*, 1996, **263**, 297-310 (*struct*)

μ-Conotoxin Sm IIIA C-821

5-OxoPro-Arg-Cys-Cys-Asn-Gly-Arg-Arg-Gly-Cys-Ser-Ser-Arg-Trp-Cys-Arg-Asp-His-Ser-Arg-Cys-Cys

$C_{97}H_{152}N_{44}O_{30}S_6$ 2606.941

Peptide of the conotoxin M-superfamily. Isol. from the venom of *Conus stercusmuscarum*. Sodium channel blocker.

West, P.J. *et al., Biochemistry*, 2002, **41**, 15388-15393 (*isol*)

ω-Conotoxin SO C-822

Cys-Lys-Ala-Ala-Gly-Lys-Pro-Cys-Ser-Arg-Ile-Ala-Tyr-Asn-Cys-Cys-Thr-Gly-Ser-Cys-Arg-Ser-Gly-Lys-Cys-NH_2

Peptides; members of the conotoxin O-superfamily. Struct. of ω-Conotoxin SO3 shown. Present in venom of *Conus striatus*.

ω-Conotoxin SO3 [284480-65-5]
$C_{100}H_{166}N_{36}O_{31}S_6$ 2561.03

ω-Conotoxin SO4 [254972-77-5]
$C_{167}H_{252}N_{42}O_{51}S_8$ 3920.607

ω-Conotoxin SO5 [162429-63-2]
$C_{157}H_{231}N_{41}O_{53}S_7$ 3765.257

ω-Conotoxin SO6 [254747-99-4]
$C_{146}H_{202}N_{34}O_{43}S_6$ 3313.8

Lu, B.S. *et al., Peptides (N.Y.)*, 1999, **20**, 1139-1144 (*isol*)
Dai, Q. *et al., J. Nat. Prod.*, 2003, **66**, 1276-1279 (*ω-Conotoxin SO3, synth*)

ρ-Conotoxin T IA C-823

[381725-58-2]

Phe-Asn-Trp-Arg-Cys-Cys-Leu-Ile-Pro-Ala-Cys-Arg-Arg-Asn-His-Lys-Lys-Phe-Cys-NH_2

$C_{105}H_{160}N_{36}O_{21}S_4$ 2390.912

Isol. from the venom of *Conus tulipa*.

Sharpe, I.A. *et al., Nat. Neurosci.*, 2001, **4**, 902-907 (*isol*)

Conotoxin T VIIA C-824

[305790-23-2]

Ser-Cys-Ser-Gly-Arg-Asp-Ser-Arg-Cys-Pro-Pro-Val-Cys-Cys-Met-Gly-Leu-Met-Cys-Ser-Arg-Gly-Lys-Cys-Val-Ser-Ile-Tyr-Gly-Glu

$C_{125}H_{204}N_{40}O_{43}S_8$ 3211.757

Peptide of the conotoxin O-superfamily with 4-hydroxyproline residues at positions 10 and 11. Isol. from *Conus tulipa*.

Hill, J.M. *et al., Eur. J. Biochem.*, 2000, **267**, 4642-4648; 4649-4657 (*isol, synth, struct*)

α-Conotoxin Tx I C-825

[287956-60-9]

Pro-Glu-Cys-Cys-Ser-Asp-Pro-Arg-Cys-Asn-Ser-Ser-His-Pro-Glu-Leu-Cys-Gly-NH_2

$C_{74}H_{113}N_{25}O_{28}S_4$ 1929.121

Present in venom of *Conus textile*.

Lu, B.S. *et al., Peptides (N.Y.)*, 1999, **20**, 1139-1144 (*isol*)

Conotoxin tx 3 C-826

Cys-Cys-Ser-Trp-Asp-Val-Cys-Asp-His-Pro-Ser-Cys-Thr-Cys-Cys-Gly

Peptides of the M-conotoxin superfamily. Struct. of Conotoxin tx 3a shown. Isol. from *Conus textile*.

Conotoxin tx 3a
$C_{65}H_{89}N_{19}O_{24}S_6$ 1712.927

Conotoxin tx 3b
$C_{58}H_{92}N_{18}O_{16}S_7$ 1521.938

Conotoxin tx 3c
$C_{48}H_{72}N_{16}O_{16}S_6$ 1321.59
Contains a 4-hydroxyproline residue at position 10.

Corpuz, G.P. *et al., Biochemistry*, 2005, **44**, 8176-8178 (*isol*)

α-Conotoxin Tx II C-827

[254748-03-3]

Pro-Glu-Cys-Cys-Ser-His-Pro-Ala-Cys-Asn-Val-Asp-His-Pro-Glu-Ile-Cys-Arg

$C_{80}H_{120}N_{26}O_{27}S_4$ 2006.25
Present in venom of *Conus textile*.

Lu, B.S. *et al., Peptides (N.Y.)*, 1999, **20**, 1139-1144 (*isol*)

ϵ-Conotoxin Tx IX C-828

Conotoxin tx5A
[230292-91-8]
Gla-Cys-Cys-Gla-Asp-Gly-Trp*-Cys-Cys-Thr*-Ala-Ala-Hyp

$C_{70}H_{96}BrN_{15}O_{37}S_4$ 1947.775

Trp* = bromotryptophan, Thr* = threonine glycosylated with *N*-acetylgalactosamine-galactose. Isol. from venom of *Conus textile*.

Walker, C.S. *et al., J. Biol. Chem.*, 1999, **274**, 30664-30671 (*isol*)
Rigby, A.C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1999, **96**, 5758-5763 (*isol*)
Kalume, D.E. *et al., J. Mass Spectrom.*, 2000, **35**, 145-156 (*ms, struct*)
Kang, J. *et al., Eur. J. Biochem.*, 2004, **271**, 4939-4949 (*synth, pmr*)

ω-Conotoxin Tx VII C-829

[250689-92-0]

Cys-Lys-Gln-Ala-Asp-Glu-Pro-Cys-Asp-Val-Phe-Ser-Leu-Asp-Cys-Cys-Thr-Gly-Ile-Cys-Leu-Gly-Val-Cys-Met-Trp

$C_{118}H_{177}N_{29}O_{38}S_7$ 2834.33

Peptide of the conotoxin O-superfamily. Isol. from venom of *Conus textile*. L-type calcium channel blocker.

Fainzilber, M. *et al., Biochemistry*, 1996, **35**, 8748-8752 (*isol*)
Sasaki, T. *et al., Biochemistry*, 1999, **38**, 12876-12884 (*synth*)
Kobayashi, K. *et al., Biochemistry*, 2000, **39**, 14761-14767 (*soln struct*)

Conotoxin Tx VIIA C-830

Cys-Gly-Gly-Tyr-Ser-Thr-Tyr-Cys-Glu-Val-Asp-Ser-Glu-Cys-Cys-Ser-Asp-Asn-Cys-Val-Arg-Ser-Tyr-Cys-Thr-Leu-Phe-NH_2

$C_{124}H_{174}N_{32}O_{49}S_6$ 3089.32

Peptide of the conotoxin O-superfamily with 4-carboxyglutamate residues at positions 9 and 13. Isol. from venom of *Conus textile*.

Fainzilber, M. *et al., Eur. J. Biochem.*, 1991, **202**, 589-595 (*isol*)
Nakamura, T. *et al., Protein Sci.*, 1996, **5**, 524-530 (*struct*)

Conotoxin tx 9a C-831

π-Conotoxin Tx IXA
Gly-Cys-Asn-Asn-Ser-Cys-Gln-Glu-His-Ser-Asp-Cys-Glu-Ser-His-Cys-Ile-Cys-Thr-Phe-Arg-Gly-Cys-Gly-Ala-Val-Asn-NH_2

$C_{111}H_{163}N_{39}O_{45}S_6$ 2956.139

Peptide of the conotoxin P-superfamily containing 4-carboxyglutamate residues at positions 8 and 13. Isol. from venom of *Conus textile*.

Lirazan, M.B. *et al., Biochemistry*, 2000, **39**, 1583-1588 (*isol*)

ω-Conotoxin Tx O C-832

Cys-Leu-Asp-Ala-Gly-Glu-Val-Cys-Asp-Ile-Phe-Phe-Pro-Thr-Cys-Cys-Gly-Tyr-Cys-Ile-Leu-Leu-Phe-Cys-Ala

Peptides of the conotoxin O-superfamily. Struct. of ω-Conotoxin TxO 1 shown. Present in venom of *Conus textile*.

ω-Conotoxin TxO 1 [254748-05-5]
$C_{121}H_{173}N_{25}O_{34}S_6$ 2714.241

ω-Conotoxin TxO 2 [254748-07-7]
$C_{104}H_{148}N_{28}O_{36}S_6$ 2558.875

ω-Conotoxin TxO 3 [254748-09-9]
$C_{107}H_{146}N_{26}O_{35}S_6$ 2548.88

ω-Conotoxin TxO 4 [254748-11-3]
$C_{138}H_{188}N_{32}O_{37}S_7$ 3111.657

ω-Conotoxin TxO 5 [254748-13-5]
$C_{130}H_{181}N_{31}O_{37}S_6$ 2962.441

ω-Conotoxin TxO 6 [254972-79-7]
$C_{173}H_{233}N_{39}O_{46}S_6$ 3787.373

Lu, B.S. *et al., Peptides (N.Y.)*, 1999, **20**, 1139-1149 (*isol*)

κ-Conotoxin ViTx C-833

Ser-Arg-Cys-Phe-Pro-Pro-Gly-Ile-Tyr-Cys-Thr-Ser-Tyr-Leu-Pro-Cys-Cys-Trp-Gly-Ile-Cys-Cys-Ser-Thr-Cys-Arg-Asn-Val-Cys-His-Leu-Arg-Ile-Gly-Lys

$C_{169}H_{255}N_{49}O_{44}S_8$ 3933.703

Peptide of the conotoxin O-superfamily. Isol. from *Conus virgo*. Inhibitor of voltage-sensitive potassium channels.

Kauferstein, S. *et al., Toxicon*, 2003, **42**, 43-52 (*isol*)

Conotoxins C-834

Conopeptides

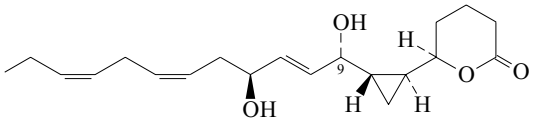
Peptides, mostly having 10-25 residues and showing a wide variety of primary struct. and 0-3 disulfide bridges. Up to 50,000 different conotoxins may exist (approx. 100 toxins in each of 500 known spp., with v. little duplication). Those on which the most work has been done have individual entries. A few conotoxins have been called Conantokins, Contulakins, Contryphans or Conorfamides. Prod. by carnivorous marine molluscs of the genus *Conus* (Neogasteropoda). Toxic substances having different modes of action where known, e.g. potassium channel blockers. Neuropharmacological tools used in study of ion channels. Different *C.* spp. feed on worms, other molluscs or fish. The piscivorous spp. have the most powerful toxins.

▶ Some conotoxins v. highly toxic, capable of human fatality.

Myers, R.A. *et al., Chem. Rev.*, 1993, **93**, 1923-1936 (*rev*)
West, D.J. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1996, **113**, 1-10 (*rev*)
Adams, D.J. *et al., Drug Dev. Res.*, 1999, **46**, 219-334 (*rev*)
Shen, G.S. *et al., Drug Discov. Today*, 2000, **5**, 98-106 (*rev*)
Olivera, B.M. *et al., Toxicon*, 2001, **39**, 7-14 (*rev*)
Terlau, H. *et al., Physiol. Rev.*, 2004, **84**, 41-68 (*rev*)
Armishaw, C.J. *et al., Curr. Protein Pept. Sci.*, 2005, **6**, 221-240 (*rev*)

Constanolactone C C-835

6-[2-(1,4-Dihydroxy-2,6,9-dodecatrienyl)cyclopropyl]tetrahydro-2H-pyran-2-one, 9CI



$C_{20}H_{30}O_4$ 334.455
Metab. of red alga *Constantinea simplex*. Oil (as di-Ac). $[\alpha]_D^{23}$ -3.8 (c, 1.3 in $CHCl_3$) (di-Ac).

9-Epimer: ***Constanolactone D***
$C_{20}H_{30}O_4$ 334.455
Metab. of *Constantinea simplex*. Oil (as di-Ac). $[\alpha]_D$ -4.7 (c, 0.3 in $CHCl_3$) (di-Ac).

17,18-Dihydro: ***Constanolactone A***
[130223-05-1]
$C_{20}H_{32}O_4$ 336.47
Metab. of *Constantinea simplex*. Oil. $[\alpha]_D$ -3.8 (c, 1.3 in $CHCl_3$). $[\alpha]_D$ +1.4 (c, 1 in MeOH).

17,18-Dihydro, 9-Me ether: ***9-O-Methylconstanolactone A***
$C_{21}H_{34}O_4$ 350.497
Metab. of *Constantinea simplex*. Oil. $[\alpha]_D$ +7.3 (c, 0.2 in MeOH).

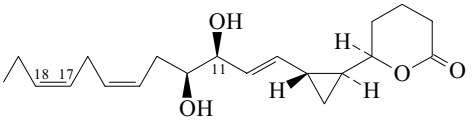
9-Epimer, 17,18-dihydro: ***Constanolactone B***
[130320-78-4]
$C_{20}H_{32}O_4$ 336.47
Metab. of *Constantinea simplex*. Oil. $[\alpha]_D^{23}$ +10.2 (c, 1 in MeOH).

9-Epimer, 17,18-dihydro, 9-Me ether: ***9-O-Methylconstanolactone B***
$C_{21}H_{34}O_4$ 350.497
Metab. of *Constantinea simplex*. Oil.

Gerwick, W.H. *et al., Chem. Rev.*, 1993, **93**, 1807-1823 (*rev*)
Nagle, D.G. *et al., J.O.C.*, 1994, **59**, 7227 (*isol, pmr, cmr, abs config*)
White, J.D. *et al., J.A.C.S.*, 1995, **117**, 6224 (*synth*)
Barloy-Da Silva, C. *et al., Tet. Lett.*, 2000, **41**, 3077-3081 (*synth*)
Yu, J. *et al., Tet. Lett.*, 2002, **43**, 3939-3941 (*synth*)

Constanolactone G C-836

[160523-31-9]



$C_{20}H_{30}O_4$ 334.455
Metab. of red alga *Constantinea simplex*. Oil (as di-Ac).

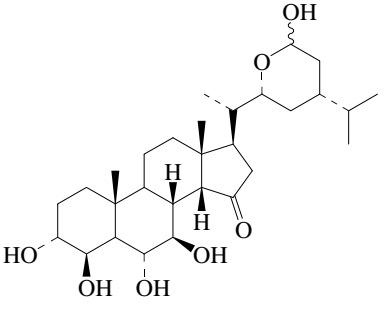
17,18-Dihydro: ***Constanolactone F***
[160552-58-9]
$C_{20}H_{32}O_4$ 336.47
Metab. of *Constantinea simplex*. Oil. $[\alpha]_D$ +55 (c, 0.2 in MeOH) (as di-Ac).

11-Epimer, 17,18-dihydro: ***Constanolactone E***
[160523-30-8]
$C_{20}H_{32}O_4$ 336.47
Metab. of *Constantinea simplex*. Oil. $[\alpha]_D$ +33 (c, 0.2 in MeOH).

Nagle, D.G. *et al., J.O.C.*, 1994, **59**, 7227 (*isol, pmr, cmr, abs config*)
Miyaoka, H. *et al., Tet. Lett.*, 1996, **37**, 7407 (*synth, Constanolactone E*)
Miyaoka, H. *et al., Heterocycles*, 1998, **47**, 415-428 (*synth*)

Contignasterol C-837

[137571-30-3]



$C_{29}H_{48}O_7$ 508.694

24-Config. revised in 2002. Constit. of *Petrosia contignata*. Antiasthma and antialleric agent. Histamine release inhibitor. Under development (1998, Inflazyme) but prob. superseded by

more active semisynthetic analogues. Cryst. (MeOH aq.). Mp 239-241°.

Burgoyne, D.L. *et al., J.O.C.*, 1992, **57**, 525 (*isol, pmr, cmr*)
Yang, L. *et al., J. Nat. Prod.*, 2002, **65**, 1924-1926 (*abs config*)

Contractin A C-838

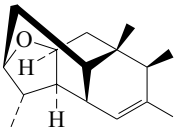
[132579-38-5]

Protein with 138 amino acid residues. Isol. from the pedicellarial venom of the sea urchin *Toxopneustes pileolus*. Muscle contractor.

Nakagawa, H. *et al., Arch. Biochem. Biophys.*, 1991, **284**, 279-284 (*isol*)

Contrunculin A C-839

[152221-13-1]

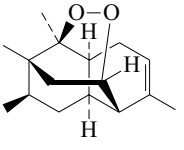


$C_{16}H_{24}O$ 232.365
Constit. of *Latrunculia conulosa*. Oil. $[\alpha]_D$ +151.3 (c, 3.99 in $CHCl_3$).

Butler, M.S. *et al., Aust. J. Chem.*, 1993, **46**, 1363 (*isol, pmr, cmr*)

Contrunculin B C-840

[152244-01-4]



$C_{16}H_{24}O_2$ 248.364
Constit. of *Latrunculia conulosa*. Unstable oil. $[\alpha]_D$ -35.9 (c, 1.7 in $CHCl_3$).

Butler, M.S. *et al., Aust. J. Chem.*, 1993, **46**, 1363 (*isol, pmr, cmr*)

Contryphans C-841

Gly-Cys-Hyp-D-Trp-Asp-Pro-Trp-Cys-NH_2

Short peptides characterised by the presence of 4-hydroxyproline (O) and D-tryptophan residues and a disulfide bond; struct. of Contryphan P shown. Biol. function unknown.

Contryphan P [206262-12-6]
$C_{44}H_{53}N_{11}O_{11}S_2$ 976.102
Isol. from *Conus purpurascens*.

Contryphan R [183428-21-9]
$C_{45}H_{55}N_{11}O_{11}S_2$ 990.129
Isol. from *Conus radiatus*. D-Trp at position 4.

Contryphan Sm [206262-14-8]
$C_{45}H_{56}N_{12}O_{10}S_2$ 989.144
Isol. from *Conus stercusmuscarum*. D-Trp at position 4.

Contryphan Tx [354530-26-0]
$C_{43}H_{55}N_{11}O_{11}S_2$ 966.107
Isol. from *Conus textile*. D-Trp at position 4.

Contryphan Vn [388122-35-8]
$C_{50}H_{65}N_{12}O_{11}S_2$ 1074.269
D-Trp at position 5. Isol. from *Conus ventricosus*.

Jimenez, E.C. *et al., J. Biol. Chem.*, 1996, **271**, 28002-28005 (*Contryphan P, Contryphan Sm*)
Jacobsen, R. *et al., J. Pept. Res.*, 1998, **51**, 173-179 (*Contryphan R*)
Pallaghy, P.K. *et al., Biochemistry*, 1999, **38**, 11553-11559 (*Contryphan R, soln struct*)
Massilia, G.R. *et al., Biochem. Biophys. Res. Commun.*, 2001, **288**, 908-913; 2003, **303**, 238-246 (*Contryphan Vn*)
Jimenez, E.C. *et al., Toxicon*, 2001, **39**, 803-808 (*Contryphan Tx*)
Eliseo, T. *et al., Biopolymers*, 2004, **74**, 189-198 (*Contryphan Vn, soln struct*)

Contulakin G C-842

[229180-41-0]

5-OxoPro-Ser-Glu-Glu-Gly-Gly-Ser-Asn-Ala-^{10}Thr-Lys-Lys-Pro-Tyr-Ile-Leu-OH

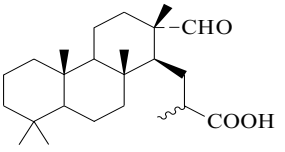
$C_{88}H_{140}N_{20}O_{37}$ 2070.186

Glycopeptide; the major glycosylated form incorporates the disaccharide β-D-Galp-(1→3)-α-D-GalpNAc-(1→) attached to the OH of ^{10}Thr. Isol. from the venom of *Conus geographus*. Neurotensin.

Craig, A.G. *et al., J. Biol. Chem.*, 1999, **274**, 13752-13759 (*isol, struct*)
Kindahl, L. *et al., Aust. J. Chem.*, 2002, **80**, 1022-1031 (*pmr, conformn*)

Conulosin A C-843

[150627-35-3]

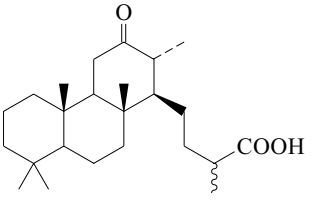


$C_{24}H_{40}O_3$ 376.578
Constit. of *Latrunculia conulosa*. Unstable oil (as Me ester). $[\alpha]_D$ -10.3 (c, 1.7 in $CHCl_3$) (Me ester).

Butler, M.S. *et al., Nat. Prod. Lett.*, 1992, **1**, 171 (*isol, pmr, cmr*)

Conulosin B C-844

[150627-36-4]

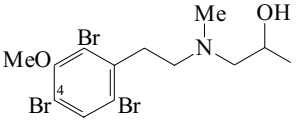


$C_{24}H_{40}O_3$ 376.578
Constit. of *Latrunculia conulosa*. Unstable oil (as Et ester).

Butler, M.S. *et al., Nat. Prod. Lett.*, 1992, **1**, 171 (*isol, pmr, cmr*)

Convolutamine A C-845

[161099-50-9]



$C_{13}H_{18}Br_3NO_2$ 460.003
Alkaloid from the marine bryozoan *Amathia convoluta*. Exhibits cytotoxicity against murine P388 lymphocytic leukaemia. Oil. Racemic. λ_{max} 212 (ϵ 27900) (MeOH) (Berdy).

N-*De-Me:* ***Convolutamine C***
[161099-52-1]
$C_{12}H_{16}Br_3NO_2$ 445.976
From *Amathia convoluta*. Oil. Stereochem. unknown.

N-*De(2-hydroxypropyl):* ***Convolutamine F***
[243858-10-8]
$C_{10}H_{12}Br_3NO$ 401.923

Alkaloid from *Amathia convoluta*. Oil. $[\alpha]_D^{20}$ +24.3 (c, 0.4 in $CHCl_3$). λ_{max} 213 (ϵ 21800) (MeOH).

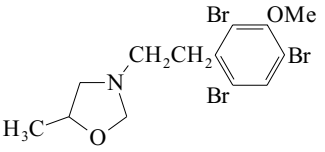
4-Debromo: ***Convolutamine B***
[161099-51-0]
$C_{13}H_{19}Br_2NO_2$ 381.107
From *Amathia convoluta*. Exhibits cytotoxicity against murine P388 lymphocytic leukaemia. Oil. Racemic. λ_{max} 211 (ϵ 20100) (MeOH) (Berdy).

4-Debromo, N-*de(2-hydroxypropyl):* ***Convolutamine G***
[243858-11-9]
$C_{10}H_{13}Br_2NO$ 323.027
Alkaloid from *Amathia convoluta*. Oil. λ_{max} 206 (ϵ 8910); 229 (ϵ 1930) (MeCN).

Zhang, H. *et al., Chem. Lett.*, 1994, 2271-2274 (*isol, uv, ir, pmr, cmr, ms, struct*)
Kamano, Y. *et al., Coll. Czech. Chem. Comm.*, 1999, **64**, 1147-1153 (*Convolutamines F,G*)
Hashima, H. *et al., Bioorg. Med. Chem.*, 2000, **8**, 1757-1766 (*synth*)

Convolutamine D C-846

[161099-53-2]

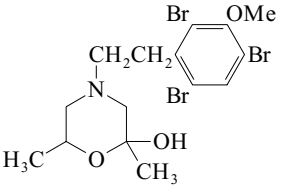


$C_{13}H_{16}Br_3NO_2$ 457.987
Alkaloid from the marine bryozoan *Amathia convoluta*. Exhibits cytotoxicity against murine P388 lymphocytic leukaemia. Oil.

Zhang, H. *et al., Chem. Lett.*, 1994, 2271-2274 (*isol, pmr, cmr, struct*)

Convolutamine E C-847

[161099-54-3]

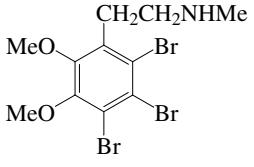


$C_{15}H_{20}Br_3NO_3$ 502.04
Alkaloid from the marine bryozoan *Amathia convoluta*. Oil.

Zhang, H. *et al., Chem. Lett.*, 1994, 2271 (*isol, pmr, cmr, struct*)

Convolutamine H C-848

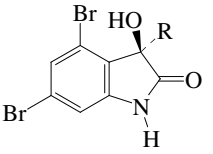
N-*Methyl-2-(2,3,4-tribromo-5,6-dimethoxyphenyl)ethylamine.*
2,3,4-Tribromo-5,6-dimethoxy-N-*methylbenzeneethanamine, 9CI*
[443355-92-8]



$C_{11}H_{14}Br_3NO_2$ 431.949
Alkaloid from the marine bryozoan *Amathia convoluta*. Pale yellow oil. λ_{max} 217 (log ϵ 4.4) (MeOH).

Narkowicz, C.K. *et al., J. Nat. Prod.*, 2002, **65**, 938-941 (*isol, pmr, cmr, ms*)

Convolutamydines C-849



Absolute Configuration

Convolutamydine A; R = CH_2COCH_3
B; R = CH_2CH_2Cl
C; R = CH_3
D; R = $CH{=}CH_2$
E; R = CH_2CH_2OH

Convolutamydine A
*4,6-Dibromo-1,3-dihydro-3-hydroxy-3-(2-oxopropyl)-2*H-*indol-2-one, 9CI*
[163564-85-0]
[184587-77-7]
$C_{11}H_9Br_2NO_3$ 363.005
Alkaloid from the marine bryozoan *Amathia convoluta*. Cell differentiation and growth inhibitor. Amorph. solid (MeOH). Mp 190-195°. $[\alpha]_D^{26}$ +27.4 (c, 0.06 in MeOH). λ_{max} 224 (ϵ 21600); 262 (ϵ 5200); 291 (ϵ 3100) (MeOH) (Berdy).

Convolutamydine B
*4,6-Dibromo-3-(2-chloroethyl)-1,3-dihydro-3-hydroxy-2*H-*indol-2-one, 9CI*
[163564-86-1]
$C_{10}H_8Br_2ClNO_2$ 369.439
Alkaloid from the marine bryozoan *Amathia convoluta*. Amorph. solid (Me_2CO).
Mp 225-227°. $[\alpha]_D^{25}$ +18.1 (c, 0.42 in MeOH).

Convolutamydine C
*4,6-Dibromo-1,3-dihydro-3-hydroxy-3-methyl-2*H-*indol-2-one, 9CI*
[163564-87-2]
$C_9H_7Br_2NO_2$ 320.968
Alkaloid from the marine bryozoan *Amathia convoluta*. Amorph. solid (Me_2CO).
Mp 175-180°. $[\alpha]_D^{25}$ +32.4 (c, 0.03 in MeOH).

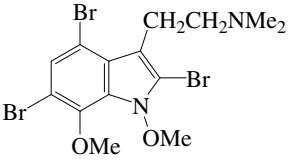
Convolutamydine D
*4,6-Dibromo-3-ethenyl-1,3-dihydro-3-hydroxy-2*H-*indol-2-one, 9CI*
[163564-94-1]
$C_{10}H_7Br_2NO_2$ 332.979
Alkaloid from the marine bryozoan *Amathia convoluta*. Cell differentiation and growth inhibitor. Amorph. solid. $[\alpha]_D^{26}$ +14 (c, 0.04 in MeOH). λ_{max} 220 (ϵ 7488); 290 (ϵ 1475) (MeOH) (Berdy).

Convolutamydine E
*4,6-Dibromo-1,3-dihydro-3-hydroxy-3-(2-hydroxyethyl)-2*H-*indol-2-one, 9CI*
[243858-13-1]
$C_{10}H_9Br_2NO_3$ 350.994
Alkaloid from the marine bryozoan *Amathia convoluta*. Oil. λ_{max} 223 (ϵ 16870); 298 (ϵ 850) (MeCN).

Kamano, Y. *et al., Tet. Lett.*, 1995, **36**, 2783-2784 (*Convolutamydine A, isol*)
Zhang, H. *et al., Tetrahedron*, 1995, **51**, 5523-5528 (*isol, uv, ir, pmr, cmr, cd, struct*)
Miah, S. *et al., J.C.S. Perkin 1*, 1997, 2405-2412 (*synth, Convolutamydine C*)
Kamano, Y. *et al., Coll. Czech. Chem. Comm.*, 1999, **64**, 1147-1163 (*Convolutamydine E*)
Jnaneshwara, G.K. *et al., Synth. Commun.*, 1999, **29**, 3627-3633 (*Convolutamydine A*)
Takayama, H. *et al., Tetrahedron*, 1999, **55**, 6841-6846 (*abs config*)
Kawasaki, T. *et al., Tetrahedron*, 2004, **60**, 3493-3503 (*synth*)
Nakamura, T. *et al., Org. Lett.*, 2006, **8**, 677-679 (*synth*)

Convolutindole A C-850

2,4,6-Tribromo-1,7-dimethoxy-N,N-*dimethyl-1*H-*indole-3-ethanamine. 2,4,6-Tribromo-3-(2-dimethylaminoethyl)-1,7-dimethoxyindole*
[443356-86-3]



$C_{14}H_{17}Br_3N_2O_2$ 485.013
Alkaloid from the marine bryozoan *Amathia convoluta*. Amorph. solid.
Mp 61.5-62.5°. λ_{max} 235 (log ϵ 4.7); 289 (log ϵ 4.1); 305 (log ϵ 4) (MeOH).

Narkowicz, C.K. *et al., J. Nat. Prod.*, 2002, **65**, 938-941 (*isol, pmr, cmr, ms*)

Conus textile Convulsant peptide C-851

Textile convulsant peptide
Asn-Cys-Pro-Tyr-Cys-Val-Val-Tyr-Cys-Cys-Pro-Pro-Ala-Tyr-Cys-Glu-Ala-Ser-Gly-Cys-Arg-Pro-Pro-NH_2
$C_{106}H_{150}N_{28}O_{30}S_6$ 2488.917
Isol. from venom of *Conus textile*.

Cruz, L.J. *et al., Biol. Bull. (Woods Hole, Mass.)*, 1992, **183**, 159-164 (*isol*)

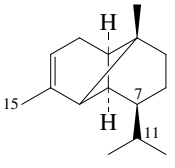
Cooliatoxin C-852

[172308-32-6]
Polyether toxin probably related to Yessotoxin, Y-7. Isol. from the dinoflagellate *Coolia monotis*.

Holmes, M.J. *et al., Nat. Toxins*, 1995, **3**, 355-362

3-Copaene C-853

1,3-Dimethyl-8-(1-methylethyl)tricyclo[4.4.0.0^{2,7}]dec-3-ene, 9CI. 8-Isopropyl-1,3-dimethyltricyclo[4.4.0.0^{2,7}]dec-3-ene



(1α*H*,6α*H*,7α*H*)-*form*

$C_{15}H_{24}$ 204.355

(1α*H*,6α*H*,7α*H*)-*form*
Ylangene. *α-Ylangene*
[14912-44-8]
Isol. from various essential oils, esp. *Schizandra chinensis*.
Oil. $[\alpha]_D^{20}$ +50.5.

(1β*H*,6β*H*,7α*H*)-*form*
α-Copaene. *Aglaiene. Copaene*
[3856-25-5]
Constit. of the oils of African Copaiva balsam and *Sindora wallichii*. Also from various other higher plant oils and from the brown alga *Dictyopteris divaricata*. Shows antibacterial activity.
Oil. Bp 246-251°. $[\alpha]_D$ -13.3 ($CHCl_3$). n_D^{20} 1.4722.

11-Hydroxy: 3-Copaen-11-ol. ***α-Copaen-11-ol***
[41370-56-3]
$C_{15}H_{24}O$ 220.354
Constit. of the essential oil of *Parabenzoin praecox*. Cryst.
Mp 99.5-100.5°. $[\alpha]_D$ +9.2 ($CHCl_3$).

15-Hydroxy: 3-Copaen-15-ol. ***15-Copaenol***
[41610-70-2]
$C_{15}H_{24}O$ 220.354
Constit. of *Brachylaena hutchinsii* and *Pilgerodendron uniferum*.
Oil. $[\alpha]_D^{25}$ -28.6 (c, 0.2 in $CHCl_3$).

$\Delta^{4,15}$-Isomer: 4(15)-Copaene. ***β-Copaene***
[18252-44-3]
$C_{15}H_{24}$ 204.355
Present in various plant oils. Oil. $[\alpha]_D$ -7.6 (c, 2 in $CHCl_3$).

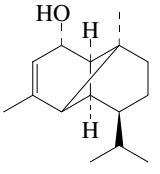
(1β*H*,6β*H*,7β*H*)-*form*
(-)-α-Ylangene
[947-59-1]
Constit. of *Aristolochia triangularis* and *Scapania undulata*.

$\Delta^{4,15}$-Isomer: ***(+)-β-Ylangene***
[28129-91-1]
$C_{15}H_{24}$ 204.355
Constit. of *Pseudoplexaura porosa* and *Angelica archangelica*.

[41530-63-6, 41530-64-7, 115728-41-1]

Motl, O. *et al., Coll. Czech. Chem. Comm.*, 1962, **27**, 987 (*isol, Ylangene*)
Irie, T. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 1053 (*isol, α-Copaene*)
Kapadia, V.H. *et al., Tetrahedron*, 1965, **21**, 607 (*pmr*)
De Mayo, P. *et al., Tetrahedron*, 1965, **21**, 619 (*ir*)
Westfelt, L. *et al., Acta Chem. Scand.*, 1966, **20**, 2841; 1967, **21**, 152 (*β-Copaene*)
Veldhuis, M.K. *et al., J. Food Sci.*, 1967, **32**, 697 (*nomencl*)
Weinheimer, A.J. *et al., Drugs Sea Trans. Symp.*, 1968, 135-140; *CA*, **72**, 70562 (*(+)-β-Ylangene*)
Ohta, Y. *et al., Tet. Lett.*, 1969, 1601 (*struct, abs config, Ylangene*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 1907 (*occur*)
Ohara, K. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 641 (*α-Copaen-11-ol*)
Corey, E.J. *et al., J.A.C.S.*, 1973, **95**, 2303 (*synth*)
Andersen, N.H. *et al., Phytochemistry*, 1977, **16**, 1731-1751 (*(-)-α-Ylangene*)
Ruecker, G. *et al., Planta Med.*, 1981, **41**, 143-149 (*(-)-α-Ylangene*)
Snider, B.B. *et al., J.O.C.*, 1987, **52**, 1568 (*β-Copaene*)
Kulkarni, Y.S. *et al., J.O.C.*, 1987, **52**, 1568-1576 (*synth, cmr*)
Oyarzún, M.L. *et al., Phytochemistry*, 1988, **27**, 1121 (*15-Copaenol*)
De Buyck, L.F. *et al., Flavour Fragrance J.*, 1989, **4**, 53-57 (*cmr*)
Vieira, P.C. *et al., J. Nat. Prod.*, 1991, **54**, 416 (*15-Copaenol*)
Wenkert, E. *et al., J.A.C.S.*, 1992, **114**, 644 (*synth*)
Flath, R.A. *et al., J. Chem. Ecol.*, 1994, **20**, 1969-1984 (*(+)-β-Ylangene*)
Melching, S. *et al., Phytochemistry*, 1997, **44**, 1291 (*pmr*)
Dos Santos, M.H. *et al., Rev. Bras. Cienc. Farm.*, 1999, **35**, 297-300 (*activity*)

3-Copaen-2-ol C-854



2α-*form*

$C_{15}H_{24}O$ 220.354

2α-*form* [182684-49-7]
Constit. of *Entandrophragma cylindricum*.
Cryst.
Mp 57°. $[\alpha]_D^{20}$ -47.6 (c, 0.5 in $CHCl_3$).

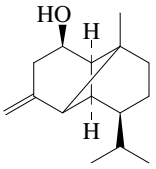
2-Ketone: ***3-Copaen-2-one***. ***Mustakone***. *4-Oxo-α-ylangene*
[1209-91-2]
Constit. of *Cyperus rotundus* (nutgrass), *Cyperus articulatus* and *Lemnalia cervicorni*.
Oil. Bp_1 128-129°. $[\alpha]_D^{25}$ -42.5 (c, 1.85 in $CHCl_3$). Stereochem. revised in 2004.

2-Ketone, 2,4-dinitrophenylhydrazone:
Cryst. (EtOH). Mp 141-142°.

2β-*form*
Isolemnalol
[771534-40-8]
Constit. of *Lemnalia cervicorni*.
Oil. $[\alpha]_D^{25}$ +3.33 (c, 0.66 in $CHCl_3$). λ_{max} 212 (log ϵ 3.56) (MeOH).

Kapadia, V.H. *et al., Tetrahedron*, 1965, **21**, 607 (*ketone*)
Nyasse, B. *et al., Phytochemistry*, 1988, **27**, 3319 (*ketone*)
Daniewski, W.M. *et al., Phytochemistry*, 1996, **43**, 811-814 (*isol, pmr, cmr*)
Duh, C.Y. *et al., J. Nat. Prod.*, 2004, **67**, 1650-1653 (*Lemnalia cervicorni constits*)

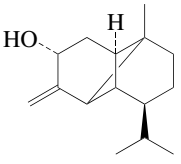
4(15)-Copaen-2-ol C-855



$C_{15}H_{24}O$ 220.354

2β-*form*
Cervicol
[771534-39-5]
Constit. of *Lemnalia cervicorni*.
Oil. $[\alpha]_D^{25}$ -70.8 (c, 0.8 in $CHCl_3$). λ_{max} 212 (log ϵ 3.88) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 2004, **67**, 1650-1653 (*isol, pmr, cmr*)

4(15)-Copaen-3-ol C-856



Absolute Configuration

$C_{15}H_{24}O$ 220.354

3α-*form*
Lemnalol
[82570-34-1]
Constit. of *Lemnalia tenuis* and *Lemnalia cervicorni*. Membrane permeability enhancer. Cryst.
Mp 46-47°. $[\alpha]_D^{20}$ -9.3 (c, 0.01 in $CHCl_3$). λ_{max} 227 (ϵ 9000) (EtOH). λ_{max} 214 (log ϵ 3.5) (MeOH).
Kikuchi, H. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1086 (*cryst struct*)
Kulkarni, Y.S. *et al., J.O.C.*, 1987, **52**, 1568-1576 (*synth*)
Duh, C.Y. *et al., J. Nat. Prod.*, 2004, **67**, 1650-1653 (*isol, pmr, cmr*)

Copper chloride hydroxide ($Cu_2Cl(OH)_3$), 9CI C-857

Copper chloride hydroxide
[1332-65-6]
$Cu_2Cl(OH)_3$
$ClCu_2H_3O_3$ 213.567
Mineral.

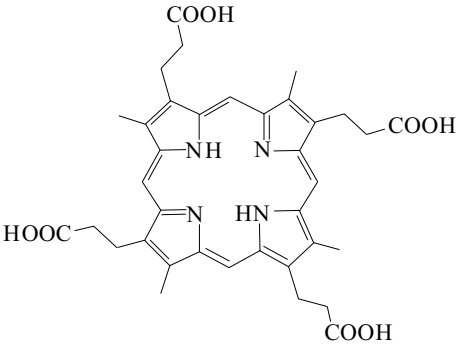
Mineral-*form*
Botallackite, 9CI
[12015-74-6]
Rare secondary mineral. Occurs associated with atacamite and paratacamite at the Botallack mine, St. Just, Cornwall, UK. Pale green monoclinic cryst. α-form.

Mineral-*form*
Paratacamite, 9CI
[12186-00-4]
Secondary mineral. Widespread in the oxidn. zone of copper deposits. Green-rhombohedral cryst. γ-form.

Mineral-*form*
Atacamite, 9CI
[1306-85-0]
Secondary mineral. Widespread in the oxidn. zone of copper deposits. Structural component of the jaws of marine bloodworm *Glycera dibranchiata*. Light green orthorhombic cryst. δ-form.
Palache, C. *et al., Dana's System of Mineralogy*, Wiley, 7th Edn., 1951, **2**, 69 (*mineralogy*)
Osward, H.R. *et al., Helv. Chim. Acta*, 1964, **47**, 272 (*synth*)
Fleet, M.E. *et al., Acta Cryst. B*, 1975, **31**, 183 (*cryst struct, paratacamite*)
Hawthorne, F.C. *et al., Mineral. Mag.*, 1985, **49**, 87 (*cryst struct, botallackite*)
Parise, J.B. *et al., Acta Cryst. C*, 1986, **42**, 1277 (*cryst struct, atacamite*)
Pollard, A.M. *et al., Mineral. Mag.*, 1989, **53**, 557 (*synth*)
Lichtenegger, H.C. *et al., Science (Washington, D.C.)*, 2002, **298**, 389-392 (*Glycera dibranchiata, constit*)

Coproporphyrin I C-858

*3,8,13,18-Tetramethyl-21*H*,23*H*-porphine-2,7,12,17-tetrapropanoic acid, 9CI*
[531-14-6]
[27121-71-7]



$C_{36}H_{38}N_4O_8$ 654.718
Minor component of free porphyrins found in urine, faeces, blood, yeast, marine organisms, etc. Violet cryst.
Mp 286-289°. The amount excreted may increase in certain types of abnormal metabolism.

Tetra-Me ester: [25767-20-8]
$C_{40}H_{46}N_4O_8$ 710.825
Violet cryst. ($CHCl_3$/MeOH). Mp 252-253°. λ_{max} 400; 498; 532; 566; 594; 621 (no solvent reported).

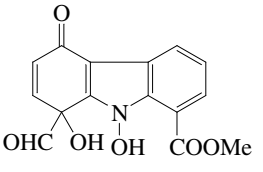
5,10,15,20,22,24-Hexahydro: ***Coproporphyrinogen I***
[31110-56-2]
$C_{36}H_{44}N_4O_8$ 660.766
Prod. of enzymic decarboxylation of Uroporphyrinogen I.

[69477-27-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 577A (*ir*)
Fischer, H. *et al., Annalen*, 1928, **466**, 147
MacDonald, S.F. *et al., J.A.C.S.*, 1953, **75**, 3040 (*synth*)
Abraham, R.J. *et al., J.C.S.(B)*, 1966, 620 (*pmr*)
Jackson, A.H. *et al., J.C.S. Perkin 1*, 1972, 1475 (*synth*)
With, T.K. *et al., Int. J. Biochem.*, 1978, **9**, 887 (*cryst struct*)
Janson, J.R. *et al., The Porphyrins*, (Dolphin, D., Ed.), Academic Press, N.Y., Vol. II, 1979, 1 (*pmr, cmr*)
Battersby, A.R. *et al., J.C.S. Perkin 1*, 1981, 2786 (*synth*)
Lim, C.K. *et al., Methods Enzymol.*, 1986, **123**, 383 (*hplc*)
Abraham, R.J. *et al., Magn. Reson. Chem.*, 1990, **28**, 1051 (*pmr*)
Ono, N. *et al., Tetrahedron*, 1990, **46**, 7483 (*synth, pmr*)
Cheng, L. *et al., Org. Prep. Proced. Int.*, 1995, **27**, 224 (*tetra-Me ester, synth*)

Coproverdine C-859

*Methyl 1-formyl-4,9-dihydro-1,9-dihydroxy-4-oxo-1*H*-carbazole-8-carboxylate, 9CI. Methyl 8-formyl-8,9-dihydro-8,9-dihydroxy-5-oxo-5*H*-carbazole-1-carboxylate*
[437702-23-3]



$C_{15}H_{11}NO_6$ 301.255
Alkaloid from a New Zealand tunicate. Antitumour agent. Yellow oil. $[\alpha]_D^{20}$ -8 (c, 0.36 in EtOH). λ_{max} 208 (ϵ 20000); 270 (ϵ 6700); 302 (ϵ 4800); 382 (ϵ 16000) (EtOH).

Urban, S. *et al., J. Nat. Prod.*, 2002, **65**, 1371-1373 (*isol, pmr, cmr, ms*)

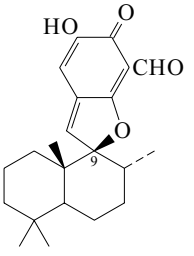
Corallan C-860

Sulfated glycoprotein containing D-Glc, D-Gal, L-Gal, D-Ara, L-Fuc and D-Glucuronic acid residues. Struct. has been partially determined. Isol. from the Caribbean soft coral *Pseudopterogorgia americana*. Sol. H_2O; poorly sol. MeOH, hexane.

Molchanova, V.I. *et al., Carbohydr. Res.*, 1985, **141**, 289

Corallidictyal A C-861

[160632-45-1]



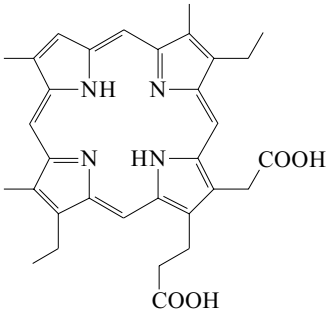
$C_{22}H_{28}O_4$ 356.461
Constit. of *Aka coralliphagum*. λ_{max} 209 (ϵ 5100); 266 (ϵ 10400); 322 (ϵ 16000) (MeOH) (Berdy).

9-Epimer: ***Corallidictyal B***
[160708-03-2]
$C_{22}H_{28}O_4$ 356.461
Constit. of *Aka coralliphagum*. λ_{max} 209; 266; 322 (MeOH) (Berdy).

Chan, J.A. *et al., J. Nat. Prod.*, 1994, **57**, 1543 (*isol, pmr, cmr*)

Corallistin A C-862

[125398-29-0]

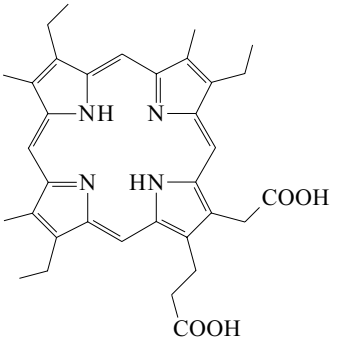


$C_{32}H_{34}N_4O_4$ 538.645
Isol. from a Coral Sea demosponge *Corallistes* sp. Phototherapeutic agent. Rare example of a free porphyrin from a natural organism. λ_{max} 400; 498; 538; 569; 618 (MeOH) (Berdy).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1989, **72**, 1451 (*isol, uv, pmr, cmr, struct*)

Corallistin B C-863

*3-Carboxy-7,12,18-triethyl-8,13,17-trimethyl-21*H,*23*H-*porphine-2-propanoic acid, 9CI*
[151484-69-4]

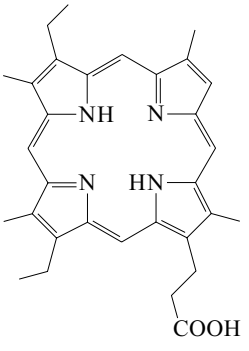


$C_{34}H_{38}N_4O_4$ 566.699
Isol. from the sponge *Corallistes* sp. Red solid (as di-Me ester). Mp 216-218° (di-Me ester). λ_{max} 400 (ϵ 126300); 500 (ϵ 14500); 534 (ϵ 12500); 566 (ϵ 10000); 620 (ϵ 7700) (CH_2Cl_2) (di-Me ester).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1993, **76**, 1489 (*isol, pmr, cmr*)
Pandey, R.K. *et al., Tet. Lett.*, 1994, **35**, 8093 (*synth*)
Pandey, R.K. *et al., ARKIVOC*, 2002, **vi**, 264-278 (*synth, pmr*)

Corallistin C C-864

*12,18-Diethyl-3,8,13,17-tetramethyl-21*H,*23*H-*porphine-2-propanoic acid, 9CI*
[151484-70-7]

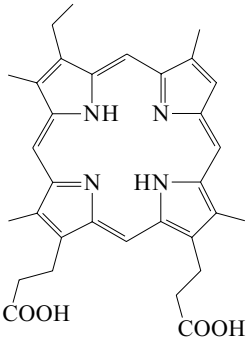


$C_{31}H_{34}N_4O_2$ 494.635
Isol. from the sponge *Corallistes* sp.
Mp 192-194° (as di-Me ester). λ_{max} 399 (ϵ 12000); 496 (ϵ 18900); 530 (ϵ 15900); 566 (ϵ 14100); 618 (ϵ 12380) (CH_2Cl_2) (di-Me ester).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1993, **76**, 1489 (*isol, pmr, cmr*)
Pandey, R.K. *et al., Tet. Lett.*, 1994, **35**, 8093 (*synth*)
Pandey, R.K. *et al., ARKIVOC*, 2002, **vi**, 264-278 (*synth, pmr*)

Corallistin D C-865

*8-Ethyl-3,7,12,17-tetramethyl-21*H,*23*H-*porphine-2,18-dipropanoic acid, 9CI. 3-Ethyldeuteroporphyrin IX*
[151484-71-8]

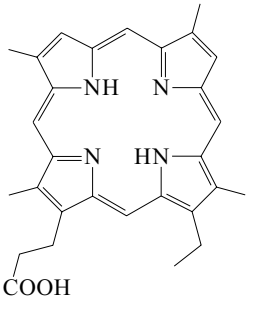


$C_{32}H_{34}N_4O_4$ 538.645
Isol. from the sponge *Corallistes* sp. Isol. as di-Me ester.

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1993, **76**, 1489 (*isol, pmr, cmr*)

Corallistin E C-866

*18-Ethyl-3,7,12,17-tetramethyl-21*H,*23*H-*porphine-2-propanoic acid, 9CI*
[151484-78-5]

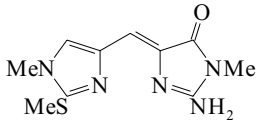


$C_{29}H_{30}N_4O_2$ 466.582
Isol. from the sponge *Corallistes* sp.
Mp 204-206° (as di-Me ester). λ_{max} 398 (ϵ 131100); 496 (ϵ 17300); 530 (ϵ 14100); 564 (ϵ 12700); 618 (ϵ 9900) (CH_2Cl_2) (di-Me ester).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1993, **76**, 1489 (*isol, pmr, cmr*)
Pandey, R.K. *et al., Tet. Lett.*, 1994, **35**, 8093 (*synth*)
Pandey, R.K. *et al., ARKIVOC*, 2002, **vi**, 264-278 (*synth, pmr*)

Corallistine† C-867

[121098-71-3]

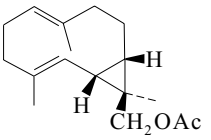


$C_{10}H_{13}N_5OS$ 251.312
Isol. from the New Caledonian sponge *Corallistes fulvodesmus.*
Light yellow cryst. (MeOH).
Mp 192° dec.

Debitus, C. *et al., Tet. Lett.*, 1989, **30**, 1535-1538 (*isol, uv, ir, pmr, cmr, cryst struct*)

Coralloidin B C-868

[105708-64-3]

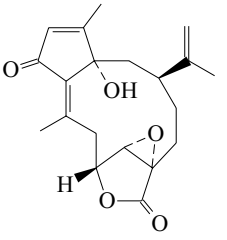


$C_{17}H_{26}O_2$ 262.391
Constit. of *Alcyonium coralloides.* Oil. $[\alpha]_D^{20}$ -33.2 (c, 0.3 in cyclohexane).

Guierriero, A. *et al., J. Nat. Prod.*, 1986, **49**, 608

Coralloidolide C C-869

[125185-54-8]

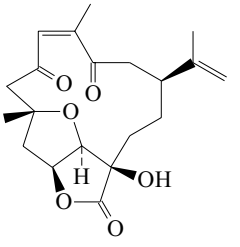


$C_{20}H_{24}O_5$ 344.407
Constit. of *Alcyonium coralloides.* Needles (MeOH).
Mp 266° dec. $[\alpha]_D^{20}$ +3.1 (c, 0.065 in EtOH).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1989, **72**, 1590 (*isol, pmr, cmr*)

Coralloidolide D C-870

[125185-55-9]

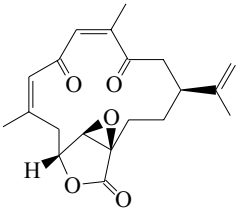


$C_{20}H_{26}O_6$ 362.422
Constit. of *Alcyonium coralloides.* Needles (EtOH).
Mp 209-211°. $[\alpha]_D^{20}$ +41 (c, 0.105 in EtOH).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1989, **72**, 1590 (*isol, pmr, cmr*)
Rowley, M. *et al., J.A.C.S.*, 1989, **111**, 2735 (*synth*)

Coralloidolide E C-871

[125185-56-0]

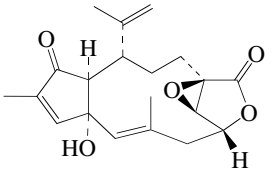


$C_{20}H_{24}O_5$ 344.407
Constit. of *Alcyonium coralloides.* Needles (Me_2CO).
Mp 190-192°. $[\alpha]_D^{20}$ +12.8 (c, 0.21 in Me_2CO).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1989, **72**, 1590 (*isol, pmr, cmr*)

Coralloidolide F C-872

[129622-86-2]

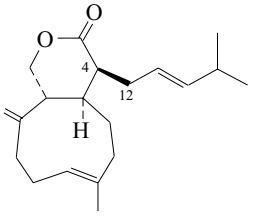


$C_{20}H_{24}O_5$ 344.407
Isol. from the coral *Alcyonium coralloides*.
$[\alpha]_D^{20}$ +76 (c, 0.05 in EtOH). λ_{max} 224 (ϵ 6000) (EtOH).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1990, **73**, 804-807 (*isol, uv, pmr, cmr, ms*)

Coraxeniolide A C-873

[80388-48-3]



$C_{20}H_{30}O_2$ 302.456
Constit. of *Corallium* spp. Cryst. (CH_2Cl_2).
Mp 88-91°. $[\alpha]_D^{25}$ +82 (c, 0.95 in $CHCl_3$). Coraxeniolide D is a semisynthetic prod.

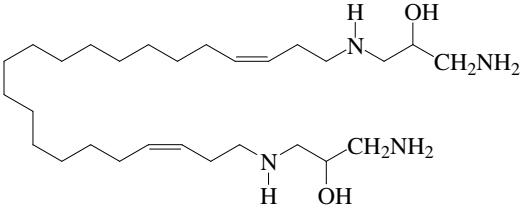
*4,12-Didehydro(*E-*):* ***Coraxeniolide B***
[80388-47-2]
$C_{20}H_{28}O_2$ 300.44
Constit. of *Corallium* spp. Oil. $[\alpha]_D^{27}$ +35 (c, 1.4 in CH_2Cl_2). λ_{max} 270 (ϵ 12000) (MeOH) (Derep).

[80433-13-2]

Schwartz, R.E. *et al., Tetrahedron*, 1981, **37**, 2725

Coriacenine A C-874

[182011-67-2]



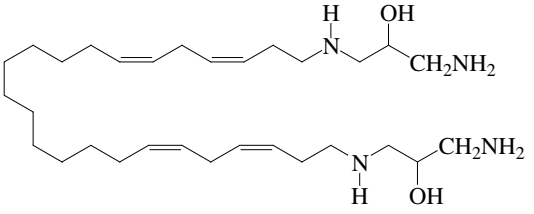
$C_{28}H_{58}N_4O_2$ 482.792
Alkaloid from the sponge *Clathrina coriacea*. Yellow oil (as per-Ac). $[\alpha]_D$ -6.1 (c, 0.24 in $CHCl_3$) (per-Ac).

Didehydro: ***Coriacenine B***
[182265-33-4]
$C_{28}H_{56}N_4O_2$ 480.776
Alkaloid from *Clathrina coriacea*. Yellow oil (as per-Ac). $[\alpha]_D$ -6.3 (c, 0.08 in $CHCl_3$) (per-Ac). Posn. of double bond not known, but is located between the other 2 double bonds.

Casapullo, A. *et al., J.O.C.*, 1996, **61**, 7415-7419

Coriacenine D C-875

[182011-68-3]



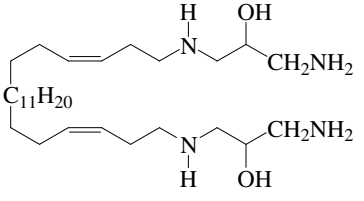
$C_{30}H_{58}N_4O_2$ 506.814
Alkaloid from the sponge *Clathrina coriacea*. Yellow oil (as per-Ac). $[\alpha]_D$ -10 (c, 0.36 in $CHCl_3$).

Dihydro: ***Coriacenine C***
[182149-41-3]
$C_{30}H_{60}N_4O_2$ 508.83
Alkaloid from *Clathrina coriacea*. Yellow oil (as per-Ac). $[\alpha]_D$ -6.2 (c, 0.16 in $CHCl_3$). Posn. of one double bond not determined.

Casapullo, A. *et al., J.O.C.*, 1996, **61**, 7415-7419

Coriacenine E C-876

[182149-43-5]

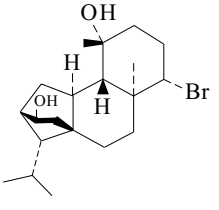


$C_{29}H_{58}N_4O_2$ 494.803
Posn. of one double bond not determined. Alkaloid from the sponge *Clathrina coriacea*. Yellow oil.

Casapullo, A. *et al., J.O.C.*, 1996, **61**, 7415-7419 (*isol, struct*)

Coronopifoliol C-877

[97415-92-4]

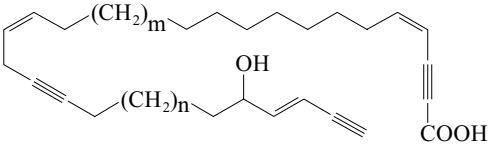


$C_{20}H_{33}BrO_2$ 385.383
Constit. of *Sphaerococcus coronopifolius*. Oil. $[\alpha]_D$ -28.6.

Cafieri, F. *et al., J.O.C.*, 1985, **50**, 3982

Corticatic acid C C-878

[160337-75-7]



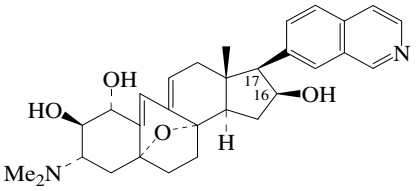
$m + n = 6$

$C_{31}H_{44}O_3$ 464.687

Isol. from the marine sponge *Petrosia corticata*. Antifungal agent. Oil. $[\alpha]_D^{23}$ +7 (c, 0.05 in $CHCl_3$). λ_{max} 226 (ϵ 18900); 238 (ϵ 8700); 245 (ϵ 11500); 255 (ϵ 8700) (MeOH) (Berdy).

Li, H.-Y. *et al., J. Nat. Prod.*, 1994, **57**, 1464 (*isol, pmr*)

Cortistatin B C-879



$C_{30}H_{36}N_2O_4$ 488.625
Alkaloid from the sponge *Corticium simplex*. Anti-angiogenic agent. $[\alpha]_D^{20}$ +15.6 (c, 0.27 in MeOH). λ_{max} 224 (ϵ 44400) (MeOH).

16-Ketone: ***Cortistatin C***
$C_{30}H_{34}N_2O_4$ 486.61
Alkaloid from *Corticium simplex*.
$[\alpha]_D^{20}$ -45 (c, 0.71 in MeOH). λ_{max} 222 (ϵ 49800) (MeOH).

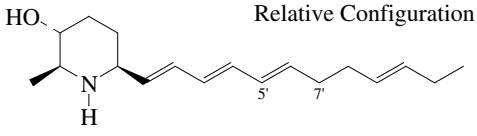
16-Deoxy: ***Cortistatin A***
$C_{30}H_{36}N_2O_3$ 472.626
Alkaloid from *Corticium simplex*.
$[\alpha]_D^{20}$ +30.1 (c, 0.56 in MeOH). λ_{max} 219 (ϵ 45600) (MeOH).

17α-Hydroxy, 16-ketone: ***Cortistatin D***
$C_{30}H_{34}N_2O_5$ 502.609
Alkaloid from *Corticium simplex*.
$[\alpha]_D^{20}$ -37.1 (c, 0.45 in MeOH). λ_{max} 219 (ϵ 48900) (MeOH).

Aoki, S. *et al., J.A.C.S.*, 2006, **128**, 3148-3149 (*isol, pmr, cmr, cryst struct*)

Corydendramine A C-880

6-(1,3,5,9-Dodecatetraenyl)-2-methyl-3-piperidinol
[291764-44-8]



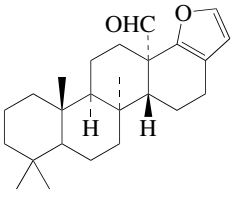
$C_{18}H_{29}NO$ 275.433
Defence compd. isol. from the marine hydroid *Corydendrium parasiticum*. Pale yellow oil. $[\alpha]_D$ -24.3 (c, 0.17 in MeOH). λ_{max} 258 (ϵ 24200); 268 (ϵ 32700); 278 (ϵ 25600) (MeOH).

*7′,8′-Didehydro(*E-*), 5′,6′-dihydro: 6-(1,3,7,9-Dodecatetraenyl)-2-methyl-3-piperidinol.* ***Corydendramine B***
[291764-45-9]
$C_{18}H_{29}NO$ 275.433
Defence compd. isol. from *Corydendrium parasiticum*. Amorph. powder. $[\alpha]_D$ +83.7 (c, 0.08 in MeOH). λ_{max} 236 (ϵ 40400) (MeOH).

Lindquist, N. *et al., J. Nat. Prod.*, 2000, **63**, 1290-1291 (*Corydendramines A,B*)

Coscinafuran C-881

[221012-79-9]

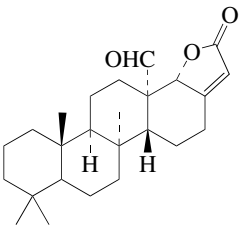


$C_{25}H_{36}O_2$ 368.558
Constit. of *Coscinoderma mathewsi*.

Kimura, J. *et al., Chem. Lett.*, 1999, 61-62 (*isol, pmr, cmr*)

Coscinalactone C-882

[221012-78-8]

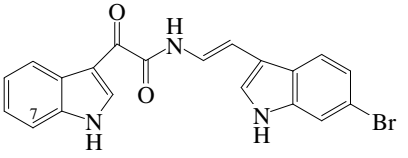


$C_{25}H_{36}O_3$ 384.558
Constit. of *Coscinoderma mathewsi*.

Kimura, J. *et al., Chem. Lett.*, 1999, 61-62 (*isol, pmr, cmr*)

Coscinamide A C-883

[298196-72-2]



$C_{20}H_{14}BrN_3O_2$ 408.254
Isol. from the marine sponge *Coscinoderma* sp. Yellow solid. $[\alpha]_D$ -1.9 (c, 1.3 in MeOH). λ_{max} 207 (log ϵ 4.47); 256 (log ϵ 4.12); 335 (log ϵ 3.96) (MeOH).

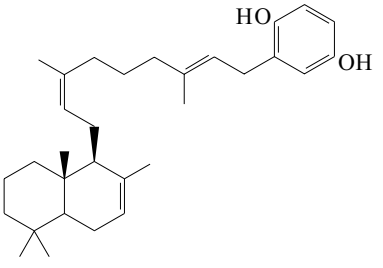
Debromo: ***Coscinamide B***
[298196-73-3]
$C_{20}H_{15}N_3O_2$ 329.357
Isol. from *Coscinoderma* sp. Orange solid.
Mp 228-230° dec. $[\alpha]_D$ +23.6 (c, 0.83 in MeOH). λ_{max} 207 (log ϵ 4.53); 229 (log ϵ 4.29); 267 (log ϵ 4.26); 347 (log ϵ 4.17) (MeOH).

7-Hydroxy: ***Coscinamide C***
[298196-74-4]
$C_{20}H_{14}BrN_3O_3$ 424.253
Isol. from *Coscinoderma* sp. Yellow solid. $[\alpha]_D$ -9.9 (c, 0.14 in MeOH). λ_{max} 213 (log ϵ 4.09); 261 (log ϵ 3.77); 363 (log ϵ 3.6) (MeOH).

Bokesch, H.R. *et al., Tet. Lett.*, 2000, **41**, 6305-6308 (*Coscinamides, isol, pmr, cmr*)
Chakrabarty, M. *et al., Synthesis*, 2003, 2011-2014 (*Coscinamide B, synth*)

Coscinoquinol C-884

[154071-70-2]

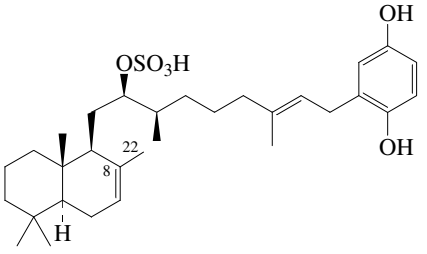


$C_{31}H_{46}O_2$ 450.703
Constit. of a *Coscinoderma* sp. Oil. $[\alpha]_D$ +8.2 (c, 0.27 in $CHCl_3$).

Alea, G.V. *et al., Aust. J. Chem.*, 1994, **47**, 191 (*isol, pmr, cmr*)

Coscinosulfate C-885

[381226-93-3]



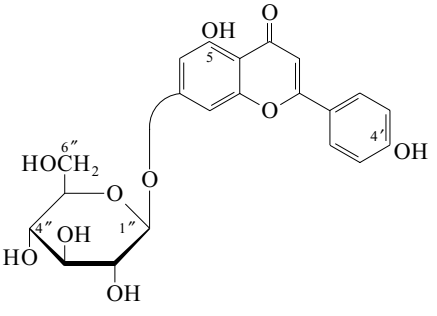
$C_{31}H_{48}O_6S$ 548.783
Constit. of the New Caledonian sponge *Coscinoderma matthewsi*. CDC25 phosphatase inhibitor. Antimitotic agent. Amorph. solid. Mp 129-130°. $[\alpha]_D^{22}$ +5 (c, 1.4 in MeOH).

$\Delta^{8(22)}$-Isomer: [393870-33-2]
$C_{31}H_{48}O_6S$ 548.783
Constit. of *Coscinoderma matthewsi*. Isol. as dimethylguanidine salt.

Loukaci, A. *et al., Bioorg. Med. Chem.*, 2001, **9**, 3049-3054 (*isol, pmr, cmr*)
Poigny, S. *et al., J.O.C.*, 2001, **66**, 7263-7269 (*synth, abs config*)

Cosmosiin C-886

7-O-β-D-Glucopyranosyloxy-4′,5-dihydroxyflavone. Apigenin 7-O-glucoside. Cosmetin. Apigetrin
[578-74-5]



$C_{21}H_{20}O_{10}$ 432.383
Constit. of flowers of *Cosmos bipinnatus, Zinnia elegans* and other plant spp. Anti-HIV agent. Yellow needles (EtOH or Me_2CO). Mp 178° Mp 203° Mp 229-232°. $[\alpha]_D$ -64 (Py). Forms a dihydrate, Mp 218-220°.

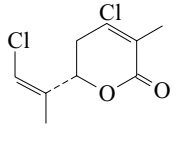
2″-Sulfate: ***Thalassiolin C***
$C_{21}H_{20}O_{13}S$ 512.447
Constit. of the sea grass *Thalassia testudinum*. Inhibitor of HIV integrase. Yellow amorph. solid. $[\alpha]_D$ -54 (c, 0.2 in MeOH). λ_{max} 207 (ε 23400); 268 (ε 12300); 334 (ε 13600) (MeOH).

[36790-49-5, 86546-87-4, 105815-90-5]

Rowley, D.C. *et al., Bioorg. Med. Chem.*, 2002, **10**, 3619-3625 (*Thalassiolin C*)

Costatolide† C-887

[63023-58-5]



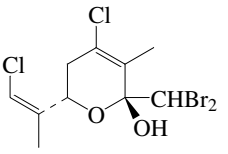
Absolute configuration

$C_9H_{10}Cl_2O_2$ 221.082
Constit. of *Plocamium costatum*. Oil. $[\alpha]_D$ -152 (c, 0.87 in $CHCl_3$). λ_{max} 228 (ε 22200); 284 (ε 22800); 325 (ε 13700) (MeOH) (Derep).

Stierle, D.B. *et al., Tet. Lett.*, 1976, 4455 (*isol, struct*)
Williard, P.G. *et al., J.O.C.*, 1983, **48**, 1123 (*synth*)

Costatone C-888

[63023-59-6]



Absolute Configuration

$C_{10}H_{12}Br_2Cl_2O_2$ 394.917
Constit. of *Plocamium costatum*. Cryst. (hexane). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 70°. $[\alpha]_D$ -52.4 (c, 1 in $CHCl_3$).

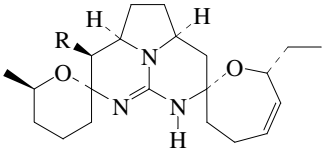
Kazlauskas, R. *et al., Tet. Lett.*, 1976, 4451 (*isol, struct*)
Stierle, D.B. *et al., Tet. Lett.*, 1976, 4455 (*cryst struct*)
Williard, P.G. *et al., Tet. Lett.*, 1984, **25**, 5009 (*synth*)

CPA 1 C-889

Glycoprotein containing 5.6% carbohydrates and consisting of 2 subunits. Isol. from the red alga *Cystoclonium purpureum*. Agglutinin.

Kamiya, H. *et al., J. Nat. Prod.*, 1980, **43**, 136-139 (*isol*)

Crambescidin 359 C-890



Absolute Configuration

R = H

$C_{21}H_{33}N_3O_2$ 359.511
Alkaloid from the sponge *Monanchora unguiculata*. Gum. $[\alpha]_{577}$ -9 (c, 0.18 in CH_2Cl_2).

Braekman, J.C. *et al., J. Nat. Prod.*, 2000, **63**, 193-196
Nagasawa, K. *et al., Org. Lett.*, 2002, **4**, 177-180 (*synth*)
Moore, C.G. *et al., Tet. Lett.*, 2003, **44**, 251-254 (*synth*)
Aron, Z.D. *et al., J.A.C.S.*, 2005, **127**, 3380-3390 (*synth*)

Crambescidin 431 C-891

As Crambescidin 359, C-890 with
R = -COOEt

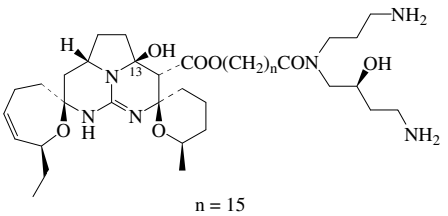
$C_{24}H_{37}N_3O_4$ 431.574
Alkaloid from the sponge *Monanchora unguiculata*. Gum. $[\alpha]_{577}$ +12 (c, 0.19 in CH_2Cl_2).

Parent acid: ***Crambescidin acid***
$C_{22}H_{33}N_3O_4$ 403.52
Alkaloid from *Monanchora unguiculata*.
$[\alpha]_D^{25}$ -19 (c, 0.04 in MeOH). λ_{max} 231 (log ε 3.2); 268 (log ε 2.84) (MeOH).

Braekman, J.C. *et al., J. Nat. Prod.*, 2000, **63**, 193-196 (*Crambescidin 431*)
Meragelman, K.M. *et al., J. Nat. Prod.*, 2004, **67**, 1165-1167 (*Crambescidin acid*)
Aron, Z.D. *et al., J.A.C.S.*, 2005, **127**, 3380-3390 (*synth*)

Crambescidin 816 C-892

[135257-45-3]



Absolute Configuration

n = 15

$C_{45}H_{80}N_6O_7$ 817.163

Alkaloid from the sponges *Crambe crambe* and *Batzella* sp. Possesses antiviral and cytotoxic props. Ca antagonist, ichthyotoxin. Oil. $[\alpha]_D^{25}$ -20.14 (c, 0.4 in MeOH).

13-Deoxy: ***Crambescidin 800***

[135257-46-4]

$C_{45}H_{80}N_6O_6$ 801.164

From the sponges *Crambe crambe* and *Batzella* sp. Possesses antiviral and cytotoxic props. Ichthyotoxin. Oil.

13-Deoxy, 13,14,15-triepimer: ***Isocrambescidin 800***

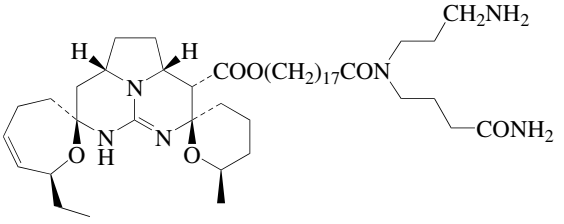
[151121-78-7]

$C_{45}H_{80}N_6O_6$ 801.164

Alkaloid from *Crambe crambe*. Ichthyotoxin. Oil. $[\alpha]_D^{25}$ -48 (c, 0.53 in MeOH).

Jares-Erijman, E.A. *et al., J.O.C.*, 1991, **56**, 5712-5715; 1993, **58**, 4805-4808 (*isol, pmr, cmr, struct, derivs*)
Berlinck, R.G.S. *et al., J. Nat. Prod.*, 1993, **56**, 1007-1015 (*isol*)
Coffey, D.S. *et al., J.A.C.S.*, 1999, **121**, 6944-6945; 2000, **122**, 4893-4903; 4904-4914 (*synth, Isocrambescidin 800*)

Crambescidin 826 C-893



$C_{47}H_{82}N_6O_6$ 827.201

Alkaloid from the sponge *Monanchora* sp. Inhibitor of HIV-1 fusion. Glassy solid. $[\alpha]_D^{20}$ -7.7 (c, 0.09 in MeOH). λ_{max} 207 (log ϵ 4.04); 274 (log ϵ 3.24) (MeOH).

Chang, L.C. *et al., J. Nat. Prod.*, 2003, **66**, 1490-1494 (*isol, pmr, cmr*)

Crambescidin 830 C-894

[135257-47-5]

As Crambescidin 816, C-892 with

n = 16

$C_{46}H_{82}N_6O_7$ 831.19

Alkaloid from the sponge *Crambe crambe*. Possesses antiviral and cytotoxic props. Oil.

Jares-Erijman, E.A. *et al., J.O.C.*, 1991, **56**, 5712 (*isol, pmr, cmr, struct*)

Crambescidin 844 C-895

[135283-73-7]

As Crambescidin 816, C-892 with

n = 17

$C_{47}H_{84}N_6O_7$ 845.217

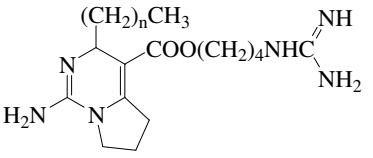
Alkaloid from the sponge *Crambe crambe*. Possesses antiviral and cytotoxic props. Oil. $[\alpha]_D^{25}$ -10.32 (c, 0.19 in MeOH).

Jares-Erijman, E.A. *et al., J.O.C.*, 1991, **56**, 5712 (*isol, pmr, cmr, struct*)

Crambescin A† C-896

Crambine A

[132210-62-9]



n = 10

$C_{24}H_{44}N_6O_2$ 448.651

Major component of bis-guanidine complex where in addition *n* = 9, 11 and 12. Alkaloids from the sponge *Crambe crambe*. Glassy solid. $[\alpha]_D$ +2 (c, 0.7 in MeOH). λ_{max} 204 (ϵ 10600); 286 (ϵ 5500) (MeOH) (Derep).

Lower homologue (n = 4): ***Antibiotic Sch 575948***. *Sch 575948*

$C_{18}H_{32}N_6O_2$ 364.49

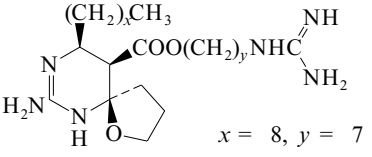
Isol. from the marine sponge *Ptilocaulis spiculifer*. Antibacterial agent.

Berlinck, R.G.S. *et al., Tet. Lett.*, 1990, **31**, 6531-6534 (*isol, pmr, struct*)
Yang, S.W. *et al., J. Antibiot.*, 2003, **56**, 970-972 (*Sch 575948*)

Crambescin B C-897

Crambine B

[132210-63-0]



x = 8, *y* = 7

$C_{25}H_{48}N_6O_3$ 480.693

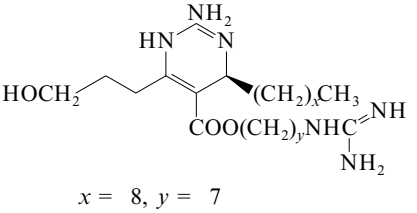
Major component of bis-guanidine complex where in addition *x* + *y* = 14, 16, 17. Struct. revised in 1993; originally descr. as having *x* = 10, *y* = 5. Alkaloids from the sponge *Crambe crambe*. Cytotoxic against L1210 murine leukaemia cells. Cell reaggregation inhibitor. Ichthyotoxin. Glassy solid. $[\alpha]_D$ +52 (c, 0.9 in MeOH).

Berlinck, R.G.S. *et al., Tet. Lett.*, 1990, **31**, 6531 (*isol, pmr*)
Snider, B.B. *et al., J.O.C.*, 1992, **57**, 2526 (*stereochem*)
Jares-Erijman, E.A. *et al., J. Nat. Prod.*, 1993, **56**, 2186 (*isol, pmr, cmr, struct*)

Crambescin C1 C-898

Crambine C1

[142605-06-9]



x = 8, *y* = 7

$C_{25}H_{48}N_6O_3$ 480.693

Major homologue of bis-guanidine complex where in addn. *x* + *y* = 14, 16 and 17. Struct revised in 1993; originally descr. as the compd. with *x* = 10, *y* = 5. Alkaloid from the Mediterranean sponge *Crambe crambe*. Ichthyotoxic agent. Glassy solid. Sol. MeOH, $CHCl_3$. $[\alpha]_{404}$ +13.7 (c, 0.8 in MeOH). λ_{max} 207 (ϵ 4600); 279 (ϵ 2200) (MeOH) (Derep).

Berlinck, R.G.S. *et al., J. Nat. Prod.*, 1992, **55**, 528 (*isol, uv, ir, pmr, cmr, cd*)
Jares-Erijman, E.A. *et al., J. Nat. Prod.*, 1993, **56**, 2186 (*struct*)

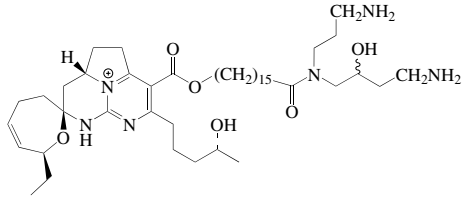
Crambescin C2 C-899

Crambine C2
[142605-07-0]
As Crambescin C1, C-898 with
x + y = 14
$C_{24}H_{46}N_6O_3$ 466.666
Originally descr. as the compd. with x = 10 and y = 4 but this is doubtful in view of the revised struct. of Crambescin C1. Alkaloid from the sponge *Crambe crambe*. Ichthyotoxic agent. Glassy solid. Sol. MeOH, $CHCl_3$. $[\alpha]_D$ -30 (c, 0.2 in MeOH). λ_{max} 204 (ϵ 10600); 286 (ϵ 5500) (MeOH) (Derep). λ_{max} 203 (ϵ 6000); 281 (ϵ 2500) (MeOH) (Berdy).

Berlinck, R.G.S. *et al., J. Nat. Prod.*, 1992, **55**, 528 (*isol, uv, pmr*)
Jares-Erijman, E.A. *et al., J. Nat. Prod.*, 1993, **56**, 2186 (*nomencl*)

Crambidine C-900

[151271-96-4]



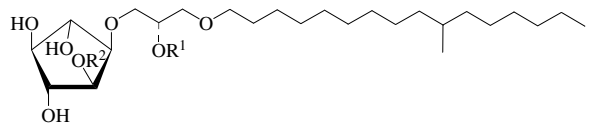
Absolute Configuration

$C_{45}H_{79}N_6O_6^{\oplus}$ 800.156
Alkaloid from the marine sponge *Crambe crambe*. Shows ichthyotoxic props. Glassy solid (as per-Ac, chloride).

Berlinck, R.G.S. *et al., J. Nat. Prod.*, 1993, **56**, 1007-1015 (*isol, uv, pmr, cmr*)
Overman, L.E. *et al., J.A.C.S.*, 2005, **127**, 15652-15658 (*synth, abs config*)

Crasserides C-901

Keruffarides
[146908-95-4]



Crasserides R^1 = Acyl, R^2 = H
Isocrasserides R^1 = H, R^2 = Acyl

A group of cyclitol glycolipid analogues. Keruffarides are considered to be identical with Crasserides. Present in all sponges examined incl. *Aplysina* spp., *Luffariella* sp. and *Pseudoceratina crassa*. It is proposed that these compounds are the distinguishing metabolite of the phylum Porifera. Exhibit fish antifeedant activity.

Tetradecanoylcrasseride [147102-98-5]
$C_{39}H_{76}O_8$ 673.025

Pentadecanoylcrasseride
$C_{40}H_{78}O_8$ 687.051

9-Methyltetradecanoylcrasseride [147102-99-6]
$C_{40}H_{78}O_8$ 687.051

10-Methyltetradecanoylcrasseride
$C_{40}H_{78}O_8$ 687.051

12-Methyltetradecanoylcrasseride [147103-01-3]
$C_{40}H_{78}O_8$ 687.051

13-Methyltetradecanoylcrasseride [147103-00-2]
$C_{40}H_{78}O_8$ 687.051

Hexadecanoylcrasseride
$C_{41}H_{80}O_8$ 701.078

9-Methylpentadecanoylcrasseride
$C_{41}H_{80}O_8$ 701.078

10-Methylpentadecanoylcrasseride
$C_{41}H_{80}O_8$ 701.078

14-Methylpentadecanoylcrasseride [147103-02-4]
$C_{41}H_{80}O_8$ 701.078

10-Methylhexadecanoylcrasseride [147103-03-5]
$C_{42}H_{82}O_8$ 715.105

Tetradecanoylisocrasseride
$C_{39}H_{76}O_8$ 673.025

Pentadecanoylisocrasseride
$C_{40}H_{78}O_8$ 687.051

9-Methyltetradecanoylisocrasseride
$C_{40}H_{78}O_8$ 687.051

10-Methyltetradecanoylisocrasseride
$C_{40}H_{78}O_8$ 687.051

12-Methyltetradecanoylisocrasseride
$C_{40}H_{78}O_8$ 687.051

13-Methyltetradecanoylisocrasseride
$C_{40}H_{78}O_8$ 687.051

Hexadecanoylisocrasseride
$C_{41}H_{80}O_8$ 701.078

9-Methylpentadecanoylisocrasseride
$C_{41}H_{80}O_8$ 701.078

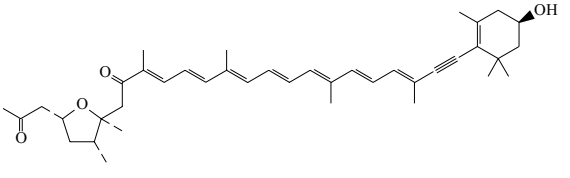
10-Methylpentadecanoylisocrasseride
$C_{41}H_{80}O_8$ 701.078

14-Methylpentadecanoylisocrasseride
$C_{41}H_{80}O_8$ 701.078

10-Methylhexadecanoylisocrasseride
$C_{42}H_{82}O_8$ 715.105

Kobayashi, J. *et al., Chem. Comm.*, 1993, 79
Ishibashi, M *et al., J. Nat. Prod.*, 1993, **56**, 1856 (*isol, pmr*)
Costantino, V. *et al., J.O.C.*, 1993, **58**, 186-191 (*isol, pmr, ms, struct*)
Costantino, V. *et al., J. Nat. Prod.*, 1994, **57**, 1726 (*stereochem*)
Costantino, V. *et al., J. Nat. Prod.*, 2002, **65**, 883-886 (*Isocrasserides*)

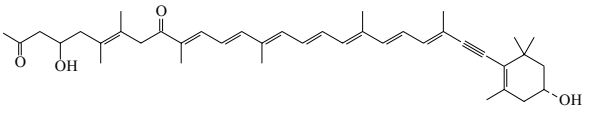
Crassostreaxanthin A C-902



$C_{40}H_{54}O_4$ 598.864
Constit. of *Crassostrea gigas*.

Fujiwara, Y. *et al., Tet. Lett.*, 1992, **33**, 4941-4944 (*isol, pmr, cmr*)

Crassostreaxanthin B C-903

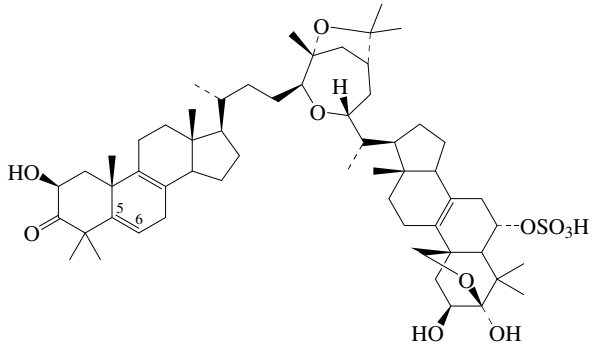


$C_{40}H_{54}O_4$ 598.864
Constit. of *Crassostrea gigas.*

Fujiwara, Y. *et al., Tet. Lett.*, 1992, **34**, 4941-4944 (*isol, pmr, cmr*)
Tode, C. *et al., J.C.S. Perkin 1*, 1999, 1625-1626 (*synth*)
Tode, C. *et al., J.C.S. Perkin 1*, 2001, 3338-3345 (*synth*)

Crellastatin I C-904

[252741-11-0]



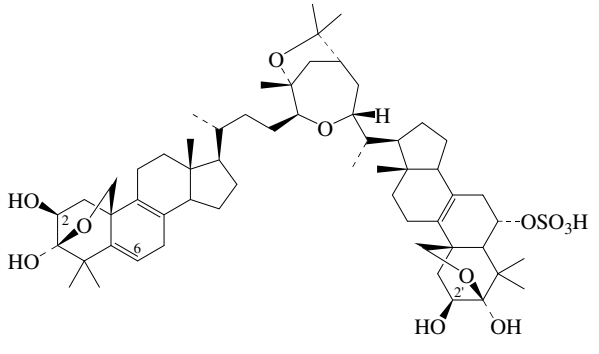
$C_{58}H_{88}O_{11}S$ 993.393
Constit. of a *Crella* sp. Amorph. powder. $[\alpha]_D^{20}$ +40.7 (c, 0.005 in MeOH).

*6α-Hydroxy, 5,6-dihydro, 6-*O*-sulfate:* ***Crellastatin H***
[225235-75-6]
$C_{58}H_{90}O_{15}S_2$ 1091.472
Constit. of a *Crella* sp. Cytotoxic. Amorph. powder. $[\alpha]_D$ +27.8 (c, 0.001 in MeOH).

Zampella, A. *et al., Eur. J. Org. Chem.*, 1999, 949-953 (*Crellastatin H*)
Giannini, C. *et al., Tetrahedron*, 1999, **55**, 13749-13756 (*isol, pmr, cmr*)

Crellastatin A C-905

[214778-08-2]



$C_{58}H_{88}O_{12}S$ 1009.392
Constit. of a *Crella* sp. Amorph. powder. $[\alpha]_D$ +55 (c, 1 in MeOH). λ_{max} 208 (ε 7000) (MeOH).

*5,6-Dihydro, 6α-hydroxy, 6-*O*-sulfate:* ***Crellastatin F***
[225235-73-4]
$C_{58}H_{90}O_{16}S_2$ 1107.471
Constit. of a *Crella* sp. Cytotoxic. Amorph. powder. $[\alpha]_D$ +60.3 (c, 0.001 in MeOH).

2-Deoxy: ***Crellastatin B***
[225235-66-5]
$C_{58}H_{88}O_{11}S$ 993.393
Constit. of a *Crella* sp. Cytotoxic. Amorph. powder. $[\alpha]_D$ +32 (c, 0.001 in MeOH).

2′-Deoxy: ***Crellastatin C***
[225235-68-7]
$C_{58}H_{88}O_{11}S$ 993.393
Constit. of a *Crella* sp. Cytotoxic. Amorph. powder. $[\alpha]_D$ +50.9 (c, 0.001 in MeOH).

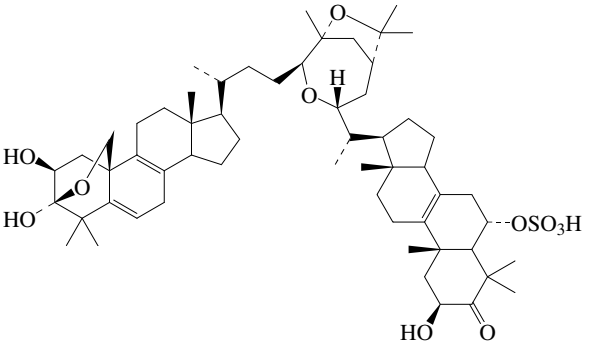
*2′-Deoxy, 5,6-dihydro, 6α-hydroxy, 6-*O*-sulfate:* ***Crellastatin G***
[225235-74-5]
$C_{58}H_{90}O_{15}S_2$ 1091.472
Constit. of a *Crella* sp. Cytotoxic. Amorph. powder. $[\alpha]_D$ +68.7 (c, 0.001 in MeOH).

2,2′-Dideoxy: ***Crellastatin D***
[225235-70-1]
$C_{58}H_{88}O_{10}S$ 977.393
Constit. of a *Crella* sp. Cytotoxic. Amorph. powder. $[\alpha]_D$ +51.6 (c, 0.001 in MeOH).

D'Auria, M.V. *et al., J.O.C.*, 1998, **63**, 7382-7388 (*Crellastatin A*)
Zampella, A. *et al., Eur. J. Org. Chem.*, 1999, 949-953 (*Crellastatins B,C,D,F,G*)

Crellastatin E C-906

[225235-72-3]

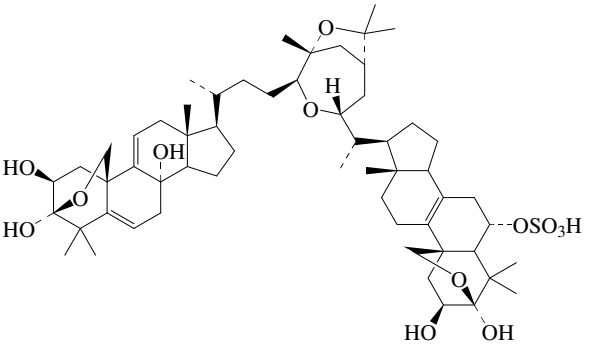


$C_{58}H_{88}O_{11}S$ 993.393
Constit. of a *Crella* sp. Cytotoxic. Amorph. powder. $[\alpha]_D$ +11.4 (c, 0.001 in MeOH).

Zampella, A. *et al., Eur. J. Org. Chem.*, 1999, 949-954 (*isol, pmr, cmr*)

Crellastatin J C-907

[252741-12-1]

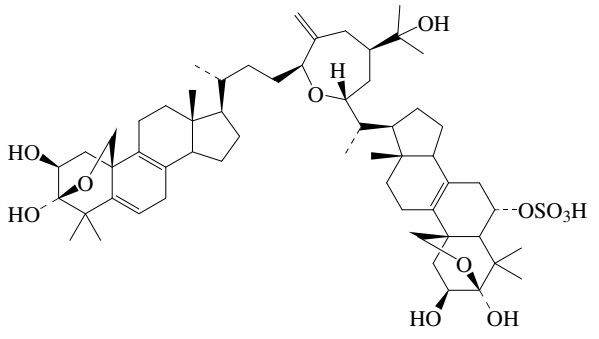


$C_{58}H_{88}O_{13}S$ 1025.391
Constit. of a *Crella* sp. Amorph. powder.

Giannini, C. *et al., Tetrahedron*, 1999, **55**, 13749-13756 (*isol, pmr, cmr*)

Crellastatin K C-908

[252741-13-2]

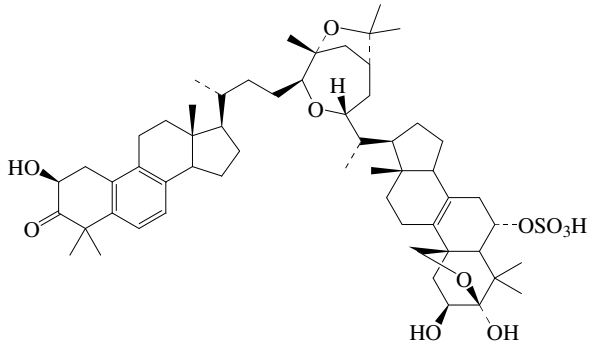


$C_{58}H_{88}O_{12}S$ 1009.392
Constit. of a *Crella* sp. Amorph. powder. $[\alpha]_D^{20}$ +22.3 (c, 0.002 in MeOH).

Giannini, C. *et al., Tetrahedron*, 1999, **55**, 13749-13756 (*isol, pmr, cmr*)

Crellastatin L C-909

[252741-14-3]

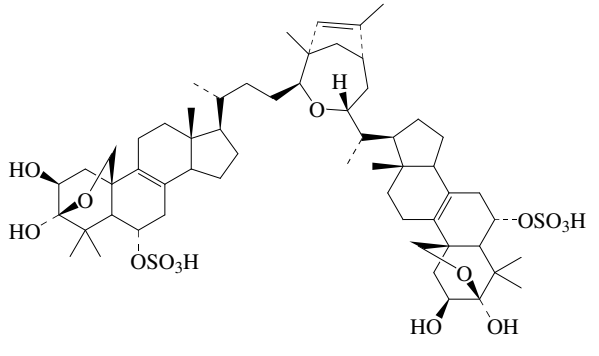


$C_{57}H_{84}O_{11}S$ 977.35
Constit. of a *Crella* sp. Amorph. powder. $[\alpha]_D^{20}$ +6.11 (c, 0.003 in MeOH).

Giannini, C. *et al., Tetrahedron*, 1999, **55**, 13749-13756 (*isol, pmr, cmr*)

Crellastatin M C-910

[252741-15-4]

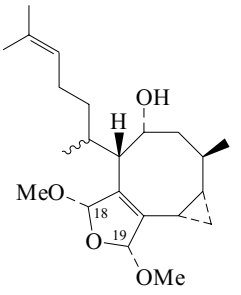


$C_{58}H_{88}O_{15}S_2$ 1089.456
Constit. of a *Crella* sp. Amorph. powder. $[\alpha]_D^{20}$ +48 (c, 0.001 in MeOH).

Giannini, C. *et al., Tetrahedron*, 1999, **55**, 13749-13756 (*isol, pmr, cmr*)

Crenulacetal A C-911

[99798-71-7]



$C_{22}H_{36}O_4$ 364.524
Constit. of *Dictyota dichotoma*. Oil. $[\alpha]_D$ +5.1 (c, 0.4 in $CHCl_3$).

19-Epimer: ***Crenulacetal B***
[99880-99-6]
$C_{22}H_{36}O_4$ 364.524
From *Dictyota dichotoma*. Oil. $[\alpha]_D$ +69.9 (c, 0.33 in $CHCl_3$).

18,19-Diepimer, 4-Ac: ***Crenulacetal C***
[99798-72-8]
$C_{24}H_{38}O_5$ 406.561
From *Dictyota dichotoma*. Oil. $[\alpha]_D$ -6.15 (c, 0.65 in $CHCl_3$).

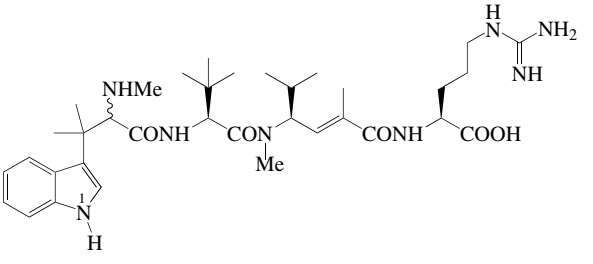
18-Epimer, 4-Ac: ***Crenulacetal D***
[99881-00-2]
$C_{24}H_{38}O_5$ 406.561
From *Dictyota dichotoma*. Oil. $[\alpha]_D$ +14.1 (c, 1.7 in $CHCl_3$).

18,19-Di-de-Me, 4-Ac, stereoisomer: ***Crenuladial***
[118225-54-0]
$C_{22}H_{34}O_5$ 378.508
Metab. of *Dilophus ligulatus*. Oil. $[\alpha]_D$ +27.3 ($CHCl_3$). Diterpenoid antibiotic. Shows antibacterial activity. Config. at 18 and 19 unassigned.

Kusumi, T. *et al., J.O.C.*, 1986, **51**, 384
Tringali, C. *et al., Can. J. Chem.*, 1988, **66**, 2799 (*Crenuladial*)

Criamide A C-912

[169181-26-4]



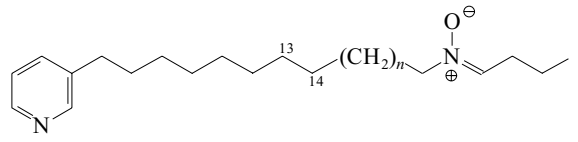
$C_{35}H_{56}N_8O_5$ 668.878
Peptide antibiotic. Isol. from the sponge *Cymbastela* sp. Cytotoxic agent. Microtubule formation inhibitor. Amorph. solid. Sol. MeOH. $[\alpha]_D$ +97 (c, 0.02 in MeOH). Related to Hemiasterlin, H-113.

N^1*-Me:* ***Criamide B***
[169181-27-5]
$C_{36}H_{58}N_8O_5$ 682.905
Isol. from *Cymbastela* sp. Cytotoxic agent. Amorph. solid. Sol. MeOH.

Coleman, J.E. *et al., Tetrahedron*, 1995, **51**, 10653-10662 (*isol, pmr, cmr*)

Cribrochalinamine oxide A C-913

[152273-70-6]



n = 3

$C_{21}H_{36}N_2O$ 332.528
Alkaloid from the marine sponge *Cribrochalina* sp. Shows antifungal activity. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 255 (ϵ 2100); 270 (ϵ 1900) (MeOH) (Derep).

Matsunaga, S. *et al., Tet. Lett.*, 1993, **34**, 5953 (*isol, uv, pmr, cmr, struct*)

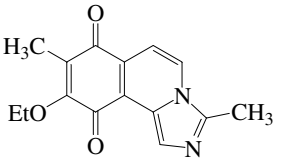
Cribrochalinamine oxide B C-914

[152273-71-7]
As Cribrochalinamine oxide A, C-913 with
n = 5, $\Delta^{13,14}$(*Z*-)
$C_{23}H_{38}N_2O$ 358.566
Alkaloid from the marine sponge *Cribrochalina* sp. H_2O. λ_{max} 255 (ϵ 2100); 270 (ϵ 1900) (MeOH) (Derep). λ_{max} 255 (ϵ 1700); 271 (ϵ 1500) (MeOH) (Berdy).

Matsunaga, S. *et al., Tet. Lett.*, 1993, **34**, 5953 (*isol, uv, pmr, cmr, struct*)

Cribrostatin 6 C-915

[518056-45-6]

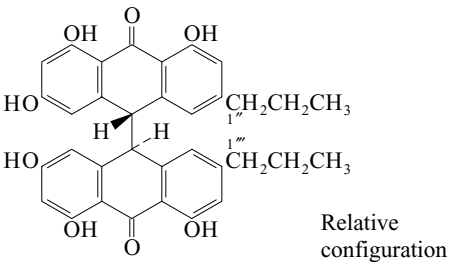


$C_{15}H_{14}N_2O_3$ 270.287
Isol. from the marine sponge *Cribrochalina* sp. Cancer cell growth inhibitor. Antibacterial agent. Dark blue needles (Me_2CO).
Mp 169-171°. λ_{max} 203 (ϵ 26760); 266 (ϵ 24430); 323 (ϵ 5600); 552 (ϵ 1480) (no solvent reported).

Pettit, G.R. *et al., J. Nat. Prod.*, 2003, **66**, 544-547 (*isol, uv, pmr, cmr, ms, cryst struct*)
Nakahara, S. *et al., Heterocycles*, 2004, **63**, 2355-2362; 2006, **68**, 515-520 (*synth, pmr, cmr*)
Pettit, R.K. *et al., J. Med. Microbiol.*, 2004, **53**, 61-65 (*activity*)

Crinemodin bianthrone C-916

*2,2′,4,4′,5,5′-Hexahydroxy-7,7′-dipropyl-[9,9′-bianthracene]-10,10′(9*H*,9′*H*)-dione, 9CI*
[97888-13-6]



Relative configuration

$C_{34}H_{30}O_8$ 566.606
Constit. of the crinoid *Lamprometra palmata gyges*. Yellow microneedles (toluene/EtOAc).
Mp 234-235° dec. $[\alpha]_{579}$ -14 (c, 0.1 in Me_2CO). λ_{max} 277 (log ϵ 4.31); 361 (log ϵ 4.42) (MeOH).

1″-Hydroxy: ***Crinemodin-rhodoptilometrin bianthrone***
[97888-15-8]
$C_{34}H_{30}O_9$ 582.606
Constit. of *Lamprometra palmata gyges*. Yellow microcryst. (toluene/EtOAc).
Mp 190-193° dec. Stereochem. not defined. λ_{max} 277 (log ϵ 4.24); 361 (log ϵ 4.39) (MeOH).

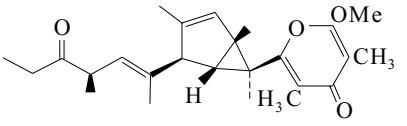
1″,1‴-Dihydroxy: ***Rhodoptilometrin bianthrone***
[97888-14-7]
$C_{34}H_{30}O_{10}$ 598.605
Constit. of *Lamprometra palmata gyges*. Cryst. (toluene/EtOAc).
Mp 195-200° dec. Stereochem. not defined. λ_{max} 277 (log ϵ 4.24); 361 (log ϵ 4.41) (MeOH).

[97948-90-8]

Rideout, J.A. *et al., Aust. J. Chem.*, 1985, **38**, 793-808 (*isol, synth, uv, ir, pmr*)

Crispatene C-917

[79495-60-6]

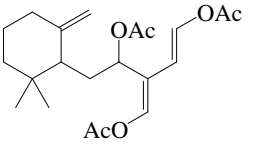


$C_{25}H_{34}O_4$ 398.541
Constit. of *Elysia crispata* (formerly *Tridachia crispata*). Cytotoxic. Oil. Sol. MeOH, Me_2CO, Et_2O, $CHCl_3$; poorly sol. H_2O.
$[\alpha]_D$ -92.8 (c, 0.12 in $CHCl_3$). λ_{max} 256 (ϵ 5700) (MeOH) (Berdy).

Ireland, C. *et al., Tetrahedron, Suppl.*, No. 1, 1981, **37**, 233-240 (*isol*)
Ksebati, M.B. *et al., J.O.C.*, 1985, **50**, 5637-5642 (*isol*)
Miller, A.K. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2004, **101**, 12019-12023 (*synth, pmr, cmr*)

Crispatenine C-918

[194224-62-9]

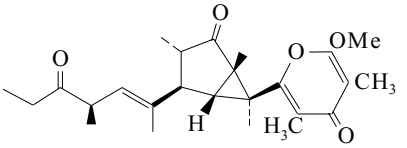


$C_{21}H_{30}O_6$ 378.464
Constit. of *Laurencia viridis*. Oil. $[\alpha]_D$ +5 (c, 2.1 in $CHCl_3$). λ_{max} 246 (ϵ 15800) (no solvent reported).

Gavagnin, M. *et al., Nat. Prod. Lett.*, 1997, **10**, 151-156 (*isol, pmr, cmr*)

Crispatone C-919

[70117-21-4]



$C_{25}H_{34}O_5$ 414.541
Constit. of *Tridachia crispata*. Cytotoxic agent, ichthyotoxin. Cryst. (hexane). Sol. MeOH, Et_2O, $CHCl_3$, Me_2CO; poorly sol. H_2O.
Mp 164.5-166.5°. $[\alpha]_D$ -84.7 (c, 0.03 in $CHCl_3$). λ_{max} 253 (ϵ 6000) (MeOH) (Derep). λ_{max} 257 (ϵ 5800) (MeOH) (Berdy).

Ireland, C. *et al., J.A.C.S.*, 1979, **101**, 1275-1276 (*isol*)
Ireland, C. *et al., Tetrahedron, Suppl.*, No. 1, 1981, 223 (*cryst struct*)
Ksebati, M.B. *et al., J.O.C.*, 1985, **50**, 5637

Crustacean cardioactive peptide C-920

CCAP. CAP_{2a}. Cama-CCAP. Manduca CCAP
[107090-96-0]
H-Pro-Phe-Cys-Asn-Ala-Phe-Thr-Gly-Cys-NH_2
$C_{42}H_{57}N_{11}O_{11}S_2$ 956.111

Peptide. Reduced form shown. Isol. from the pericardial organs of the shore crab *Carcinus maenas*. Also obt. from the moth *Manduca sexta*, the mealworm *Tenebrio molitor*, the southern armyworm *Spodoptera eridania*, the stick insect *Carausius morosus* and the fruitfly *Drosophila melanogaster*.

[145874-64-2]

Stangier, J. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1987, **84**, 575-579 (*isol, Carcinus constit, synth*)
Cheung, C.C. *et al., FEBS Lett.*, 1992, **313**, 165-168 (*isol, Manduca constit*)
Furuya, K. *et al., Biol. Chem. Hoppe-Seyler*, 1993, **374**, 1065-1074 (*isol, Tenebrio constit, Spodoptera constit*)
Lehman, H.K. *et al., Peptides (Pergamon)*, 1993, **14**, 735-741 (*isol, Manduca constit, struct*)
Predel, R. *et al., Eur. J. Entomol.*, 1999, **96**, 275-278 (*isol, Carausius constit*)
Broeck, J.V. *et al., Peptides (N.Y.)*, 2001, **23**, 241-254 (*isol, Drosophila constit*)

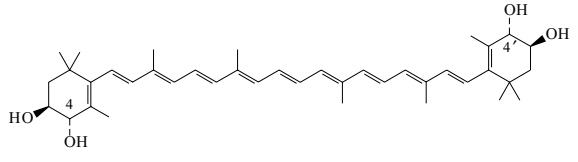
Crustacean hyperglycaemic hormone C-921

Peptide containing 72 amino acid residues and 6 disulfide bonds. Present in the haemolymph of crabs (e.g. *Carcinus maenas*), crayfish (e.g. *Orconectes limosus*) and lobsters (e.g. *Homarus americanus*). Neuropeptide involved in the regulation of haemolymph glucose.

De Kleijn, D.P.V. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1995, **112**, 573-579 (*rev*)
Soyez, D. *et al., Ann. N.Y. Acad. Sci.*, 1997, **814**, 319-323 (*rev*)
Chang, E.S. *et al., Am. Zool.*, 2001, **41**, 380-382 (*rev*)

Crustaxanthin C-922

β,β-Carotene-3,3′,4,4′-tetrol
[6094-35-5]



$C_{40}H_{56}O_4$ 600.88

Abs. config. of natural compd. uncertain; *cis,cis*- and *trans,trans*-isomers have been synthesized. Isol. from the crustacean *Arctodiaptomus salinus*, also from the copepod *Euchaeta russelli* and in aplanospores of *Haematococcus pluvialis* and fish skins. Mp 172-173°.

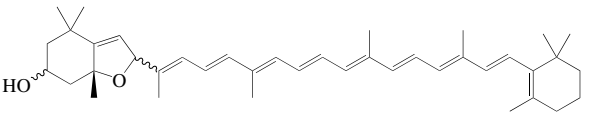
4,4′-Diketone: See Astaxanthin, A-721

Tetraketone: ***Astacene***. *β,β-Carotene-3,3′,4,4′-tetrone. Astacin. Euglenarhodone*
[514-76-1]
$C_{40}H_{48}O_4$ 592.817
Found in fish, crustaceans, bacteria (*Mycobacterium laticolum*) and algae (*Euglena*). Purple-red cryst. (Py).
Mp 243°.

Bodea, C. *et al., Annalen*, 1963, **666**, 189 (*ir*)
Bartlett, L. *et al., J.C.S.(C)*, 1969, 2527 (*ord*)
Andrewes, A.G. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 730 (*synth, struct, uv*)
Kienzle, F. *et al., Helv. Chim. Acta*, 1975, **58**, 198 (*derivs*)
Englert, G. *et al., Helv. Chim. Acta*, 1975, **58**, 2367; 1977, **60**, 1209 (*cmr, pmr*)
Cooper, R.D.G. *et al., J.C.S. Perkin 1*, 1975, 2195 (*synth*)
Andrewes, A.G. *et al., Phytochemistry*, 1976, **15**, 1003 (*biosynth*)
Hall, E.A.H. *et al., Chem. Comm.*, 1978, 387
Widmer, E. *et al., Helv. Chim. Acta*, 1981, **64**, 2405; 1982, **65**, 671 (*synth*)
Bandaranayake, W.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **72**, 409; *CA*, **98**, 14534n (*isol*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 197; 398; 406 (*bibl*)
Buschor, D.J. *et al., Helv. Chim. Acta*, 1990, **73**, 1002 (*synth, pmr, cmr, cd, uv*)
Choi, S. *et al., J.O.C.*, 2005, **70**, 3328-3331 (*synth*)

Cryptoflavin C-923

5,8-Epoxy-5,8-dihydro-β,β-caroten-3-ol
[30311-63-8]

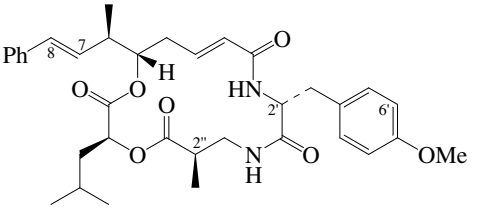


$C_{40}H_{56}O_2$ 568.881
Prod. by acid isom. of Violaxanthin (Violaxanthin, V-52). Constit. of persimmon (*Diospyros kaki*), star fruit (*Averrhoa carambola*), orange (*Citrus sinensis*) and alfalfa (*Medicago*) spp. Poss. isol. from peach (*Prunus persica*). Red cryst. (MeOH).
Mp 171° Mp 177° (sealed tube). Natural occurrence poorly document, poss. artifact. λ_{max} 459; 490 (CS_2). λ_{max} 439; 470 (C_6H_6).

Ignasiak, T. *et al., Biochem. Syst. Ecol.*, 1973, **1**, 97; 1975, **2**, 177 (*isol*)
Ebert, G. *et al., Helv. Chim. Acta*, 1985, **24**, 29 (*isol*)

Cryptophycin 4 C-924

Cryptophycin D
[155645-51-5]



$C_{35}H_{44}N_2O_7$ 604.742

Depsipeptide antibiotic. Prod. by *Nostoc* sp. GSV 224. Cytotoxic agent. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{25}$ +36.7 (c, 1.9 in MeOH). λ_{max} 206 (ϵ 41800); 228 (ϵ 25000); 240 (ϵ 21200); 248 (ϵ 22500); 280 (ϵ 3000); 290 (ϵ 1230) (MeOH) (Derep). λ_{max} 204 (ϵ 34500); 228 (ϵ 16600); 250 (ϵ 14700); 282 (ϵ 2000) (neutral solvent not reported) (Derep).

O-*De-Me:* ***Cryptophycin 43***
[162473-78-1]
$C_{34}H_{42}N_2O_7$ 590.715
$[\alpha]_D$ +20 (c, 0.2 in $CHCl_3$). λ_{max} 250 (ϵ 20150); 282 (ϵ 4080); 294 (ϵ 1730) ($CHCl_3$). λ_{max} 250 (ϵ 20512); 282 (ϵ 4053); 294 (ϵ 1734) (MeOH) (Berdy).

*7*R,*8*R-*Epoxide:* ***Cryptophycin 2***. *Cryptophycin B*
[155645-50-4]
$C_{35}H_{44}N_2O_8$ 620.741
Prod. by *Nostoc* sp. GSV 224. Cytotoxic agent. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{25}$ +20.4 (c, 0.5 in MeOH). λ_{max} 206 (ϵ 43800); 218 (ϵ 37500); 232 (ϵ 22900); 278 (ϵ 2410) (MeOH) (Derep).

6′-Chloro: ***Cryptophycin 3***. *Cryptophycin C*
[124689-64-1]
$C_{35}H_{43}ClN_2O_7$ 639.187
Prod. by *Nostoc* sp. GSV 224. Cytotoxic agent. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{25}$ +20.3 (c, 1.1 in MeOH). λ_{max} 206 (ϵ 51700); 218 (ϵ 31200); 230 (ϵ 22900); 246 (ϵ 18800); 280 (ϵ 3230) (MeOH) (Derep).

6′-Chloro, O-*de-Me:* ***Cryptophycin 17***
[171674-91-2]
$C_{34}H_{41}ClN_2O_7$ 625.16
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +27.8 (c, 0.37 in $CHCl_3$). λ_{max} 208 (ϵ 55100); 232 (ϵ 21700); 248 (ϵ 21800); 282 (ϵ 3200) (MeOH).

*6′-Chloro, 7*R,*8*R-*epoxide:* ***Cryptophycin 1***. *Cryptophycin A*
[124689-65-2]
$C_{35}H_{43}ClN_2O_8$ 655.186
Prod. by *Nostoc* sp. GSV 224. Cytotoxic agent. $[\alpha]_D^{25}$ +33.8 (c, 1.8 in MeOH). λ_{max} 208 (ϵ 42400); 218 (ϵ 33700); 228 (ϵ 23800); 280 (ϵ 2210) (MeOH) (Derep).

*6′-Chloro, 7*R*,8*R*-epoxide,* O*-de-Me:* ***Cryptophycin 16***
[169181-93-5]
$C_{34}H_{41}ClN_2O_8$ 641.159
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +41.3 (c, 5.2 in MeOH). λ_{max} 206 (ϵ 38300); 218 (ϵ 28200); 248 (ϵ 2950); 282 (ϵ 1820) (MeOH).

*6′-Chloro, 7*R*,8*R *epoxide, 2′′-Me: Cryptophycin 52. LY 355703*
[186256-68-8]
$C_{36}H_{45}ClN_2O_8$ 669.213
Antimitotic, antitumour agent. Solid. $[\alpha]_D$ +19.9 (c, 0.5 in $CHCl_3$). Synthetic.

6′-Chloro, 3α-hydroxy, 2,3-dihydro: ***Cryptophycin 30***
[168569-18-4]
$C_{35}H_{45}ClN_2O_8$ 657.202
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ -12.3 (c, 1.53 in $CHCl_3$). λ_{max} 204 (ϵ 51100); 232 (ϵ 15500); 252 (ϵ 17300); 280 (ϵ 3200) (MeOH) (Berdy).

6′,8′-Dichloro: ***Cryptophycin 175***
[186593-83-9]
$C_{35}H_{42}Cl_2N_2O_7$ 673.631
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +32.8 (c, 0.81 in $CHCl_3$). λ_{max} 208 (ϵ 84800); 210 (ϵ 78700); 228 (sh) (no solvent reported).

6′,8′-Dichloro, O*-de-Me:* ***Cryptophycin 45***
[168569-19-5]
$C_{34}H_{40}Cl_2N_2O_7$ 659.605
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +72 (c, 0.2 in MeOH). λ_{max} 250 (ϵ 25500); 284 (ϵ 5300) ($CHCl_3$). λ_{max} 250 (ϵ 25500); 284 (ϵ 5300) (MeOH) (Berdy).

*6′,8′-Dichloro, 7*R*,8*R*-epoxide:* ***Cryptophycin 31***
[171674-92-3]
$C_{35}H_{42}Cl_2N_2O_8$ 689.631
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +50.6 (c, 1.13 in MeOH). λ_{max} 206 (ϵ 45500); 220 (ϵ 28300); 280 (ϵ 600) (MeOH).

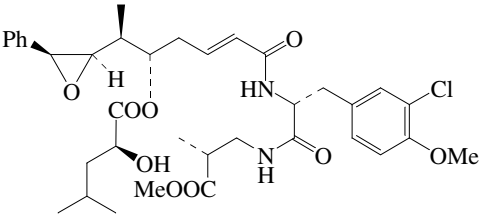
*6′,8′-Dichloro, 7*R*,8*R*-epoxide,* O*-de-Me:* ***Cryptophycin 23***
[168569-16-2]
$C_{34}H_{40}Cl_2N_2O_8$ 675.604
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +47 (c, 1.55 in MeOH). λ_{max} 208 (ϵ 44200); 252 (ϵ 3530); 290 (ϵ 1860) (MeOH).

2′-Epimer, 6′-chloro: ***Cryptophycin 46***
[162679-35-8]
$C_{35}H_{43}ClN_2O_7$ 639.187
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ -62.1 (c, 0.66 in $CHCl_3$).

Trimurtulu, G. *et al., J.A.C.S.*, 1994, **116**, 4729-4737 (*isol, uv, ir, cd, pmr, cmr*)
Barrow, R.A. *et al., J.A.C.S.*, 1995, **117**, 2479 (*synth, struct*)
Golatoki, T. *et al., J.A.C.S.*, 1995, **117**, 12030-12049 (*isol, uv, ir, pmr, cmr, ms*)
De Muys, J.M. *et al., Bioorg. Med. Chem. Lett.*, 1996, **6**, 1111 (*synth*)
Rej, R. *et al., J.O.C.*, 1996, **61**, 6289 (*synth*)
Salamonczyk, G.M. *et al., J.O.C.*, 1996, **61**, 6893 (*synth*)
Pat. Coop. Treaty (WIPO), 1996, (*Univ. Hawaii*)96 40 184; *CA*, **126**, 118201q (*Cryptophycin 52, synth, isomers, pharmacol*)
Subbaraju, G.V. *et al., J. Nat. Prod.*, 1997, **60**, 302-305 (*Cryptophycin 46, Cryptophycin 175*)
Wagner, M.M. *et al., Cancer Chemother. Pharmacol.*, 1999, **43**, 115-125 (*Cryptophycin 52, pharmacol*)
Patel, V.F. *et al., J. Med. Chem.*, 1999, **42**, 2588-2563 (*Cryptophycin 52, synth*)
White, J.D. *et al., J.O.C.*, 1999, **64**, 6206-6216 (*synth*)
Liang, J. *et al., J.O.C.*, 2000, **65**, 3143-3147 (*Cryptophycin 52, synth*)
Stevenson, J.P. *et al., Clin. Cancer Res.*, 2002, **8**, 2524-2529 (*Cryptophycin 52, pharmacol*)
Li, L.-H. *et al., Org. Lett.*, 2002, **4**, 1637-1640 (*synth*)
Tius, M.A. *et al., Tetrahedron*, 2002, **58**, 4343-4367 (*rev, synth*)
Ghosh, A.K. *et al., J.O.C.*, 2003, **68**, 9823-9826 (*Cryptophycin 52, synth*)
Ghosh, A.K. *et al., Eur. J. Org. Chem.*, 2004, 2131-2141 (*Cryptophycin 2, synth*)
Danner, P. *et al., Eur. J. Org. Chem.*, 2005, 3317-325 (*Cryptophycin 3, synth*)

Cryptophycin 5 C-925

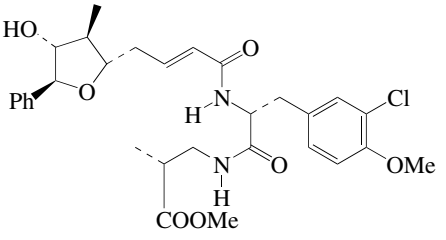
Cryptophycin E methyl ester
[125546-14-7]
[155486-20-7]



$C_{36}H_{47}ClN_2O_9$ 687.228
Peptide antibiotic. Artifact. Prod. by *Nostoc* sp. (GSV 224; ATCC55483). Cytotoxic agent. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D$ +36 (c, 0.55 in MeOH). λ_{max} 206 (ϵ 45600); 218 (ϵ 37700); 280 (ϵ 3790); 286 (ϵ 3480); 325 (ϵ 2080) (MeOH) (Derep).
Golakoti, T. *et al., J.A.C.S.*, 1995, **117**, 12030-12049 (*struct*)

Cryptophycin 6 C-926

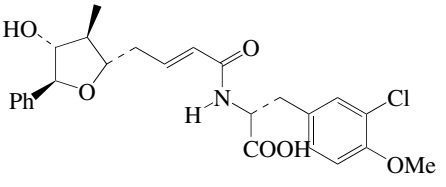
Cryptophycin F methyl ester
[168482-34-6]
[155379-98-9]



$C_{30}H_{37}ClN_2O_7$ 573.084
Peptide antibiotic. Artifact. Prod. by *Nostoc* sp. GSV 224. Cytotoxic agent. $[\alpha]_D^{25}$ +17.1 (c, 1.1 in MeOH).
Golakoti, T. *et al., J.A.C.S.*, 1995, **117**, 12030-12049 (*struct*)

Cryptophycin 7 C-927

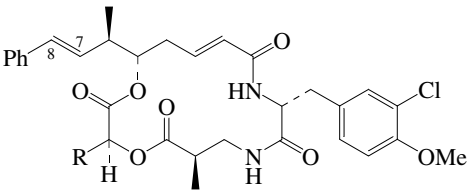
Cryptophycin G
[168482-35-7]
[155645-53-7]



$C_{25}H_{28}ClNO_6$ 473.952
Peptide antibiotic. Artifact. Prod. by *Nostoc* sp. GSV 224. Cytotoxic agent. $[\alpha]_D^{25}$ -51.9 (c, 0.9 in MeOH). λ_{max} 206 (ϵ 23400); 220 (ϵ 14900); 282 (ϵ 1670) (MeOH).
Golakoti, T. *et al., J.A.C.S.*, 1995, **117**, 12030-12049 (*struct*)

Cryptophycin 18 C-928

[168569-14-0]



R = -CH(CH$_3$)CH$_2$CH$_3$

$C_{35}H_{43}ClN_2O_7$ 639.187
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +54.9 (c, 0.93 in MeOH). λ_{max} 208 (ϵ 59000); 228 (ϵ 30100); 248 (ϵ 27000); 280 (ϵ 4150) (MeOH).

7β,8β-Epoxide: ***Cryptophycin 54***
[168569-20-8]
$C_{35}H_{43}ClN_2O_8$ 655.186
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +20.7 (c, 0.73 in MeOH). λ_{max} 204 (ϵ 37730); 218 (ϵ 24660); 234 (ϵ 11950); 284 (ϵ 1980) (MeOH).

Golakoti, T. *et al., J.A.C.S.*, 1995, **117**, 12030-12049 (*isol, uv, ir, pmr, cmr, ms*)

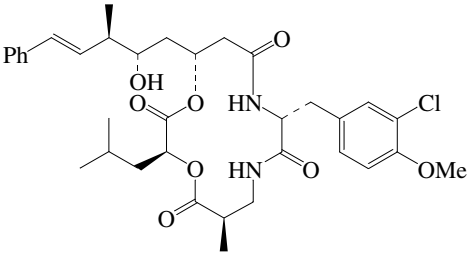
Cryptophycin 19 C-929

[168482-37-9]
As Cryptophycin 18, C-928 with
R = CH(CH$_3$)$_2$
$C_{34}H_{41}ClN_2O_7$ 625.16
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +62.6 (c, 0.67 in MeOH). λ_{max} 204 (ϵ 44900); 230 (ϵ 17000); 248 (ϵ 15600); 280 (ϵ 2500) (MeOH).

Golakoti, T. *et al., J.A.C.S.*, 1995, **117**, 12030-12049 (*isol, uv, ir, pmr, cmr, ms*)

Cryptophycin 26 C-930

[168482-38-0]

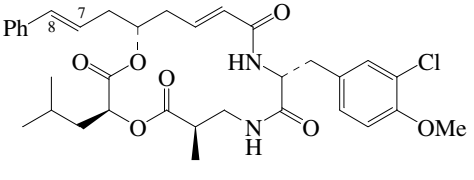


$C_{35}H_{45}ClN_2O_8$ 657.202
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +28.2 (c, 1.31 in $CHCl_3$). λ_{max} 206 (ϵ 40200); 232 (ϵ 13700); 252 (ϵ 16400); 282 (ϵ 3540) (MeOH).

Golakoti, T. *et al., J.A.C.S.*, 1995, **117**, 12030-12049 (*isol, uv, ir, pmr, cmr, ms*)

Cryptophycin 28 C-931

[168482-39-1]



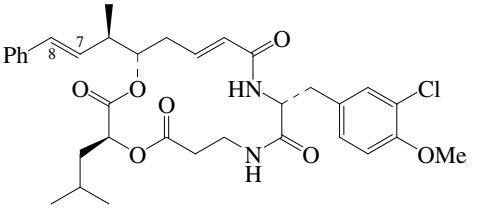
$C_{34}H_{41}ClN_2O_7$ 625.16
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +65.6 (c, 0.93 in MeOH). λ_{max} 204 (ϵ 48000); 230 (ϵ 19300); 248 (ϵ 18700); 280 (ϵ 3400) (MeOH).

7β,8β-Epoxide: ***Cryptophycin 40***
[168482-41-5]
$C_{34}H_{41}ClN_2O_8$ 641.159
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +41.6 (c, 0.31 in $CHCl_3$). λ_{max} 242 (ϵ 4970); 266 (ϵ 3910); 274 (ϵ 3670); 286 (ϵ 3560); 328 (ϵ 510) (MeOH).

Golakoti, T. *et al., J.A.C.S.*, 1995, **117**, 12030-12049 (*isol, uv, ir, pmr, cmr, ms*)

Cryptophycin 29 C-932

[168569-17-3]



$C_{34}H_{41}ClN_2O_7$ 625.16
Prod. by *Nostoc* sp. ATCC 53789.
$[\alpha]_D$ +22.2 (c, 1.13 in $CHCl_3$). λ_{max} 204 (ϵ 45600); 230 (ϵ 17200); 248 (ϵ 16500); 280 (ϵ 2600) (MeOH).

*7*R*,8*R*-Epoxide:* ***Cryptophycin 21***
[168569-15-1]
$C_{34}H_{41}ClN_2O_8$ 641.159
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +40.2 (c, 0.72 in $CHCl_3$). λ_{max} 204 (ϵ 44190); 218 (ϵ 32320); 244 (ϵ 5190); 284 (ϵ 1630) (MeOH).

*7*R*,8*R*-Epoxide,* O*-de-Me:* ***Cryptophycin 176***
[186593-86-2]
$C_{33}H_{39}ClN_2O_8$ 627.132
Prod. by *Nostoc* sp. ATCC 53789.
$[\alpha]_D$ +40.5 (c, 0.38 in MeOH). λ_{max} 206 (39900); 220 (sh) (26600); 282 (MeOH).

*Dechloro, 7*R*,8*R*-epoxide:* ***Arenastatin A***. *Cryptophycin 24*
[162600-54-6]
[162473-79-2]
$C_{34}H_{42}N_2O_8$ 606.714
Constit. of the marine sponge *Dysidea arenaria* and of the alga *Nostoc* sp. ATCC 53789. Cytotoxic and antimitotic agent. Microtubule assembly inhibitor. Shows selective antifungal activity. Amorph. solid. Sol. MeOH, EtOAc, Me_2CO; poorly sol. hexane. $[\alpha]_D$ +19 (c, 0.1 in MeOH). $[\alpha]_D$ +48.8 (c, 0.63 in $CHCl_3$). λ_{max} 230 (ϵ 12500); 270 (ϵ 2400); 285 (ϵ 1900) (MeOH) (Berdy). λ_{max} 228 (ϵ 19000); 242 (ϵ 8250); 274 (ϵ 2350) ($CHCl_3$).

*5′-Chloro, 7*R*,8*R*-epoxide:* ***Cryptophycin 326***
[741730-84-7]
$C_{34}H_{40}Cl_2N_2O_8$ 675.604
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +9 (c, 0.4 in $CHCl_3$). λ_{max} 208 (ϵ 39660); 218 (ϵ 25255); 280 (ϵ 1370) (MeOH).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 2196-2198; 2394-2396; 1995, **43**, 1598-1600 (*Arenastatin A, pmr, cmr, struct, abs config, synth*)
Golakoti, T. *et al., J.A.C.S.*, 1995, **117**, 12030-12049 (*Arenastatin A, Cryptophycins, isol, uv, ir, pmr, cmr, ms*)
De Muys, J.M. *et al., Bioorg. Med. Chem. Lett.*, 1996, **6**, 1111-1116 (*synth*)
Koiso, Y. *et al., Chem. Biol. Interact.*, 1996, **102**, 183-191 (*Arenastatin A, activity*)
Subbaraju, G.V. *et al., J. Nat. Prod.*, 1997, **60**, 302-305 (*Cryptophycin 176*)
Iwasaki, S. *et al., Yakugaku Zasshi*, 1998, **118**, 111-126 (*rev, Arenastatin A, activity*)
White, J.D. *et al., J.O.C.*, 1999, **64**, 6206-6216 (*synth*)
Eggen, M. *et al., J.O.C.*, 2000, **65**, 7792-7799 (*synth*)
Vidya, R. *et al., J.O.C.*, 2003, **68**, 9687-9693 (*synth*)
Ghosh, A.K. *et al., Eur. J. Org. Chem.*, 2004, 2131-2141 (*synth, pmr, cmr*)
Chaganty, S. *et al., J. Nat. Prod.*, 2004, **67**, 1403-1406 (*Cryptophycin 326*)
Tripathy, N.K. *et al., Tet. Lett.*, 2004, **45**, 5309-5311 (*Arenastatin A, synth*)

Cryptophycin 49 C-933

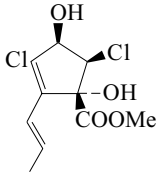
[168482-42-6]
As Cryptophycin 18, C-928 with
R = $CH_2CH_2CH_3$
$C_{34}H_{41}ClN_2O_7$ 625.16
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +68.1 (c, 0.07 in MeOH). Cryptophycins 49 and 50 are confused in the lit. including CAS. λ_{max} 246 (ϵ 25500); 284 (ϵ 5200) ($CHCl_3$).

7β,8β-Epoxide: ***Cryptophycin 50***
[168482-43-7]
$C_{34}H_{41}ClN_2O_8$ 641.159
Prod. by *Nostoc* sp. GSV 224.
$[\alpha]_D$ +32 (c, 0.44 in $CHCl_3$). λ_{max} 242 (ϵ 4930); 262 (ϵ 3996); 274 (ϵ 3720); 286 (ϵ 2430); 332 (ϵ 360) ($CHCl_3$).

Golakoti, T. *et al., J.A.C.S.*, 1995, **117**, 12030-12049 (*isol, uv, ir, pmr, cmr, ms*)

Cryptosporiopsinol C-934

3,5-Dichloro-1,4-dihydroxy-2-(1-propenyl)-2-cyclopentene-1-carboxylic acid, methyl ester, 9CI
[26312-75-4]



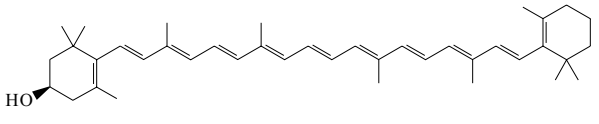
$C_{10}H_{12}Cl_2O_4$ 267.108
Metab. of *Periconia macrospinosa* and the marine *Coniothyrium* sp. 193H77. Cryst. (Et_2O/petrol).
Mp 121-122°. $[\alpha]_D^{25}$ -90 (c, 0.56 in MeOH). λ_{max} 247 (ϵ 22500) (MeOH) (Berdy).

4-Ketone: See Cryptosporiopsin in *The Combined Chemical Dictionary.*

Giles, D. *et al., J.C.S.(C)*, 1969, 2187 (*isol, struct*)
Holker, J.S.E. *et al., Chem. Comm.*, 1975, 525 (*biosynth*)
Henderson, G.B. *et al., J.C.S. Perkin 1*, 1982, 3037 (*biosynth*)
Höller, U. *et al., Dissertation*, Univ. of Braunschweig, 1999, (*isol, pmr, cmr*)

β-Cryptoxanthin C-935

β,β-Caroten-3-ol. Cryptoxanthin. 3-Hydroxy-β-carotene. Caricaxanthin. Neocryptoxanthin. β-Krypoxanthin. Cryptoxanthol
[472-70-8]



$C_{40}H_{56}O$ 552.882
Isol. from papaya (*Carica papaya*) and many other higher plants, also from fungi, diatoms blue-green algae and fish eggs. Cryst. (C_6H_6/EtOH), metallic prisms or needles (C_6H_6).
Mp 172-173° (169°). λ_{max} 452; 480 (no solvent reported).

O-*[9-Methyldecanoyl-(→6)-β-D-glucopyranoside]:* ***Thermocryptoxanthin 11***
[173355-94-7]
$C_{57}H_{86}O_7$ 883.302
Constit. of *Thermus thermophilus.*

O-*[11-Methyldodecanoyl-(→6)-β-D-glucopyranoside]:* ***Thermocryptoxanthin 13***
[173355-95-8]
$C_{59}H_{90}O_7$ 911.356
Constit. of *Thermus thermophilus.*

O-*[13-Methyltetradecanoyl-(→6)-β-D-glucopyranoside]:* ***Thermocryptoxanthin 15***
[173355-96-9]
$C_{61}H_{94}O_7$ 939.409
Constit. of *Thermus thermophilus.*

Hexadecanoyl: β-Cryptoxanthin palmitate
[25671-24-3]
$C_{56}H_{86}O_2$ 791.294
Isol. from *Physalis akekengi* and *Physalis franchetti*. Cryst. (C_6H_6/MeOH).
Mp 114°.

5R,6S-Epoxide: 5,6-Epoxy-5,6-dihydro-β,β-caroten-3-ol. ***Cryptoxanthin epoxide***
[188116-19-0]
[29291-23-4]
$C_{40}H_{56}O_2$ 568.881
Isol. from yellow paprika (*Capsicum annuum* var. *lycopersiforme*), peel of ripe persimmon (*Diospyros kaki*), mature fruit of peach (*Prunus persica*) and ripe peel of a mandarin hybrid (*Citrus reticulata*). Cryst. (C_6H_6/petrol).
Mp 154°. Absolute stereochem. of isolate from *C. annuum* determined by Molnar *et al*. (1997). Stereochem. of isolates and synthetic epoxide prior to this date unknown.

5′ξ,6′ξ-Epoxide: 5′,6′-Epoxy-5′,6′-dihydro-β,β-caroten-3-ol
[29291-23-4]
$C_{40}H_{56}O_2$ 568.881
Isol. from *Citrus reticulata* (mandarin). Cryst. (C_6H_6/hexane).
Mp 158-160°.

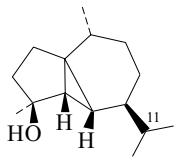
5,5′:6,6′-Diepoxide: See Violaxanthin, V-52

7′,8′-Dihydro: ***7′,8′-Dihydro-β,β-caroten-3-ol****. 7′,8′-Dihydro-β-cryptoxanthin*
[82890-05-9]
$C_{40}H_{58}O$ 554.898
Isol. from *Ecklonia cava*, *Enteromorpha intestinalis* and the catfish *Parasilurus* spp.

7,8-Didehydro: 7,8-Didehydro-β,β-caroten-3-ol, 9CI. 7,8-Didehydrocryptoxanthin. ***Allobetaxanthin***
[76207-91-5]
[162302-60-5]
$C_{40}H_{54}O$ 550.866
Isol. from *Microciona prolifera*. Cryst. (MeOH/Et_2O).
Mp 173°. λ_{max} 452 (ϵ 155000) (Me_2CO).

Karrer, P. *et al., Helv. Chim. Acta*, 1946, **29**, 229-233 (*epoxide, synth*)
Isler, O. *et al., Helv. Chim. Acta*, 1957, **40**, 456-467 (*synth*)
Entschel, R. *et al., Helv. Chim. Acta*, 1958, **41**, 983-987 (*palmitate*)
Bodea, C. *et al., Annalen*, 1963, **666**, 189-191 (*ir*)
Subbarayan, C. *et al., Anal. Biochem.*, 1965, **12**, 275-281 (*epoxide*)
De Ville, T.E. *et al., Chem. Comm.*, 1969, 1311-1312 (*abs config*)
Bartlett, L. *et al., J.C.S.(C)*, 1969, 2527-2544 (*struct*)
Loeber, D.E. *et al., J.C.S.(C)*, 1971, 404-408 (*synth*)
Pfander, H. *et al., Chimia*, 1972, **27**, 103-104 (*isol*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 1837 (*occur*)
Cooper, R.D.G. *et al., J.C.S. Perkin 1*, 1975, 2195-2204 (*synth*)
Lassertois, D. *et al., Phytochemistry*, 1978, **17**, 411-415 (*epoxide, isol*)
Litchfield, C. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **66**, 359-365 (*Allobetaxanthin*)
Shimizu, T. *et al., CA*, 1982, **97**, 108729m (*7′,8′-Dihydrocryptoxanthin*)
Farin, D. *et al., Phytochemistry*, 1983, **22**, 403-408 (*5,6-epoxide, 5′,6′-epoxide, isol*)
Ebert, G. *et al., Phytochemistry*, 1985, **24**, 29-32 (*epoxide, isol*)
Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **83**, 335 (*isol*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 55 (*bibl*)
Godoy, H.T. *et al., Food Chem.*, 1990, **36**, 281-286 (*5,6-epoxide*)
Haugan, J.A. *et al., Acta Chem. Scand.*, 1994, **48**, 899-904 (*Allobetaxanthin, synth*)
Yokoyama, A. *et al., Arch. Microbiol.*, 1996, **165**, 342-345 (*Thermocryptoxanthins 11,13,15*)
Molnar, P. *et al., Helv. Chim. Acta*, 1997, **80**, 221-229 (*epoxide*)
Tsushima, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2002, **133**, 331-336; 2003, **136**, 147-148 (*7′,8′-Dihydrocryptox nthin*)
Yamano, Y. *et al., J.C.S. Perkin 1*, 2002, 2006-2013 (*synth*)

4-Cubebanol C-936



(4β,5β,6β,10α*H*)–*form*

$C_{15}H_{26}O$ 222.37

(4β,5β,6β,10α*H*)-*form*
Cubebol. *Cubeb camphor*
[23445-02-5]
Constit. of fruits of false cubeb (*Piper lowong*).
Cryst. (petrol).
Mp 61-62°. $[\alpha]_D^{20}$ -61.6 ($CHCl_3$). $[\alpha]_D^{20}$ -48.3.

(4α,5β,6β,10α*H*)-*form*
4-Epicubebol
[182267-63-6]
Constit. of *Taonia atomaria*.
$[\alpha]_D$ -46 (c, 0.005 in $CHCl_3$).

O-*β-D-Fucopyranoside:* ***Arvoside A***
[112543-27-8]
$C_{21}H_{36}O_5$ 368.512
Constit. of *Calendula arvensis*.
$[\alpha]_D$ -27.6.

(4α,5α,6β,10α)-*form*

O-*[4-O-(2-Methylpropanoyl)-β-D-xylopyranoside]:* [108888-32-0]
$C_{24}H_{40}O_6$ 424.576
Constit. of *Aster tanacetifolius*.

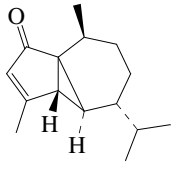
O-*[4-O-(2-Methylbutanoyl)-β-D-xylopyranoside]:* [108888-30-8]
$C_{25}H_{42}O_6$ 438.603
Constit. of *Aster tanacetifolius*.

O-*(4-O-Angeloyl-6-deoxy-β-D-glucopyranoside):*
$C_{26}H_{42}O_6$ 450.614
Constit. of *Osteospermum auriculatum*. Gum. $[\alpha]_D^{24}$ +67 (c, 0.6 in $CHCl_3$).

(4β,5β,6β,10β*H*)-*form*
10-Epicubebol
[176589-53-0]
Constit. of *Chamaecyparis obtusa*.
Cryst.
Mp 100°. $[\alpha]_D$ -72.3 (c, 3.3 in $CHCl_3$).

Tanaka, A. *et al., J.C.S. Perkin 1*, 1972, 1721-1727 (*synth, stereochem*)
Torii, S. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 771-774 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1983, **22**, 1645-1651 (*angeloyldeoxyglucoside*)
Dominguez, X.A. *et al., Rev. Latinoam. Quim.*, 1986, **17**, 207-209 (*isol, glycosides*)
Pizza, C. *et al., J. Nat. Prod.*, 1987, **50**, 784-789 (*Arvoside A*)
De Rosa, S. *et al., Phytochemistry*, 1994, **37**, 1327-1330 (*4-Epicubebol, Cubebol, cmr*)
Hieda, T. *et al., Phytochemistry*, 1996, **42**, 159-162 (*10-Epicubebol*)
Thiel, R. *et al., Phytochemistry*, 2002, **59**, 269-274 (*biosynth*)

3-Cubeben-2-one C-937



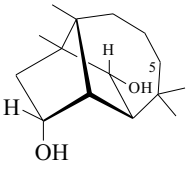
$C_{15}H_{22}O$ 218.338

(5β,6α,7α,10β)-*form*
Cubebenone
[369380-51-8]
Constit. of *Leminda millecra* and *Leptogorgia palma*.
Yellow oil. $[\alpha]_D^{23}$ +126 (c, 0.67 in $CHCl_3$).

McPhail, K.L. *et al., J. Nat. Prod.*, 2001, **64**, 1183-1190 (*isol, pmr, cmr*)

Culmorin C-938

[18374-83-9]



Absolute configuration

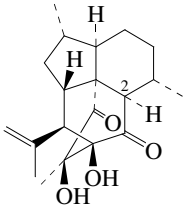
$C_{15}H_{26}O_2$ 238.369
Metab. of *Fusarium* spp. Cytotoxic, shows DNA-binding properties. Implicated in competition between lignicolous marine fungi. Cryst.
Mp 175°. $[\alpha]_D^{20}$ -14.5.

*5*R-*Hydroxy:* ***5-Hydroxyculmorin***
[139680-64-1]
$C_{15}H_{26}O_3$ 254.369
Metab. of *Fusarium graminearum*. Cryst. (MeOH).
Mp 217-218°.

Barton, D.H.R. *et al., Chem. Comm.*, 1967, 30-31 (*struct*)
Roberts, B.W. *et al., J.A.C.S.*, 1969, **91**, 3400-3401 (*synth*)
Hanson, J.R. *et al., J.C.S. Perkin 1*, 1976, 2471-2475 (*biosynth*)
Reddy, R.T. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 457-461 (*synth*)
Cohen, H. *et al., J. Nat. Prod.*, 1992, **55**, 326-332 (*5-Hydroxyculmorin*)
Meier, A. *et al., J. Antibiot.*, 1999, **52**, 952-959 (*activity*)
Pedersen, P.B. *et al., Nat. Toxins*, 1999, **7**, 305-309 (*rev, activity*)
Takasu, K. *et al., J.O.C.*, 2000, **65**, 4112-4119 (*synth*)

Cumbiasin A C-939

[303963-84-0]



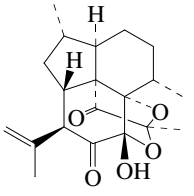
$C_{20}H_{28}O_4$ 332.439
Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{25}$ +6.7 (c, 1.78 in $CHCl_3$).

2α-Hydroxy: ***Cumbiasin B***
[303963-85-1]
$C_{20}H_{28}O_5$ 348.438
Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{25}$ -29 (c, 1.56 in $CHCl_3$). λ_{max} 208 (ε 7800) (MeOH).

Rodríguez, A.D. *et al., J.O.C.*, 2000, **65**, 6682-6687 (*isol, pmr, cmr*)

Cumbiasin C C-940

[303963-86-2]

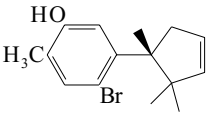


$C_{20}H_{26}O_5$ 346.422
Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{25}$ +20.8 (c, 1.78 in $CHCl_3$). λ_{max} 214 (ε 14100) (MeOH).

Rodríguez, A.D. *et al., J.O.C.*, 2000, **65**, 6682-6687 (*isol, pmr, cmr*)

Cupalaurenol C-941

4-Bromo-2-methyl-5-(1,2,2-trimethyl-3-cyclopenten-1-yl)phenol, 9CI
[103439-84-5]

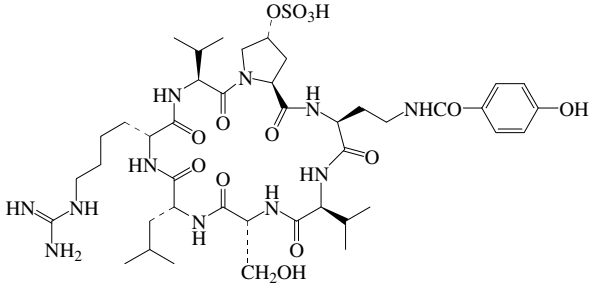


$C_{15}H_{19}BrO$ 295.218
Constit. of *Aplysia dactylomela*. Ichthyotoxic, antimicrobial, antifungal. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{19}$ +87.9 (c, 1 in $CHCl_3$). λ_{max} 206 (ϵ 14200); 224 (sh) (ϵ 6550); 282 (ϵ 1530) (EtOH) (Derep).

Ac: ***Cupalaurenol acetate***
[103456-69-5]
$C_{17}H_{21}BrO_2$ 337.256
From *Aplysia dactylomela*. Ichthyoxoic, antimicrobial, antifungal. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{19}$ +65.1 (c, 1 in $CHCl_3$). λ_{max} 206 (ϵ 14200); 224 (sh) (ϵ 6550); 282 (ϵ 1530) (EtOH) (Derep). λ_{max} 205 (ϵ 21000); 222 (ϵ 10000); 280 (ϵ 3000) (EtOH) (Berdy).
Ichiba, T. *et al., J.O.C.*, 1986, **51**, 3364

Cupolamide A C-942

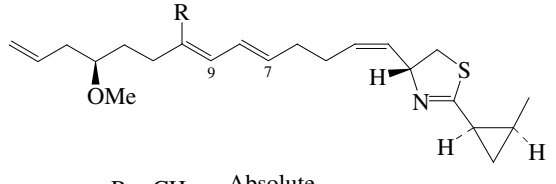
[197357-74-7]



$C_{42}H_{67}N_{11}O_{14}S$ 982.123
Cyclic peptide antibiotic. Isol. from the sponge *Theonella cupola*. Cytotoxic agent. Amorph. solid (as Na salt). $[\alpha]_D$ -34.3 (c, 1.9 in MeOH) (Na salt). λ_{max} 253 (ϵ 11000) (MeOH).
Bonnington, L.S. *et al., J.O.C.*, 1997, **62**, 7765-7767 (*isol, uv, pmr, cmr*)

Curacin A C-943

[155233-30-0]



R = CH_3 Absolute Configuration

$C_{23}H_{35}NOS$ 373.602
Isol. from the marine cyanobacterium *Lyngbya majuscula*. Antimitotic agent. Also possesses exceptional brine shrimp toxic and antiproliferative activities. Shows herbicidal props. Sol. MeOH, $CHCl_3$; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D$ +62 (c, 1.10 in $CHCl_3$) (a higher value of +86 was originally reported). Unstable when stored neat. λ_{max} 242 (hexane) (Berdy).

7Z-Isomer: ***Curacin B***
[157319-51-2]
$C_{23}H_{35}NOS$ 373.602
Isol. from the marine cyanobacterium *Lyngbya majuscula*. Antimitotic and antiinflammatory agent. Immunosuppressant. Possesses brine shrimp toxic and antiproliferative activities. $[\alpha]_D^{25}$ +62 (c, 0.84 in $CHCl_3$). λ_{max} 242 (ϵ 22000) (hexane) (Berdy).

9Z-Isomer: ***Curacin C***
[164454-35-7]
$C_{23}H_{35}NOS$ 373.602
From *Lyngbya majuscula*. Potent antimitotic agent. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{25}$ +56 (c, 0.15 in $CHCl_3$). λ_{max} 242 (ϵ 25000) (MeOH) (Berdy).
Gerwick, W.H. *et al., J.O.C.*, 1994, **59**, 1243 (*isol, pmr, cmr, struct*)
U.S. Pat., 1994, 5 324 739; *CA*, **121**, 149068c (*isol, pmr*)
Yoo, H.D. *et al., J. Nat. Prod.*, 1995, **58**, 1961 (*Curacins B and C*)
Nagle, D.G. *et al., Tet. Lett.*, 1995, **36**, 1189 (*abs config*)
Wipf, P. *et al., J.O.C.*, 1996, **61**, 6556 (*synth*)
White, J.D. *et al., J.A.C.S.*, 1997, **119**, 103 (*synth, abs config*)
Hoemann, M.Z. *et al., Tetrahedron*, 1997, **53**, 11087 (*synth*)
Muir, J.C. *et al., Tet. Lett.*, 1998, **39**, 2861-2864 (*synth*)

Curacin D C-944

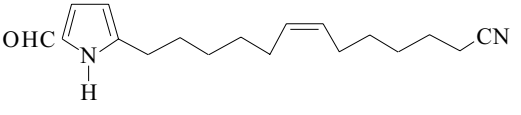
[164454-36-8]
As Curacin A, C-943 with
R = H
$C_{22}H_{33}NOS$ 359.575
Absolute configuration has not been confirmed. Isol. from *Lyngbya majuscula*. Antimitotic agent, tubulin polymerisation inhibitor. Pale yellow oil. $[\alpha]_D$ +33 (c, 0.14 in $CHCl_3$). The name Curacin D also refers to a semisynthetic stereoisomer of Curacin A. λ_{max} 224 (ϵ 9000) (hexane).
Marquez, B. *et al., Phytochemistry*, 1998, **49**, 2387-2389 (*isol, uv, ir, pmr, cmr, ms*)

Cyanocobalamin reductase (cyanide-eliminating) C-945

E.C. 1.16.1.6. Cob(I)alamin, cyanide:NADP⊕ oxidoreductase. E.C. 1.6.99.12 (transferred)
[131145-00-1]
FAD-dependent oxidoreductase enzyme. Isol. from *Euglena gracilis*. Catalyses the reaction of cyanocob(*III*)-alamin with NADPH to give Vitamin B_{12s}, $NADP^{\oplus}$ and $CN^{\ominus}$.
Watanabe, F. *et al., J. Nutr. Sci. Vitaminol.*, 1988, **34**, 1-10 (*Euglena gracilis*)

5-(12-Cyano-6-dodecenyl)-2-pyrrolecarboxaldehyde C-946

13-(5-Formyl-1H-pyrrol-2-yl)-7-tridecenenitrile, 9CI

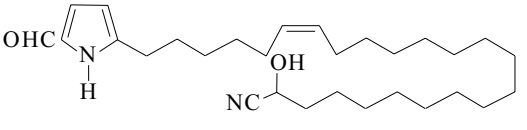


$C_{18}H_{26}N_2O$ 286.416

(Z)-form [75234-01-4]
Metab. of the marine sponge *Laxosuberites* sp.
Stierle, D.B. *et al., J.O.C.*, 1980, **45**, 4980 (*isol, uv, ir, pmr, cmr, ms, struct*)

5-(23-Cyano-23-hydroxy-6-tricosenyl)-1*H*-pyrrole-2-carboxaldehyde C-947

24-(5-Formyl-1H-pyrrol-2-yl)-2-hydroxy-18-tetracosenenitrile, 9CI



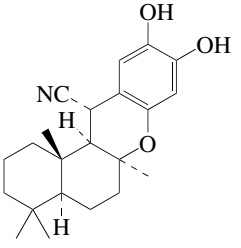
$C_{29}H_{48}N_2O_2$ 456.71

(Z)-form [75234-02-5]
Metab. of the marine sponge *Laxosuberites* sp.
Mp 38-40°. Unusually stable to normal isol. and storage procedures. λ_{max} 297 (ϵ 16100) (MeCN) (Derep).

*23-Deoxy: 5-(23-Cyano-6-tricosenyl)-1*H*-pyrrole-2-carboxaldehyde*
[290817-49-1]
$C_{29}H_{48}N_2O$ 440.711
Isol. from the sponge *Mycale tenuispiculata*.
Mp 56-58°. λ_{max} 297 (ϵ 15300) (MeCN).
Stierle, D.B. *et al., J.O.C.*, 1980, **45**, 4980-4982 (*isol, uv, ir, pmr, cmr, ms, struct*)
Venkatesham, U. *et al., J. Nat. Prod.*, 2000, **63**, 1318-1320 (*23-deoxy*)

15-Cyanopuupehenol C-948

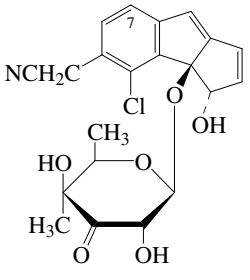
*1,2,3,4,4*a*,5,6,6*a*,12*a*,12*b*-Decahydro-9,10-dihydroxy-4,4,6*a*,2*b*-tetramethyl-2*H*-benzo[*a*]xanthene-12-carbonitrile, 9CI*
[137856-42-9]



$C_{22}H_{29}NO_3$ 355.476
Isol. from a Verongid sponge. Antiviral agent, immunomodulator.
Light tan glass. $[\alpha]_D$ -22 (c, 0.37 in MeOH). λ_{max} 206 (ϵ 20000); 230 (ϵ 5010); 346 (ϵ 1000) (MeOH) (Derep).

15-Decyano, 15α-methoxy: ***15-Methoxypuupehenol***
$C_{22}H_{32}O_4$ 360.492
Isol. from the sponge *Hyrtios* sp. Cytotoxic agent. Needles.
Mp 124°. $[\alpha]_D^{20}$ -17 (c, 0.8 in $CHCl_3$). Originally thought to be an artifact. λ_{max} 206 (ϵ 23725); 298 (ϵ 5652) (MeOH).
Hamann, M.T. *et al., Tet. Lett.*, 1991, **32**, 5671 (*isol, struct*)
Urban, S. *et al., J. Nat. Prod.*, 1996, **59**, 900-901 (*abs config*)
Bourguet-Kondracki, M.-L. *et al., J. Nat. Prod.*, 1999, **62**, 1304-1305 (*15-Methoxypuupehenol*)

Cyanosporoside A C-949

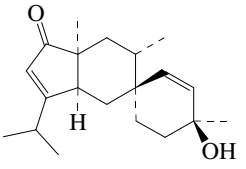


$C_{21}H_{20}ClNO_6$ 417.845
Alkaloid from *Salinospora pacifica* (CNS103). Oil. $[\alpha]_D$ +25 (c, 0.19 in MeCN). λ_{max} 242 (log ϵ 4.1); 298 (log ϵ 3.9); 324 (log ϵ 3.6) (MeCN).

Dechloro, 7-chloro: ***Cyanosporoside B***
$C_{21}H_{20}ClNO_6$ 417.845
Alkaloid from *Salinospora pacifica* (CNS103). Oil. $[\alpha]_D$ +21 (c, 0.2 in MeCN). λ_{max} 244 (log ϵ 4); 301 (log ϵ 3.9); 328 (log ϵ 3.6) (MeCN).
Oh, D.-C. *et al., Org. Lett.*, 2006, **8**, 1021-1024 (*isol, cd, pmr, cmr*)

Cyanthiwigin AC C-950

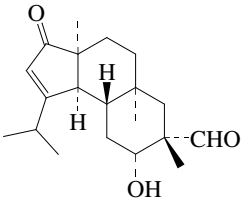
[632344-15-1]



$C_{20}H_{30}O_2$ 302.456
Rearranged cyathane. Isol. from *Myrmekioderma styx*.
Peng, J. *et al., Org. Lett.*, 2003, **5**, 4575-4578 (*isol, pmr, cmr*)
Reddy, T.J. *et al., Org. Lett.*, 2006, **8**, 5585-5588 (*synth*)

Cyanthiwigin AD C-951

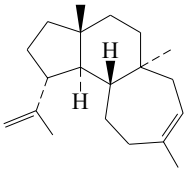
[632344-16-2]



$C_{20}H_{30}O_3$ 318.455
Rearranged cyathane. Isol. from *Myrmekioderma styx*.
$[\alpha]_D$ +30 (c, 0.12 in MeOH). λ_{max} 240 (ϵ 3708) (MeOH).
Peng, J. *et al., Org. Lett.*, 2003, **5**, 4575-4578 (*isol, pmr, cmr*)

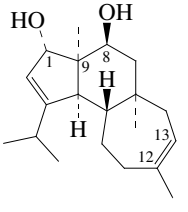
12,18-Cyathadiene C-952

[151670-37-0]



$C_{20}H_{32}$ 272.473
Constit. of a *Higginsia* sp. Oil. $[\alpha]_D$ -28 (c, 0.4 in $CHCl_3$).
Cassidy, M.P. *et al., J. Nat. Prod.*, 1993, **56**, 1190 (*isol, pmr, cmr*)

2,12-Cyathadiene-1,8-diol C-953



$C_{20}H_{32}O_2$ 304.472

(1α,8β,9α)-*form*
Cyanthiwigin D
[150999-00-1]
Constit. of sponge *Epipolasis reiswigi* and of *Myrmekioderma styx*.
Amorph. powder. $[\alpha]_D$ +17 (c, 0.04 in EtOAc).

1-Ketone: 8-Hydroxy-2,12-cyathadien-1-one. ***Cyanthiwigin E***
[481643-40-7]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Myrmekioderma styx*. Powder. $[\alpha]_D$ +90 (c, 0.1 in MeOH). λ_{max} 238 (ϵ 5903) (MeOH).

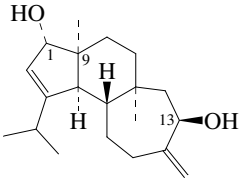
Diketone: 2,12-Cyathadiene-1,8-dione. ***Cyanthiwigin B***
[150998-99-5]
$C_{20}H_{28}O_2$ 300.44
Constit. of *Epipolasis reiswigi* and *Myrmekioderma styx*. Amorph. powder. $[\alpha]_D$ -128 (c, 0.5 in CH_2Cl_2).

12β,13β-Epoxide: 12,13-Epoxy-2-cyathene-1,8-diol. ***Cyanthiwigin J***
[481643-45-2]
$C_{20}H_{32}O_3$ 320.471
Constit. of *Myrmekioderma styx*. Powder. $[\alpha]_D$ +50 (c, 0.1 in MeOH). λ_{max} 208 (ϵ 6550) (MeOH).

12β,13β-Epoxide, 1-ketone: 12,13-Epoxy-8-hydroxy-2-cyathen-1-one. ***Cyanthiwigin AB***
[632344-14-0]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Myrmekioderma styx*. Cryst.

Green, D. *et al., Nat. Prod. Lett.*, 1992, **1**, 193 (*Cyanthiwigins B and D*)
Peng, J. *et al., Tetrahedron*, 2002, **58**, 7809-7819 (*Cyanthiwigins E and J*)
Peng, J. *et al., Org. Lett.*, 2003, **5**, 4575-4578 (*Cyanthiwigin AB*)

2,12(15)-Cyathadiene-1,13-diol C-954

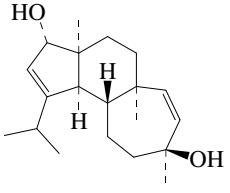


$C_{20}H_{32}O_2$ 304.472

(1α,9α,13β)-*form*
Cyanthiwigin L
[481643-47-4]
Constit. of *Myrmekioderma styx*.
Powder. $[\alpha]_D$ +14 (c, 0.11 in MeOH). λ_{max} 206 (ϵ 10236) (MeOH).

1-Ketone: 13-Hydroxy-2,12(15)-cyathadien-1-one. ***Cyanthiwigin I***
[481643-44-1]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Myrmekioderma styx*. Powder. $[\alpha]_D$ +17 (c, 0.06 in MeOH). λ_{max} 238 (ϵ 11164) (MeOH).
Peng, J. *et al., Tetrahedron*, 2002, **58**, 7809-7819 (*isol, pmr, cmr*)

2,13-Cyathadiene-1,12-diol C-955

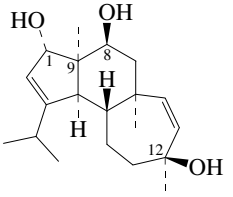


$C_{20}H_{32}O_2$ 304.472

(1α,9α,12β)-*form*
Cyanthiwigin W
[481643-58-7]
Constit. of *Myrmekioderma styx*.
Powder. $[\alpha]_D$ +97 (c, 0.08 in MeOH). λ_{max} 206 (ϵ 7184) (MeOH).

1-Ketone: 12-Hydroxy-2,13-cyathadien-1-one. ***Cyanthiwigin U***
[481643-56-5]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Myrmekioderma styx*. Cryst. $[\alpha]_D$ +131 (c, 0.1 in MeOH). λ_{max} 238 (ϵ 9621) (MeOH).
Peng, J. *et al., Tetrahedron*, 2002, **58**, 7809-7819 (*isol, pmr, cmr*)
Pfeiffer, M.W.B. *et al., J.A.C.S.*, 2005, **127**, 5334-5335 (*synth*)

2,13-Cyathadiene-1,8,12-triol C-956



$C_{20}H_{32}O_3$ 320.471

(1α,8β,9α,12β)-*form*
Cyanthiwigin X
[481643-59-8]
Constit. of *Myrmekioderma styx*.
Cryst. $[\alpha]_D$ +87 (c, 0.1 in MeOH). λ_{max} 206 (ϵ 6050) (MeOH).

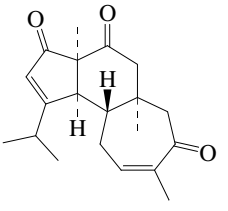
8-Ketone: 1,12-Dihydroxy-2,13-cyathadien-8-one. ***Cyanthiwigin V***
[481643-57-6]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Myrmekioderma styx*. Gum. $[\alpha]_D$ +8 (c, 0.1 in MeOH). λ_{max} 206 (ϵ 7184) (MeOH).

1-Ketone, 12-hydroperoxide: 12-Hydroperoxy-8-hydroxy-2,13-cyathadien-1-one. ***Cyanthiwigin T***
[481643-55-4]
$C_{20}H_{30}O_4$ 334.455
Constit. of *Myrmekioderma styx*. Cryst. $[\alpha]_D$ +110 (c, 0.02 in MeOH). λ_{max} 238 (ϵ 12689) (MeOH).

1,8-Diketone: 12-Hydroxy-2,13-cyathadiene-1,8-dione. ***Cyanthiwigin S***
[481643-54-3]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Myrmekioderma styx*. Cryst. $[\alpha]_D$ -50 (c, 0.09 in MeOH). λ_{max} 236 (ϵ 6481) (MeOH).

1,8-Diketone, 12-hydroperoxide: 12-Hydroperoxy-2,13-cyathadiene-1,8-dione. ***Cyanthiwigin R***
[481643-53-2]
$C_{20}H_{28}O_4$ 332.439
Constit. of *Myrmekioderma styx*. Cryst. $[\alpha]_D$ -118 (c, 0.1 in MeOH). λ_{max} 238 (ϵ 9524) (MeOH).
Peng, J. *et al., Tetrahedron*, 2002, **58**, 7809-7819 (*isol, pmr, cmr*)

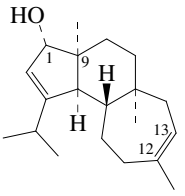
2,11-Cyathadiene-1,8,13-trione C-957



$C_{20}H_{26}O_3$ 314.424

9α-form
Cyanthiwigin AA
[481643-62-3]
Constit. of *Myrmekioderma styx*.
Gum. $[\alpha]_D$ -98 (c, 0.1 in MeOH). λ_{max} 238 (ϵ 9016) (MeOH).
Peng, J. *et al., Tetrahedron*, 2002, **58**, 7809-7819 (*isol, pmr, cmr*)

2,12-Cyathadien-1-ol C-958



$C_{20}H_{32}O$ 288.472

(1α,9α)-*form*

Cyanthiwigin C

[151063-13-7]

Constit. of the sponge *Epipolasis reiswigi* and of *Myrmekioderma styx*.

Amorph. powder. $[\alpha]_D$ +25 (c, 0.02 in EtOAc). $[\alpha]_D^{22}$ +38.5 (c, 0.05 in CH_2Cl_2). λ_{max} 229 (ϵ 762) (EtOH).

1-Ketone: 2,12-Cyathadien-1-one. ***Cyanthiwigin A***

[150998-98-4]

$C_{20}H_{30}O$ 286.456

Constit. of *Epipolasis reiswigi*. Cryst.

Mp 84-85°. $[\alpha]_D$ +7 (c, 0.5 in CH_2Cl_2).

12β,13β-Epoxide: 12,13-Epoxy-2-cyathen-1-ol. ***Cyanthiwigin K***

[481643-46-3]

$C_{20}H_{32}O_2$ 304.472

Constit. of *Myrmekioderma styx*. Powder. $[\alpha]_D$ +33 (c, 0.06 in MeOH). λ_{max} 206 (ϵ 14482) (MeOH).

12β,13β-Epoxide, 1-Ac: [144967-85-1]

$C_{22}H_{34}O_3$ 346.509

Constit. of *Myrmekioderma styx*.

$[\alpha]_D^{22}$ +69.4 (c, 0.018 in CH_2Cl_2).

12β,13β-Epoxide, 1-ketone: 12,13-Epoxy-2-cyathen-1-one. ***Cyanthiwigin H***

[481643-43-0]

$C_{20}H_{30}O_2$ 302.456

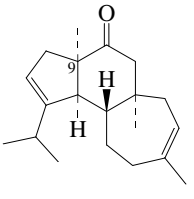
Constit. of *Myrmekioderma styx*. Powder. $[\alpha]_D$ +37 (c, 0.03 in MeOH). λ_{max} 236 (ϵ 16280) (MeOH).

Sennett, S.H. *et al., J. Nat. Prod.*, 1992, **55**, 1421 (*isol, epoxide Ac*)

Green, D. *et al., Nat. Prod. Lett.*, 1992, **1**, 193 (*Cyanthiwigin A, Cyanthiwigin C, isol, pmr, cmr, cryst struct*)

Peng, J. *et al., Tetrahedron*, 2002, **58**, 7809-7819 (*Cyanthiwigins*)

2,12-Cyathadien-8-one C-959



$C_{20}H_{30}O$ 286.456

9α-*form*

Cyanthiwigin F

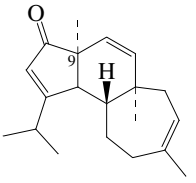
[481643-41-8]

Constit. of *Myrmekioderma styx*.

Cryst. $[\alpha]_D$ -128 (c, 0.03 in MeOH). λ_{max} 216 (ϵ 2437) (MeOH).

Peng, J. *et al., Tetrahedron*, 2002, **58**, 7809-7819 (*isol, pmr, cmr*)

2,7,12-Cyathatrien-1-one C-960



$C_{20}H_{28}O$ 284.441

9α-*form*

Cyanthiwigin G

[481643-42-9]

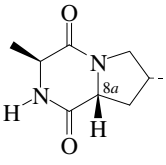
Constit. of *Myrmekioderma styx*.

Powder. $[\alpha]_D$ -9 (c, 0.1 in MeOH). λ_{max} 236 (ϵ 7343) (MeOH).

Peng, J. *et al., Tetrahedron*, 2002, **58**, 7809-7819 (*isol, pmr, cmr*)

Cyclo(alanyl-4-hydroxyprolyl) C-961

Hexahydro-7-hydroxy-3-methylpyrrolo[1,2-a]pyrazine-1,4-dione, 9CI



(3*S*,7*R*,8*aR*)-*form*

$C_8H_{12}N_2O_3$ 184.194

(3*S*,7*R*,8*aR*)-*form*

Prod. by a strain of *Ruegeria* sp. isol. from the sponge *Suberites domuncula*.

Amorph. solid. $[\alpha]_D^{25}$ +17.8 (c, 0.001 in MeOH).

(3*S*,7*R*,8*aS*)-*form*

Prod. by a strain of *Ruegeria* sp. from *Suberites domuncula*. Also isol. from *Streptomyces fradiae.*

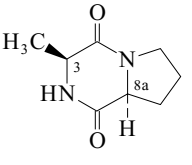
Amorph. solid. $[\alpha]_D^{25}$ -4.2 (c, 0.002 in MeOH).

Hoffmeister, D. *et al., Chem. Biol.*, 2000, **7**, 821-831 (*isol*)

Mitova, M. *et al., J. Nat. Prod.*, 2004, **67**, 1178-1181 (*isol, pmr, cmr, ms*)

Cyclo(alanylprolyl) C-962

Hexahydro-3-methylpyrrolo[1,2-a]pyrazine-1,4-dione, 9CI



(3*S*,8a*S*)–*form*

$C_8H_{12}N_2O_2$ 168.195

(3*S*,8*aS*)-*form*

*L,L-form. (3*S-trans*)-form*

[36357-32-1]

Isol. from cocoa; metab. product of the Caribbean sponge *Tedania ignis.*

Mp 153-156°. $[\alpha]_{Hg}^{20}$ -160 (c, 1 in EtOH).

(3*S*,8*aR*)-*form*

*D,L-form. (3*S-cis*)-form*

[19943-29-4]

From *Beauveria bassiana*.

Mp 162-166°. $[\alpha]_D^{22}$ -85.

(3*R*,8*aS*)-*form*

*L,D-form. (3*R-cis*)-form*

[36238-64-9]

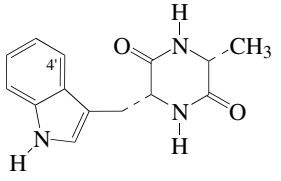
Mp 139-142°.

[19943-28-3, 65556-33-4]

Westley, J.W. *et al., Anal. Chem.*, 1968, **40**, 1888 (*glc, chromatog, pmr*)
Siemion, I.Z. *et al., Org. Magn. Reson.*, 1971, **3**, 545 (*synth, pmr*)
Young, P.E. *et al., J.A.C.S.*, 1976, **98**, 5365 (*synth, pmr, cmr*)
Izumiya, N. *et al., Pept. Chem.*, 1977, **15**, 49 (*pharmacol*)
Cotrait, M. *et al., Cryst. Struct. Commun.*, 1979, **8**, 819 (*cryst struct*)
Grove, J.F. *et al., Phytochemistry*, 1981, **20**, 815 (*isol*)
Schmitz, F.J. *et al., J.O.C.*, 1983, **48**, 3941 (*isol, pmr, ms*)
Langhammer, M. *et al., Fresenius' Z. Anal. Chem.*, 1986, **324**, 5 (*ms*)

Cyclo(alanyltryptophyl) C-963

*3-(1*H*-Indol-3-ylmethyl)-6-methyl-2,5-piperazinedione, 9CI. Cyclo(tryptophylalanyl). Alanine tryptophan anhydride*
[26384-48-5]



(3*R*,6*R*)-*form*

$C_{14}H_{15}N_3O_2$ 257.291

(3*R*,6*R*)-*form*
D,D-form. *(-)*-cis-*form*
[22839-21-0]
Cryst. (EtOH/EtOAc). Mp 281-283°. $[\alpha]_D^{25}$ -10.2 (c, 0.048 in EtOH).

*3,6-Bis(methylthio): 3-(1*H*-Indol-3-ylmethyl)-6-methyl-3,6-bis(methylthio)-2,5-piperazinedione, 9CI*
[240140-70-9]
$C_{16}H_{19}N_3O_2S_2$ 349.477
Isol. from a marine *Penicillium* sp. CNC-350. Solid. Possesses (3*S*,6*S*)-config. λ_{max} 215; 269; 277; 286 (no solvent reported).

(3*R*,6*S*)-*form*
D,L-form. *(+)*-trans-*form*
[22839-23-2]
Cryst. (EtOH/EtOAc). Mp 265-267° dec. $[\alpha]_D^{25}$ +75.6 (c, 0.049 in EtOH).

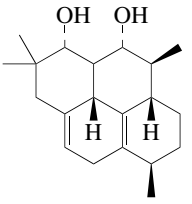
(3*S*,6*R*)-*form*
L,D-form. *(-)*-trans-*form*
[22839-22-1]
Cryst. (EtOH/EtOAc). Mp 264-267° dec. $[\alpha]_D^{25}$ -74.2 (c, 0.051 in EtOH).

(3*S*,6*S*)-*form*
L,L-form. *(+)*-cis-*form*
[17079-37-7]
Prod. by *Aspergillus chevalieri*. Intermed. in Echinulin biosynth. Needles ($MeOH/Me_2CO$).
Mp 290-292°. $[\alpha]_D^{25}$ +36 (c, 0.5 in AcOH).

(3ξ,6ξ)-*form*
4′-Methoxy: Cyclo(alanyl-4-methoxytryptophyl). ***Cortinarin C***
[88025-85-8]
$C_{15}H_{17}N_3O_3$ 287.318
Isol. from *Cortinarius* spp. Considered to be an intermed. in the biosynth. of Cortinarin A. Nontoxic. Simple cyclic peptide antibiotic. λ_{max} 268 (MeOH) (Berdy).

Nakashima, R. *et al., Can. J. Chem.*, 1967, **47**, 2069 (*synth, ord*)
Houghton, E. *et al., J.C.S.(C)*, 1969, 1003 (*synth*)
Hope, A. *et al., Tet. Lett.*, 1972, 2261 (*synth*)
Marchelli, R. *et al., Chem. Comm.*, 1975, 779 (*biosynth*)
Hamasaki, T. *et al., Agric. Biol. Chem.*, 1976, **40**, 203; 2487 (*isol*)
Kanmera, T. *et al., Tet. Lett.*, 1979, 4483 (*synth*)
Tebbett, I.R. *et al., Experientia*, 1982, **38**, 1439; 1984, **40**, 441 (*Cortinarin C*)
Son, B.W. *et al., Nat. Prod. Lett.*, 1999, **13**, 213-222 (*bismethylthio*)

8(13),10-Cycloamphilectadiene-2,14-diol C-964



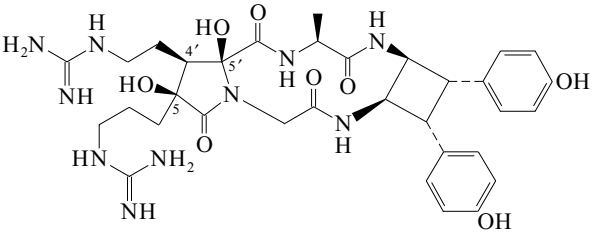
$C_{20}H_{30}O_2$ 302.456

(2α,14α)-*form*
Di-Ac: ***Sinulobatin D***
[189456-09-5]
$C_{24}H_{34}O_4$ 386.53
Constit. of *Sinularia nanolobata*. Amorph. $[\alpha]_D^{26}$ +30.6 (c, 0.07 in $CHCl_3$).

Yamada, K. *et al., Tetrahedron*, 1997, **53**, 4569-4578 (*isol, pmr, cmr*)

Cycloanchinopeptolide C C-965

[160433-76-1]

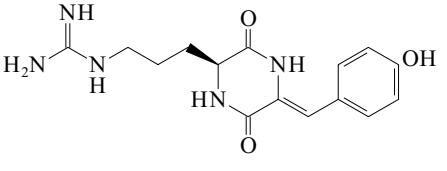


$C_{33}H_{44}N_{10}O_8$ 708.773
Stereochem. at C-5, C-4′, C-5 and around the cyclobutane ring is relative. Alkaloid from the Mediterranean marine sponge *Anchinoe tenacior*.
$[\alpha]_D$ +18.6 (c, 0.5 in MeOH). λ_{max} 215 (ε 21000); 282 (ε 8080) (MeOH) (Berdy).

Casapullo, A. *et al., J. Nat. Prod.*, 1994, **57**, 1227 (*isol, uv, pmr, cmr, cd, struct*)

Cyclo(arginyldehydrotyrosyl) C-966

[3-[5-[(4-Hydroxyphenyl)methylene]-3,6-dioxo-2-piperazinyl]-propyl]guanidine, 9CI



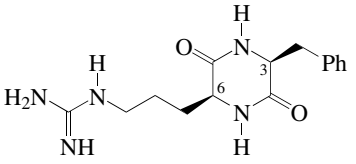
$C_{15}H_{19}N_5O_3$ 317.347

(S)*-*form [164727-33-7]
Isol. from the marine sponge *Anthosigmella* aff. *raromicrosclera*. Induces larval metamorphosis in ascidians. Yellowish oil. $[\alpha]_D^{24}$ -78.8 (c, 1.00 in MeOH). λ_{max} 223 (ε 4700); 318 (ε 6000) (MeOH) (Berdy).

Tsukamoto, S. *et al., Tetrahedron*, 1995, **51**, 6687 (*isol, uv, ir, pmr, cmr, struct*)

Cyclo(arginylphenylalanyl) C-967

[3-[3,6-Dioxo-5-(phenylmethyl)-2-piperazinyl]propyl]guanidine, 9CI. Arginyl phenylalanyl anhydride



$C_{15}H_{21}N_5O_2$ 303.363

(3*S*,6*S*)-*form* [115074-71-0]
Isol. from the Chinese soft coral *Sinularia* sp. Antitumour agent.

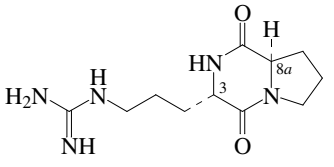
Monohydrochloride: [85717-89-1]
Cryst. + 1½ H_2O (H_2O). Mp 183-186° (dec.). $[\alpha]_D$ +13.7 (c, 0.7 in MeOH aq.).

Acetate salt: [74838-84-9]
Cryst. Mp 217°. $[\alpha]_D$ -10 (c, 1 in H_2O).

Sasaki, Y. *et al., Chem. Pharm. Bull.*, 1982, **30**, 4435-4443 (*synth*)
Ishibashi, N. *et al., Agric. Biol. Chem.*, 1988, **52**, 819-827 (*synth*)
Lin, Y. *et al., CA*, 1994, **120**, 54936z (*isol, synth*)

Cyclo(arginylprolyl) C-968

3-[3-(Aminoiminomethyl)propyl]hexahydropyrrolo[1,2-a]pyrazine-1,4-dione. 3-(3-Guanidinylpropyl)hexahydropyrrolo[1,2-a]pyrazine-1,4-dione



(3*S*,8*aR*)-*form*

$C_{11}H_{19}N_5O_2$ 253.303

(3*S*,8*aR*)-*form*
L-D-*form*. ***Antibiotic CI 4***. *CI 4*
[173524-51-1]
Prod. by the marine-derived *Pseudomonas* sp. Chitinase inhibitor.
Powder. $[\alpha]_D^{29}$ +42 (c, 0.2 in H_2O).

(3*S*,8*aS*)-*form*
L-L-*form*. ***Verpacamide A***
[74838-83-8]
Isol. from *Axinella vaceleti*.
$[\alpha]_D^{24}$ -69.2 (c, 0.4 in MeOH).

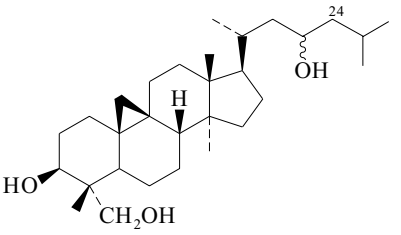
Monohydrochloride: [115181-61-8]
Mp 245-250°. $[\alpha]_D^{23}$ -72 (c, 1 in H_2O).

*8,8*a-*Didehydro:* ***Verpacamide B***
$C_{11}H_{17}N_5O_2$ 251.288
Isol. from *Axinella vaceleti*. Oil (as formate salt). $[\alpha]_D^{24}$ -5.7 (c, 0.32 in MeOH) (formate). Prob. config. is (3*S*-).

Ishibashi, N. *et al., Agric. Biol. Chem.*, 1988, **52**, 819-827 (*synth*)
Izumida, H. *et al., J. Antibiot.*, 1996, **49**, 76-80 (*Antibiotic CI 4*)
Vergne, C. *et al., Org. Lett.*, 2006, **8**, 2421-2424 (*Verpacamides*)

Cycloartane-3,23,28-triol C-969

9,19-Cyclolanostane-3,23,28-triol



$C_{30}H_{52}O_3$ 460.739

(3β,23ξ)-*form*

3,28-Disulfate: [154496-86-3]
$C_{30}H_{52}O_9S_2$ 620.867
Constit. of *Tydemania expeditionis*. Solid.
Mp 203-204° dec. $[\alpha]_D$ +20.5 (c, 0.002 in MeOH). Isol. as Na salt.

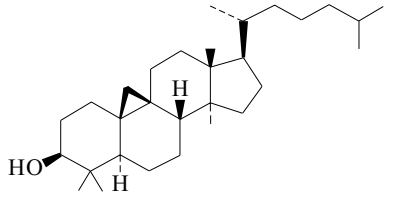
23-Ketone, 3,28-disulfate: [154496-87-4]
$C_{30}H_{50}O_9S_2$ 618.852
Constit. of *Tydemania expeditionis*. Solid.
Mp 198-199° dec. $[\alpha]_D$ +23.6 (c, 0.005 in MeOH). Isol. as Na salt.

24,25-Didehydro, 23-ketone, 3,28-disulfate: [154496-88-5]
$C_{30}H_{48}O_9S_2$ 616.836
Constit. of *Tydemania expeditionis*. Solid.
Mp 230-232° dec. Isol. as Na salt.

Govindan, M. *et al., J. Nat. Prod.*, 1994, **57**, 74 (*isol, pmr, cmr*)

Cycloartan-3-ol C-970

9,19-Cyclolanostan-3-ol



$C_{30}H_{52}O$ 428.74
Log P 10.8 (uncertain value) (calc).

3β-*form*
Cycloartanol
[4657-58-3]
Minor constit. of rice bran oil and of the rhizomes of *Polypodium vulgare*. Antiinflammatory agent. Cryst. (MeOH aq.).
Mp 101-102°. $[\alpha]_D$ +45 (c, 3.59 in $CHCl_3$).

3-O-*Sulfate:* [151890-93-6]
$C_{30}H_{52}O_4S$ 508.804
Constit. of *Eupentacta fraudatrix*.

3-O-*β*-D-*Xylopyranoside:* [151890-79-8]
$C_{35}H_{60}O_5$ 560.856
Constit. of *Eupentacta fraudatrix*.

Ac: [4575-74-0]
$C_{32}H_{54}O_2$ 470.777
Isol. from ferns *Polypodium* spp. Cryst. ($CHCl_3$/MeOH).
Mp 132-133°. $[\alpha]_D$ +57 (c, 5.31 in $CHCl_3$).

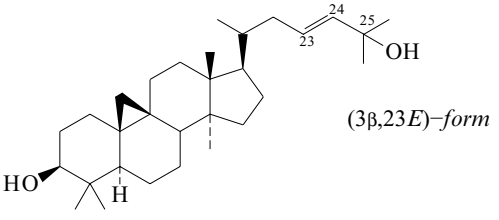
2-R-*Methylbutanoyl:* [207606-42-6]
$C_{35}H_{60}O_2$ 512.858
Constit. of *Espeletia argentea* and *Espeletia barclayana*. Cryst.
Mp 123-124°. $[\alpha]_D^{20}$ +67 ($CHCl_3$).

4-Hydroxy-3-methoxycinnamoyl: Cycloartanyl ferulate
[20972-10-5]
$C_{40}H_{60}O_4$ 604.912
Constit. of rice bran oil. Component of Mi Pi Kang.

3-Ketone: Cycloartan-3-one. ***Cycloartanone***
[4936-10-1]
$C_{30}H_{50}O$ 426.724
Constit. of *Costus tonkinensis.*
Shimizu, M. *et al., Chem. Pharm. Bull.*, 1960, **8**, 108 (*isol*)
Altenburger, E. *et al., Helv. Chim. Acta*, 1965, **48**, 704 (*synth*)
Audier, H.E. *et al., Tet. Lett.*, 1966, 4341 (*ms*)
Berti, G. *et al., Tet. Lett.*, 1967, 125 (*isol*)
Endo, T. *et al., CA*, 1968, **69**, 37319n (*isol, ferulate*)
Imhof, R. *et al., Chem. Comm.*, 1969, 852 (*synth*)
Khuong-Huu, F. *et al., Tet. Lett.*, 1975, 1787 (*cmr*)
Ageta, H. *et al., Phytochemistry*, 1984, **23**, 2875 (*isol, acetate*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Böhme, F. *et al., Phytochemistry*, 1997, **45**, 1041-1044 (*Cycloartanone, ms*)
Tellez, N. *et al., Molecules*, URL:http://www.mdpi.org/molbank/m0049.htm, 1998, **3**, M49; *CA*, **129**, 14430j (*2-methylbutanoate*)

Cycloart-23-ene-3,25-diol C-971

9,19-Cyclolanost-23-ene-3,25-diol, 9CI



(3β,23*E*)*–form*

$C_{30}H_{50}O_2$ 442.724

(3β,23E)-form [14599-48-5]
Isol. from *Tillandsia usneoides*, *Tricholepis glaberrima* and many other plant spp.
Prisms (EtOAc).
Mp 200-204°. $[\alpha]_D^{27}$ +38 (c, 0.85 in $CHCl_3$).

3-O-[β-D-Glucopyranosyl-(1→4)-β-D-glucopyranoside]: ***Acanthoside K_3***
[119259-75-5]
$C_{42}H_{70}O_{12}$ 767.008
Constit. of the root of *Acanthopanax sessiliflorus.*

3-Ac: [26531-71-5]
$C_{32}H_{52}O_3$ 484.761
Isol. from roots of *Sapium insigne.* Prisms (hexane).
Mp 148-150°. $[\alpha]_D^{22}$ +43 (c, 0.75 in $CHCl_3$).

Di-Ac:
Cryst. (Et_2O). Mp 105-108°.

3-Dodecanoyl: [691894-72-1]
$C_{42}H_{72}O_3$ 625.029
Constit. of *Sapium haematospermum.* Powder. $[\alpha]_D^{25}$ +22.7 (c, 0.1 in Py).

25-Me ether: ***25-Methoxycycloart-23-en-3β-ol***
[287100-42-9]
$C_{31}H_{52}O_2$ 456.751
Isol. from *Tillandsia usneoides* and a *Galaxaura* red alga species.
Needles (MeOH/Et_2O) (as acetate).
Mp 152-154° (acetate). $[\alpha]_D^{28}$ +48 (c, 0.75 in $CHCl_3$) (acetate).

3-Ketone: ***25-Hydroxycycloart-23-en-3-one***
[148044-47-7]
$C_{30}H_{48}O_2$ 440.708
Constit. of *Guarea trichiloides.* Cryst.
Mp 116-118°. $[\alpha]_D^{25}$ +15.3 (c, 1.9 in $CHCl_3$).

3-Ketone, 25-Me ether: 25-Methoxycycloart-23-en-3-one
[173866-02-9]
$C_{31}H_{50}O_2$ 454.735
Constit. of *Tillandsia usneoides.* Amorph. solid. $[\alpha]_D^{25}$ +14 (c, 0.07 in $CHCl_3$). λ_{max} 220 (log ε 3.1) (MeCN).

25-Hydroperoxide: ***25-Hydroperoxycycloart-23-en-3-ol***
[173740-54-0]
$C_{30}H_{50}O_3$ 458.723
Constit. of *Tillandsia recurvata* and *Xanthosoma robustum* (Araceae). Needles (Et_2O/hexane).
Mp 138-139° (127-128°). $[\alpha]_D^{25}$ +32 (c, 0.43 in $CHCl_3$).

25-Hydroperoxide, 3-ketone: 25-Hydroperoxycycloart-23-en-3-one
[173866-03-0]
$C_{30}H_{48}O_3$ 456.707
Constit. of *Tillandsia usneoides.* Amorph. solid.
Mp 25°. $[\alpha]_D^{25}$ +19 (c, 0.13 in $CHCl_3$). λ_{max} 222 (log ε 2.6) (MeCN).

(3β,23Z)-form
Sterculin A
[149252-09-5]
Constit. of *Euphorbia chamaesyce*, *Juncus effusus* and *Pterospermum lanceaefolium.*
Cryst. (MeOH/$CHCl_3$).
Mp 199.5-202°. $[\alpha]_D^{23}$ +43.6 (c, 0.73 in $CHCl_3$).

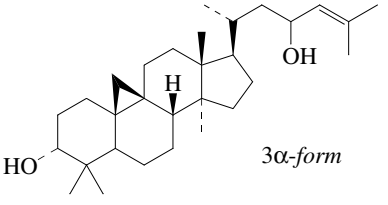
3-Ac: [215380-51-1]
Constit. of *Ficus pumila.*
Needles.
Mp 145-146°. $[\alpha]_D^{23}$ +44.1 (c, 2.3 in $CHCl_3$).

*3-(4-Hydroxy-3-methoxycinnamoyl)(*E*-):* [832095-91-7]
$C_{40}H_{58}O_5$ 618.895
Constit. of rice bran. Powder. $[\alpha]_D^{25}$ +22.4 (c, 0.25 in $CHCl_3$).

Djerassi, C. *et al., J.C.S.*, 1962, 4034 (*isol, ir, pmr, struct*)
Fourrey, J.L. *et al., Tetrahedron*, 1970, **26**, 3839 (*synth*)
Chawla, A.S. *et al., Planta Med.*, 1978, **34**, 109 (*isol*)
Srivastava, S.K. *et al., J. Nat. Prod.*, 1985, **48**, 496 (*Ac*)
De Pascual Teresa, J. *et al., Phytochemistry*, 1987, **26**, 1767 (*pmr, cmr*)
Kong, L. *et al., Zhongcaoyao*, 1988, **19**, 482; *CA*, **110**, 132187r (*Acanthoside K_3*)
Zhong, Y. *et al., CA*, 1993, **119**, 91181z (*Sterculin A*)
Furlan, M. *et al., Phytochemistry*, 1993, **32**, 1519-1522 (*3-ketone*)
Greca, M.D. *et al., Phytochemistry*, 1994, **35**, 1017-1022 (*isol, pmr, cmr*)
Singh, M. *et al., Fitoterapia*, 1995, **66**, 383 (*cmr*)
Cabrera, G.M. *et al., J. Nat. Prod.*, 1995, **58**, 1920-1920 (*hydroperoxide*)
Cabrera, G.M. *et al., J. Nat. Prod.*, 1996, **59**, 343-347 (*ketone derivs, isol, pmr, cmr*)
Tanaka, R. *et al., Phytochemistry*, 1996, **41**, 1163-1168 (*isol*)
Kato, T. *et al., Phytochemistry*, 1996, **41**, 1191 (*hydroperoxide*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1408-1411 (*Ac*)
Woldemichael, G.M. *et al., J. Nat. Prod.*, 2004, **67**, 598-603 (*3-dodecanoyl*)
Zhang, W.-H. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 59-65 (*Me ether*)
Luo, H.-F. *et al., J. Nat. Prod.*, 2005, **68**, 94-97 (*ferulate*)

Cycloart-24-ene-3,23-diol C-972

9,19-Cyclolanost-24-ene-3,23-diol



3α*-form*

$C_{30}H_{50}O_2$ 442.724

3α-form

23-Ketone: Constit. of *Monocyclanthus vignei.*
Cryst. (Me_2CO).
Mp 111-113°. $[\alpha]_D^{21}$ +15 (c, 0.4 in $CHCl_3$).

(3β,23R)-form [479679-49-7]
Constit. of *Guarea guidonia.*
Amorph. solid. $[\alpha]_D^{24}$ +35 (c, 0.21 in $CHCl_3$).

3-O-Sulfate:
$C_{30}H_{50}O_5S$ 522.788
Constit. of *Tricleocarpa fragilis.* Amorph. solid. $[\alpha]_D^{27}$ +35 (c, 0.24 in MeOH). λ_{max} 201 (MeOH).

23-Ketone: 3-Hydroxycycloart-24-en-23-one
$C_{30}H_{48}O_2$ 440.708
Constit. of *Monocyclanthus vignei.* Cryst. (Me_2CO).
Mp 130°. $[\alpha]_D^{21}$ +18 (c, 0.9 in $CHCl_3$).

23-Ketone, 3-O-sulfate: [260559-94-2]
$C_{30}H_{48}O_5S$ 520.772

Constit. of *Tricleocarpa fragilis*. Amorph. solid. $[\alpha]_D^{28}$ +20 (c, 0.54 in MeOH). λ_{max} 239 (MeOH).

Diketone: ***Cycloart-24-ene-3,23-dione****. 9,19-Cyclolanost-24-ene-3,23-dione*
$C_{30}H_{46}O_2$ 438.692
Constit. of *Monocyclanthus vignei* and *Gardenia* spp. Cryst. ($CHCl_3$/MeOH).
Mp 137-138°. $[\alpha]_D^{21}$ +6 (c, 0.85 in $CHCl_3$).

(3β,23*S*)-*form* [479679-46-4]
Constit. of *Guarea guidonia*.
Amorph. solid. $[\alpha]_D^{24}$ +23 (c, 0.15 in $CHCl_3$).

23ξ(1)-*form*

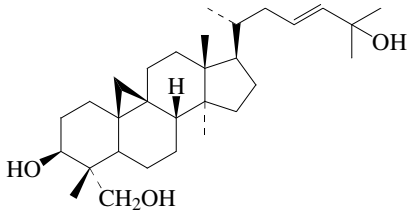
3-Ketone: 23-Hydroxycycloart-24-en-3-one
$C_{30}H_{48}O_2$ 440.708
Constit. of *Guarea trichiloides*. Cryst.
Mp 154-156°. $[\alpha]_D$ +27 (c, 1.01 in $CHCl_3$).

23ξ(2)-*form*

3-Ketone: Constit. of *Guarea trichilioides*.
Cryst.
Mp 134-136°. $[\alpha]_D^{25}$ +52.7 (c, 1.27 in $CHCl_3$). 23-Epimer of the isomer above.

Davies, N.W. *et al., Phytochemistry*, 1992, **31**, 159 (*isol, pmr, ms, ketone*)
Achenbach, H. *et al., Phytochemistry*, 1992, **31**, 4263 (*isol, pmr, cmr, ketones*)
Furlan, M. *et al., Phytochemistry*, 1993, **32**, 1519 (*isol, pmr, cmr, ketones*)
Horgen, F.D. *et al., J. Nat. Prod.*, 2000, **63**, 210-216 (*23-ketone-3-sulfate*)
Lago, J.H.G. *et al., Phytochemistry*, 2002, **60**, 333-338 (*Guarea guidonia constits*)

Cycloart-23-ene-3,25,28-triol C-973



$C_{30}H_{50}O_3$ 458.723

(3β,23*E*)-*form* [270918-16-6]
Constit. of *Aglaia rubiginosa*.

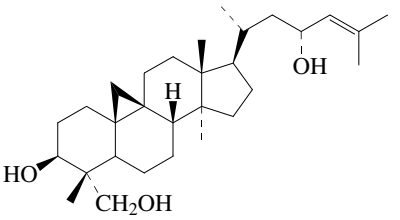
25-Me ether: ***Galaxaurol D***
[859501-80-7]
$C_{31}H_{52}O_3$ 472.75
Constit. of a *Galaxaura* red alga sp. Powder.
Mp 225-226°. $[\alpha]_D^{25}$ +30.3 (c, 0.026 in MeOH).

28-Carboxylic acid: 3,25-Dihydroxycycloart-23-en-28-oic acid
$C_{30}H_{48}O_4$ 472.707

28-Carboxylic acid, 25-Me ether, Me ester: ***Galaxaurol B***
[859501-78-3]
$C_{32}H_{52}O_4$ 500.76
Constit. of a *Galaxaura* red alga sp. Powder.
Mp 174-175°. $[\alpha]_D^{25}$ +34.2 (c, 0.023 in $CHCl_3$).

Weber, S. *et al., J. Nat. Prod.*, 2000, **63**, 636-642 (*isol, pmr, cmr*)
Zhang, W.-H. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 59-65 (*Galaxaurols*)

Cycloart-24-ene-3,23,28-triol C-974



(3β,23*R*)-*form*

$C_{30}H_{50}O_3$ 458.723

(3β,23*R*)-*form*
Galaxaurol E
[859501-81-8]
Constit. of a *Galaxaura* red alga sp.
Powder.
Mp 213-214°. $[\alpha]_D^{25}$ +62.2 (c, 0.037 in MeOH).

*3-*O*-Sulfate:* [260559-91-9]
$C_{30}H_{50}O_6S$ 538.787
Constit. of *Tricleocarpa fragilis*. Amorph. solid. $[\alpha]_D^{27}$ +35 (c, 0.14 in MeOH). λ_{max} 208 (MeOH).

23-Ketone: 3,28-Dihydroxycycloart-24-en-23-one
$C_{30}H_{48}O_3$ 456.707

*23-Ketone, 3-*O*-sulfate:* [260559-92-0]
$C_{30}H_{48}O_6S$ 536.772
Constit. of *Tricleocarpa fragilis*. Amorph. solid. $[\alpha]_D^{23}$ +28 (c, 0.12 in MeOH). λ_{max} 238 (MeOH).

28-Carboxylic acid: 3,23-Dihydroxycycloart-24-en-28-oic acid
$C_{30}H_{48}O_4$ 472.707

*28-Carboxylic acid, 3-*O*-sulfate, 28-Me ester:*
$C_{31}H_{50}O_7S$ 566.798
Constit. of *Tricleocarpa fragilis*. Amorph. solid. $[\alpha]_D^{27}$ +53 (c, 0.1 in MeOH). λ_{max} 208 (MeOH).

28-Carboxylic acid, 23-ketone: ***Gardenolic acid A****. 3-Hydroxy-23-oxocycloart-24-en-28-oic acid*
[123941-58-2]
$C_{30}H_{46}O_4$ 470.691
Constit. of *Gardenia jasminoides*. Cryst.
Mp 212-214°. $[\alpha]_D^{17}$ +38.3.

28-Carboxylic acid, 23-ketone, Me ester: ***Methyl gardenolate A****. Galaxaurol A*
[488737-14-0]
$C_{31}H_{48}O_4$ 484.718
Constit. of *Combretum woodii* and *Galaxaura* red alga sp. Powder.
Mp 165-166°. $[\alpha]_D^{25}$ +26 (c, 0.038 in $CHCl_3$). λ_{max} 252 (log ϵ 2.8) ($CHCl_3$).

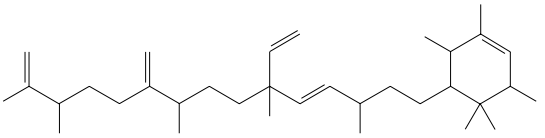
*28-Carboxylic acid, 23-ketone, 3-*O*-sulfate, Me ester:* [260559-90-8]
$C_{31}H_{48}O_7S$ 564.782
Constit. of *Tricleocarpa fragilis*.

3α-form

*23-Ketone, 28-*O*-sulfate:* [192943-02-5]
$C_{30}H_{48}O_6S$ 536.772
Constit. of *Tuemoya* sp. Amorph. powder. $[\alpha]_D$ +17 (c, 0.23 in MeOH). λ_{max} 238 (no solvent reported).

Qin, G. *et al., CA*, 1989, **111**, 228956n (*Gardenolic acid A*)
Patil, A.D. *et al., Nat. Prod. Lett.*, 1997, **9**, 209-215 (*24-ketone 28-sulfate*)
Horgen, F.D. *et al., J. Nat. Prod.*, 2000, **63**, 210-216 (*Tricleocarpa derivs*)
Coombes, P.H. *et al., Nat. Prod. Lett.*, 2002, **16**, 301-304 (*Methyl gardenolate A*)
Zhang, W.-H. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 59-65 (*Galaxaurols A,E*)

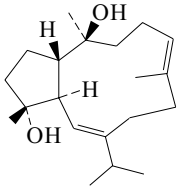
C_{34} Cyclobotryococcene C-975



$C_{34}H_{58}$ 466.832
Metab. of the alga *Botryococcus braunii*.
Metzger, P. *et al., Phytochemistry*, 1985, **24**, 2995 (*struct*)

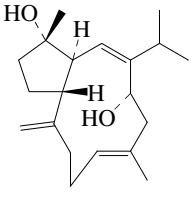
3,7-Cyclo-1,11-cembradiene-4,8-diol C-976

[103197-39-3]



$C_{20}H_{34}O_2$ 306.487
Constit. of *Cespitularia* spp. Cryst.
Mp 109-110°. $[\alpha]_D$ +93 (c, 0.046 in $CHCl_3$).
Bowden, B.F. *et al., Aust. J. Chem.*, 1986, **39**, 803 (*isol, cryst struct*)

3,7-Cyclo-1,8(19),11-cembratriene-4,14-diol C-977

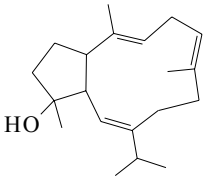


$C_{20}H_{32}O_2$ 304.472

(1*Z*,3*S*,4*S*,7*R*,11*E*,14*S*)-*form* [124616-93-9]
Constit. of *Sarcophyton glaucum*.
Kobayashi, M. *et al., Tennen Yuki Kagobutsu Toronkai Koen Yoshishu*, 1988, **30**, 212-219; *CA*, **112**, 56331g (*isol, pmr, cmr*)

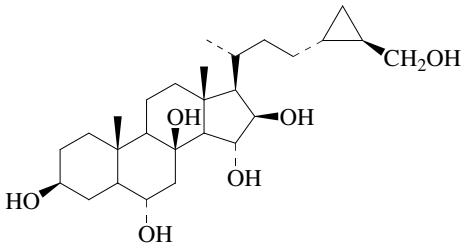
3,7-Cyclo-1,8,11-cembratrien-4-ol C-978

[103197-40-6]



$C_{20}H_{32}O$ 288.472
Constit. of *Cespitularia* spp. Oil.
Bowden, B.F. *et al., Aust. J. Chem.*, 1986, **39**, 803

24,26-Cyclocholestane-3,6,8,15,16,27-hexol C-979

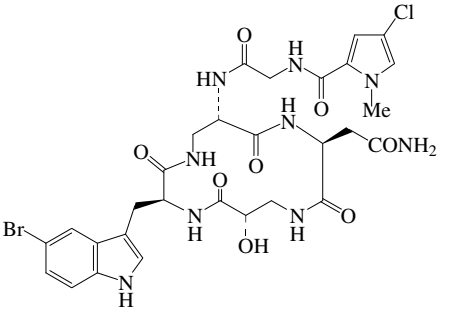


$C_{27}H_{46}O_6$ 466.657

(3β,5α,6α,8β,15α,16β,24*R*,25*R*)-*form*
Phrygiasterol
[868860-63-3]
Constit. of *Hippasteria phrygiana*.
Amorph. solid. $[\alpha]_D^{25}$ +33.2 (c, 0.25 in MeOH).
Levina, E.V. *et al., J. Nat. Prod.*, 2005, **68**, 1541-1544 (*Phrygiasterol*)

Cyclocinamide A C-980

[194427-76-4]

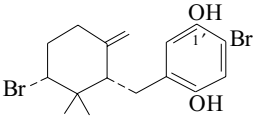


Absolute Configuration

$C_{29}H_{33}BrClN_9O_8$ 750.992
Cyclic peptide antibiotic. Isol. from the sponge *Psammocinia* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D$ +29 (c, 0.1 in MeOH).
Clark, W.D. *et al., J.A.C.S.*, 1997, **119**, 9285-9286 (*isol, pmr, cmr*)
Grieco, P.A. *et al., Tet. Lett.*, 1998, **39**, 8925-8928 (*synth, abs config*)

Cyclocymopol C-981

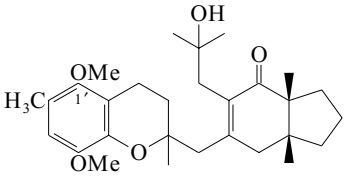
[62008-15-5]



$C_{16}H_{20}Br_2O_2$ 404.141
Metab. of *Cymopolia barbata*. Phospholipase A_2 inhibitor. Oil. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 303 (ε 8650) (MeOH) (Berdy).

1′-Me ether: [62008-00-8]
$C_{17}H_{22}Br_2O_2$ 418.168
Metab. of *Cymopolia barbata*. Viscous gum.
Högberg, H.E. *et al., J.C.S. Perkin 1*, 1976, 1696 (*isol*)
McConnell, O.J. *et al., Phytochemistry*, 1982, **21**, 2139 (*isol, struct*)
Tanaka, A. *et al., Agric. Biol. Chem.*, 1990, **54**, 121 (*synth*)

Cyclocystalgerone C-982



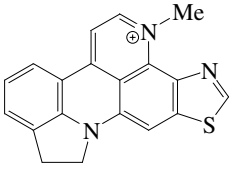
$C_{29}H_{42}O_5$ 470.648

1′-O-*De-Me:* ***Cyclo-1′-demethylcystalgerone***
[161300-11-4]
$C_{28}H_{40}O_5$ 456.621
Constit. of *Cystoseira baccata*. λ_{max} 223 (ϵ 9772); 232 (ϵ 9200); 248 (ϵ 8900); 284 (ϵ 4409) (MeOH) (Berdy).

Basabe, P. *et al., Stud. Chem.*, 1992, **17**, 101-107; *CA*, **122**, 182858d (*isol, pmr, cmr*)

Cyclodercitine C-983

[125236-61-5]

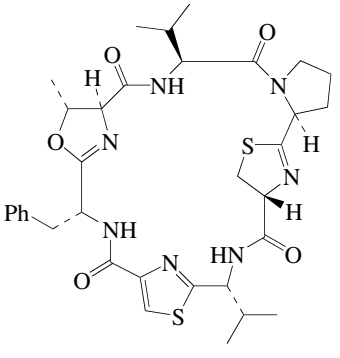


$C_{19}H_{14}N_3S^{\oplus}$ 316.406
Struct. revised in 1992. Related to *N*-Deacetylkuanoniamine D, D-30. Alkaloid from the marine sponges *Dercitus* sp. and *Stelletta* sp. Inhibits proliferation of P388 murine leukaemia cells *in vitro*. Blue powder (as chloride).
Mp 298° (chloride). λ_{max} 245 (ϵ 13800); 307 (ϵ 16900); 361 (ϵ 3900) (MeOH) (Derep).

Gunawardana, G.P. *et al., Tet. Lett.*, 1989, **30**, 4359-4362 (*isol, uv, pmr, cmr*)
Gunawardana, G.P. *et al., J.O.C.*, 1992, **57**, 1523-1526 (*struct*)

Cyclodidemnamide C-984

[170894-38-9]

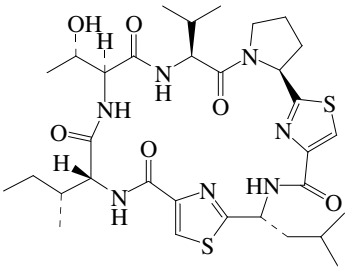


$C_{34}H_{43}N_7O_5S_2$ 693.89
Cyclic peptide antibiotic. Stereochem. revised in 1998. Isol. from *Didemnum molle*. Weak cytotoxic agent. Solid. Sol. MeOH.
Mp 114-118°. $[\alpha]_D$ +128.8 (c, 2.6 in MeOH). λ_{max} 202 (log ϵ 4.46); 248 (log ϵ 4.04) (MeOH).

Toske, S.G. *et al., Tet. Lett.*, 1995, **36**, 8355-8358 (*isol, uv, ir, pmr, cmr*)
Norley, M.C. *et al., Tet. Lett.*, 1998, **39**, 3087-3090 (*synth, struct*)
Boden, C.D.J. *et al., J.C.S. Perkin 1*, 2000, 883-888 (*synth, struct*)

Cyclodidemnamide B C-985

[446821-87-0]

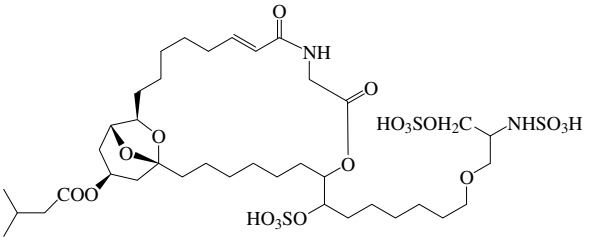


$C_{32}H_{47}N_7O_6S_2$ 689.899
Isol. from *Didemnum molle*. Amorph. solid. $[\alpha]_D$ +8.6 (c, 0.28 in $CHCl_3$).

Arrault, A. *et al., Tet. Lett.*, 2002, **43**, 4041-4044 (*isol, synth, pmr, cmr*)

Cyclodidemniserinol C-986

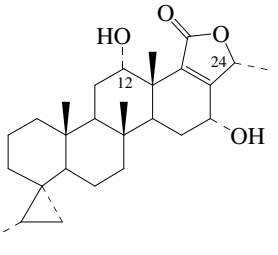
[276673-10-0]



$C_{38}H_{66}N_2O_{19}S_3$ 951.139
Isol. from the ascidian *Didemnum guttatum*. HIV-1 integrase inhibitor. Oil (as tri-Na salt). $[\alpha]_D$ -26.6 (tri-Na salt). λ_{max} 210 (ϵ 4500) (MeOH).

Mitchell, S.S. *et al., Org. Lett.*, 2000, **2**, 1605-1607

19,20-Cyclo-12,16-dihydroxy-20,24-dimethyl-17-scalaren-25,24-olide C-987



(12α,16α,24α)-*form*

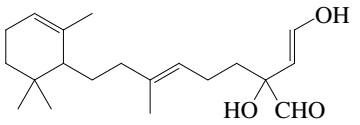
$C_{27}H_{40}O_4$ 428.611

(12α,16α,24α)-*form*
12-(3-Hydroxybutanoyl): ***Honulactone H***
[306971-13-1]
$C_{31}H_{46}O_6$ 514.701
Constit. of *Strepsichordaia aliena*. Cryst. $[\alpha]_D$ +78.3 (c, 0.75 in CH_2Cl_2).

(12α,16α,24β)-*form*
12-(3-Hydroxybutanoyl): ***Honulactone G***
[306971-12-0]
$C_{31}H_{46}O_6$ 514.701
Constit. of *Strepsichordaia aliena*. Cryst. $[\alpha]_D$ +85.7 (c, 0.85 in CH_2Cl_2).

Jiménez, J.I. *et al., J.O.C.*, 2000, **65**, 6837-6840 (*isol, pmr, cmr*)

10,15-Cyclo-1,3-dihydroxy-1,6,11-phytatrien-20-al C-988

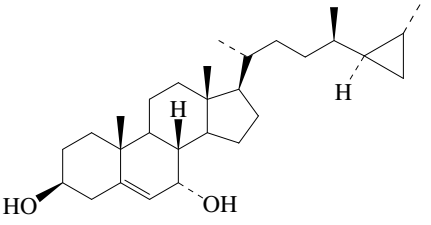


$C_{20}H_{32}O_3$ 320.471
Enol.

(1*E*,3ξ,6*E*,10ξ)-*form*
Di-Ac: [849475-56-5]
$C_{24}H_{36}O_5$ 404.545
Constit. of *Caulerpa brownii*. Oil. $[\alpha]_D$ -103 (c, 0.79 in EtOH).
Handley, J.T. *et al., Aust. J. Chem.*, 2005, **58**, 39-46 (*isol, pmr, cmr*)

26,27-Cyclo-24,26-dimethylcholest-5-ene-3,7-diol C-989

24-(2-Methylcyclopropyl)-26,27-dinorcholest-5-ene-3,7-diol

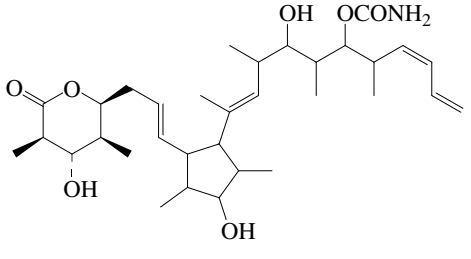


$C_{29}H_{48}O_2$ 428.697

(3β,7α,24*R*,25*R*,26*R*)-*form*
7α-Hydroxypetrosterol
[306967-76-0]
Constit. of *Strongylophora corticata*.
Amorph. powder.
Mp 124-127°. $[\alpha]_D^{21}$ -55.3 (c, 0.11 in MeOH).
7-Ketone: 26,27-Cyclo-3-hydroxy-24,26-dimethylcholest-5-en-7-one. 3-Hydroxy-24-(2-methylcyclopropyl)-26,27-dinorcholest-5-en-7-one. ***7-Oxopetrosterol***
[306967-75-9]
$C_{29}H_{46}O_2$ 426.681
Constit. of *Strongylophora corticata*. Amorph. powder.
Mp 107-110°. $[\alpha]_D^{21}$ -65.4 (c, 0.62 in MeOH). λ_{max} 238 (log ϵ 3.93) (MeOH).
Umeyama, A. *et al., J. Nat. Prod.*, 2000, **63**, 1540-1542 (*isol, pmr, cmr*)

9(13)-Cyclodiscodermolide C-990

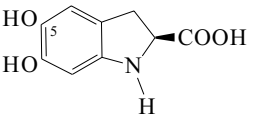
[476172-88-0]



$C_{33}H_{53}NO_7$ 575.784
Isol. from a *Discodermia* sp. Solid. $[\alpha]_D^{21}$ +24 (c, 0.01 in MeOH).
Gunasekera, S.P. *et al., J. Nat. Prod.*, 2002, **65**, 1643-1648 (*isol, pmr, cmr*)

Cyclodopa C-991

*2,3-Dihydro-5,6-dihydroxy-1*H*-indole-2-carboxylic acid, 9CI. Leucodopachrome*
[18791-20-3]



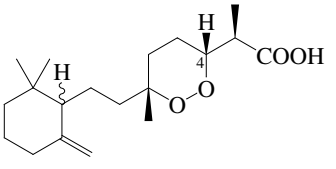
$C_9H_9NO_4$ 195.174

(*S*)-*form* [18766-67-1]
Degradn. prod. of Betanidin. $[\alpha]_D^{25}$ -92 (c, 1.65 in 20% HCl).
5-O-β-D-Glucopyranoside: ***Cyclodopa glucoside***
[71242-23-4]
$C_{15}H_{19}NO_9$ 357.316
Occurs in red beet cabbage juice. Prob. intermed. in biosynth. of Betanidin.
Mp 159.5-162.5°. $[\alpha]_D^{20.5}$ -110.7 (H_2O, pH 3). pK_{a1} 1.58; pK_{a2} 4.75; pK_{a3} 9.42.
Tri-Ac, Me ester: Mp 94-96° (after drying). $[\alpha]_D^{20}$ -61 (c, 1.03 in $CHCl_3$).

(±)-*form*
Tri-Ac, Me ester: Mp 157.5-158.5°.

(ξ)-*form*
O^5,N,N-*Tri-Me:* [165329-95-3]
$C_{12}H_{15}NO_4$ 237.255
Metab. of the Caribbean sponge *Pseudoceratina crassa*.
$[\alpha]_D^{25}$ -12 (c, 0.001 in MeOH). Zwitterion.
Wyler, H. *et al., Helv. Chim. Acta*, 1962, **45**, 638; 1968, **51**, 1476; 1984, **67**, 1348
Ciminiello, P. *et al., J. Nat. Prod.*, 1995, **58**, 689 (*tri-Me*)

10,15-Cyclo-4,7-epidioxy-1-nor-11(18)-phyten-2-oic acid C-992

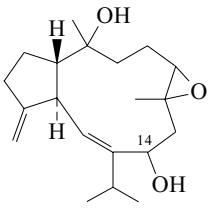


$C_{19}H_{32}O_4$ 324.459

(3*R*,4*R*,7*R*,10ξ)-*form* [204500-39-0]
Constit. of *Diacarnus* cf. *spinopoculum*.
Oil. $[\alpha]_D$ +45 (c, 0.46 in $CHCl_3$).
Me ester: ***Nuapapuin B***
[204500-40-3]
$C_{20}H_{34}O_4$ 338.486
Constit. of *Diacarnus* cf. *spinopoculum*. Oil. $[\alpha]_D$ +39 (c, 1.74 in $CHCl_3$).

(3*R*,4*S*,7*R*,10ξ)-*form*
Me ester: ***Epinuapapuin B***
$C_{20}H_{34}O_4$ 338.486
Constit. of *Diacarnus* cf. *spinopoculum*. Oil. $[\alpha]_D$ -41.6 (c, 1.5 in $CHCl_3$).
Sperry, S. *et al., J. Nat. Prod.*, 1998, **61**, 241-247 (*isol, pmr, cmr*)

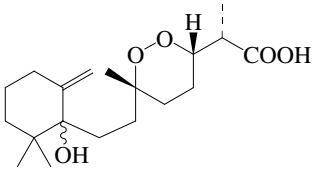
3,7-Cyclo-11,12-epoxy-1,4(18)-cembradiene-8,14-diol C-993



$C_{20}H_{32}O_3$ 320.471
Constit. of *Sarcophyton trocheliphorum*.

14-Ac:
Cryst. Mp 77-79°. $[\alpha]_D$ -120 (c, 0.42 in $CHCl_3$).
Venkateswarlu, Y. *et al., Nat. Prod. Lett.*, 1994, **5**, 131 (*isol, pmr, cmr*)

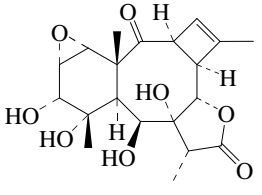
10,15-Cyclo-4,7-epoxy-10-hydroxy-1-nor-11(18)-phyten-2-oic acid C-994



$C_{19}H_{32}O_5$ 340.459

(3*S*,4*S*,7*S*,10ξ)-*form*
Me ester: ***Aikupikoxide B***
[377088-39-6]
$C_{20}H_{34}O_5$ 354.486
Constit. of Red Sea sponge *Diacarnus erythraenus*. Oil. $[\alpha]_D$ +76 (c, 0.5 in CH_2Cl_2).
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2001, **64**, 1332-1335 (*isol, pmr, cmr*)

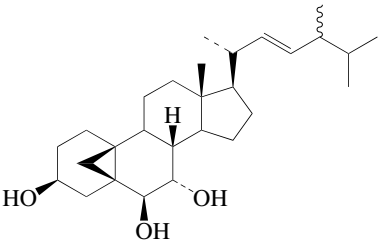
3,6-Cyclo-13,14-epoxy-8,9,11,12-tetrahydroxy-2-oxo-4-briaren-18,7-olide C-995



$C_{20}H_{26}O_8$ 394.421

(3α*H*,6α*H*,7α,8α,9β,11α,12α,13α,14α)-*form*
12-Butanoyl, 9-Ac: ***Cyclobutenbriarein A***
[446823-27-4]
$C_{26}H_{34}O_{10}$ 506.549
Constit. of *Briareum asbestinum*. Solid. $[\alpha]_D^{27}$ -22.8 (c, 0.22 in $CHCl_3$). λ_{max} 222 (log ϵ 3.44); 264 (log ϵ 2.73) (MeOH).
González, N. *et al., J.O.C.*, 2002, **67**, 5117-5123 (*isol, pmr, cmr*)

5,19-Cycloergost-22-ene-3,6,7-triol C-996

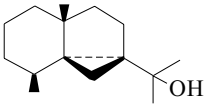


$C_{28}H_{46}O_3$ 430.67

(3β,5β,6β,7α,22*E*,24ξ)-*form*
Hatomasterol
[848132-38-7]
Constit. of a *Stylissa* sp.
Powder.
Mp 188-192°. $[\alpha]_D^{25}$ +10.5 (c, 1.1 in MeOH).
Mitome, H. *et al., Steroids*, 2005, **70**, 63-70 (*Hatomasterol*)

Cycloeudesmol C-997

Isocycloeudesmol
[75744-72-8]

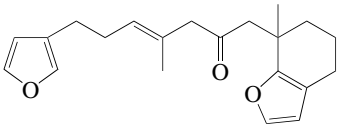


$C_{15}H_{26}O$ 222.37
Isol. from *Laurencia nipponica* and *Chondria oppositiclada*. Shows antibiotic props. Cryst. (hexane/isopropyl ether). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 99.5-100.5°. $[\alpha]_D$ +21.5 (c, 2.1 in $CHCl_3$).

Suzuki, T. *et al., Chem. Lett.*, 1980, 1267 (*isol, struct*)
Suzuki, T. *et al., Tet. Lett.*, 1981, **22**, 3423 (*cryst struct, abs config*)
Chen, E.Y. *et al., Tet. Lett.*, 1982, **23**, 4769 (*synth*)
Chen, E.Y. *et al., J.O.C.*, 1984, **49**, 3245 (*synth*)
Ando, M. *et al., J.O.C.*, 1985, **50**, 251 (*struct*)
Ando, M. *et al., Tet. Lett.*, 1985, **26**, 235 (*synth*)

Cyclofurospongin 2 C-998

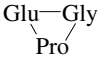
[192223-14-6]



$C_{21}H_{26}O_3$ 326.435
Constit. of *Spongia officinalis*. Oil. $[\alpha]_D^{25}$ -6 (c, 0.1 in $CHCl_3$). λ_{max} 207 (ϵ 18452) (MeOH).

Garrido, L. *et al., J. Nat. Prod.*, 1997, **60**, 794-797 (*isol, pmr, cmr*)

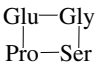
Cyclo(glutamylglycylprolyl) C-999



$C_{12}H_{17}N_3O_5$ 283.283
Prod. by a strain of *Ruegeria* sp. isol. from the sponge *Suberites domuncula*. Antibacterial agent. Amorph. solid. $[\alpha]_D^{25}$ -27.8 (c, 0.001 in MeOH).

Mitova, M. *et al., J. Nat. Prod.*, 2004, **67**, 1178-1181 (*isol, pmr, cmr, ms*)

Cyclo(glutamylglycylserylprolyl) C-1000



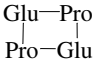
$C_{15}H_{22}N_4O_7$ 370.361

Prod. by a strain of *Ruegeria* sp. isol. from the sponge *Suberites domuncula*. Antibacterial agent. Amorph. solid. $[\alpha]_D^{25}$ -26.9 (c, 0.002 in MeOH).

Mitova, M. *et al., J. Nat. Prod.*, 2004, **67**, 1178-1181 (*isol, pmr, cmr, ms*)

Cyclo(glutamylprolylglutamylprolyl) C-1001

[82081-23-0]



$C_{20}H_{28}N_4O_8$ 452.463

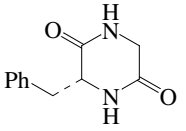
Prod. by a strain *Ruegeria* sp. isol. from the sponge *Suberites domuncula*. Amorph. solid. $[\alpha]_D^{25}$ -14.9 (c, 0.002 in MeOH).

Fusaoka, Y. *et al., Int. J. Pept. Protein Res.*, 1989, **34**, 104-110 (*synth*)
Mitova, M. *et al., J. Nat. Prod.*, 2004, **67**, 1178-1181 (*isol, ms*)

Cyclo(glycylphenylalanyl) C-1002

3-(Phenylmethyl)-2,5-piperazinedione, 9CI. 3-Benzyl-2,5-piperazinedione, 8CI. Cyclo(phenylalanylglycyl)

[5037-75-2]
[23927-19-7]



$C_{11}H_{12}N_2O_2$ 204.228

(*S*)-*form* [10125-07-2]

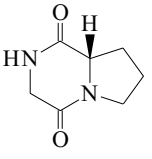
Prod. by a marine endophytic fungus.
Mp 273-275° dec. $[\alpha]_D^{20}$ +100.8 (c, 1 in AcOH).

Nitecki, D.E. *et al., J.O.C.*, 1968, **33**, 864-866 (*synth*)
Deslauriers, R. *et al., J.A.C.S.*, 1975, **97**, 5093-5100 (*cmr, conformn*)
Shin, C.-G. *et al., Heterocycles*, 1980, **14**, 1767-1770 (*synth*)
Kricheldorf, H.R. *et al., Org. Magn. Reson.*, 1980, **13**, 52-58 (*cmr, N-15 nmr*)
Suzuki, K. *et al., Chem. Pharm. Bull.*, 1981, **29**, 233-237 (*synth*)
Van der Greef, J. *et al., J. Chromatogr.*, 1987, **394**, 77-88 (*isol*)
Chen, G. *et al., Tetrahedron*, 2003, **59**, 4907-4909 (*marine isol*)

Cyclo(glycylprolyl) C-1003

Hexahydropyrrolo[1,2-a]pyrazine-1,4-dione, 9CI. 3,6-Dioxohexahydropyrrolo[1,2-a]pyrazine (incorr.). Cyclo(prolylglycyl). 1,4-Diazabicyclo[4.3.0]nonane-2,5-dione

[19179-12-5]



(*S*)−*form*

$C_7H_{10}N_2O_2$ 154.168

(*S*)-*form*

L-form

[3705-27-9]

Prod. by cultures of *Fusarium* spp. Isol. from the echinoderm *Luidia clathrata*. Constit. of *Pinellia pedatisecta*. Prod. by the marine bacteria *Ruegeria* sp. SDC-1 and *Pseudoalteromonas luteoviolacea*.

Cryst. (MeOH/Me_2CO).
Mp 216-218°. $[\alpha]_D^{20}$ -217.4 (c, 7.5 in H_2O).

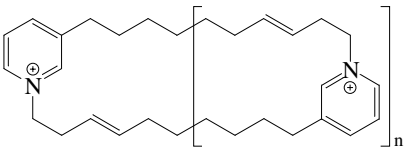
(±)-*form* [62057-47-0]

Cryst. (MeOH/Me_2CO). Mp 216-218°.

[96193-26-9]

Vičar, J. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 4060; 1973, **38**, 1940; 1957 (*synth, ir, pmr, bibl*)
Blaha, K. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 4660 (*synth*)
White, E.P. *et al., N.Z. J. Sci.*, 1972, **15**, 178; *CA*, **77**, 98731b (*isol*)
Blaha, K. *et al., Tet. Lett.*, 1972, 1437 (*synth*)
Pettit, G.R. *et al., Experientia*, 1973, **29**, 521 (*isol, ms, struct*)
Von Dreele, R.B. *et al., Acta Cryst. B*, 1975, **31**, 966 (*cryst struct*)
Johnstone, R.A.W. *et al., J.C.S. Perkin 2*, 1975, 1297 (*ms*)
Siemion, I.Z. *et al., Org. Magn. Reson.*, 1976, **8**, 432 (*cmr*)
Qin, W. *et al., Zhongcaoyao*, 1984, **15**, 490; *CA*, **102**, 109774f (*isol*)
de Costa, B.R. *et al., J. Med. Chem.*, 1993, **36**, 2311 (*synth, pmr*)
Jiang, Z. *et al., Nat. Prod. Lett.*, 2000, **14**, 435-440 (*isol, pmr, cmr*)
Mitova, M. *et al., J. Nat. Prod.*, 2004, **67**, 1178-1181 (*isol*)

Cyclohaliclonamines C-1004



Cyclohaliclonamide	A	n = 1
"	B	n = 2
"	C	n = 3
"	D	n = 4
"	E	n = 5

Alkaloids from the sponge *Haliclona* sp.

Cyclohaliclonamine A

$C_{30}H_{44}N_2^{\oplus}$ 432.691

Cyclohaliclonamine B

$C_{45}H_{66}N_3^{\oplus}$ 649.037

Cyclohaliclonamine C

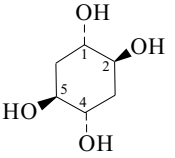
$C_{60}H_{88}N_4^{\oplus}$ 865.382

Cyclohaliclonamine D

Cyclohaliclonamine E

Teruya, T. *et al., J. Nat. Prod.*, 2006, **69**, 135-137 (*isol, pmr, cmr, ms*)

1,2,4,5-Cyclohexanetetrol, 9CI C-1005



(1*S*,2*S*,4*S*,5*S*)−*form*

$C_6H_{12}O_4$ 148.158

5 Stereoisomeric forms possible, 3 *meso* and 2 (±). All are known.

(1*S*,2*S*,4*S*,5*S*)-*form*

(1α,2β,4α,5β)-(+)-form. D-form (obsol.)

Constit. of the alga *Monochrysis lutheri*.
Prisms (EtOH).
Mp 205-207° dec. (after sintering at 131-132°). $[\alpha]_D^{21}$ +22.5 (c, 1.06 in H_2O).

Tetra-Ac:

$C_{14}H_{20}O_8$ 316.307
Viscous oil. $[\alpha]_D^{21}$ +10.1 (c, 1.53 in $CHCl_3$).

Tetrabenzoyl:
$C_{34}H_{28}O_8$ 564.59
Viscous oil. $[\alpha]_D^{21}$ -28.3 (c, 1.06 in $CHCl_3$).

*Tetrakis-*O*-trifluoroacetyl:*
$C_{14}H_8F_{12}O_8$ 532.193
Mp 104-106°.

*Tetrakis-*O*-trimethylsilyl:*
$C_{18}H_{44}O_4Si_4$ 436.885
Mp 57-59°.

(1*RS*,2*RS*,4*RS*,5*RS*)-*form*
(1α,2β,4α,5β)-(±)-form. D,L*-form (obsol.)*
Cryst. (EtOH). Mp 208°.

Tetra-Ac:
Cryst. (EtOH). Mp 148°.

Tetrabenzoyl: Mp 181°.

(1*RS*,2*SR*,4*RS*,5*SR*)-*form*
(1α,2α,2α,3α,4α)-form. all-cis-*form*
Cryst. (EtOH). Mp 224-225°. Opt. inactive (*meso*-).

Tetra-Ac:
Cryst. (EtOH). Mp 127-128°.

(1*RS*,2*SR*,4*SR*,5*RS*)-*form*
(1α,2α,4β,5β)-form
[45775-30-2]
Cryst. (EtOH). Mp 240-241°. Opt. inactive (*meso*-).

Tetra-Ac:
Cryst. (EtOH). Mp 169-170°.

(1*RS*,2*RS*,4*SR*,5*SR*)-*form*
(1α,2β,4β,5α)-form
Cryst. (EtOH). Mp 284-285° dec. Opt. inactive (*meso*-).

Tetrabenzoyl:
Cryst. ($CHCl_3$/EtOH). Mp 266-267°.

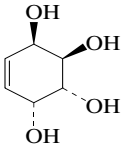
(1*RS*,2*SR*,4*RS*,5*RS*)-*form*
(1α,2α,4α,5β)-(±)-form
Cryst. (EtOH). Mp 208-209°.

Tetrabenzoyl:
Cryst. (EtOH/C_6H_6). Mp 172-173°.

McCasland, G.E. *et al., J.A.C.S.*, 1954, **76**, 1654; 2373 (*synth*)
Shoolery, J.N. *et al., J.O.C.*, 1963, **28**, 894 (*synth, pmr*)
Ramanathan, J.D. *et al., Tet. Lett.*, 1966, 1527 (*isol, abs config*)
Tschamber, T. *et al., Helv. Chim. Acta*, 1992, **75**, 1052 (*synth*)
Maras, A. *et al., Carbohydr. Res.*, 1998, **308**, 435-437 (*1RS,2RS,4RS,5RS-form, !synth*)
Mehta, G. *et al., Acta Cryst. C*, 2005, **61**, 358-360 (*cryst struct*)

5-Cyclohexene-1,2,3,4-tetrol C-1006

3,4,5,6-Tetrahydroxycyclohexene. ***Conduritol***



(1*R*S,2*R*S,3*R*S,4*R*S)-*form*

$C_6H_{10}O_4$ 146.143

(1*RS*,2*RS*,3*RS*,4*RS*)-*form*
(1α,2α,3β,4β)-form. Conduritol E
[4942-62-5]
Mp 179-180°. A racemate. Known also in opt. active forms ((+)-form, Mp 193°, $[\alpha]_D$ +332 (H_2O)).

*Tetra-Ac: Tetra-*O*-acetylconduritol E*
[143615-78-5]
$C_{14}H_{18}O_8$ 314.291
Cryst. (EtOAc/hexane). Mp 156° (153°). $Bp_{0.6}$ 165°.

*1,2:3,4-Di-*O*-isopropylidene: 1,2:3,4-Di-*O*-isopropylideneconduritol E*
[142129-09-7]
$C_{12}H_{18}O_4$ 226.272
Mp 60-61°.

(1*RS*,2*RS*,3*RS*,4*SR*)-*form*
(1α,2α,3β,4α)-form. ***Conduritol F****. Leucanthemitol*
[4782-76-7]
[6090-98-8]
Constit. of *Chrysanthemum leucanthemum, Chrysanthemum maximum, Hoya carnosa, Thuja occidentalis*, and *Chlorella fusca*. Found in opt. active form in nearly all green plants in small amts.. Mp 103-104°. A racemate, to which the Mp given refers. The naturally occurring isomer is the (+)-form having Mp 134°, $[\alpha]_D$+101.5 (H_2O).

*Tetra-Ac: Tetra-*O*-acetylconduritol F*
[6216-24-6]
$C_{14}H_{18}O_8$ 314.291
Mp 92°.

*2-*O*-β-*D*-Glucopyranoside:* [209542-57-4]
$C_{12}H_{20}O_9$ 308.285
Constit. of *Marsdenia tomentosa*. Solid. $[\alpha]_D^{25}$ -22.5 (c, 1.2 in H_2O).

*3-*O*-β-*D*-Glucopyranoside:*
$C_{12}H_{20}O_9$ 308.285
Constit. of *Asclepias curassavica* and *Cynanchum liukiuense.* Amorph solid. $[\alpha]_D^{25}$ -30 (c, 0.25 in H_2O).

*4-*O*-β-*D*-Glucopyranoside:*
$C_{12}H_{20}O_9$ 308.285
Constit. of *Cynanchum liukiuense*. Amorph. solid. $[\alpha]_D^{26}$ -4.6 (c, 0.34 in MeOH).

(1*RS*,2*RS*,3*SR*,4*RS*)-*form*
(1α,2α,3α,4β)-form. Conduritol C
[4942-61-4]
Mp 150-152° (146-148°). A racemate. Known also in opt. active forms. ((-)-form, Mp 146-148°, $[\alpha]_D^{25}$ -209 (H_2O)).

*Tetra-Ac: Tetra-*O*-acetylconduritol C*
[143615-79-6]
$C_{14}H_{18}O_8$ 314.291
Mp 92°.

(1*RS*,2*RS*,3*SR*,4*SR*)-*form*
(1α,2α,3α,4α)-form. Conduritol D
[4782-75-6] Opt. inactive (*meso*-).

*Tetra-Ac: Tetra-*O*-acetylconduritol D*
[123354-99-4]
$C_{14}H_{18}O_8$ 314.291
Mp 102-104°.

*Tetrabenzoyl: Tetra-*O*-benzoylconduritol D*
$C_{34}H_{26}O_8$ 562.575
Mp 184°.

*1,2:3,4-Di-*O*-isopropylidene:*
$C_{12}H_{18}O_4$ 226.272
Mp 67-68°. Cryst. with difficulty.

(1*RS*,2*SR*,3*RS*,4*SR*)-*form*
(1α,2β,3β,4α)-form. ***Conduritol A***
[526-87-4]
Constit. of condurango bark (*Marsdenia condurango*), four genera of Aselepiadaceae, and six families of Dicotyledons.
Large tetragonal prisms.
Mp 118° Mp 142-143°. Opt. inactive (*meso*-).

*1-*O*-α-*D*-Galactopyranoside:* [209542-55-2]
$C_{12}H_{20}O_9$ 308.285
Constit. of *Marsdenia tomentosa*. Solid. $[\alpha]_D^{24}$ +106.5 (c, 0.8 in MeOH).

*2- or 3-*O*-β-*D*-Glucopyranoside:*
$C_{12}H_{20}O_9$ 308.285
Constit. of *Marsdenia tomentosa*. Solid. $[\alpha]_D^{26}$ +21.3 (c, 0.5 in H_2O).

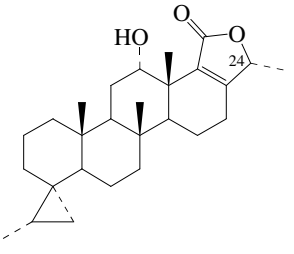
(1*RS*,2*SR*,3*SR*,4*RS*)-*form*
(1α,2β,3α,4β)-form. Conduritol B
[25348-64-5]
Mp 205°. A racemate. Known also in opt. active forms. ((-)-form, Mp 179.2°, $[\alpha]_D^{20}$ -156.0 (MeOH)).

*Tetra-Ac: Tetra-*O*-acetylconduritol B*
[25348-63-4]

$C_{14}H_{18}O_8$ 314.291
Mp 92-93° (85-85.5°).

Nakajima, M. *et al., Chem. Ber.*, 1957, **90**, 246-250 (*Conduritol A, Conduritol B, Conduritol C, Conduritol E, synth*)
Angyal, S.J. *et al., J.C.S.*, 1958, 375-379 (*Conduritol D, synth*)
Posternak, Th. *et al., The Cyclitols*, Holden-Day, San Francisco, 1965, 145
Kindl, H. *et al., Monatsh. Chem.*, 1966, **97**, 1783-1786 (*Leucanthemitol, isol*)
Sütbeyaz, Y. *et al., Chem. Comm.*, 1988, 1330-1331 (*Conduritol A, synth*)
Le Drian, C. *et al., Helv. Chim. Acta*, 1989, **72**, 338; 1990, **73**, 161-168 (*Conduritol C, Conduritol B, Conduritol F, synth, bibl, abs config*)
Cambie, R.C. *et al., Synth. Commun.*, 1989, **19**, 537-546 (*Conduritol A, synth*)
Balci, M. *et al., Tetrahedron*, 1990, **46**, 3715-3742 (*rev*)
Carless, H.A.J. *et al., Chem. Comm.*, 1992, 234-235 (*Conduritol C, synth*)
Tschamber, T. *et al., Helv. Chim. Acta*, 1992, **75**, 1052-1060 (*Conduritol C, Conduritol D, Conduritol E, synth, pmr*)
Dumortier, L. *et al., Synlett*, 1992, 243-245 (*Conduritol C, Conduritol E, Conduritol F, synth*)
Secen, H. *et al., Synth. Commun.*, 1992, **22**, 2613-2619 (*Conduritol C, Conduritol E, synth*)
Akiyama, T. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 3760-3767 (*Conduritol B, Conduritol F, synth*)
Chretien, F. *et al., Nat. Prod. Lett.*, 1993, **2**, 69-75 (*Conduritol E, Conduritol F, synth*)
Guo, Z.X. *et al., Carbohydr. Res.*, 1994, **264**, 147-153 (*Conduritol B, !synth*)
Mereyala, H.B. *et al., J.C.S. Perkin 1*, 1994, 2187-2190 (*Conduritol A, Conduritol C, synth*)
Takano, S. *et al., J.O.C.*, 1994, **59**, 54-57 (*Conduritol E, synth*)
Secen, H. *et al., Synth. Commun.*, 1994, **24**, 2103-2108 (*Conduritol F, synth, cmr*)
Patti, A. *et al., J.O.C.*, 1996, **61**, 6458-6461 (*Conduritol F, synth*)
Balci, M. *et al., Pure Appl. Chem.*, 1997, **69**, 97-104 (*rev, synth*)
Yoshizaki, H. *et al., J.O.C.*, 1998, **63**, 9339-9341 (*Conduritol C, synth, pmr, cmr*)
Abe, F. *et al., Phytochemistry*, 1998, **47**, 1297-1301 (*isol, glycosides*)
Angelaud, R. *et al., J.O.C.*, 1999, **64**, 9613-9624 (*Conduritol E, synth, pmr*)
Abe, F. *et al., Chem. Pharm. Bull* , 2000, **48**, 1090-1092 (*glucosides*)
Mehta, G. *et al., Tet. Lett.*, 2000, **41**, 3509-3512 (*Conduritol E, synth*)
Cere, V. *et al., Tetrahedron*, 2000, **56**, 1225-1231 (*synth*)
Kwon, Y.-U. *et al., J.O.C.*, 2002, **67**, 3327-3338 (*synth*)
De Souza, S.E. *et al., Tetrahedron*, 2002, **58**, 4643-4654 (*Conduritol F, synth, tetra-Ac*)
Gultekin, M.S. *et al., Curr. Org. Chem.*, 2004, **8**, 1159-1186 (*rev*)
Finn, K.J. *et al., Tetrahedron*, 2006, **62**, 7471-7476 (*Conduritol E, synth*)

19,20-Cyclo-12-hydroxy-20,24-dimethyl-17-scalaren-25,24-olide C-1007



(12α,24α)-*form*

$C_{27}H_{40}O_3$ 412.611

(12α,24α)-*form*

12-(3-Hydroxybutanoyl): ***Honulactone B***
[306971-07-3]
$C_{31}H_{46}O_5$ 498.701
Constit. of *Strepsichordaia aliena*. Cryst. $[\alpha]_D$ +77 (c, 0.66 in CH_2Cl_2).

12-(3-Hydroxypentanoyl): ***Honulactone F***
[306971-11-9]
$C_{32}H_{48}O_5$ 512.728
Constit. of *Strepsichordaia aliena*. Cryst. $[\alpha]_D$ +81.5 (c, 1.1 in CH_2Cl_2).

(12α,24β)-*form*

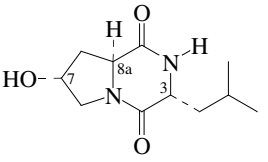
12-(3-Hydroxybutanoyl): ***Honulactone A***
[306971-06-2]
$C_{31}H_{46}O_5$ 498.701
Constit. of *Strepsichordaia aliena*. Cryst. $[\alpha]_D$ +73.2 (c, 0.71 in CH_2Cl_2).

12-(3-Hydroxypentanoyl): ***Honulactone E***
[306971-10-8]
$C_{32}H_{48}O_5$ 512.728
Constit. of *Strepsichordaia aliena*. Cryst. $[\alpha]_D$ +105.2 (c, 1.5 in CH_2Cl_2).

Jiménez, J.I. *et al., J.O.C.*, 2000, **65**, 6837-6840 (*isol, pmr, cmr, cryst struct*)

Cyclo(4-hydroxyprolylleucyl) C-1008

Hexahydro-7-hydroxy-3-(2-methylpropyl)pyrrolo[1,2-a]pyrazine-1,4-dione, 9CI. Hydroxyproline leucine anhydride
[308368-99-2]



(3*R*,7*R*,8*aS*)-*form*

$C_{11}H_{18}N_2O_3$ 226.275

(3*R*,7*R*,8*aS*)-*form*

L-D-form
[208850-33-3]
Isol. from a marine bacterium associated with a *Palythoa* sp.
Solid. $[\alpha]_D$ +14.7 (c, 0.34 in MeOH). λ_{max} 230 (MeOH).

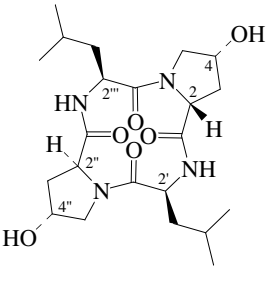
(3*S*,7*R*,8*aR*)-*form* [205648-55-1]
Metab. of the marine yeast *Aureobasidium pullulans* and two marine bacteria associated with the sponge *Ircinia variabilis.*
Amorph. solid. $[\alpha]_D^{24}$ +40.5 (c, 1 in MeOH).

(3*S*,7*R*,8*aS*)-*form*

7-Hydroxygancidin W. *L-L*-form
[115006-86-5]
Isol. from rabbit skin tissue. Also from a marine bacterium associated with a *Palythoa* sp. and two marine bacteria associated with the sponge *Ircinia variabilis.* Plant growth regulator.
Mp 178-179°. $[\alpha]_D^{28}$ -148.2 (c, 1 in H_2O). λ_{max} 232 (MeOH).

Ienaga, K. *et al., Tet. Lett.*, 1987, **28**, 1285-1286 (*3S,7R,8aS-form, isol, pmr, cmr, struct*)
Shigemori, H. *et al., J. Nat. Prod.*, 1998, **61**, 696-698 (*3S,7R,8aR-form, isol, ir, pmr, cmr*)
Cronan, J.M. *et al., Nat. Prod. Lett.*, 1998, **11**, 271-278 (*Palythoa sp, isol, uv, pmr, cmr*)
De Rosa, S. *et al., Biomol. Eng.*, 2003, **20**, 311-316 (*Ircinia variabilis constits*)
Mitova, M. *et al., Z. Naturforsch., C*, 2003, **58**, 740-745 (*Ircinia variabilis constit*)

Cyclo(4-hydroxyprolylleucyl-4-hydroxyprolylleucyl) C-1009



$C_{22}H_{36}N_4O_6$ 452.55

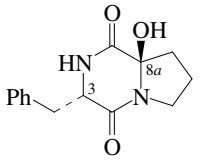
(2*R*,2′*S*,2″*S*,2‴*S*,4*R*,4″*R*)-*form*

Prod. by a *Pseudomonas* sp. strain IM-1 associated with the sponge *Ircinia muscarum*.
Amorph. solid. $[\alpha]_D$ -18.1 (c, 0.01 in MeOH).

Mitova, M. *et al., Z. Naturforsch., C*, 2003, **58**, 740-745 (*isol, pmr, cmr*)

Cyclo(2-hydroxyprolylphenylalanyl) C-1010

*Hexahydro-8*a*-hydroxy-3-(phenylmethyl)pyrrolo[1,2-*a*]pyrazine-1,4-dione, 9CI*



(3*S*,8*aR*)-*form*

$C_{14}H_{16}N_2O_3$ 260.292

(3*S*,8*aR*)-*form*

D,L-form

Prod. by the marine-derived *Chromocleista* sp. strain R721. $[\alpha]_D^{25}$ -26.1 (c, 0.03 in MeOH). λ_{max} 198 (log ϵ 3.5); 257 (log ϵ 0.3) (MeOH).

*8*a*-Deoxy, 8,8*a*-didehydro: 2,3,6,7-Tetrahydro-3-(phenylmethyl)-pyrrolo[1,2-*a*]pyrazine-1,4-dione, 9CI*

$C_{14}H_{14}N_2O_2$ 242.277

Prod. by *Chromocleista* sp. strain R721. $[\alpha]_D^{25}$ -31.9 (c, 0.05 in MeOH). Dec. prod. of parent. λ_{max} 200 (log ϵ 3.7); 257 (log ϵ 0.5); 330 (log ϵ 0.2) (MeOH).

(3*S*,8*aS*)-*form*

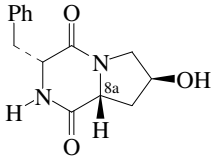
L,L-form

Prod. by the marine-derived *Chromocleista* sp. strain R721. λ_{max} 200 (log ϵ 3.7); 257 (log ϵ 0.4) (MeOH).

Park, Y.C. *et al., J. Nat. Prod.*, 2006, **69**, 580-584 (*isol, pmr, cmr*)

Cyclo(4-hydroxyprolylphenylalanyl) C-1011

*Hexahydro-7-hydroxy-3-(phenylmethyl)pyrrolo[1,2-*a*]pyrazine-1,4-dione, 9CI. 3-Benzylhexahydro-7-hydroxypyrrolo[1,2-*a*]pyrazine-1,4-dione*



(3*R*,7*S*,8*aR*)-*form*

$C_{14}H_{16}N_2O_3$ 260.292

(3*R*,7*S*,8*aR*)-*form* [631922-77-5]

Prod. by the marine bacterial strains CF-20 and C-148 obt. from the mollusc *Pecten maximus*. Active against *Vibrio anguillarum*. $[\alpha]_D$ +7.3 (c, 0.02 in MeOH). Error in struct. diag. in ref.

(3*S*,7*R*,8*aR*)-*form* [205648-54-0]

Metab. of the marine yeast *Aureobasidium pullulans* and two strains of microorganism isol. from the marine sponge *Ircinia variabilis*.

Amorph. solid. $[\alpha]_D^{24}$ +34.7 (c, 1 in MeOH). λ_{max} 208 (ϵ 28000); 281 (ϵ 2900) (MeOH).

(3*S*,7*R*,8*aS*)-*form* [118477-06-8]

Metab. of an undescr. Fijian marine sponge (Jaspidae), the marine bacterium *Pseudoalteromonas luteoviolacea* and two strains of microorganism isol. from the marine sponge *Ircinia variabilis*. Plant growth regulator. Viscous oil. $[\alpha]_D^{20}$ -6.7 (c, 0.016 in MeOH).

Adamczeski, M. *et al., J.A.C.S.*, 1989, **111**, 647-654 (*isol, ir, pmr, cmr, ms, struct, Jaspidae constit*)

Shigemori, H. *et al., J. Nat. Prod.*, 1998, **61**, 696-698 (*Aureobasidium pullulans constit*)

Cronan, J.M. *et al., Nat. Prod. Lett.*, 1998, **11**, 271-278 (*3S,7R,8aS-form, isol*)

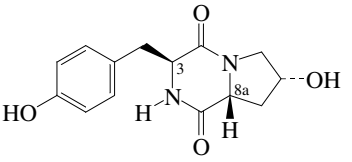
Jiang, Z. *et al., Nat. Prod. Lett.*, 2000, **14**, 435-440 (*Pseudoalteromonas luteoviolacea constit*)

De Rosa, S. *et al., Biomol. Eng.*, 2003, **20**, 311-316 (*Ircinia variabilis constit*)

Fdhila, F. *et al., J. Nat. Prod.*, 2003, **66**, 1299-1301 (*3R,7S,8aR-form, isol*)

Cyclo(4-hydroxyprolyltyrosyl) C-1012

*Hexahydro-7-hydroxy-3-[(4-hydroxyphenyl)methyl]pyrrolo[1,2-*a*]pyrazine-1,4-dione, 9CI*



(3*S*,7*R*,8*aR*)-*form*

$C_{14}H_{16}N_2O_4$ 276.291

(3*S*,7*R*,8*aR*)-*form* [813461-20-0]

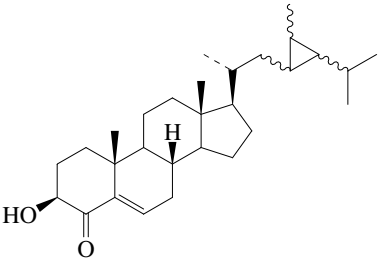
Prod. by a *Ruegeria* sp. isol. from the sponge *Suberites domuncula*. $[\alpha]_D$ +82.3 (c, 0.001 in MeOH).

(3*S*,7*R*,8*aS*)-*form* [813461-21-1]

Prod. by a *Ruegeria* sp. isol. from *Suberites domuncula*. $[\alpha]_D$ -10.4 (c, 0.003 in MeOH).

Mitova, M. *et al., Mar. Biotechnol.*, 2004, **6**, 95-103 (*isol*)

23,28-Cyclo-3-hydroxystigmast-5-en-4-one C-1013



$C_{29}H_{46}O_2$ 426.681

3β-*form* [283176-13-6]

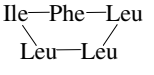
Constit. of *Ulva lactua*.

Cryst. (MeOH).

Mp 148-150°.

Xu, S. *et al., Yaoxue Xuebao*, 2000, **35**, 76-78 (*isol, pmr, cmr*)

Cyclo(isoleucylphenylalanylleucylleucylleucyl) C-1014



$C_{33}H_{53}N_5O_5$ 599.812

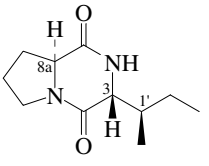
Prod. by an endophytic fungus No. 2524 isol. from the seeds of the mangrove *Avicennia marina*. Amorph. powder. $[\alpha]_D^{20}$ -56 (c, 0.13 in MeOH). λ_{max} 225 (ϵ 1400) (MeOH).

Li, H.-J. *et al., J. Asian Nat. Prod. Res.*, 2004, **6**, 185-191 (*isol, pmr, cmr*)

Cyclo(isoleucylprolyl) C-1015

*Hexahydro-3-(1-methylpropyl)pyrrolo[1,2-*a*]pyrazine-1,4-dione, 9CI*

[58917-56-9]



(1'*R*,3*R*,8*aS*)-*form*

$C_{11}H_{18}N_2O_2$ 210.275

(1′*R*,3*R*,8*aS*)-*form*
L-D-allo-*form*
[61117-55-3]
Cryst. (hexane/Et_2O/Me_2CO). Mp 107-108°.

(1′*S*,3*R*,8*aS*)-*form*
L-D-*form*
[61117-54-2]
Cryst. (Me_2CO). Mp 143-145°.

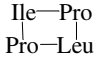
(1′*S*,3*S*,8*aR*)-*form* [162830-28-6]
Isol. from the sponge *Calyx* cf. *podatypa*.
Amorph. powder. $[\alpha]_D^{23}$ +98 (c, 0.1 in EtOH). Config. of nat. prod. revised in 1998.

(1′*S*,3*S*,8*aS*)-*form* [57089-60-8]
Isol. from *Calyx* cf. *podatypa*. Prod. by marine-derived *Pseudomonas aeruginosa* and *Vibrio parahaemolyticus*. Constit. of *Schizandra chinensis*.
Amorph. solid. $[\alpha]_D^{20}$ -173.5 (c, 0.16 in EtOH).

(1′ξ,3*R*,8*aR*)-*form* [631922-76-4]
Prod. by the marine bacterial strains CF-20 and C-148 isol. from cultures of the larvae of the mollusc *Pecten maximus*. Active against *Vibrio anguillarum*. $[\alpha]_D$ +168.1 (c, 0.13 in EtOH).

Bycroft, B.W. *et al., Chem. Comm.*, 1975, 988-989 (*synth*)
Young, P.E. *et al., J.A.C.S.*, 1976, **98**, 5358-5364; 5365-5371 (*synth, conformn*)
Suzuki, K. *et al., Chem. Pharm. Bull.*, 1981, **29**, 233-237 (*synth*)
Adamczeski, M. *et al., J. Nat. Prod.*, 1995, **58**, 201-208 (*isol, pmr, cmr*)
Jayatilake, G.S. *et al., J. Nat. Prod.*, 1996, **59**, 293-296 (*isol*)
Bull, S.D. *et al., J.C.S. Perkin 1*, 1998, 2313-2320 (*synth, pmr*)
Ginz, M. *et al., J. Agric. Food Chem.*, 2000, **48**, 3528-3532 (*isol, coffee*)
Fdhila, F. *et al., J. Nat. Prod.*, 2003, **66**, 1299-1301 (*isol, pmr, cmr*)
Pedras, M.S.C. *et al., Z. Naturforsch., C*, 2005, **60**, 717-722 (*isol, synth, pmr, cmr*)

Cyclo(isoleucylprolylleucylprolyl) C-1016

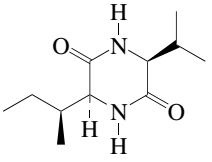


$C_{22}H_{36}N_4O_4$

(*all*-L)-*form*
Antibiotic MK 349A. *MK 349A*
Prod. by a marine-derived *Nocardiopsis* sp. Cytotoxic. Gum. $[\alpha]_D^{25}$ -41.3 (c, 0.12 in MeOH).
Shin, J. *et al., J. Nat. Prod.*, 2003, **66**, 883-884 (*isol, pmr, cmr*)

Cyclo(isoleucylvalyl) C-1017

3-(1-Methylethyl)-6-(1-methylpropyl)-2,5-piperazinedione, 9CI. 3-Isopropyl-6-(1-methylpropyl)-2,5-piperazinedione. Isoleucyl valyl anhydride



(*all-S*)-*form*

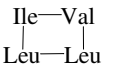
$C_{11}H_{20}N_2O_2$ 212.291

(1′*S*,3*S*,6*S*)-*form* [35590-75-1]
Metab. of *Beauveria bassiana*, *Cordyceps sinensis* and *Phytophthora cinnamoni*. Prod. by *Cytophaga marinoflava* sp. AM13.1.
Mp 276-278° dec. $[\alpha]_D$ -53.3 (c, 1 in AcOH).

(1′ξ,3ξ,6ξ)-*form*
N,N′-*Dihydroxy:* ***Terramide B***
[104187-49-7]
$C_{11}H_{20}N_2O_4$ 244.29
Prod. by *Aspergillus terreus*. Cryst. (MeOH).
Mp 179-184°. $[\alpha]_D^{22}$ -137 (c, 0.13 in EtOH). $[\alpha]_D^{22}$ -223 (c, 0.30 in MeOH). Biol. activity not investigated.
[35590-76-2]

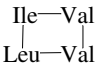
Eriksen, S. *et al., J. Agric. Food Chem.*, 1976, **24**, 1242 (*ms*)
Suzuki, K. *et al., Chem. Pharm. Bull.*, 1981, **29**, 233 (*synth*)
Grove, J.F. *et al., Phytochemistry*, 1981, **20**, 815 (*isol*)
Garson, M.J. *et al., J.C.S. Perkin 1*, 1986, 901 (*Terramide B*)
Trigos, A. *et al., CA*, 1995, **123**, 309992w (*isol*)
Shaaban, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*isol, Cytophaga*)
Jia, J.-M. *et al., Chem. Pharm. Bull.*, 2005, **53**, 582-583 (*isol*)

Cyclo(isoleucylvalylleucylleucyl) C-1018



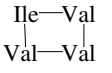
$C_{23}H_{42}N_4O_4$ 438.609
Isol. from an unidentified marine-derived fungus.
Yin, W. *et al., Zhongshan Daxue Xuebao Ziran Kexueban*, 2002, **41**, 56-58

Cyclo(isoleucylvalylvalylleucyl) C-1019



$C_{22}H_{40}N_4O_4$ 424.582
Isol. from an unidentified marine-derived fungus.
Yin, W. *et al., Zhongshan Daxue Xuebao Ziran Kexueban*, 2002, **41**, 56-58

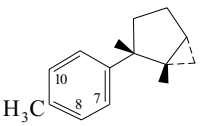
Cyclo(isoleucylvalylvalylvalyl) C-1020



$C_{21}H_{38}N_4O_4$ 410.556
Isol. from an unidentified marine-derived fungus.
Yin, W. *et al., Zhongshan Daxue Xuebao Ziran Kexueban*, 2002, **41**, 56-58

Cyclolaurene C-1021

1,2-Dimethyl-2-(4-methylphenyl)bicyclo[3.1.0]hexane, 9CI
[103439-82-3]



$C_{15}H_{20}$ 200.323
Constit. of *Aplysia dactylomela*. Ichthyotoxic, antimicrobial and antifungal agent. Oil. $[\alpha]_D$ -9 (c, 0.22 in $CHCl_3$).

7-Hydroxy: ***Debromolaurinterol***
Constit. of *Laurencia intermedia*, *Laurencia okamurai* and *Laurencia johnstonii*. Shows weak antimycobacterial activity. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D^{20}$ -12.2 ($CHCl_3$). λ_{max} 276 (ϵ 3500); 282 (ϵ 3400) (EtOH) (Berdy).

8-Hydroxy: ***Isodebromolaurinterol***. *Cyclolauren-2-ol. 6,8,10-Cyclolauratrien-8-ol*
[861251-22-1]
$C_{15}H_{20}O$ 216.322
Constit. of *Laurencia tristicha* and *Laurencia okamurai*. Gum or oil. $[\alpha]_D^{20}$ +2.1 (c, 0.22 in MeOH). $[\alpha]_D^{20}$ +3 (c, 0.11 in $CHCl_3$). λ_{max} 202 (log ϵ 4.78); 249 (log ϵ 3.51) (MeOH).

7-Bromo, 10-hydroxy: ***Cyclolaurenol***
[103439-83-4]
$C_{15}H_{19}BrO$ 295.218
Constit. of *Aplysia dactylomela*. Ichthyotoxic agent. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 109-109.5°. $[\alpha]_D^{21}$ -9.3 (c, 4.04 in $CHCl_3$). λ_{max} 206 (ϵ 12000); 269 (ϵ 570); 278 (ϵ 700) (EtOH) (Derep).

7-Bromo, 10-acetoxy: Cyclolaurenol acetate
[103456-68-4]
$C_{17}H_{21}BrO_2$ 337.256
From *Aplysia dactylomela*. Ichthyotoxic agent. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{19}$ -9.2 (c, 0.82 in $CHCl_3$). λ_{max} 206 (ϵ 12000); 269 (ϵ 570); 278 (ϵ 700) (EtOH) (Derep).

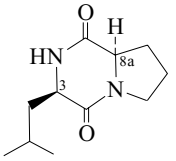
8-Bromo, 7-hydroxy: ***Neolaurinterol***
[68773-09-1]
$C_{15}H_{19}BrO$ 295.218
Constit. of *Laurencia okamurai*. Cryst.
Mp 62-63°. $[\alpha]_D$ -14 (c, 0.57 in $CHCl_3$). λ_{max} 240 (ϵ 30000) (EtOH) (Derep).

10-Bromo, 7-hydroxy: ***Laurinterol***
[10539-87-4]
$C_{15}H_{19}BrO$ 295.218
Constit. of *Laurencia intermedia*, *Laurencia nidifica*, *Marginisporum aberrans*, *Amphiroa nidifica*, *Corallina pilulifera*, *Corallina chilensis*, *Aplysia* sp., *Rhodomela californica* and *Laurencia okamurai*. Reverse transcriptase inhibitor. Cryst. (MeOH). Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 54-55°. $[\alpha]_D$ +13.3 (c, 1.9 in $CHCl_3$). λ_{max} 240 (ϵ 30000) (EtOH) (Derep). λ_{max} 225 (ϵ 7100); 283 (ϵ 2200); 289 (ϵ 2100) (EtOH) (Berdy).

Cameron, A.F. *et al., J.C.S.(B)*, 1969, 692 (*Laurinterol, abs config*)
Irie, T. *et al., Tetrahedron*, 1970, **26**, 3271 (*Laurinterol, Debromolaurinterol, isol*)
Feutrill, G.I. *et al., Aust. J. Chem.*, 1973, **26**, 345 (*Laurinterol, synth*)
Suzuki, M. *et al., Tet. Lett.*, 1978, 2503 (*Neolaurinterol*)
Ichiba, T. *et al., J.O.C.*, 1986, **51**, 3364 (*Cyclolaurene, Cyclolaurenol, Cyclolaurenol acetate*)
Srikrishna, A. *et al., Tetrahedron*, 1992, **48**, 3429 (*synth*)
Koenig, G.M. *et al., Planta Med.*, 2000, **66**, 337-342 (*Debromolaurinterol, activity*)
Okamoto, Y. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 474-476 (*Laurinterol, Debromolaurinterol, isol, pmr, cmr*)
Mao, S.-C. *et al., Helv. Chim. Acta*, 2005, **88**, 1034-1039 (*Isodebromolaurinterol*)
Sun, J. *et al., J. Nat. Prod.*, 2005, **68**, 915-919 (*Cyclolauren-2-ol*)

Cyclo(leucylprolyl) C-1022

Hexahydro-3-(2-methylpropyl)pyrrolo[1,2a]pyrazine-1,4-dione. Prolylleucyldiketopiperazine. Gancidin W. Maculosin 6
[5654-86-4]



(3*R*,8a*R*)–*form*

$C_{11}H_{18}N_2O_2$ 210.275

(3*R*,8*aR*)-*form*
D,D-form
[162872-80-2]
Prod. by the marine bacterial strains CF-20 and C-148 obt. from molluscs.
Amorph. solid. $[\alpha]_D$ +128.3 (c, 0.11 in EtOH).

(3*R*,8*aS*)-*form* [36238-67-2]
Cryst. Sol. MeOH, EtOAc. Mp 148-149° (119-122°). $[\alpha]_D^{31}$ -105.5 (c, 0.5 in EtOH).

(3*S*,8*aR*)-*form* [32510-93-3]
Isol. from the sponges *Calyx* cf. *podatypa* and *Stelletta clavosa*. Solid. $[\alpha]_D^{25}$ +35 (c, 0.11 in EtOH).

(3*S*,8*aS*)-*form*
L,L-form
[2873-36-1]
Prod. by *Streptomyces gancidicus*, *Nocardia restricta*, *Candida albicans*, *Guignardia laricina* and several *Ceratocystis* spp. Also from the sponges *Calyx* cf. *podatypa* and *Tedania ignis*. Shows antitumour and antifungal props. Phytotoxin associated with fungal diseases of trees. Cryst.
Mp 168-172° (158-159°). $[\alpha]_D^{25}$ -133 (c, 1 in EtOH) (lit. gives a temp. range). $[\alpha]_D^{21}$ -144 (c, 0.5 in H_2O).
▶ LD_{50} (mus, ivn) 80 mg/kg. UY8708800

[19943-30-7, 43041-29-8]

Kodaira, Y. *et al., Agric. Biol. Chem.*, 1961, **25**, 261
Nitecki, D.E. *et al., J.O.C.*, 1968, **33**, 864 (*synth*)
Siemion, I.Z. *et al., Org. Magn. Reson.*, 1971, **3**, 545 (*synth, nmr*)
Vicar, J. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 4060; 1973, **38**, 1940 (*synth, ir, pmr*)
Karle, I.L. *et al., J.A.C.S.*, 1972, **94**, 81 (*cryst struct*)
Takahashi, K. *et al., Agric. Biol. Chem.*, 1974, **38**, 927
Bycroft, B.W. *et al., Chem. Comm.*, 1975, 988 (*synth*)
Davies, D.B. *et al., J.C.S. Perkin 2*, 1976, 187 (*conformn*)
Pancoska, P. *et al., Coll. Czech. Chem. Comm.*, 1977, **44**, 1296 (*cd*)
Jain, T.C. *et al., Heterocycles*, 1977, **7**, 341 (*isol, struct, uv, ms*)
Bjoerkman, S. *et al., J. Med. Chem.*, 1979, **22**, 931 (*synth*)
Suzuki, K. *et al., Chem. Pharm. Bull.*, 1981, **29**, 233 (*synth*)
Schmidtz, F.J. *et al., J.O.C.*, 1983, **48**, 3941 (*isol, ms, pmr, synth, bibl*)
Ayer, W.A. *et al., Can. J. Chem.*, 1986, **64**, 904 (*isol*)
Kricheldorf, H.R. *et al., Magn. Reson. Chem.*, 1986, **24**, 21 (*cmr*)
Adamczeski, M. *et al., J. Nat. Prod.*, 1995, **58**, 201 (*isol, pmr, cmr, bibl*)
Bull, S.D. *et al., J.C.S. Perkin 1*, 1998, 2313-2320 (*config, biosynth*)
Fdhila, F. *et al., J. Nat. Prod.*, 2003, **66**, 1299-1301 (*isol, pmr, cmr*)
Wegerski, C.J. *et al., Bioorg. Med. Chem.*, 2004, **12**, 5631-5637 (*isol*)
Pedras, M.S.C. *et al., Z. Naturforsch., C*, 2005, **60**, 717-722 (*isol, synth, pmr, cmr*)

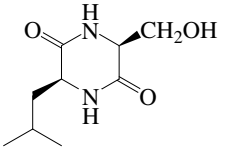
Cyclo(leucylprolylleucylprolyl) C-1023

$C_{22}H_{36}N_4O_4$ 420.551
λ_{max} 259 (ϵ 492) (EtOH) (Berdy).

(all-L)-form [135086-71-4]
Isol. from the marine ascidian *Cystodytes dellechiajei*.
Aracil, J.-M. *et al., Tet. Lett.*, 1991, **32**, 2609-2612 (*isol, pmr, cmr, struct*)

Cyclo(leucylseryl) C-1024

3-Hydroxymethyl-6-(2-methylpropyl)-2,5-piperazinedione, 9CI. Cyclo(serylleucyl)



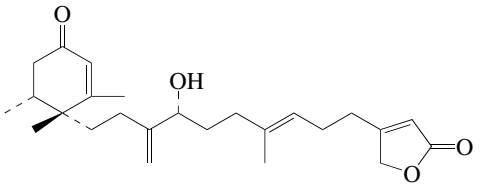
$C_9H_{16}N_2O_3$ 200.237

(3*S*,6*S*)-*form*
L-L-form
[65519-48-4]
Isol. from a marine endophytic fungus. Constit. of the roots of *Panax notoginseng* (sanchi).
Mp 231-233° dec. $[\alpha]_D^{25}$ -54.5 (c, 0.6 in DMF).

Lee, S. *et al., Int. J. Pept. Protein Res.*, 1979, **13**, 207-217 (*synth*)
Falorni, M. *et al., Synthesis*, 1994, 391-395 (*synth, pmr, cmr*)
Chen, G. *et al., Tetrahedron*, 2003, **59**, 4907-4909 (*marine isol*)
Tan, N. *et al., Yunnan Zhiwu Yanjiu*, 2003, **25**, 366-368; *CA*, **142**, 370710m (*Panax, isol*)

Cyclolinteinol C-1025

[191789-76-1]



$C_{25}H_{36}O_4$ 400.557

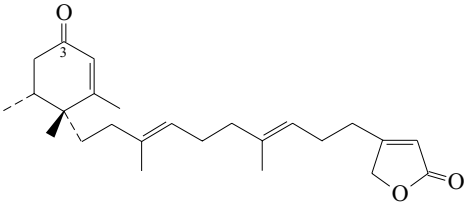
Constit. of *Cacospongia* cf. *linteiformis*. Macrophage activation modulator. Nitric oxide production and synthase induction inhibitor. $[\alpha]_D^{25}$ +63 (c, 0.03 in $CHCl_3$).

Ac: [191789-78-3]
$C_{27}H_{38}O_5$ 442.594
Constit. of *Cacospongia* cf. *linteiformis*. Macrophage activation modulator. Nitric oxide production and synthase induction inhibitor. $[\alpha]_D^{25}$ +61 (c, 0.003 in $CHCl_3$).

Carotenuto, A. *et al., Tetrahedron*, 1997, **53**, 7305-7310 (*isol, pmr, cmr*)

Cyclolinteinone C-1026

[159934-16-4]



$C_{25}H_{36}O_3$ 384.558

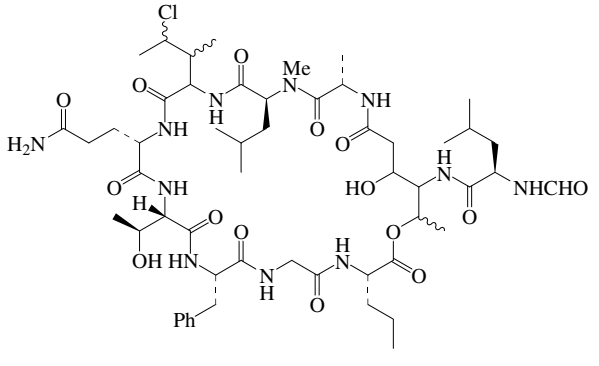
Constit. of *Cacospongia* cf. *linteiformis*. Inhibits NO (nitrogen oxide) generation. Ichthyotoxic and antiinflammatory agent. Macrophage activation modulator. INOS and Cox-2 expression regulator. Oil. $[\alpha]_D^{25}$ +53 (c, 0.04 in $CHCl_3$).

3-Deoxo: ***3-Deoxocyclolinteinone***
$C_{25}H_{38}O_2$ 370.574
Constit. of *Cacospongia* cf. *linteiformis*. Antifeedant. Ichthyotoxic agent. Macrophage activation modulator. $[\alpha]_D^{25}$ +89 (c, 0.03 in $CHCl_3$).

Conte, M.R. *et al., Tetrahedron*, 1994, **50**, 13469 (*isol, pmr, cmr*)
Carotenuto, A. *et al., Tetrahedron*, 1995, **51**, 10751 (*3-Deoxocyclolinteinone*)
Carotenuto, A. *et al., Tetrahedron*, 1997, **53**, 7305-7310 (*activity*)
D'Acquisto, *et al., Biochem. J.*, 2000, **346**, 793-798 (*activity*)

Cyclolithistide A C-1027

[218899-71-9]



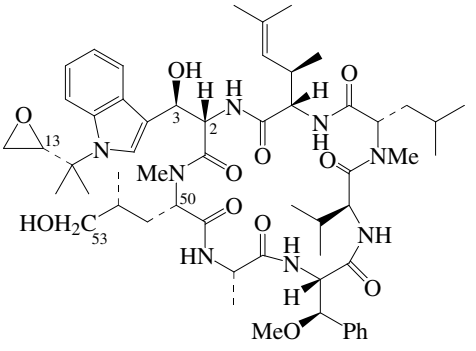
$C_{54}H_{86}ClN_{11}O_{15}$ 1164.791

Depsipeptide antibiotic. Isol. from the sponge *Theonella swinhoei*. Antifungal agent. Amorph. solid.
Mp 174° (dec.). $[\alpha]_D$ -29.3 (c, 0.01 in MeOH). λ_{max} 220; 266 (MeOH).

Clark, D.P. *et al., J.O.C.*, 1998, **63**, 8757-8764 (*isol, pmr, cmr, ms*)

Cyclomarin A C-1028

Marinovir
[169062-92-4]



$C_{56}H_{82}N_8O_{11}$ 1043.311

Cyclic peptide antibiotic. Prod. by a marine *Streptomyces* sp. Antiinflammatory and antiviral agent. Cryst. (Me_2CO/Et_2O). Sol. MeOH. $[\alpha]_D$ -51.7 (c, 0.48 in $CHCl_3$). λ_{max} 222 (log ϵ 4.36); 287 (log ϵ 3.99); 293 (log ϵ 4.05) (MeOH).

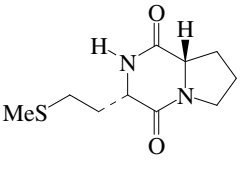
53-Deoxy: ***Cyclomarin B***
[255705-66-9]
$C_{56}H_{82}N_8O_{10}$ 1027.311
Prod. by a marine *Streptomyces* sp. Solid. $[\alpha]_D^{20}$ -30.4 (c, 0.9 in $CHCl_3$). C-50 config. not confirmed. λ_{max} 220 (ϵ 32900); 275 (ϵ 3200) (MeOH).

13,14-Deepoxy, 13,14-didehydro: ***Cyclomarin C***
[255705-67-0]
$C_{56}H_{82}N_8O_{10}$ 1027.311
Prod. by a marine *Streptomyces* sp. Solid. $[\alpha]_D^{20}$ -19.7 (c, 1 in $CHCl_3$). C-3 config. not confirmed. λ_{max} 220 (ϵ 16400) (MeOH).

Renner, M.K. *et al., J.A.C.S.*, 1999, **121**, 11273-11276 (*Cyclomarins A-C, cryst struct*)
Wen, S.-J. *et al., Tetrahedron*, 2005, **61**, 4931-4938 (*Cyclomarin C, synth*)

Cyclo(methionylprolyl) C-1029

Hexahydro-3-[2-(methylthio)ethyl]pyrrolo[1,2-a]pyrazine-1,4-dione, 9CI. Cyclo(prolylmethionyl)

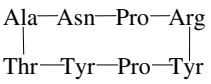


$C_{10}H_{16}N_2O_2S$ 228.315

(3S,8aS)-form
L-L-form
[53049-06-2]
Prod. by *Pseudomonas aeruginosa* isol. from an Antarctic sponge. Amorph. solid. $[\alpha]_D^{20}$ -82.2 (c, 0.14 in EtOH).

Padmanabhan, V.M. *et al., Acta Cryst. C*, 1987, **43**, 349-351 (*cryst struct*)
Jayatilake, G.S. *et al., J. Nat. Prod.*, 1996, **59**, 293-296 (*isol, synth, pmr, cmr*)

Cyclonellin C-1030



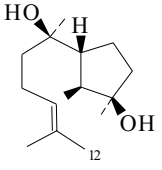
$C_{45}H_{62}N_{12}O_{12}$ 963.058

Cyclic peptide. Isol. from the sponge *Axinella carteri*. Amorph. solid. $[\alpha]_D$ -92.8 (c, 0.25 in MeOH). λ_{max} 218 (log ϵ 4.44); 276 (log ϵ 3.88) (EtOH).

Milanowski, D.J. *et al., J. Nat. Prod.*, 2004, **67**, 441-444 (*isol, pmr, cmr, ms*)

Cyclonerodiol C-1031

[28834-06-2]



$C_{15}H_{28}O_2$ 240.385

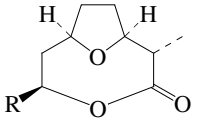
Metab. of *Trichothecium* spp., *Fusarium culmorum, Gibberella fujikuroi*, *Trichoderma polysporum* and an unidentified marine fungus. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ -20.

12-Hydroxy: ***Cyclonerotriol***
[57689-00-6]
$C_{15}H_{28}O_3$ 256.384
Metab. of *Fusarium culmorum*. Cryst. (Et_2O/petrol). Mp 113-114°. $[\alpha]_D$ -27.8 (c, 0.2 in MeOH).

Evans, R. *et al., J.C.S. Perkin 1*, 1976, 1214 (*Cyclonerotriol*)
Cane, D.E. *et al., Tet. Lett.*, 1977, 3511 (*abs config*)
Cane, D.E. *et al., J.A.C.S.*, 1981, **103**, 914 (*biosynth*)
Fujita, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 4419 (*isol, bibl*)
Cutler, H.G. *et al., Agric. Biol. Chem.*, 1991, **55**, 243 (*isol, pmr, cmr, bibl*)
Li, X. *et al., Bull. Korean Chem. Soc.*, 2004, **25**, 607-608 (*isol, pmr, cmr*)

Cyclononactic acid C-1032

2,5-Dimethyl-4,10-dioxabicyclo[5.2.1]decan-3-one



Relative Configuration

R = CH_3

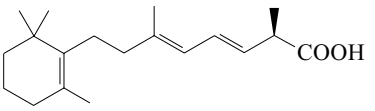
$C_{10}H_{16}O_3$ 184.235

Prod. by Actinomycete strain BS 1465.

Homologue (R = CH_2CH_3): ***Cyclohomononactic acid***. *Boralactin A*. *Borolactin A*
$C_{11}H_{18}O_3$ 198.261
Prod. by Actinomycete strain BS 1465 the marine-derived *Streptomyces* sp. B5375.

Stadler, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 2001, **334**, 143-147 (*isol, pmr, cmr*)
Laatsch, H. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

10,15-Cyclo-1-nor-4,6,10-phytatrien-2-oic acid C-1033



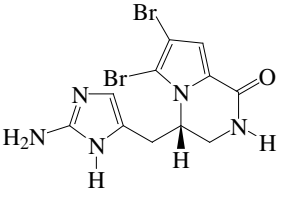
$C_{19}H_{30}O_2$ 290.445

(3R,4E,6E)-form [133883-12-2]
Constit. of *Latrunculia brevis*.
Unstable pale yellow oil. $[\alpha]_D$ -27.5 (c, 4.94 in $CHCl_3$).

Me ester: [133883-14-4]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Latrunculia brevis*. Unstable pale yellow oil. $[\alpha]_D$ -42.7 (c, 4.78 in $CHCl_3$).

Butler, M.S. *et al., Aust. J. Chem.*, 1991, **44**, 77 (*isol, pmr, cmr*)

Cyclooroidin C-1034



Absolute Configuration

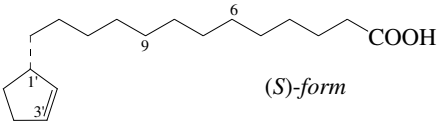
$C_{11}H_{11}Br_2N_5O$ 389.049

Alkaloid from the sponge *Agelas oroides*. Pale yellow solid. $[\alpha]_D$ -12 (c, 0.02 in MeOH).

Fattorusso, E. *et al., Tet. Lett.*, 2000, **41**, 9917-9922 (*isol, pmr, cmr*)
Papeo, G. *et al., Tet. Lett.*, 2005, **46**, 8635-8638 (*synth*)
Patel, J. *et al., Tet. Lett.*, 2006, **47**, 5561-5563 (*synth*)

13-(2-Cyclopentenyl)tridecanoic acid C-1035

2-Cyclopentene-1-tridecanoic acid, 9CI. ***Chaulmoogric acid***. *Chaulmoogrina*
[502-30-7]



(*S*)-*form*

$C_{18}H_{32}O_2$ 280.45

Antileprotic agent. Log P 7.19 (uncertain value) (calc).

(S)-form [29106-32-9]
Constit. of oils of *Hydnocarpus wightii*, *Carpotroche brasiliensis*, *Asteriastigma macrocarpa* (preferred genus name *Hydnocarpus*), *Caloncoba* spp., *Lindackeria dentata* and *Buchnerodendron speciosum*.
Shiny leaflets (EtOH or petrol).
Mp 67-68°. $[\alpha]_D^{26}$ +61.7 (c, 4.82 in $CHCl_3$). Pharmacol. active enantiomer.

Me ester: [24828-59-9]
$C_{19}H_{34}O_2$ 294.476
Mp 22°. Bp_{20} 227°. $[\alpha]_D$ +50 ($CHCl_3$).

Et ester: Antileprol. *Chaulmestrol*. *Chaulmoogrol*. *Hyrganol*. *Moogrol*
[623-32-5]

$C_{20}H_{36}O_2$ 308.503
Leprostatic agent. Bp_{20} 230°. $[\alpha]_D$ +50.7. Log P 8.14 (uncertain value) (calc).

Chloride:
$C_{18}H_{31}ClO$ 298.895
Mp 20-25°.

Amide:
$C_{18}H_{33}NO$ 279.465
Mp 106°. $[\alpha]_D$ +57.3 ($CHCl_3$).

Nitrile:
$C_{18}H_{31}N$ 261.45
$Bp_{3.5}$ 158-160°. $[\alpha]_D$ +55.2 (c, 0.3 in $CHCl_3$).

6,7-Didehydro: 13-(2-Cyclopentenyl)-6-tridecenoic acid. ***Gorlic acid***
[502-31-8]
$C_{18}H_{30}O_2$ 278.434
Isol. from *Oncoba echinata* and others in Flacourtiaceae. Oil. Mp 6°. Bp 232.5°. $[\alpha]_D^{25}$ +60.7 (c, 25 in $CHCl_3$).

6,7-Didehydro, Me ester: Fp -10. Bp_{10} 209°. $[\alpha]_D^{25}$ +57.7 (c, 25 in $CHCl_3$).

6,7-Didehydro, amide:
Cryst. (Me_2CO). Mp 95°.

Δ^1-Isomer, 3-oxo: 3-Oxo-1-cyclopentenetridecanoic acid. ***Ketochaulmoogric acid***
$C_{18}H_{30}O_3$ 294.433
Isol. from *Symplocos racemosa* and the seed oil of *Carpotroche brasiliensis* (sapucainha oil). Light yellow granules (EtOH). Mp 116°. $[\alpha]_D^{23}$ -8.3 (c, 0.17 in MeOH). Prob. artifact of autoxidn. λ_{max} 202 (log ϵ 2.08); 228 (log ϵ 2.77) (MeOH).

(±)-form
Cryst. (EtOAc). Mp 68.5°.

Amide:
Cryst. (EtOH). Mp 106°.

Nitrile: $Bp_{2.5}$ 155-158°.

ξ-form

2′,3′-Dihydro: Cyclopentanetridecanoic acid. 13-Cyclopentyltridecanoic acid. ***Dihydrochaulmoogric acid***
[6053-47-0]
[24828-61-3]
$C_{18}H_{34}O_2$ 282.465
Constit. of *Hydnocarpus anthelmintica* and various red algae of the Solieriaceae. Cryst. (EtOH aq.).
Mp 70-72°.

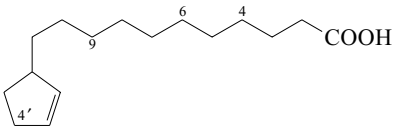
4,5-Didehydro(Z-): 13-(2-Cyclopentenyl)-4-tridecenoic acid
[119903-67-2]
[120727-01-7]
$C_{18}H_{30}O_2$ 278.434
Constit. of the seed oil of *Hydnocarpus anthelmintica*.

9,10-Didehydro: 13-(2-Cyclopentenyl)-9-tridecenoic acid
$C_{18}H_{30}O_2$ 278.434
Isol. from *Caloncoba echinata*, *Hydnocarpus anthemintica* and *Hydnocarpus wightiana* seeds. Prob. opt. active and with (*Z*)-config.

Paget, H. *et al., J.C.S.*, 1937, 955 (*Ketochaulmoogric acid*)
Cole, H.I. *et al., J.A.C.S.*, 1938, **60**, 612 (*Gorlic acid*)
Mislow, K. *et al., J.A.C.S.*, 1955, **77**, 3807 (*synth, abs config, bibl*)
Buchta, E. *et al., Annalen*, 1962, **655**, 81-85 (*synth, dihydrochaulmoogric acid*)
Mani, V.V.S. *et al., J. Chromatogr.*, 1969, **39**, 182 (*isol, chromatog*)
Christie, W.W. *et al., Lipids*, 1969, **4**, 229 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 978 (*occur*)
Spencer, F. *et al., Biochemistry*, 1974, **13**, 2241 (*deriv*)
Levy, L. *et al., Am. Rev. Respir. Dis.*, 1975, **111**, 703 (*props*)
Kaneda, T. *et al., Biochem. Biophys. Res. Commun.*, 1981, **99**, 1226 (*biosynth*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 6557
Christie, W.W. *et al., Lipids*, 1989, **24**, 116-120 (*derivs, isol*)
Miralles, J. *et al., Phytochemistry*, 1990, **29**, 2161-2163 (*isol, dihydrochaulmoogric acid*)
Seemann, M. *et al., Eur. J. Org. Chem.*, 2003, 2122-2127 (*synth*)
Abbasi, M.A. *et al., Nat. Prod. Res.*, 2005, **19**, 509-515 (*Ketochaulmoogric acid*)

11-(2-Cyclopentenyl)undecanoic acid C-1036

2-Cyclopentene-1-undecanoic acid, 9CI. Hydnocarpic acid
[459-67-6]



$C_{16}H_{28}O_2$ 252.396
Antileprotic agent. Log P 6.13 (calc).

(+)-form
Constit. of chaulmoogra oil and seed oils of other Flacourtiaceae spp., *Hydnocarpus*, *Asteriastigma* (preferred genus name *Hydnocarpus*), *Carpotroche*, *Caloncoba* and *Lindackeria* spp.
Cryst. (EtOH).
Mp 58-59°. $[\alpha]_D^{25}$ +68 ($CHCl_3$).

Me ester: [28046-99-3]
Mp 8°. Bp_{19} 200-203°. $[\alpha]_D^{25}$ +62.4 ($CHCl_3$).

Et ester: [3552-12-3]
[146763-61-3 general CAS no] Bp_{19} 211°. $[\alpha]_D$ +51.6 ($CHCl_3$).

Amide: Mp 111-112°. $[\alpha]_D^{25}$ +69.4.

2′,3′-Dihydro: Cyclopentaneundecanoic acid, 9CI. 13-Cyclopentylundecanoic acid. ***Dihydrohydnocarpic acid***
[6053-49-2]
[25779-85-5]
$C_{16}H_{30}O_2$ 254.412
Constit. of *Hydnocarpus anthelmintica* and various red algae of the Solieriaceae. Cryst. (petrol/EtOAc or EtOH aq.).
Mp 64-66°. Bp_{16} 238-240°. Opt. inactive achiral compd.

4,5-Didehydro: 11-(2-Cyclopentenyl)-4-undecenoic acid
[52904-23-1]
$C_{16}H_{26}O_2$ 250.38
Isol. from *Caloncoba echinata* seeds. Prob. opt. active and with (*Z*)-config.

6,7-Didehydro: 11-(2-Cyclopentenyl)-6-undecenoic acid. ***Manoaic acid***
[52904-22-0]
$C_{16}H_{26}O_2$ 250.38
Isol. from seeds of *Caloncoba echinata*. Prob. opt. active and with *Z*-config.

9,10-Didehydro: 11-(2-Cyclopentenyl)-9-undecenoic acid
$C_{16}H_{26}O_2$ 250.38
Isol. from *Caloncoba echinata* seeds. Prob. opt. active and with *Z*-config.

4′-Oxo: ***Ketohydnocarpic acid***
$C_{16}H_{26}O_3$ 266.38
Minor constit. of oil of *Carpotroche brasiliensis*. Presumably artifact of autoxidn.

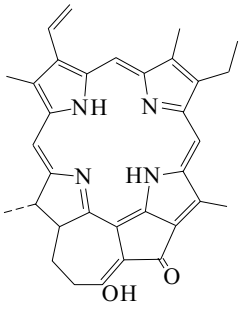
(±)-form
Cryst. (petrol). Mp 58-59°.

Nitrile: Bp_3 155-156°.

Hinegardner, W.S. *et al., J.A.C.S.*, 1933, **55**, 2831-2834 (*synth*)
Paget, H. *et al., J.C.S.*, 1937, 955-960 (*Ketohydnocarpic acid*)
Adriaens, L. *et al., CA*, 1946, **40**, 6754 (*isol*)
Buchta, E. *et al., Annalen*, 1962, **655**, 81-85 (*synth, dihydrohydnocarpic acid*)
Christie, W.W. *et al., Lipids*, 1969, **4**, 229-231 (*ms*)
Sengupta, A. *et al., J. Sci. Food Agric.*, 1973, **24**, 669-674 (*isol*)
Spener, F. *et al., Biochemistry*, 1974, **13**, 2241-2248 (*Calonocoba echinata constits*)
Spener, F. *et al., Chem. Phys. Lipids*, 1974, **12**, 344-355 (*Hydnocarpus anthelmintica constits*)
Christie, W.W. *et al., Lipids*, 1989, **24**, 116-120 (*Dihydrohydnocarpic acid*)
Mirallès, J. *et al., Phytochemistry*, 1990, **29**, 2161-2163 (*red algae constit*)

$13^2,17^3$-Cyclophaeophorbide enol C-1037

*6-Ethenyl-11-ethyl-15,19,20,21-tetrahydro-18-hydroxy-5,10,22,23-tetramethyl-4,7-imino-2,21-methano-14,16-metheno-9,12-nitrilo-17*H*-azuleno[1,8-*bc*][1,5]diazacyclooctadecin-17-one, 9CI*
[103538-56-3]

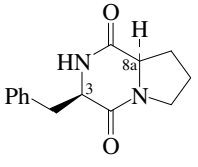


$C_{33}H_{32}N_4O_2$ 516.641
Chlorophyll a deriv. isol. from *Darwinella oxeata*, first porphyrin from a sponge. Lustrous black needles (hexane/CH_2Cl_2).
Mp 360°. Opt. active but accurate $[\alpha]_D$ could not be determined. λ_{max} 287 (ϵ 4300); 359 (ϵ 4800); 426 (ϵ 4800); 452 (ϵ 4700); 626 (ϵ 4000); 686 (ϵ 4500) (solvent not reported) (Derep).

Karuso, P. *et al., Tet. Lett.*, 1986, **27**, 2177 (*isol, uv, ir, cryst struct*)

Cyclo(phenylalanylprolyl) C-1038

*Hexahydro-3-(phenylmethyl)pyrrolo[1,2-*a*]pyrazine-1,4-dione, 9CI. 3-Benzylhexahydropyrrolo[1,2-*a*]pyrazine-1,4-dione, 8CI. Phenylalanylproline anhydride*
[14705-60-3]



(3*R*,8*aR*)-*form*

$C_{14}H_{16}N_2O_2$ 244.293

(3*R*,8*aR*)-*form*
D-D-form
[5654-85-3]
Prod. by the marine bacterial strains CF-20 and C-148 obt. from molluscs.
Amorph. solid. $[\alpha]_D$ +88.7 (c, 0.22 in EtOH).

(3*R*,8*aS*)-*form* [26488-24-4]
Prod. by *Alternaria alternata* and *Streptomyces rochei*. Phytotoxic.
Mp 150-153°. $[\alpha]_D^{25}$ -94.2 (c, 0.2 in H_2O).

(3*S*,8*aR*)-*form* [32021-26-4]
Isol. from the sponge *Calyx* cf. *podatypa*. Prod. by *Aspergillus flavipes*.
Cryst. (EtOAc).
Mp 150-151°. $[\alpha]_D^{20}$ +99 (c, 0.23 in H_2O).

(3*S*,8*aS*)-*form*
L-L-form
[3705-26-8]
Prod. by *Alternaria alternata, Candida albicans* and *Rosellinia necatrix*. Isol. from the sponge *Stelletta clavosa*. Shows broad spectrum antibacterial and gastrointestinal cell maturation enhancing activity.
Mp 133°. $[\alpha]_D$ -89 (c, 0.3 in H_2O).

[43041-16-3, 43041-30-1, 52645-32-6]

Ott, H. *et al., Tetrahedron*, 1963, **19**, 1675 (*synth*)
Lingappa, B.T. *et al., Science (Washington, D.C.)*, 1969, **163**, 192 (*isol*)
Poisel, H. *et al., Chem. Ber.*, 1973, **106**, 3408 (*synth*)
Vicar, J. *et al., Coll. Czech. Chem. Comm.*, 1973, **38**, 1940 (*synth, pmr*)
Ramani, R. *et al., Acta Cryst. B*, 1976, **32**, 1051 (*cryst struct*)
Young, P.E. *et al., J.A.C.S.*, 1976, **98**, 5365 (*pmr, cmr*)
Suzuki, K. *et al., Chem. Pharm. Bull.*, 1981, **29**, 233 (*synth*)
Mazza, F. *et al., Acta Cryst. C*, 1984, **40**, 1974 (*cryst struct*)
Sleeckx, J.J.M. *et al., Bull. Soc. Chim. Belg.*, 1985, **94**, 187 (*pmr, conformn*)
Stierle, A.C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1988, **85**, 8008 (*isol*)
Adamczeski, M. *et al., J. Nat. Prod.*, 1995, **38**, 201-208 (*isol, pmr, cmr*)
Bull, S.D. *et al., J.C.S. Perkin 1*, 1998, 2313-2320 (*config, biosynth*)
Graz, M. *et al., Pharmazie*, 1999, **54**, 772 (*activity*)
Fdhila, F. *et al., J. Nat. Prod.*, 2003, **66**, 1299-1301 (*isol, pmr, cmr*)
Wegerski, C.J. *et al., Bioorg. Med. Chem.*, 2004, **12**, 5631-5637 (*isol*)

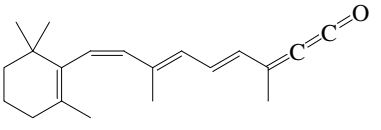
Cyclo(phenylalanylprolylphenylalanylprolyl) C-1039

$C_{28}H_{32}N_4O_4$ 488.585

(*all*-L)-*form* [135213-04-6]
Isol. from the marine ascidian *Cystodytes dellechiajei*. λ_{max} 259 (ϵ 492) (EtOH) (Derep).

Aracil, J.-M. *et al., Tet. Lett.*, 1991, **32**, 2609-2612 (*isol, pmr, cmr, struct*)

10,15-Cyclo-1,2,4,6,8,10-phytahexaen-1-one C-1040

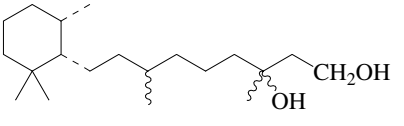


$C_{20}H_{26}O$ 282.425

(4*E*,6*E*,8*Z*)-*form*
Irciniketene
[352674-33-0]
Constit. of marine sponge *Ircinia selaginea*.

Yan, S.-J. *et al., Gaodeng Xuexiao Huaxue Xuebao*, 2001, **22**, 949-951; *CA*, **135**, 150110f (*isol, pmr, cmr*)

10,15-Cyclo-1,3-phytanediol C-1041



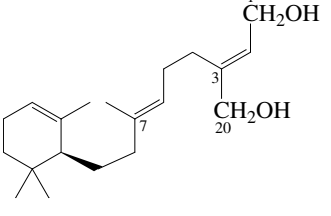
$C_{20}H_{40}O_2$ 312.535

(3ξ,7ξ,10*S*,11*S*)-*form*
Viridiol B
[183585-28-6]
Constit. of *Laurencia viridis*.
Oil. $[\alpha]_D^{25}$ +3.18 (c, 0.22 in $CHCl_3$).

Norte, M. *et al., Nat. Prod. Lett.*, 1996, **8**, 263-269 (*isol, pmr, cmr*)

10,15-Cyclo-2,6,10-phytatriene-1,20-diol C-1042

9,10-Seco-1(10),8,13-labdatriene-15,16-diol



(2*E*,6*E*,10*S*)-*form*

$C_{20}H_{34}O_2$ 306.487

(2*E*,6*E*,10*S*)-*form*

Di-Ac:
$C_{24}H_{38}O_4$ 390.562
Constit. of *Caulerpa brownii*. Oil. $[\alpha]_D$ -150 (c, 0.5 in EtOH). λ_{max} 212 (ϵ 3900) (EtOH).

20-Aldehyde, 1-Ac: [278605-20-2]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Caulerpa trifaria*. Pale yellow oil. $[\alpha]_D$ -49 (EtOH). λ_{max} 203 (ϵ 6055) (EtOH).

Dialdehyde: ***10,15-Cyclo-2,6,10-phytatriene-1,20-dial***. *9,10-Seco-1(10),8,13-labdatriene-15,16-dial*
[278605-18-8]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Caulerpa trifaria*. Pale yellow oil. $[\alpha]_D$ -71 (EtOH). λ_{max} 227 (ϵ 6700) (EtOH).

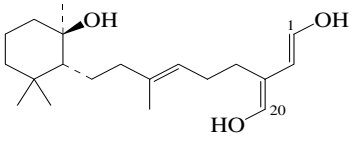
(2*Z*,6*E*,10*S*)-*form*

Di-Ac: [278605-19-9]
Constit. of *Caulerpa trifaria*.
Pale yellow oil. $[\alpha]_D$ -51 (EtOH). λ_{max} 203 (ϵ 11300) (EtOH).

1-Aldehyde, 20-Ac: [849475-58-7]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Caulerpa brownii*.
Handley, J.T. *et al., Aust. J. Chem.*, 2000, **53**, 67-71; 2005, **58**, 39-46

10,15-Cyclo-1,3(20),6-phytatriene-1,11,20-triol C-1043

9,10-Seco-8,13(16),14-labdatriene-10,15,16-triol. *10-Hydroxy-9,10-seco-8-labdene-15,16-dial*

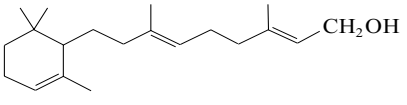


$C_{20}H_{34}O_3$ 322.487
Enolised dialdehyde, notional parent of isolated di-Ac.

(1*E*,3(20)*E*,6*E*,10*R*,11*R*)-*form*

1,20-Di-Ac: 1,20-Diacetoxy-10,15-cyclo-1,3(20),6-phytatrien-11-ol. *15,16-Diacetoxy-9,10-seco-8,13(16),14-labdatrien-10-ol*
[99695-01-9]
$C_{24}H_{38}O_5$ 406.561
Constit. of the alga *Caulerpa brownii*.
$[\alpha]_D^{25}$ -0.5 (c, 1 in $CHCl_3$). λ_{max} 249 (ϵ 16000) (MeOH).
Paul, V.J. *et al., Phytochemistry*, 1985, **24**, 2239-2243 (*isol, pmr, cmr*)

10,15-Cyclo-2,6,11-phytatrien-1-ol C-1044



$C_{20}H_{34}O$ 290.488

(2*E*,6*E*,10ξ)-*form*
Caulerpol
[62123-23-3]
Constit. of *Caulerpa brownii*. $Bp_{0.1}$ 120°. $[\alpha]_D$ -84.8 (MeOH).

O-*(9Z,12Z,15-Hexadecatrienoyl):* [849475-66-7]
$C_{36}H_{58}O_2$ 522.853
Constit. of *Caulerpa brownii*.

O-*(9Z-Octadecenoyl):* [849475-63-4]
$C_{38}H_{66}O_2$ 554.938
Constit. of *Caulerpa brownii*.

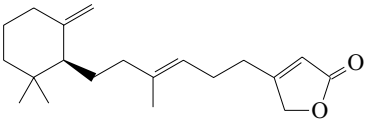
O-*(9Z,12Z-Octadecadienoyl):* [849475-64-5]
$C_{38}H_{64}O_2$ 552.922
Constit. of *Caulerpa brownii*.

O-*(9Z,12Z,15Z-Octadecatrienoyl):* [849475-65-6]
$C_{38}H_{62}O_2$ 550.907
Constit. of *Caulerpa brownii*.

O-*(5Z,8Z,11Z,14Z-Eicosatetraenoyl):* [849475-60-1]
$C_{40}H_{64}O_2$ 576.944
Constit. of *Caulerpa brownii*.

O-*(5Z,8Z,11Z,14Z,17Z-Eicosapentaenoyl):* [849475-62-3]
$C_{40}H_{62}O_2$ 574.929
Constit. of *Caulerpa brownii*.
Blackman, A.J. *et al., Tet. Lett.*, 1976, 2729-2730
Handley, J.T. *et al., Aust. J. Chem.*, 2005, **58**, 39-46 (*esters*)

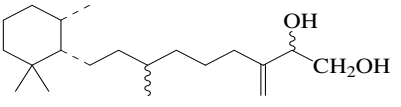
10,15-Cyclo-2,6,11(18)-phytatrien-1,20-olide C-1045



$C_{20}H_{30}O_2$ 302.456

(6*E*,10*S*)-*form*
Luffarin W
[145398-73-8]
Constit. of *Luffariella geometrica*.
Oil. $[\alpha]_D^{20}$ +13.2 (c, 0.7 in $CHCl_3$).
Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705 (*isol, pmr, cmr*)

10,15-Cyclo-3(20)-phytene-1,2-diol C-1046

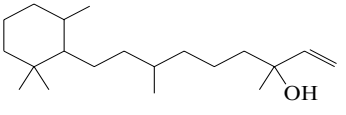


$C_{20}H_{38}O_2$ 310.519

(2ξ,7ξ,10*S*,11*S*)-*form*
Viridiol A
[183585-27-5]
Constit. of *Laurencia viridis*.
Oil. $[\alpha]_D^{25}$ +0.16 (c, 0.64 in $CHCl_3$).
Norte, M. *et al., Nat. Prod. Lett.*, 1996, **8**, 263-269 (*isol, pmr, cmr*)

10,15-Cyclo-1-phyten-3-ol C-1047

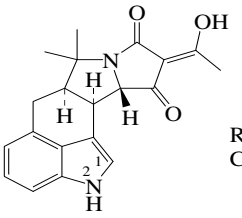
Callyspinol
[171828-75-4]



$C_{20}H_{38}O$ 294.52
Constit. of *Callyspongia spinosissima*.
$[\alpha]_D^{28}$ +1.2 (CH_2Cl_2).
Garg, H.S. *et al., Tet. Lett.*, 1995, **36**, 9035 (*isol, pmr, cmr*)

α-Cyclopiazonic acid C-1048

[18172-33-3]
[83136-88-3]



Relative Configuration

$C_{20}H_{20}N_2O_3$ 336.39

Enolised β-triketone. CAS numbering shown. Toxic alkaloid from *Penicillium cyclopium*, *Penicillium camemberti*, *Penicillium duclauxii* MF2831, *Aspergillus versicolor*, *Aspergillus flavus*, *Aspergillus oryzae* ATCC20235 and *Aspergillus tamarii* IAM1465. Antioxidant. Mycotoxin. Inhibits sarcoplasmic reticulum Ca^{2+}-ATPase and ATP-dependent Ca^{2+} transport. Pharmacol. tool for studying intracellular Ca^{2+} homeostasis. Exerts negative inotropic effects on adult myocardium. Mp 245-246°. $[\alpha]_D^{18}$ -74 (c, 1 in $CHCl_3$). λ_{max} 225 (ϵ 39800); 253 (ϵ 16600); 275 (sh) (ϵ 19100); 284 (ϵ 20400); 292 (sh) (ϵ 17400) (MeOH) (Derep). λ_{max} 224 (ϵ 32360); 282 (ϵ 17780); 290 (ϵ 14125) (MeOH) (Berdy). λ_{max} 223 (ϵ 39400); 281 (ϵ 19300) (EtOH) (Berdy). λ_{max} 222 (ϵ 40800); 252 (ϵ 16300); 281 (ϵ 19300) (EtOH/NaOH) (Berdy).

▶ Exp. reprod. and teratogenic effects. Tremorgenic toxin. Adverse effects incl. muscle incoordination, hypokinesia, convulsions; LD_{50} (mus, ipr) 2.3 mg/kg. LD_{50} (rat, orl) 36 mg/kg. UY8587000

Hydrazone: Mp 189-190°.

1-Hydroxy, 2-Me: ***Speradine A***

[566943-74-6]

$C_{21}H_{22}N_2O_4$ 366.416

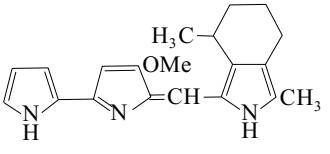
Alkaloid from a marine-derived *Aspergillus tamarii*. Pale yellow solid. $[\alpha]_D^{18}$ -79 (c, 1 in $CHCl_3$). Exists in 1-oxo-2*NH*-form. λ_{max} 210 (ϵ 15000); 253 (ϵ 7700); 280 (ϵ 6400) (MeOH).

Holzapfel, C.W. *et al., Tetrahedron*, 1968, **24**, 2101-2119 (*isol, uv, ir, ms, pmr, cd, struct*)
Holzapfel, C.W. *et al., Phytochemistry*, 1971, **10**, 351-358 (*biosynth*)
Purchase, I.F.H. *et al., Toxicol. Appl. Pharmacol.*, 1971, **18**, 114-123 (*tox*)
Steyn, P.S. *et al., Chem. Comm.*, 1975, 465-466 (*biosynth*)
De Jesus, A.E. *et al., J.C.S. Perkin 1*, 1981, 3292-3294 (*biosynth*)
Chalmers, A.A. *et al., Chem. Comm.*, 1982, 1367-1368 (*biosynth*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2220-2284 (*uv, ir, pmr, ms, cd*)
Somei, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2153-2156 (*synth*)
Kozikowski, A.P. *et al., J.A.C.S.*, 1984, **106**, 6873-6874 (*synth*)
Nishie, K. *et al., Food Chem. Toxicol.*, 1985, **23**, 831-839; 1069-1076 (*tox, metab*)
Muratake, H. *et al., Heterocycles*, 1985, **23**, 1111 (*synth*)
Norred, W.P. *et al., J. Agric. Food Chem.*, 1988, **36**, 113-116
Seidler, N.W. *et al., J. Biol. Chem.*, 1989, **264**, 17816-17823 (*pharmacol*)
Agata, N. *et al., Br. J. Pharmacol.*, 1993, **108**, 571-572 (*pharmacol*)
Bradburn, N. *et al., Phytochemistry*, 1994, **35**, 817 (*activity*)
Plenge-Tellechea, F. *et al., J. Biol. Chem.*, 1997, **272**, 2794-2800 (*pharmacol*)
Schwinger, R.H.G. *et al., J. Pharmacol. Exp. Ther.*, 1997, **283**, 286-292 (*pharmacol*)
Tsuda, M. *et al., Tetrahedron*, 2003, **59**, 3227-3230 (*Speradine A*)
Haskins, C.M. *et al., Chem. Comm.*, 2005, 3162-3164 (*synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 497
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, CQD000

Cycloprodigiosin C-1049

*4,5,6,7-Tetrahydro-3-[[3-methoxy-5-(1*H*-pyrrol-2-yl)-2*H*-pyrrol-2-ylidene]methyl]-1,4-dimethyl-2*H*-isoindole, 9CI*

[86797-91-3]

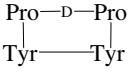


$C_{20}H_{23}N_3O$ 321.421

Pyrrole antibiotic. Revised struct. Minor red pigment from cultures of the aerobic marine bacterium *Alteromonas rubra*. Also isolated from *Pseudoalteromonas denitrificans* and *Beneckea gazogenes*. Shows antibacterial, antifungal, immunosuppressant, antiarteriosclerotic and antiosteoporotic activities. λ_{max} 216 (ϵ 8660); 275 (sh) (ϵ 6440); 296 (ϵ 12200); 371 (ϵ 7750); 382 (sh) (ϵ 7240); 510 (sh) (ϵ 54400); 541 (ϵ 132000) (EtOH, pH 2.9) (Derep). λ_{max} 226 (ϵ 10800); 289 (ϵ 9820); 337 (ϵ 7590); 471 (ϵ 41600); 539 (ϵ 17200) (EtOH, pH 7.4) (Derep). λ_{max} 257 (ϵ 7950); 281 (ϵ 9520); 336 (ϵ 7860); 469 (ϵ 42400) (EtOH,pH 11) (Derep). λ_{max} 544 (ϵ 110000) ($CHCl_3$/HCl) (Berdy). λ_{max} 540 (EtOH/HCl) (Berdy).

Laatsch, H. *et al., Tet. Lett.*, 1983, **24**, 2701 (*isol, uv, pmr, ms, struct*)
Gerber, N.N. *et al., Tet. Lett.*, 1983, **24**, 2797 (*cmr, pmr*)
Wassermann, H.H. *et al., Tet. Lett.*, 1984, 1387 (*synth*)
Japan. Pat., 1998, 98 80 293; *CA*, **128**, 294012d (*isol, activity*)

Cyclo(prolyl-D-prolyltyrosyltyrosyl) C-1050



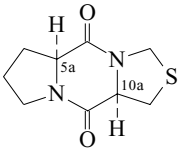
$C_{28}H_{32}N_4O_6$ 520.584

Isol. from a *Pseudomonas* sp. strain IM-1 associated with the marine sponge *Ircinia muscarum*. Amorph. solid. $[\alpha]_D$ -7.6 (c, 0.003 in MeOH).

Mitova, M. *et al., Z. Naturforsch., C*, 2003, **58**, 740-745 (*isol, pmr, cmr*)

Cyclo(prolylthioprolyl) C-1051

*Hexahydro-3*H*,5*H*,10*H*-pyrrolo[1,2-*a*]thiazolo[3,4-*d*]pyrazine-5,10-dione, 9CI*



$C_9H_{12}N_2O_2S$ 212.272

CA numbering shown.

(5aS,10aR)-form

(-)-cis-*form*

[136849-41-7]

Alkaloid from the sponge *Tedania ignis*.

Cryst.

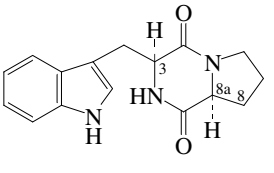
Mp 168-170°. $[\alpha]_D^{23}$ -114.3 (c, 0.14 in $CHCl_3$).

Dillman, R.L. *et al., J. Nat. Prod.*, 1991, **54**, 1159 (*isol, synth, pmr, cmr*)

Cyclo(prolyltryptophyl) C-1052

*Hexahydro-3-(1*H*-indol-3-ylmethyl)pyrrolo[1,2-*a*]pyrazine-1,4-dione, 9CI. Cyclo(tryptophanylprolyl). Cyclo(tryptophylprolyl)*

[67889-75-2]



$C_{16}H_{17}N_3O_2$ 283.329

(3R,8aS)-form

D-L-form

[41222-71-3]

Cryst. (Me_2CO). Mp 204-206°. $[\alpha]_D^{22}$ -101 (c, 1.78 in AcOH).

(3S,8aR)-form

L-D-form

[73136-47-7]
Cryst. (Me_2CO/petrol). Mp 191-193°. $[\alpha]_D^{20}$ +120 (c, 1.3 in AcOH).

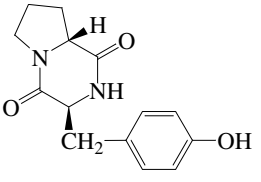
(3*S*,8*aS*)-*form*
L-L-form. ***Brevianamide F***
[38136-70-8]
Prod. by *Penicillium brevi-compactum*, *Penicillium piscarium* and *Alteromonas distincta* He169. Also prod. by a *Vibrio* sp. isol. from the sponge *Hyrtios altum*. Shows broad spectrum antibacterial and gastrointestinal cell maturation enhancing activity.
Mp 173-175°. $[\alpha]_D^{24}$ -99 (c, 1.2 in AcOH). λ_{max} 220 (ϵ 11000); 276 (ϵ 1900); 281 (ϵ 2000); 290 (ϵ 1700) (MeOH) (Berdy).

*8,8*a-*Didehydro: 12,13-Dehydroprolyltryptophyldiketopiperazine. Cyclo(dehydroprolyltryptophyl)*
[290348-28-6]
$C_{16}H_{15}N_3O_2$ 281.313
Prod. by *Penicillium piscarium*.

Birch, A.J. *et al., Tetrahedron*, 1972, **28**, 2999 (*isol, uv, ir, ms, pmr, synth*)
Steyn, P.S. *et al., Tetrahedron*, 1973, **29**, 107
Sammes, P.G. *et al., J.C.S. Perkin 1*, 1979, 3048 (*synth, bibl*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 2449-2451 (*Vibrio, isol*)
Grant, G.D. *et al., J. Chem. Crystallogr.*, 1999, **29**, 435-447 (*cryst struct*)
Graz, M. *et al., Pharmazie*, 1999, **54**, 772 (*activity*)
Kozlovskii, A.G. *et al., Prikl. Biokhim. Mikrobiol.*, 2000, **36**, 317-321 (*isol*)
Williams, R.M. *et al., Chem. Pharm. Bull.*, 2002, **50**, 711-740 (*rev, synth, biosynth*)
Shabaan, M. *et al., Dissertation*, Univ. of Gottingen, 2004, (*Alteromonas, isol*)

Cyclo(prolyltyrosyl) C-1053

*Hexahydro-3-(4-hydroxybenzyl)pyrrolo[1,2-*a*]pyrazine-1,4-dione*
[74345-23-6]



(3*S*,8a*R*)-*form*

$C_{14}H_{16}N_2O_3$ 260.292

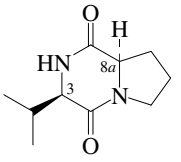
(3*S*,8*aR*)-*form*
L,D-form
[61117-56-4]
Isol. from two strains of microorganisms isol. from the marine sponge *Ircinia variabilis* and the fungus *Aspergillus flavipes*.
Cryst. (Et_2O/Me_2CO).
Mp 218-220°.

(3*S*,8*aS*)-*form*
L,L-form. ***Maculosin 1***. *ML 1532II. A 19C. Antibiotic A 19C. Antibiotic ML 1532II*
[4549-02-4]
Prod. by *Alternaria alternata*, *Aspergillus flavipes*, *Streptomyces gelaticus*, *Streptomyces* sp. ML1532, *Fusarium nivale*, a fungal growth on *Zinnia elegans* and *Bacillus licheniformis*. Isol. from the sponges *Jaspis digonoxea* and *Tedania anhelans*, a marine-derived *Pseudomonas aeruginosa*, marine *Penicillium* sp., marine bacterium *Vibrio parahaemolyticus* and pathogenic fungus *Pestalotia palmarum*. Present in coml. peptone. Cytotoxic. Inhibits SV-40 transformed cells and germination. Plant growth regulator. Possesses pesticidal props. Plates.
Mp 152-154° (140°). $[\alpha]_D$ -148 (c, 1 in H_2O).

Tamura, S. *et al., Agric. Biol. Chem.*, 1964, **28**, 650-652 (*3S,8aS-form, isol*)
Tatsuno, T. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1498-1500 (*3S,8aS-form, isol*)
Madison, V. *et al., J.A.C.S.*, 1976, **98**, 5365-5371 (*synth, cd, pmr, cmr*)
Kamikawa, T. *et al., Agric. Biol. Chem.*, 1980, **44**, 691-692 (*3S,8aS-form, isol*)
Munekata, M. *et al., Agric. Biol. Chem.*, 1981, **45**, 2613-2618 (*3S,8aS-form, isol*)
Sasaki, Y. *et al., Chem. Pharm. Bull.*, 1982, **30**, 4435-4443 (*3S,8aS-form, synth*)
Stierle, A.C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1988, **85**, 8008-8011 (*Maculosin 1*)
Milne, P.J. *et al., J. Crystallogr. Spectrosc. Res.*, 1992, **22**, 643-649 (*cryst struct, conformn*)
Barrow, C.J. *et al., J. Nat. Prod.*, 1994, **57**, 471-476 (*Aspergillus flavipes constit*)
Rudi, A. *et al., J. Nat. Prod.*, 1994, **57**, 829-836 (*isol, pmr, cmr*)
Jayatilake, G.S. *et al., J. Nat. Prod.*, 1996, **59**, 293-296 (*isol, pmr, cmr*)
De Rosa, S. *et al., Biomol. Eng.*, 2003, **20**, 311-316 (*Ircinia variabilis constit*)

Cyclo(prolylvalyl) C-1054

*Hexahydro-3-(1-methylethyl)pyrrolo[1,2*a*]pyrazine-1,4-dione, 9CI. Hexahydro-3-isopropylpyrrolo[1,2-*a*]pyrazine-1,4-dione. Prolylvaline anhydride. Maculosine 5. Antibiotic K 73. K 73*
[5654-87-5]



(3*R*,8*aR*)-*form*

$C_{10}H_{16}N_2O_2$ 196.249
Diketopiperazine antibiotic.

(3*R*,8*aR*)-*form*
D-D-form
Prod. by the marine bacterial strains CF-20 and C-148 obt. from molluscs. Active against *Vibrio anguillarum*. $[\alpha]_D$ +120.1 (c, 0.1 in EtOH).

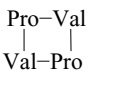
(3*R*,8*aS*)-*form* [27483-18-7]
Cryst. (EtOAc/hexane). Mp 154-156°. $[\alpha]_D^{20}$ -96.4 (c, 0.25 in H_2O).

(3*S*,8*aR*)-*form* [156617-55-9]
Prod. by *Aspergillus* sp. F70609 and *Aspergillus flavipes*. Specific β-glucosidase inhibitor. Cryst. (EtOAc/hexane).
Mp 147-149°. $[\alpha]_D^{20}$ +88 (c, 1 in H_2O).

(3*S*,8*aS*)-*form*
L-L-form
[2854-40-2]
Prod. by *Aspergillus, Streptomyces, Oospora* spp. and *Pinellia pedatisecta*. Alkaloid from the Caribbean sponges *Calyx* cf. *podatypa* and *Tedania ignis*. Also from the alga *Scenedesmus* sp. and the fungi *Rhizoctonia solani* and *Rosellinia necatrix*. Shows antibiotic and phytotoxic props. Needles (butanol).
Mp 189.5° (169-172°). $[\alpha]_D^{20}$ -157 (c, 1 in $CHCl_3$). $[\alpha]_D^{20}$ -180.5 (c, 1 in EtOH).

Luedemann, G. *et al., J.O.C.*, 1961, **26**, 4128-4130 (*isol*)
Siemion, I.Z. *et al., Org. Magn. Reson.*, 1971, **3**, 545-550 (*synth, nmr*)
Ogura, H. *et al., Chem. Pharm. Bull.*, 1975, **23**, 2474-2477 (*isol*)
Munekata, M. *et al., Agric. Biol. Chem.*, 1981, **45**, 2613-2618 (*isol*)
Schmidtz, F.J. *et al., J.O.C.*, 1983, **48**, 3941-3945 (*isol, pmr, ms, synth, bibl*)
Giralt, E. *et al., Synthesis*, 1985, 181-184 (*synth*)
Stierle, A.C. *et al., Experientia*, 1988, **44**, 1021 (*isol*)
Barrow, C.J. *et al., J. Nat. Prod.*, 1994, **57**, 471-476 (*isol*)
Adamczeski, M. *et al., J. Nat. Prod.*, 1995, **58**, 201-208 (*isol, pmr, cmr*)
Jayatilake, G.S. *et al., J. Nat. Prod.*, 1996, **59**, 293-296 (*isol, cmr*)
Bull, S.D. *et al., J.C.S. Perkin 1*, 1998, 2313-2320 (*configs, biosynth*)
Kwon, O.S. *et al., J. Antibiot.*, 2001, **54**, 179-181 (*isol, pmr, cmr*)
Fdhila, F. *et al., J. Nat. Prod.*, 2003, **66**, 1299-1301 (*isol, pmr, cmr*)
Pedras, M.S.C. *et al., Z. Naturforsch., C*, 2005, **60**, 717-722 (*isol, synth, pmr, cmr*)

Cyclo(prolylvalylprolylvalyl) C-1055



$C_{20}H_{32}N_4O_4$ 392.497
λ_{max} 259 (ϵ 492) (EtOH) (Berdy).

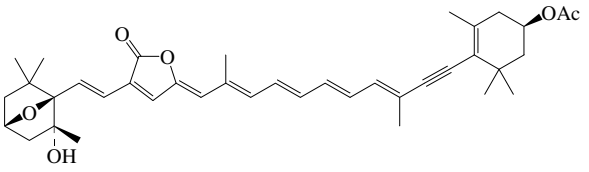
(*all*-L)-*form* [88927-74-6]
Isol. from the marine ascidian *Cystodytes dellechiajei*. Cytotoxic.

[97644-10-5]

Ueda, T. *et al., Int. J. Pept. Protein Res.*, 1985, **25**, 475-480 (*synth*)
Aracil, J.-M. *et al., Tet. Lett.*, 1991, **32**, 2609-2612 (*isol, pmr, cmr, struct*)

Cyclopyrrhoxanthin C-1056

[866025-62-9]

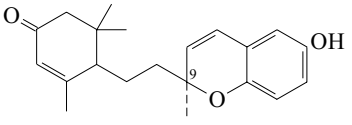


$C_{39}H_{48}O_6$ 612.805
Constit. of the corbicula clam (Shijimi), *Corbicula japonica*, from brackish water. λ_{max} 455; 475 (Et_2O).

Maoka, T. *et al., J. Nat. Prod.*, 2005, **68**, 1341-1344 (*Cyclopyrrhoxanthin*)

Cyclorenierin A C-1057

[164672-55-3]



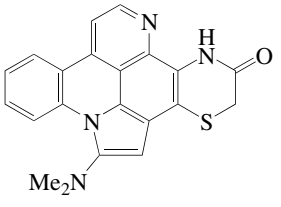
$C_{21}H_{26}O_3$ 326.435
Constit. of a *Haliclona* sp.

9-Epimer: ***Cyclorenierin B***
[164906-29-0]
$C_{21}H_{26}O_3$ 326.435
Constit. of a *Haliclona* sp.

Jaspars, M. *et al., J. Nat. Prod.*, 1995, **58**, 609 (*isol, pmr, cmr*)

Cycloshermilamine D C-1058

[272118-05-5]

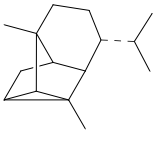


$C_{21}H_{16}N_4OS$ 372.45
Alkaloid from the tunicate *Cystodytes violatinctus.* Amorph. yellow powder. λ_{max} 208 (log ϵ 4.18); 215 (log ϵ 4.16); 262 (log ϵ 4.04); 299 (log ϵ 3.88); 391 (log ϵ 3.35); 480 (log ϵ 3.19) (MeOH).

Koren-Goldschlager, G. *et al., J. Nat. Prod.*, 2000, **63**, 830-831 (*isol, uv, pmr*)

Cyclosinularane C-1059

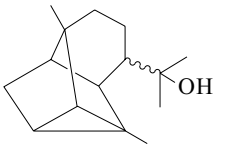
[79383-64-5]



$C_{15}H_{24}$ 204.355
Constit. of *Clavularia viridis.* Oil. $[\alpha]_D$ +22.2 (c, 0.1 in $CHCl_3$).

Yasumoto, M. *et al., J. Nat. Prod.*, 2000, **63**, 1534-1536 (*isol, pmr, cmr*)

Cyclosinularan-12-ol C-1060

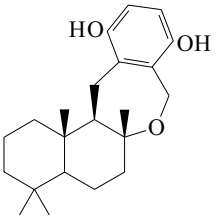


$C_{15}H_{24}O$ 220.354

Ac: ***12-Acetoxycyclosinularane***
$C_{17}H_{26}O_2$ 262.391
Constit. of *Clavularia inflata*. Oil. $[\alpha]_D$ +20.5 (c, 0.4 in $CHCl_3$).

Braekman, J.C. *et al., Tetrahedron*, 1981, **37**, 179-186 (*cryst struct*)

Cyclosiphonodictyol A C-1061



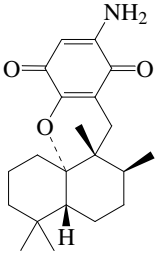
$C_{22}H_{32}O_3$ 344.493

Disulfate: ***Bis(sulfato)cyclosiphonodictyol A***
[167172-98-7]
$C_{22}H_{32}O_9S_2$ 504.621
Constit. of *Siphonodictyon coralliphagum*. Amorph. solid. $[\alpha]_D^{24}$ +12 (c, 0.2 in MeOH). λ_{max} 203 (ϵ 9400); 217 (ϵ 42000); 262 (ϵ 410); 266 (ϵ 410) (MeOH) (Berdy).

Killday, K.B. *et al., J. Nat. Prod.*, 1995, **58**, 958 (*isol, pmr, cmr*)

Cyclosmenospongine C-1062

[501691-51-6]

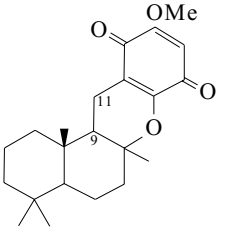


$C_{21}H_{29}NO_3$ 343.465
Isol. from the Australian sponge *Spongia* sp. Wine-coloured oil. $[\alpha]_D^{25}$ -18 (c, 0.12 in $CHCl_3$). λ_{max} 211 (log ϵ 3.01); 313 (log ϵ 2.84) (EtOH).

Utkina, N.K. *et al., J. Nat. Prod.*, 2003, **66**, 1263-1265 (*abs config*)
Utkina, N.K. *et al., Tet. Lett.*, 2003, **44**, 101-102 (*isol, pmr, cmr*)

Cyclospongiaquinone 1 C-1063

[69672-68-0]



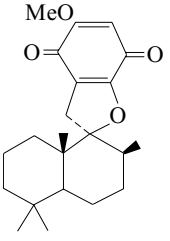
$C_{22}H_{30}O_4$ 358.477
Constit. of *Stelospongia conulata*. Yellow cryst. (hexane). Mp 196-196.5°. $[\alpha]_D^{20}$ -2.15 (c, 1 in $CHCl_3$). λ_{max} (no change in UV reported) (Derep). λ_{max} 300 (ϵ 15500); 440 (ϵ 324) (EtOH) (Derep).

9,11-Didehydro: ***Dehydrocyclospongiaquinone 1***
[69672-70-4]
$C_{22}H_{28}O_4$ 356.461
Constit. of *Stelospongia conulata*. Red cryst. (EtOH). Mp 90.5-92°. $[\alpha]_D^{20}$ -140 (c, 0.2 in $CHCl_3$). λ_{max} (no shifts reported) (Derep). λ_{max} 266 (ϵ 12000); 280 (sh) (ϵ 10500); 295 (sh) (ϵ 9330); 310 (sh) (ϵ 7410); 496 (ϵ 708) (MeOH) (Derep).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1978, **31**, 2685

Cyclospongiaquinone 2 C-1064

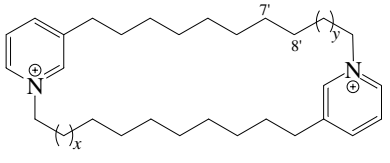
[69672-69-1]



$C_{22}H_{30}O_4$ 358.477
Constit. of *Stelospongia conulata*. Orange cryst. (hexane). Mp 196-197°. $[\alpha]_D^{20}$ +11.7 (c, 1 in $CHCl_3$). λ_{max} 285 (ϵ 21900); 406 (ϵ 372) (EtOH) (Derep).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1978, **31**, 2685-2697 (*isol, pmr, cmr, ms, uv*)

Cyclostellettamines C-1065



Cyclostellettamine A, $x = 3, y = 3$
B, $x = 3, y = 4$
C, $x = 4, y = 4$
D, $x = 3, y = 5$
E, $x = 4, y = 5$
F, $x = 5, y = 5$
G, $x = 2, y = 3$
H, $x = 1, y = 3$
I, $x = 1, y = 4$
K, $x = 1, y = 5$
L, $x = 2, y = 5$

Muscarinic receptor binding inhibitors.

Cyclostellettamine A [156953-85-4]
$C_{34}H_{56}N_2$ 492.83
Alkaloid from the marine sponge *Stelletta maxima*. Sol. MeOH, butanol. λ_{max} 266 (MeOH) (Berdy).

Cyclostellettamine B [156953-87-6]
$C_{35}H_{58}N_2$ 506.857
From *Stelletta maxima*. Sol. MeOH, butanol. λ_{max} 268 (MeOH) (Berdy).

Cyclostellettamine C [156953-91-2]
[181212-11-3]
$C_{36}H_{60}N_2$ 520.883
From *Stelletta maxima*. Amorph. solid (EtOAc/hexane) (as bis(trifluoromethanesulfonate)). Sol. MeOH, butanol. Mp 123-124° (bis(trifluoromethanesulfonate)). λ_{max} 266 (ϵ 6320) (MeOH).

Cyclostellettamine D [156953-89-8]
$C_{36}H_{60}N_2$ 520.883
From *Stelletta maxima*. Sol. MeOH, butanol. λ_{max} 267 (MeOH) (Berdy).

7′,8′Z-Didehydro: ***Dehydrocyclostellettamine D***
[706784-72-7]
$C_{36}H_{58}N_2$ 518.868
Isol. from *Xestospongia* sp. Amorph. solid. CAS No. refers to trifluoroacetic acid salt.

Cyclostellettamine E [156953-93-4]
$C_{37}H_{62}N_2$ 534.91
From *Stelletta maxima*. Sol. MeOH, butanol. λ_{max} 268 (MeOH) (Berdy).

7′,8′Z-Didehydro: ***Dehydrocyclostellettamine E***
[706784-74-9]
$C_{37}H_{60}N_2$ 532.894
Isol. from a *Xestospongia* sp. Amorph. solid. CAS No. refers to trifluoroacetic acid salt. λ_{max} 204 (ϵ 19000); 215 (sh) (ϵ 9400); 269 (ϵ 8600); 274 (sh) (ϵ 7200) (MeOH).

Cyclostellettamine F [156953-95-6]
$C_{38}H_{64}N_2$ 548.937
From *Stelletta maxima*. Sol. MeOH, butanol. λ_{max} 267 (MeOH) (Berdy).

Cyclostellettamine G [708255-98-5]
$C_{33}H_{54}N_2$ 478.803
Isol. from a *Xestospongia* sp. and from *Pachychalina* sp. Amorph. solid. CAS No. refers to trifluoroacetic acid salt. λ_{max} 203 (ϵ 13000); 216 (sh) (ϵ 6400); 268 (ϵ 4700); 274 (sh) (ϵ 4000) (MeOH).

Cyclostellettamine H
$C_{32}H_{52}N_2$ 464.776
From *Pachychalina* sp.

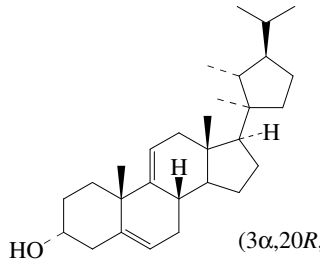
Cyclostellettamine I
$C_{33}H_{54}N_2$ 478.803
From *Pachychalina* sp.

Cyclostellettamine K
$C_{34}H_{56}N_2$ 492.83
From *Pachychalina* sp.

Cyclostellettamine L
$C_{35}H_{58}N_2$ 506.857
From *Pachychalina* sp.

Fusetani, N. *et al., Tet. Lett.*, 1994, **35**, 3967-3970 (*Cyclostellettamines A-F, isol, uv, pmr, struct*)
Fusetani, N. *et al., Tetrahedron*, 1996, **52**, 10849-10860 (*synth, Cyclostellettamine C, pmr, cmr, uv*)
Wanner, M.J. *et al., Eur. J. Org. Chem.*, 1998, 889-895 (*synth*)
Matzanke, N. *et al., Org. Prep. Proced. Int.*, 1998, **30**, 3-51 (*rev*)
Baldwin, J.E. *et al., Tetrahedron*, 1998, **54**, 13655-13680 (*synth*)
Oku, N. *et al., Bioorg. Med. Chem. Lett.*, 2004, **14**, 2617-2620 (*Cyclostellettamine G, Dehydrocyclostellettamines*)
De Oliveira, J.H.H.L. *et al., J. Nat. Prod.*, 2004, **67**, 1685-1689 (*Cyclostellettamines G-L*)
Grube, A. *et al., Eur. J. Org. Chem.*, 2006, 1285-1295 (*Cyclostellettamine H, I, K, L, synth, ms*)
De Oliveira, J.H.H.L. *et al., Mar. Drugs*, 2006, **4**, 1-8 (*activity*)

20,28-Cyclostigmasta-5,9(11)-dien-3-ol C-1066



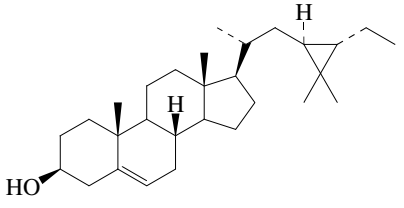
(3α,20*R*,24*R*,28*R*)-*form*

$C_{29}H_{46}O$ 410.682

(3α,20*R*,24*R*,28*R*)-*form*
3-Epilappasterol
[780755-38-6]
Constit. of *Saussurea lappa* roots.
Cryst. ($CHCl_3$/MeOH).
Mp 126-128°. $[\alpha]_D^{28}$ +345.2 (c, 0.04 in $CHCl_3$).

(3β,20*R*,24*R*,28*R*)-*form*
Lappasterol
[780755-37-5]
Constit. of *Saussurea lappa* roots.
Cryst. ($CHCl_3$/MeOH).
Mp 130-132°. $[\alpha]_D^{28}$ 0 (c, 0.14 in $CHCl_3$).
Singh, V. *et al., Indian J. Chem., Sect. B*, 2004, **43**, 655-659 (*isol, pmr, cmr*)

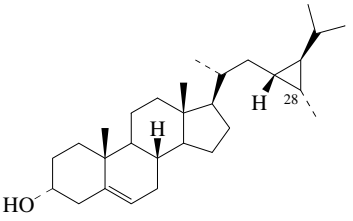
23,25-Cyclostigmast-5-en-3-ol C-1067



$C_{29}H_{48}O$ 412.698

(3β,23*S*,24*S*)-*form*
Nicasterol
[96363-06-3]
Constit. of *Calyx nicaeensis*.
Mp 132-134°. $[\alpha]_D^{20}$ -25.8 (c, 1.55 in $CHCl_3$).
Proudfoot, J.R. *et al., J.O.C.*, 1985, **50**, 2026-2030 (*isol, synth*)

23,28-Cyclostigmast-5-en-3-ol C-1068



(3α,23*S*,24*S*,28*R*)-*form*

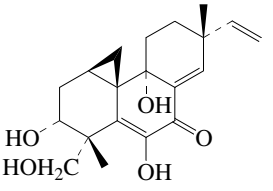
$C_{29}H_{48}O$ 412.698

(3α,23*S*,24*S*,28*R*)-*form*
5β,6-Dihydro: ***3α,5β-Dihydrocalystanol***
[123238-27-7]
$C_{29}H_{50}O$ 414.713
Isol. from sponge *Calyx nicaeensis*, prob. as endobacterial metab.

(3β,23*R*,24*S*,28*R*)-*form*
23-Epidihydrocalysterol
[132438-14-3]
Constit. of *Cribrochalina vasculum*.

(3β,23*S*,24*S*,28*R*)-*form*
Dihydrocalysterol
[83542-16-9]
Constit. of *Calyx nicaensis*, *Petrosia ficiformis* and *Petrosia hebes*.
Cryst.
Mp 159-161°. $[\alpha]_D^{20}$ -56 (c, 0.8 in CH_2Cl_2).
5α,6-Dihydro: ***5α-Dihydrocalystanol***
[106566-87-4]
$C_{29}H_{50}O$ 414.713
Isol. from sponges *Petrosia ficiformis* and *Calyx nicaensis*, prob. as endobacterial metab. Constit. of *Petrosia hebes*.
Mp 119-120°.
Seidel, S.B. *et al., Steroids*, 1986, **47**, 49-62 (*Dihydrocalystanol*)
Proudfoot, J.R. *et al., J.C.S. Perkin 1*, 1987, 1283-1290 (*isol, synth, pmr*)
Cho, J.H. *et al., J.C.S. Perkin 1*, 1987, 1307-1318 (*5α-Dihydrocalystanol, isol*)
Doss, G.A. *et al., J.A.C.S.*, 1988, **110**, 8124-8128 (*isol, pmr, cmr*)
Tam Ha, T.B. *et al., Steroids*, 1989, **53**, 487-499 (*Dihydro-5β-calystan-3α-ol*)
Giner, J.-L. *et al., Steroids*, 1992, **57**, 258-261 (*isol, pmr*)

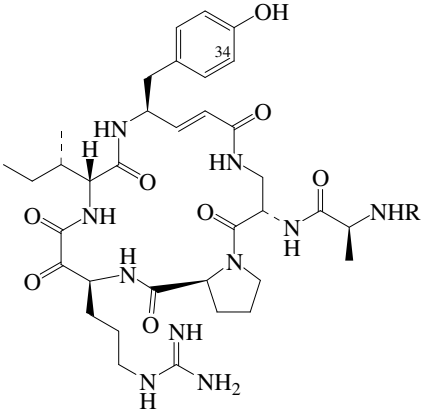
1,20-Cyclo-3,6,9,18-tetrahydroxy-5,8(14),15-isopimaratrien-7-one C-1069



$C_{20}H_{26}O_5$ 346.422

(3α,9α)-*form*
18-Ac: ***Libertellenone D***
[866413-31-2]
$C_{22}H_{28}O_6$ 388.46
Metab. of a marine-derived *Libertella* sp. Oil. $[\alpha]_D$ -145.1 (c, 0.247 in MeCN). λ_{max} 216 (log ϵ 3.83); 267 (log ϵ 3.71); 327 (log ϵ 3.73) (no solvent reported).
Oh, D.-C. *et al., Bioorg. Med. Chem.*, 2005, **13**, 5267-5273 (*Libertellenone D*)

Cyclotheonamide C-1070



Cyclotheonamide E R = -$COCH_2Ph$
" E2 R = -COPh
" E3 R = -$COCH_2CH(CH_3)_2$
" E4 R = -$COCH_2CH(CH_3)CH_2CH_3$

Cyclotheonamide E [170129-81-4]

$C_{43}H_{58}N_{10}O_9$ 858.993

Cyclic peptide antibiotic. Isol. from the sponges *Theonella swinhoei* and *Ircinia* sp. Thrombin inhibitor. Amorph. solid. $[\alpha]_D^{23}$ -17.6 (c, 0.07 in MeOH). λ_{max} 273 (ϵ 2700); 323 (ϵ 400) (MeOH).

Cyclotheonamide E2

$C_{42}H_{56}N_{10}O_9$ 844.966

Isol. from a *Theonella* sp. Amorph. pale brown solid. $[\alpha]_D^{26}$ -37.3 (c, 0.1 in MeOH). λ_{max} 274 (ϵ 4020) (MeOH).

Cyclotheonamide E3

$C_{40}H_{60}N_{10}O_9$ 824.976

Isol. from a *Theonella* sp. Amorph. pale brown solid. $[\alpha]_D^{26}$ -40.2 (c, 0.1 in MeOH). λ_{max} 272 (ϵ 2140) (MeOH).

Cyclotheonamide E4

$C_{41}H_{62}N_{10}O_9$ 839.002

Isol. from the sponge *Ircinia* sp. Pale yellow solid. $[\alpha]_D^{25}$ -101 (c, 0.04 in MeOH). λ_{max} 287 (ϵ 1367) (MeOH).

34-Hydroxy: ***Cyclotheonamide E5***

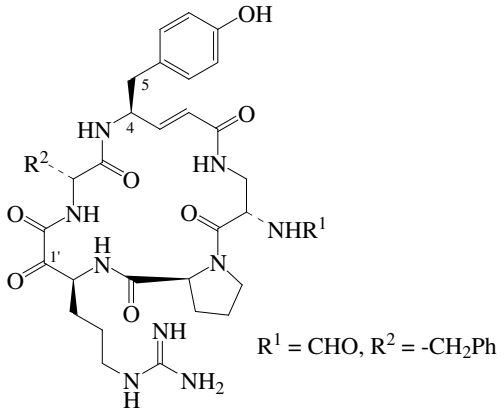
$C_{41}H_{62}N_{10}O_{10}$ 855.002

Isol. from an *Ircinia* sp. Pale yellow solid. $[\alpha]_D^{25}$ -64.5 (c, 0.03 in MeOH). λ_{max} 285 (ϵ 3780) (MeOH).

Nakoa, Y. *et al., Bioorg. Med. Chem.*, 1995, **3**, 1115-1122 (*isol, uv, pmr, cmr*)
Nakoa, Y. *et al., J. Nat. Prod.*, 1998, **61**, 667-670 (*isol, uv, pmr, cmr*)
Murakami, Y. *et al., J. Nat. Prod.*, 2002, **65**, 259-261 (*Cyclotheonamide E4,E5*)
Wasserman, H.H. *et al., Tetrahedron*, 2002, **58**, 6277-6283 (*synth*)

Cyclotheonamide A **C-1071**

MS 1144. Antibiotic MS 1144
[129033-04-1]



R^1 = CHO, R^2 = $-CH_2Ph$

$C_{36}H_{45}N_9O_8$ 731.807

Cyclic peptide. Isol. from the marine sponge *Theonella swinhoei*. Potent thrombin inhibitor. $[\alpha]_D^{23}$ -13 (c, 0.2 in MeOH). λ_{max} 278 (ϵ 1940) (MeOH) (Derep).

1′β-Alcohol: ***Dihydrocyclotheonamide A***

$C_{36}H_{47}N_9O_8$ 733.823

Isol. from *Theonella swinhoei*. Serine protease inhibitor. Amorph. solid. $[\alpha]_D^{29}$ +37 (c, 0.25 in MeOH). λ_{max} 225 (sh) (ϵ 15000); 243 (sh) (ϵ 4800); 278 (sh) (ϵ 1400) (MeOH).

4,5-Didehydro(Z-): ***Cyclotheonamide C***

[170034-94-3]

$C_{36}H_{43}N_9O_8$ 729.791

Isol. from *Theonella swinhoei*. Thrombin and trypsin inhibitor. Amorph. yellow solid. $[\alpha]_D^{23}$ +42.4 (c, 1 in MeOH). λ_{max} 271 (ϵ 7000); 332 (ϵ 12000) (MeOH).

Fusetani, N. *et al., J.A.C.S.*, 1990, **112**, 7053 (*isol, struct*)
Hagihara, M. *et al., J.A.C.S.*, 1992, **114**, 6570 (*struct*)
Nakao, Y. *et al., Bioorg. Med. Chem.*, 1995, **3**, 1115-1122 (*Cyclotheonamide C*)
Maryanoff, B.E. *et al., J.A.C.S.*, 1995, **117**, 1225 (*synth*)
Nakao, Y. *et al., J.A.C.S.*, 1999, **121**, 2425-2431 (*Dihydrocyclotheonamide A*)

Cyclotheonamide B **C-1072**

[129033-05-2]

As Cyclotheonamide A, C-1071 with

R^1 = Ac, R^2 = $-CH_2Ph$

$C_{37}H_{47}N_9O_8$ 745.834

Cyclic peptide. Isol. from the marine sponge *Theonella swinhoei*. Potent thrombin inhibitor. $[\alpha]_D^{23}$ -13.5 (c, 0.2 in MeOH) (synthetic). λ_{max} (solvent not reported) (Derep). λ_{max} 278 (ϵ 1940) (MeOH) (Derep).

Fusetani, N. *et al., J.A.C.S.*, 1990, **112**, 7053 (*isol, struct*)
Hagihara, M. *et al., J.A.C.S.*, 1992, **114**, 6570 (*synth*)
Maryanoff, B.E. *et al., Bioorg. Med. Chem.*, 1995, **3**, 1025-1038 (*pharmacol*)
Maryanoff, B.E. *et al., J.A.C.S.*, 1995, **117**, 1225 (*synth*)
Deng, J. *et al., Tet. Lett.*, 1996, **37**, 2261 (*synth*)
Bastiaans, H.M.M. *et al., J.O.C.*, 1997, **62**, 3880 (*synth*)

Cyclotheonamide D **C-1073**

[170129-80-3]

As Cyclotheonamide A, C-1071 with

R^1 = -CHO, R^2 = $-CH_2CH(CH_3)_2$

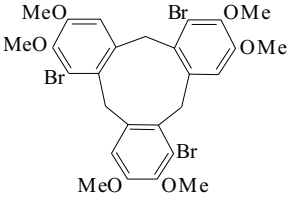
$C_{33}H_{47}N_9O_8$ 697.79

Cyclic peptide antibiotic. Isol. from the marine sponge *Theonella swinhoei*. Thrombin inhibitor. Amorph. solid. $[\alpha]_D^{23}$ -16.7 (c, 0.27 in MeOH).

Nakao, Y. *et al., Bioorg. Med. Chem.*, 1995, **3**, 1115-1122 (*isol, pmr, cmr*)

Cyclotribromoveratrylene **C-1074**

*1,6,11-Tribromo-10,15-dihydro-2,3,7,8,12,13-hexamethoxy-5*H*-tribenzo[*a,d,g*]cyclononene*
[68040-66-4]

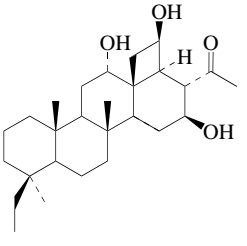


$C_{27}H_{27}Br_3O_6$ 687.219

Isol. from *Halopytis pinastroides*. Cryst. ($CHCl_3$/EtOH). Mp 222°. *Halopytis* may be an error for *Halopitys*.

Combaut, G. *et al., Phytochemistry*, 1978, **17**, 1791-1792 (*isol, struct*)
Combaut, G. *et al., Tet. Lett.*, 1978, 1699 (*conformn*)
Al-Farhan, E. *et al., Tet. Lett.*, 1992, **33**, 5846 (*synth*)

23,25-Cyclo-12,16,25-trihydroxy-20,24-dimethyl-24-scalaranone **C-1075**



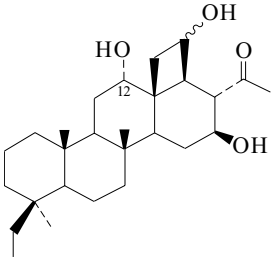
$C_{27}H_{44}O_4$ 432.642

(12α,16β,25β)-*form*

16-(2-Hydroxybutanoyl), 12-Ac: [221163-30-0]
$C_{33}H_{52}O_7$ 560.77
Constit. of *Strepsichordaia lendenfeldi*. Oil. $[\alpha]_D^{25}$ +31.4 (c, 2.07 in $CHCl_3$).
Jahn, T. *et al., J. Nat. Prod.*, 1999, **62**, 375-377 (*isol, pmr, cmr*)

23,25-Cyclo-12,16,25-trihydroxy-20,24-dimethyl-24-scalaranone C-1076

12,16,25-Trihydroxy-23,25-cyclo-20,24-dimethyl-24-scalaranone

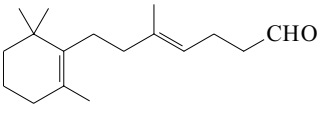


$C_{27}H_{44}O_4$ 432.642

(12α,16β,25ξ)-*form*

12-Ac: [99617-45-5]
$C_{29}H_{46}O_5$ 474.679
Constit. of sponge *Carteriospongia foliascens*. Ichthyotoxin. Cryst. Mp 190-193°. $[\alpha]_D$ +46 (c, 1.46 in $CHCl_3$).
Braekman, J.C. *et al., Tetrahedron*, 1985, **41**, 4603

10,15-Cyclo-1,2,20-trinor-6,10-phytadien-3-al C-1077

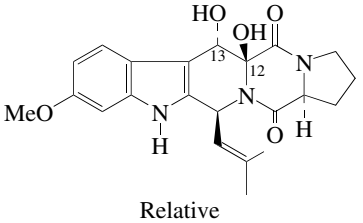


$C_{17}H_{28}O$ 248.408

Di-Me acetal: [160157-96-0]
$C_{19}H_{34}O_2$ 294.476
Constit. of *Fasciospongia cavernosa*. Oil. Poss. artifact as the biol. sample was stored in MeOH.
Venkateswarlu, Y. *et al., J. Nat. Prod.*, 1994, **57**, 1578 (*isol, pmr, cmr*)

Cyclotryprostatin A C-1078

[111468-06-5]



Relative Configuration

$C_{22}H_{25}N_3O_5$ 411.457
Prod. by *Aspergillus fumigatus*. Mammalian cell cycle inhibitor; microtubule polymerisation inhibitor. Pale yellow cryst. powder. Mp 180-185° dec. $[\alpha]_D^{23}$ +104.3 (c, 0.07 in $CHCl_3$). Closely related to Fumitremorgin C, F-131. λ_{max} 226 (ε 27660); 259 (ε 7230); 265 (sh) (ε 6860); 294 (ε 7070); 303 (sh) (ε 5510) (MeOH).

13-Me ether: ***Cyclotryprostatin B***
[184305-67-7]
$C_{23}H_{27}N_3O_5$ 425.483
From *Aspergillus fumigatus*. Mammalian cell cycle inhibitor; microtubule polymerisation inhibitor. Pale yellow cryst.
Mp 159-165° dec. $[\alpha]_D^{24}$ +95.7 (c, 0.36 in $CHCl_3$). λ_{max} 224 (ε 41690); 262 (ε 7180); 267 (ε 7180); 295 (ε 8290); 303 (sh) (ε 6590) (MeOH).

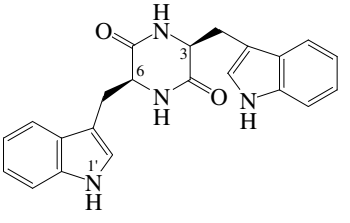
Demethoxy, 12-epimer: ***Cyclotryprostatin C***
[111427-97-5]
$C_{21}H_{23}N_3O_4$ 381.43
From *Aspergillus fumigatus*. Mammalian cell cycle inhibitor; microtubule polymerisation inhibitor. Needles.
Mp 221-223° dec. $[\alpha]_D^{25}$ +23.4 (c, 1.0 in $CHCl_3$). λ_{max} 224 (ε 19680); 272 (ε 6570); 280 (sh) (ε 6325); 290 (sh) (ε 5220) (MeOH).

Demethoxy, 12-epimer, 13-ketone: ***Cyclotryprostatin D***
[184305-68-8]
$C_{21}H_{21}N_3O_4$ 379.415
From *Aspergillus fumigatus*. Mammalian cell cycle inhibitor. Pale yellow amorph. powder. $[\alpha]_D^{26}$ +88 (c, 0.10 in $CHCl_3$). λ_{max} 216 (ε 18290); 240 (sh) (ε 12320); 247 (ε 15310); 264 (ε 9720); 267 (sh) (ε 9570); 301 (ε 8550) (MeOH).

Cui, C.-B. *et al., Tetrahedron*, 1997, **53**, 59 (*isol, uv, ir, pmr, cmr, ms, struct*)
Kondoh, M. *et al., J. Antibiot.*, 1998, **51**, 801-804 (*activity*)
Afiyatullov, S.S. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2004, **40**, 615-617 (*isol, pmr, cmr*)

Cyclo(tryptophyltryptophyl) C-1079

3,6-Bis(1H-indol-3-ylmethyl)-2,5-piperazinedione, 9CI. ***Fellutanine A***
[90243-53-1]
[21361-74-0]



$C_{22}H_{20}N_4O_2$ 372.426

(3*S*,6*S*)-*form*

L-L-form
[20829-55-4]
Prod. by *Penicillium fellutanum* and *Penicillium simplicissimum*. Microcryst. (MeCN).
Mp 270-272° (265-268°). $[\alpha]_D^{20}$ -139 (c, 0.2 in MeOH). λ_{max} 217 (log ε 4.61); 274 (log ε 3.96); 280 (log ε 3.99); 289 (log ε 3.92) (MeOH).

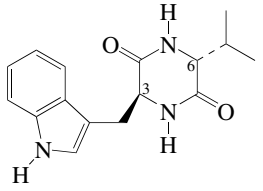
N^1,N^4*-Di-Me:* ***Antibiotic Sch 725418***. *Sch 725418*
$C_{24}H_{24}N_4O_2$ 400.479
Prod. by a *Micromonospora* sp. Stereochem. not confirmed.

$N^{1'}$*-(1,1-Dimethyl-2-propenyl):* ***Cyclo[N$^{1'}$-(1,1-dimethyl-2-propenyl)tryptophyltryptophyl]***
[244066-05-5]
$C_{27}H_{28}N_4O_2$ 440.544
Prod. by *Penicillium simplicissimum*. Powder.
Mp 171-173°. $[\alpha]_D^{20}$ -89 (c, 0.19 in MeOH). λ_{max} 222 (ε 54100); 282 (ε 10600); 290 (ε 9600) (MeOH).

Deslauriers, R. *et al., J.A.C.S.*, 1975, **97**, 5093-5100 (*cmr, conformn*)
Hope, A.P. *et al., Aust. J. Chem.*, 1976, **29**, 1591-1603 (*synth*)
Shiono, Y. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 1910-1920 (*isol, pmr, cmr*)
Kozlovsky, A.G. *et al., J. Nat. Prod.*, 2000, **63**, 698-700 (*isol, uv, pmr, cmr*)
Yang, S.-W. *et al., J. Antibiot.*, 2004, **57**, 345-347 (*Sch 725418*)

Cyclo(tryptophylvalyl) C-1080

*3-(1*H*-Indol-3-ylmethyl)-6-(1-methylethyl)-2,5-piperazinedione. Tryptophan valine anhydride. Valyltryptophan anhydride. Cyclo(-valyltryptophyl) (incorr.)*



(3*S*,6*R*)-*form*

$C_{16}H_{19}N_3O_2$ 285.345

(3*S*,6*R*)-*form*

L-D-form. (-)-trans-*form*
[29478-47-5]
Prod. by *Aspergillus chevalieri.*
Cryst.
Mp 278-280°. $[\alpha]_D$ -15 (c, 1 in DMF).

(3*S*,6*S*)-*form*

L-L-form. (-)-cis-*form*. ***Polanrazine A***
[29552-08-7]
Prod. by *Phoma lingam*. Phytotoxic.
Mp 294-298°. $[\alpha]_D^{20}$ -98 (c, 1 in DMF).

3,6-Dihydroxy: ***Polanrazine F***
[394221-04-6]
$C_{16}H_{19}N_3O_4$ 317.344
Prod. by *Phoma lingum*.
$[\alpha]_D$ -10 (c, 0.26 in MeOH). Possesses (3*R*,6*R*)-config. λ_{max} 219 (log ϵ 4.2); 281 (log ϵ 3.5) (no solvent reported).

6-Methoxy, 3-hydroxy: ***Polanrazine E***
[394421-03-5]
$C_{17}H_{21}N_3O_4$ 331.371
Prod. by *Phoma lingum*.
$[\alpha]_D$ -6 (c, 0.07 in MeOH). Possesses (3*R*,6*R*)-config. λ_{max} 222 (log ϵ 4.3); 282 (log ϵ 3.7) (no solvent reported).

3-(Methylthio), 6-hydroxy: ***Polanrazine D***
[394221-02-4]
$C_{17}H_{21}N_3O_3S$ 347.437
Prod. by *Phoma lingum*.
$[\alpha]_D$ -8.2 (c, 0.18 in MeOH). Possesses (3*R*,6*R*)-config. λ_{max} 219 (log ϵ 4) (no solvent reported).

6-(Methylthio), 3-hydroxy: ***Polanrazine C***
[394221-01-3]
$C_{17}H_{21}N_3O_3S$ 347.437
Prod. by *Phoma lingum*.
$[\alpha]_D$ +16 (c, 0.18 in MeOH). Possesses (3*R*,6*R*)-config. λ_{max} 219 (log ϵ 4.3) (no solvent reported).

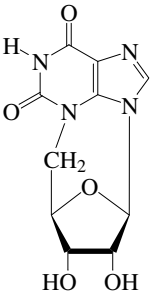
3,6-Bis(methylthio): ***Polanrazine B***
[394221-00-2]
$C_{18}H_{23}N_3O_2S_2$ 377.531
Prod. by *Phoma lingum*.
$[\alpha]_D$ -60 (c, 0.2 in $CHCl_3$). Possesses (3*R*,6*R*)-config. λ_{max} 218 (log ϵ 4.5) (no solvent reported).

$N^{1'}$*-(3-Methyl-2-butenyl):* ***Antibiotic M3***†. *M3*
$C_{21}H_{27}N_3O_2$ 353.463
Prod. by the marine ascomycete fungus M-3 isol. from *Porphyra yezoensis.* Antifungal agent. Solid. $[\alpha]_D^{25}$ -16 (c, 0.05 in MeOH). Tentative stereochem. assigned. CAS no. not found CA **138**.
λ_{max} 222; 288 (MeOH).

Schlessinger, J. *et al., J.A.C.S.*, 1974, **96**, 7396-7400 (*uv, cd*)
Siemion, I.Z. *et al., Rocz. Chem.*, 1975, **49**, 781-789 (*synth, pmr*)
Stipanovic, R.D. *et al., J. Nat. Prod.*, 1976, **39**, 158-159 (*isol, synth*)
Bergman, J. *et al., Tet. Lett.*, 1989, **30**, 4597-4600 (*synth*)
Funasaki, N. *et al., Anal. Chem.*, 1993, **65**, 1861-1867 (*synth, hplc, pmr*)
Pedras, M.S.C. *et al., Phytochemistry*, 1998, **49**, 1575-1577 (*Polanrazine A, pmr, cmr, ms, activity*)
Pedras, M.S.C. *et al., Phytochemistry*, 2001, **58**, 905-909 (*Polanrazines*)
Byun, H.-G. *et al., J. Antibiot.*, 2003, **56**, 102-106 (*Antibiotic M3*)

3,5′-Cycloxanthosine C-1081

[10380-93-5]

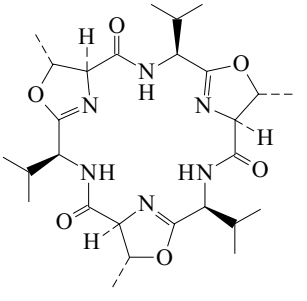


$C_{10}H_{10}N_4O_5$ 266.213
Alkaloid from the marine sponge *Erylus* sp. Cryst. (H_2O).
Mp 310-314°. $[\alpha]_D$ -18 (c, 0.02 in DMSO). λ_{max} 236 (log ϵ 3.91); 266 (log ϵ 3.99) (H_2O).

Hampton, A. *et al., J.O.C.*, 1967, **32**, 1688-1691 (*synth*)
Chen, G.S. *et al., Nucleosides Nucleotides*, 2004, **23**, 347-359 (*synth*)
Capon, R.J. *et al., J. Nat. Prod.*, 2005, **68**, 1689-1691 (*isol, pmr, cmr, ms*)

Cycloxazoline C-1082

Trisoxazoline. Westiellamide
[131998-54-4]

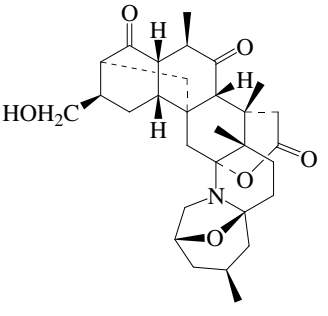


$C_{27}H_{42}N_6O_6$ 546.665
Isol. from the ascidian *Lissoclinum bistratum* and *Westiellopsis prolifica*. Cytotoxic. Amorph. $[\alpha]_D$ +30 (c, 0.1 in MeOH).

Prinsep, M.R. *et al., J. Nat. Prod.*, 1992, **55**, 140-142 (*isol, pmr, cmr, struct*)
Hambley, T.W. *et al., Tetrahedron*, 1992, **48**, 341-348 (*isol, pmr, cmr, struct*)
Wipf, P. *et al., Tetrahedron*, 2000, **56**, 9143-9150 (*synth*)

Cyclozoanthamine C-1083

[159509-35-0]

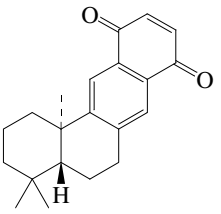


$C_{30}H_{41}NO_6$ 511.657
Alkaloid from *Zoanthus* sp. Cytotoxic agent. Oil.

Japan. Pat., 1994, 94 199 867; *CA*, **122**, 9777d
Fukuzawa, S. *et al., Heterocycl. Commun.*, 1995, **1**, 207-214

Cyclozonarone C-1084

[173693-48-6]



$C_{21}H_{24}O_2$ 308.419

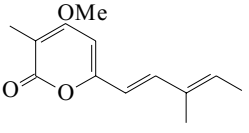
Constit. of *Dictyopteris undulata*. Feeding deterrent. Oil. $[\alpha]_D^{19}$ -89.1 (c, 0.33 in $CHCl_3$). λ_{max} 257 (ϵ 22800); 348 (ϵ 3200) (MeOH) (Berdy).

Kurata, K. *et al., Phytochemistry*, 1996, **41**, 749-752 (*isol, pmr, cmr*)
Cortés, M. *et al., J. Nat. Prod.*, 2001, **64**, 348-349 (*synth, abs config*)
Schröder, J. *et al., Tet. Lett.*, 2001, **42**, 8151-8152 (*synth*)

Cyercene 1 C-1085

*4-Methoxy-3-methyl-6-(3-methyl-1,3-pentadienyl)-2*H*-pyran-2-one*

[136669-16-4]



$C_{13}H_{16}O_3$ 220.268

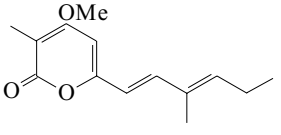
Constit. of *Cyerce cristallina*. Ichthyotoxin. λ_{max} 248 (ϵ 16000); 340 (ϵ 8500) (MeOH) (Berdy).

Vardaro, R.R. *et al., Tetrahedron*, 1991, **47**, 5569 (*isol, pmr, cmr*)

Cyercene 2 C-1086

*4-Methoxy-3-methyl-6-(3-methyl-1,3-hexadienyl)-2*H*-pyran-2-one*

[136669-17-5]



$C_{14}H_{18}O_3$ 234.294

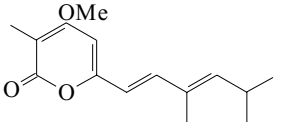
Constit. of *Cyerce cristallina*. Ichthyotoxin. λ_{max} 253 (ϵ 19200); 356 (ϵ 9400) (MeOH) (Berdy).

Vardaro, R.R. *et al., Tetrahedron*, 1991, **47**, 5569 (*isol, pmr, cmr*)

Cyercene 3 C-1087

*6-(3,5-Dimethyl-1,3-hexadienyl)-4-methoxy-3-methyl-2*H*-pyran-2-one*

[136669-18-6]



$C_{15}H_{20}O_3$ 248.321

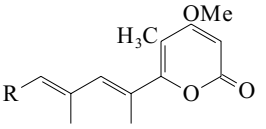
Constit. of *Cyerce cristallina*. Ichthyotoxin. λ_{max} 252 (ϵ 15000); 353 (ϵ 7960) (MeOH) (Berdy).

Vardaro, R.R. *et al., Tetrahedron*, 1991, **47**, 5569 (*isol, pmr, cmr*)

Cyercene 4 C-1088

*6-(1,3-Dimethyl-1,3-pentadienyl)-4-methoxy-5-methyl-2*H*-pyran-2-one*

[136669-19-7]



R = CH_3

$C_{14}H_{18}O_3$ 234.294

Isol. from the mollusc *Cyerce cristallina*. Ichthyotoxin. λ_{max} 238 (ϵ 8900); 304 (ϵ 10200) (MeOH) (Berdy).

Vardaro, R.R. *et al., Tetrahedron*, 1991, **47**, 5569 (*isol, pmr, cmr*)

Cyercene 5 C-1089

*6-(1,3-Dimethyl-1,3-hexadienyl)-4-methoxy-5-methyl-2*H*-pyran-2-one*

[136669-20-0]

As Cyercene 4, C-1088 with

R = CH_2CH_3

$C_{15}H_{20}O_3$ 248.321

Isol. from the mollusc *Cyerce cristallina*. Ichthyotoxin. λ_{max} 240 (ϵ 7500); 298 (ϵ 8800) (MeOH) (Berdy).

3′Z-Isomer: [127848-76-4]

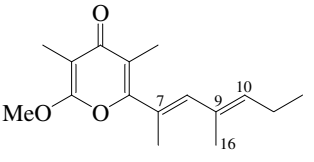
$C_{15}H_{20}O_3$ 248.321

Isol. from *Cyerce cristallina* and *Cyerce nigricans*.

Roussis, V. *et al., Experientia*, 1990, **46**, 327 (*isol*)
Vardaro, R.R. *et al., Tetrahedron*, 1991, **47**, 5569-5576 (*isol, pmr, cmr*)

Cyercene A C-1090

[136669-14-2]



$C_{16}H_{22}O_3$ 262.348

Authors' numbering shown. Constit. of *Cyerce cristallina*. Ichthyotoxic, tissue regeneration stimulant. λ_{max} 260 (ϵ 11200) (base in MeOH) (Derep). λ_{max} 262 (ϵ 9400) (acidic MeOH) (Derep). λ_{max} 264 (ϵ 14000) (MeOH) (Berdy).

7Z-Isomer: ***Placidene A***

[142878-34-0]

$C_{16}H_{22}O_3$ 262.348

Constit. of *Placida dendritica*. Ichthyotoxin. λ_{max} 260 (ϵ 11200) (base in MeOH) (Derep). λ_{max} 262 (ϵ 9400) (acidic MeOH) (Derep). λ_{max} 262 (ϵ 9400) (MeOH) (Berdy).

7Z,9Z-Isomer: ***Isoplacidene A***

[142878-35-1]

$C_{16}H_{22}O_3$ 262.348

Constit. of *Placida dendritica*. ichthyotoxin. λ_{max} 254 (ϵ 10300) (MeOH) (Derep). λ_{max} 254 (ϵ 10340) (MeOH) (Berdy).

$\Delta^{9(16)}$-Isomer, 10ξ-hydroperoxy: ***2-(4-Hydroperoxy-1-methyl-3-methylene-1-hexenyl)-6-methoxy-3,5-dimethyl-4H-pyran-4-one***

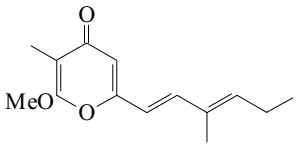
$C_{16}H_{22}O_5$ 294.347

Constit. of *Placida dendritica*. Amorph. solid.

Vardaro, R.R. *et al., Tetrahedron*, 1991, **47**, 5569-5576 (*isol, pmr, cmr*)
Vardaro, R.R. *et al., Tet. Lett.*, 1992, **33**, 2875-2878 (*Placidenes*)
Cutignano, A. *et al., J. Nat. Prod.*, 2003, **66**, 1399-1401 (*$\Delta^{9(16)}$-isomer 10-hydroperoxy*)
Moses, J.E. *et al., Tet. Lett.*, 2004, **45**, 6447-6448 (*synth*)
Zuidema, D.R. *et al., J. Nat. Prod.*, 2005, **68**, 481-486 (*synth, uv, props*)
Liang, G. *et al., Org. Lett.*, 2005, **7**, 819-821 (*synth*)

Cyercene B C-1091

[136669-15-3]



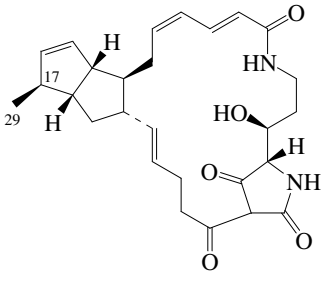
$C_{14}H_{18}O_3$ 234.294

Constit. of *Cyerce cristallina* and *Ercolania funerea*. Ichthyotoxic. λ_{max} 239 (ϵ 12100); 302 (ϵ 11400) (MeOH) (Berdy).

Vardaro, R.R. *et al., Tetrahedron*, 1991, **47**, 5569; 1992, **48**, 9561 (*isol, pmr, cmr*)

Cylindramide C-1092

[147362-39-8]



Relative Configuration

$C_{27}H_{34}N_2O_5$ 466.576

Tetramic acid antibiotic. Shows enol tautomerism over the dioxopyrrolidinecarbonyl system. Isol. from the sponge *Halichondria cylindrata*. Cytotoxic agent. Wax. $[\alpha]_D^{25}$ +167 (c, 0.4 in MeOH). λ_{max} 265 (ϵ 22000) (MeOH).

17,29-Didehydro, Mg salt (2:1): ***Geodin A***

$C_{54}H_{62}MgN_4O_{10}$ 951.41

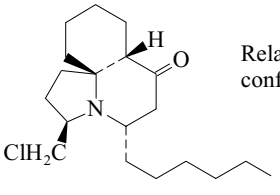
Isol. from the sponge *Geodia* sp. Nematocide. Amorph. solid. Mp 173° dec. $[\alpha]_D^{20}$ +179 (c, 1 in DMSO). Stereochem. not fully determined. Mg coordinated to the dioxopyrrolidinecarbonyl chromophore with charge/bond delocalisation. λ_{max} 264 (ϵ 19100) (DMSO).

[153175-60-1]

Kanazawa, S. *et al., Tet. Lett.*, 1993, **34**, 1065 (*Cylindramide*)
Capon, R.J. *et al., J. Nat. Prod.*, 1999, **62**, 1256-1259 (*Geodin A*)
Cramer, N. *et al., Chem. Eur. J.*, 2006, **12**, 2488-2503 (*synth, pmr, cmr*)
Hart, A.C. *et al., J.A.C.S.*, 2006, **128**, 1094-1095 (*synth*)

Cylindricine A C-1093

[152273-89-7]



Relative configuration

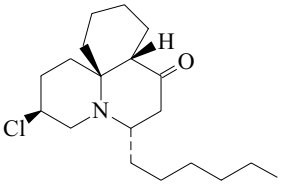
$C_{19}H_{32}ClNO$ 325.921

Alkaloid from the ascidian *Clavelina cylindrica*. Light yellow oil.

Blackman, A.J. *et al., Tetrahedron*, 1993, **49**, 8645-8656 (*isol, pmr, cmr, ms, cryst struct*)
Snider, B. B. *et al., J.O.C.*, 1997, **62**, 5630-5633 (*synth*)
Liu, J.F. *et al., J.O.C.*, 1999, **64**, 8263-8266 (*synth*)

Cylindricine B C-1094

[152273-68-2]



Relative configuration

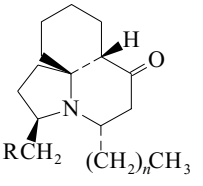
$C_{19}H_{32}ClNO$ 325.921

Alkaloid from the ascidian *Clavelina cylindrica*. Light yellow oil.

Blackman, A.J. *et al., Tetrahedron*, 1993, **49**, 8645-8656 (*isol, pmr, cmr, ms, cryst struct*)
Liu, J.F. *et al., J.O.C.*, 1999, **64**, 8263-8266 (*synth*)

Cylindricine C C-1095

[156953-77-4]



Relative configuration

R = OH, *n* = 5

$C_{19}H_{33}NO_2$ 307.475

Alkaloid from the ascidian *Clavelina cylindrica*. Light yellow oil.

Ac: ***Cylindricine E***

[156953-79-6]

$C_{21}H_{35}NO_3$ 349.512

From *Clavelina cylindrica*. Light yellow oil.

Me ether: ***Cylindricine D***

[156953-78-5]

$C_{20}H_{35}NO_2$ 321.502

From *Clavelina cylindrica*. Light yellow oil.

Li, C. *et al., Aust. J. Chem.*, 1994, **47**, 1355-1361 (*isol, ir, pmr, cmr, ms*)
Snider, B.B. *et al., J.O.C.*, 1997, **62**, 5630-5633 (*synth*)
Molander, G.A. *et al., J.O.C.*, 1999, **64**, 5183-5187 (*synth*)
Trost, B.M. *et al., Org. Lett.*, 2003, **5**, 4599-4602 (*synth*)
Canesi, S. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 4336-4338 (*synth*)
Arai, T. *et al., Tet. Lett.*, 2004, **45**, 5921-5924 (*synth*)
Abe, H. *et al., J.A.C.S.*, 2005, **127**, 1473-1480 (*synth*)
Liu, J. *et al., J.O.C.*, 2005, **70**, 3898-3902 (*synth*)
Shibuguchi, T. *et al., Angew. Chem., Int. Ed.*, 2006, **45**, 4635-4637 (*synth*)
Swidorski, J.J. *et al., Org. Lett.*, 2006, **8**, 777-780 (*synth*)

Cylindricine F C-1096

[156953-80-9]

As Cylindricine C, C-1095 with

R = SCN, *n* = 5

$C_{20}H_{32}N_2OS$ 348.552

Alkaloid from the ascidian *Clavelina cylindrica*. Light yellow oil.

Li, C. *et al., Aust. J. Chem.*, 1994, **47**, 1355-1361 (*isol, ir, pmr, cmr, ms, struct*)

Cylindricine G C-1097

[156953-81-0]

As Cylindricine C, C-1095 with

R = SCN, *n* = 3

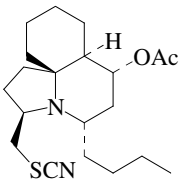
$C_{18}H_{28}N_2OS$ 320.498

Alkaloid from the ascidian *Clavelina cylindrica*. Light yellow oil.

Li, C. *et al., Aust. J. Chem.*, 1994, **47**, 1355-1361 (*isol, pmr, cmr, ms, struct*)

Cylindricine H C-1098

[164740-25-4]



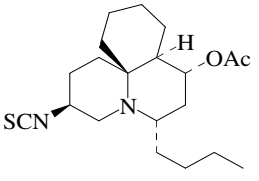
$C_{20}H_{32}N_2O_2S$ 364.551
Alkaloid from the ascidian *Clavelina cylindrica*. Oil. CA name is incorrect.

Isothiocyanate: ***Cylindricine I***
[164740-26-5]
$C_{20}H_{32}N_2O_2S$ 364.551
Alkaloid from *Clavelina cylindrica*. Oil. Has -NCS replacing -SCN. CA name is incorrect.

Li, C. *et al., Aust. J. Chem.*, 1995, **48**, 955-965 (*isol, ir, pmr, cmr, ms*)

Cylindricine J C-1099

[164740-27-6]

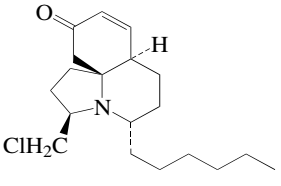


$C_{20}H_{32}N_2O_2S$ 364.551
Alkaloid from the ascidian *Clavelina cylindrica*. Oil.

Li, C. *et al., Aust. J. Chem.*, 1995, **48**, 955-965 (*isol, ir, pmr, cmr, ms*)

Cylindricine K C-1100

[164740-28-7]

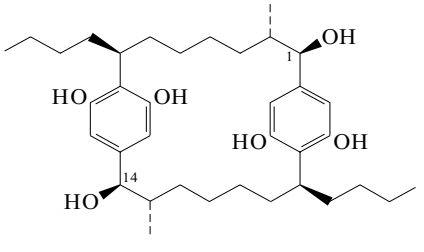


$C_{19}H_{30}ClNO$ 323.905
Alkaloid from the ascidian *Clavelina cylindrica*. Light yellow oil.

Li, C. *et al., Aust. J. Chem.*, 1995, **48**, 955-965 (*isol, ir, pmr, cmr, ms*)

Cylindrocyclophane A C-1101

[126693-92-3]



$C_{36}H_{56}O_6$ 584.835
Constit. of cyanobacterium *Cylindrospermum licheniforme*. Cytotoxic agent. Cryst.
Mp 276-278°. $[\alpha]_D$ -20 (c, 0.5 in MeOH). λ_{max} (solvent not reported) (Derep). λ_{max} 212 (ϵ 47200); 226 (ϵ 15800); 276 (ϵ 3000); 283 (ϵ 2960) (MeOH) (Derep). λ_{max} 208 (ϵ 6400); 222 (ϵ 6100); 248 (ϵ 200); 278 (ϵ 2300) (MeOH) (Berdy).

14-Ac: ***Cylindrocyclophane B***
[141854-65-1]
$C_{38}H_{58}O_7$ 626.872
Constit. of *Cylindrospermum licheniforme*.
$[\alpha]_D$ +25 (c, 0.6 in MeOH). λ_{max} 215 (ϵ 6800); 231 (ϵ 4700); 279 (ϵ 1600) (MeOH) (Berdy).

1,14-Di-Ac: ***Cylindrocyclophane D***
[141854-67-3]
$C_{40}H_{60}O_8$ 668.909
Constit. of *Cylindrospermum licheniforme*.
$[\alpha]_D$ +83 (c, 0.2 in MeOH). λ_{max} 218 (ϵ 17000); 228 (ϵ 9700); 231 (ϵ 10600); 281 (ϵ 1500) (MeOH) (Berdy).

14-Deoxy: ***Cylindrocyclophane C***
[141854-66-2]
$C_{36}H_{56}O_5$ 568.835
Constit. of *Cylindrospermum licheniforme*.
$[\alpha]_D$ -40 (c, 0.1 in MeOH). λ_{max} 208 (ϵ 6700); 231 (ϵ 4300); 250 (ϵ 2000); 279 (ϵ 1300) (MeOH) (Berdy).

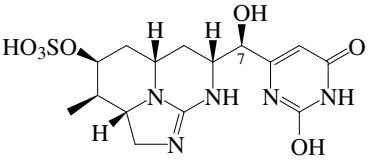
14-Deoxy, 1-Ac: ***Cylindrocyclophane E***
[141854-68-4]
$C_{38}H_{58}O_6$ 610.873
Constit. of *Cylindrospermum licheniforme*.
$[\alpha]_D$ +10 (c, 0.1 in MeOH). λ_{max} 216 (ϵ 10000); 231 (ϵ 4100); 255; 279 (ϵ 700) (MeOH) (Berdy).

1,14-Dideoxy: ***Cylindrocyclophane F***
[141854-69-5]
$C_{36}H_{56}O_4$ 552.836
Constit. of *Cylindrospermum licheniforme*.
$[\alpha]_D$ -72 (c, 0.9 in MeOH). λ_{max} 209 (ϵ 9200); 234 (ϵ 6900); 251 (ϵ 500); 256 (ϵ 200); 275 (ϵ 600) (MeOH) (Berdy).

Moore, B.S. *et al., J.A.C.S.*, 1990, **112**, 4061-4063 (*isol*)
Moore, B.S. *et al., Tetrahedron*, 1992, **48**, 3001 (*isol, pmr, cmr*)
Bobzin, S.C. *et al., Tetrahedron*, 1993, **49**, 7615 (*biosynth*)
Smith, A.B. *et al., J.A.C.S.*, 2001, **123**, 5925-5937 (*synth*)

Cylindrospermopsin C-1102

[143545-90-8]



Absolute Configuration

$C_{15}H_{21}N_5O_7S$ 415.426
Exists as prototropic zwitterion. C-7 config. revised in 2001.
Alkaloid from the cyanobacteria *Aphanizomenon ovalisporum*, *Cylindrospermopsis raciborskii* and *Umezikia natans*. Potent hepatotoxin, glutathione synthesis inhibitor. Off-white microcryst. $[\alpha]_D$ -31 (c, 0.1 in H_2O). λ_{max} 262 (ϵ 5800); 290 (sh) (ϵ 2100) (H_2O) (Derep).
▶ LD_{50} (mus, ipr) 0.2 mg/kg , LD_{50} (mus, ipr) 2.1 mg/kg.

7-Epimer: ***7-Epicylindrospermopsin***
[265652-18-4]
$C_{15}H_{21}N_5O_7S$ 415.426
Alkaloid from *Aphanizomenon ovalisporum*. Hepatotoxin.
Amorph. solid. $[\alpha]_D^{25}$ -20.5 (c, 0.06 in H_2O).

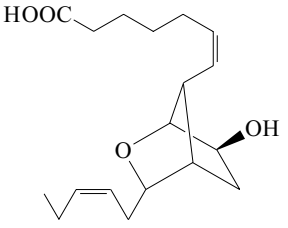
7-Deoxy: ***7-Deoxycylindrospermopsin***
[221554-69-4]
$C_{15}H_{21}N_5O_6S$ 399.427
Alkaloid from *Cylindrospermopsis raciborskii*.

Ohtani, I. *et al., J.A.C.S.*, 1992, **114**, 7941-7942 (*isol, uv, pmr, cmr, ms, struct*)
Norris, R.L. *et al., Environ. Toxicol.*, 1999, **14**, 163-165 (*7-Deoxycylindrospermopsin*)
Banker, R. *et al., J. Nat. Prod.*, 2000, **63**, 387-389 (*7-epimer*)
Xie, C. *et al., J.A.C.S.*, 2000, **122**, 5018-5024 (*synth*)
Burgoyne, D.L. *et al., J.O.C.*, 2000, **65**, 152-156 (*biosynth*)

Heintzelman, G.R. *et al., J.A.C.S.*, 2002, **124**, 3939-3945 (*synth, abs config*)
White, J.D. *et al., J.O.C.*, 2005, **70**, 1963-1977 (*synth, abs config*)
Looper, R.E. *et al., Tetrahedron*, 2006, **62**, 4549-4562 (*synth, abs cofig*)

Cymathere ether A C-1103

[144118-07-0]

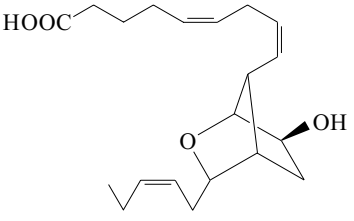


$C_{18}H_{28}O_4$ 308.417
Constit. of *Cymathere triplicata*. Oil. $[\alpha]_D^{15}$ +39 (c, 0.41 in Me_2CO).

Proteau, P.J. *et al., Tet. Lett.*, 1992, **33**, 4393-4396 (*isol, pmr, cmr, ms*)

Cymathere ether B C-1104

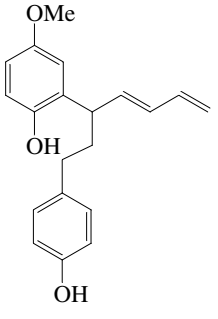
[144118-08-1]



$C_{20}H_{30}O_4$ 334.455
Constit. of *Cymathere triplicata*. Oil. $[\alpha]_D^{19.5}$ +5.1 (c, 0.77 in Me_2CO).

Proteau, P.J. *et al., Tet. Lett.*, 1992, **33**, 4393-4396 (*isol, pmr, cmr, ms*)

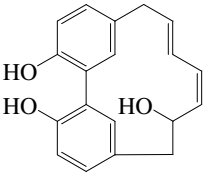
Cymodiene C-1105



$C_{20}H_{22}O_3$ 310.392
Constit. of the sea grass *Cymodocea nodosa*. Oil. $[\alpha]_D$ -17 (c, 0.1 in CH_2Cl_2). λ_{max} 245 (log ϵ 2.92); 260 (log ϵ 2.16); 286 (log ϵ 2.73) (CH_2Cl_2).

Kontiza, I. *et al., Tet. Lett.*, 2005, **46**, 2845-2847 (*isol, pmr, cmr*)

Cymodienol C-1106



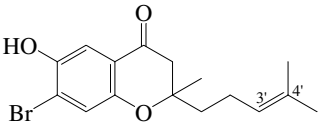
$C_{19}H_{18}O_3$ 294.349

Constit. of the sea grass *Cymodocea nodosa*. Cytotoxic. Greenish oil. $[\alpha]_D$ -181 (c, 0.5 in CH_2Cl_2). λ_{max} 279 (log ϵ 1.75); 300 (log ϵ 1.84); 386 (log ϵ 1.26) (CH_2Cl_2).

Kontiza, I. *et al., Tet. Lett.*, 2005, **46**, 2845-2847 (*isol, pmr, cmr*)

Cymopochromanone C-1107

*7-Bromo-2,3-dihydro-6-hydroxy-2-methyl-2-(4-methyl-3-pentenyl)-4*H*-1-benzopyran-4-one*



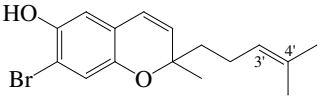
$C_{16}H_{19}BrO_3$ 339.228
Parent not known.

3′,4′-Dihydro, 4′-hydroxy: ***7-Hydroxycymopochromanone***
[413597-29-2]
$C_{16}H_{21}BrO_4$ 357.244
Constit. of *Cymopolia barbata*. Yellow cryst.
Mp 123.5-124.5°. $[\alpha]_D^{25}$ -13.2 (c, 0.2 in $CHCl_3$).

Dorta, E. *et al., J. Nat. Prod.*, 2002, **65**, 329-333 (*isol, pmr, cmr, ms*)

Cymopochromenol C-1108

*7-Bromo-2-methyl-2-(4-methyl-3-pentenyl)-2*H*-1-benzopyran-6-ol, 9CI. 7-Bromo-6-hydroxy-2-methyl-2-(4-methyl-3-pentenyl)-3-chromene*
[62042-44-8]



$C_{16}H_{19}BrO_2$ 323.229
Constit. of *Cymopolia barbata*. Oil. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. λ_{max} 235 (ϵ 13490); 267 (ϵ 3020); 335 (ϵ 3390) (EtOH) (Berdy).

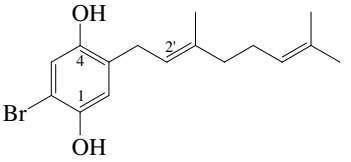
3′,4′-Dihydro, 4′-hydroxy: ***7-Hydroxycymopochromenol***
[413597-31-6]
$C_{16}H_{21}BrO_3$ 341.244
Constit. of *Cymopolia barbata*. Yellow oil. $[\alpha]_D^{25}$ -9.1 (c, 0.2 in $CHCl_3$). Misleading name.

Δ4′-Isomer, 3′-hydroxy: 6-Hydroxycymopochromenol
[413597-33-8]
$C_{16}H_{19}BrO_3$ 339.228
Constit. of *Cymopolia barbata*. Yellow oil. $[\alpha]_D^{25}$ -12.8 (c, 0.2 in $CHCl_3$). Relative config. known. Synonym is misleading.

Högberg, H.-E. *et al., J.C.S. Perkin 1*, 1976, 1696-1701 (*uv, pmr, ms*)
Dorta, E. *et al., J. Nat. Prod.*, 2002, **65**, 329-333 (*isol, pmr, cmr, ms*)

Cymopol C-1109

2-Bromo-5-(3,7-dimethyl-2,6-octadienyl)-1,4-benzenediol, 9CI. 2-Bromo-5-geranyl-1,4-benzenediol
[62008-14-4]



$C_{16}H_{21}BrO_2$ 325.245
Isol. from the green calcareous alga *Cymopolia barbata*. Antioxidant. Phospholipase A2 inhibitor, antifeedant. Solid (hexane).
Mp 59-61°. λ_{max} 299 (ϵ 7650) (EtOH) (Berdy).

▶ Shows mutagenic props.

1-Me ether: 5-Bromo-2-(3,7-dimethyl-2,6-octadienyl)-4-methoxyphenol, 9CI. ***6′-Methoxycymopol***
[62008-01-9]
$C_{17}H_{23}BrO_2$ 339.271
Isol. from *Cymopolia barbata*. Oil. Misleading synonym.

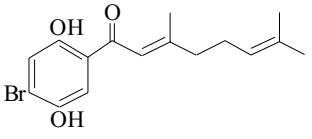
6′,7′-Dihydro, 7′-hydroxy: 2-Bromo-5-(7-hydroxy-3,7-dimethyl-2-octenyl)-1,4-benzenediol. ***7-Hydroxycymopol***
$C_{16}H_{23}BrO_3$ 343.26
Isol. from *Cymopolia barbata*. Antioxidant. Oil. λ_{max} 296 (log ϵ 3.5) (MeOH).

6′,7′-Dihydro, 7′-hydroxy, 4-Me ether: 7-Hydroxy-3′-methoxycymopol
[413579-33-6]
$C_{17}H_{25}BrO_3$ 357.287
Constit. of *Cymopolia barbata*. Yellow oil.

Högberg, H.E. *et al., J.C.S. Perkin 1*, 1976, 1696-1701 (*isol*)
Reynolds, P.W. *et al., Chem. Comm.*, 1977, 499 (*synth*)
Chenard, B.L. *et al., J.O.C.*, 1980, **45**, 378-384 (*synth, ir, pmr, ms*)
Dorta, E. *et al., J. Nat. Prod.*, 2002, **65**, 329-333 (*isol, pmr, cmr*)
Takamatsu, S. *et al., J. Nat. Prod.*, 2003, **66**, 605-608 (*7-Hydroxycymopol*)

Cymopolone C-1110

1-(4-Bromo-2,5-dihydroxyphenyl)-3,7-dimethyl-2,6-octadien-1-one, 9CI



(*E*)–*form*

$C_{16}H_{19}BrO_3$ 339.228

(*E*)-*form* [62008-12-2]
Constit. of *Cymopolia barbata*.
Yellow cryst. (hexane). Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O.
Mp 79-81°. λ_{max} 380 (ϵ 6760) (MeOH) (Berdy). λ_{max} 280 (ϵ 19950) (EtOH) (Berdy).

2,3-Dihydro, 3ξ-hydroxy: 1-(4-Bromo-2,5-dihydroxyphenyl)-3-hydroxy-3,7-dimethyl-6-octen-1-one. ***3-Hydroxycymopolone***
[413597-26-9]
$C_{16}H_{21}BrO_4$ 357.244
Constit. of *Cymopolia barbata*. Yellow oil. $[\alpha]_D^{25}$ -10 (c, 0.2 in $CHCl_3$).

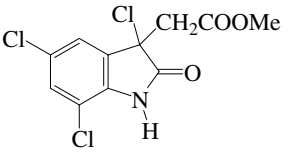
6,7-Dihydro, 7-hydroxy: 1-(4-Bromo-2,5-dihydroxyphenyl)-7-hydroxy-3,7-dimethyl-2-octen-1-one. ***7-Hydroxycymopolone***
[111625-69-5]
$C_{16}H_{21}BrO_4$ 357.244
Constit. of *Cymopolia barbata*. Yellow cryst. (hexane/CH_2Cl_2). Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O.
Mp 126-128°. λ_{max} 280 (log ϵ 4.35); 380 (log ϵ 3.9) (EtOH).

2,3,7,8-Tetrahydro, 3ξ,7-dihydroxy: 1-(4-Bromo-2,5-dihydroxyphenyl)-3,7-dihydroxy-3,7-dimethyl-1-octanone. ***3,7-Dihydroxycymopolone***
[413597-27-0]
$C_{16}H_{23}BrO_5$ 375.259
Constit. of *Cymopolia barbata*. Yellow oil. $[\alpha]_D^{25}$ -14.6 (c, 0.2 in $CHCl_3$).

(*Z*)-*form*
Isocymopolone
[62008-13-3]
Constit. of *Cymopolia barbata*.
Yellow needles. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O.
Mp 55-56° (hexane). λ_{max} 375 (ϵ 1620) (MeOH) (Berdy). λ_{max} 283 (ϵ 16500) (EtOH) (Berdy).

Högberg, H.E. *et al., J.C.S. Perkin 1*, 1976, 1696-1701 (*isol, uv, ir, pmr, ms*)
Estrada, D.M. *et al., J. Nat. Prod.*, 1987, **50**, 735-737 (*7-Hydroxycymopolone*)
Dorta, E. *et al., J. Nat. Prod.*, 2002, **65**, 329-333 (*isol, pmr, cmr, ms*)

Cynthichlorine C-1111



$C_{11}H_8Cl_3NO_3$ 308.547

(ξ)-*form*
Isol. from the tunicate *Cynthia savignyi*. Antifungal and antibacterial agent. Cytotoxic.

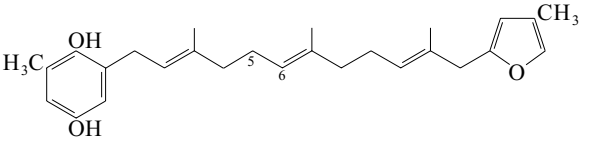
Abourriche, A. *et al., Farmaco*, 2003, **58**, 1351-1354 (*isol, pmr*)

Cystatin C-1112

[153891-65-7]
Polypeptide of 111 amino acid residues. For struct. see ref. Isol. from pituitary gland of the salmon, *Oncorhynchus keta* and from chestnut. Cysteine proteinase inhibitor. Shows antibacterial activity against *Porphyromonas gingivalis*. Shows antifungal activity.

Koide, Y. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 164 (*isol, hplc*)
Blaukenvoorde, M.F.J. *et al., Biol. Chem.*, 1998, **379**, 1371-1375 (*activity*)
Pernas, M. *et al., Mol. Plant-Microbe Interact.*, 1999, **12**, 624-627; *CA*, **131**, 182179 (*activity*)

Cystofuranoquinol C-1113



$C_{27}H_{36}O_3$ 408.58

5-Hydroxy: ***5-Hydroxycystofuranoquinol***
[115788-00-6]
$C_{27}H_{36}O_4$ 424.579
Constit. of the brown alga *Cystoseira spinosa* var. *squarrosa*. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{20}$ +1.2 (c, 2.8 in EtOH). λ_{max} 221 (ϵ 12500); 290 (ϵ 2800) (EtOH) (Berdy).

5-Oxo: ***5-Oxocystofuranoquinol***
[115787-99-0]
$C_{27}H_{34}O_4$ 422.563
Constit. of *Cystoseira spinosa* var. *squarrosa*. Oil.

1′,4′-Quinone, 5-oxo: ***5-Oxocystofuranoquinone***
[592533-87-4]
$C_{27}H_{32}O_4$ 420.547
Constit. of *Cystoseira crinita*. Oil. λ_{max} 250 (ϵ 25500) (EtOH).

6Z-Isomer, 5-oxo: ***5-Oxoisocystofuranoquinol***
[115787-98-9]
$C_{27}H_{34}O_4$ 422.563
Constit. of *Cystoseira spinosa* var. *squarrosa*. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. λ_{max} 218 (ϵ 30000); 246 (ϵ 14600); 287 (ϵ 4800) (EtOH) (Berdy).

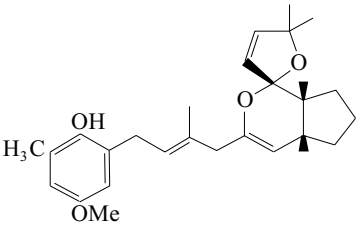
6Z-isomer, 1′,4′-quinone, 5-oxo: ***5-Oxoisocystofuranoquinone***
[592533-88-5]
$C_{27}H_{32}O_4$ 420.547
Constit. of *Cystoseira crinata*. Oil. λ_{max} 250 (ϵ 9400) (EtOH).

[115787-96-7, 115787-97-8]

Amico, V. *et al., Phytochemistry*, 1988, **27**, 1327-1331 (*isol, pmr, cmr, ms*)
Fisch, K.M. *et al., J. Nat. Prod.*, 2003, **66**, 968-975 (*quinones*)

Cystoketal C-1114

[96253-60-0]

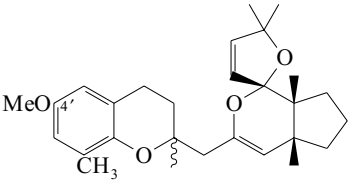


$C_{28}H_{38}O_4$ 438.606
Metab. of *Cystoseira balearica*. Oil. $[\alpha]_D$ +11.5 (c, 1 in EtOH).

Z-Isomer: ***Isocystoketal***
[110351-76-3]
$C_{28}H_{38}O_4$ 438.606
From *Cystoseira stricta*. Oil. $[\alpha]_D^{20}$ +24.9 (c, 0.54 in EtOH).

Amico, V. *et al., J. Nat. Prod.*, 1984, **47**, 947 (*Cystoketal*)
Amico, V. *et al., Phytochemistry*, 1987, **26**, 1719 (*Isocystoketal*)
Valls, R. *et al., Phytochemistry*, 1996, **41**, 1367-1371 (*isol, pmr, cmr*)

Cystoketalchromane C-1115



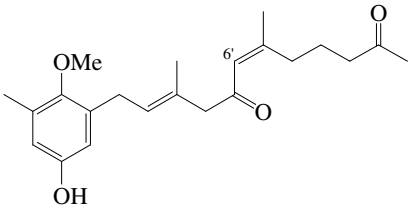
$C_{28}H_{38}O_4$ 438.606
Constit. of *Cystoseira amentacea*. Oil.

4′-O-De-Me: ***Demethylcystoketalchromane***
[175673-58-2]
$C_{27}H_{36}O_4$ 424.579
Constit. of *Cystoseira amentacea*. Oil.

Amico, V. *et al., J. Nat. Prod.*, 1984, **47**, 947 (*isol, pmr*)
Valls, R. *et al., Phytochemistry*, 1996, **41**, 1367 (*isol, pmr, cmr*)

Cystomexicone A C-1116

[220702-85-2]



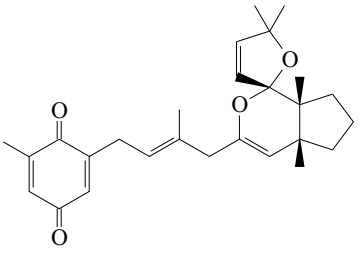
$C_{22}H_{30}O_4$ 358.477
Constit. of *Cystoseira abies*. Oil. λ_{max} 208 (ϵ 11300); 280 (ϵ 2385) (EtOH).

6′E-Isomer: ***Cystomexicone B***
[220702-86-3]
$C_{22}H_{30}O_4$ 358.477
Constit. of *Cystoseira abies*. Oil. λ_{max} 209 (ϵ 11320); 280 (ϵ 2339) (EtOH).

Fernández, J.J. *et al., Nat. Prod. Lett.*, 1998, **12**, 285-291 (*isol, pmr, cmr*)

Cystoquinone C-1117

[175702-36-0]

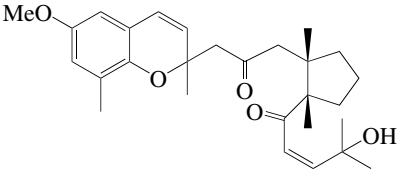


$C_{27}H_{34}O_4$ 422.563
Constit. of *Cystoseira amentacea* var. *stricta*. Oil. $[\alpha]_D^{25}$ +11.2 (c, 1.3 in CH_2Cl_2).

Valls, R. *et al., Phytochemistry*, 1996, **41**, 1367-1371 (*isol, pmr, cmr*)

Cystoseirachromene, 9CI C-1118

*4-Hydroxy-1-[2-[3-(6-methoxy-2,8-dimethyl-2*H*-1-benzopyran-2-yl)-2-oxopropyl]-1,2-dimethylcyclopentyl]-4-methyl-2-penten-1-one*

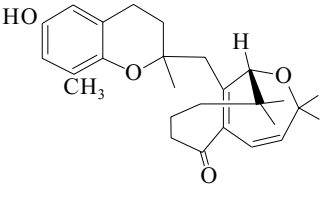


$C_{28}H_{38}O_5$ 454.605
Not named in paper. Metab. of *Cystoseira amentacea* var. *stricta*. Oil.

Mesguiche, V. *et al., Phytochemistry*, 1997, **45**, 1489-1494 (*isol, pmr, cmr*)

Cystoseirol A C-1119

[102396-17-8]

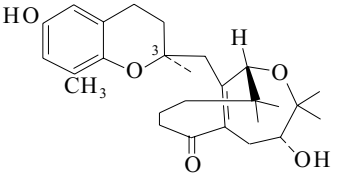


$C_{27}H_{36}O_4$ 424.579
C-2 config. not established. Constit. of brown algae *Cystoseira mediterranea, Cystoseira stricta* and *Cystoseira tamariscifolia*. $[\alpha]_D$ +15 (c, 1.6 in CCl_4). λ_{max} 241 (ϵ 4600); 296 (ϵ 4400) ($CHCl_3$) (Derep).

Francisco, C. *et al., Tet. Lett.*, 1985, **26**, 4919-4922 (*isol, uv, ir, pmr, cmr, struct*)

Cystoseirol B C-1120

[102396-15-6]

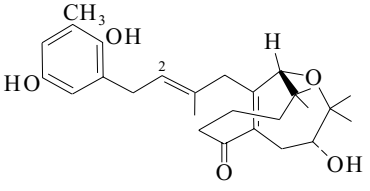


$C_{27}H_{38}O_5$ 442.594
Constit. of *Cystoseira* spp. Oil. $[\alpha]_D$ +20 (c, 0.3 in MeOH). λ_{max} 230 (ϵ 8800); 295 (ϵ 3960) (MeOH) (Derep).

3-Epimer: ***Cystoseirol C***
[102491-66-7]
$C_{27}H_{38}O_5$ 442.594
From *Cystoseira* spp. Oil. $[\alpha]_D$ +36 (c, 0.5 in MeOH). λ_{max} 230 (ϵ 8800); 295 (ϵ 3960) (MeOH) (Derep).
Francisco, C. *et al., J.O.C.*, 1986, **51**, 2707

Cystoseirol D C-1121

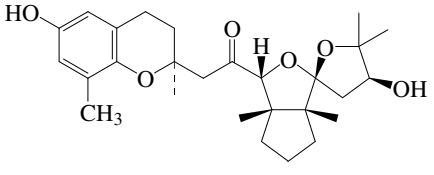
[102396-16-7]



$C_{27}H_{38}O_5$ 442.594
Constit. of *Cystoseira* spp. Oil. $[\alpha]_D$ -4 (c, 1 in MeOH). λ_{max} 230 (ϵ 8800); 295 (ϵ 3960) (MeOH) (Derep).

2Z-Isomer: ***Cystoseirol E***
[102490-77-7]
$C_{27}H_{38}O_5$ 442.594
From *Cystoseira* spp. Oil. $[\alpha]_D$ +10 (c, 0.4 in MeOH). λ_{max} 230 (ϵ 8800); 295 (ϵ 3960) (MeOH) (Derep).
Francisco, C. *et al., J.O.C.*, 1986, **51**, 2707

Cystoseirone C-1122

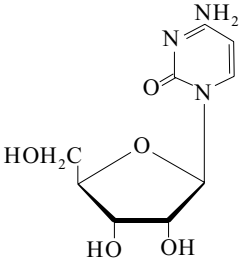


$C_{27}H_{38}O_6$ 458.594
Constit. of a *Cystoseira* sp.

Di-Ac: [676339-97-2]
Oil. $[\alpha]_D^{25}$ +26.9 (c, 0.125 in $CHCl_3$). λ_{max} 205 (log ϵ 4.05); 280 (log ϵ 3.38) (MeOH).
Navarro, G. *et al., J. Nat. Prod.*, 2004, **67**, 495-499 (*isol, pmr, cmr*)

Cytidine, 9CI, 8CI C-1123

1-β-D-Ribofuranosylcytosine, 9CI. 4-Amino-1-β-D-ribofuranosyl-2(1H)-pyrimidinone
[65-46-3]



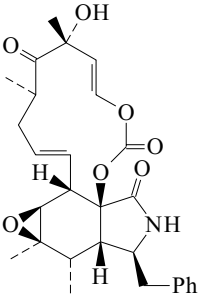
$C_9H_{13}N_3O_5$ 243.219
Constit. of nucleic acids. Isol. from yeast nucleic acid. Needles. Mp 230° dec. $[\alpha]_D^{21}$ +29.6 (H_2O). λ_{max} 280 (ϵ 13400) (pH 2.2). λ_{max} 271 (ϵ 9100) (pH 8.2).
▶ LD_{50} (mus, ipr) 2700 mg/kg. UW7370000

3N-Me: ***3-Methylcytidine***
[2140-64-9]
$C_{10}H_{15}N_3O_5$ 257.246
Found in yeast soluble RNA. Isol. from the marine sponge *Geodia baretti*.
Mp 193-194° (as methanesulfonate). pK_a 8.7. λ_{max} 254 (H_2O) (Berdy). λ_{max} 278 (ϵ 11800) (pH 4). λ_{max} 266 (ϵ 900) (pH 12).
[7607-04-7, 21028-20-6, 26524-60-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 831A; 832C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 387A; 389B; 389C (*nmr*)
Hancock, R.L. *et al., J. Chromatogr. Sci.*, 1969, **7**, 366 (*N-methyl*)
Lee, G.C.Y. *et al., Biochem. Biophys. Res. Commun.*, 1971, **43**, 435 (*N-methyl*)
Ueda, T. *et al., Chem. Pharm. Bull.*, 1974, **22**, 2377 (*N-methyl*)
Kaito, A. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 3073 (*N-methyl*)
Yamauchi, K. *et al., J.C.S. Perkin 1*, 1989, 13 (*N-methyl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CQM500

Cytochalasin E C-1124

[36011-19-5]



$C_{28}H_{33}NO_7$ 495.571
Metab. of *Rosellinia necatrix* and *Aspergillus clavatus*. Also from the marine-derived *Spicaria elegans*. Antibiotic and cytotoxic agent. Fibroblast inhibitor, lipid droplet formation inhibitor, cholesteryl ester synthesis inhibitor. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O.
Mp 206-208° dec. $[\alpha]_D^{25}$ -25.6 (MeOH). Log P 1.25 (uncertain value) (calc). λ_{max} 252 (ϵ 5370); 257 (ϵ 6025); 263 (ϵ 3890) (MeOH) (Berdy).
▶ LD_{50} (rat, orl) 9.1 mg/kg; LD_{50} (rat, ipr) 2.6 mg/kg. Exp. teratogen. HA5360000

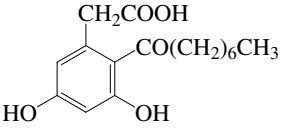
4′-Methoxy: 4′-Methoxycytochalasin E. ***Phenochalasin B.*** *Antibiotic Mer-WF 1726. Mer-WF 1726*
[207679-46-7]
$C_{29}H_{35}NO_8$ 525.597
Prod. by *Daldinia concentrica*, *Phomopsis* sp. FT-0211 and *Libertella* sp. Mer-WF 1726. Cytotoxic agent. Powder.
Mp 130-132°. $[\alpha]_D^{22}$ -5.7 (c, 0.53 in MeOH). Contains a 4-methoxyphenyl group. λ_{max} 200 (ϵ 24500); 225 (ϵ 14400); 275 (ϵ 3200); 283 (ϵ 2900) (MeOH).

4′-Hydroxy, 6,7-deepoxy, 6,7-didehydro: ***Phenochalasin A***
$C_{28}H_{33}NO_7$ 495.571
Prod. by *Phomopsis* sp. FT-0211. Powder.
Mp 143-145°. $[\alpha]_D^{22}$ -4.3 (c, 0.53 in MeOH). λ_{max} 200 (ϵ 27800); 225 (ϵ 10900); 285 (ϵ 3000); 300 (ϵ 2100) (MeOH).

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1111F (*ir*)
Aldridge, D.C. *et al., Chem. Comm.*, 1973, 551 (*struct, pmr, cmr*)
Büchi, G. *et al., J.A.C.S.*, 1973, **95**, 5423 (*struct, ms, ir, pmr, cryst struct*)
Kajimoto, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2212 (*pmr, cmr*)
Japan. Pat., 1998, 98 114 776; *CA*, **129**, 15357c (*Mer-WF 1726*)
Tomoda, H. *et al., J. Antibiot.*, 1999, **52**, 851-856; 857-861 (*Phenochalasins*)
Quang, D.N. *et al., J. Nat. Prod.*, 2002, **65**, 1869-1874 (*Phenochalasin B, isol*)
Liu, R. *et al., J. Nat. Prod.*, 2006, **69**, 871-875 (*Spicaria isol, pmr, cmr*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 266
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CQM250

Cytochalasin K† C-1125

[460085-82-9]
[81657-79-6]



$C_{28}H_{33}NO_7$ 495.571

Related to Cytochalasin E, C-1124 and not to confused with Cytochalasin K. Prod. by *Aspergillus clavatus* MCR1181 and *Mycotypha* sp. UMF-006. Also isol. from the marine-derived *Spicaria elegans*. Shows antibiotic and cytotoxic props. Cryst. (hexane/Me_2CO). Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane. Mp 246-248°. λ_{max} 257 (MeOH) (Berdy).

$\Delta^{6,12}$-Isomer: [460085-83-0]
$C_{28}H_{33}NO_7$ 495.571
Prod. by *Mycotypha* sp. UMF-006.

Steyn, P.S. *et al., J.C.S. Perkin 1*, 1982, 541-544 (*isol, struct*)
Takamatsu, S. *et al., J. Antibiot.*, 2002, **55**, 585-592 (*$\Delta^{6,12}$-isomer*)
Liu, R. *et al., J. Nat. Prod.*, 2006, **69**, 871-875 (*isol, pmr, cmr*)

[Cytochrome *c*]-methionine *S*-methyltransferase C-1126

E.C. 2.1.1.123. S-*Adenosyl-*L*-methionine:[cytochrome-*c*]-methionine* S-*methyltransferase*
[93585-98-9]

Enzyme. Isol. from *Euglena gracilis*. Catalyses the reaction of *S*-adenosyl-L-methionine and a L-methionine residue in cytochrome *c* to give *S*-adenosyl-L-homocysteine and a *S*-methyl-L-methionine residue.

Farooqui, J.-Z. *et al., J. Biol. Chem.*, 1985, **260**, 537-545 (*isol*)

Sagartia rosea Cytolysin C-1127

Src I

Protein. Isol. from the sea anemone *Sagartia rosea*. Shows haemolytic activity.

Jiang, X. *et al., Biochem. Biophys. Res. Commun.*, 2003, **312**, 562-570 (*isol*)

Cytolysin Or-A C-1128

Or-A

Protein of the Actinoporin group. Partial struct. determined. MW approx. 18kDa. Isol. from the sea anemone *Oulactis orientalis*. Cytolytic toxin.

Ilina, A.P. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2005, **31**, 34-42 (*isol, struct*)

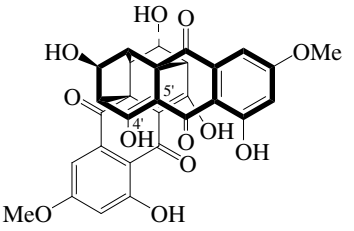
Cytolysin Or-G C-1129

Or-G

Protein of the Actinoporin group. Partial struct. determined. MW approx. 18kDa. Isol. from the sea anemone *Oulactis orientalis*. Cytolytic toxin.

Ilina, A.P. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2005, **31**, 34-42 (*isol, struct*)

Cytoskyrin A C-1130



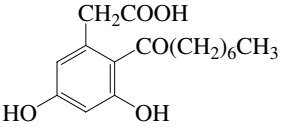
$C_{30}H_{22}O_{12}$ 574.497
Prod. by a *Cytospora* sp. and from the fungus *Curvularia lunata* isol. from the marine sponge *Niphates olemda*. Antibiotic. Cryst. (Me_2CO).

5′ξ-Hydroxy (4′-oxo tautomer): ***Cytoskyrin B***
$C_{30}H_{22}O_{13}$ 590.496
Prod. by a *Cytospora* sp.

Brady, S.F. *et al., Org. Lett.*, 2000, **2**, 4047-4049 (*isol, pmr, cmr, cryst struct*)
Jadulco, R. *et al., J. Nat. Prod.*, 2002, **65**, 730-733 (*isol*)

Cytosporone A C-1131

3,5-Dihydroxy-2-(1-oxooctyl)benzeneacetic acid. 3,5-Dihydroxy-2-octanoylphenylacetic acid
[97902-31-3]



$C_{16}H_{22}O_5$ 294.347
Prod. by *Cytospora* sp., *Diaporthe* sp. and a *Phoma* sp. Cryst. Mp 130°. λ_{max} 219; 270 (MeCN).

Et ester: ***Cytosporone B***
$C_{18}H_{26}O_5$ 322.4
Prod. by *Cytospora* sp., *Diaporthe* sp. and *Dothiorella* sp. λ_{max} 219; 268 (MeCN).

6′ξ-Hydroxy, Et ester: ***Dothiorelone B***
[849758-67-4]
$C_{18}H_{26}O_6$ 338.4
Prod. by the mangrove fungus *Dothiorella* sp. Cytotoxic.

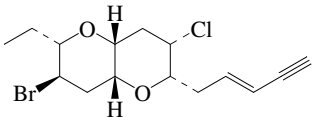
7′ξ-Hydroxy, Et ester: ***Dothiorelone A***
[849758-66-3]
$C_{18}H_{26}O_6$ 338.4
Prod. by *Dothiorella* sp. Cytotoxic.

8′-Hydroxy, Et ester: ***Dothiorelone C***
[849758-68-5]
$C_{18}H_{26}O_6$ 338.4
Prod. by *Dothiorella* sp. Cytotoxic.

Voblikova, V.D. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 362-365 (*isol*)
Brady, S.F. *et al., Org. Lett.*, 2000, **2**, 4043-4046 (*isol, pmr, cmr*)
Xu, Q. *et al., Acta Oceanol. Sin.*, 2004, **23**, 541-547; *CA*, **142**, 388784y (*Dothiorelones*)

Dactomelyne D-1

3-Bromo-7-chloro-2-ethyloctahydro-6-(2-penten-4-ynyl)pyrano[3,2-b]pyran, 9CI



(*E*)-*form* Absolute Configuration

$C_{15}H_{20}BrClO_2$ 347.678

Closely related to Elatenyne, E-61.

(*E*)-*form* [79373-29-8]

Isol. from *Aplysia dactylomela* and *Laurencia obtusa*.
Cryst. (hexane).
Mp 74-75°. $[\alpha]_D$ -15.9 (c, 0.6 in $CHCl_3$). λ_{max} 225 (ϵ 15800) (EtOH).

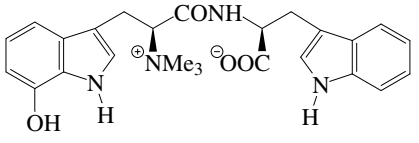
(*Z*)-*form* [79433-83-3]

Isol. from *Aplysia dactylomela*.
Cryst. (hexane).
Mp 119-120°. $[\alpha]_D$ -21.3 (c, 1.6 in $CHCl_3$). λ_{max} 221 (ϵ 13700) (EtOH).

Gopichand, Y. *et al., J.O.C.*, 1981, **46**, 5192-5197 (*isol, pmr, ms, cryst struct*)
Lee, E. *et al., J.A.C.S.*, 1995, **117**, 8017-8018 (*synth*)
Aydogmuş, Z. *et al., Nat. Prod. Res.*, 2004, **18**, 43-49 (*isol, pmr, cmr*)

Dactylamide A D-2

[398143-15-2]



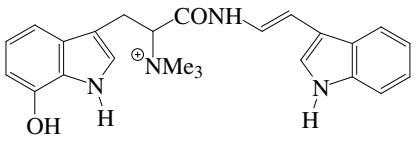
Absolute Configuration

$C_{25}H_{28}N_4O_4$ 448.521
Isol. from *Aplysia dactylomela*. Amorph. solid.
Mp 204-210° dec. $[\alpha]_D^{20}$ +7 (c, 0.68 in MeOH aq.). λ_{max} 220 (log ϵ 4.34); 272 (log ϵ 3.56); 286 (log ϵ 3.53); 290 (log ϵ 3.45) (MeOH).

Appleton, D.R. *et al., Tetrahedron*, 2001, **57**, 10181-10189 (*isol, pmr, cmr, uv*)

Dactylamide B D-3

[398143-16-3]

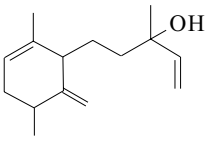


$C_{24}H_{27}N_4O_2^{\oplus}$ 403.503
Isol. from *Aplysia dactylomela*. Pale yellow solid.
Mp 160-163° dec. $[\alpha]_D^{20}$ +160 (c, 0.4 in MeOH). Counterion not specified. λ_{max} 219 (log ϵ 4.44); 282 (log ϵ 3.85); 292 (log ϵ 3.83); 313 (log ϵ 3.85) (MeOH).

Appleton, D.R. *et al., Tetrahedron*, 2001, **57**, 10181-10189 (*isol, pmr, cmr, uv*)

Dactylenol D-4

[58542-82-8]



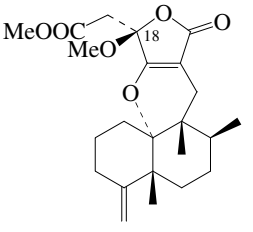
$C_{15}H_{24}O$ 220.354
Constit. of *Aplysia dactylomela*. Oil. $[\alpha]_D$ +203.8 (neat).

Ac:
$C_{17}H_{26}O_2$ 262.391
Constit. of *Aplysia dactylomela*. Oil. $[\alpha]_D$ +168 (c, 2.5 in $CHCl_3$).

Schmitz, F.J. *et al., J.O.C.*, 1978, **43**, 4220-4225 (*isol*)

Dactylolactone A D-5

[487016-15-9]



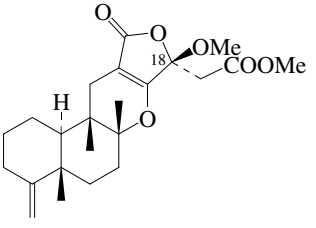
$C_{23}H_{32}O_6$ 404.502
Constit. of *Dactylospongia elegans*. Amorph. solid. $[\alpha]_D$ +10 (c, 0.1 in $CHCl_3$). λ_{max} 242 (log ϵ 3.3) (EtOH).

18-Epimer: ***Dactylolactone B***
[487016-16-0]
$C_{23}H_{32}O_6$ 404.502
Constit. of *Dactylospongia elegans*. Amorph. solid. $[\alpha]_D^{28}$ +12.5 (c, 0.2 in $CHCl_3$). λ_{max} 241 (log ϵ 3.5) (EtOH).

Mitome, H. *et al., J. Nat. Prod.*, 2003, **66**, 46-50 (*isol, pmr, cmr*)

Dactylolactone C D-6

[487016-17-1]

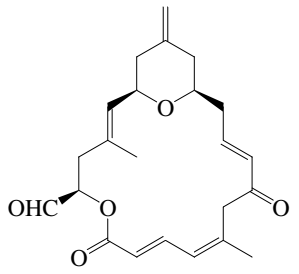


$C_{23}H_{32}O_6$ 404.502
Constit. of *Dactylospongia elegans*. Amorph. solid. $[\alpha]_D^{28}$ -23.1 (c, 0.13 in $CHCl_3$). λ_{max} 239 (log ϵ 3.5) (EtOH).

18-Epimer: ***Dactylolactone D***
[487016-18-2]
$C_{23}H_{32}O_6$ 404.502
Constit. of *Dactylospongia elegans*. Amorph. solid. $[\alpha]_D^{28}$ -22.7 (c, 0.22 in $CHCl_3$). λ_{max} 240 (log ϵ 3.7) (EtOH).

Mitome, H. *et al., J. Nat. Prod.*, 2003, **66**, 46-50 (*isol, pmr, cmr*)

Dactylolide D-7



Absolute Configuration

$C_{23}H_{28}O_5$ 384.471
Isol. from the sponge *Dactylospongia* sp. Cytotoxic. Amorph. solid. $[\alpha]_D$ +30 (c, 1 in MeOH). λ_{max} 222 (ϵ 11000); 266 (ϵ 16000); 317 (ϵ 800) (no solvent reported).

Cutignano, A. *et al., Eur. J. Org. Chem.*, 2001, 775-778 (*isol*)
Smith, A.B. *et al., J.A.C.S.*, 2002, **124**, 11102-11113 (*synth, abs config*)
Hoye, T.R. *et al., J.A.C.S.*, 2003, **125**, 9576-9577 (*synth*)
Aubele, D.L. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 3485-3488 (*synth*)
Sanchez, C.C. *et al., Org. Lett.*, 2005, **7**, 3053-3056 (*synth*)
Louis, I. *et al., Org. Lett.*, 2006, **8**, 1117-1120 (*synth*)

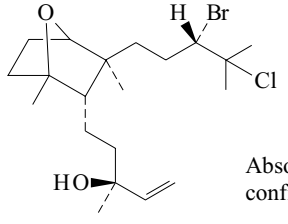
Dactylomelin P D-8

Protein. Isol. from purple gland of the sea hare *Aplysia dactylomela*. Antibacterial and haemagglutinating agent.

Melo, V.M. *et al., Toxicon*, 2000, **38**, 1415-1427 (*isol, struct*)

Dactylomelol D-9

[126739-08-0]



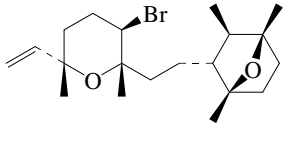
Absolute configuration

$C_{20}H_{34}BrClO_2$ 421.844
Metab. of *Aplysia dactylomela*. Toxic to brine shrimp. Cryst. (CH_2Cl_2/hexane).
Mp 85-86°. $[\alpha]_D^{20}$ -34.3 (c, 0.7 in $CHCl_3$).

Estrada, D.M. *et al., Tet. Lett.*, 1989, **30**, 6219-6220 (*cryst struct*)
Wessels, M. *et al., J. Nat. Prod.*, 2000, **63**, 920-928 (*activity*)

Dactylopyranoid D-10

[288858-56-0]

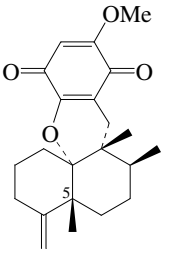


$C_{20}H_{33}BrO_2$ 385.384
Constit. of *Aplysia dactylomela*.
$[\alpha]_D$ -14 (c, 0.42 in $CHCl_3$).

Wessels, M. *et al., J. Nat. Prod.*, 2000, **63**, 920-928 (*isol, pmr, cmr*)

Dactyloquinone A D-11

[385822-20-8]



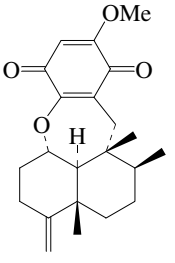
$C_{22}H_{28}O_4$ 356.461
Constit. of *Dactylospongia elegans*. Pale yellow powder.
Mp 183-185°. $[\alpha]_D^{26}$ -28.3 (c, 0.6 in $CHCl_3$). λ_{max} 279 (log ϵ 4.2); 285 (log ϵ 4.2); 396 (log ϵ 3.3) (EtOH).

5-Epimer: ***Dactyloquinone B***
[385822-22-0]
$C_{22}H_{28}O_4$ 356.461
Constit. of *Dactylospongia elegans*. Pale yellow powder.
Mp 178-180°. $[\alpha]_D^{26}$ -33.1 (c, 1.5 in $CHCl_3$). λ_{max} 278 (log ϵ 4.2); 287 (log ϵ 4.2); 398 (log ϵ 2.1) (EtOH).

Mitome, H. *et al., J. Nat. Prod.*, 2001, **64**, 1506-1508 (*isol, pmr, cmr*)

Dactyloquinone C D-12

[432551-98-9]

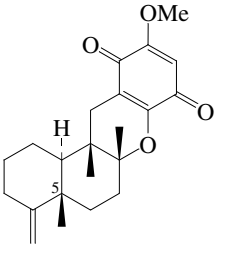


$C_{22}H_{28}O_4$ 356.461
Constit. of *Dactylospongia elegans*. Pale yellow amorph. solid.
$[\alpha]_D^{27}$ -22.7 (c, 0.22 in $CHCl_3$). λ_{max} 286 (log ϵ 3.7) (EtOH).

Mitome, H. *et al., Tetrahedron*, 2002, **58**, 1693-1696 (*isol, pmr, cmr*)

Dactyloquinone D D-13

[432551-99-0]



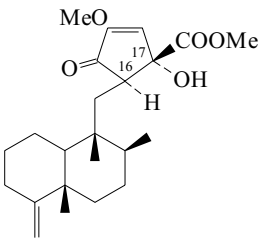
$C_{22}H_{28}O_4$ 356.461
Constit. of *Dactylospongia elegans*. Pale yellow amorph. solid.
$[\alpha]_D^{27}$ -26.7 (c, 0.15 in $CHCl_3$). λ_{max} 291 (log ϵ 4.1) (EtOH).

5-Epimer: ***Dactyloquinone E***
[432552-05-1]
$C_{22}H_{28}O_4$ 356.461
Constit. of *Dactylospongia elegans*. Pale yellow amorph. solid.
$[\alpha]_D^{27}$ +33.3 (c, 0.09 in $CHCl_3$). λ_{max} 290 (log ϵ 4.2) (EtOH).

Mitome, H. *et al., Tetrahedron*, 2002, **58**, 1693-1696 (*isol, pmr, cmr*)

Dactylospongenone A D-14

[123062-42-0]



$C_{23}H_{34}O_5$ 390.519
Metab. of *Dactylospongia* sp. Cryst. Sol. MeOH, EtOAc; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D$ -167.7 (c, 0.062 in MeOH). λ_{max} 248 (ϵ 7620) (MeOH) (Berdy).

16-Epimer: ***Dactylospongenone D***
[123123-36-4]
$C_{23}H_{34}O_5$ 390.519
Metab. of *Dactylospongia* sp. Sol. MeOH, EtOAc; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D$ -121.7 (c, 0.14 in MeOH). λ_{max} 249 (ϵ 5594) (MeOH) (Berdy).

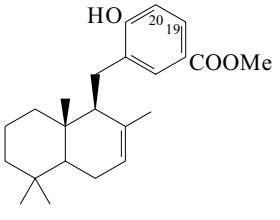
17-Epimer: ***Dactylospongenone C***
[123123-35-3]
$C_{23}H_{34}O_5$ 390.519
Metab. of *Dactylospongia* sp. Sol. MeOH, EtOAc; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D$ +25.5 (c, 0.20 in MeOH). λ_{max} 251 (ϵ 4845) (MeOH) (Berdy).

16,17-Diepimer: ***Dactylospongenone B***
[123123-34-2]
$C_{23}H_{34}O_5$ 390.519
Metab. of *Dactylospongia* sp. Sol. MeOH, EtOAc; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D$ +96.4 (c, 0.22 in MeOH). λ_{max} 249 (ϵ 6751) (MeOH) (Berdy).

Kushlan, D.M. *et al., Tetrahedron*, 1989, **45**, 3307 (*cryst struct*)
Rodríguez, J. *et al., Tetrahedron*, 1992, **48**, 6667-6680 (*cmr*)

Dactylosponol D-15

[144335-14-8]



$C_{23}H_{32}O_3$ 356.504
Constit. of *Dactylospongia elegans.* Cryst.
Mp 145-147°. $[\alpha]_D$ -14 (c, 0.05 in CH_2Cl_2).

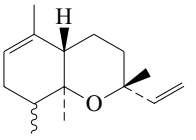
20-Hydroxy: ***Smenodiol***
[135823-98-2]
$C_{23}H_{32}O_4$ 372.503
Isol. from the sponge *Smenospongia sp.* Cryst. (MeOH).
Mp 164-166°. $[\alpha]_D$ +53.5 (c, 0.4 in MeOH). $[\alpha]_D$ -46.7 (c, 0.3 in CH_2Cl_2). λ_{max} 254; 280 (MeOH).

19,20-Dihydroxy: ***Dactylospontriol***
[144335-15-9]
$C_{23}H_{32}O_5$ 388.503
Isol. from *Dactylospongia elegans.* Cryst.
Mp 167-169°. $[\alpha]_D$ -18 (c,0.1 in CH_2Cl_2).

Venkateswarlu, Y. *et al., J.O.C.*, 1991, **56**, 6271 (*Smenodiol*)
Rodríguez, J. *et al., Tetrahedron*, 1992, **48**, 6667-6680 (*isol, pmr, cmr*)

Dactyloxene A D-16

[54990-54-4]

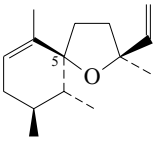


$C_{15}H_{24}O$ 220.354
Constit. of *Aplysia dactylomela.* Oil. $[\alpha]_D$ -5.9 (c, 1.4 in $CHCl_3$).

Schmitz, F.J. *et al., J.O.C.*, 1978, **43**, 4220-4225

Dactyloxene B D-17

[54928-03-9]



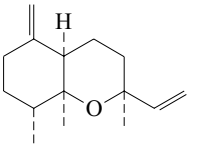
$C_{15}H_{24}O$ 220.354
Constit. of *Aplysia dactylomela.* Oil. $[\alpha]_D$ +106 (c, 0.7 in $CHCl_3$).

5-Epimer: ***Dactyloxene C***
[54990-55-5]
$C_{15}H_{24}O$ 220.354
Constit. of *Aplysia dactylomela.* Oil. $[\alpha]_D$ +45.8 (c, 0.9 in $CHCl_3$).

Schmitz, F.J. *et al., J.O.C.*, 1978, **43**, 4220 (*isol, struct*)
Maurer, B. *et al., Helv. Chim. Acta*, 1980, **63**, 2503 (*synth, abs config*)
Paquette, L.A. *et al., Tet. Lett.*, 1993, **34**, 5693 (*synth*)

Dactyloxene D D-18

[157110-32-2]

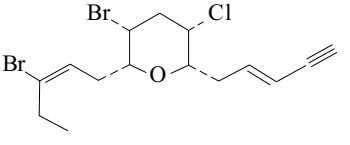


$C_{15}H_{24}O$ 220.354
Constit. of *Laurencia obtusa.* Oil.

Ayyad, S.N. *et al., Phytochemistry*, 1994, **36**, 1077 (*isol, pmr, cmr*)

Dactylyne D-19

[55306-12-2]



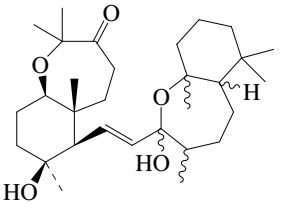
Absolute configuration

$C_{15}H_{19}Br_2ClO$ 410.575
Constit. of *Aplysia dactylomela* and a *Laurencia* sp. Cryst. Sol. MeOH, hexane; poorly sol. H_2O.
Mp 62.2-63.3°. $[\alpha]_D^{25}$ -36 (c, 15.2 in $CHCl_3$). λ_{max} 223 (ϵ 12000) (isooctane) (Derep). λ_{max} 222 (ϵ 12000) (isooctane) (Berdy).

McDonald, F.J. *et al., J.O.C.*, 1975, **40**, 665-666 (*isol*)
Gao, L.-X. *et al., Heterocycles*, 1996, **42**, 745 (*synth, ir, pmr*)
Suzuki, M. *et al., Phytochemistry*, 1999, **51**, 657-662 (*isol, cmr*)

Dahabinone A D-20

[329050-25-1]

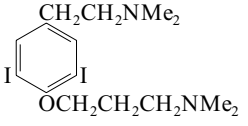


$C_{30}H_{50}O_5$ 490.722
Constit. of *Siphonochalina siphonella*. Amorph. powder.

Kashman, Y. *et al., J. Nat. Prod.*, 2001, **64**, 175-180 (*isol, pmr, cmr*)

Dakaramine D-21

[173075-47-3]

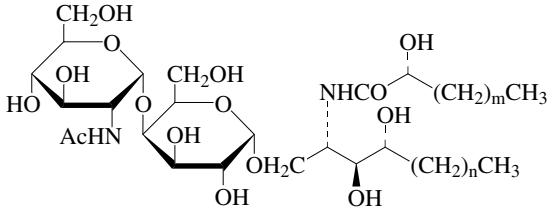


$C_{15}H_{24}I_2N_2O$ 502.176
Metab. from the Senegalese sponge *Ptilocaulis spiculifer*. Isol. with, O-*Sulfate as counterion.*

Diop, M. *et al., J. Nat. Prod.*, 1996, **59**, 271-272 (*isol, uv, ir, pmr, cmr, struct*)

Damicoside D-22

[871125-59-6]

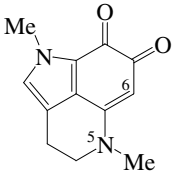


α-Galactoglycosphingolipid complex. Constit. of the sponge *Axinella damicornis.* Amorph. solid. $[\alpha]_D^{25}$ +55 (c, 0.66 in MeOH).

Costantino, V. *et al., J. Med. Chem.*, 2005, **48**, 7411-7417 (*isol, pmr, cmr*)

Damirone A D-23

*1,3,4,5-Tetrahydro-1,5-dimethylpyrrolo[4,3,2-*de*]quinoline-7, 8-dione, 9CI*
[138683-66-6]



$C_{12}H_{12}N_2O_2$ 216.239
Alkaloid from the sponges *Damiria* sp. and *Zyzzya* sp. Purple solid.
Mp 240-242° dec. λ_{max} 242 (ϵ 12600); 347 (ϵ 10200); 518 (ϵ 912) (MeOH) (Derep). λ_{max} 214 (ϵ 9000); 245 (ϵ 21000); 347 (ϵ 7200); 516 (ϵ 500) (MeOH) (Derep).

N^1*-De-Me:* ***Damirone B***
[138683-67-7]
$C_{11}H_{10}N_2O_2$ 202.212
Alkaloid from the sponges *Damiria* sp. and *Zyzzya fuliginosa*. Purple solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 250°. λ_{max} 242 (ϵ 7080); 350 (ϵ 4470); 498 (ϵ 257) (MeOH) (Derep). λ_{max} 242 (ϵ 29500); 347 (ϵ 19500) (MeOH) (Berdy). λ_{max} 242 (ϵ 19000); 347 (ϵ 19300) (MeOH/NaOH) (Berdy). λ_{max} 243; 348; 492 (EtOH) (Berdy).

N^5*-De-Me:* ***6-Dechlorobatzelline C***
[138683-68-8]
$C_{11}H_{10}N_2O_2$ 202.212
Isol. from *Zyzzya fuliginosa*.

N^1,N^5*-Di-de-Me:* ***Damirone C***
[157669-64-2]
$C_{10}H_8N_2O_2$ 188.185
Alkaloid from the sponge *Zyzzya fuliginosa*. Red-brown solid.

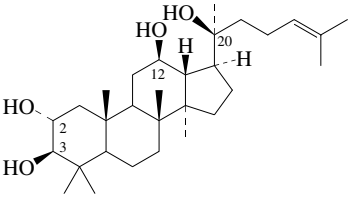
N^1,N^5*-Di-de-Me,* N^1*-β-*D*-ribofuranosyl:* ***N^1-β-D-Ribofuranosyldamirone C***
$C_{15}H_{16}N_2O_6$ 320.301
Alkaloid from the sponge *Strongylodesma aliwaliensis.* Red amorph. solid. $[\alpha]_D^{14}$ +5 (c, 0.06 in MeOH). λ_{max} 246 (ϵ 14100); 334 (ϵ 7990); 526 (ϵ 650) (MeOH).

6-Bromo, N^5*-de-Me:* ***Makaluvone***
[146555-84-2]
$C_{11}H_9BrN_2O_2$ 281.108
Isol. from the sponge *Zyzzya fuliginosa*. Grey solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 246 (ϵ 9800); 330 (ϵ 6300) (MeOH/NaOH) (Derep). λ_{max} 246 (ϵ 10100); 330 (ϵ 5500) (MeOH) (Derep).

6-Bromo, N^1,N^5*-di-de-Me: 6-Bromo-1,3,4,5-tetrahydropyrrolo[4,3,2-*de*]quinoline-7,8-dione, 9CI.* ***Makaluvamine O***
$C_{10}H_7BrN_2O_2$ 267.082
Alkaloid from the sponge *Smenospongia* sp. Purple solid.
Mp 282-283° dec. λ_{max} 222 (log ϵ 3.81); 244 (log ϵ 3.28); 328 (log ϵ 2.94); 362 (sh) (log ϵ 2.86); 542 (log ϵ 2.06) (MeOH). λ_{max} 244 (log ϵ 4.01); 337 (log ϵ 3.75) (MeOH).

Stierle, D.B. *et al., J. Nat. Prod.*, 1991, **54**, 1131 (*isol, uv, ir, pmr, ms, struct, cmr*)
Baumann, C. *et al., Angew. Chem., Int. Ed.*, 1993, **105**, 1087 (*synth*)
Radisky, D.C. *et al., J.A.C.S.*, 1993, **115**, 1632 (*isol, Damirone B*)
Sadanandan, E.V. *et al., Tet. Lett.*, 1993, **34**, 2405 (*synth*)
Yamada, F. *et al., Heterocycles*, 1995, **41**, 1905 (*synth*)
Schmidt, E.W. *et al., J. Nat. Prod.*, 1995, **58**, 1861 (*Damirone C*)
Roue, N. *et al., J. Pharm. Belg.*, 1995, **50**, 94 (*synth*)
Peat, A.J. *et al., J.A.C.S.*, 1996, **118**, 1028 (*synth*)
Roberts, D. *et al., J.O.C.*, 1997, **62**, 568 (*synth*)
Hu, J.F. *et al., J. Nat. Prod.*, 2002, **65**, 476-480 (*Makaluvamine O*)
Tasdemir, D. *et al., Z. Naturforsch., C*, 2002, **57**, 914-922 (*Makaluvamine O*)
Keyzers, R.A. *et al., Tet. Lett.*, 2004, **45**, 9415-9418 (*N-Ribofuranosyldamirone C*)
Dijoux, M.-G. *et al., Bioorg. Med. Chem.*, 2005, **13**, 6035-6044 (*isol, cmr, activity*)

Dammar-24-ene-2,3,12,20-tetrol D-24



(2α,3β,12β,20*R*)-*form*

$C_{30}H_{52}O_4$ 476.738

(2α,3β,12β,20*R*)-*form*

3-O-*[β-*D*-Glucopyranosyl-(1→2)-β-*D*-glucopyranoside]:* ***Gypenoside LI***
[94987-10-7]
$C_{42}H_{72}O_{14}$ 801.022
Constit. of *Gynostemma pentaphyllum*.
$[\alpha]_D$ 0 (c, 1.4 in MeOH).

(2α,3β,12β,20*S*)-*form*

3-O-*β-*D*-Glucopyranoside, 20*-O-*[β-*D*-xylopyranosyl-(1→6)-β-*D*-glucopyranoside]:* ***Gypenoside LVII***

[105239-70-1]
$C_{47}H_{80}O_{18}$ 933.138
Isol. from *Gynostemma pentaphyllum*.
Mp 189-191°. $[\alpha]_D^{22}$ +11.8 (c, 3.8 in MeOH).

3-O-*β*-D-Glucopyranoside, *20*-O-[*α*-L-rhamnopyranosyl-(1→6)-*β*-D-glucopyranoside]: ***Gypenoside XLV***
[94729-05-2]
$C_{48}H_{82}O_{18}$ 947.165
Isol. from *Gynostemma pentaphyllum* and the leaves of *Gymnema sylvestre*. Cryst. + $3H_2O$.
Mp 196-198°. $[\alpha]_D^{22}$ +9.3 (c, 4.1 in MeOH).

3-O-*β*-D-Glucopyranoside, *20*-O-[*β*-D-glucopyranosyl-(1→6)-*β*-D-glucopyranoside]: ***Gypenoside XLIV***
[94705-69-8]
$C_{48}H_{82}O_{19}$ 963.164
Isol. from *Gynostemma pentaphyllum*. Cryst. + $3H_2O$.
Mp 185-187°. $[\alpha]_D^{22}$ +10.4 (c, 2.3 in MeOH).

20-O-*β*-D-Glucopyranoside: ***Gynosaponin TN1***
[77658-94-7]
$C_{36}H_{62}O_9$ 638.88
Constit. of *Gynostemma pentaphyllum*. Cryst. (EtOH aq.).
Mp 168-173°. $[\alpha]_D^{23}$ +34.5 (c, 0.9 in MeOH).

20-O-*α*-L-Rhamnopyranosyl-(1→6)-*β*-D-glucopyranoside: ***Gynosaponin TN2***
[77658-95-8]
$C_{42}H_{72}O_{13}$ 785.023
Constit. of *Gynostemma pentaphyllum*. Cryst. (MeOH/$CHCl_3$/EtOAc).
Mp 236-240°. $[\alpha]_D^{24}$ +11.6 (c, 1 in MeOH).

3-O-[*β*-D-Glucopyranosyl-(1→2)-*β*-D-glucopyranoside], *20*-O-*β*-D-glucopyranoside: ***Gypenoside XLVI***
[94705-70-1]
$C_{48}H_{82}O_{19}$ 963.164
Isol. from *Gynostemma pentaphyllum*. Cryst. + $3H_2O$.
Mp 190-192°. $[\alpha]_D^{22}$ +20.1 (c, 3.1 in MeOH).

3-O-[*β*-D-Glucopyranosyl-(1→2)-*β*-D-glucopyranoside], *20*-O-[*β*-D-xylopyranosyl-(1→6)-*β*-D-glucopyranoside]: ***Gypenoside LVI***
[105214-48-0]
$C_{53}H_{90}O_{23}$ 1095.28
Isol. from *Gynostemma pentaphyllum*. Cryst. + $2.5H_2O$.
Mp 212-214°. $[\alpha]_D^{22}$ +7.9 (c, 3.8 in MeOH).

3-O-[*β*-D-Glucopyranosyl-(1→2)-*β*-D-glucopyranoside], *20*-O-[*α*-L-rhamnopyranosyl-(1→6)-*β*-D-glucopyranoside]: ***Gypenoside XLIII***
[94705-68-7]
$C_{54}H_{92}O_{23}$ 1109.307
Isol. from *Gynostemma pentaphyllum*. Cryst. + $1H_2O$.
Mp 202-204°. $[\alpha]_D^{22}$ +6.6 (c, 2.1 in MeOH).

3-O-[*β*-D-Glucopyranosyl-(1→2)-*β*-D-glucopyranoside], *20*-O-[*β*-D-glucopyranosyl-(1→6)-*β*-D-glucopyranoside]: ***Gypenoside XLII***
[94705-67-6]
$C_{54}H_{92}O_{24}$ 1125.306
Isol. from *Gynostemma pentaphyllum*. Cryst. + $1H_2O$.
Mp 188-190°. $[\alpha]_D^{22}$ +2.5 (c, 3.8 in MeOH).

12-Ketone: ***2,3,20-Trihydroxydammar-24-en-12-one***
$C_{30}H_{50}O_4$ 474.723
Sapogenin from *Gynostemma pentaphyllum*.

12-Ketone, 3-O-[*β*-D-glucopyranosyl-(1→2)-*β*-D-glucopyranoside], *20*-O-[*β*-D-xylopyranosyl-(1→6)-*β*-D-glucopyranoside]:
$C_{53}H_{88}O_{23}$ 1093.264
Constit. of *Gynostemma pentaphyllum*. Amorph. powder.
$[\alpha]_D^{18.5}$ -2.32 (c, 0.03 in MeOH).

12-Ketone, 3-O-[*β*-D-glucopyranosyl-(1→2)-*β*-D-glucopyranoside], *20*-O-[*α*-L-rhamnopyranosyl-(1→6)-*β*-D-glucopyranoside]:
$C_{54}H_{90}O_{23}$ 1107.291
Constit. of *Gynostemma pentaphyllum*. Amorph. powder.
$[\alpha]_D^{18.5}$ -6 (c, 0.02 in MeOH).

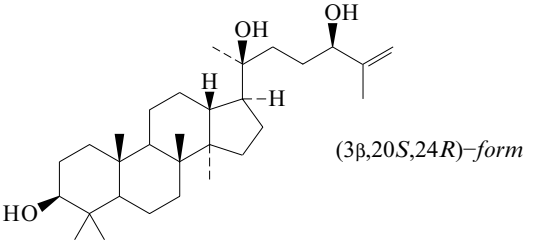
20-O-[*β*-D-Xylopyranosyl-(1→6)-*β*-D-glucopyranoside]: ***Gypenoside LXXVII***
[110925-28-5]
$C_{41}H_{70}O_{13}$ 770.996
Constit. of *Gynostemma pentaphyllum*. Cryst.
Mp 216-218°. $[\alpha]_D^{22}$ +9 (c, 6.7 in MeOH).

20-O-[*β*-D-Glucopyranosyl-(1→6)-*β*-D-glucopyranoside]: ***Gypenoside LXXIV***
[110261-97-7]
$C_{42}H_{72}O_{14}$ 801.022
Constit. of *Gynostemma pentaphyllum*. Cryst.
Mp 173-175°. $[\alpha]_D$ +13.7 (c, 6.4 in MeOH).

3-O-[*β*-D-Glucopyranosyl-(1→2)-*β*-D-glucopyranoside]: ***Gypenoside L***
[94987-09-4]
$C_{42}H_{72}O_{14}$ 801.022
Constit. of *Gynostemma pentaphyllum*.
$[\alpha]_D^{22}$ +15.2 (c, 1.8 in MeOH).

Nagai, M. *et al., Chem. Pharm. Bull.*, 1981, **29**, 779
Takemoto, T. *et al., Yakugaku Zasshi*, 1984, **104**, 1043-1049; 1155-1162; 1986, **106**, 664-670; 1987, **107**, 361-366 (*Gypenosides XLIII - XLV, L-LI, LVI-LVII, LXXIV-LXXVII*)
Yoshikawa, K. *et al., Chem. Pharm. Bull.*, 1989, **37**, 852 (*Gypenoside XLIII, Gypenoside XLV*)
Hu, L. *et al., J. Nat. Prod.*, 1996, **59**, 1143 (*12-ketone derivs*)
Razmovski-Naumovski, V. *et al., Acta Cryst. E*, 2005, **61**, o1239-o1241 (*Gynosaponin TN1, cryst struct*)

Dammar-25-ene-3,20,24-triol D-25



(3β,20*S*,24*R*)-*form*

$C_{30}H_{52}O_3$ 460.739

(3β,20*S*,24*R*)-*form*
Fouquierol
[53822-98-3]
Constit. of *Fouquieria splendens*.
Cryst.
Mp 163-165°. $[\alpha]_D$ +29 ($CHCl_3$).

3-Ketone: 20,24-Dihydroxydammar-25-en-3-one. ***Fouquierone***
[366479-04-1]
$C_{30}H_{50}O_3$ 458.723
Constit. of root bark of *Rhus javanica*. Powder. $[\alpha]_D^{25}$ +58 (c, 0.16 in $CHCl_3$).

3-Dodecanoyl:
[825631-05-8 (mixt. of 24-epimers)]
$C_{42}H_{74}O_4$ 643.044
Constit. of *Arnica lonchophylla*.

3-Tetradecanoyl:
[825631-22-9 (mixt. of 24-epimers)]
$C_{44}H_{78}O_4$ 671.098
Constit. of *Arnica lonchophylla*.

3-Hexadecanoyl:
[825631-23-0 (mixt. of 24-epimers)]
$C_{46}H_{82}O_4$ 699.151
Constit. of *Arnica lonchophylla*.

3-Octadecanoyl:
[825631-24-1 (mixt. of 24-epimers)]
$C_{48}H_{86}O_4$ 727.205
Constit. of *Arnica lonchophylla*.

(3β,20*S*,24*S*)-*form*
24-Epifouquierol
Constit. of *Arnica lonchophylla*.

3-Dodecanoyl:
$C_{42}H_{74}O_4$ 643.044
Constit. of *Arnica lonchophylla*.

3-Tetradecanoyl:
$C_{44}H_{78}O_4$ 671.098
Constit. of *Arnica lonchophylla*.

3-Hexadecanoyl:
$C_{46}H_{82}O_4$ 699.151
Constit. of *Arnica lonchophylla*.

3-Octadecanoyl:
$C_{48}H_{86}O_4$ 727.205
Constit. of *Arnica lonchophylla*.

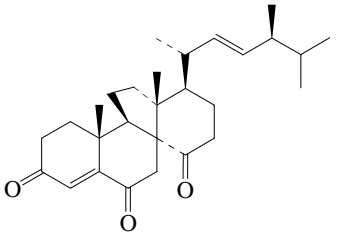
(3β,20*S*,24ξ)-*form*

24-Hydroperoxide: 24-Hydroperoxydammar-25-ene-3,20-diol.
Cereotagaloperoxide
[57082-36-7]
$C_{30}H_{52}O_4$ 476.738
Constit. of the mangrove *Ceriops tagal*. Amorph. powder.
Mp 183-185°. $[\alpha]_D^{27}$ +54.1 (c, 0.04 in MeOH).

Butruille, D. *et al., Tet. Lett.*, 1974, 639 (*struct*)
Butruille, D. *et al., Rev. Latinoam. Quim.*, 1976, **7**, 96 (*biosynth*)
Lee, I.S. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1024-1026 (*Fouquierone*)
Schmidt, T.J. *et al., Planta Med.*, 2004, **70**, 967-977 (*acyl derivs*)
Pakhathirathien, C. *et al., J. Nat. Prod.*, 2005, **68**, 1787-1789 (*Cereotagaloperoxide*)

Dankasterone D-26

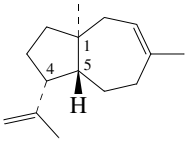
[244303-77-3]



$C_{28}H_{40}O_3$ 424.622
A 13(14→8)-Abeoergostane. Metab. of *Gymnascella dankaliensis* from the sponge *Halichondria japonica*. Shows cytotoxicity against tumour cells. Cryst. (MeOH).
Mp 133-134°. $[\alpha]_D^{26}$ +57.8 (c, 0.7 in $CHCl_3$). λ_{max} 254 (log ϵ 4.02) (EtOH).

Amagata, T. *et al., Chem. Comm.*, 1999, 1321-1322 (*isol, pmr, cmr, cryst struct*)

8,11-Daucadiene D-27



(1α,4α,5β)-*form*

$C_{15}H_{24}$ 204.355

(1α,4α,5β)-*form* [395070-75-4]
Constit. of *Cupressocyparis leylandii*.

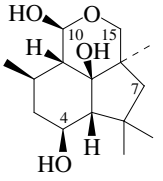
(1β,4α,5α)-*form* [85431-47-6]
Constit. of a *Higginsia* sp. and *Plagiomnium undulatum*.
Oil. $[\alpha]_D$ -7 (c, 1.1 in $CHCl_3$).

(1β,4β,5α)-*form* [142878-08-8]
Constit. of *Vernonia galpinii*.
Oil. $[\alpha]_D^{24}$ +13 (c, 1.1 in $CHCl_3$). Struct. revised in 2001.

Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 2263-2267 (*Vernonia galpinii constit*)
Cassidy, M.P. *et al., J. Nat. Prod.*, 1993, **56**, 1190-1193 (*Higginsia constit*)
Saritas, Y. *et al., Phytochemistry*, 2001, **57**, 443-457 (*Plagiomnium undulatum, bibl*)
Cool, L.G. *et al., Phytochemistry*, 2001, **58**, 969-972 (*Cupressocyparis leylandii constit*)

Deacetyldihydrobotrydial D-28

[97165-22-5]



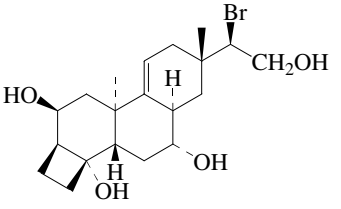
$C_{15}H_{26}O_4$ 270.368
Metab. of *Botrytis squamosa*. Phytotoxic, plant growth regulator. Prisms.
Mp 163-165°. $[\alpha]_D^{28}$ +22.4 (c, 1.2 in MeOH).

4-Ac: ***Dihydrobotrydial***
[54433-86-2]
$C_{17}H_{28}O_5$ 312.405
Metab. of *Botrytis cinerea*, *Hymenoscyphus epiphyllus* and the marine-derived *Emericellopsis minima* H7-65. Cytotoxic agent, phytotoxin. Cryst. (petrol).
Mp 158-160°. $[\alpha]_D^{22}$ +56 (c, 0.94 in petrol). λ_{max} 200 (hexane) (Berdy).

Höller, U. *et al., Dissertation*, Univ. of Braunschweig, 1999, (*Dihydrobotrydial, marine isol*)
Durán-Patrón, R. *et al., Tetrahedron*, 1999, **55**, 2389-2400 (*activity, Dihydrobotrydial*)

Deacetylisoparguerol D-29

[132309-62-7]



$C_{20}H_{31}BrO_4$ 415.366
Isol. from *Laurencia obtusa*. Feeding deterrent. Glassy solid. $[\alpha]_D$ +5 (c, 0.46 in MeOH).

2-Ac: ***Isoparguerol***
[83115-46-2]
$C_{22}H_{33}BrO_5$ 457.404
Constit. of *Aplysia dactylomela*. Cytotoxic agent. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 139-141°. $[\alpha]_D$ +3.6 (c, 0.14 in $CHCl_3$).

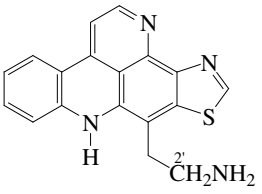
2,16-Di-Ac: [83115-48-4]
$C_{24}H_{35}BrO_6$ 499.441
Isol. from *Aplysia dactylomela*. Cytotoxic agent. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 180-182°. $[\alpha]_D$ -18.8 (c, 0.09 in $CHCl_3$).

2,7,16-Tri-Ac: [83115-47-3]
$C_{26}H_{37}BrO_7$ 541.478
Constit. of *Laurencia saitoi*. Feeding deterrent.

Schmitz, F.J. *et al., J.A.C.S.*, 1982, **104**, 6415-6423 (*Isoparguerol, 2,16-di-Ac*)
Takeda, S. *et al., Bull. Chem. Soc. Jpn.*, 1990, **63**, 3066-3072 (*Deacetylisoparguerol*)
Kurata, K. *et al., Phytochemistry*, 1998, **47**, 363-369 (*tri-Ac*)
Tsukamoto, S. *et al., Mar. Drugs*, 2004, **2**, 170-175 (*Isoparguerol, pmr, activity*)

N-Deacetylkuanoniamine D D-30

[202932-14-7]



$C_{18}H_{14}N_4S$ 318.401

Alkaloid from the sponge *Oceanapia* sp. Cytotoxic agent. DNA intercalator. Amorph. orange powder. λ_{max} 201 (log ϵ 4.14); 239 (log ϵ 4.33); 264 (log ϵ 4.11); 295 (log ϵ 4.08); 304 (log ϵ 4.05); 342 (log ϵ 3.82); 355 (log ϵ 3.85) (MeOH). λ_{max} 201 (ϵ 13800); 223 (ϵ 26900); 295 (ϵ 12000); 342 (ϵ 6600); 365 (ϵ 3550) (MeOH) (Berdy).

N$^{2'}$-*Ac:* ***Kuanoniamine D***

[133401-13-5]

$C_{20}H_{16}N_4OS$ 360.439

Alkaloid from a tunicate and its mollusc predator *Chelynotus semperi*. Also isol. from a purple tunicate tentatively identified as *Cystodytes* sp. Topoisomerase II inhibitor, chelating agent., adenosine and GABA receptor binding agent; cytotoxic agent; insecticide, toxic to brine shrimp. Amorph. yellow powder ($CHCl_3$). Mp 300°. λ_{max} 206 (ϵ 14100); 240 (ϵ 16600); 270 (ϵ 11700); 306 (ϵ 18600); 360 (ϵ 5620); 526 (ϵ 2450) (MeOH/HCl) (Derep). λ_{max} 206 (ϵ 17400); 240 (ϵ 20900); 264 (ϵ 15800); 294 (sh) (ϵ); 344 (ϵ 7590); 358 (ϵ 7410); 452 (ϵ 2400) (MeOH) (Derep). λ_{max} 206; 240; 270; 360; 526 (MeOH/NaOH) (Berdy).

N$^{2'}$-*Propanoyl:* ***Kuanoniamine C****. Dercitamide*

[133401-12-4]

$C_{21}H_{18}N_4OS$ 374.465

Alkaloid from a tunicate and its mollusc predator *Chelynotus semperi*. Also isol. from a purple tunicate tentatively identified as *Cystodytes* sp. and from a deep water marine sponge *Stelletta* sp. Cytotoxic. Inhibits proliferation of P388 murine leukaemia cells in vitro. Also displays immunosuppressive activity. Amorph. yellow powder ($CHCl_3$).
Mp 300° (192°). λ_{max} 206 (ϵ 14100); 240 (ϵ 16600); 270 (ϵ 11700); 306 (ϵ 18600); 360 (ϵ 5620); 526 (ϵ 2450) (MeOH/HCl) (Derep). λ_{max} 245 (ϵ 13800); 307 (ϵ 16900); 361 (ϵ 3900); 541 (ϵ 1800) (MeOH) (Derep). λ_{max} 206 (ϵ 17400); 240 (ϵ 20900); 264 (ϵ 15800); 294 (sh); 344 (ϵ 7590); 358 (ϵ 7410); 452 (ϵ 2400) (MeOH) (Derep).

N$^{2'}$-*(2-Methylpropanoyl):* ***Kuanoniamine E***

[445471-59-0]

$C_{22}H_{20}N_4OS$ 388.492

Alkaloid from a Singaporean ascidian. Yellow gum. λ_{max} 204 (log ϵ 4.27); 241 (log ϵ 4.52); 265 (log ϵ 4.3); 296 (sh) (log ϵ 3.97); 346 (log ϵ 4.07); 362 (log ϵ 4.08); 452 (log ϵ 3.67) (MeOH).

N$^{2'}$-*(2-Methylbutanoyl):* ***Kuanoniamine F***

[445471-61-4]

$C_{23}H_{22}N_4OS$ 402.519

Alkaloid from a Singaporean ascidian. Yellow gum. $[\alpha]_D$ +105 (c, 0.18 in MeOH). λ_{max} 206 (log ϵ 4.26); 242 (log ϵ 4.49); 262 (log ϵ 4.29); 296 (sh) (log ϵ 3.98); 346 (log ϵ 4.04); 363 (log ϵ 4.05); 455 (log ϵ 3.38) (MeOH).

N$^{2'}$-*(3-Methylbutanoyl):* ***Kuanoniamine B***

[133401-11-3]

$C_{23}H_{22}N_4OS$ 402.519

Alkaloid from a tunicate and its mollusc predator *Chelynotus semperi*. Cytotoxic agent. Amorph. yellow powder ($CHCl_3$).
Mp 300°. λ_{max} 204 (ϵ 17400); 240 (ϵ 20900); 264 (ϵ 15100); 294 (sh) (ϵ 7760); 344 (ϵ 7410); 360 (ϵ 7410); 450 (ϵ 2750) (MeOH) (Derep).

N$^{2'}$-*(3-Methyl-2-butenoyl):* ***Dehydrokuanoniamine B***

[158734-24-8]

$C_{23}H_{20}N_4OS$ 400.503

Alkaloid from *Cystodytes* sp. Antitumour agent; DNA intercalator; topoisomerase II inhibitor. Orange solid. λ_{max} 237 (ϵ 50970); 261 (ϵ 30120); 344 (ϵ 16410); 359 (ϵ 16950); 452 (ϵ 6050) (MeOH).

N$^{2'}$-*Me:* ***Dercitamine***

[125236-60-4]

$C_{19}H_{16}N_4S$ 332.428

Alkaloid from *Stelletta* sp. Inhibits proliferation of P388 murine leukaemia cells *in vitro*. Also displays immunosuppressive activity. Orange solid.
Mp 135°. Regiochem. revised in 1992. Genus name incorr. given as Stelleta. λ_{max} 245 (ϵ 13800); 307 (ϵ 16900); 361 (ϵ 3900) (MeOH) (Derep).

N$^{2'}$,N$^{2'}$-*Di-Me:* ***Nordercitin***

[125236-59-1]

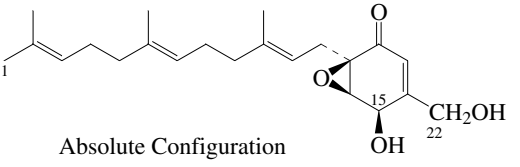
$C_{20}H_{18}N_4S$ 346.455

Alkaloid from a deep water marine sponge *Stelletta* sp. Inhibits proliferation of P388 murine leukaemia cells *in vitro*. Also displays immunosuppressive activity. Yellow solid.
Mp 176°. λ_{max} 245 (ϵ 13800); 307 (ϵ 16900); 361 (ϵ 3900) (MeOH) (Derep).

Gunawardana, G.P. *et al., Tet. Lett.*, 1989, **30**, 4359-4362 (*Dercitamine, Nordercitin*)
Carroll, A.R. *et al., J.O.C.*, 1990, **55**, 4426-4431 (*Kuanoniamines A-D, isol, uv, ir, pmr, cmr, ms, struct*)
Bishop, M.J. *et al., J.A.C.S.*, 1992, **114**, 10081-10082 (*synth*)
Gunawardana, G.P. *et al., J.O.C.*, 1992, **57**, 1523-1526 (*Kuanoniamine D, Dercitamine, Nordercitin, struct*)
Eldredge, G.S. *et al., J. Med. Chem.*, 1994, **37**, 3819-3827 (*Dehydrokuoniamine B*)
Ciufolini, M.A. *et al., J.A.C.S.*, 1995, **117**, 12460-12469 (*synth*)
Eder, C. *et al., J. Nat. Prod.*, 1998, **61**, 301-305 (*Deacetylkuanoniamine D*)
Nilar, *et al., J. Nat. Prod.*, 2002, **65**, 1198-1200 (*Kuanoniamines E-F*)
Sidebottom, N.P.J. *et al., J. Nat. Prod.*, 2002, **65**, 1198-1200 (*Kuanoniamine E,F*)

22-Deacetylyanuthone A D-31

[307001-93-0]



Absolute Configuration

$C_{22}H_{32}O_4$ 360.492

Prod. by a marine *Aspergillus niger* F97S11 isol. from an *Aplidium* sp. Closely related to Oligosporol A. λ_{max} 238 (log ϵ 4.21); 302 (log ϵ 2.68) (MeOH).

15-Ac: ***Yanuthone C***

[307304-26-3]

$C_{24}H_{34}O_5$ 402.53

Prod. by *Aspergillus niger* F97S11. Oil. λ_{max} 232 (log ϵ 4.12); 280 (log ϵ 3.31); 322 (log ϵ 3.03) (MeOH).

22-Ac: ***Yanuthone A***

[307304-24-1]

$C_{24}H_{34}O_5$ 402.53

Prod. by *Aspergillus niger* F97S11. Pale yellow oil. λ_{max} 232 (log ϵ 3.9); 310 (log ϵ 2.7) (MeOH).

22-O-*(4-Carboxy-3-hydroxy-3-methylbutanoyl)(*R-*):* ***Yanuthone E***

[307304-28-5]

$C_{28}H_{40}O_8$ 504.619

Prod. by *Aspergillus niger* F97S11. Yellow-brown oil. λ_{max} 234 (log ϵ 3.96); 280 (log ϵ 3); 340 (log ϵ 2.65) (MeOH).

15-Ketone, 22-Ac: ***Yanuthone B***

[307304-25-2]

$C_{24}H_{32}O_5$ 400.514

Prod. by *Aspergillus niger* F97S11. Pale yellow oil. λ_{max} 244 (log ϵ 3.65); 290 (log ϵ 3.29); 338 (log ϵ 2.92) (MeOH).

15-Ketone, 22-O-*(4-carboxy-3-hydroxy-3-methylbutanoyl)(*R-*):* ***Yanuthone D***

[307304-27-4]

$C_{28}H_{38}O_8$ 502.603

Prod. by *Aspergillus niger* F97S11. λ_{max} 226 (log ϵ 3.9); 254 (log ϵ 3.57); 298 (log ϵ 3.06) (MeOH).

22-Deoxy: ***22-Deacetoxyyanuthone A****. 7-Deacetoxyyanuthone A*
$C_{22}H_{32}O_3$ 344.493
Metab. of a marine-derived *Penicillium* sp. Yellow oil. $[\alpha]_D$ +3.1 (c, 0.5 in $CHCl_3$). Numbering systems differ. λ_{max} 203 (log ϵ 4.6); 238 (log ϵ 4.2) (MeOH).

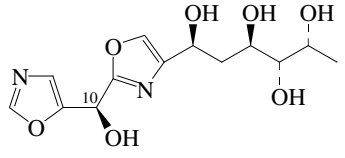
1-Hydroxy, 15-Ac: ***1-Hydroxyyanuthone C***
[307304-30-9]
$C_{24}H_{34}O_6$ 418.529
Prod. by *Aspergillus niger* F97S11. Oil. λ_{max} 232 (log ϵ 3.67); 282 (log ϵ 2.67) (MeOH).

1-Hydroxy, 22-Ac: ***1-Hydroxyyanuthone A***
[307304-29-6]
$C_{24}H_{34}O_6$ 418.529
Prod. by *Aspergillus niger* F97S11. Oil. λ_{max} 234 (log ϵ 3.93); 290 (log ϵ 2.34) (MeOH).

13,14-Deepoxy, 13β,14α-dihydroxy, 22-deoxy: [635682-46-1]
$C_{22}H_{34}O_4$ 362.508
Metab. of a marine-derived *Penicillium* sp. Oil. $[\alpha]_D$ -2.1 (c, 0.3 in $CHCl_3$). λ_{max} 203 (log ϵ 4.2); 238 (log ϵ 4) (MeOH).

Bugni, T.S. *et al., J.O.C.*, 2000, **65**, 7195-7200 (*Aspergillus niger isolates*)
Li, X. *et al., J. Nat. Prod.*, 2003, **66**, 1499-1500 (*Penicillium metabs*)
Mehta, G. *et al., Tet. Lett.*, 2005, **46**, 5219-5223 (*synth*)

Deacylbengazole C D-32



Absolute Configuration

$C_{13}H_{18}N_2O_7$ 314.294

O^{10}-*Tridecanoyl:* ***Bengazole C***
[147512-35-4]
$C_{26}H_{42}N_2O_8$ 510.626
Isol. from a *Jaspis* sp. Anthelmintic agent. Oil. λ_{max} 217 (MeOH aq.).

O^{10}-*Tetradecanoyl:* ***Bengazole A***
[112549-08-3]
$C_{27}H_{44}N_2O_8$ 524.653
Isol. from a Jaspidae marine sponge from Fiji. Exhibits anthelminthic activity. Antifungal agent. Viscous oil. $[\alpha]_D^{20}$ +5 (c, 0.107 in MeOH). λ_{max} 209 (ϵ 1400) (MeOH) (Derep).

O^{10}-*(12-Methyltridecanoyl):* ***Bengazole D***
[147362-22-9]
$C_{27}H_{44}N_2O_8$ 524.653
Isol. from a *Jaspis* sp. Anthelmintic agent. Oil. λ_{max} 217 (MeOH aq.).

O^{10}-*Pentadecanoyl:* ***Bengazole E***
[147362-23-0]
$C_{28}H_{46}N_2O_8$ 538.68
Isol. from a *Jaspis* sp. Anthelmintic agent. Oil. λ_{max} 217 (MeOH aq.).

O^{10}-*(12-Methyltetradecanoyl):* ***Bengazole B1***
[147391-82-0]
$C_{28}H_{46}N_2O_8$ 538.68
Isol. from a Great Barrier Reef sponge *Jaspis* sp. Inseparable 1:5 mixt. with Bengazole B.

O^{10}-*(13-Methyltetradecanoyl):* ***Bengazole B***
[112549-09-4]
$C_{28}H_{46}N_2O_8$ 538.68
Isol. from a Jaspidae marine sponge from Fiji and from an Australian *Jaspis* sp. (as an inseparable mixt. with Bengazole B1). Exhibits anthelminthic and antifungal activity. Viscous oil. $[\alpha]_D^{20}$ +4.7 (c, 0.024 in MeOH). λ_{max} 209 (ϵ 1400) (MeOH) (Derep).

O^{10}-*Hexadecanoyl:* ***Bengazole G***
[147362-24-1]
$C_{29}H_{48}N_2O_8$ 552.707
Isol. from a *Jaspis* sp. Anthelminthic agent. Oil. λ_{max} 217 (MeOH aq.).

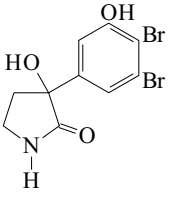
O^{10}-*(13-Methylpentadecanoyl):* ***Bengazole F***
[147391-83-1]
$C_{29}H_{48}N_2O_8$ 552.707
Isol. from a *Jaspis* sp. Anthelminthic agent. Oil. λ_{max} 217 (MeOH aq.).

10-Deoxy: See Bengazole Z, B-50

Adamczeski, M. *et al., J.A.C.S.*, 1988, **110**, 1598 (*isol, uv, ir, pmr, cmr, ms, struct*)
Molinski, T.F. *et al., J. Nat. Prod.*, 1993, **56**, 1 (*biochem*)
Searle, P.A. *et al., J.O.C.*, 1996, **61**, 4073-4079 (*abs config*)
Mulder, R.J. *et al., J.O.C.*, 1999, **64**, 4995-4998; 2000, **65**, 8126 (*synth*)
Chittari, P. *et al., Heterocycles*, 2003, **59**, 465-472 (*synth*)

Deacylconvolutamide D-33

3-(3,4-Dibromo-5-hydroxyphenyl)-3-hydroxy-2-pyrrolidinone



$C_{10}H_9Br_2NO_3$ 350.994

N-*Tetradecanoyl:* ***Convolutamide A***
[158182-21-9]
$C_{24}H_{35}Br_2NO_4$ 561.353
Isol. from the marine bryozoan *Amathia convoluta*. Exhibits cytotoxicity against L1210 murine leukaemia and KB human epidermoid carcinoma cells. Amorph. solid. $[\alpha]_D^{20}$ -6 (c, 0.4 in $CHCl_3$). Opt. rotn. and biol. activity refer to a 1:1.7 insep. mixt. with Convolutamide B. λ_{max} 225 (ϵ 34000) (MeOH) (Berdy).

N-*(9Z-Hexadecenoyl):* ***Convolutamide B***
[158182-22-0]
$C_{26}H_{37}Br_2NO_4$ 587.391
From *Amathia convoluta*. See statement under Convolutamide A above.

N-*Hexadecanoyl:* ***Convolutamide C***
[158182-23-1]
$C_{26}H_{39}Br_2NO_4$ 589.406
From *Amathia convoluta*. Shows no cytotoxicity. Amorph. solid. $[\alpha]_D^{20}$ -5.1 (c, 0.4 in $CHCl_3$). Opt. rotn. refers to a 1.8:1 insep. mixt. with Convolutamide D.

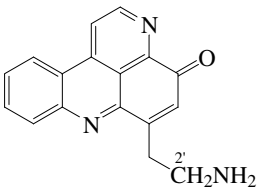
N-*(9Z-Octadecenoyl):* ***Convolutamide D***
[158182-24-2]
$C_{28}H_{41}Br_2NO_4$ 615.444
From *Amathia convoluta*. See statement under Convolutamide C above.

N-*Octadecanoyl:* ***Convolutamide E***
[158182-25-3]
$C_{28}H_{43}Br_2NO_4$ 617.46
From *Amathia convoluta*. Shows no cytotoxicity. Amorph. solid. $[\alpha]_D^{20}$ -25 (c, 0.1 in $CHCl_3$). Opt. rotn. refers to a 7.9:1 insep. mixt. with Convolutamide F.

N-*(8-Eicosenoyl):* ***Convolutamide F***
[158182-26-4]
$C_{30}H_{45}Br_2NO_4$ 643.498
From *Amathia convoluta*. See statement under Convolutamide E above. Geometry of side chain double bond not assigned.

Zhang, H. *et al., Tetrahedron*, 1994, **50**, 10201-10206 (*isol, uv, ir, pmr, cmr, ms, struct*)

N-Deacylcystodytin D-34



$C_{17}H_{13}N_3O$ 275.309

$N^{2'}$-*Ac:* ***Cystodytin J***
[158734-25-9]
$C_{19}H_{15}N_3O_2$ 317.346
Isol. from a *Cystodytes* sp. Cytotoxic agent. Inhibitor of topoisomerase II. DNA intercalator. Yellow solid. λ_{max} 218 (ϵ 12414); 277 (ϵ 6033); 300 (ϵ 7491); 318 (ϵ 8123); 359 (ϵ 1708); 382 (ϵ 1716); 538 (ϵ 1423) (MeOH) (Berdy).

$N^{2'}$-*(3-Methyl-2-butenoyl):* ***Cystodytin A***
[113321-71-4]
$C_{22}H_{19}N_3O_2$ 357.411
Isol. from *Cystodytes dellechiajei.* Topoisomerase II inhibitor. Calcium release agent. Yellow cryst. Sol. MeOH, toluene, $CHCl_3$; poorly sol. H_2O.
Mp 181-183°. Inseparable mixt. with Cystodytin B. λ_{max} 214 (ϵ 37000); 274 (ϵ 30000); 384 (ϵ 11000) (MeOH) (Derep). λ_{max} 226 (ϵ 35000); 272 (ϵ 26000); 380 (ϵ 11500) (MeOH) (Derep).

$N^{2'}$-*(3-Hydroxy-3-methylbutanoyl):* ***Cystodytin C***
[113351-76-1]
$C_{22}H_{21}N_3O_3$ 375.426
Isol. from *Cystodytes dellechiajei.* Calcium release agent. Light yellow cryst. Sol. MeOH, $CHCl_3$, toluene; poorly sol. H_2O.
Mp 257-259°. λ_{max} 214 (ϵ 37000); 274 (ϵ 30000); 384 (ϵ 11000) (MeOH) (Derep). λ_{max} 226 (ϵ 35000); 272 (ϵ 26000); 380 (ϵ 11500) (MeOH) (Derep). λ_{max} 228 (ϵ 29900); 272 (ϵ 29100); 380 (ϵ 11800) (MeOH) (Berdy).

$N^{2'}$-*Tigloyl:* ***Cystodytin B***
[113351-75-0]
$C_{22}H_{19}N_3O_2$ 357.411
Isol. from *Cystodytes dellechiajei.* Shows calcium release activity. Sol. MeOH, $CHCl_3$, toluene; poorly sol. H_2O. Obt. only in admixture with Cystodytin A. λ_{max} 214 (ϵ 37000); 274 (ϵ 30000); 384 (ϵ 11000) (MeOH) (Derep). λ_{max} 226 (ϵ 35000); 272 (ϵ 26000); 380 (ϵ 11500) (MeOH) (Derep).

1′-Hydroxy, $N^{2'}$-*(3-methyl-2-butenoyl):* ***Cystodytin D***
[141544-60-7]
$C_{22}H_{19}N_3O_3$ 373.41
Isol. from *Cystodytes dellechiajei*. Sol. MeOH; poorly sol. hexane, H_2O. λ_{max} 214 (ϵ 37000); 274 (ϵ 30000); 384 (ϵ 11000) (MeOH) (Derep). λ_{max} 226 (ϵ 35000); 272 (ϵ 26000); 380 (ϵ 11500) (MeOH) (Derep).

1′-Hydroxy, $N^{2'}$-*tigloyl:* ***Cystodytin E***
[141544-61-8]
$C_{22}H_{19}N_3O_3$ 373.41
Alkaloid from *Cystodytes dellechiajei*. λ_{max} 214 (ϵ 37000); 274 (ϵ 30000); 384 (ϵ 11000) (MeOH) (Derep). λ_{max} 226 (ϵ 35000); 272 (ϵ 26000); 380 (ϵ 11500) (MeOH) (Derep).

1′-(9-Octadecenoyloxy), $N^{2'}$-*(3-methyl-2-butenoyl):* ***Cystodytin H***
[141544-64-1]
$C_{40}H_{51}N_3O_4$ 637.861
Alkaloid from *Cystodytes dellechiajei*. Sol. MeOH; poorly sol. hexane, H_2O. λ_{max} 225 (ϵ 37000); 273 (ϵ 25000); 382 (ϵ 10000) (MeOH) (Derep).

1′-(9-Octadecenoyloxy), $N^{2'}$-*tigloyl:* ***Cystodytin I***
[141657-37-6]
$C_{40}H_{51}N_3O_4$ 637.861
Alkaloid from *Cystodytes dellechiajei.* λ_{max} 225 (ϵ 37000); 273 (ϵ 25000); 382 (ϵ 10000) (MeOH) (Derep).

1′-Methoxy, $N^{2'}$-*Ac:* ***Cystodytin K***
[496909-76-3]
$C_{20}H_{17}N_3O_3$ 347.373
Isol. from *Lissoclinum notti*. Yellow solid. $[\alpha]_D^{20}$ -292 (c, 0.06 in MeOH). λ_{max} 207 (log ϵ 4.57); 272 (log ϵ 4.17); 382 (log ϵ 3.67) (MeOH/trifluoroacetate).

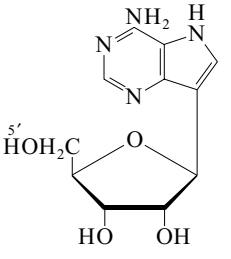
1′-Methoxy, $N^{2'}$-*(3-methyl-2-butenoyl):* ***Cystodytin F***
[141544-62-9]
$C_{23}H_{21}N_3O_3$ 387.437
Alkaloid from *Cystodytes dellechiajei.* Sol. MeOH; poorly sol. hexane, H_2O. λ_{max} 225 (ϵ 30000); 272 (ϵ 23000); 380 (ϵ 11000) (MeOH) (Derep).

1′-Methoxy, $N^{2'}$-*tigloyl:* ***Cystodytin G***
[141544-63-0]
$C_{23}H_{21}N_3O_3$ 387.437
Alkaloid from *Cystodytes dellechiajei.* λ_{max} 225 (ϵ 30000); 272 (ϵ 23000); 380 (ϵ 11000) (MeOH) (Derep).

Kobayashi, J. *et al., J.O.C.*, 1988, **53**, 1800-1804 (*Cystodytins A-C, isol, uv, ir, pmr, cmr, ms, struct*)
Kobayashi, J. *et al., J. Nat. Prod.*, 1991, **54**, 1634-1638 (*Cystodytins D-I*)
Ciufolini, M.A. *et al., J.A.C.S.*, 1991, **113**, 8016-8024 (*Cystodytins A,B, synth*)
Eldredge, G.S. *et al., J. Med. Chem.*, 1994, **37**, 3819-3827 (*Cystodytin J*)
Ciufolini, M.A. *et al., Tet. Lett.*, 1995, **36**, 4709-4712 (*Cystodytin A, synth*)
Appleton, D.R. *et al., Tetrahedron*, 2002, **58**, 9779-9783 (*Cystodytin K*)

9-Deazaadenosine D-35

1-C-*(4-Amino-5*H*-pyrrolo[3,2-*d*]pyrimidin-7-yl)-1,4-dihydro-*D*-ribitol, 9CI*
[77691-03-3]



$C_{11}H_{14}N_4O_4$ 266.256
Isol. from the cyanobacterium *Anabaena affinis.* Cytotoxic agent, molluscicide. Sol. H_2O, MeOH; poorly sol. EtOAc, hexane.

Hydrochloride: [77699-40-2]
Cryst. (EtOH). Mp 179-183°.

5′-O-α-D-Glucopyranoside: [146445-11-6]
$C_{17}H_{24}N_4O_9$ 428.398
Isol. from *Anabaena affinis.* Sol. H_2O, MeOH; poorly sol. EtOAc, hexane. $[\alpha]_D^{28}$ +21.9 (c, 0.05 in H_2O). λ_{max} 229; 268; 276 (H_2O) (Berdy). λ_{max} 235; 272 (HCl) (Berdy).

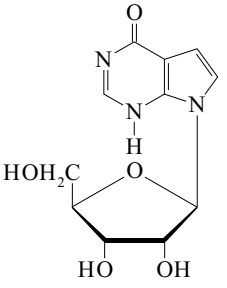
[77699-39-9]

Lim, M.-I. *et al., Tet. Lett.*, 1981, **22**, 25 (*synth, pmr*)
Chu, M.Y. *et al., Biochem. Pharmacol.*, 1984, **33**, 1229 (*props*)
Namikoshi, M. *et al., J.A.C.S.*, 1993, **115**, 2504 (*isol, struct*)

7-Deazainosine D-36

*1,7-Dihydro-7-β-D-ribofuranosyl-4*H*-pyrrolo[2,3-*d*]pyrimidin-4-one, 9CI. XK 101-2. Antibiotic XK 101-2. B 15645. Antibiotic B 15645*

[2862-16-0]



$C_{11}H_{13}N_3O_5$ 267.241

Nucleoside antibiotic. Identity with B 15645 not certain. Prod. by *Micromonospora chalcea tubercidica* and *Streptomyces griseolus*. Also isol. from the ascidian *Aplidium pantherinum*. Cytotoxic. Needles (H_2O).

Mp 241-244°. $[\alpha]_D^{18}$ -6.72 (c, 0.5 in H_2O). $[\alpha]_D^{21}$ -47.5 (c, 0.5 in H_2O).

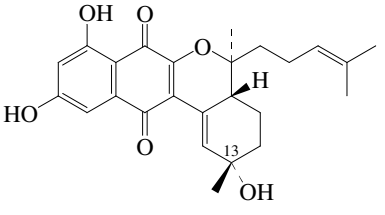
▶ UY9450000

Mizuno, Y. *et al., J.O.C.*, 1963, **28**, 3331 (*synth*)
Japan. Pat., 1970, 20 559; *CA*, **73**, 108248h (*B 15645*)
Chenon, M.T. *et al., J.A.C.S.*, 1975, **97**, 4627 (*cmr*)
Japan. Pat., 1978, 78 124 685; *CA*, **90**, 136241v (*isol*)
Seela, F. *et al., Chem. Ber.*, 1980, **113**, 3389 (*synth, uv, pmr*)
Kim, J. *et al., J. Nat. Prod.*, 1993, **56**, 1813-1816 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DAE200

Debromohydroxymarinone D-37

Hydroxydebromomarinone

[272458-33-0]



$C_{25}H_{28}O_6$ 424.493

Misleading name. Related to Marinone, M-108. Prod. by a marine actinomycete (CNH-099). Moderate cytotoxic agent. $[\alpha]_D^{25}$ +280 (c, 0.2 in MeOH). λ_{max} 211 (ϵ 18900); 228 (ϵ 16000); 275 (ϵ 17000); 283 (ϵ 18100); 328 (ϵ 7000); 392 (ϵ 2800); 460 (ϵ 2600) (MeOH/HCl). λ_{max} 238 (ϵ 20300); 249 (ϵ 20700); 299 (ϵ 13400); 358 (ϵ 8100); 525 (ϵ 4700) (MeOH/KOH).

13-Me ether: ***Debromomethoxymarinone****. Methoxydebromomarinone*

[272458-34-1]

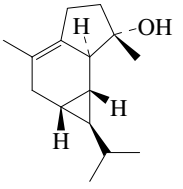
$C_{26}H_{30}O_6$ 438.519

Prod. by a marine actinomycete (CNH-099). Moderate cytotoxic agent. $[\alpha]_D^{25}$ +140 (c, 0.1 in MeOH). λ_{max} 208 (ϵ 17800); 228 (sh) (ϵ 13200); 275 (ϵ 12000); 283 (ϵ 12400); 308 (ϵ 5900); 325 (sh) (ϵ 5300); 385 (ϵ 2700); 455 (ϵ 2100) (MeOH/HCl). λ_{max} 250 (ϵ 15900); 298 (ϵ 10000); 354 (ϵ 6000); 525 (ϵ 3000) (MeOH/KOH).

Hardt, I.H. *et al., Tet. Lett.*, 2000, **41**, 2073-2076 (*isol, pmr, cmr*)

Debromoisocalenzanol D-38

[661476-06-8]



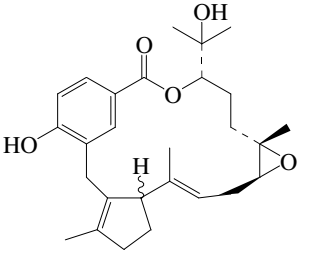
$C_{15}H_{24}O$ 220.354

Constit. of *Laurencia microcladia*. Oil. $[\alpha]_D^{20}$ -15.8 (c, 0.04 in MeOH).

Guella, G. *et al., Chem. Eur. J.*, 2003, **9**, 5770-5777 (*isol, pmr, cmr*)

Debromophycolide A D-39

[869860-00-4]



$C_{27}H_{36}O_5$ 440.578

Constit. of *Callophycus serratus*. Amorph. solid. $[\alpha]_D^{23}$ -7 (c, 0.012 in $CHCl_3$). λ_{max} 265 (log ϵ 3.46) (MeOH).

Kubanek, J. *et al., Org. Lett.*, 2005, **7**, 5261-5264 (*Debromophycolide A*)

4,7-Decadien-1-ol D-41

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH_2CH_2OH$

$C_{10}H_{18}O$ 154.252

(4Z,7E)-form

O-*Sulfate:* [160116-62-1]
$C_{10}H_{18}O_4S$ 234.316
Isol. from the ascidian *Halocynthia roretzi*. Antibacterial and antifungal agent.

(4Z,7Z)-form [104188-11-6]
Constit. of the oil of *Acorus calamus* (sweet flag).

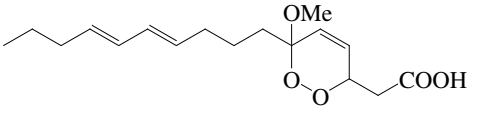
O-*Sulfate:* [160116-61-0]
Isol. from *Halocynthia roretzi*. Antibacterial and antifungal agent.

Van Lier, F.P. *et al., Perfum. Essent. Oil Res.*, 1985, 215; *CA*, **106**, 72677f (*isol, synth*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 1994, **57**, 1606-1609 (*sulfates*)

6-(4,6-Decadienyl)-3,6-dihydro-6-methoxy-1,2-dioxin-3-acetic acid, 9CI D-42

6-Methoxy-3,6-peroxy-4,10,12-hexadecatrienoic acid

[154702-55-3]



$C_{17}H_{26}O_5$ 310.389

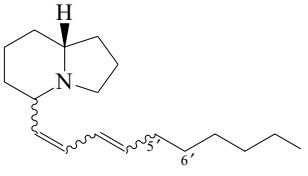
Isol. from the sponge *Plakortis simplex*.

$[\alpha]_D$ +60 (c, 0.25 in $CHCl_3$).

Me ester: [154702-56-4]
$C_{18}H_{28}O_5$ 324.416
Isol. from *Plakortis simplex*.

$[\alpha]_D^{23}$ +52 (c, 0.25 in $CHCl_3$).
Rudi, A. *et al., J. Nat. Prod.*, 1993, **56**, 2178-2182 (*isol*)

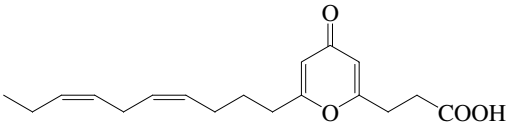
5-(1,3-Decadienyl)octahydroindolizine **D-43**
5-(1,3-Decadienyl)indolizidine. ***Piclavine B***
[142609-25-4]



$C_{18}H_{31}N$ 261.45
Alkaloid from the tunicate *Clavelina picta*. Exhibits antimicrobial props. Oil. $[\alpha]_D$ +33.5 (c, 1 in CH_2Cl_2). Obt. as a mixt. of stereoisomers. λ_{max} 232 (ϵ 12500) (EtOH) (Derep). λ_{max} 232 (ϵ 12500) (MeOH) (Berdy).

5′,6′-Didehydro: 5-(1,3,5-Decatrienyl)octahydroindolizine. 5-(1,3,5-Decatrienyl)indolizidine. ***Piclavine C***
[142609-26-5]
$C_{18}H_{29}N$ 259.434
Isol. from *Clavelina picta*. Exhibits antimicrobial props. Pale yellow oil. $[\alpha]_D$ +36 (c, 5 in CH_2Cl_2). Obt. as a mixt. of stereoisomers. λ_{max} 262 (ϵ 11800); 267 (ϵ 15000); 281 (ϵ 11800) (EtOH) (Derep). λ_{max} 262 (ϵ 11800); 267 (ϵ 15000); 281 (ϵ 11800) (MeOH) (Berdy).
Raub, M.F. *et al., Tet. Lett.*, 1992, **33**, 2257-2260 (*isol, struct*)

6-(4,7-Decadienyl)-4-oxo-4*H*-pyran-2-propanoic acid **D-44**
4,8-Epoxy-6-oxo-4,7,12,15-octadecatetraenoic acid

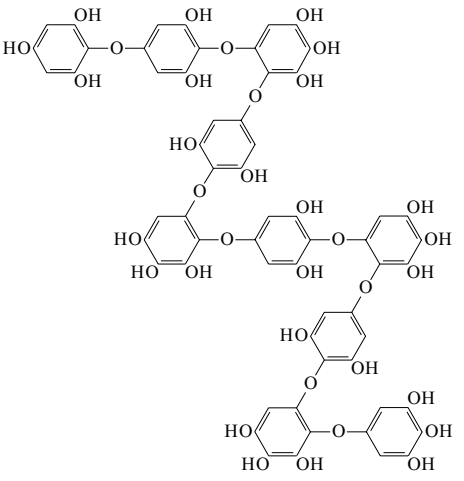


$C_{18}H_{24}O_4$ 304.385

(all-Z)-form

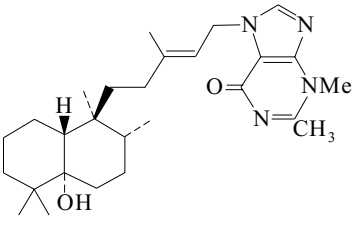
Me ester: ***Peyssopyrone***
$C_{19}H_{26}O_4$ 318.412
Constit. of the red alga *Peyssonnelia caulifera*. Oil. λ_{max} 212 (log ϵ 3.18); 246 (log ϵ 3.19) (MeOH).
McPhail, K.L. *et al., J. Nat. Prod.*, 2004, **67**, 1010-1013 (*isol, pmr, cmr*)

Decafuhalol A **D-45**
[164176-31-2]



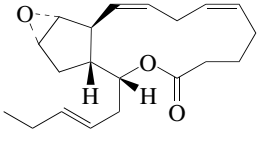
$C_{60}H_{42}O_{35}$ 1322.971
Constit. of the brown algae *Sargassum spinuligerum* and *Carpophyllum angustifolium*. Unstable. Obt. as per-Ac.
Glombitza, K.-W. *et al., Phytochemistry*, 1995, **38**, 987-995 (*isol, pmr, cmr, ms*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

7-[5-(Decahydro-4*a*-hydroxy-1,2,5,5-tetramethyl-1-naphthalenyl)-3-methyl-2-pentenyl]-3,7-dihydro-2,3-dimethyl-6*H*-purin-6-one, 9CI **D-46**
[90162-26-8]



$C_{27}H_{42}N_4O_2$ 454.654
Isol. from the marine sponge *Agelas mauritiana*. Cryst. (C_6H_6) (as Ac). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 95-98° (Ac). Seemingly an artifact; the struct. of the true sponge metab. is unknown. λ_{max} 221 (ϵ 9400); 267 (ϵ 3300); 344 (ϵ 200) (MeOH) (Berdy).
Nakatsu, T. *et al., Tet. Lett.*, 1984, **25**, 935 (*isol, uv, pmr, ms, cryst struct*)

1*a*,2,2*a*,3,6,7,8,11,13*a*,13*b*-Decahydro-3-(2-pentenyl)-5*H*-oxireno[3,4-*b*]cyclopent[1,2-*c*]oxacyclotridecin-5-one **D-47**



$C_{20}H_{28}O_3$ 316.439
Tentative struct. assigned. Isol. from *Laurencia hybrida* with co-metab. Hybridalactone, H-425.
Higgs, M.D. *et al., Tetrahedron*, 1981, **37**, 4259-4262 (*isol*)

Decanal, 9CI D-48

Decyl aldehyde. Capraldehyde. Caprinaldehyde. FEMA 2362
[112-31-2]
$H_3C(CH_2)_8CHO$
$C_{10}H_{20}O$ 156.267
Constit. of Cassia, Neroli and other oils esp. citrus peel oils. Also present in coriander leaf or seed, caviar, roast turkey, roast filbert, green tea, fish oil, hop oil and beer. Used in perfumery and flavour industries. Liq. with strong orange-peel odour. d_4^{20} 0.85.
Mp -5° approx. Bp 208-209° Bp_7 81°. n_D^{20} 1.4887.
▶ Skin irritant. LD_{50} (rat, orl) 3730 mg/kg. HD6000000

Di-Me acetal: 1,1-Dimethoxydecane. FEMA 2363
[7779-41-1]
$C_{12}H_{26}O_2$ 202.336
Flavouring ingredient. Liq. $d^{15.5}$ 0.83. Bp 218°. n_D^{24} 1.4244.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 469A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 732B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 555C (*ir*)
Pickard, K.J. *et al., J.C.S.*, 1913, **103**, 1947
Mathis, C. *et al., Phytochemistry*, 1964, **3**, 377 (*isol*)
Attaway, J.A. *et al., Phytochemistry*, 1966, **5**, 141 (*isol*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 477 (*rev, tox*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir, pmr*)
Stanley, J.B. *et al., J. Food Sci.*, 1975, **40**, 1134 (*ms*)
Org. Synth., 1976, **55**, 84 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DAG000; DAG200
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 145 (*di-Me acetal*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 772-774 (*props, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DAG000; DAG200

2,4,7-Decatrienal, 9CI D-49

[51325-37-2]
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH{=}CHCHO$
$C_{10}H_{14}O$ 150.22

(2E,4Z,7Z)-form [43108-49-2]
Isol. from the diatom *Thalassiosira rotula*. Also results from n-3 polyene acyl chains. $Bp_{0.4}$ 65-67°.

[38664-37-8, 66642-86-2]

Meijboom, P.W. *et al., J. Am. Oil Chem. Soc.*, 1972, **49**, 555 (*occur, synth*)
Harkes, P.D. *et al., J. Am. Oil Chem. Soc.*, 1974, **51**, 356 (*occur*)
Seifert, R.M. *et al., J. Agric. Food Chem.*, 1980, **28**, 68 (*synth*)
d'Ippolito, G. *et al., Phytochemistry*, 2006, **67**, 314-322 (*isol, biosynth*)

2,4,7-Decatrienoic acid D-50

[78417-28-4]
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH{=}CHCOOH$
$C_{10}H_{14}O_2$ 166.219

(2E,4E,7Z)-form

Me ester: [150922-04-6]
$C_{11}H_{16}O_2$ 180.246
Constit. of the marine green alga *Cladophora columbiana*.

Et ester: [28290-88-2]
[78417-28-4]
$C_{12}H_{18}O_2$ 194.273
Constit. of various fruits incl. *Durio zibethinus* and pears. Aroma compound used in food flavouring.

(2E,4Z,7Z)-form [244274-82-6]
Prod. by *Streptomyces viridochromogenes*. Herbicide.

Et ester: [142676-19-5]
[78417-28-4]
Constit. of various fruits incl. *Durio zibethinus* and pears. Aroma compound present in durian and pears. Used for imparting a note of pear, greenery and violet leaves in perfumes.

Creveling, R.K. *et al., J. Agric. Food Chem.*, 1970, **18**, 19-24 (*isol, ester*)
Eur. Pat., 1992, 482 385; *CA*, **117**, 76268y (*2E,4Z,7Z-form-Et ester, use*)
Gerwick, W.H. *et al., Hydrobiologia*, 1993, **260-261**, 653-665 (*Cladophora columbiana constit*)
Naef, R. *et al., Flavour Fragrance J.*, 1996, **11**, 295-303 (*isol, ester*)
Maier, A. *et al., Pestic. Sci.*, 1999, **55**, 733-739 (*isol*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 532 (*Et ester*)

3,6,9-Decatrien-1-ol D-51

$H_2C{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH_2OH$
$C_{10}H_{16}O$ 152.236

(3Z,6Z)-form

O-*Sulfate:* [160116-63-2]
$C_{10}H_{16}O_4S$ 232.3
Isol. from the ascidian *Halocynthia roretzi*. Antibacterial and antifungal agent.

Tsukamoto, S. *et al., J. Nat. Prod.*, 1994, **57**, 1606-1609 (*sulfate*)

3-Decenoic acid D-52

[15469-77-9]
$H_3C(CH_2)_5CH{=}CHCH_2COOH$
$C_{10}H_{18}O_2$ 170.251
Occurs in squid oil. Comly. available flavour ingredient. (*E/Z*) composition of natural isolates not detd.

(E)-form [53678-20-9]
Liq. Bp_1 110-112°.

Et ester: [82561-67-9]
$C_{12}H_{22}O_2$ 198.305
Liq. $Bp_{0.5}$ 80-82°. n_D^{20} 1.4372.

(Z)-form [2430-93-5]
Sex pheromone of the furniture carpet beetle *Athrenus flavipes*. Liq. or solid with fatty odour.
Mp 18°. Bp_{11} 154-163°.

Tulus, R. *et al., CA*, 1940, **40**, 3722 (*synth*)
Gorge, M. *et al., Ann. Chim. (Paris)*, 1951, **6**, 648 (*synth*)
Fukui, H. *et al., Tet. Lett.*, 1974, 3563 (*isol*)
Brown, H.C. *et al., J.O.C.*, 1986, **51**, 3398-3400 (*E-form, Et ester, synth, ir, pmr, cmr*)
Shirakawa, T. *et al., Dev. Food Sci.*, 1988, **18**, 915 (*occur, bibl*)
Sharma, M.L. *et al., Coll. Czech. Chem. Comm.*, 1991, **56**, 1744 (*synth, ir, pmr*)
Ragoussis, N. *et al., J.C.S. Perkin 1*, 1998, 3529-3533 (*E-form, synth, Et ester, ir, pmr, cmr, ms*)

9-Decenoic acid D-53

Caproleic acid. FEMA 3660
[14436-32-9]
$H_2C{=}CH(CH_2)_7COOH$
$C_{10}H_{18}O_2$ 170.251
Minor constit. of milk fats. Also detected in clams, snails and human adipose tissue. Commercially available flavouring agent. Liq. with fatty odour. Bp_{21} 158-163°.

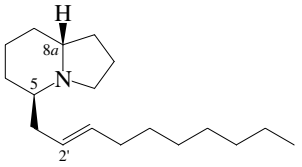
Me ester:
$C_{11}H_{20}O_2$ 184.278
Oil. Bp_{20} 120°.

4-Bromophenacyl ester:
Cryst. (EtOH aq.). Mp 58°.

Black, H.K. *et al., J.C.S.*, 1953, 1785 (*synth*)
Renner, E. *et al., Milchwissenschaft*, 1978, **33**, 489 (*isol*)
Hase, T.A. *et al., Synth. Commun.*, 1979, **9**, 63 (*synth*)
Shirakawa, T. *et al., Dev. Food Sci.*, 1988, **18**, 915 (*occur, props*)
Bartra, M. *et al., J.O.C.*, 1991, **56**, 5132 (*synth, pmr, cmr, ir*)

5-(2-Decenyl)octahydroindolizine D-54

5-(2-Decenyl)indolizidine. ***Piclavine A***



(2'*E*,5*R*,8*aR*)-*form*

$C_{18}H_{33}N$ 263.465
Shows antimicrobial props. Oil. $[\alpha]_D$ +15 (c, 1 in CH_2Cl_2). Data given is for the mixt. of isomers.

(2′*E*,5*R*,8*aR*)-*form*
Piclavine A₁
[142609-24-3]
Isol. from the tunicate *Clavelina picta*.
$[\alpha]_D^{26}$ -5.6 (c, 0.84 in CH_2Cl_2).

(2′*E*,5*R*,8*aS*)-*form*
Piclavine A₃
[142696-98-8]
From *Clavelina picta*.
$[\alpha]_D^{26}$ -73.6 (c, 1.3 in CH_2Cl_2).

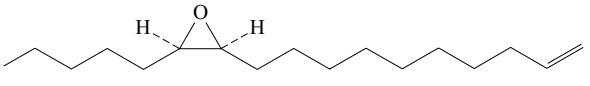
(2′*Z*,5*R*,8*aR*)-*form*
Piclavine A₂
[142696-99-9]
From *Clavelina picta*.
$[\alpha]_D^{27}$ +4 (c, 0.21 in CH_2Cl_2).

(2′*Z*,5*R*,8*aS*)-*form*
Piclavine A₄
[142697-00-5]
From *Clavelina picta*.
$[\alpha]_D^{27}$ -76.4 (c, 0.63 in CH_2Cl_2).

Raub, M.F. *et al., Tet. Lett.*, 1992, **33**, 2257-2260 (*isol, struct*)
Jefford, C.W. *et al., Helv. Chim. Acta*, 1995, **78**, 1511-1524 (*synth*)
Takahata, H. *et al., Bioorg. Med. Chem. Lett.*, 2000, **10**, 1799-1801 (*synth*)
McAlonan, H. *et al., Tet. Lett.*, 2000, **41**, 5411-5414 (*synth*)

2-(9-Decenyl)-3-pentyloxirane, 9CI D-55

11,12-Epoxy-1-heptadecene



$C_{17}H_{32}O$ 252.439

(2*S*,3*R*)-*form* [129436-95-9]
Isol. from the brown alga *Notheia anomala*.
Unstable oil. $[\alpha]_D$ +2 (c, 0.25 in $CHCl_3$).
Barrow, R.A. *et al., Aust. J. Chem.*, 1990, **43**, 895 (*isol, pmr, cmr*)

Mytilus Defensin D-56

Peptides. Isol. from the blood of *Mytilus edulis* (blue mussel). Shows antimicrobial activity.

Mytilus defensin A
Contains 37 amino acid residues.

Mytilus defensin B
Charlet, M. *et al., J. Biol. Chem.*, 1996, **271**, 21808-21813

Mytilus galloprovincialis Defensins D-57

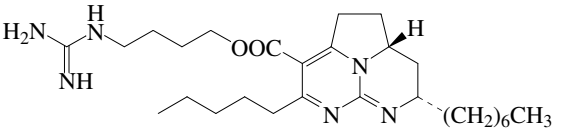
Isol. from the edible Mediterranean mussel *Mytilus galloprovincialis*. Defensins.

MGD 1
Peptide consisting 39 amino acid residues including 8 cysteines.

MGD 2
An isoform of MGD 1 differing in 5 positions.

Hubert, F. *et al., Eur. J. Biochem.*, 1996, **240**, 302-306 (*MGD 1, isol, struct*)
Mitta, G. *et al., J. Cell Biol.*, 1999, **112**, 4233-4242 (*MGD 2, isol*)
Yang, Y.S. *et al., Biochemistry*, 2000, **39**, 14436-14447 (*MGD 2, synth, pmr, struct*)

Dehydrobatzelladine C D-58

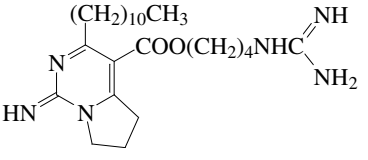


$C_{27}H_{46}N_6O_2$ 486.699
Alkaloid from the sponge *Monanchora arbuscula*. Pale brown gum. λ_{max} 206 (ϵ 8500); 258 (ϵ 7500); 303 (ϵ 1600) (MeOH).

Braekman, J.C. *et al., J. Nat. Prod.*, 2000, **63**, 193-196
Collins, S.K. *et al., Org. Lett.*, 2004, **6**, 1253-1255 (*synth*)

Dehydrocrambine A D-59

Dehydrocrambescin A

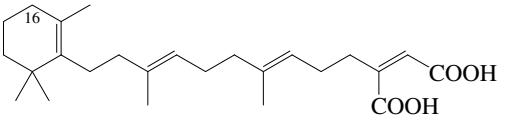


$C_{24}H_{42}N_6O_2$ 446.635
Alkaloid from the sponge *Monanchora* sp. Brown gum. $[\alpha]_D^{20}$ -12.1 (c, 0.09 in MeOH). λ_{max} 206 (log ϵ 3.83); 259 (log ϵ 3.53); 289 (log ϵ 3.18) (MeOH).

Chang, L.C. *et al., J. Nat. Prod.*, 2003, **66**, 1490-1494 (*isol, pmr, cmr*)

Dehydroluffariellolide diacid D-60

[132911-46-7]

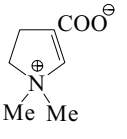


$C_{25}H_{38}O_4$ 402.573
Isol. from *Fascaplysinopsis reticulata*. Oil.

16-Oxo: ***16-Oxodehydroluffarielolide diacid***
$C_{25}H_{36}O_5$ 416.556
Isol. from *Fascaplysinopsis reticulata*.

Jiménez, C. *et al., J.O.C.*, 1991, **56**, 3403 (*isol, uv, ir, pmr, cmr, ms, struct*)

2,3-Dehydro-β-stachydrine D-61

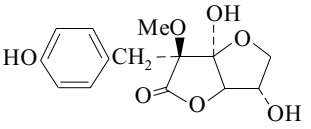


$C_7H_{11}NO_2$ 141.169
Isol. from the red alga *Pterocladia capillacea*. Off-white amorph. powder.

Sciuto, S. *et al., J. Nat. Prod.*, 1988, **51**, 322

Delesserine D-62

[82198-78-5]



Relative configuration

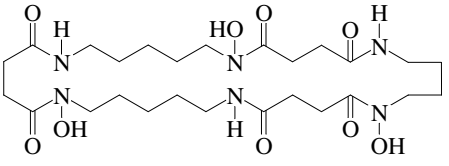
$C_{14}H_{16}O_7$ 296.276

Isol. from the marine alga *Delesseria sanguinea*. Anticoagulant. Cryst. (MeOH). Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 117°. $[\alpha]_D^{20}$ +36 (c, 0.72 in MeOH). Exists partially in an open form in soln. λ_{max} 225 (ϵ 13000); 277 (ϵ 4300) (EtOH) (Berdy). λ_{max} 220 (ϵ 35000); 293 (ϵ 3000) (MeOH/NaOH) (Berdy).

Yvin, J.-C. *et al., J.A.C.S.*, 1982, **104**, 4497 (*isol, ms, uv, pmr, cmr, ir, cryst struct*)

Demethylenenocardamine D-63

1,12,22-Trihydroxy-1,6,12,17,22,27-hexaazacyclodotriacontane-2,5,13,16,23,26-hexone

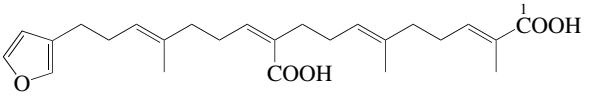


$C_{26}H_{46}N_6O_9$ 586.684

Lower homologue of Nocardamine, N-133. Prod. by a marine-derived *Streptomyces* sp. strain M1087. Amorph. solid. Mp 179-181°.

Lee, H.-S. *et al., J. Nat. Prod.*, 2005, **68**, 623-625 (*isol, pmr, cmr*)

Demethylfurospongin 3 D-64



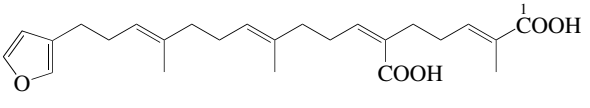
$C_{25}H_{34}O_5$ 414.541

The parent sesterterpenoid does not yet appear to have been characterised (cf. Demethylfurospongin 4, D-65).

1-Me ester: ***Furospongin 3***
[41060-10-0]
$C_{26}H_{36}O_5$ 428.567
Constit. of *Spongia officinalis*. Oil.

Cimino, G. *et al., Tetrahedron*, 1972, **28**, 5983

Demethylfurospongin 4 D-65



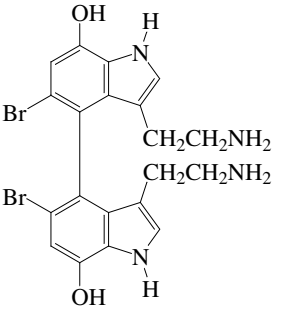
$C_{25}H_{34}O_5$ 414.541
Constit. of *Spongia officinalis*. Oil. λ_{max} 207 (ϵ 13174) (MeOH).

1-Me ester: ***Furospongin 4***
[41060-11-1]
$C_{26}H_{36}O_5$ 428.567
Constit. of *Spongia officinalis*. Oil.

Cimino, G. *et al., Tetrahedron*, 1972, **28**, 5983 (*Furospongin 4*)
Garrido, L. *et al., J. Nat. Prod.*, 1997, **60**, 794-797 (*Demethylfurospongin 4*)

Dendridine A D-66

*3,3′-Bis(2-aminoethyl)-5,5′-dibromo-4,4′-bi-1*H*-indole-7,7′-diol*



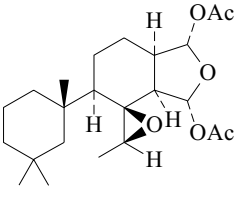
$C_{20}H_{20}Br_2N_4O_2$ 508.212

Isol. from the marine sponge *Dictyodendrilla* sp. Antibacterial and antifungal agent. Yellowish solid. λ_{max} 282 (ϵ 5700); 292 (ϵ 5800); 303 (ϵ 4000) (no solvent reported).

Tsuda, M. *et al., J. Nat. Prod.*, 2005, **68**, 1277-1278 (*isol*)

Dendrillin D-67

[170475-13-5]



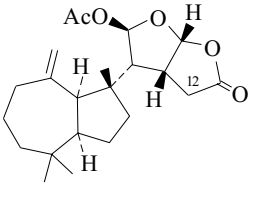
$C_{23}H_{36}O_6$ 408.534

Constit. of *Dendrilla membranosa*. Oil.

Baker, B.J. *et al., J. Nat. Prod.*, 1995, **58**, 1459 (*isol, pmr, cmr*)

Dendrillolide A D-68

[91158-68-8]



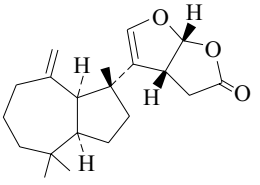
$C_{22}H_{32}O_5$ 376.492

Constit. of a *Dendrilla* sp. and *Chelonaplysilla violacea*. Oil. $[\alpha]_D^{20}$ +83.51 (c, 3.8 in $CHCl_3$). Formerly this struct. was assigned to Dendrillolide B. The struct. of Dendrillolide B has not been reassigned.

Sullivan, B. *et al., J.O.C.*, 1984, **49**, 3204-3206 (*isol, pmr*)
Molinski, T.F. *et al., J.O.C.*, 1986, **51**, 4564-4567 (*struct*)
Bobzin, S.C. *et al., J.O.C.*, 1989, **54**, 5727-5731 (*struct*)

Dendrillolide C D-69

[91158-70-2]

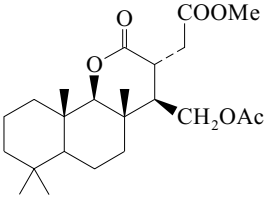


$C_{20}H_{28}O_3$ 316.439
Constit. of *Dendrilla* sp. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
$[\alpha]_D$ +130.9 (c, 0.3 in $CHCl_3$) .

Sullivan, B. *et al., J.O.C.*, 1984, **49**, 3204

Dendrillolide D D-70

[123332-86-5]

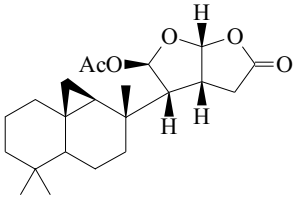


$C_{23}H_{36}O_6$ 408.534
Metab. of *Dendrilla* spp. and *Chelonaplysilla* spp. Cryst. (Et_2O/hexane).
Mp 120°. $[\alpha]_D$ +35.8 (c, 0.35 in $CHCl_3$).

Bobzin, S.C. *et al., J.O.C.*, 1989, **54**, 5727 (*isol, pmr, cmr*)

Dendrillolide E D-71

[123332-87-6]

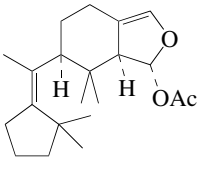


$C_{22}H_{32}O_5$ 376.492
Metab. of *Dendrilla* spp. Oil. $[\alpha]_D$ +21.4 (c, 0.25 in $CHCl_3$).

Bobzin, S.C. *et al., J.O.C.*, 1989, **54**, 5727 (*isol, pmr, cmr*)

Dendrinolide D-72

[188064-74-6]

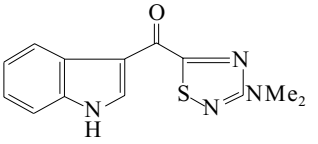


$C_{21}H_{32}O_3$ 332.482
Related to Glaciolide, G-85. Constit. of *Dendrilla membranosa*. Yellow oil. $[\alpha]_D^{25}$ +89 (c, 0.7 in $CHCl_3$).

Fontana, A. *et al., J. Nat. Prod.*, 1997, **60**, 475-477 (*isol, pmr, cmr*)

Dendrodoine D-73

[75351-10-9]

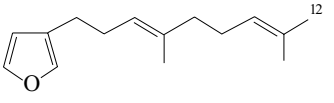


$C_{13}H_{12}N_4OS$ 272.33
Isol. from the marine tunicate *Dendrodoa grossularia*. Cytotoxic. Cryst. (EtOAc). Sol. Et_2O; poorly sol. H_2O.
Mp 280-285° Mp 192-197° (as Ac). λ_{max} 250 (ϵ 15000); 270 (ϵ 12000); 300 (ϵ 8000) (MeOH) (Derep).

Heitz, S. *et al., Tet. Lett.*, 1980, **21**, 1457-1458 (*ir, pmr, ms, cryst struct*)
Hogan, I.T. *et al., Tetrahedron*, 1984, **40**, 681 (*synth, ir, pmr, cmr, ms*)

Dendrolasin D-74

3-(4,8-Dimethyl-3,7-nonadienyl)furan, 9CI
[23262-34-2]



$C_{15}H_{22}O$ 218.338
Constit. of the ant *Lasius (Dendrolasius) fuliginosus* and the wood of *Torreya nucifera*. Also in sweet potato. Found in molluscs *Hypselodoris californiensis*, *Hypselodoris ghiselini*, *Hypselodoris cantabrica*, *Hypselodoris tricolor* and *Hypselodoris villafranca*. Feeding deterrent. Oil. Bp_{16} 148-150°. n_D^{20} 1.4860.

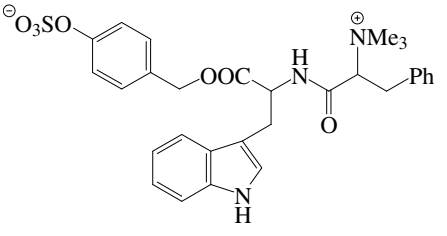
12-Hydroxy: See Neotorreyol in *The Combined Chemical Dictionary.*

9-Oxo: See 9-(3-Furanyl)-2,6-dimethyl-2,6-nonadien-4-one in *The Combined Chemical Dictionary.*

Bernadi, R. *et al., Tet. Lett.*, 1967, 3893 (*isol*)
Waldner, E.E. *et al., Helv. Chim. Acta*, 1969, **52**, 15 (*biosynth*)
Vanderah, D.J. *et al., Lloydia*, 1975, **38**, 271 (*struct*)
Kobayashi, M. *et al., J.O.C.*, 1980, **45**, 5225 (*synth*)
Lee, E. *et al., Tet. Lett.*, 1981, **22**, 2671 (*synth*)
Araki, S. *et al., Chem. Lett.*, 1982, 177 (*synth, bibl*)
Hochlowski, J.E. *et al., J.O.C.*, 1982, **47**, 88
Janis, S.P. *et al., Tet. Lett.*, 1982, **23**, 3115 (*synth*)
Belardini, M. *et al., J. Nat. Prod.*, 1983, **46**, 481 (*synth, bibl*)
Mandai, T. *et al., J.O.C.*, 1983, **48**, 5183 (*synth*)
Kraus, G.A. *et al., J.O.C.*, 1983, **48**, 5356 (*synth*)
Fontana, A. *et al., J. Chem. Ecol.*, 1993, **19**, 339-356 (*isol*)
Chakraborty, A. *et al., Tetrahedron*, 1997, **53**, 8513-8518 (*synth*)

Denticin A D-75

[157078-50-7]

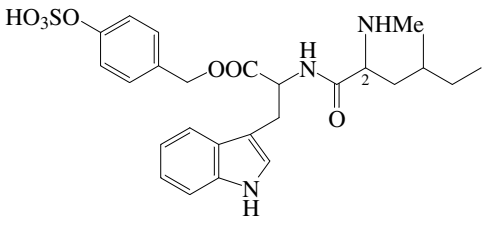


$C_{30}H_{33}N_3O_7S$ 579.673
Isol. from seaweed *Martensia denticulata*. Lipid peroxidation inhibitor. λ_{max} 219 (ϵ 30200); 273 (ϵ 36100); 290 (ϵ 28200) (MeOH).

Murakami, H. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 535-538

Denticin B D-76

[157078-51-8]



$C_{26}H_{33}N_3O_7S$ 531.629

Isol. from the seaweed *Martensia denticulata*. Lipid peroxidation inhibitor. λ_{max} 222 (ϵ 22800); 281 (ϵ 30500); 290 (ϵ 26700) (MeOH).

N^2-*Me:* ***Denticin C***

[157078-52-9]

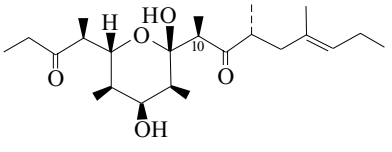
$C_{27}H_{35}N_3O_7S$ 545.655

Isol. from *Martensia denticulata*. Lipid peroxidation inhibitor. λ_{max} 220 (ϵ 23400); 282 (ϵ 31400); 290 (ϵ 27400) (MeOH).

Murakami, H. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 535-538

Denticulatin A D-77

[87697-98-1]



$C_{23}H_{40}O_5$ 396.566

Metab. of *Siphonaria denticulata*. Ichthyotoxin. Oil. $[\alpha]_D$ -30.7 (c, 1.49 in $CHCl_3$).

10-Epimer: ***Denticulatin B***

[87758-52-9]

$C_{23}H_{40}O_5$ 396.566

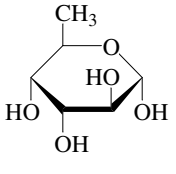
Metab. of *Siphonaria denticulata*. Cryst.

Mp 137-141°. $[\alpha]_D$ -26.4 (c, 0.39 in $CHCl_3$).

Hochlowski, J.E. *et al., J.A.C.S.*, 1983, **105**, 7413-7415 (*isol, cryst struct*)
Manker, D.C. *et al., Chem. Comm.*, 1988, 1061 (*biosynth*)
Ziegler, F.E. *et al., J.O.C.*, 1990, **55**, 2800 (*synth*)
Andersen, M.W. *et al., Chem. Ber.*, 1991, **124**, 2127 (*synth*)
Paterson, I. *et al., Tet. Lett.*, 1992, **33**, 801 (*synth, bibl*)
Oppolzer, W. *et al., Tet. Lett.*, 1995, **36**, 4413 (*synth*)
Paterson, I. *et al., Tetrahedron*, 1996, **52**, 1811 (*synth*)
De Brabander, J. *et al., Tetrahedron*, 1997, **53**, 9169 (*synth*)

6-Deoxyaltrose D-78

Altromethylose



α-D-*form*

$C_6H_{12}O_5$ 164.158

An aq. soln. at 30° contains 33.3% α-Pyr, 38.5% β-Pyr, 15.4% α-Fur and 12.8% β-Fur. Only 6-deoxyhexose and fucose found in glycoproteins. Residue present in some strains of *Eubacterium saburreum* and lipopolysaccharide of *Yersinia enterocolitica*.

β-D-Pyranose-*form*

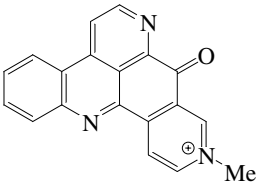
Found in polysialoglycoprotein of *Salvelinus leucomaenis* eggs.

Iwasaki, M. *et al., Eur. J. Biochem.*, 1987, **168**, 185-192 (*isol*)

Deoxyamphimedine D-79

*10-Methyl-8-oxo-8*H*-benzo[*b*]pyrido[4,3,2-de][1,8]phenanthrolinium. Deoxoamphimedine*

[340774-96-1]



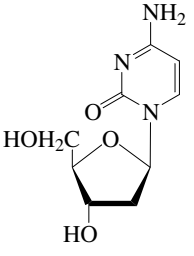
$C_{19}H_{12}N_3O^{\oplus}$ 298.323

Quaternary alkaloid from two *Xestospongia* spp. Cytotoxic. Yellow-brown amorph. solid. Counterion not specified. λ_{max} 206 (log ϵ 3.92); 244 (log ϵ 3.93); 294 (sh) (log ϵ 3.52); 388 (log ϵ 3.51); 478 (log ϵ 2.59) (MeOH).

Tasdemir, D. *et al., J.O.C.*, 2001, **66**, 3246-3248

2′-Deoxycytidine, 9CI, 8CI D-80

Cytosine deoxyriboside. Cytosine deoxyribonucleoside



β-D-*form*

$C_9H_{13}N_3O_4$ 227.219

β-D-*form*

*1-(2-Deoxy-β-D-*erythro*-pentofuranosyl)cytosine, 9CI*

[951-77-9]

Mp 207-210°. $[\alpha]_D$ +57.6 (H_2O).

► Exp. reprod. effects. HA3800000

*3*N*-Me: 2′-Deoxy-3-methylcytidine, 9CI*

[5040-21-1]

$C_{10}H_{15}N_3O_4$ 241.246

Isol. from *Geodia barettii*. Cryst. (MeOH) (as hydrochloride).

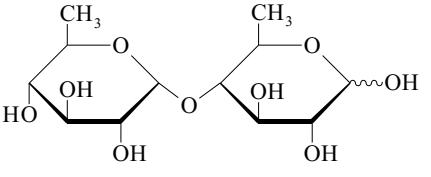
Mp 160° (hydrochloride).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 832B; 838D; 839C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 396A; 396C (*nmr*)
Ulbricht, T.L.V. *et al., J.C.S.*, 1965, 6134-6135 (*3*N*-Me*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DAQ850

6-Deoxy-4-*O*-(6-deoxy-α-D-glucopyranosyl)-D-glucose, 9CI D-81

4-O-*α-D-Quinovopyranosyl-D-quinovose. 6-Deoxy-D-glucobiose*

[39669-45-9]



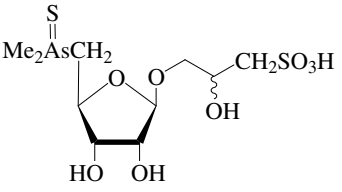
Pyranose–*form*

$C_{12}H_{22}O_9$ 310.3

Reducing disaccharide. Isol. from Asterosaponin A from starfish *Asterias amurensis*. Needles ($CHCl_3$/MeOH).
Mp 192-193.8°. $[\alpha]_D^{25}$ +29.8 (5 min) → +6.4 (48h) (c, 0.05 in H_2O).

Ikegami, S. *et al., Agric. Biol. Chem.*, 1972, **36**, 1843; 2449 (*isol, ms*)
Koto, S. *et al., Bull. Chem. Soc. Jpn.*, 2000, **73**, 967-976 (*synth, pmr*)

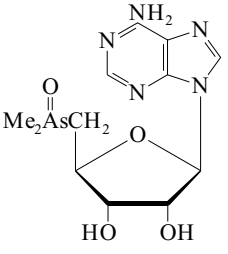
3-[[5-Deoxy-5-(dimethylarsinothioyl)-β-D-ribofuranosyl]oxy]-2-hydroxy-1-propanesulfonic acid, 9CI **D-82**
[865197-11-1]



$C_{10}H_{21}AsO_8S_2$ 408.325
Isol. from the gonads and muscles of *Pecten maximus* (giant scallop).

Kahn, M. *et al., Environ. Chem.*, 2005, **2**, 171-176 (*isol*)

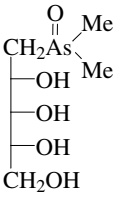
5′-Deoxy-5′-(dimethylarsinoyl)adenosine, 9CI **D-83**
[137138-03-5]



$C_{12}H_{18}AsN_5O_4$ 371.227
Isol. from the kidney of the giant clam, *Tridacna maxima*.
$[\alpha]_D$ +54.2 (c, 3 in MeOH). λ_{max} 260 (ϵ 10000) (MeOH) (Derep).

Francesconi, K.A. *et al., Chem. Comm.*, 1991, 928-929 (*isol*)

1-Deoxy-1-(dimethylarsinoyl)ribitol **D-84**
[194858-47-4]

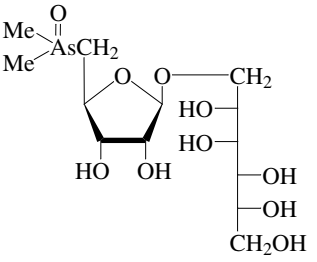


$C_7H_{17}AsO_5$ 256.13

5-O-*Sulfate:* [194858-44-1]
$C_7H_{17}AsO_8S$ 336.194
Isol. from *Chondria crassicaulis* and other red algae.

Edmonds, J.S. *et al., Tet. Lett.*, 1997, **38**, 5819-5828 (*synth, struct*)

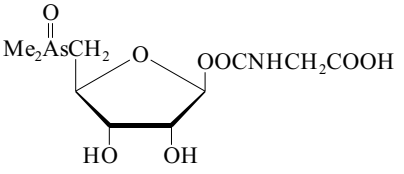
1-*O*-[5-Deoxy-5-(dimethylarsinoyl)-β-D-ribofuranosyl]-D-mannitol **D-85**
[138328-62-8]



$C_{13}H_{27}AsO_{10}$ 418.272
Isol. from the brown alga *Sargassum lacerifolium*. Syrup.

Francesconi, K. *et al., J.C.S. Perkin 1*, 1991, 2707-2716 (*isol, pmr, cmr*)

***N*-[[5-Deoxy-5-(dimethylarsinoyl)ribofuranosyl]oxycarbonyl]glycine** **D-86**

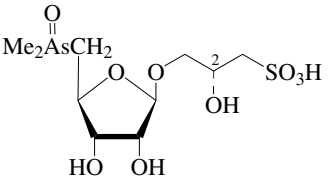


$C_{10}H_{18}AsNO_8$ 355.176

β-D-*form* [142732-39-6]
Constit. of the kidney of *Tridacna maxima*.

Francesconi, K.A. *et al., J.C.S. Perkin 1*, 1992, 1349-1357 (*isol*)

3-[5-Deoxy-5-(dimethylarsinoyl)ribofuranosyloxy]-2-hydroxy-1-propanesulfonic acid **D-87**
[77939-92-5]



(2*R*-β-D)-*form*

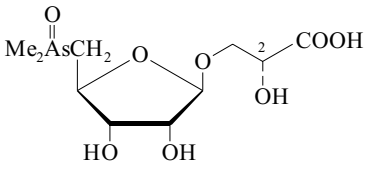
$C_{10}H_{21}AsO_9S$ 392.258

(2*R*-β-D)-*form* [142794-41-0]
Isol. from edible brown seaweeds *Hizikia fusiforme* and *Laminaria japonica*, and the giant clam, *Tridacna maxima*.

(2*S*-β-D)-*form* [142794-40-9]
Isol. from brown kelp *Ecklonia radiata*, the brown alga *Sargassum lacerifolium* and from the edible brown seaweeds *Sphaerotrichia divaricata*, *Laminaria japonica* and *Hizikia fusiforme*. Also from kidney of the giant clam *Tridacna maxima*.
Syrup. Possible metab. in formn. of Arsenobetaine, A-683 in marine fauna.

Edmonds, J.S. *et al., Nature (London)*, 1981, **289**, 602 (*isol, pmr, ir*)
Edmonds, J.S. *et al., J.C.S. Perkin 1*, 1983, 2375-2382; 1987, 577-580 (*isol, pmr, ir, cmr, struct*)
Shibata, Y. *et al., Agric. Biol. Chem.*, 1987, **51**, 391 (*isol, pmr, hplc*)
Jin, K. *et al., Agric. Biol. Chem.*, 1988, **52**, 1965-1971 (*isol, pmr*)
Francesconi, K.A. *et al., J.C.S. Perkin 1*, 1991, 2707-2716; 1992, 1349-1357 (*pmr, struct*)
Edmonds, J.S. *et al., Nat. Prod. Rep.*, 1993, **10**, 421-428 (*isol, rev*)

3-[[5-Deoxy-5-(dimethylarsinoyl)ribofuranosyl]oxy]-2-hydroxypropanoic acid D-88



(2*R*)–β–D–*form*

$C_{10}H_{19}AsO_8$ 342.177

(2*R*)-β-D-*form* [142732-41-0]
Constit. of the kidney of *Tridacna maxima*.
Syrup (as NH_4 salt). $[\alpha]_D$ +6.2 (c, 4 in H_2O) (as NH_4 salt).

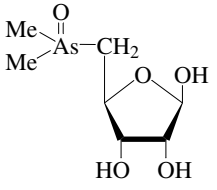
(2*S*)-β-D-*form* [142732-40-9]
Constit. of the kidney of *Tridacna maxima*.
Syrup (as NH_4 salt).

[142808-61-5, 142808-62-6]

Francesconi, K.A. *et al., J.C.S. Perkin 1*, 1992, 1349-1357 (*isol, synth, pmr*)

5-Deoxy-5-(dimethylarsinoyl)ribose D-89

[144161-79-5]



$C_7H_{15}AsO_5$ 254.114

β-D-Furanose-*form*

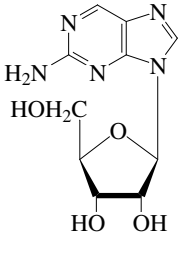
Me glycoside: Methyl 5-deoxy-5-(dimethylarsinoyl)-β-D-ribofuranoside
[138328-61-7]
$C_8H_{17}AsO_5$ 268.141
Isol. from *Sargassum lacerifolium*. Syrup. $[\alpha]_D$ +3.9 (c, 4.1 in MeOH). Poss. artifact.

Me glycoside, 2,3-isopropylidene: [138328-63-9]
Hygroscopic prisms. Mp 144-146°. $[\alpha]_D$ +0.4 (c, 4.8 in MeOH).

Francesconi, K.A. *et al., J.C.S. Perkin 1*, 1991, 2707-2716 (*isol, synth, pmr, cmr*)

6-Deoxyguanosine D-90

*9-β-D-Ribofuranosyl-9*H*-purin-2-amine. 2-Amino-9-β-D-ribofuranosylpurine*
[4546-54-7]



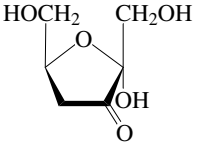
$C_{10}H_{13}N_5O_4$ 267.244
Potent inhibitor of several purine metabolising enzymes, incorporated in *E. coli* and phage T4 DNA. Cryst. (EtOH aq.). Mp 164-166°. $[\alpha]_D^{23}$ -39 (c, 1.2 in H_2O).

N^2-(2,3-Dibromo-4,5-dihydroxybenzyl):
$C_{17}H_{17}Br_2N_5O_6$ 547.159
Isol. from the red alga *Rhodomela confervoides*. Brown powder. Mp 205-207°. $[\alpha]_D^{20}$ +7 (c, 4.4 in DMSO).

Nair, V. *et al., J.O.C.*, 1987, **52**, 1344 (*synth, pmr, cmr, uv, bibl*)
Virta, P. *et al., Org. Biomol. Chem.*, 2004, **2**, 821-827 (*synth*)
Zhao, J. *et al., J. Nat. Prod.*, 2005, **68**, 691-694 (*2,3-dibromo-4,5-dihydroxybenzyl*)

4-Deoxy-*glycero*-hexo-2,3-diulose D-91

*Dihydro-2-hydroxy-2,5-bis(hydroxymethyl)-3(2*H*)-furanone, 9CI*
[211864-27-6]



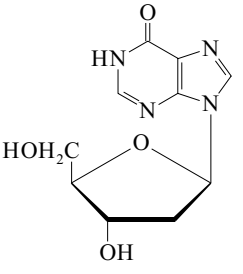
$C_6H_{10}O_5$ 162.142

DL-*form*
Isol. from the red alga *Gracilariopsis lemaneiformis*.

Broberg, A. *et al., Carbohydr. Res.*, 1998, **306**, 171-175 (*isol, synth, pmr, cmr*)
Broberg, A. *et al., Anal. Biochem.*, 1999, **268**, 35-42 (*anal*)

2′-Deoxyinosine D-92

9-(2-Deoxyribofuranosyl)hypoxanthine. Hypoxanthine 2-deoxyriboside
[29868-32-4]
[890-38-0]



$C_{10}H_{12}N_4O_4$ 252.229
Isol. from herring sperm DNA, from *Phaseolus vulgaris* (kidney bean), *Laminaria saccharina, Furcellaria fastigiata, Lactobacillus* spp. etc. Also from the starfish *Asterias rollestoni*. Ambiguous nucleoside forming base pairs with all four conventional nucleosides. Needles (MeOH), cryst. (H_2O).
Mp 218° dec. $[\alpha]_D^{27}$ +7.92 (c, 0.53 in 0.1*M* NaOH). $[\alpha]_D^{30}$ -21 (c, 1 in H_2O).

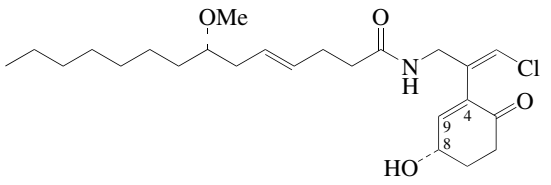
Oxime: [51385-49-0]
Mp 139-140°. $[\alpha]_D$ -21.8 (c, 1 in MeOH). Softens at 110-115° and 130-135°.

3′-Ac: [229326-13-0]
$C_{12}H_{14}N_4O_5$ 294.266
Mp 116°. $[\alpha]_D^{25}$ -22.5 (c, 1 in MeOH).

Brown, D.M. *et al., J.C.S.*, 1950, 1990-1991 (*struct*)
Manson, L.A. *et al., J. Biol. Chem.*, 1951, **191**, 87-93 (*isol*)
Banhidi, Z.G. *et al., Acta Chem. Scand.*, 1953, **7**, 713-720 (*isol*)
Venner, H. *et al., Chem. Ber.*, 1960, **93**, 140-149 (*synth*)
Robins, M.J. *et al., J.A.C.S.*, 1965, **87**, 4934-4940 (*pmr*)
Rousseau, R.J. *et al., J. Het. Chem.*, 1970, **7**, 367-372 (*synth, uv*)
Robins, M.J. *et al., Can. J. Chem.*, 1973, **51**, 3161-3169 (*synth*)
Yamazaki, A. *et al., Chem. Pharm. Bull.*, 1973, **21**, 1143-1146 (*synth*)
Mengel, R. *et al., Annalen*, 1977, 1585-1596 (*synth*)
Ciuffreda, P. *et al., Tetrahedron*, 2000, **56**, 3239-3243 (*3′-Ac, synth, pmr*)
Li, G.-Q. *et al., J. Chin. Pharm. Sci.*, 2004, **13**, 81-86 (*Asterias, isol*)

Deoxymalyngamide C D-93

[96845-20-4]



$C_{24}H_{38}ClNO_4$ 440.021

Minor constit. of a shallow-water variety of the marine blue-green alga *Lyngbya majuscula*. Oil. $[\alpha]_D$ -23 (c, 6.6 in EtOH). λ_{max} 235 (ϵ 6300) (EtOH) (Derep).

4α,9α-Epoxide: ***Malyngamide C***
[70622-52-5]
$C_{24}H_{38}ClNO_5$ 456.021
Metab. of a shallow-water variety of the marine blue-green alga *Lyngbya majuscula*. Oil. $[\alpha]_D^{23.5}$ -19.6 (c, 1.4 in $CHCl_3$). $[\alpha]_D$ -27.4 (c, 5.8 in EtOH).

4α,9α-Epoxide, Ac: ***Malyngamide C acetate***
[96845-19-1]
$C_{26}H_{40}ClNO_6$ 498.058
Minor constit. of *Lyngbya majuscula*. Oil. $[\alpha]_D$ -32.4 (c, 1.4 in EtOH).

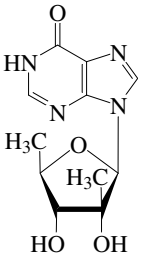
Deoxy: ***Malyngamide K***. *Dideoxymalyngamide C*
[96845-21-5]
$C_{24}H_{38}ClNO_3$ 424.022
Isol. from *Lyngbya majuscula*.
$[\alpha]_D$ -8.4 (c, 0.3 in $CHCl_3$). λ_{max} 223 (ϵ 8900) (MeOH).

Deoxy, 4α,9α-epoxide: ***8′-Deoxymalyngamide C***
[132362-43-7]
$C_{24}H_{38}ClNO_4$ 440.021
Isol. from a shallow-water variety of a blue-green alga, *Lyngbya* sp. Yellow oil. $[\alpha]_D^{20}$ +5.8 (c, 0.8 in $CHCl_3$). Erroneously named 8′-Deacetoxymalyngamide C in the paper based on an incorr. struct. shown for Malyngamide C.

Cardellina, J.H. *et al., Phytochemistry*, 1978, **17**, 2091-2095 (*isol, pmr, ms*)
Ainslie, R.D. *et al., J.O.C.*, 1985, **50**, 2859-2862 (*Malyngamide C, Malyngamide C acetate, Deoxymalyngamide C*)
Wright, A.D. *et al., J. Nat. Prod.*, 1990, **53**, 845-861 (*Deoxymalyngamide C*)
Wu, M. *et al., Tetrahedron*, 1997, **53**, 15983-15990 (*Malyngamide K*)

5′-Deoxy-2′-*C*-methylinosine, 9CI D-94

Trachycladine B
[164803-17-2]

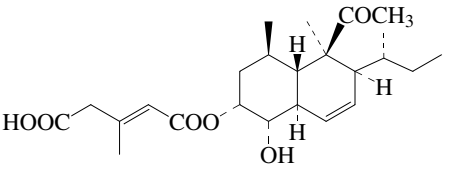


$C_{11}H_{14}N_4O_4$ 266.256

Isol. from the marine sponge *Trachycladus laevispirulifer*.
Amorph. solid. Sol. MeOH, butanol; fairly sol. H_2O; poorly sol. hexane. λ_{max} 249 (ϵ 15000) (MeOH).

Searle, P.A. *et al., J.O.C.*, 1995, **60**, 4296-4298 (*isol, uv, pmr, ms*)

Deoxynortrichoharzin D-95



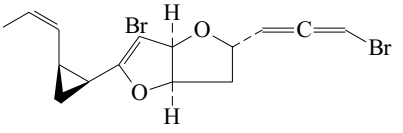
$C_{24}H_{36}O_6$ 420.545

Isol. from a sponge-derived fungus, *Paecilomyces* cf. *javanica*.
Glassy solid. $[\alpha]_D$ +26 (c, 0.16 in MeOH). λ_{max} 217 (log ϵ 4.29) (MeOH).

Rahbaek, L. *et al., J. Nat. Prod.*, 1998, **61**, 1571-1573 (*isol, uv, ir, pmr, cmr*)

Deoxyokamurallene D-96

Deepoxyokamurallene
[81474-94-4]



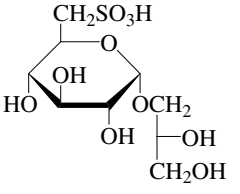
$C_{15}H_{16}Br_2O_2$ 388.098

Constit. of *Laurencia okamurai*. Oil. $[\alpha]_D^{23}$ +220 (c, 0.84 in $CHCl_3$).

Suzuki, M. *et al., Chem. Lett.*, 1982, 289; 1991, 33 (*isol, abs config*)
Suzuki, M. *et al., Phytochemistry*, 1989, **28**, 2145 (*struct*)

1-*O*-(6-Deoxy-6-sulfoglucopyranosyl)glycerol D-97

2,3-Dihydroxypropyl 6-deoxy-6-sulfoglucopyranoside, 9CI.
6-Sulfoquinovopyranosyl-(1→1)-glycerol



$C_9H_{18}O_{10}S$ 318.301

α-D-*form* [2308-53-4]
Isol. from nitrogen-fixing *Rhizobium* bacteria. Biosynth. intermediate for 1,2-Diacylglycerol 6-sulfoquinovosides, D-111.
$[\alpha]_D^{22}$ +55 (c, 0.5 in H_2O).

Na salt: [84271-27-2]
$[\alpha]_D^{15}$ +58 (c, 0.6 in H_2O).

Cyclohexylamine salt:
Cryst. (EtOH/EtOAc). Mp 151.5-153°. $[\alpha]_D^{25}$ +74.5 (c, 1.8 in H_2O, pH 4). No CAS no found 8-14 CI.

3-Tetradecanoyl: [71932-07-5]
$C_{23}H_{44}O_{11}S$ 528.66
Isol. from shell of the sea urchin *Anthocidaris crassispina* and from New Zealand spinach *Tetragonia expansa*. Isol. as mixt. with 1-hexadecanoyl (4:96).

3-Hexadecanoyl: [71963-28-5]
$C_{25}H_{48}O_{11}S$ 556.714
Isol. from shell of the sea urchin *Anthocidaris crassispina* and brown algae *Sargassum thunbergii* and *Sargassum wightii*.

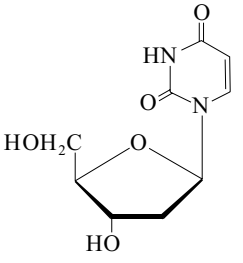
3-Octadecanoyl: [267900-56-1]
$C_{27}H_{52}O_{11}S$ 584.767
Isol. from brown alga *Sargassum thunbergii* and from *Amphidinium carterae*. Isol. as a mixt. with 1-hexadecanoyl (4:96).

Diacyl derivs: See 1,2-Diacylglycerol 6-sulfoquinovosides, D-111

Lepage, M. *et al., J.A.C.S.*, 1961, **83**, 157-159 (*isol*)
Miyano, M. *et al., J.A.C.S.*, 1962, **84**, 59-62 (*synth*)
Okaya, Y. *et al., Acta Cryst.*, 1964, 1276-1282 (*cryst struct*)
Anderson, R. *et al., Biochim. Biophys. Acta*, 1978, **528**, 89-106 (*Nitzchia alba*)
Sato, N. *et al., Biochim. Biophys. Acta*, 1979, **572**, 19-28 (*Anabaena varialulis Anacystis vidulous*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1979, **27**, 1934-1937 (*3-hexadecanoyl, 3-tetradecanoyl, 3-octadecanoyl*)
Harwood, J.L. *et al., Biochem. Plants*, 1980, **4**, 1-55 (*rev*)
Mudd, J.B. *et al., Chemistry*, 1981, **94**, 61720 (*biosynth, rev*)
Son, B.W. *et al., Phytochemistry*, 1990, **29**, 307-309 (*Gracilaria verucosa*)
Son, B.W. *et al., Bull. Korean Chem. Soc.*, 1992, **13**, 584-586 (*3-octadecanoyl, 3-hexadecanoyl*)
Sahara, H. *et al., Br. J. Cancer*, 1997, **75**, 324-332 (*Strongylocentrus intermedius*)
Wang, J. *et al., Carbohydr. Res.*, 1998, **307**, 347-350 (*isol, pmr*)
Arunkumar, K. *et al., Bot. Mar.*, 2005, **48**, 441-445 (*3-hexadecanoyl, isol, Sargassum*)
Wu, J. *et al., Chem. Pharm. Bull.*, 2005, **53**, 330-332 (*Amphidinium carterae sulfoglucoside*)

2′-Deoxyuridine, 9CI D-98

*1-(2-Deoxy-β-D-*erythro*-pentofuranosyl)uracil. 1-(2-Deoxy-β-D-ribofuranosyl)uracil*
[951-78-0]



$C_9H_{12}N_2O_5$ 228.204
Isol. from *Acanthaster planci, Aplidium pantherinum, Chara globularis* and *Ptychodera flava*. Cryst. (MeOH).
Mp 167° (163.5°). $[\alpha]_D$ +30 (H_2O). $[\alpha]_D$ +50 (1*M* NaOH).
λ_{max} 262 (ϵ 10200) (pH7).

▶ YU7490000

5′-Phosphate: 2′-Deoxy-5′-uridylic acid, 9CI
[964-26-1]
$C_9H_{13}N_2O_8P$ 308.184

5′-Ac:
$C_{11}H_{14}N_2O_6$ 270.241
Mp 96°.

5′-Trityl: [14270-73-6]
$C_{28}H_{26}N_2O_5$ 470.524
Mp 204-205°.

N-*Me:* ***2′-Deoxy-3-methyluridine, 9CI***
[24514-32-7]
$C_{10}H_{14}N_2O_5$ 242.231
Isol. from the marine sponge *Geodia baretti*. Plates (EtOAc).
Mp 98-100°.

5′-Carboxylic acid: ***2′-Deoxyuridine-5′-carboxylic acid***
[3180-30-1]
$C_9H_{10}N_2O_6$ 242.188
Constit. of the ascidian *Aplidium fuscum*. Plates (H_2O).
Mp 226-227° dec. (222-223°).

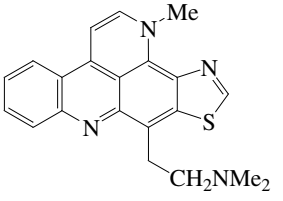
5′-Carboxylic acid amide: 2′-Deoxyuridine-5′-carboxamide
[68382-10-5]
$C_9H_{11}N_3O_5$ 241.203
Mp 257-258° dec.

5′-Triphosphate: [1173-82-6]
$C_9H_{15}N_2O_{14}P_3$ 468.144
Cell nucleic acid constit.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 816A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 374B (*nmr*)
Dekker, C.A. *et al., Nature (London)*, 1950, **166**, 557-558 (*synth*)
Brown, D.M. *et al., J.C.S.*, 1958, 3035-3038 (*synth*)
Fox, J.J. *et al., Adv. Carbohydr. Chem.*, 1959, **14**, 283-380 (*rev*)
U.S. Pat., 1966, 3 280 104; *CA*, **66**, 38207y (*5-trityl, 5-phosphate*)
Kikugawa, K. *et al., Chem. Pharm. Bull.*, 1969, **17**, 785-797 (*synth, N-Me*)
Rahman, A. *et al., Acta Cryst. B*, 1972, **28**, 2260-2270 (*cryst struct*)
Hruska, F.E. *et al., Can. J. Chem.*, 1974, **52**, 497-508 (*conformn, pmr*)
Sprecher, C.A. *et al., Biopolymers*, 1977, **16**, 2243-2264 (*cd*)
Schinazi, R.F. *et al., J. Med. Chem.*, 1978, **21**, 1141-1146 (*synth, acid*)
Brokes, J. *et al., Coll. Czech. Chem. Comm.*, 1979, **44**, 439-447 (*synth*)
Akhrem, A.A. *et al., Org. Magn. Reson.*, 1979, **12**, 247-253 (*cmr*)
Komori, T. *et al., Annalen*, 1980, 653-668 (*isol*)
Barr, P.J. *et al., Tetrahedron*, 1980, **36**, 1269-1273 (*cryst struct*)
Ludwig, J. *et al., Synthesis*, 1982, 32-34 (*5′-phosphate*)
Sakema, S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **82**, 107-109 (*isol*)
Dematte, N. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **84**, 11-13 (*isol, acid*)
Lidgren, G. *et al., J. Nat. Prod.*, 1988, **51**, 1277-1280 (*2′-Deoxy-3-methyluridine*)
Rimerman, R.A. *et al., J. Chromatogr., B: Biomed. Appl.*, 1993, **619**, 29-35 (*5′-triphosphate*)

Dercitine D-99

[115141-47-4]



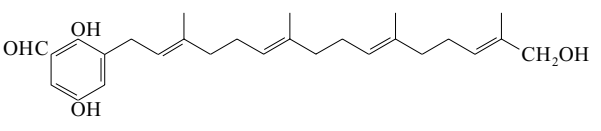
$C_{21}H_{20}N_4S$ 360.482
Regiochemistry of the thiazole moiety revised in 1992. Alkaloid from a deep water marine sponge *Dercitus* sp. and *Stelletta* sp. Exhibits antitumour, antiviral and immunosuppressive activities. Hygroscopic deep violet powder.
Mp 168°. λ_{max} 245 (ϵ 13800); 307 (ϵ 16900); 361 (ϵ 3900); 541 (ϵ 1800) (MeOH) (Derep). λ_{max} 234 (ϵ 13800); 245 (ϵ 14500); 307 (ϵ 19500); 354 (ϵ 4500); 515 (ϵ 3300) (MeOH/HCl) (Berdy). λ_{max} 238 (ϵ 12600); 261 (ϵ 11750); 293 (ϵ 14450); 405 (ϵ 6000); 527 (ϵ 2050); 558 (ϵ 1750); 610 (ϵ 1550) (MeOH/NaOH) (Berdy).

▶ UV1198950

Gunawardana, G.P. *et al., J.A.C.S.*, 1988, **110**, 4856 (*isol, pmr, cmr, ms*)
Burres, N.S. *et al., Cancer Res.*, 1989, **49**, 5267-5274 (*activity*)
Bishop, M.J. *et al., J.A.C.S.*, 1992, **114**, 10081 (*synth*)
Gunawardana, G.P. *et al., J.O.C.*, 1992, **57**, 1523 (*struct*)
Ciufolini, M.A. *et al., J.A.C.S.*, 1995, **117**, 12460 (*synth*)

Desmarestial D-100

[130756-36-4]

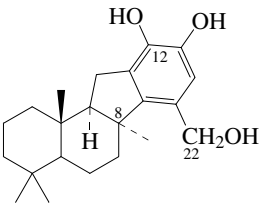


$C_{27}H_{38}O_4$ 426.595
Constit. of *Desmarestia menziesii*. Amorph. solid.
Mp 98-100°.

Rivera, P. *et al., Can. J. Chem.*, 1990, **68**, 1399 (*isol, pmr, cmr*)

O-Desulfoakaol B D-101

O-*Demethylakaol A*



$C_{22}H_{32}O_3$ 344.493

12-O-Sulfate: ***Akaol B***
[539843-00-0]
$C_{22}H_{32}O_6S$ 424.557
Constit. of an *Aka* sp.
$[\alpha]_D$ -36 (c, 0.05 in MeOH).

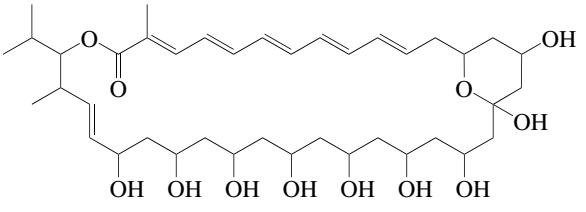
22-Me ether: ***Akaol A***
[539842-98-3]
$C_{23}H_{34}O_3$ 358.52
Constit. of an *Aka* sp.
$[\alpha]_D$ -12 (c, 0.15 in MeOH).

8-Epimer, 22-carboxylic acid, Me ester: ***Pelorol***
[287974-44-1]
$C_{23}H_{32}O_4$ 372.503
Constit. of *Dactylospongia elegans* and *Petrosaspongia metachromia*. Amorph. solid. $[\alpha]_D^{23}$ -72.1 (c, 0.33 in CH_2Cl_2). λ_{max} 218 (ϵ 12362); 260 (ϵ 4033); 292 (ϵ 1687) (MeOH).

Goclik, E. *et al., J. Nat. Prod.*, 2000, **63**, 1150-1152 (*Pelorol*)
Kwak, J.H. *et al., J. Nat. Prod.*, 2000, **63**, 1153-1156 (*Pelorol*)
Mukku, V.J.R.V. *et al., J. Nat. Prod.*, 2003, **66**, 686-689 (*Akaols*)
Yang, L. *et al., Org. Lett.*, 2005, **7**, 1073-1076 (*synth*)

Dhanyabadomycin D-102

Antibiotic TG 488. TG 488
[171370-53-9]



$C_{40}H_{64}O_{12}$ 736.938

Pentaene antibiotic. Prod. by *Streptomyces* sp. T-920488 and a marine-derived *Streptomyces* sp. B 8905. Antifungal agent. Yellow cryst. Sol. MeOH, Me_2CO. $[\alpha]_D$ -58 (MeOH). λ_{max} 260; 358 (MeOH). λ_{max} 260 (E1%/1cm 220); 358 (E1%/1cm 1000) (MeOH) (Berdy).

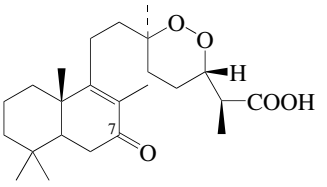
Japan. Pat., 1995, 95 238 082; *CA*, **124**, 7185b (*isol*)
Maskey, R.P. *et al., Dissertation*, Univ. of Göttingen, 2001, (*marine, isol*)

Diabolin D-103

Protein similar to lectin. Isol. from the kelp *Laminaria diabolica*. Defence chemical inducing false fertilisation in sea urchin eggs.

Nomura, K. *et al., Biochem. Biophys. Res. Commun.*, 2000, **272**, 691-693 (*isol*)

Diacarnoic acid B D-104



$C_{24}H_{38}O_5$ 406.561

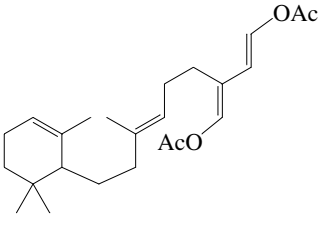
Me ester: ***Methyl diacarnoate B***
[211239-49-5]
$C_{25}H_{40}O_5$ 420.588
Constit. of *Diacarnus levii*.
$[\alpha]_D^{25}$ -2.8 (c, 0.32 in $CHCl_3$).

7-Deoxo, benzyl ester: ***Benzyl deoxydiacarnoate B***
[211239-56-4]
$C_{31}H_{46}O_4$ 482.702
Constit. of *Diacarnus levii*.
$[\alpha]_D^{25}$ 0 (c, 0.3 in $CHCl_3$).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1998, **81**, 1285-1292 (*isol, pmr, cmr*)

1,20-Diacetoxy-10,15-cyclo-1,3(20),6,11-phytatetraene D-105

15,16-Diacetoxy-9,10-seco-1(10),8,13(16),14-labdatetraene



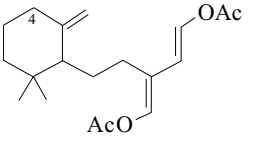
$C_{24}H_{36}O_4$ 388.546

(1E,3(20)E,11E)-form [278605-17-7]
Constit. of *Caulerpa trifaria*.
Pale yellow oil. $[\alpha]_D$ -75 (EtOH). λ_{max} 251 (ϵ 22500) (EtOH).

Handley, J.T. *et al., Aust. J. Chem.*, 2000, **53**, 67-71 (*isol, pmr, cmr*)

1,4-Diacetoxy-2-[2-(2,2-dimethyl-6-methylenecyclohexyl)ethyl]-1,3-butadiene D-106

2-[2-(2,2-Dimethyl-6-methylenecyclohexyl)ethyl]-1,3-butadiene-1,4-diol diacetate, 9CI
[85654-09-7]



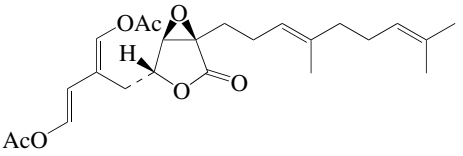
$C_{19}H_{28}O_4$ 320.428
Constit. of marine alga *Caulerpa bikinensis*. Cytotoxin, ichthyotoxin and antifeedant. Viscous oil. $[\alpha]_D$ -3 (c, 0.9 in $CHCl_3$). λ_{max} 245 (ϵ 26000) (solvent not reported) (Derep).

Δ^4-Isomer: ***1,4-Diacetoxy-2-[2-(2,6,6-trimethyl-2-cyclohexenyl)ethyl]-1,3-butadiene***. *2-[2-(2,6,6-Trimethyl-2-cyclohexen-1-yl)ethyl]-1,3-butadiene-1,4-diol diacetate*
[79689-22-8]
Constit. of *Caulerpa flexilis*.
Oil. $Bp_{0.25}$ 125°. $[\alpha]_D$ -47 (c, 9.5 in MeOH).

Capon, R.J. *et al., Aust. J. Chem.*, 1981, **34**, 1775
Paul, V.J. *et al., Tet. Lett.*, 1982, **23**, 5017 (*isol, struct*)

1,20-Diacetoxy-6,7-epoxy-1,3(20),10,14-phytatetraen-19,5-olide D-107

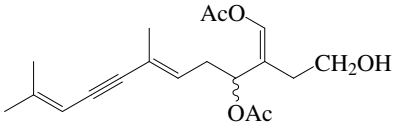
[99694-97-0]



$C_{24}H_{32}O_7$ 432.513
Constit. of the alga *Udotea argentea*.
$[\alpha]_D^{25}$ +7 (c, 1.5 in $CHCl_3$). λ_{max} 245 (ϵ 10400) (MeOH).

Paul, V.J. *et al., Phytochemistry*, 1985, **24**, 2239-2243 (*isol, uv, ir, pmr, cmr*)

4,15-Diacetoxy-3(15),6,10-farnesatrien-8-yn-1-ol D-108



$C_{19}H_{26}O_5$ 334.411

(3(15)*Z*,4ξ,6*E*)-*form*

1-O-*Hexadecanoyl:* [488730-08-1]
$C_{35}H_{56}O_6$ 572.824
Constit. of *Caulerpa prolifera*.

1-O-*(7Z,10Z,13Z-Hexadecatrienoyl):* [488730-14-9]
$C_{35}H_{50}O_6$ 566.776
Constit. of *Caulerpa prolifera*.

1-O-*Octadecanoyl:* [488730-11-6]
$C_{37}H_{60}O_6$ 600.877
Constit. of *Caulerpa prolifera*.

1-O-*(9Z,12Z-Octadecadienoyl):* [488730-07-0]
$C_{37}H_{56}O_6$ 596.846
Constit. of *Caulerpa prolifera*.

1-O-*(9Z,12Z,15Z-Octadecatrienoyl):* [488730-09-2]
$C_{37}H_{54}O_6$ 594.83
Constit. of *Caulerpa prolifera*.

1-O-*(6Z,9Z,12Z,15Z-Octadecatetraenoyl):* [488730-15-0]
$C_{37}H_{52}O_6$ 592.814
Constit. of *Caulerpa prolifera*.

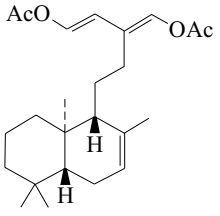
1-O-*(11Z-Eicosenoyl):* [488730-12-7]
$C_{39}H_{62}O_6$ 626.915
Constit. of *Caulerpa prolifera*.

1-O-*(5Z,8Z,11Z,14Z-Eicosatetraenoyl):* [488730-13-8]
$C_{39}H_{56}O_6$ 620.868
Constit. of *Caulerpa prolifera*.

1-O-*(5Z,8Z,11Z,14Z,17Z-Eicosapentaenoyl):* [488730-10-5]
$C_{39}H_{54}O_6$ 618.852
Constit. of *Caulerpa prolifera*.

Smyrniotopoulos, V. *et al., J. Nat. Prod.*, 2003, **66**, 21-24 (*isol, pmr, cmr*)

15,16-Diacetoxy-7,13(16),14-labdatriene D-109



$C_{24}H_{36}O_4$ 388.546

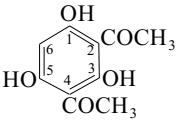
(*ent*-13*E*,14*E*)-*form*

Metab. of *Caulerpa trifaria*.
Rods (CH_2Cl_2/petrol).
Mp 62.5-63°. $[\alpha]_D$ -8 (c, 6.6 in $CHCl_3$).

Capon, R.J. *et al., Phytochemistry*, 1983, **22**, 1465

2,4-Diacetyl-1,3,5-benzenetriol D-110

1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bisethanone, 9CI. 2,4-Diacetylphloroglucinol, 8CI
[2161-86-6]



$C_{10}H_{10}O_5$ 210.186
Isol. from *Pseudomonas fluorescens*. Active against gram-positive bacteria and actinomycetes (Anti-MRSA). Cryst. (C_6H_6/petrol). Mp 173-174°. λ_{max} 288 (ϵ 26800) (MeOH/NaOH) (Derep). λ_{max} 270 (ϵ 26200) (MeOH) (Derep).

▶ LD_{50} (mus, scu) 0.16 mg/kg. SY1100000

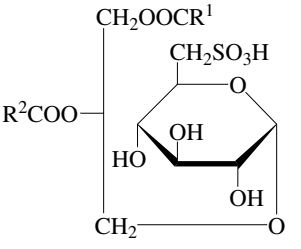
1-Me ether: 2,4-Diacetyl-5-methoxy-1,3-benzenediol
[3098-38-2]
$C_{11}H_{12}O_5$ 224.213
Needles. Mp 106°.

1,5-Di-Me ether: 2,6-Diacetyl-3,5-dimethoxyphenol
$C_{12}H_{14}O_5$ 238.24
Needles (petrol). Mp 128°. No CAS no. assigned 1967-2001 (8-14CI).

Dean, F.M. *et al., J.C.S.*, 1953, 1241-1249 (*synth*)
Reddi, T.K. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1969, **5**, 116 (*isol, uv, ir, nmr*)
Broadbent, D. *et al., Phytochemistry*, 1976, **15**, 1785 (*isol, synth, props*)
Nowak-Thompson, B. *et al., Can. J. Microbiol.*, 1994, **40**, 1064-1066 (*isol, pmr*)
Marchand, P.A. *et al., J. Agric. Food Chem.*, 2000, **48**, 1882-1887 (*synth, uv, pmr, cmr, ms*)
Isnansetyo, A. *et al., J. Antimicrob. Chemother.*, 2001, **47**, 724-725 (*isol, activity*)

1,2-Diacylglycerol 6-sulfoquinovosides D-111

1,2-Diacylglycerol 3-(6-deoxy-6-sulfo-α-D-glucopyranosides). 6-Sulfoquinovose diacylglycerides. Sulfoquinovosyldiglycerides. SQDG



A specialised class of glycosides of Glycerol 1,2-dialkanoates, G-121. See also 1-*O*-(6-Deoxy-6-sulfoglucopyranosyl)glycerol, D-97 for further refs. and general information. All examples so far characterised have R^2 = hexadecanoyl, with 2*S*-(≡1,2-diacyl-*sn*-glycerol) abs. config. Isol. from cultured cyanobacteria (blue-green algae) *Lyngbya lagerheimii* and *Phormidium tenue* and from *Rhizobium* nitrogen-fixing bacteria. Incompletely characterised diacyl mixtures have also been isol. from the non-photosynthetic diatom *Nitzschia alba*, blue-green algae *Anabaena variabilis* and *Anacystis nidulans*, red alga *Gracilaria verrucosa*, marine sponge *Phyllospongia foliascens* and the sea urchin *Strongylocentrotus intermedius*. Occur in the organelle membranes involved in CO_2 fixation. Show anti-HIV-1 activity *in vitro*.

2-*O*-Hexadecanoyl-1-*O*-(9-hexadecenoyl)glycerol 3-(6-deoxy-6-sulfo-α-D-glucopyranoside) [122991-49-5]
$C_{41}H_{76}O_{12}S$ 793.11

2-*O*-Hexadecanoyl-1-*O*-(9-octadecenoyl)glycerol 3-(6-deoxy-6-sulfo-α-D-glucopyranoside) [123016-84-2]
$C_{43}H_{80}O_{12}S$ 821.164
Also isol. from the brown alga *Dictyota ciliolata*.

2-*O*-Hexadecanoyl-1-*O*-(9*Z*,12*Z*-octadecadienoyl)glycerol 3-(6-deoxy-6-sulfo-α-D-glucopyranoside) [123016-83-1]
$C_{43}H_{78}O_{12}S$ 819.148
$[\alpha]_D$ +62.8 (c, 0.83 in MeOH).

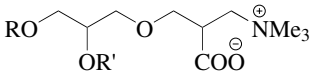
2-*O*-Hexadecanoyl-1-*O*-(9*Z*,12*Z*,15*Z*-octadecatrienoyl)glycerol 3-(6-deoxy-6-sulfo-α-D-glucopyranoside) [123036-44-2]
[130193-67-8] $[\alpha]_D^{22}$ +42.8 (c, 1 in MeOH) (as Na salt).

1,2-Di-*O*-hexadecanoylglycerol 3-(6-deoxy-6-sulfo-α-D-glucopyranoside) [169048-28-6]
$C_{41}H_{78}O_{12}S$ 795.126
Isol. from *Laurencia pedicularioides* (as tri-Ac). CAS no. refers to tri-Ac.

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1979, **27**, 1934-1937 (*isol, sea urchin*)
Gustafson, K.R. *et al., J. Natl. Cancer Inst.*, 1989, **81**, 1254-1258 (*isol, pmr, cmr, activity*)
Adebodun, F. *et al., Biochemistry*, 1992, **31**, 4502-4509 (*pmr, cmr*)
Gordon, D.M. *et al., J.A.C.S.*, 1992, **114**, 659-663 (*isol, struct*)
Siddhanta, A.K. *et al., Bot. Mar.*, 1995, **38**, 329-331 (*dihexadecanoyl*)
Kim, Y.H. *et al., J. Mass Spectrom.*, 1997, **32**, 968-977 (*ms*)
Bourne, D.J. *et al., Aust. J. Chem.*, 1999, **52**, 69-70 (*isol, Dictyota, pmr, cmr, bibl*)

1,2-Diacylglyceryl-*O*-2′-(hydroxymethyl)-*N*,*N*,*N*-trimethyl-β-alanine D-112

DGTA

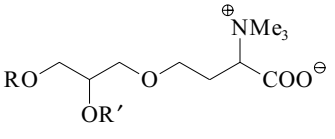


R and R′ are long chain acyl residues. Isol. from various marine algae.

Kato, M. *et al., Phytochemistry*, 1996, **42**, 1341
Vaskovsky, V.E. *et al., Phytochemistry*, 1996, **42**, 1347

4-*O*-(1,2-Diacylglyceryl)-*N*,*N*,*N*-trimethylhomoserine D-113

DGTS

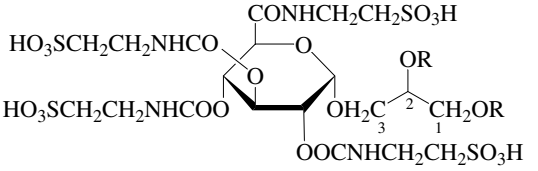


R and R′ are long-chain acyl residues. Betaine lipid present in fungi, lichens, most ferns, some higher plants and green algae.

Sato, N. *et al., Phytochemistry*, 1984, **23**, 1625-1627 (*bibl*)
Dembitsky, V.M. *et al., Prog. Lipid Res.*, 1996, **35**, 1-51 (*rev*)
Kuenzler, K. *et al., Phytochemistry*, 1997, **46**, 883-892 (*occur*)
Vaskovsky, V.E. *et al., Phytochemistry*, 1998, **47**, 755-760 (*occur*)
Rozentsvet, O.A. *et al., Phytochemistry*, 2000, **54**, 401-407 (*occur*)

1,2-Diacyl-3-(2,3,4,6-tetra-*N*-taurinamido-α-D-glucopyranosyl)glycerol D-114

1,2-Diacyl-3-(α-D-glucuronopyranosylglycero)taurinamide

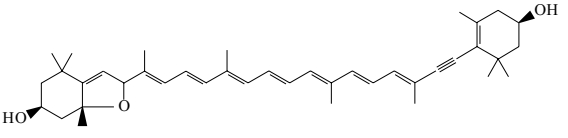


$R^1 = R^2$ = long-chain acyl groups

Constit. of the marine bacterium *Hyphomonas jannaschiana*.
Batrakov, S.G. *et al., Biochim. Biophys. Acta*, 1996, **1302**, 167-176

Diadinochrome D-115

7′,8′-Didehydro-5,8-epoxy-5,8-dihydro-β,β-carotene-3,3′-diol
[24381-84-8]

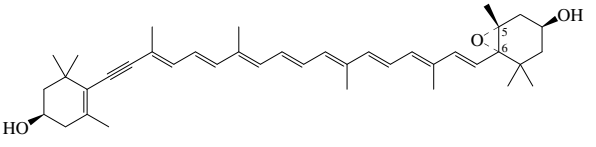


$C_{40}H_{54}O_3$ 582.865
Constit. of *Pelagococcus subviridis*, *Phaeodactylum tricornutum, Lamprometra klunzingeri* and the sea squirt *Halocynthia roretzi*.
Orange needles (petrol).
Mp 127-130°.

Gross, J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1975, **52**, 459 (*isol*)
Carreto, J.L. *et al., Mar. Biol. (Berlin)*, 1976, **36**, 105 (*isol*)
Matsuno, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 4309 (*occur*)
Bjornland, T. *et al., Phytochemistry*, 1989, **28**, 3347 (*isol, pmr*)

Diadinoxanthin A D-116

7′,8′-Didehydro-5,6-epoxy-5,6-dihydro-β,β-carotene-3,3′-diol
[18457-54-0]

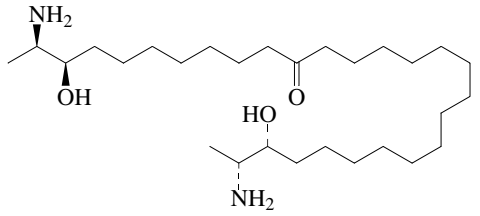


$C_{40}H_{54}O_3$ 582.865
Constit. of diatoms, e.g. *Euglena gracilis*. Cryst.
Mp 158-162°.

5,6-Diepimer: ***Diadinoxanthin B***
[280774-91-6]
$C_{40}H_{54}O_3$ 582.865
Constit. of the common freshwater goby (*Rhinogobius brunneus*).
λ_{max} 420; 445; 475 (Et_2O).

Aitzetmüller, K. *et al., Chem. Comm.*, 1968, 32 (*isol*)
Buchecker, R. *et al., Phytochemistry*, 1977, **16**, 729 (*abs config*)
Swift, I.E. *et al., Phytochemistry*, 1982, **21**, 2859 (*biosynth*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 230 (*bibl*)
Bjornland, J. *et al., Phytochemistry*, 1989, **28**, 3347 (*isol, pmr, ms*)
Tsushima, M. *et al., J. Nat. Prod.*, 2000, **63**, 960-964 (*Diadinoxanthin B*)
Kim, D. *et al., J. Nat. Prod.*, 2004, **67**, 1067-1069 (*biosynth*)

2,27-Diamino-3,26-dihydroxy-11-octacosanone D-117



$C_{28}H_{58}N_2O_3$ 470.778

(2R,3R,26R,27R)-form

26-O-*β*-D-Glucopyranoside: ***Rhizochalin***
[125342-59-8]
$C_{34}H_{68}N_2O_8$ 632.92
Constit. of the sponge *Rhizochalina incrustata*. Antibacterial and cytotoxic agent. Cryst. (EtOH/EtOAc). Sol. MeOH, H_2O.
Mp 124-126°. $[\alpha]_{578}$ -5.

N^2-*Ethoxycarbonyl, 26*-O-*β*-D-*galactopyranoside:* ***Rhizochalin A***
$C_{37}H_{72}N_2O_{10}$ 704.983
Constit. of *Rhizochalina incrustata*.
$[\alpha]_D^{18}$ +15 (c, 0.22 in EtOH) (as per-Ac).

Makarieva, T.N. *et al., Tet. Lett.*, 1989, **30**, 6581-6584 (*Rhizochalin*)
Makarieva, T.N. *et al., J. Nat. Prod.*, 2005, **68**, 255-257 (*Rhizochalin A*)

3,3′-Diaminodipropylamine, 8CI D-118

N-*(3-Aminopropyl)-1,3-propanediamine, 9CI. Bis(3-aminopropyl) amine. Dipropylenetriamine. 1,7-Diamino-4-azaheptane. Iminobispropylamine. 1,5,9-Triazanonane. Norspermidine. Caldine*
[56-18-8]
$(H_2NCH_2CH_2CH_2)_2NH$
$C_6H_{17}N_3$ 131.22
Metab. of various bacteria and plant spp. Isol. from the green alga *Codium fragile*. Colorimetric reagent for nitro compds. Cross-linking agent for epoxy resins. Liq. Sol. H_2O, polar org. solvs.
d_{20}^{20} 0.93.
Mp -14°. Bp 240° Bp_2 100°. n_D^{20} 1.4810.
▶ Skin and severe eye irritant. LD_{50} (rat, orl) 810 mg/kg. LD_{50} (skn, rbt) 110 mg/kg. JL9450000

Hydrochloride (1:3):
Cryst. (MeOH aq. or EtOH/Et_2O). Mp 270° (259°).

Tripicrate:
Cryst. (H_2O). Mp 226-227°.

$N^3,N^{3'}$-*Bis(2,3-dihydroxybenzoyl):* [88381-35-5]
$C_{20}H_{25}N_3O_6$ 403.434
Isol. from *Vibrio fluvialis*. Siderophore. λ_{max} 248 (E1%/1cm 12.8); 316 (E1%/1cm 8.1) (MeOH) (Berdy).

N^1-*Me:* N-*(3-Aminopropyl)*-N-*methyl-1,3-propanediamine. 3,3′-Diamino*-N-*methylpropylamine.* N,N-*Bis(3-aminopropyl)-methylamine*
[105-83-9]
$C_7H_{19}N_3$ 145.247
Monomer for polyamides and polyureas. Liq. Bp_{12} 112-114°.
▶ Skin and severe eye irritant. LD_{50} (rat, orl) 1540 mg/kg. JL9625000

$N^1,N^3,N^{3'}$-*Tri-Me:* N,N′-*Dimethyl*-N-*[3-(methylamino)propyl]-1,3-propanediamine.* N-*Methyl-3,3′-bis(methylamino)propylamine*
[123-70-6]
$C_9H_{23}N_3$ 173.301
No phys. props. reported.

$N^3,N^3,N^{3'},N^{3'}$-*Tetra-Me:* N′-*[3-(Dimethylamino)propyl]*-N,N-*dimethyl-1,3-propanediamine. 3,3′-Bis(dimethylamino)dipropylamine*
[6711-48-4]
$C_{10}H_{25}N_3$ 187.328
Mp -78°. Bp_{20} 128-131°. n_D^{20} 1.4490.
▶ JM1925000

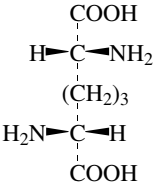
N-*Penta-Me:* N-*[3-(Dimethylamino)propyl]*-N,N′,N′-*trimethyl-1,3-propanediamine, 9CI. 3,3′-Bis(dimethylamino)*-N-*methyldipropylamine, 8CI.* N,N,N′,N″,N″-*Pentamethyldipropylenetriamine*
[3855-32-1]
$C_{11}H_{27}N_3$ 201.354
Catalyst for polyurethane foam production; auxiliary for lithiation reactions. Liq. Bp_{11} 100-102°.

[27708-70-9, 72864-15-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 309C; 310B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 500B; 500C; 501A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 397A; 397B (*ir*)
Wiedeman, D.F. *et al., J.A.C.S.*, 1945, **67**, 1994 (*synth*)
Terent'ev, A.P. *et al., Zh. Obshch. Khim.*, 1950, **20**, 1073; *CA*, **44**, 9350a (*synth*)
Marxer, A. *et al., Helv. Chim. Acta*, 1951, **34**, 924-931 (*N-penta-Me*)
Israel, M. *et al., J. Med. Chem.*, 1964, **7**, 710 (*synth*)
Schrier, M. *et al., Mikrochim. Acta*, 1965, 1091; 1967, 218 (*use*)
Ger. Pat., 1978, 2 739 353; *CA*, **89**, 111389r (*N-penta-Me*)
Bergeron, R.J. *et al., Synthesis*, 1981, 732 (*synth*)
Canadian Pat., 1982, 1 132 292; *CA*, **98**, 55043v (*N-penta-Me*)
Murahashi, S. *et al., J.A.C.S.*, 1983, **105**, 5002 (*synth, pmr, ir*)
Dagnall, S.P. *et al., J.C.S. Perkin 2*, 1984, 435 (*cmr*)
Hamana, K. *et al., J. Biochem. (Tokyo)*, 1985, **97**, 1595; 1991, **109**, 444 (*occur*)
Tanaka, Y. *et al., CA*, 1988, **109**, 232044q (*crosslinking*)
Carboni, B. *et al., Tet. Lett.*, 1988, **29**, 1279 (*synth*)
Yamamato, S. *et al., J. Biochem. (Tokyo)*, 1993, **113**, 538 (*bisdihydroxybenzoyl*)
Thurner, A. *et al., Synth. Commun.*, 1998, **28**, 443-449 (*N-penta-Me, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AIX250; BGU750; TDP750

2,6-Diaminoheptanedioic acid, 9CI D-119

2,6-Diaminopimelic acid
[583-93-7]



(2*R*,6*R*)-*form*

$C_7H_{14}N_2O_4$ 190.199
The *meso*-form and occasionally the chiral isomers are constits. of the polymeric peptidoglycans present in the cell walls of algae and all bacteria, except Halobacteria.

(2R,6R)-form

D,D-*form*
[17121-19-6]
Mp 309-310°. $[\alpha]_D^{16}$ -30.4 (6*M* HCl).

Hydrochloride: Mp 288°.

N,N′-*Dibenzoyl, dianilide:* Mp 307° dec.

(2S,6S)-form

L,L-*form*
[14289-34-0]
Mp 310-312°. $[\alpha]_D$ +44 (c, 0.96 in 1*M* HCl).

Hydrochloride: Mp 288°.

N,N′-*Dibenzoyl, dianilide:* Mp 307° dec.

N-*Succinoyl: 2-Amino-6-[(3-carboxy-1-oxopropyl)amino]heptanedioic acid, 9CI. 2-Amino-6-(carboxypropionamido)heptanedioic acid, 8CI*
[26605-36-7]
$C_{11}H_{18}N_2O_7$ 290.272
Precursor of lysine in *E. coli*.

(2RS,6SR)-form

meso-*form*
[922-54-3]

Lysine precursor. Cross-linking agent in bacterial peptidoglycans esp. in gram-negative bacteria. Needles (H_2O). Mp 313-315° dec.

Hydrochloride:
Plates. Mp 264-265° (240°) dec.

N,N′-*Dibenzoyl:*
$C_{21}H_{22}N_2O_6$ 398.415
Needles (EtOAc/petrol). Mp 194-195°.

N,N′-*Dibenzoyl, monoanilide:* Mp 220-221°.

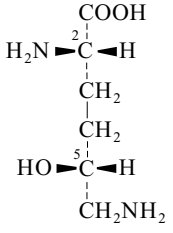
N,N,N-*Tri-Me, betaine:* ***6-Amino-6-carboxy-2-trimethylammoniohexanoate***
$C_{10}H_{20}N_2O_4$ 232.279
Isol. from red alga *Schottera nicaeensis*. Off-white hygroscopic powder. $[\alpha]_D^{25}$ -6.4 (c, 1.6 in H_2O). A quasi-meso compd. showing opt. activity. Abs. config. of nat. compd. not determined.

[2577-62-0]

Izumi, Y. *et al., Nippon Kagaku Zasshi*, 1954, **75**, 993-995; 1152-1155; *CA*, **49**, 11550 (*synth*)
Hoare, D.S. *et al., Biochem. J.*, 1957, **65**, 441-447 (*isol*)
Nakayama, K. *et al., Agric. Biol. Chem.*, 1970, **34**, 282-288 (*succinoyl*)
Arendt, A. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1974, **48**, 883-885; *CA*, **81**, 63946f (*synth*)
Hull, S.E. *et al., Acta Cryst. B*, 1977, **33**, 3832-3837 (*cryst struct*)
Sciuto, S. *et al., J. Nat. Prod.*, 1985, **48**, 602-605 (*N-tri-Me betaine*)
Bouchaudon, J. *et al., J.C.S. Perkin 1*, 1989, 695-701 (*synth*)
Bold, G. *et al., Helv. Chim. Acta*, 1992, **75**, 865-882 (*synth*)
Williams, R.M. *et al., J.O.C.*, 1992, **57**, 6519-6527 (*synth, pmr, bibl*)
Pavelka, M.S. *et al., J. Bacteriol.*, 1996, **178**, 6496-6507 (*biosynth*)
Arakawa, Y. *et al., Chem. Pharm. Bull.*, 1998, **46**, 674-680 (*synth, ir, pmr, cmr*)
Gao, Y. *et al., J.O.C.*, 1998, **63**, 2133-2143 (*synth*)
Hiebl, J. *et al., J.O.C.*, 1999, **64**, 1947-1952 (*synth*)
Davis, F.A. *et al., J.O.C.*, 2000, **65**, 3248-3251 (*synth*)
Hernandez, N. *et al., J.O.C.*, 2001, **66**, 4934-4938 (*derivs, synth, bibl*)
Collier, P.N. *et al., Tet. Lett.*, 2001, **42**, 5953-5954 (*synth*)
Wang, W. *et al., Synthesis*, 2002, 94-98 (*synth*)

2,6-Diamino-5-hydroxyhexanoic acid D-120

5-Hydroxylysine, 9CI. α,ε-Diamino-δ-hydroxycaproic acid
[504-91-6]



(2*S*,5*R*)–*form*

$C_6H_{14}N_2O_3$ 162.188

(2S,5R)-form
L-erythro-*form*
[1190-94-9]
One of the natural protein-bound amino acids. Occurs free in plant tissues, e.g. *Viscum album, Medicago sativa* (alfalfa).
$[\alpha]_D^{25}$ +17.8 (c, 2 in 6*M* HCl).

N^6-*Tri-Me, betaine:* [29259-54-9]
$C_9H_{20}N_2O_3$ 204.269
Component of the cell walls of *Nitzschia angularis*, *Nitzschia incerta*, *Cylindrotheca fusiformis*, *Cyclotella cryptica*, *Phaeodactylum tricornutum* and *Navicula pelliculosa*. Isol. from rat urine.

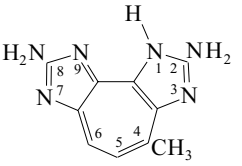
N^6-*Tri-Me* O^5-*phosphate:*
$C_9H_{21}N_2O_6P$ 284.249
Component of the cell walls of *Nitzschia angularis*, *Nitzschia incerta*, *Cylindrotheca fusiformis*, *Cyclotella cryptica*, *Phaeodactylum tricornutum* and *Navicula pelliculosa*. CAS no. not found 8-14CI.

[6000-08-4, 18899-30-4, 18899-31-5, 78088-29-6]

Nakajima, T. *et al., Biochem. Biophys. Res. Commun.*, 1970, **39**, 28-33 (N^6-*tri-Me betaine,* N^6-*tri-Me* O^5-*phosphate, isol, occur*)

2,8-Diamino-4-methyl-1*H*-cyclohepta[1,2-*d*:3,4-*d*′]diimidazole D-121

*4-Methyl-1*H*-cyclohepta[1,2-*d*:3,4-*d*′]diimidazole-2,8-diamine, 9CI.* ***Pseudozoanthoxanthin A***
[60049-47-0]



$C_{10}H_{10}N_6$ 214.229
Tautomeric with 9*H*-form. Note that when the 1-posn. is substd., CA numbering is reversed and derivs. become 6-methyl instead of 4-methyl. Isol. from *Parazoanthus axinellae* and other Zoanthidea. Cryst. (EtOH).
Mp 280° dec.

1-Me: ***3-Norpseudozoanthoxanthin***
[94080-60-1]
$C_{11}H_{12}N_6$ 228.256
From *Parazoanthus gracilis* and *Epizoanthus arenaceus*. Yellow needles (MeOH).
Mp 300°.

9-Me: ***Norpseudozoanthoxanthin***
[55827-12-8]
$C_{11}H_{12}N_6$ 228.256
Pigment from *Epizoanthus arenaceus*. Yellow prisms (MeOH). Darkens >230°.

N^8-*Di-Me:* ***N^8,N^8-Dimethylpseudozoanthoxanthin A***
[94080-62-3]
$C_{12}H_{14}N_6$ 242.283
From *Parazoanthus gracilis*. Yellow needles (MeOH).
Mp 300°.

1,N^8-*Di-Me:* ***1,N^8-Dimethylpseudozoanthoxanthin A***
[71337-50-3]
$C_{12}H_{14}N_6$ 242.283
Isol. from the coral *Gerardia* sp. Amorph. yellow powder. Dec. at *ca.* 180°.

1,3-Di-Me: ***Pseudozoanthoxanthin***
[55827-11-7]
$C_{12}H_{14}N_6$ 242.283
Pigment from *Parazoanthus axinellae*, *Parazoanthus gracilis*, *Epizoanthus arenaceus*, *Zoanthus sociatus* and *Palythoa mammillosa*. Yellow prisms (MeOH).
Mp 310°. Imino-tautomer on C-2. λ_{max} 290 (ε 75900); 335 (ε 5890); 348 (ε 6030); 399 (ε 21400) (MeOH/HCl) (Derep). λ_{max} 281 (ε 30200); 307 (ε 46800); 367 (ε 11700); 421 (ε 8510) (MeOH) (Derep).

N^2,N^8-*Di-Me:* ***N^2,N^8-Dimethylpseudozoanthoxanthin A***. *Norparagracine*
[94080-61-2]
[71827-21-9 (tautomer)]
$C_{12}H_{14}N_6$ 242.283
From *Parazoanthus gracilis* and *Epizoanthus arenaceus*. Yellow needles (MeOH/CH_2Cl_2).
Mp 190-192° dec.

1,3,N^8-*Tri-Me:* ***Homopseudozoanthoxanthin***
[71827-22-0]
$C_{13}H_{16}N_6$ 256.31
Trace pigment from *Palythoa* sp. and *Zoanthus sociatus*. Yellow prisms (MeOH).
Mp 256-259°. Imino-tautomer on C-2. λ_{max} 226 (ε 10500); 261 (ε 10500); 306 (ε 38900); 317 (sh) (ε 30900); 377 (ε 10000); 416 (ε 15100) (MeOH) (Derep).

1,N^8,N^8-Tri-Me: ***1,N^8,N^8-Trimethylpseudozoanthoxanthin A***
[68395-65-3]
$C_{13}H_{16}N_6$ 256.31
From *Gerardia* sp., *Palythoa* sp. and *Parazoanthus* sp. Cryst. (EtOH aq.) or amorph. yellow powder. Dec. at *ca.* 200°. Imino-tautomer on C-2.

N^2,N^8,N^8-*Tri-Me:* ***Paragracine***
[57695-32-6]
$C_{13}H_{16}N_6$ 256.31
Isol. from *Parazoanthus gracilis* together with *Dentitheca habereri* (the former is parasitic on the latter). Also from *Epizoanthus* sp. Shows papaverine-like activity and antihistamine activity. Selective Na channel blocker in squid axon membranes. Yellow needles (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 258-262° dec. Strong yellow-green fluor. in soln. λ_{max} 230 (sh) (ϵ 15000); 252 (ϵ 13000); 305 (sh) (ϵ 47900); 316 (ϵ 62200); 373 (ϵ 15000); 409 (ϵ 14400); 428 (sh) (ϵ 3800) (EtOH) (Derep). λ_{max} 252 (ϵ 11900); 314 (ϵ 52000); 372 (ϵ 12600); 409 (ϵ 13100) (MeOH) (Berdy). λ_{max} 245 (ϵ 13500); 301 (ϵ 54800); 363 (ϵ 6900); 410 (ϵ 21300) (MeOH/HCl) (Berdy).

N^2,N^8,N^8-*Tri-Me, dihydrobromide:*
Yellow needles + $3H_2O$. Mp 280-282° dec.

1,N^2,N^8,N^8-*Tetra-Me:* ***9-Methylparagracine***
[81904-42-9]
$C_{14}H_{18}N_6$ 270.336
Isol. from *Parazoanthus gracilis*. Yellow prisms.
Mp 269-271° dec. λ_{max} 251 (ϵ 1875); 309 (ϵ 8250); 369 (ϵ 1625); 409 (ϵ 2125) (MeOH).

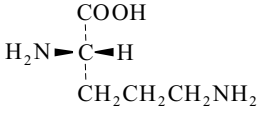
1,3,N^8,N^8-*Tetra-Me:* ***Dimethylpseudozoanthoxanthin***
$C_{14}H_{18}N_6$ 270.336
Pigment from *Palythoa* sp. Yellow needles (MeOH).
Mp 310°. Imino-tautomer on C-2.

1,N^2,N^2,N^8,N^8-*Penta-Me:* ***N^2,N^2,N^8,N^8,1,4-Hexamethyl-1H-cyclohepta[1,2-d:3,4-d′]diimidazole-2,8-diamine, 9CI***
[71337-51-4]
$C_{15}H_{20}N_6$ 284.363
Minor constit. of *Gerardia* sp. Oily yellow solid.
Mp 115° dec. approx.

Cariello, L. *et al., Tetrahedron*, 1974, **30**, 4191-4196 (*Epizoanthus arenaceus constits*)
Komoda, Y. *et al., Chem. Pharm. Bull.*, 1975, **23**, 2464 (*uv, pmr, cryst struct*)
Braun, M. *et al., J.A.C.S.*, 1978, **100**, 4208-4213 (*synth*)
Schwartz, R.E. *et al., Tet. Lett.*, 1978, 2235-2238 (*1,N^8,N^8-tri-Me, isol, cryst struct*)
Schwartz, R.E. *et al., Can. J. Chem.*, 1979, **57**, 1707-1711 (*Gerardia constits, isol, cryst struct*)
Cariello, L. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1979, **63**, 77-82 (*Zoanthus constits, Palythoa constits*)
Komoda, Y. *et al., Chem. Pharm. Bull.*, 1982, **30**, 502; 1984, **32**, 3873-3879 (*Parazoanthus gracilis constits, uv, pmr, cmr, ms*)
Jiménez, C. *et al., J. Nat. Prod.*, 1993, **56**, 9-14 (*9-Methylparagracine, isol*)

2,5-Diaminopentanoic acid D-122

Ornithine, 9CI, INN. 5-Aminonorvaline. Orn
[7006-33-9]



(*S*)–*form*

$C_5H_{12}N_2O_2$ 132.162

(R)-form
D-form
[348-66-3]
Residue present in Gramicidins.

Hydrochloride: [16682-12-5]
Leaflets (EtOH aq.). Mp 239-240° dec. $[\alpha]_D^{26}$ -11 (c, 2 in H_2O). $[\alpha]_D^{25}$ -24.5 (c, 0.5 in 6*M* HCl).

N^5-*Ac:* [81397-94-6]
$C_7H_{14}N_2O_3$ 174.199
Cryst. (EtOH aq.). Mp 233-234° dec. $[\alpha]_D^{20}$ -24.6 (c, 1 in 5*M* HCl).

N^2,N^5-*Bis(benzyloxycarbonyl):* [13594-49-5]
$C_{21}H_{24}N_2O_6$ 400.43
Cryst. (Et_2O/petrol). Mp 112-113°.

(S)-form
L-form
[70-26-8]
Component of proteins, esp. of fungi; found in small amts. in plants in free state. Isol. from green algae *Codium decorticatum*, *Enteromorpha intestinalis* and *Ulva lactuca*. Manuf. by fermentation. Used in treatment of hyperammonaemia and liver disorders. Cryst. (EtOH/Et_2O). Sol. H_2O, EtOH; spar. sol. Et_2O.
Mp 140°. $[\alpha]_D^{25}$ +11.5.

▶ RM2980820
Hydrochloride: [3184-13-2]
Cryst. Mp 245° (233°) dec. $[\alpha]_D^{25}$ +28.3 (c, 2 in 5*M* HCl) $[\alpha]_D^{24}$ +23.6 (c, 4 in 6*N* HCl).

▶ RM2985000
Hydrochloride (1:2): [6211-16-1]
Cryst. (MeOH/Et_2O). Mp 202-203° Mp 230-232° dec. $[\alpha]_D^{25}$ +16.5 (c, 4 in H_2O).

N^2-*Ac:* N^{α}-*Acetylornithine*
[6205-08-9]
$C_7H_{14}N_2O_3$ 174.199
Intermed. in biosynth. of ornithine from Glutamic acid, G-113 in bacteria. Cryst.
Mp 226-227°. $[\alpha]_D^{25}$ +6.5 (c, 5 in H_2O).

N^5-*Ac:* N^{δ}-*Acetylornithine*
[2185-16-2]
Isol. from various plants, e.g. *Asplenium* spp. and grasses. Plates (MeOH).
Mp 266° (229°) dec. $[\alpha]_D^{24}$ +13.1 (H_2O). $[\alpha]_D^{25}$ +24 (c, 1 in 5*M* HCl).

N^2,N^5-*Di-Ac:* N^{α},N^{δ}-*Diacetylornithine, 9CI.* ***Bisorcic, INN***
[39825-23-5]
$C_9H_{16}N_2O_4$ 216.236
Hepatoprotective agent, psychostimulant. Log P -1.86 (calc).

N^5-*Benzoyl:* ***N^{δ}-Benzoylornithine***
[15647-43-5]
$C_{12}H_{16}N_2O_3$ 236.27
Constit. of the seeds of *Vicia pseudo-orobus*. Cryst. (H_2O).
Mp 205-213° dec. $[\alpha]_D^{20}$ +22.1 (c, 1 in 3*M* HCl).

N^2,N^5-*Dibenzoyl: Ornithuric acid*
[495-46-5]
$C_{19}H_{20}N_2O_4$ 340.378
Needles or plates (EtOH). Spar. sol. H_2O, EtOAc, hot EtOH; insol. Et_2O. Mp 188-189°. $[\alpha]_D^{20}$ +8.5 (EtOH aq.). $[\alpha]_D^{25}$ +24 (c, 1 in 5*M* HCl).

N^2,N^5-*Dibenzoyl, Me ester:* [70548-49-1]
$C_{20}H_{22}N_2O_4$ 354.405
Cryst. (EtOAc). Mp 148-150° (145.6°). $[\alpha]_D^{17}$ -13.2 (c, 1.4 in MeOH).

N^2,N^5-*Dibenzoyl, Et ester:*
$C_{21}H_{24}N_2O_4$ 368.432
Mp 155°.

N^2-*Benzyloxycarbonyl:* [2640-58-6]
$C_{13}H_{18}N_2O_4$ 266.296
Cryst. (H_2O). Mp 209-210°. $[\alpha]_D$ -8.4 (c, 1 in 5*M* HCl).

N^5-*Benzyloxycarbonyl:* [3304-51-6]
$C_{13}H_{18}N_2O_4$ 266.296
Cryst. (EtOH/HCl). Mp 254-255°.

N^5-*Benzyloxycarbonyl,* N^2-*Ac, Me ester:* [148824-34-4]
$C_{16}H_{22}N_2O_5$ 322.36
Cryst. (CH_2Cl_2/petrol). Mp 133°. $[\alpha]_D^{23}$ +28 ($CHCl_3$).

N^5-*Benzyloxycarbonyl,* N^2-tert-*butyloxycarbonyl:* [2480-93-5]
$C_{18}H_{26}N_2O_6$ 366.413
Cryst. Mp 95-97°. $[\alpha]_D^{20}$ -3.1 (c, 1.0 in AcOH).

N^5-*Benzyloxycarbonyl,* N^2-tert-*butyloxycarbonyl, Me ester:* [2480-95-7]
$C_{19}H_{28}N_2O_6$ 380.44

Cryst. (Et_2O/petrol). Mp 70-71°. $[\alpha]_D$ -10.5 (c, 1.0 in MeOH).

N^5-*Benzyloxycarbonyl,* N^2-tert-*butyloxycarbonyl,* tert-*butyl ester:* [53054-02-7]
$C_{22}H_{34}N_2O_6$ 422.52
Viscous oil. $[\alpha]_D$ -14.66 (c, 1.03 in MeOH).

N^5-*Benzyloxycarbonyl,* N^2-tert-*butyloxycarbonyl, 2,4,6-trichlorophenyl ester:* [70830-95-4]
$C_{24}H_{27}Cl_3N_2O_6$ 545.845
Cryst. (Et_2O/petrol). Mp 114-115°. $[\alpha]_D^{20}$ -24 (c, 1 in MeOH).

N^2,N^5-*Bis(benzyloxycarbonyl):* [2274-58-0]
Cryst. (Et_2O/petrol). Mp 112-114°. $[\alpha]_D^{20}$ -4 (c, 3 in MeOH).

N^2,N^5-*Bis(benzyloxycarbonyl), Me ester:*
$C_{22}H_{26}N_2O_6$ 414.457
Cryst. ($CHCl_3$/petrol). Mp 71-72°.

N^5-*Me:* [3485-66-3]
$C_6H_{14}N_2O_2$ 146.189
Present in *Atropa belladonna*. Alkaloid precursor.

N^5-*Me; hydrochloride:* [37149-01-2]
Mp 252°. $[\alpha]_D^{25}$ +34.3 (c, 0.5 in 6*M* HCl).

N^5-*Tri-Me; 4-Amino-4-carboxy*-N,N,N-*trimethyl-1-butanaminium*. **N^5-*Trimethylornithine***
[66101-16-4]
$C_8H_{18}N_2O_2$ 174.242
Constit. of the red alga *Vidalia volubilis*. Zwitterionic. Config. of nat. prod. not confirmed.

N^5-*Tri-Me,* N^2-*Ac: 4-(Acetylamino)-4-carbonyl*-N,N,N-*trimethyl-1-butanaminium*. **N^2-*Acetyl*-N^5-*trimethylornithine***
[147427-23-4]
$C_{10}H_{20}N_2O_3$ 216.28
Constit. of the red alga *Digenea simplex*.
$[\alpha]_D^{25}$ +16 (c, 0.43 in H_2O). Zwitterion.

N-*Hexa-Me:* ***Miokinine***
$C_{11}H_{25}N_2O_2^{\oplus}$ 217.331
Isol. from mammalian muscle.

(±)-*form* [616-07-9] pK_{a2} 8.98; pK_{a3} 10.73 (25°, 0.1*M* KNO_3). pK_{a1} 1.71; pK_{a2} 8.69; pK_{a3} 10.76 (25°).

Hydrochloride: [1069-31-4]
Cryst. (EtOH aq.). Mp 225°.

Hydrochloride (1:2): [15160-12-0]
Mp 230-232° dec.

N^5-*Benzoyl:* [69980-44-5]
Cryst. (H_2O). Mp 285-288°.

N^5-*Benzoyl,* N^2-*(4-methylbenzenesulfonyl):*
Needles (EtOH aq.). Mp 185°.

N^2,N^5-*Dibenzoyl:* [2478-55-9]
Needles (EtOH). Mp 187-188°.

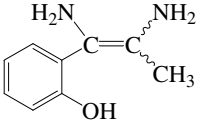
N^5-*Me; hydrochloride:*
Cryst. (EtOH aq.). Mp 242-243°.

[15647-44-6]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 494C; 494D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 587A; 587B (*ir*)
Karrer, P. *et al., Helv. Chim. Acta*, 1926, **9**, 301 (*derivs, synth*)
Hunter, A. *et al., Biochem. J.*, 1939, **33**, 29
Albertson, N.F. *et al., J.A.C.S.*, 1945, **67**, 2043 (*synth*)
Synge, R.C.M. *et al., Biochem. J.*, 1948, **42**, 99
Biochem. Prep., 1953, **3**, 96
Gaudry, R. *et al., Can. J. Chem.*, 1953, **31**, 1060 (*synth*)
Fowden, L. *et al., Nature (London)*, 1958, **182**, 406 (*occur, acetylornithine*)
Thompson, J.F. *et al., Arch. Biochem. Biophys.*, 1962, **99**, 326
Schröder, E. *et al., Annalen*, 1964, **679**, 221-223 (*N^5-benzyloxycarbonyl N^2-tert-butyloxycarbonyl Me ester*)
Katzin, L.I. *et al., J.A.C.S.*, 1964, **86**, 1655 (*ord*)
Lipson, M.A. *et al., J.O.C.*, 1964, **29**, 2392 (*bis(benzyloxycarbonyl), synth*)
Nakamura, A. *et al., Nippon Kagaku Zasshi*, 1965, **86**, 780 (*pmr*)
Gilbertson, T.J. *et al., J.A.C.S.*, 1967, **89**, 7085 (*synth, deriv*)
Ger. Pat., 1973, 2 219 874; *CA*, **78**, 98010t (*Bisorcic*)
Widmer, J. *et al., Helv. Chim. Acta*, 1974, **57**, 657-664 (*N^5-benzyloxycarbonyl N^2-tert-butyloxycarbonyl derivs, synth, ir, pmr*)
Gohring, W. *et al., Annalen*, 1975, 1765-1775 (*N^5-benzyloxycarbonyl N^2-tert-butyloxycarbonyl*)
Rabenstein, D.L. *et al., J. Magn. Reson.*, 1976, **24**, 27 (*cmr*)
Paik, W.K. *et al., Biochem. Med.*, 1978, **19**, 39 (*N^5-trimethylornithine*)
Kawai, M. *et al., Biopolymers*, 1978, **17**, 1549-1565 (*N^5-benzyloxycarbonyl N^2-tert-butyloxycarbonyl*)
Lammek, B. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1979, **53**, 333-342 (*N^5-benzyloxycarbonyl N^2-tert-butyloxycarbonyl derivs, synth, ir*)
Hedges, S.H. *et al., Phytochemistry*, 1981, **20**, 2064 (*isol, deriv*)
Hatanaka, S. *et al., Phytochemistry*, 1981, **20**, 2291 (*N^5-benzoylornithine*)
Chan, S.I. *et al., J.A.C.S.*, 1982, **104**, 6953 (*gramicidin, pmr*)
Dhaon, IM.K. *et al., J.O.C.*, 1982, **47**, 1962-1965 (*N^5-benzyloxycarbonyl N^2-tert-butyloxycarbonyl derivs*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 608
Kulik, W. *et al., Biomed. Environ. Mass Spectrom.*, 1988, **15**, 419 (*ms*)
Milewska, M.J. *et al., Synthesis*, 1990, 233 (*derivs, synth*)
Amino, Y. *et al., Bull. Chem. Soc. Jpn.*, 1991, **64**, 613 (*synth*)
Patti, A. *et al., J. Nat. Prod.*, 1992, **55**, 53; 1993, **56**, 432 (*N^5-Trimethylornithine, N^2-Acetyl-N^5-trimethylornithine*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OJU000

2-(1,2-Diamino-1-propenyl)phenol, 9CI D-123

1,2-Diamino-1-(2-hydroxyphenyl)propene
[173559-57-4]

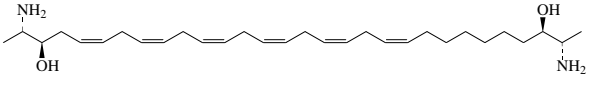


$C_9H_{12}N_2O$ 164.207
Present in shrimp shell (*Pandalus jordani*) waste. Antioxidant. Characterised spectroscopically.

Seymour, T.A. *et al., J. Agric. Food Chem.*, 1996, **44**, 682-685 (*isol, ms, uv, pmr*)

2,29-Diamino-5,8,11,14,17,20-triacontahexaene-3,28-diol, 9CI D-124

Leucettamol A
[145940-90-5]
[151124-32-2]

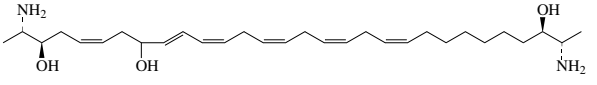


$C_{30}H_{52}N_2O_2$ 472.753
Isol. from *Leucetta microraphis*. Pale yellow oil. Probably racemic.

Kong, F. *et al., J.O.C.*, 1993, **58**, 970-971 (*isol*)

2,29-Diamino-5,9,11,14,17,20-triacontahexaene-3,8,28-triol D-125

Leucettamol B
[145940-91-6]
[151124-31-1]

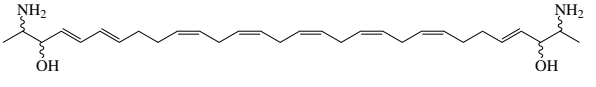


$C_{30}H_{52}N_2O_3$ 488.752
Isol. from *Leucetta microraphis*. Pale yellow oil. Probably racemic.

Kong, F. *et al., J.O.C.*, 1993, **58**, 970-971 (*isol*)

2,29-Diamino-4,6,10,13,16,19,22,26-triacontaoctaene-3,28-diol D-126

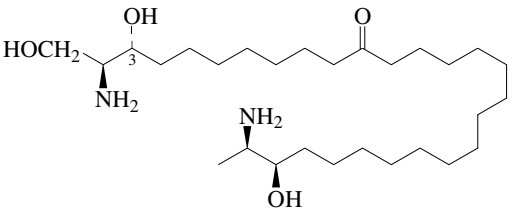
BRS 1



$C_{30}H_{48}N_2O_2$ 468.721

(2ξ,3ξ,4*E*,6*E*,10*Z*,13*Z*,16*Z*,19*Z*,22*Z*,26*E*,28ξ,29ξ)-*form* [193749-72-3]
Isol. from the Australian sponge *Leucetta microraphis*. Protein kinase C inhibitor.
Willis, R.H. *et al., Toxicon*, 1997, **35**, 1125-1129 (*isol*)
Kehraus, S. *et al., J.O.C.*, 2002, **67**, 4989-4992 (*isol*)

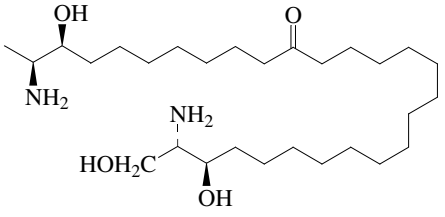
2,27-Diamino-1,3,26-trihydroxy-11-octacosanone D-127
Oceanin



$C_{28}H_{58}N_2O_4$ 486.777

(2*S*,3*R*,26*R*,27*R*)-*form* [276879-24-4]
Glass. $[\alpha]_D$ +14.7 (c, 0.3 in MeOH).
3-O-*β*-D-*Glucopyranoside:* ***Oceanapiside***
[251319-53-6]
$C_{34}H_{68}N_2O_9$ 648.919
Isol. from the sponge *Oceanapia phillipensis*. Antifungal agent. Amorph. solid. $[\alpha]_D$ -5.5 (c, 1.2 in MeOH).
Nicholas, G.M. *et al., J. Nat. Prod.*, 1999, **62**, 1678-1681 (*isol*)
Nicholas, G.M. *et al., J.A.C.S.*, 2000, **122**, 4011-4019 (*abs config*)

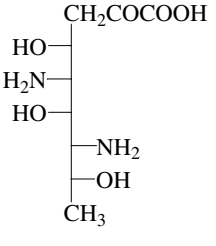
2,27-Diamino-3,26,28-trihydroxy-11-octacosanone D-128
Calyxinin



$C_{28}H_{58}N_2O_4$ 486.777

(2*S*,3*S*,26*R*,27*S*)-*form* [392688-08-3]
Gum. $[\alpha]_D$ -2.2 (c, 0.23 in MeOH).
28-O-*β*-D-*Glucopyranoside:* ***Calyxoside***
[392688-06-1]
$C_{34}H_{68}N_2O_9$ 648.919
Isol. from the sponge *Calyx* sp. Gel-like substance. $[\alpha]_D^{25}$ -15.8 (c, 0.32 in MeOH).
Zhou, B.-N. *et al., Tetrahedron*, 2001, **57**, 9549-9554 (*isol, pmr, cmr*)

5,7-Diamino-4,6,8-trihydroxy-2-oxononanoic acid D-129
5,7-Diamino-3,5,7,9-tetradeoxynon-2-ulosonic acid



(4*R*,5*R*,6*S*,7*R*,8*R*)-*form*

$C_9H_{18}N_2O_6$ 250.251
Exists mainly in pyranose forms.

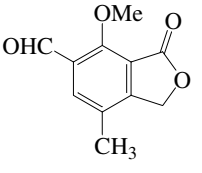
(4*R*,5*R*,6*S*,7*R*,8*R*)-*form*
D-glycero-D-talo-*form*. *4-Epilegionamic acid*
Obt. by mild hydrol. of *Legionella pneumophila* lipopolysaccharides. Formerly assigned as the L-*glycero*-D-*talo*- isomer.
N,N′-*Di-Ac:* $[\alpha]_D$ -3.9 (c, 0.2 in H_2O).

(4*S*,5*R*,6*S*,7*R*,8*R*)-*form*
D-glycero-D-galacto-*form*. ***Legionamic acid***
Isol. from lipopolysaccharides of *Legionella pneumophila*, *Pseudomonas fluorescens*, *Vibrio salmonicida*, *Vibrio alginolyticus* and *Acinetobacter baumannii*. Formerly assigned to either the L-*glycero*-D-*galacto*- or D-*glycero*-L-*galacto*- stereochem.
N,N′-*Di-Ac:* $[\alpha]_D$ +25.2 (c, 0.5 in H_2O).

(4*S*,5*R*,6*S*,7*R*,8*S*)-*form*
L-glycero-D-galacto-*form*. *8-Epilegionamic acid*
Isol. from lipopolysaccharides of *Pseudomonas aeruginosa*, *Salmonella arizonae* and *Yersinia ruckeri*. Formerly assigned as the enantiomeric D-*glycero*-L-*galacto*-form.
N^5-*(1-Iminoethyl),* N^7-*Ac: 5-Acetamidino-7-acetamido-3,5,7,9-tetradeoxy*-L-glycero-D-galacto-*non-2-ulosonic acid*
$C_{13}H_{23}N_3O_7$ 333.341
Component of the lipopolysaccharides of *Morganella morganii*.

(4*S*,5*S*,6*S*,7*S*,8*S*)-*form*
L-glycero-L-manno-*form*. ***Pseudaminic acid***
[93973-64-9]
Residue present in some O-specific polysaccharides of *Shigella boydii* and *Pseudomonas aeruginosa*.
N^5-*Ac,* N^7-*formyl: 5-Acetamido-3,5,7,9-tetradeoxy-7-formamido*-L-glycero-L-manno-*nonulosonic acid*
$C_{12}H_{20}N_2O_8$ 320.299
Isol. from polysaccharides of the marine *Pseudoalteromonas distincta* KMM 638. Residue present in O-specific side chain of *Pseudomonas aeruginosa* type 6 lipopolysaccharides.
N^5,N^7-*Di-Ac:*
$C_{13}H_{22}N_2O_8$ 334.325
Residue present in *Pseudomonas aeruginosa* O13 and *Proteus vulgaris* O39 polysaccharides.
N^7-*(3-Hydroxybutanoyl),* N^5-*Ac:*
$C_{15}H_{26}N_2O_9$ 378.378
Larger fragment present in *Shigella boydii* and *Pseudomonas aeruginosa* polysaccharides.
Knirel, Y.A. *et al., Carbohydr. Res.*, 1985, **141**, C1; 1986, **145**, C1; 2001, **333**, 241-249 (*Pseudaminic acid derivs*)
Muldoon, J. *et al., Carbohydr. Res.*, 2001, **330**, 231-239 (*N-Ac-N-formyl, isol*)
Tsvetkov, Y.E. *et al., Carbohydr. Res.*, 2001, **331**, 233-237; **335**, 221-243 (*synth, abs config, bibl*)
Kilcoyne, M. *et al., Carbohydr. Res.*, 2002, **337**, 1697-1702 (*iminoethyl Ac*)

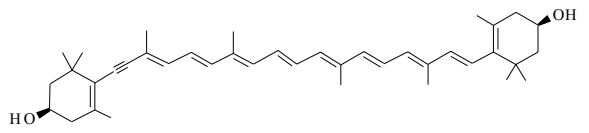
Diaporthelactone D-130
1,3-Dihydro-4-methoxy-7-methyl-3-oxo-5-isobenzofurancarboxaldehyde, 9CI. 6-Formyl-7-methoxy-4-methylphthalide
[876609-25-5]



$C_{11}H_{10}O_4$ 206.198
Prod. by a marine *Diaporthe* sp. strain HLY2. Cytotoxic. Cryst. (EtOAc).
Lin, X. *et al., FEMS Microbiol. Lett.*, 2005, **251**, 53-58 (*isol, pmr, cmr, ms*)

Diatoxanthin D-131

7,8-Didehydro-β,β-carotene-3,3′-diol
[31063-73-7]



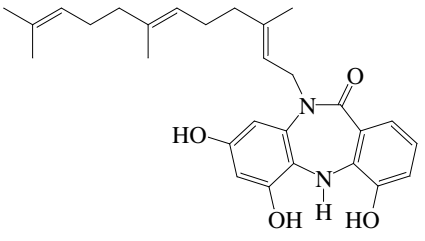
$C_{40}H_{54}O_2$ 566.865
Constit. of diatoms, algae and fish. Red needles (Me_2CO/petrol). Mp 201°.

5α,6α-Epoxide: See Diadinoxanthin A, D-116

Chapman, D.J. *et al., Phytochemistry*, 1966, **5**, 1331 (*isol*)
Mallams, A.K. *et al., Chem. Comm.*, 1967, 301 (*struct*)
de Ville, T.E. *et al., Chem. Comm.*, 1969, 1311 (*abs config*)
Nitsche, H. *et al., Tet. Lett.*, 1976, 4913 (*synth*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 118 (*bibl*)
Bjørnland, J. *et al., Phytochemistry*, 1989, **28**, 3347 (*isol, pmr*)
Haugen, J.A. *et al., Acta Chem. Scand.*, 1994, **48**, 899 (*synth*)

Diazepinomicin D-132

*5,10-Dihydro-4,6,8-trihydroxy-10-(3,7,11-trimethyl-2,6,10-dodecatrienyl)-11*H*-dibenzo[*b,e*][1,4]diazepin-11-one, 9CI*
[733035-26-2]

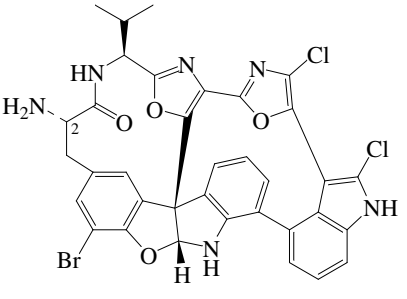


$C_{28}H_{34}N_2O_4$ 462.588
Closely related to Antibiotic BU 4664L. Prod. by *Micromonospora* sp. (strain DPJ12) isol. from *Didemnum proliferum*. Antimicrobial agent. λ_{max} 212; 230; 298 (MeOH aq.).

Charan, R.D. *et al., J. Nat. Prod.*, 2004, **67**, 1431-1433 (*isol, pmr, cmr, ms*)

Diazonamide B D-133

[131703-15-6]



Absolute Configuration

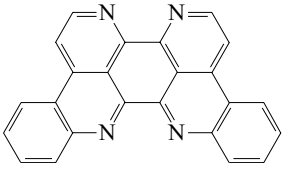
$C_{35}H_{25}BrCl_2N_6O_4$ 744.43
Struct. revised in 2001. Alkaloid from the marine ascidian *Diazona chinensis*. Cytotoxic. Amorph. λ_{max} 205 (ε 110000); 222 (ε 4700); 350 (sh) (MeOH/NaOH) (Derep). λ_{max} 215 (ε 21000); 281 (sh); 290 (ε 4900); 297 (sh) (MeOH) (Derep). λ_{max} 220 (ε 110000); 292 (ε 4700) (MeOH/NaOH) (Berdy).

Debromo, N^2*-(2S-hydroxy-3-methylbutanoyl):* ***Diazonamide A***
[131727-01-0]
$C_{40}H_{34}Cl_2N_6O_6$ 765.651
Alkaloid from *Diazona chinensis*. Cytotoxic. Glass. $[\alpha]_D$ -217.3 (c, 8.8 in MeOH). λ_{max} 204 (ε 101000); 296 (ε 4500); 350 (sh) (MeOH/NaOH) (Derep). λ_{max} 216 (ε 19200); 280 (sh); 290 (ε 5300); 298 (sh) (MeOH) (Derep).

Lindquist, N. *et al., J.A.C.S.*, 1991, **113**, 2303-2304 (*isol, struct*)
Li, J. *et al., Angew. Chem., Int. Ed.*, 2001, **40**, 4770-4773 (*struct*)
Ritter, T. *et al., Angew. Chem., Int. Ed.*, 2002, **41**, 2489-2495 (*rev*)
Burgett, A.W.G. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 4961-4966 (*synth*)
Nicolaou, K.C. *et al., J.A.C.S.*, 2004, **126**, 12888-12896; 12897-12906; 15316 (*synth*)

Dibenzo[*b,j*]dipyrido[4,3,2-*de*:2′,3′,4′-*gh*][1,10] phenanthroline, 9CI D-134

Eilatin
[120154-96-3]



$C_{24}H_{12}N_4$ 356.386
Alkaloid from the Red Sea tunicate *Eudistoma* sp. and by *Cystodytes* sp. Topoisomerase inhibitor, Ni chelating agent. Bright yellow cryst. ($CHCl_3$/MeOH/H_2O).
Mp 310°. λ_{max} 305 (ε 39800); 440 (ε 21500) (MeOH/HCl) (Derep). λ_{max} 242 (ε 48200); 286 (ε 36700); 363 (ε 11500); 388 (ε 21000); 408 (ε 30400); 434 (ε 27000) (MeOH) (Derep). λ_{max} 240 (ε 47600); 275 (ε 35400); 284 (ε 37700); 295 (ε 24800); 367 (ε 13200); 385 (ε 21700); 407 (ε 30500); 432 (ε 27100) (EtOH) (Berdy).

Rudi, A. *et al., Tet. Lett.*, 1988, **29**, 6655-6656 (*uv, ir, pmr, cmr, ms, cryst struct*)
Rudi, A. *et al., J.O.C.*, 1989, **54**, 5331-5337 (*isol, uv, ir, pmr, cmr, ms*)
Nakahara, S. *et al., Heterocycles*, 1993, **36**, 1139-1144 (*synth*)
Gellerman, G. *et al., Tet. Lett.*, 1993, **34**, 1827-1830 (*synth*)

Dibenzyl disulfide D-135

Bis(phenylmethyl) disulfide, 9CI. Benzyl disulfide, 8CI. FEMA 3617
[150-60-7]
$PhCH_2$-S-S-CH_2Ph
$C_{14}H_{14}S_2$ 246.397
Isol. from the sponge *Crella spinulata*. Constit. of the roots of *Petiveria alliacea*. Lubricating oil additive, corrosion inhibitor. Flavouring agent. Reference material used in elemental microanalysis. Pale yellow leaflets (EtOH) with burnt caramel odour. Mp 71-72°. Exposure to sunlight causes conversion to a second form, Mp 69-70°. λ_{max} 239 (ε 9200); 279 (ε 340) (MeOH).

▶ Skin and eye irritant. LD_{50} (rat, orl) 3780 mg/kg. JO1750000

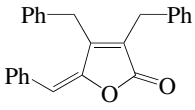
S-*Oxide:* S-*Phenylmethyl phenylmethanesulfinothioate.* S-*Benzyl benzylsulfinothioate.* ***Petivericin***
$C_{14}H_{14}OS_2$ 262.396
Constit. of the roots of *Petiveria alliacea*. Solid.
Mp 77-78°. λ_{max} 208 (log ε 4.43); 226 (log ε 4.3); 266 (log ε 3.36) (EtOH).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1184D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 445A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1104C (*ir*)
Cumper, C.W.N. *et al., J.C.S.*, 1965, 5323 (*synth*)
Bowie, J.H. *et al., J.C.S.(B)*, 1966, 946 (*ms*)
Voronkov, M.G. *et al., Zh. Strukt. Khim.*, 1968, **9**, 627 (*pmr*)
Reiter, G.F. *et al., J. Appl. Phys.*, 1970, **41**, 1368 (*uv*)
Srinivasan, R. *et al., Acta Cryst. B*, 1972, **28**, 2615 (*cryst struct*)
Analyst (London), 1972, **97**, 740 (*microanal*)
Subrahmanyan, B. *et al., Chem. Age India*, 1975, **26**, 333 (*synth, use*)
Meshram, H.M. *et al., Org. Prep. Proced. Int.*, 1993, **25**, 232 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 59
Bandaranayake, W.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1996, **113**, 499-502 (*isol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 267
Benevides, P.J.C. *et al., Phytochemistry*, 2001, **57**, 743-747 (*isol, pmr, cmr*)
Kubec, R. *et al., Phytochemistry*, 2002, **61**, 675-680 (*Petivericin*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DXH200

3,4-Dibenzyl-5-benzylidene-2(5*H*)-furanone D-136

*3,4-Bis(phenylmethyl)-5-(phenylmethylene)-2(5*H*)-furanone*



(*E*)-*form*

$C_{25}H_{20}O_2$ 352.432

(*E*)-*form*

Maculalactone C

[199600-35-6]

Isol. from the cyanobacterium *Kyrtuthrix maculans.*

Oil.

(*Z*)-*form*

Maculalactone B

[199600-34-5]

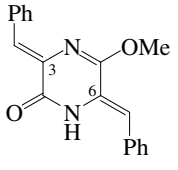
Isol. from *Kyrtuthrix maculans.*

Oil.

Lee, S.-C. *et al., J. Nat. Prod.*, 1998, **61**, 29-33 (*isol, ir, pmr, cmr*)
Brown, G.D. *et al., Tetrahedron*, 2004, **60**, 5439-5451 (*synth*)
Kar, A. *et al., Tetrahedron*, 2005, **61**, 5297-5302 (*synth*)

3,6-Dibenzylidene-3,6-dihydro-5-methoxy-2-pyrazinone D-137

*3,6-Dihydro-5-methyl-3,6-bis(phenylmethylene)-2(1*H*)-pyrazinone, 9CI*



$C_{19}H_{16}N_2O_2$ 304.348

(3*Z*,6*Z*)-*form*

Neihumicin

[111451-12-8]

Isol. from *Micromonospora neitmensis.* Exhibits antifungal and cytotoxic props. Yellow cryst. (EtOH). Sol. DMSO; fairly sol. MeOH; poorly sol. C_6H_6, hexane, H_2O.

Mp 175-176°. λ_{max} 243 (log ϵ 3.73); 364 (log ϵ 4.54) (MeOH).

4′-Methoxy: 6-Benzylidene-3,6-dihydro-5-methoxy-3-(4-methoxybenzylidene)-2-pyrazinone. ***4′-Methoxyneihumicin***

$C_{20}H_{18}N_2O_3$ 334.374

Prod. by an unidentified marine bacterium NPS0002/0014.

Yang, L.M. *et al., J. Antibiot.*, 1988, **41**, 481-487; 488-493; 494-501 (*isol, struct, synth*)
Laatsch, H. *et al., Dissertation*, Univ. or Göttingen, 2005, (*4′-Methoxyneihumicin*)

Dibromoacetaldehyde, 9CI, 8CI D-138

[3039-13-2]

Br_2CHCHO

$C_2H_2Br_2O$ 201.845

Isol. from the algae *Asparagopsis taxiformis* and *Falkenbergia rufolanosa.* Liq. V. sol. H_2O, EtOH. Bp 142°. Polymerises on standing.

Covalent hydrate: 2,2-Dibromo-1,1-ethanediol

Mp 58-60°.

Di-Et acetal: 1,1-Dibromo-2,2-diethoxyethane

[761-17-1]

$C_6H_{12}Br_2O_2$ 275.968

Bp_{12} 94-97°.

Mylo, B. *et al., Ber.*, 1912, **45**, 645 (*synth*)
Dworzak, R. *et al., Monatsh. Chem.*, 1925, **46**, 253 (*synth*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)

Dibromoacetic acid, 9CI, 8CI D-139

[631-64-1]

$Br_2CHCOOH$

$C_2H_2Br_2O_2$ 217.845

Deliquescent cryst. Sol. EtOH, Et_2O. Mp 48°. Bp 232-234° dec. Bp_{15} 75°. pK_a 1.48 (25°).

Me ester: [6482-26-4]

$C_3H_4Br_2O_2$ 231.871

Bp 182-184°.

Et ester: [617-33-4]

$C_4H_6Br_2O_2$ 245.898

Synthetic reagent. d_{20}^{20} 1.9. Bp 194° Bp_{74} 121°. n_D^{13} 1.5017.

Bromide:

C_2HBr_3O 280.741

Fuming liq. Bp 194°.

Amide: Dibromoacetamide

[598-70-9]

$C_2H_3Br_2NO$ 216.86

Constit. of *Asparagopsis taxiformis.*

Mp 156°.

Nitrile: Dibromoacetonitrile. Dibromocyanomethane

[3252-43-5]

C_2HBr_2N 198.845

Used with aldehydes and ketones to prepare α-bromoesters. Bp_{24} 67-69°.

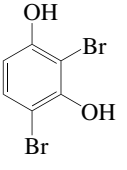
▶ AL8450000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 509A; 849A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 792B; 1367A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 807B (*ir*)
Genvresse, M.P. *et al., Bull. Soc. Chim. Fr.*, 1892, **7**, 365 (*synth*)
Org. Synth., Coll. Vol., 4, 1963, 254 (*nitrile*)
Parrot, J. *et al., Bull. Soc. Chim. Fr.*, 1964, 1063 (*synth*)
Netherlands Pat., 1965, 6 401 521; *CA*, **64**, 3360 (*synth*)
Elvidge, J.A. *et al., J.C.S.(C)*, 1968, 2188 (*use, nitrile*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 195; 1975, **5**, 186 (*use*)
Legris, C. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1974, **278**, 77 (*use, nitrile*)
Woolard, F.X. *et al., Tetrahedron*, 1976, **32**, 2843-2846 (*amide, isol*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **3**, 1543-1544 (*nitrile, use*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2423-2424 (*Et ester, use*)

2,4-Dibromo-1,3-benzenediol, 9CI D-140

2,4-Dibromoresorcinol, 8CI

[18011-67-1]



$C_6H_4Br_2O_2$ 267.904

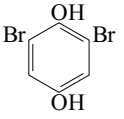
Isol. from an acorn worm *Ptychodera* sp. Needles (H_2O).

Mp 93-94°.

Davis, T.L. *et al., J.A.C.S.*, 1934, **56**, 129-132 (*synth*)
Higa, T. *et al., Tetrahedron*, 1987, **43**, 1063-1070 (*isol, ms*)
Kiehlmann, E. *et al., Can. J. Chem.*, 1989, **67**, 335-344 (*synth, cmr*)
Weisz, A. *et al., Org. Mass Spectrom.*, 1992, **27**, 891-895 (*ms*)
Sijbesma, R.P. *et al., J.A.C.S.*, 1993, **115**, 8999-9005 (*pmr*)

2,6-Dibromo-1,4-benzenediol, 9CI D-141

2,6-Dibromohydroquinone, 8CI. 2,6-Dibromoquinol. 1,3-Dibromo-2,5-dihydroxybenzene
[3333-25-3]



$C_6H_4Br_2O_2$ 267.904
Isol. from the marine acorn worms *Ptychodera* spp. and from the sponge *Verongia aurea*. Cryst. (toluene).
Mp 166-167° (164°).

4-Ac: 4-Acetoxy-2,6-dibromophenol
[150900-94-0]
$C_8H_6Br_2O_3$ 309.942
Isol. from *Ptychodera bahamensis.*

Di-Ac:
$C_{10}H_8Br_2O_4$ 351.979
Mp 116.5°.

1-Me ether: 3,5-Dibromo-4-methoxyphenol, 9CI
[13670-73-0]
$C_7H_6Br_2O_2$ 281.931
Constit. of the sponges *Axinella* sp. and *Verongia* sp.
Mp 149-151°.

4-Me ether: 2,6-Dibromo-4-methoxyphenol, 9CI
[2423-74-7]
$C_7H_6Br_2O_2$ 281.931
Isol. from *Verongia aurea*. Cryst. (heptane).
Mp 88-89°.

Di-Me ether: 1,3-Dibromo-2,5-dimethoxybenzene, 9CI
[74076-59-8]
$C_8H_8Br_2O_2$ 295.958
Mp 56°.

Ungnade, H.E. *et al., J.O.C.*, 1951, **16**, 64-69 (*synth*)
Terent'ev, A.P. *et al., Zh. Obshch. Khim.*, 1954, **24**, 1433-1435; *J. Gen. Chem. USSR (Engl. Transl.)*, 1954, **24**, 1415-1417 (*synth*)
Linneaus, C.D. *et al., J.O.C.*, 1966, **31**, 3666-3671 (*mono-Me ethers, synth, ir*)
Goo, Y.M. *et al., CA*, 1980, **92**, 169100t (*isol*)
Higa, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **65**, 525-530 (*isol*)
Kajigaeshi, S. *et al., Chem. Lett.*, 1987, 627-630 (*synth, 4-Me ether*)
Norte, M. *et al., Tetrahedron*, 1988, **44**, 4973-4980 (*1-Me ether, synth, ir, pmr*)
Corgiat, J.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1993, **106**, 83-86 (*isol, 4-Ac*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 148-151 (*1-Me ether, isol*)

3,5-Dibromo-1,2-benzenediol, 9CI D-142

3,5-Dibromocatechol
[111167-61-4]
$C_6H_4Br_2O_2$ 267.904
Metab. of the sponge *Dysidea* sp. 15-Lipoxygenase inhibitor.
Mp 58-60°.

Di-Ac:
$C_{10}H_8Br_2O_4$ 351.979
Mp 96°.

1-Me ether: 2,4-Dibromo-6-methoxyphenol, 9CI
[53948-36-0]
$C_7H_6Br_2O_2$ 281.931
Cryst. Mp 66-67°.

2-Me ether: 3,5-Dibromo-2-methoxyphenol, 9CI
[79893-39-3]
$C_7H_6Br_2O_2$ 281.931
Cryst. Mp 67-68°. $Bp_{0.24}$ 120°.

Cousin, H. *et al., Ann. Chim. (Paris)*, 1898, **13**, 480-555 (*synth*)
Kakinami, T. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 3373-3375 (*1-Me ether, synth*)
Broderick, J.B. *et al., Biochemistry*, 1991, **30**, 7349-7358 (*synth*)
Green, K. *et al., J.O.C.*, 1991, **56**, 4325-4326 (*2-Me ether, synth, pmr, cmr*)
Fu, X. *et al., J. Nat. Prod.*, 1995, **58**, 1384-1391 (*isol*)

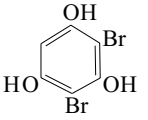
4,5-Dibromo-1,3-benzenediol, 9CI D-143

4,5-Dibromoresorcinol
[170473-58-2]
$C_6H_4Br_2O_2$ 267.904
Metab. of the sponge *Dysidea* sp.

Fu, X. *et al., J. Nat. Prod.*, 1995, **58**, 1384-1391 (*isol, ir, pmr, ms, props*)

2,4-Dibromo-1,3,5-benzenetriol D-144

Dibromophloroglucinol
[84743-75-9]



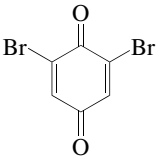
$C_6H_4Br_2O_3$ 283.904
Constit. of *Rhabdonia verticillata*. Cryst. (H_2O).
Mp 146°.

Tri-Me ether: 2,4-Dibromo-1,3,5-trimethoxybenzene, 9CI
[5876-90-4]
$C_9H_{10}Br_2O_3$ 325.984
Constit. of *Rytiphloea tinctoria*. Cryst. (hexane).
Mp 130°. Genus name incorrectly given as Rhytiphlea.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 128C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 946A (*ir*)
Yanovskaya, L.A. *et al., Zh. Obshch. Khim.*, 1952, **22**, 1594; *CA*, **47**, 8032 (*synth*)
Chevolot-Magueur, A.-M. *et al., Phytochemistry*, 1976, **15**, 767 (*isol, struct, synth*)
Blackman, A.J. *et al., Phytochemistry*, 1982, **21**, 2141 (*isol*)

2,6-Dibromo-1,4-benzoquinone D-145

2,6-Dibromo-2,5-cyclohexadiene-1,4-dione, 9CI
[19643-45-9]

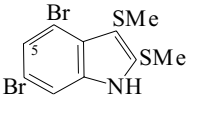


$C_6H_2Br_2O_2$ 265.889
Constit. of the sponge *Verongia aurea*. Also isol. from *Aplysina fistularis.* Shows antibacterial activity. Yellow needles (EtOH).
Mp 131°.

4-Oxime:
$C_6H_3Br_2NO_2$ 280.903
Yellow cryst. Mp 170°.

Hodgson, H.H. *et al., J.C.S.*, 1930, 1085 (*synth*)
Ramart-Lucas, P. *et al., Bull. Soc. Chim. Fr.*, 1949, 901 (*deriv*)
Flaig, W. *et al., Annalen*, 1958, **618**, 117 (*uv*)
Nagara, K.V. *et al., Arch. Biochem. Biophys.*, 1982, **215**, 544 (*isol*)
Saá, J.M. *et al., Tet. Lett.*, 1986, **27**, 5125 (*synth*)
Omura, K. *et al., Synthesis*, 1998, 1145-1148 (*synth*)

4,6-Dibromo-2,3-bis(methylthio)-1*H*-indole D-146



$C_{10}H_9Br_2NS_2$ 367.128
Isol. from the red algae *Laurencia brongniartii* and *Laurencia grevilleana*.
Mp 108.5-110°.

2-S-*Oxide: 4,6-Dibromo-2-(methylsulfinyl)-3-(methylthio)-1*H-*indole.* ***Itomanindole A***
[119340-95-3]
$C_{10}H_9Br_2NOS_2$ 383.127
Isol. from *Laurencia brongniartii*. Cryst. ($CHCl_3$).
Mp 134-136°. $[\alpha]_D$ +8 (c, 1.56 in $CHCl_3$). Partial racemate.

3-S-*Oxide: 4,6-Dibromo-3-(methylsulfinyl)-2-(methylthio)-1*H-*indole.* ***Itomanindole B***
[119340-97-5]
$C_{10}H_9Br_2NOS_2$ 383.127
Isol. from *Laurencia brongniartii*. Cryst. ($CHCl_3$/MeOH).
Mp 104-106°. $[\alpha]_D$ -38 (c, 0.33 in $CHCl_3$/MeOH 1:1). Partial racemate.

2,3-Di-S-*oxide: 4,6-Dibromo-2,3-bis(methylsulfinyl)-1*H-*indole*
$C_{10}H_9Br_2NO_2S_2$ 399.127
Isol. from *Laurencia brongniartii*.
Mp 132-134°. λ_{max} 230 (log ϵ 4.4); 310 (log ϵ 4) (MeOH).

N-*Me, 2*-S-*oxide:* Mp 117.5-118.5°. $[\alpha]_D$ -6.9 (c, 0.54 in $CHCl_3$).

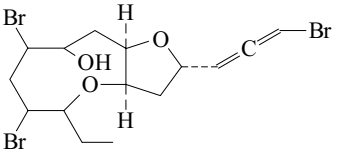
5-Bromo: ***4,5,6-Tribromo-2,3-bis(methylthio)-1H-indole***
[128351-86-0]
$C_{10}H_8Br_3NS_2$ 446.024
Isol. from *Laurencia brongniartii* and *Laurencia grevilleana*.

5-Bromo, 2-S-*oxide: 4,5,6-Tribromo-2-(methylsulfinyl)-3-(methylthio)-1*H-*indole*
$C_{10}H_8Br_3NOS_2$ 462.023
Isol. from *Laurencia brongniartii*.
Mp 142-144°. λ_{max} 234 (log ϵ 4.6); 315 (log ϵ 4.2) (MeOH).

Christophersen, C. *et al., Alkaloids (N.Y.)*, 1985, **24**, 25
Tanaka, J. *et al., Tetrahedron*, 1989, **45**, 7301-7310 (*isol, pmr, cmr, cryst struct*)
El-Gamal, A.A. *et al., J. Nat. Prod.*, 2005, **68**, 815-817 (*isol, pmr, cmr, ms*)

6,8-Dibromo-2-(3-bromo-1,2-propadienyl)-5-ethyldecahydrofuro[3,2-*b*]oxonin-9-ol, 9CI D-147

4,6,15-Tribromo-3,10:9,12-diepoxy-13,14-pentadecadien-7-ol. 1,10,12-Tribromo-4,7:6,13-diepoxy-1,2-pentadecadien-9-ol

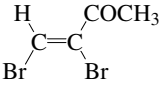


$C_{15}H_{21}Br_3O_3$ 489.041

Ac: 9-Acetoxy-1,10,12-tribromo-4,7:6,13-bisepoxy-1,2-pentadecadiene
[125092-25-3]
$C_{17}H_{23}Br_3O_4$ 531.078
Metab. of the red alga *Laurencia implicata*. Oil. $[\alpha]_D$ +2.16 (c, 0.007 in $CHCl_3$).
Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1685 (*isol, pmr, cmr, ir*)

3,4-Dibromo-3-buten-2-one, 9CI D-148

[70442-41-0]

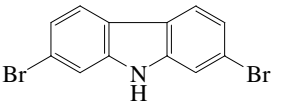


$C_4H_4Br_2O$ 227.883

(Z)-form [56020-84-9]
Isol. from *Asparagopsis taxiformis.*
Burreson, B.J. *et al., Tet. Lett.*, 1975, 473-476 (*isol*)
McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367-374 (*isol*)

2,7-Dibromo-9*H*-carbazole, 9CI D-149

[136630-39-2]

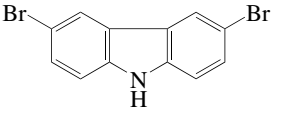


$C_{12}H_7Br_2N$ 325.002
Alkaloid from the cyanobacterium *Kyrtuthrix maculans.* Prisms (hexane/C_6H_6).
Mp 198-203° Mp 236-238°.

Yamato, T. *et al., J.O.C.*, 1991, **56**, 6248-6250 (*synth, ir, pmr*)
Lee, S.-C. *et al., Phytochemistry*, 1999, **52**, 537-540 (*isol, ir, pmr, cmr, ms*)
Dierschke, F. *et al., Synthesis*, 2003, 2471-2472 (*synth, pmr, cmr*)

3,6-Dibromo-9*H*-carbazole, 9CI D-150

[6825-20-3]



$C_{12}H_7Br_2N$ 325.002
Alkaloid from the cyanobacterium *Kyrtuthrix maculans.* Prisms or needles (EtOH). Sol. $CHCl_3$, C_6H_6, spar. sol. petrol.
Mp 212-213°.

N-*Benzoyl:*
$C_{19}H_{11}Br_2NO$ 429.11
Mp 213-214°.

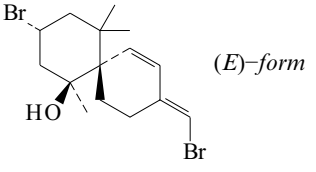
N-*Et:* [33255-13-9]
$C_{14}H_{11}Br_2N$ 353.056
Needles (EtOH). Mp 140-141°.

N-*Ph:* [57103-20-5]
$C_{18}H_{11}Br_2N$ 401.1
Needles (EtOH). Mp 66-67°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 680B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 162B (*nmr*)
McLintock, J. *et al., J.C.S.*, 1927, 1214 (*synth*)
Lopatinskii, V.P. *et al., CA*, 1966, **65**, 2203e (*synth*)
Smith, K. *et al., Tetrahedron*, 1992, **48**, 7479-7488 (*synth, pmr, cmr*)
Polivin, Y.N. *et al., Izv. Akad. Nauk, Ser. Khim.*, 1993, 234-235 (*synth*)
Park, M. *et al., Tetrahedron*, 1998, **54**, 12707-12714 (*N-Et, N-Ph, synth, pmr, cmr*)
Lee, S.-C. *et al., Phytochemistry*, 1999, **52**, 537-540 (*isol, pmr, cmr, ms*)

9,15-Dibromo-1,3(15)-chamigradien-7-ol D-151

3-Bromo-9-bromomethylene-1,5,5-trimethylspiro[5.5]undec-7-en-1-ol



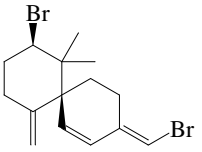
(E)–form

$C_{15}H_{22}Br_2O$ 378.146
Shows antibacterial and antifungal activity. Exhibits algicidal effect. Toxic to brine shrimp.

(E)-form [86161-35-5]
Constit. of the digestive gland of the sea hare *Aplysia dactylomela*. Shows antibacterial and antifungal activity. Exhibits algicidal effect. Toxic to brine shrimp. Cryst.
Mp 84-86°. $[\alpha]_D$ -64 (c, 0.29 in $CHCl_3$). λ_{max} 246 (ϵ 39000) (EtOH) (Derep).

(*Z*)-*form* [86105-62-6]
From *Aplysia dactylomela*.
Oil.
González, A.G. *et al., Tet. Lett.*, 1983, **24**, 847-848 (*isol, cryst struct, abs config*)
Wessels, M. *et al., J. Nat. Prod.*, 2000, **63**, 920-928 (*cmrl activity*)

10,15-Dibromo-1,3(15),7(14)-chamigratriene D-152

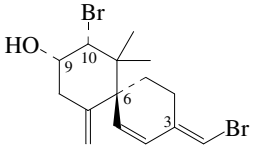


$C_{15}H_{20}Br_2$ 360.131

(*E*)-*form* [388110-04-1]
Constit. of *Laurencia scoparia*.
Oil. $[\alpha]_D^{25}$ -17.4 (c, 0.23 in $CHCl_3$).

(*Z*)-*form* [388110-03-0]
Constit. of *Laurencia scoparia*.
Oil. $[\alpha]_D^{25}$ +9 (c, 1.4 in $CHCl_3$).
Davyt, D. *et al., J. Nat. Prod.*, 2001, **64**, 1552-1555 (*isol, pmr, cmr*)

10,15-Dibromo-1,3(15),7(14)-chamigratrien-9-ol D-153
[70449-76-2, 71565-17-8, 73651-01-1]



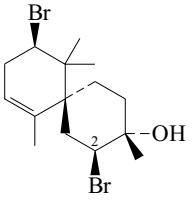
(3(15),*E*,6*S*,9*S*,10*R*)-*form*

$C_{15}H_{20}Br_2O$ 376.13

(3(15)*E*,6*S*,9*S*,10*R*)-*form* [124649-21-4]
Constit. of *Aplysia dactylomela* and *Laurencia majuscula*.
Oil. Sol. Me_2CO, C_6H_6; fairly sol. hexane; poorly sol. H_2O.
$[\alpha]_D$ -40 (c, 0.01 in $CHCl_3$). λ_{max} 247 (ϵ 16000) (EtOH).

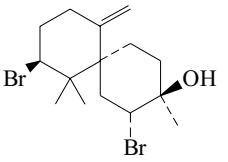
(3(15)*Z*,6*S*,9*S*,10*R*)-*form* [124649-20-3]
Constit. of *Laurencia majuscula* and *Laurencia chondrioides*.
Oil. $[\alpha]_D$ +2.7 (c, 0.002 in $CHCl_3$).
Schmitz, F.J. *et al., J.A.C.S.*, 1982, **104**, 6415-6423 (*Aplysia dactyomela constit*)
Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1591-1603; 1992, **45**, 1611-1623 (*Laurencia majuscula constits*)
Bansemir, A. *et al., Chem. Biodiversity*, 2004, **1**, 463-467 (*Laurencia chondrioides constit*)

2,10-Dibromo-7-chamigren-3-ol D-154
2,10-Dibromo-3-hydroxy-α-chamigrene
[89203-65-6]



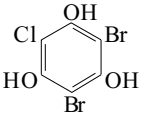
$C_{15}H_{24}Br_2O$ 380.162
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D^{18}$ -27 (c, 2.13 in $CHCl_3$).
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 3824

2,10-Dibromo-7(14)-chamigren-3-ol D-155
2,8-Dibromo-5(14)-chamigren-9-ol
[104643-38-1]



$C_{15}H_{24}Br_2O$ 380.162
Constit. of *Laurencia flexilis*. Oil.
De Nys, R. *et al., Phytochemistry*, 1993, **34**, 725-728 (*isol, pmr, cmr*)

2,4-Dibromo-6-chloro-1,3,5-benzenetriol D-156
Dibromochlorophloroglucinol. Chlorodibromophloroglucinol
[84743-78-2]

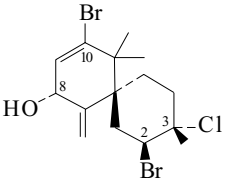


$C_6H_3Br_2ClO_3$ 318.349
Constit. of *Rhabdonia verticillata*.
Blackman, A.J. *et al., Phytochemistry*, 1982, **21**, 2141 (*isol*)

1,4-Dibromo-3-chloro-3-buten-2-one, 9CI D-157
[70442-43-2]
$BrCH{=}CClCOCH_2Br$
$C_4H_3Br_2ClO$ 262.328
Isol. from *Asparagopsis taxiformis*.
Fenical, W. *et al., Proc. Int. Seaweed Symp.*, 1977, **9**, 387-400; *CA*, **91**, 14474y (*synth*)

4,4-Dibromo-3-chloro-3-buten-2-one, 9CI D-158
[70442-44-3]
$Br_2C{=}CClCOCH_3$
$C_4H_3Br_2ClO$ 262.328
Isol. from *Asparagopsis taxiformis*.
Fenical, W. *et al., Proc. Int. Seaweed Symp.*, 1977, **9**, 387-400; *CA*, **91**, 14474y (*synth*)

2,10-Dibromo-3-chloro-7(14),9-chamigradien-8-ol D-159



$C_{15}H_{21}Br_2ClO$ 412.591
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D^{20}$ -24.2 (c, 1.88 in$CHCl_3$).

8-Ketone: ***2,10-Dibromo-3-chloro-7(14),9-chamigradien-8-one***
[98752-13-7]
$C_{15}H_{19}Br_2ClO$ 410.575
From *Laurencia nipponica*. Pale yellow oil. $[\alpha]_D^{22}$ +1.95 (c, 1.59 in $CHCl_3$).

8-Ketone, 10-debromo: ***2-Bromo-3-chloro-7(14),9-chamigradien-8-one***
[102043-63-0]
$C_{15}H_{20}BrClO$ 331.679
Constit. of *Aplysia dactylomela*. Cryst.

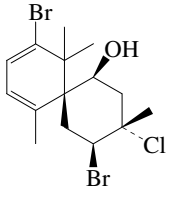
Mp 98-100°. $[\alpha]_D$ +19.6 (c, 0.64 in $CHCl_3$).

Enantiomer, 8-ketone, 10-debromo: [193077-96-2]
$C_{15}H_{20}BrClO$ 331.679
Constit. of *Laurencia majuscula*.

Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 2435
Sakai, R. *et al., Helv. Chim. Acta*, 1986, **69**, 91-105 (*isol, Aplysia*)
Masuda, M. *et al., Phycol. Res.*, 1997, **45**, 59-64; *CA*, **127**, 133150 (*Laurencia majuscula constit*)

4,10-Dibromo-3-chloro-7,9-chamigradien-1-ol D-160

[222837-29-8]

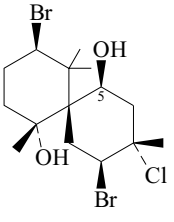


$C_{15}H_{21}Br_2ClO$ 412.591
Constit. of *Laurencia nidifica*. Oil. $[\alpha]_D$ -36 (c, 0.12 in $CHCl_3$).

Kimura, J. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 289-292 (*isol, pmr, cmr*)

2,10-Dibromo-3-chloro-5,7-chamigranediol D-161

[54462-54-3]



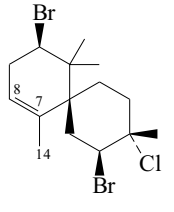
$C_{15}H_{25}Br_2ClO_2$ 432.622

5-Ac: 5-Acetoxy-2,10-dibromo-3-chloro-7-chamigranol. ***Acetoxyintricatol***
$C_{17}H_{27}Br_2ClO_3$ 474.659
Constit. of *Laurencia intricata*. Cryst.(CCl_4/hexane).

McMillan, J.A. *et al., Tet. Lett.*, 1974, 2039

2,10-Dibromo-3-chloro-7-chamigrene D-162

[57685-65-1]



$C_{15}H_{23}Br_2Cl$ 398.607
Constit. of *Laurencia glandulifera*. Oil. $[\alpha]_D$ -14 (c, 1.45 in $CHCl_3$).

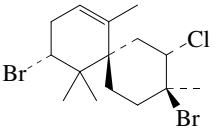
$\Delta^{7(14)}$-Isomer: 2,10-Dibromo-3-chloro-7(14)-chamigrene. ***Nidificene****. Intricatene*
[54928-01-7]
$C_{15}H_{23}Br_2Cl$ 398.607
Constit. of *Laurencia nipponica* and *Laurencia nidifica*. Cryst. (hexane).
Mp 76-77°. $[\alpha]_D^{15}$ +30.6 (c, 1.4 in $CHCl_3$).

$\Delta^{7(14)}$-Isomer, 8α-Hydroxy: ***2,10-Dibromo-3-chloro-7(14)-chamigren-8-ol****. 2,10-Dibromo-3-chloro-8-hydroxy-β-chamigrene*
[89299-70-7]
$C_{15}H_{23}Br_2ClO$ 414.607
From *Laurencia nipponica*. Oil. $[\alpha]_D^{17}$ +3.33 (c, 1.2 in $CHCl_3$).

[88586-20-3]

Waraszkiewicz, S.M. *et al., Tet. Lett.*, 1974, 2003 (*Nidificene*)
Suzuki, M. *et al., Tetrahedron*, 1979, **35**, 823 (*abs config*)
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 3824
McPhail, K.L. *et al., J. Nat. Prod.*, 1999, **62**, 1618-1623 (*Nidificene, pmr, cmr*)

3,10-Dibromo-2-chloro-7-chamigrene D-163



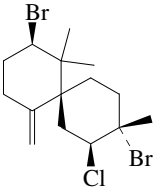
$C_{15}H_{23}Br_2Cl$ 398.607

(2S,3S,6S,10R)-form [870480-95-8]
Constit. of *Aplysia dactylomela*.
Oil. $[\alpha]_D^{20}$ -210.2 (c, 0.033 in $CHCl_3$).

Dias, T. *et al., J. Nat. Prod.*, 2005, **68**, 1677-1679 (*Aplysia dactylomela constit*)

3,10-Dibromo-2-chloro-7(14)-chamigrene D-164

Obtusane



(+)-*form*

$C_{15}H_{23}Br_2Cl$ 398.607

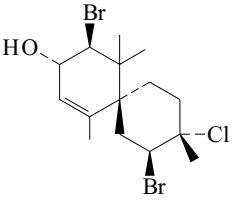
(+)-form [73436-46-1]
Constit. of *Laurencia obtusa*.
Cryst.
Mp 174-175°. $[\alpha]_D$ +38.

(-)-form
Constit. of *Laurencia nipponica*.
Cryst. (diispropyl ether). $[\alpha]_D^{22}$ -38.5 (c, 0.55 in $CHCl_3$).

González, A.G. *et al., Tet. Lett.*, 1979, 2719 (*(+)-form*)
Furusaki, A. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 3501-3502 (*(-)-form, cryst struct*)

2,10-Dibromo-3-chloro-7-chamigren-9-ol D-165

[60031-96-1]



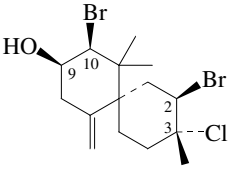
$C_{15}H_{23}Br_2ClO$ 414.607
Metab. of *Laurencia nipponica*, *Laurencia pacifica* and *Laurencia nidifica*. Cryst. (diisopropyl ether).
Mp 119-120°. $[\alpha]_D^{19}$ +25.3 (c, 1.39 in $CHCl_3$).

Ac: [76015-99-1]
$C_{17}H_{25}Br_2ClO_2$ 456.644
Isol. from *Aplysia dactylomela*.

Fenical, W. *et al., Phytochemistry*, 1976, **15**, 511-512
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 3371-3373 (*isol*)

Rovirosa, J. *et al., Bol. Soc. Chil. Quim.*, 1991, **36**, 153-156 (*Ac*)
Kimura, J. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 289-292 (*isol*)

2,10-Dibromo-3-chloro-7(14)-chamigren-9-ol D-166



(2*R*,3*R*,6*S*,9*R*,10*S*)-*form*

$C_{15}H_{23}Br_2ClO$ 414.607

(2*R*,3*R*,6*S*,9*R*,10*S*)-*form*
Cartilagineol. *Alloisoobtusol*
[185215-99-0]
Constit. of *Laurencia cartilaginea* and *Aplysia dactylomela*.
Cryst.
Mp 62-63°. $[\alpha]_D$ -32 (c, 0.25 in $CHCl_3$). Struct. revised in 1998.

(2*R*,3*R*,6*S*,9*S*,10*R*)-*form*
Rogiolol
[131683-12-0]
Oil. $[\alpha]_D^{20}$ -7.7 (c, 0.86 in $CHCl_3$).

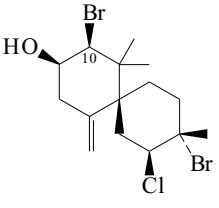
Ac: ***Rogiolol acetate***
[131683-11-9]
$C_{17}H_{25}Br_2ClO_2$ 456.644
Constit. of *Spongia zimocca*. Prisms (hexane).
Mp 129-130°. $[\alpha]_D^{20}$ +24.1 (c, 0.7 in $CHCl_3$).

(2*S*,3*S*,6*S*,9*S*,10*R*)-*form* [124649-22-5]
Metab. of *Laurencia majuscula*.
Oil. $[\alpha]_D$ -3.6 (c, 0.04 in $CHCl_3$).

Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1591 (*isol, pmr, cmr*)
Guella, G. *et al., Helv. Chim. Acta*, 1990, **73**, 1612 (*Rogiolol acetate*)
Juagdan, E.G. *et al., Tetrahedron*, 1997, **53**, 521-528 (*Alloisoobtusol*)
Francisco, M.E.Y. *et al., Tet. Lett.*, 1998, **39**, 5289-5292 (*Cartilagineol, cryst struct*)
Wessels, M. *et al., J. Nat. Prod.*, 2000, **63**, 920-928 (*Cartilagineol*)

3,10-Dibromo-2-chloro-7(14)-chamigren-9-ol D-167

Obtusol
[73494-22-1]



$C_{15}H_{23}Br_2ClO$ 414.607
Constit. of *Laurencia obtusa* and *Aplysia dactylomela*. Shows antifungal, algicidal and antimutagenic activity. Cryst. Poorly sol. hexane.
Mp 145-146°. $[\alpha]_D$ +14.3 (c, 0.38 in $CHCl_3$).

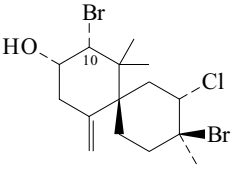
10-Debromo: ***3-Bromo-2-chloro-7(14)-chamigren-9-ol***
[73465-57-3]
$C_{15}H_{24}BrClO$ 335.711
Constit. of *Laurencia obtusa*.
Mp 81-82° (as Ac). $[\alpha]_D$ +11 (Ac).

7S,14-Epoxide: 3,10-Dibromo-2-chloro-7,14-epoxy-9-chamigranol.
Obtusol epoxide
[126005-78-5]
$C_{15}H_{23}Br_2ClO_2$ 430.606
Isol. from *Laurencia obtusa*. Needles.
Mp 103-105°. $[\alpha]_D^{25}$ +5.9 (c, 1.69 in $CHCl_3$).

González, A.G. *et al., Tet. Lett.*, 1976, 3051; 1979, 2717-2718; 2719-2722 (*isol, struct, cmr*)
Martin, J.D. *et al., Phytochemistry*, 1989, **28**, 3365 (*epoxide*)
Wessels, M. *et al., J. Nat. Prod.*, 2000, **63**, 920-928 (*isol, pmr, cmr, activity*)

3,10-Dibromo-2-chloro-7(14)-chamigren-9-ol D-168

Isoobtusol
[73494-23-2]



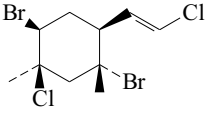
$C_{15}H_{23}Br_2ClO$ 414.607
Constit. of *Laurencia obtusa* and *Aplysia dactylomela*. Toxic to brine shrimp. Cryst. Poorly sol. hexane.
Mp 118-120°. $[\alpha]_D$ +33.

Ac: Acetylisoobtusol. Isoobtusol acetate
[73465-63-1]
[81445-90-1]
$C_{17}H_{25}Br_2ClO_2$ 456.644
Constit. of *Aplysia dactylomela*. Cytotoxic agent. $[\alpha]_D$ +57.9 (c, 0.38 in $CHCl_3$).

10-Debromo: ***3-Bromo-4-chloro-7(14)-chamigren-9-ol***
[73465-58-4]
$C_{15}H_{24}BrClO$ 335.711
Constit. of *Laurencia obtusa*. Cryst. (as Ac).
Mp 102-104° (Ac). $[\alpha]_D$ +73 (Ac).

González, A.G. *et al., Tet. Lett.*, 1976, 3051; 1979, 2717; 2719 (*isol, cryst struct, cmr*)
Schmitz, F.J. *et al., J.A.C.S.*, 1982, **104**, 6415 (*Ac, isol*)
Wessels, M. *et al., J. Nat. Prod.*, 2000, **63**, 920-928 (*isol, pmr, cmr, activity*)

1,4-Dibromo-5-chloro-2-(2-chloroethenyl)-1,5-dimethylcyclohexane, 9CI D-169

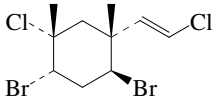


$C_{10}H_{14}Br_2Cl_2$ 364.934

(1*R*,2*S*,4*S*,5*R*)-*form* [66321-23-1]
[89254-84-2]
Constit. of *Plocamium cartilagineum* and *Aplysia punctata*. Metab. of *Aplysia dactylomela*. Shows antibacterial and antifungal activities; toxic to brine shrimp.
Mp 86-87°. $[\alpha]_D^{20}$ -36 (c, 1.13 in $CHCl_3$). $[\alpha]_D$ -46.1 (c, 0.345 in $CHCl_3$).

Norton, R.S. *et al., Tet. Lett.*, 1977, 3905 (*isol, cmr*)
Higgs, M.D. *et al., Tetrahedron*, 1977, **33**, 2775-2780 (*isol, pmr, ir, uv, ms, cmr*)
Gonzalez, A.G. *et al., Phytochemistry*, 1978, **17**, 947 (*nmr, ir, abs config*)
Wessels, M. *et al., J. Nat. Prod.*, 2000, **63**, 920-928 (*isol, activity*)

2,4-Dibromo-1-chloro-5-(2-chloroethenyl)-1,5-dimethylcyclohexane D-170



Relative Configuration

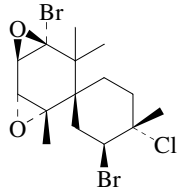
$C_{10}H_{14}Br_2Cl_2$ 364.934

(1*R,2*S**,4*S**,5*S**)-*form*** [66328-04-9]
[105017-62-7]
Constit. of *Aplysia punctata* and *Plocamium cartilagineum*.
Oil. $[\alpha]_D^{20}$ +32.3 (c, 1.75 in $CHCl_3$).

Higgs, M.D. *et al., Tetrahedron*, 1977, **33**, 2775-2780 (*isol, pmr, cmr, ms*)
Quinoa, E. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **92**, 99-101 (*isol*)

2,10-Dibromo-3-chloro-7,8:9,10-diepoxychamigrane D-171

[208756-73-4]

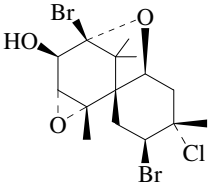


$C_{15}H_{21}Br_2ClO_2$ 428.59
Constit. of *Laurencia nidifica*. Oil. $[\alpha]_D$ +91 (c, 0.05 in $CHCl_3$).

Kimura, J. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 289-292 (*isol, pmr, cmr*)

2,10-Dibromo-3-chloro-5,10:7,8-diepoxy-9-chamigranol D-172

Johnstonol
[35671-09-1]

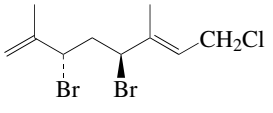


$C_{15}H_{21}Br_2ClO_3$ 444.59
Constit. of the red alga *Laurencia johnstonii*, the sea hare *Aplysia californica* and *Aplysia dactilomela*. Also from *Laurencia nidifica*. Cryst. (EtOAc).
Mp 178°.

Sims, J.J. *et al., Tet. Lett.*, 1972, **13**, 195 (*isol, struct*)
Ireland, C. *et al., J.O.C.*, 1976, **41**, 2461 (*synth*)
Kimura, J. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 289-292 (*isol*)
Kaiser, C.R. *et al., Magn. Reson. Chem.*, 2001, **39**, 147-149 (*pmr, cmr*)

3,5-Dibromo-8-chloro-2,6-dimethyl-1,6-octadiene D-173

Preplocamene A
[62743-07-1]

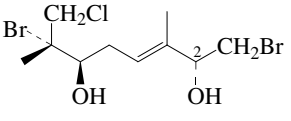


Relative Configuration

$C_{10}H_{15}Br_2Cl$ 330.489
Constit. of the marine red alga *Plocamium violaceum*. Oil. $[\alpha]_D^{20}$ -35 (c, 1.43 in $CHCl_3$).

Crews, P. *et al., J.O.C.*, 1977, **42**, 2812 (*isol, pmr, cmr, ms*)

1,7-Dibromo-8-chloro-3,7-dimethyl-3-octene-2,6-diol D-174



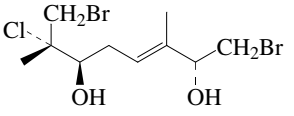
$C_{10}H_{17}Br_2ClO_2$ 364.504

(2R*,3E,6R*,7S*)-form
Plocamenol A
[419573-86-7]
Constit. of *Plocamium cartilagineum*.
Oil. $[\alpha]_D^{25}$ +22 (c, 0.2 in $CHCl_3$).

2-Ketone: 1,7-Dibromo-8-chloro-6-hydroxy-3,7-dimethyl-3-octen-2-one. ***Plocamenol C***
[419573-88-9]
$C_{10}H_{15}Br_2ClO_2$ 362.488
Constit. of *Plocamium cartilagineum*. Oil. $[\alpha]_D^{25}$ +18 (c, 0.2 in $CHCl_3$).

Díaz-Marrero, A.R. *et al., J. Nat. Prod.*, 2002, **65**, 585-588 (*isol, pmr, cmr*)

1,8-Dibromo-7-chloro-3,7-dimethyl-3-octene-2,6-diol D-175



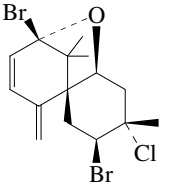
$C_{10}H_{17}Br_2ClO_2$ 364.504

(2R*,3E,6R*,7S*)-form
Plocamenol B
[419573-87-8]
Constit. of *Plocamium cartilagineum*.
Oil. $[\alpha]_D^{25}$ +14 (c, 0.2 in $CHCl_3$).

Díaz-Marrero, A.R. *et al., J. Nat. Prod.*, 2002, **65**, 585-588 (*isol, pmr, cmr*)

2,10-Dibromo-3-chloro-5,10-epoxy-7(14),8-chamigradiene D-176

Pacifidiene
[33880-92-1]

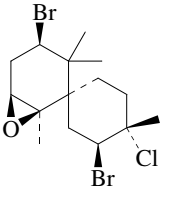


$C_{15}H_{19}Br_2ClO$ 410.575
Constit. of *Aplysia dactilomela*.

Kaiser, C.R. *et al., Magn. Reson. Chem.*, 2001, **39**, 147-149 (*isol, pmr, cmr*)

2,10-Dibromo-3-chloro-7,8-epoxychamigrane D-177

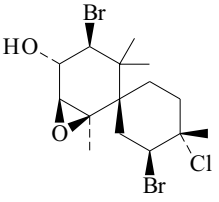
4,10-Dibromo-3-chloro-7,8-epoxy-α-chamigrene
[84847-86-9]



$C_{15}H_{23}Br_2ClO$ 414.607
Isol. from *Laurencia okamurai*. Cryst.
Mp 123.5-124°. $[\alpha]_D^{24}$ +13 (c, 0.4 in $CHCl_3$).

Howard, B.M. *et al., Tet. Lett.*, 1975, 1687 (*synth*)
Ojika, M. *et al., Phytochemistry*, 1982, **21**, 2410 (*isol*)
Bano, S. *et al., Planta Med.*, 1987, **53**, 508 (*isol, cmr*)
Cox, P.J. *et al., Z. Kristallogr.*, 1989, **188**, 1 (*abs config, cryst struct*)

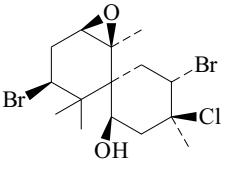
2,10-Dibromo-3-chloro-7,8-epoxy-9-chamigranol D-178
4,10-Dibromo-3-chloro-7,8-epoxy-9-hydroxy-α-chamigrane



$C_{15}H_{23}Br_2ClO_2$ 430.606
Constit. of *Laurencia glomerata*. Gum. $[\alpha]_D^{25}$ +32.7 (c, 0.91 in $CHCl_3$).

Elsworth, J.F. *et al., J. Nat. Prod.*, 1989, **52**, 893 (*isol, pmr, cmr*)

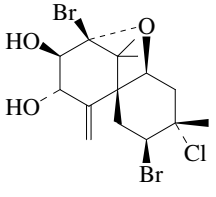
4,10-Dibromo-3-chloro-7,8-epoxy-1-chamigranol D-179
[97651-87-1]



$C_{15}H_{23}Br_2ClO_2$ 430.606
Constit. of a *Laurencia* sp.
$[\alpha]_D$ +8.8 (c, 1.5 in $CHCl_3$).

Bittner, M.L. *et al., Phytochemistry*, 1985, **24**, 987 (*isol, pmr, cmr*)

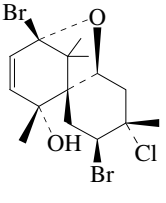
2,10-Dibromo-3-chloro-5,10-epoxy-7(14)-chamigrene-8,9-diol D-180
Pacifenediol
[55035-53-5]



$C_{15}H_{21}Br_2ClO_3$ 444.59
Constit. of *Aplysia dactilomela* and *Aplysia californica*.

Ireland, C. *et al., J.O.C.*, 1976, **41**, 2461-2465 (*isol*)
Kaiser, C.R. *et al., Magn. Reson. Chem.*, 2001, **39**, 147-149 (*isol, pmr, cmr*)

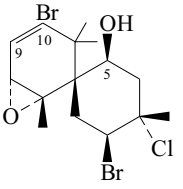
2,10-Dibromo-3-chloro-5,10-epoxy-8-chamigren-7-ol D-181
Pacifenol
[33880-90-9]



$C_{15}H_{21}Br_2ClO_2$ 428.59
Constit. of the red algae *Laurencia pacifica*, *Laurencia majuscula*, *Laurencia nidifica*, *Laurencia claviformis* and *Laurencia marianensis* and the mollusc *Aplysia dactilomela*. Feeding deterrent for aphids, insecticide, antimitotic agent. Cryst. (petrol).
Mp 149-150.5°. λ_{max} 204 (ϵ 2393) (EtOH) (Berdy).

Sims, J.J. *et al., J.A.C.S.*, 1971, **93**, 3774 (*struct*)
Rovirosa, J. *et al., Bol. Soc. Chil. Quim.*, 1991, **36**, 153 (*isol*)
De Nys, R. *et al., Aust. J. Chem.*, 1993, **46**, 933 (*isol, pmr, cmr*)
Argandoña, V.H. *et al., Phytochemistry*, 1993, **32**, 1159-1161 (*isol, pmr, cmr*)
Kimura, J. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 289-292 (*isol*)
Kaiser, C.R. *et al., Magn. Reson. Chem.*, 2001, **39**, 147-149 (*pmr, cmr*)

2,10-Dibromo-3-chloro-7,8-epoxy-9-chamigren-5-ol D-182
Prepacifenol
[41060-07-5]



$C_{15}H_{21}Br_2ClO_2$ 428.59
Constit. of *Laurencia filiformis*, *Laurencia pacifica*, *Laurencia nidifica* and *Aplysia dactyomela*. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O.
Mp 109-126° (solidifies and remelts at 147°).

Ac: ***Acetylprepacifenol***
[476371-84-3]
$C_{17}H_{23}Br_2ClO_3$ 470.628
Constit. of *Aplysia parvula* and *Laurencia filiformis*. Cryst. (petrol).
Mp 178-178.5°. $[\alpha]_D$ +62.5 (c, 0.096 in CH_2Cl_2). λ_{max} 205 (log ϵ 2.9) (CH_2Cl_2).

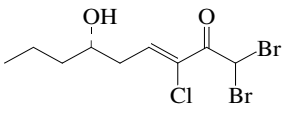
9β,10β-Epoxide: 2,10-Dibromo-7-chloro-7,8:9,10-diepoxy-5-chamigranol. ***Prepacifenol epoxide***
[55304-01-3]
$C_{15}H_{21}Br_2ClO_3$ 444.59
Constit. of *Aplysia californica*, *Aplysia dactylomela* and *Laurencia nidifida*. Cryst.
Mp 98-99°.

5-Deoxy: 2,10-Dibromo-3-chloro-7,8-epoxy-9-chamigrene. ***Deoxyprepacifenol***
[58967-05-8]
$C_{15}H_{21}Br_2ClO$ 412.591
Constit. of *Aplysia californica*, *Laurencia claviformis*, *Laurencia nipponica*, *Laurencia elata*, *Laurencia marianensis* and *Laurencia majuscula*. Shows insecticidal props. Cryst. (pentane). Sol. MeOH, $CHCl_3$.
Mp 125°. λ_{max} 212 (ϵ 4540) (EtOH) (Berdy).

5-Deoxy, 9,10-epoxide: ***Dehydroxyprepacifenol epoxide***
$C_{15}H_{21}Br_2ClO_2$ 428.59
Isol. from mollusc *Aplysia dactyomela* from Brazil. Stereochem. not assigned.

Sims, J.J. *et al., J.A.C.S.*, 1973, **95**, 972 (*isol*)
Faulkner, D.J. *et al., Tet. Lett.*, 1974, 3571-3574 (*Prepacifenol epoxide*)
Fenical, W. *et al., J. Phycol.*, 1975, **11**, 104 (*isol*)
Ireland, C. *et al., J.O.C.*, 1976, **41**, 2461-2465 (*isol, Deoxyprepacifenol*)
Fronczek, F.R. *et al., Acta Cryst. C*, 1989, **45**, 1102 (*Deoxyprepacifenol, cryst struct, abs config*)
De Nys, R. *et al., Aust. J. Chem.*, 1993, **46**, 933 (*Deoxyprepacifenol, pmr, cmr*)
Kaiser, C.R. *et al., Spectrosc. Lett.*, 1998, **31**, 573-585 (*Dehydroxyprepacifenol epoxide*)
Kimura, J. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 289-292 (*isol, struct*)
McPhail, K.L. *et al., J. Nat. Prod.*, 1999, **62**, 1618-1623 (*Prepacifenol epoxide, pmr, cmr*)
Jongaramruong, J. *et al., Aust. J. Chem.*, 2002, **55**, 275-280 (*Acetylprepacifenol, isol, pmr, cmr, cryst struct*)

1,1-Dibromo-3-chloro-6-hydroxy-3-nonen-2-one D-183

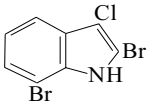


$C_9H_{13}Br_2ClO_2$ 348.461

(3*Z*,6*S*)-*form*
Constit. of the red alga *Ptilonia magellanica*.
Oil. $[\alpha]_D^{25}$ -8 (c, 0.24 in CH_2Cl_2).
Lorenzo, M. *et al., Tetrahedron*, 2005, **61**, 9550-9554 (*isol, pmr, cmr, ms*)

2,7-Dibromo-3-chloro-1*H*-indole, 9CI D-184

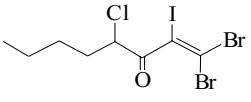
3-Chloro-2,7-dibromoindole
[68234-20-8]



$C_8H_4Br_2ClN$ 309.387
Alkaloid from the marine red alga *Rhodophyllis membranacea*.
Mp 86-87°.
Brennan, M.R. *et al., Tet. Lett.*, 1978, 1637 (*isol, pmr, struct*)
Erickson, K.L. *et al., Synth. Commun.*, 1981, **11**, 253 (*synth, ir, pmr, ms*)

1,1-Dibromo-4-chloro-2-iodo-1-octen-3-one D-185

[64785-99-5]



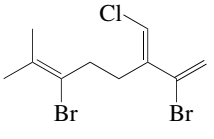
$C_8H_{10}Br_2ClIO$ 444.332
Constit. of *Delisea fimbriata*. Oil.
Rose, A.F. *et al., Tet. Lett.*, 1977, 1847

Dibromochloromethane, 9CI, 8CI D-186

Chlorodibromomethane. R 20B2
[124-48-1]
$CHBr_2Cl$
$CHBr_2Cl$ 208.28
Isol. from several marine algae. Source of bromochlorocarbene in the presence of base and crown ether. Liq.
Fp -22. Bp 121.3-121.8° (118-122°). n_D^{20} 1.5484.
▶ LD_{50} (rat, orl) 848 mg/kg. PA6360000
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 83D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 122C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 117A (*ir*)
Barrett, G.C. *et al., J.C.S.(C)*, 1971, 279 (*synth*)
Fedorynski, M. *et al., Synth. Commun.*, 1977, 287 (*synth*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CFK500

2,6-Dibromo-3-(chloromethylene)-7-methyl-1,6-octadiene D-187

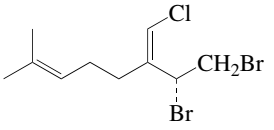
3,7-Dibromo-10-chloro-β-myrcene



$C_{10}H_{13}Br_2Cl$ 328.473
Config. probably assigned incorrectly in paper and CA.

(*E*)-*form* [55498-41-4]
Constit. of *Chondrococcus hornemanni* (*Portieria hornemannii*). Called (*Z*)- in ref.
Ichikawa, N. *et al., Chem. Lett.*, 1974, 1333-1336 (*isol, ms, pmr*)

7,8-Dibromo-6-(chloromethylene)-2-methyl-2-octene, 9CI D-188

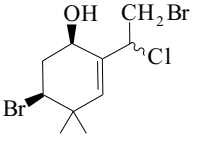


$C_{10}H_{15}Br_2Cl$ 330.489

(6*E*,7*R*)-*form* [112642-60-1]
Constit. of *Chondrococcus hornemanni* and *Portieria hornemanni*.
Oil. $[\alpha]_D$ +12.5 (c, 0.015 in $CHCl_3$).
Coll, J.C. *et al., Aust. J. Chem.*, 1987, **40**, 1893
Wright, A.D. *et al., J. Nat. Prod.*, 1990, **53**, 845-861 (*isol*)

1,6-Dibromo-2-chloro-3(8)-ochtoden-4-ol D-189

5-Bromo-2-(2-bromo-1-chloroethyl)-4,4-dimethyl-2-cyclohexen-1-ol, 9CI
[73872-77-2]

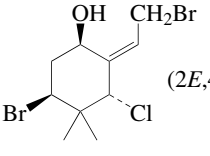


$C_{10}H_{15}Br_2ClO$ 346.489

(4*R,6*S**)-*form***
Constit. of *Ochtodes crockeri*.
Oil. $[\alpha]_D^{20}$ -26.8 (c, 1 in $CHCl_3$).
Paul, V.J. *et al., J.O.C.*, 1980, **45**, 3401

1,6-Dibromo-8-chloro-2-ochtoden-4-ol D-190

5-Bromo-2-(2-bromoethylidene)-3-chloro-4,4-dimethylcyclohexanol, 9CI



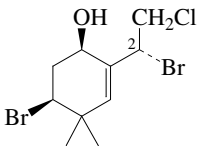
(2*E*,4β,6β,8α)-*form*

$C_{10}H_{15}Br_2ClO$ 346.489

(2*E*,4β,6β,8α)-*form*
Constit. of *Ochtodes secundiramea*.
Oil.

(2*Z*,4α,6α,8β)-*form*
Ac: [851473-81-9]
$C_{12}H_{17}Br_2ClO_2$ 388.526
Constit. of *Carpopeltis crispata*. Oil. $[\alpha]_D^{20}$ -235 (c, 0.049 in $CHCl_3$).
Crews, P. *et al., J.O.C.*, 1984, **49**, 1371 (*isol, struct, cmr*)
Kimura, J. *et al., J. Nat. Prod.*, 2005, **68**, 585-587 (*Ac*)

2,6-Dibromo-1-chloro-3(8)-ochtoden-4-ol D-191



(2*R**,4β,6β)-*form*

$C_{10}H_{15}Br_2ClO$ 346.489

(2*R,4β,6β)-*form***

Ac: [851473-83-1]
$C_{12}H_{17}Br_2ClO_2$ 388.526
Constit. of *Carpopeltis crispata*. Oil. $[\alpha]_D^{20}$ -87 (c, 0.03 in $CHCl_3$).

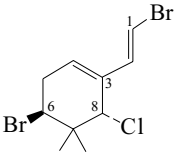
(2*S,4β,6β)-*form***

Ac: [851473-82-0]
Constit. of *Carpopeltis crispata*.
Oil. $[\alpha]_D^{20}$ -7.5 (c, 0.03 in $CHCl_3$).

Kimura, J. *et al., J. Nat. Prod.*, 2005, **68**, 585-587 (*isol, pmr, cmr*)

1,6-Dibromo-8-chloro-1,3-ochtodiene D-192

4-Bromo-1-(2-bromoethenyl)-6-chloro-5,5-dimethylcyclohexene, 9CI



$C_{10}H_{13}Br_2Cl$ 328.473

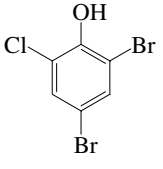
(1*E*,6*S,8*S**)-*form*** [73872-74-9]
Constit. of *Ochtodes crockeri*.
Oil. $[\alpha]_D^{20}$ +16.7 (c, 5.4 in $CHCl_3$).

[89197-93-3]

Paul, V.J. *et al., J.O.C.*, 1980, **45**, 3401

2,4-Dibromo-6-chlorophenol D-193

[4526-56-1]



$C_6H_3Br_2ClO$ 286.35
Prod. by the marine bacterium *Pseudoalteromonas luteoviolacea*.
Mp 78-79°.

Mousseron, M. *et al., Bull. Soc. Chim. Fr.*, 1951, 106-114 (*synth*)
Kakinami, T. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 3373-3375 (*synth*)
Jiang, Z. *et al., Nat. Prod. Lett.*, 2000, **14**, 435-440 (*isol, pmr, cmr*)

2,6-Dibromo-4-chlorophenol D-194

[5324-13-0]

$C_6H_3Br_2ClO$ 286.35
Isol. from the acorn worm *Ptychodera bahamensis*.
Mp 92°.

[84717-41-9]

Rondestvedt, C.S. *et al., J.A.C.S.*, 1954, **76**, 509-515 (*synth*)
Kakinami, T. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 3373-3375 (*synth*)
Corgiat, J.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1993, **106**, 83-86 (*isol*)

1,1-Dibromo-1-chloro-2-propanone, 9CI, 8CI D-195

1,1-Dibromo-1-chloroacetone
[30957-55-2]
$H_3CCOCClBr_2$
$C_3H_3Br_2ClO$ 250.317
Minor component of the essential oil of the edible Hawaiian red alga (*Asparagopsis taxiformis*). Liq. Bp 164-165° Bp_1 41-42°. n_D^{20} 1.5370.
▶ Lachrymator.

Barrett, G.C. *et al., J.C.S.(C)*, 1971, 279 (*synth, ir*)
Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*synth, pmr, ms, glc*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)

1,1-Dibromo-3-chloro-2-propanone, 9CI D-196

1,1-Dibromo-3-chloroacetone
[1578-18-3]
$Br_2CHCOCH_2Cl$
$C_3H_3Br_2ClO$ 250.317
Minor component of the red alga *Asparagopsis taxiformis* and of *Falkenbergia rufolanosa*.

Rappe, C. *et al., Ark. Kemi*, 1965, **24**, 105; *CA*, **63**, 5489a (*synth*)
Fenical, W. *et al., Tet. Lett.*, 1974, 4463 (*isol, glc, synth*)
Codomier, L. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1977, **284**, 1163 (*isol, glc*)

1,3-Dibromo-1-chloro-2-propanone, 9CI D-197

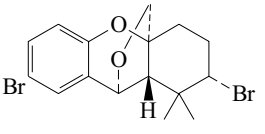
1,3-Dibromo-1-chloroacetone
[55716-00-2]
$BrCH_2COCHBrCl$
$C_3H_3Br_2ClO$ 250.317

(±)-*form*
Component of the red algae *Asparagopsis taxiformis, Asparagopsis armata* and tetrasporophyte *Falkenbergia rufolanosa*. Bp_{10} 95-97°. n_D^{25} 1.5632.

Rappe, C. *et al., Ark. Kemi*, 1965, **24**, 105; *CA*, **63**, 5489a (*synth*)
Codomier, L. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1977, **284**, 1163 (*isol*)
Bruneau, Y. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1978, **286**, 603 (*isol*)
Combaut, G. *et al., Phytochemistry*, 1978, **17**, 1661 (*isol, glc*)

Dibromocyclocacoxanthene D-198

[132244-38-3]

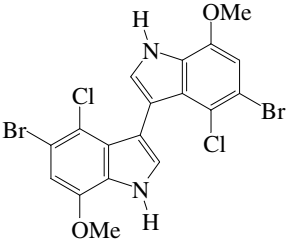


$C_{16}H_{18}Br_2O_2$ 402.125
Constit. of a *Cacospongia* sp. Oil. $[\alpha]_D$ -45.1 (c, 0.324 in $CHCl_3$).

Bali, D.K.L. *et al., Aust. J. Chem.*, 1990, **43**, 2009 (*isol, pmr, cmr*)

5,5′-Dibromo-4,4′-dichloro-7,7′-dimethoxy-3,3′-bi-1*H*-indole D-199

*3,3′-Bis(5-bromo-4-chloro-7-methoxy-1*H*-indole)*

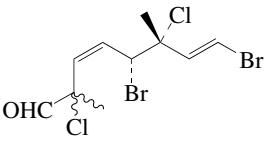


$C_{18}H_{12}Br_2Cl_2N_2O_2$ 519.018

Isol. from the green alga *Chaetomorpha basiretorsa*. Amorph. powder.

Shi, D.Y. *et al., Chin. Chem. Lett.*, 2005, **16**, 777-780 (*isol, pmr, cmr, ms*)

5,8-Dibromo-2,6-dichloro-2,6-dimethyl-3,7-octadienal D-200

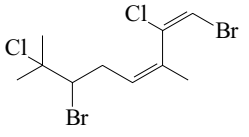


$C_{10}H_{12}Br_2Cl_2O$ 378.918

(2ξ,3*Z*,5*R,6*R**,7*E*)-*form*** [184292-58-8]
Constit. of *Plocamium cartilagineum*.
Oil.

Abreu, P.M. *et al., J. Nat. Prod.*, 1996, **59**, 1159-1162 (*isol, pmr, cmr*)

1,6-Dibromo-2,7-dichloro-3,7-dimethyl-1,3-octadiene, 9CI D-201

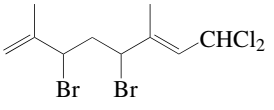


$C_{10}H_{14}Br_2Cl_2$ 364.934

(1*E*,3*Z*)-*form* [96300-26-4]
Constit. of *Plocamium cartilagineum*.
Oil.

Blunt, J.W. *et al., Aust. J. Chem.*, 1985, **38**, 319

3,5-Dibromo-8,8-dichloro-2,6-dimethyl-1,6-octadiene D-202

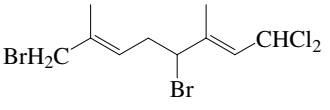


$C_{10}H_{14}Br_2Cl_2$ 364.934

(3ξ,5ξ,6*E*)-*form*
Plocoralide B
[861959-26-4]
Constit. of *Plocamium corallorhiza*.
Oil. $[\alpha]_D$ -15 (c, 0.02 in $CHCl_3$).

Knott, M.G. *et al., Phytochemistry*, 2005, **66**, 1108-1112 (*Plocoralide B*)

4,8-Dibromo-1,1-dichloro-3,7-dimethyl-2,6-octadiene D-203



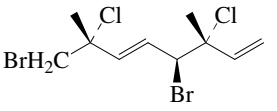
$C_{10}H_{14}Br_2Cl_2$ 364.934

(2*E*,4ξ,6*E*)-*form*
Plocoralide A
[861959-25-3]
Constit. of *Plocamium corallorhiza*.
Oil.

Knott, M.G. *et al., Phytochemistry*, 2005, **66**, 1108-1112 (*Plocoralide A*)

4,8-Dibromo-3,7-dichloro-3,7-dimethyl-1,5-octadiene D-204

[119903-44-5]



(3*R**,4*S**,5*E*,6*R**)-*form*

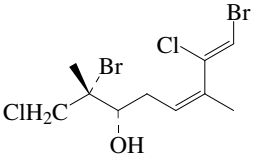
$C_{10}H_{14}Br_2Cl_2$ 364.934

(3*R*,4*S*,5*E*,6*R*)-*form*
Isol. from *Plocamium hamatum*.

(3*R*,4*S*,5*E*,6*S*)-*form*
Constit. of *Plocamium hamatum*.
Oil. $[\alpha]_D$ -7 (c, 0.006 in $CHCl_3$).

Coll, J.C. *et al., Aust. J. Chem.*, 1988, **41**, 1743
Wright, A.D. *et al., J. Nat. Prod.*, 1990, **53**, 845-861 (*isol*)
König, G.M. *et al., Phytochemistry*, 1999, **52**, 1047-1053 (*isol, pmr, cmr*)

2,8-Dibromo-1,7-dichloro-2,6-dimethyl-5,7-octadien-3-ol D-205

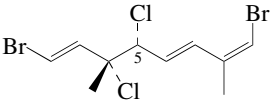


$C_{10}H_{14}Br_2Cl_2O$ 380.933

(2*R,3*S**,5*Z*,7*Z*)-*form***
Prefuroplocamioid
[460042-97-1]
Constit. of *Plocamium cartilagineum*.
Oil. $[\alpha]_D^{25}$ +34 (c, 0.6 in $CHCl_3$).

Diaz-Marrero, A.R. *et al., Org. Lett.*, 2002, **4**, 2949-2952 (*isol, pmr, cmr*)

1,8-Dibromo-5,6-dichloro-2,6-dimethyl-1,3,7-octatriene D-206



(1*Z*,3*E*,5*R*,6*R*,7*E*)-*form*

$C_{10}H_{12}Br_2Cl_2$ 362.918

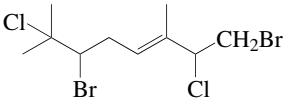
(1*Z*,3*E*,5*R*,6*R*,7*E*)-*form* [57766-75-3]
Constit. of the red algae *Plocamium cartilagineum* and *Plocamium oregonum*.

(1*Z*,3*E*,5*S*,6*R*,7*E*)-*form* [57766-76-4]
Constit. of *Plocamium cartilagineum* and *Plocamium oregonum*.

Crews, P. *et al., J.O.C.*, 1977, **42**, 2634 (*isol, cmr, ms*)
Mynderse, J.S. *et al., Phytochemistry*, 1978, **17**, 237 (*isol*)

1,6-Dibromo-2,7-dichloro-3,7-dimethyl-3-octene D-207

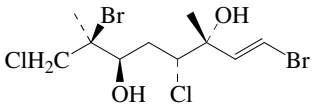
[184292-59-9]



$C_{10}H_{16}Br_2Cl_2$ 366.95
Constit. of *Plocamium cartilagineum*. Oil. $[\alpha]_D$ -53 (c, 0.67 in $CHCl_3$).

Abreu, P.M. *et al., J. Nat. Prod.*, 1996, **59**, 1159-1162 (*isol, pmr, cmr*)

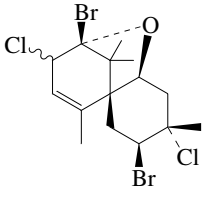
1,7-Dibromo-4,8-dichloro-3,7-dimethyl-1-octene-3,6-diol D-208



$C_{10}H_{16}Br_2Cl_2O_2$ 398.949

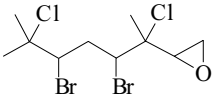
(1*E*,3*R,4*R**,6*R**,7*S**)-*form*** [479072-76-9]
Constit. of *Plocamium cartilagineum*.
Oil. $[\alpha]_D^{25}$ -143 (c, 0.03 in $CHCl_3$).
Díaz-Marrero, A.R. *et al., Tetrahedron*, 2002, **58**, 8539-8542 (*isol, pmr, cmr*)

2,10-Dibromo-3,9-dichloro-5,10-epoxy-7-chamigrene D-209
[54665-34-8]



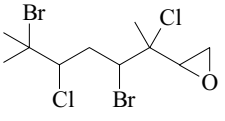
$C_{15}H_{20}Br_2Cl_2O$ 447.036
Constit. of *Aplysia californica*.
Stallard, M.O. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1974, **49**, 37-41 (*isol, pmr*)

4,6-Dibromo-3,7-dichloro-1,2-epoxy-3,7-dimethyloctane D-210
(2,4-Dibromo-1,5-dichloro-1,5-dimethylhexyl)oxirane, 9CI
[96300-29-7]



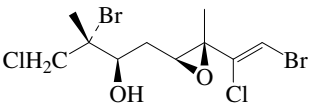
$C_{10}H_{16}Br_2Cl_2O$ 382.949
Constit. of *Plocamium cartilagineum*. Oil.
Blunt, J.W. *et al., Aust. J. Chem.*, 1985, **38**, 319

4,7-Dibromo-3,6-dichloro-1,2-epoxy-3,7-dimethyloctane D-211
(2,5-Dibromo-1,4-dichloro-1,5-dimethylhexyl)oxirane, 9CI
[96300-28-6]



$C_{10}H_{16}Br_2Cl_2O$ 382.949
Constit. of *Plocamium cartilagineum*.
Blunt, J.W. *et al., Aust. J. Chem.*, 1985, **38**, 319

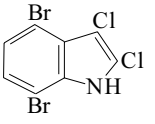
2,8-Dibromo-1,7-dichloro-5,6-epoxy-2,6-dimethyl-7-octen-3-ol D-212



$C_{10}H_{14}Br_2Cl_2O_2$ 396.933

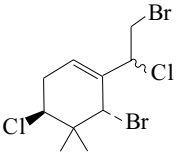
(2*R*,3*R*,5*S*,6*S*,7*Z*)-*form* [723302-04-3]
Constit. of *Plocamium cartilagineum*.
Oil. $[\alpha]_D^{25}$ +80 (c, 0.01 in $CHCl_3$).
Díaz-Marrero, A.R. *et al., Tetrahedron*, 2004, **60**, 5049-5052 (*isol, pmr, cmr*)

4,7-Dibromo-2,3-dichloro-1*H*-indole, 9CI D-213
[68234-22-0]



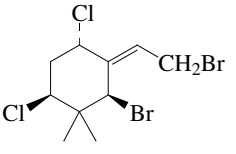
$C_8H_3Br_2Cl_2N$ 343.832
Alkaloid from the marine red alga *Rhodophyllis membranacea*.
Mp 142.5-143°.
Brennan, M.R. *et al., Tet. Lett.*, 1978, 1637 (*isol, pmr, struct*)
Ohta, T. *et al., Heterocycles*, 1989, **29**, 1663 (*synth*)

1,8-Dibromo-2,6-dichloro-3-ochtodene D-214
6-Bromo-1-(2-bromo-1-chloroethyl)-4-chloro-5,5-dimethylcyclohexene, 9CI
[58086-86-5]



$C_{10}H_{14}Br_2Cl_2$ 364.934
Constit. of *Chondrococcus hornemanni*. Oil.
Burreson, B.J. *et al., Chem. Lett.*, 1975, 1111 (*isol*)
Crews, P. *et al., J.O.C.*, 1984, **40**, 1371 (*cmr, struct*)

1,8-Dibromo-4,6-dichloro-2-ochtodene D-215

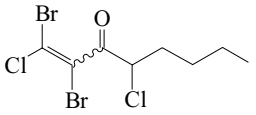


$C_{10}H_{14}Br_2Cl_2$ 364.934

(2*Z*,4α,6β,8β)-*form* [851473-80-8]
Constit. of *Carpopeltis crispata*.
Oil. $[\alpha]_D^{20}$ +280 (c, 0.028 in $CHCl_3$).
Kimura, J. *et al., J. Nat. Prod.*, 2005, **68**, 585-587 (*isol, pmr, cmr*)

1,2-Dibromo-1,4-dichloro-1-octen-3-one, 9CI D-216

[64785-89-3]



$C_8H_{10}Br_2Cl_2O$ 352.88

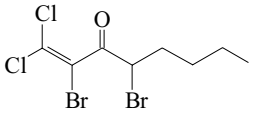
(E)-form

Constit. of *Bonnemaisonia asparagoides.*

McConnell, O.J. *et al., Tet. Lett.*, 1977, 1851 (*synth*)

2,4-Dibromo-1,1-dichloro-1-octen-3-one, 9CI D-217

[64785-88-2]



$C_8H_{10}Br_2Cl_2O$ 352.88

Constit. of *Bonnemaisonia asparagoides.*

McConnell, O.J. *et al., Tet. Lett.*, 1977, 1851 (*synth*)

1,1-Dibromo-3,3-dichloro-2-propanone, 9CI D-218

1,1-Dibromo-3,3-dichloroacetone

[62874-83-3]

$Br_2CHCOCHCl_2$

$C_3H_2Br_2Cl_2O$ 284.762

Component of the red alga *Asparagopsis armata* and tetrasporophyte *Falkenbergia rufolanosa*.

McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367 (*isol, glc, ms*)

Bruneau, Y. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1978, **286**, 603 (*isol, glc*)

Combaut, G. *et al., Phytochemistry*, 1978, **17**, 1661 (*isol, glc*)

1,3-Dibromo-1,3-dichloro-2-propanone, 9CI D-219

1,3-Dibromo-1,3-dichloroacetone

[62874-84-4]

BrCHClCOCHBrCl

$C_3H_2Br_2Cl_2O$ 284.762

Component of the red alga *Asparagopsis armata* and tetrasporophyte *Falkenbergia rufolanosa*. Yellowish liq. Bp_3 65-67°.

▶ Irritant.

McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367 (*isol, glc*)

Bruneau, Y. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1978, **286**, 603 (*isol, glc*)

Combaut, G. *et al., Phytochemistry*, 1978, **17**, 1661 (*isol, glc*)

Torsten, K. *et al., J.O.C.*, 2003, **68**, 2964-2967 (*synth, pmr*)

1,1-Dibromo-3,3-dichloro-1-propene D-220

[56020-81-6]

$Cl_2CHCH{=}CBr_2$

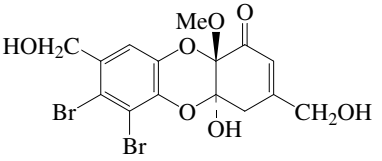
$C_3H_2Br_2Cl_2$ 268.762

Isol. from the alga *Asparagopsis taxiformis.*

Burreson, B.J. *et al., Tet. Lett.*, 1975, 473 (*isol, ms*)

Lambert, J.B. *et al., J.A.C.S.*, 1984, **106**, 3584 (*synth*)

6,7-Dibromo-4*a*,10*a*-dihydro-4*a*-hydroxy-3,8-bis(hydroxymethyl)-10*a*-methoxy-4*H*-dibenzo[*b,e*][1,4]dioxin-1-one D-221



$C_{15}H_{14}Br_2O_7$ 466.079

(4aRS,10aSR)-form

Constit. of the brown alga *Leathesia nana.*

Brown powder (Me_2CO).

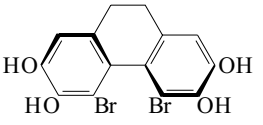
Mp 193-195°.

Xu, X. *et al., J. Nat. Prod.*, 2004, **67**, 1661-1666 (*isol, pmr, cmr, ms*)

4,5-Dibromo-9,10-dihydro-2,3,6,7-phenanthrenetetrol, 9CI D-222

4,5-Dibromo-9,10-dihydro-2,3,6,7-tetrahydroxyphenanthrene. ***Polysiphenol***

[140163-61-7]



$C_{14}H_{10}Br_2O_4$ 402.039

(R)-form

Constit. of *Polysiphonia ferulacea.*

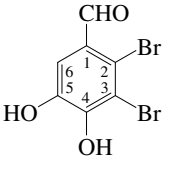
$[\alpha]_D^{25}$ -191 (MeOH).

Aknin, M. *et al., Tet. Lett.*, 1992, **33**, 555 (*isol, pmr, cmr*)

2,3-Dibromo-4,5-dihydroxybenzaldehyde, 9CI D-223

5,6-Dibromoprotocatechualdehyde

[14045-41-1]



$C_7H_4Br_2O_3$ 295.915

Isol. from the algae *Polysiphonia lanosa* and *Rhodomela larix*.

Needles (EtOAc or by subl.).

Mp 203-205°.

5-Me ether: 2,3-Dibromo-4-hydroxy-5-methoxybenzaldehyde, 9CI. 5,6-Dibromovanillin

[2973-75-3]

$C_8H_6Br_2O_3$ 309.942

Solid (MeOH). Mp 230°.

Di-Me ether: 2,3-Dibromo-4,5-dimethoxybenzaldehyde, 9CI. 5,6-Dibromoveratraldehyde

[70625-29-5]

$C_9H_8Br_2O_3$ 323.968

Needles. Mp 129-130°.

Katsui, N. *et al., Tetrahedron*, 1967, **23**, 1185-1188 (*isol*)

Pedersen, M. *et al., Phytochemistry*, 1974, **13**, 2273-2279 (*isol*)

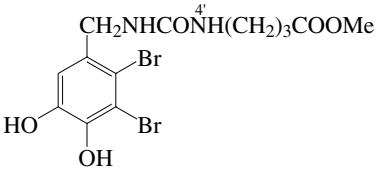
Lundgren, L. *et al., Acta Chem. Scand., Ser. B*, 1979, **33**, 105-108 (*synth, pmr, ms*)

Ford, P.W. *et al., J.O.C.*, 1994, **59**, 5955-5960 (*Me ether, synth, ir, uv, pmr, cmr*)

Shoeib, N.A. *et al., J. Nat. Prod.*, 2004, **67**, 1445-1449 (*isol, synth*)

_N_-(2,3-Dibromo-4,5-dihydroxybenzyl)-_N′_-(3-methoxycarbonylpropyl)urea D-224

Methyl N′*-(2,3-dibromo-4,5-dihydroxybenzyl) γ-ureidobutyrate*

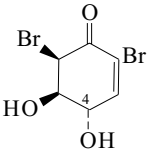


$C_{13}H_{16}Br_2N_2O_5$ 440.088
Constit. of *Rhodomela confervoides*. Amorph. powder.
Mp 155-158°.

N$^{4'}$*-(2,3-Dibromo-4,5-dihydroxybenzyl):* N,N′*-Bis(2,3-dibromo-4,5-dihydroxybenzyl)*-N-*(3-methoxycarbonylpropyl)urea*
$C_{20}H_{20}Br_4N_2O_7$ 720.003
Constit. of *Rhodomela confervoides*. Brown gum.

Ma, M. *et al., J. Nat. Prod.*, 2006, **69**, 206-210 (*isol, pmr, cmr, ms*)

2,6-Dibromo-4,5-dihydroxy-2-cyclohexen-1-one D-225



(4*S*,5*R*,6*R*)*–form*

$C_6H_6Br_2O_3$ 285.92

(4*S*,5*R*,6*R*)-*form*

4-Ac: 4-Acetoxy-2,6-dibromo-5-hydroxy-2-cyclohexen-1-one
[110850-10-7]
$C_8H_8Br_2O_4$ 327.957
Metab. of the marine acorn worm *Ptychodera* sp. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{23}$ +130 (c, 0.1 in CH_2Cl_2). λ_{max} 202 (ϵ 4400); 256 (ϵ 5500) (MeOH) (Berdy).

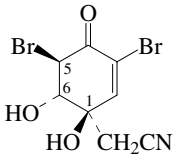
(4*S*,5*R*,6*S*)-*form*

4-Ac: [110786-60-2]
Metab. of the marine acorn worm *Ptychodera* sp.
Cryst. (EtOAc/hexane). Sol. MeOH, $CHCl_3$.
Mp 136-138°. $[\alpha]_D^{25}$ +109.7 (c, 1.24 in $CHCl_3$). λ_{max} 255 (ϵ 5200) (MeOH) (Berdy).

*1*R*-Alcohol, 4-Ac: 4-Acetoxy-2,6-dibromo-5-cyclohexene-1,3-diol*
[110786-61-3]
$C_8H_{10}Br_2O_4$ 329.973
Metab. of marine *Ptychodera* sp. Cryst. (EtOAc/hexane). Sol. MeOH, $CHCl_3$.
Mp 150.5-151.5°.

Higa, T. *et al., Tetrahedron*, 1987, **43**, 1063-1070 (*isol, uv, pmr, ms*)

3,5-Dibromo-1,6-dihydroxy-4-oxo-2-cyclohexene-1-acetonitrile, 9CI D-226



(1*R*,5*R*,6*S*)*-form*

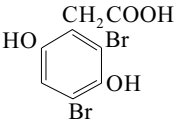
$C_8H_7Br_2NO_3$ 324.956
λ_{max} 249 (ϵ 4000); 254 (ϵ 4100) (EtOH) (Derep).

(1*R*,5*S*,6*S*)-*form* [108526-92-7]
Constit. of *Aplysina laevis*. Possesses antimicrobial activity.

(1*R*,5*R*,6*S*)-*form* [108590-99-4]
Constit. of *Aplysina laevis*. Possesses antimicrobial activity.
Capon, R.J. *et al., Aust. J. Chem.*, 1987, **40**, 341

2,4-Dibromo-3,6-dihydroxyphenylacetic acid D-227

2,4-Dibromo-3,6-dihydroxybenzeneacetic acid, 9CI



$C_8H_6Br_2O_4$ 325.941

Amide: 2,4-Dibromo-3,6-dihydroxyphenylacetamide. 2,4-Dibromo-3,6-dihydroxybenzeneacetamide, 9CI
[55895-97-1]
$C_8H_7Br_2NO_3$ 324.956
Metab. of *Verongia aurea*. Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 180-182°. λ_{max} 250 (ϵ 4000); 280 (ϵ 2900); 368 (ϵ 7200) (0.1*N* NaOH) (Derep). λ_{max} 250 (ϵ 4000); 280 (ϵ 2900); 368 (ϵ 7200) (pH 12) (Derep). λ_{max} 222 (ϵ 5400) (MeOH) (Berdy). λ_{max} 250 (ϵ 4000); 280 (ϵ 2900); 368 (ϵ 7200) (NAOH) (Berdy).

Krejcarek, G.E. *et al., Tet. Lett.*, 1975, 507 (*uv, ir, ms, cryst struct*)
Krohn, K. *et al., Tet. Lett.*, 1975, 4667 (*uv, nmr, synth*)

2,6-Dibromo-3,5-dihydroxyphenylacetic acid D-228

2,6-Dibromo-3,5-dihydroxybenzeneacetic acid
[80314-69-8]
$C_8H_6Br_2O_4$ 325.941
Constit. of the red alga *Halopytis incurvus*. Genus name given as Halopithys.

Di-O-*sulfate:* [80314-70-1]
$C_8H_6Br_2O_{10}S_2$ 486.069
Constit. of *Halopytis incurvus*. CAS no. refers to di-K salt.

De Nanteuil, G. *et al., Phytochemistry*, 1981, **20**, 1750 (*isol*)

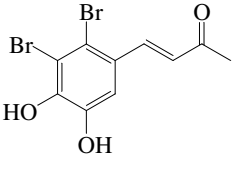
3,5-Dibromo-2,4-dihydroxyphenylacetic acid D-229

3,5-Dibromo-2,4-dihydroxybenzeneacetic acid, 9CI
[37677-03-5]
$C_8H_6Br_2O_4$ 325.941

4-Me ether, amide: 3,5-Dibromo-2-hydroxy-4-methoxyphenylacetamide
[28495-12-7]
$C_9H_9Br_2NO_3$ 338.983
Constit. of the sponges *Aplysina aerophoba*, *Aplysina thiona* and *Psammaplysilla purpurea*. Cryst. ($CHCl_3$).
Mp 174-176° (166-167°). λ_{max} 250 (sh) (ϵ 1610); 290 (ϵ 2500); 314 (sh) (ϵ 450) (MeOH) (Derep).

Fatturusso, E. *et al., J.C.S. Perkin 1*, 1972, 16 (*synth*)
Chang, C.W.J. *et al., Tet. Lett.*, 1977, 4005 (*synth*)
Kelecom, A. *et al., Ann. Acad. Bras. Cienc.*, 1979, **51**, 639 (*isol*)
Cruz, F. *et al., J. Nat. Prod.*, 1990, **53**, 543 (*isol*)

4-(2,3-Dibromo-4,5-dihydroxyphenyl)-3-buten-2-one D-230



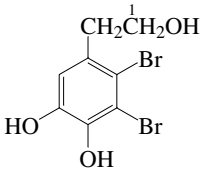
$C_{10}H_8Br_2O_3$ 335.979

(*E*)-*form*
Isol. from the red alga *Rhodomela confervoides*.
Brown cryst. (MeOH aq.).
Mp 165-166°.

Zhao, J. *et al., J. Nat. Prod.*, 2004, **67**, 1032-1035 (*isol, pmr, cmr, cryst struct*)

2-(2,3-Dibromo-4,5-dihydroxyphenyl)ethanol D-231

3,4-Dibromo-5-(2-hydroxyethyl)-1,2-benzenediol, 9CI



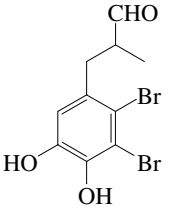
$C_8H_8Br_2O_3$ 311.957
Constit. of *Rhodomela confervoides*. Brown gum. λ_{max} 211 (log ϵ 4.1); 292 (log ϵ 3.23) (MeOH).

1-Sulfate:
$C_8H_8Br_2O_6S$ 392.022
Constit. of *Rhodomela confervoides*. Brown gum. λ_{max} 210 (log ϵ 4.39); 292 (log ϵ 3.29) (MeOH).

Ma, M. *et al., J. Nat. Prod.*, 2006, **69**, 206-210 (*isol, pmr, cmr, ms*)

3-(2,3-Dibromo-4,5-dihydroxyphenyl)-2-methylpropanal D-232

2,3-Dibromo-4,5-dihydroxy-α-methylbenzenepropanal, 9CI



$C_{10}H_{10}Br_2O_3$ 337.995

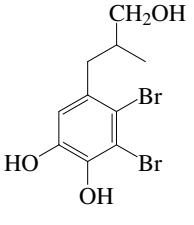
(±)-*form*
Isol. from the red alga *Rhodomela confervoides*.
Yellowish gum.

Di-Me acetal: 3,4-Dibromo-5-(3,3-dimethoxy-2-methylpropyl)-1,2-benzenediol
$C_{12}H_{16}Br_2O_4$ 384.064
Isol. from *Rhodomela confervoides*. Amorph. powder (Me_2CO). Mp 117-118°. Possible artifact.

Fan, X. *et al., Chin. Chem. Lett.*, 2003, **14**, 1045-1047 (*isol, pmr, cmr*)
Fan, X. *et al., J. Nat. Prod.*, 2003, **66**, 455-458 (*isol, pmr, cmr, ms*)

3-(2,3-Dibromo-4,5-dihydroxyphenyl)-2-methyl-1-propanol D-233

3,4-Dibromo-5-(3-hydroxy-2-methylpropyl)-1,2-benzenediol

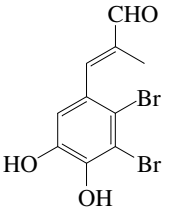


$C_{10}H_{12}Br_2O_3$ 340.011

(+)-*form*
Isol. from the brown alga *Leathesia nana*.
Gum. $[\alpha]_D^{20}$ +5 (c, 0.41 in MeOH).

Xu, X.-L. *et al., J. Asian Nat. Prod. Res.*, 2004, **6**, 217-221 (*isol, pmr, cmr*)

3-(2,3-Dibromo-4,5-dihydroxyphenyl)-2-methyl-2-propenal D-234

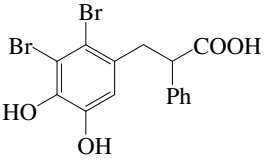


$C_{10}H_8Br_2O_3$ 335.979

(*E*)-*form*
Isol. from the brown alga *Leathesia nana*.
Red powder.
Mp 138-140°.

Xu, X.-L. *et al., Chin. Chem. Lett.*, 2004, **15**, 661-663 (*isol, pmr, cmr*)
Xu, X.-L. *et al., J. Asian Nat. Prod. Res.*, 2004, **6**, 217-221 (*isol, pmr, cmr*)

3-(2,3-Dibromo-4,5-dihydroxyphenyl)-2-phenylpropanoic acid D-235



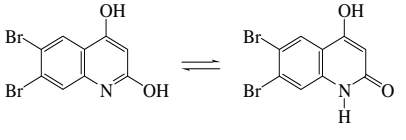
$C_{15}H_{12}Br_2O_4$ 416.065

(ξ)-*form*
Isol. from the red alga *Rhodomela confervoides*.
Brown gum.

Zhao, J. *et al., J. Nat. Prod.*, 2004, **67**, 1032-1035 (*isol, pmr, cmr*)

6,7-Dibromo-2,4-dihydroxyquinoline D-236

6,7-Dibromo-4-hydroxy-2(1H)-quinolinone, 9CI. 6,7-Dibromo-2,4-quinolinediol
[376598-45-7]

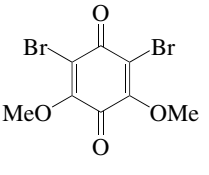


$C_9H_5Br_2NO_2$ 318.952
Isol. from the sponge *Hyrtios erecta*. Yellow powder. λ_{max} 216 (ϵ 37400) (MeOH).

Aoki, S. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1372-1374 (*isol, pmr, cmr*)

2,6-Dibromo-3,5-dimethoxy-1,4-benzoquinone D-237

2,6-Dibromo-3,5-dimethoxy-2,5-cyclohexadiene-1,4-dione
[61014-67-3]

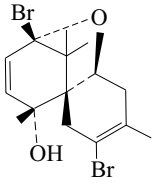


$C_8H_6Br_2O_4$ 325.941
Isol. from *Ptychodera flava laysanica*. Red plates (AcOH).
Mp 175°.

Robinson, R. *et al., J.C.S.*, 1941, 660 (*synth*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 22 (*occur*)

2,10-Dibromo-5,10-epoxy-2,8-chamigradien-7-ol D-238

[86510-24-9]



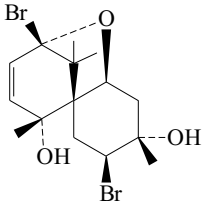
Absolute configuration

$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of red alga *Laurencia nipponica*. Oil. $[\alpha]_D$ -28.3 (c, 4.0 in $CHCl_3$).

Kurata, K. *et al., Chem. Lett.*, 1983, 561

2,10-Dibromo-5,10-epoxy-8-chamigrene-3,7-diol D-239

[74173-68-5]

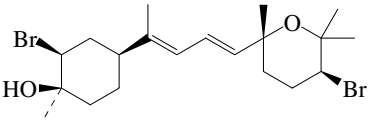


$C_{15}H_{22}Br_2O_3$ 410.145
Constit. of *Laurencia nipponica*. Cryst.
Mp 162-163°. $[\alpha]_D$ -12.8 (c, 1.25 in $CHCl_3$).

Suzuki, T. *et al., Chem. Lett.*, 1980, 541-542 (*isol, pmr, cmr*)

2,14-Dibromo-11,15-epoxy-7,9-prenylbisaboladien-3-ol D-240

[321847-10-3]

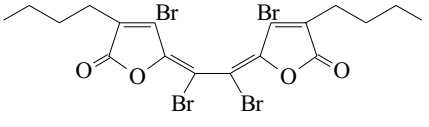


$C_{20}H_{32}Br_2O_2$ 464.28
Constit. of *Laurencia microcladia*.
$[\alpha]_D^{20}$ -33.3 (c, 0.2 in CCl_4). λ_{max} 245 (ϵ 11700) (MeOH).

Guella, G. *et al., Helv. Chim. Acta*, 2000, **83**, 2946-2952 (*isol, pmr, cmr*)

5,5′-(1,2-Dibromo-1,2-ethanediylidene)bis[4-bromo-3-butyl-2(5*H*)-furanone], 9CI D-241

[115721-46-5]

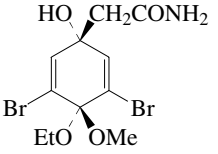


$C_{18}H_{18}Br_4O_4$ 617.954
Constit. of the red alga *Delisea elegans*. Cryst. (Et_2O/petrol).

McCombs, J.D. *et al., Tetrahedron*, 1988, **44**, 1489

3,5-Dibromo-4-ethoxy-1-hydroxy-4-methoxy-2,5-cyclohexadien-1-acetamide D-242

[41841-34-3]



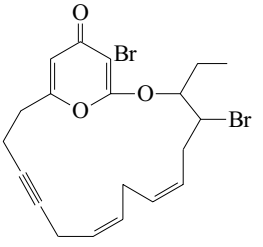
Relative Configuration

$C_{11}H_{15}Br_2NO_4$ 385.052
Related to Aplysinketal A, A-602. Alkaloid from an *Aplysina* sp. and *Pseudoceratina purpurea*. Originally thought to be an artifact.

Andersen, R.J. *et al., Tet. Lett.*, 1973, **14**, 1175-1178 (*isol*)
Kijjoa, A. *et al., Z. Naturforsch., B*, 2005, **60**, 904-908 (*isol*)

4,19-Dibromo-3-ethyl-2,20-dioxabicyclo[14.3.1]eicosa-1(19),6,9,16-tetraen-12-yn-18-one, 9CI D-243

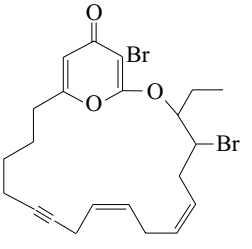
3,18-Dibromo-19-ethyl-2,6-epoxy-1-oxacyclononadeca-2,5,12,15-tetraen-9-yn-4-one
[129136-72-7]



$C_{20}H_{22}Br_2O_3$ 470.2
Isol. from the red alga *Phacelocarpus labillardieri*. Oil.

Blackman, A.J. *et al., Aust. J. Chem.*, 1990, **43**, 1133 (*isol, uv, ir, pmr, cmr, ms*)

3,20-Dibromo-21-ethyl-2,6-epoxy-1-oxa-2,5,14,17-cycloheneicosatetraen-11-yn-4-one D-244

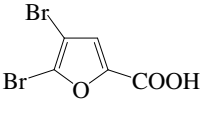


$C_{22}H_{26}Br_2O_3$ 498.254

(14Z,17Z)-form
Constit. of *Phacelocarpus labillardieri*. Cryst. (MeCN). Mp 107-109°.
Kazlauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 113

4,5-Dibromo-2-furancarboxylic acid, 9CI D-245

4,5-Dibromo-2-furoic acid, 8CI. 4,5-Dibromopyromucic acid
[2434-03-9]



$C_5H_2Br_2O_3$ 269.877
Cryst. (H_2O). Mp 170.5-171.5°.

tert-*Butyl ester:* [54113-43-8]
$C_9H_{10}Br_2O_3$ 325.984
Syrup.

Amide: ***4,5-Dibromo-2-furancarboxamide***
$C_5H_3Br_2NO_2$ 268.892
Isol. from the marine sponge *Phakellia conulus* from the Andaman Islands. Needles (MeOH aq.).
Mp 142-143°. λ_{max} 289 (ϵ 35000) (EtOH).

[54113-41-6, 54113-42-7]

Divald, S. *et al., J.O.C.*, 1976, **41**, 2835-2846 (*synth, pmr*)
Sarma, N.S. *et al., Indian J. Chem., Sect. B*, 1990, **29**, 771-772 (*amide*)
Karminski-Zamola, G. *et al., Heterocycles*, 1994, **38**, 759-767 (*synth*)
Bury, P. *et al., Tetrahedron*, 1994, **50**, 8793-8808 (*synth, ir, pmr, ms*)
Muratake, H. *et al., Chem. Pharm. Bull.*, 1997, **45**, 799-806 (*tert-butyl ester*)

1,1-Dibromo-2,4-heptanediol D-246

$H_3CCH_2CH_2CH(OH)CH_2CH(OH)CHBr_2$
$C_7H_{14}Br_2O_2$ 289.994

4-Ac: ***4-Acetoxy-1,1-dibromo-2-heptanol***
[109770-52-7]
$C_9H_{16}Br_2O_3$ 332.032
Constit. of the red alga *Ptilonia magellanica*. Pale yellow oil. Racemic.

Nicod, F. *et al., J. Nat. Prod.*, 1987, **50**, 259 (*isol, pmr, ms, ir*)

1,1-Dibromo-2-heptanol D-247

[74055-91-7]
$H_3C(CH_2)_4CH(OH)CHBr_2$
$C_7H_{14}Br_2O$ 273.995
Isol. from the red alga *Bonnemaisonia* sp.

(±)-*form*
Ac: [186344-77-4]
$C_9H_{16}Br_2O_2$ 316.032
Isol. from the alga *Delisea fimbriata*. Oil.

McConnell, O.J. *et al., Phytochemistry*, 1980, **19**, 233
Cueto, M. *et al., J. Nat. Prod.*, 1997, **60**, 279-281 (*acetate, isol*)

1,1-Dibromo-2-heptanone D-248

[14799-24-7]
$H_3C(CH_2)_4COCHBr_2$
$C_7H_{12}Br_2O$ 271.979
Isol. from *Bonnemaisonia hamifera*.

Jacobsen, N. *et al., Tet. Lett.*, 1978, **19**, 3065-3068 (*isol*)

1,3-Dibromo-2-heptanone, 9CI D-249

[1577-30-6]
$H_3C(CH_2)_3CHBrCOCH_2Br$
$C_7H_{12}Br_2O$ 271.979
Constit. of *Bonnemaisonia hamifera*. n_D^{25} 1.5043.

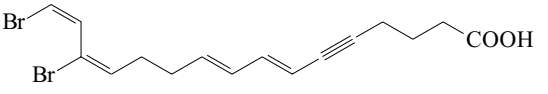
Org. Synth., 1973, **53**, 123 (*synth*)
Siuda, J.F. *et al., J.A.C.S.*, 1975, **97**, 937 (*isol*)

3,3-Dibromo-2-heptanone D-250

[69394-08-7]
$H_3C(CH_2)_3CBr_2COCH_3$
$C_7H_{12}Br_2O$ 271.979
Isol. from *Bonnemaisonia hamifera*.

Jacobsen, N. *et al., Tet. Lett.*, 1978, **19**, 3065-3068 (*isol*)

14,16-Dibromo-7,9,13,15-hexadecatetraen-5-ynoic acid D-251

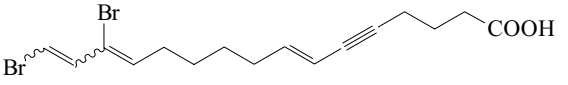


$C_{16}H_{18}Br_2O_2$ 402.125

(7*E*,9*E*,13*E*,15*Z*)-*form* [152543-03-8]
Isol. from the sponge *Oceanapia* sp. λ_{max} 204 (ϵ 15000); 268 (ϵ 37100); 278 (ϵ 28700) (MeOH) (Berdy).

Ichiba, T. *et al., Helv. Chim. Acta*, 1993, **76**, 2814 (*isol, pmr, cmr, uv, ir*)

14,16-Dibromo-7,13,15-hexadecatrien-5-ynoic acid D-252



$C_{16}H_{20}Br_2O_2$ 404.141

(7*E*,15*Z*)-*form* [70147-24-9]
Isol. from *Xestospongia muta*. Shows tumour-inhibitory and CNS activity. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 212
(ϵ 16335); 225 (ϵ 17920); 250 (ϵ 6235); 264 (ϵ 4353); 281 (ϵ 2470) (EtOH) (Berdy).

Schmitz, F.J. *et al., Tet. Lett.*, 1978, **19**, 3637-3640 (*isol, struct*)

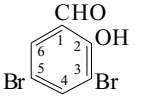
16,16-Dibromo-15-hexadecen-5-ynoic acid D-253

[162259-45-2]
$Br_2C{=}CH(CH_2)_8C{\equiv}CCH_2CH_2CH_2COOH$
$C_{16}H_{24}Br_2O_2$ 408.172
Isol. from the sponge *Xestospongia* sp.

Li, Y. *et al., J. Chem. Res., Synop.*, 1995, 126-127 (*isol*)

3,5-Dibromo-2-hydroxybenzaldehyde, 9CI D-254

3,5-Dibromosalicylaldehyde, 8CI
[90-59-5]



$C_7H_4Br_2O_2$ 279.915
Isol. from *Thelepus setosus*. Yellowish prims.
Mp 85° subl. pK_{a1} 6.54 (25°,butanol aq.). pK_{a1} 6.17 (25°,H_2O).

▶ CU5609000

Oxime: [21386-43-6]
$C_7H_5Br_2NO_2$ 294.93
Mp 218-220°.

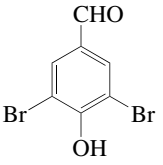
Ac: [109165-13-1]
$C_9H_6Br_2O_3$ 321.953
Mp 90°.

[61657-65-6]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 124A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 126A (*ir*)
Lindemann, H. *et al., Annalen*, 1926, **449**, 63-81 (*synth*)
Clarke, K. *et al., J.C.S.*, 1963, 245-250 (*synth, pKa*)
Ryabokobyklo, Yu.S. *et al., J. Org. Chem. USSR (Engl. Transl.)*, 1974, **10**, 1768 (*pKa*)
Higa, T. *et al., J.A.C.S.*, 1974, **76**, 2246-2248 (*isol*)
Hinterding, K. *et al., Bioorg. Med. Chem.*, 1998, **6**, 1153-1162 (*synth, pmr*)
Bandgar, B.P. *et al., Synth. Commun.*, 1998, **28**, 3225-3229 (*synth*)

3,5-Dibromo-4-hydroxybenzaldehyde, 9CI D-255

[2973-77-5]



$C_7H_4Br_2O_2$ 279.915
Isol. from *Polysiphonia urceolata, Rhodomela larix* and *Thelepus* spp. Needles (EtOH aq. or $CHCl_3$). Mp 186-187° (181°).

Oxime: Bromoxime
[25952-74-3]
$C_7H_5Br_2NO_2$ 294.93
Needles. Mp 199°.

Ac: [74849-10-8]
$C_9H_6Br_2O_3$ 321.953
Cryst. (EtOH). Mp 110-111°.

Di-Ac, oxime:
$C_{11}H_9Br_2NO_4$ 379.004
Mp 122°.

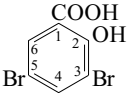
Me ether: 3,5-Dibromo-4-methoxybenzaldehyde
[108940-96-1]
$C_8H_6Br_2O_2$ 293.942
Cryst. (hexane/Et_2O). Mp 92°.

Benzyl ether:
$C_{14}H_{10}Br_2O_2$ 370.04
Needles (EtOH aq.). Mp 78-79°.

Wentworth, V. *et al., J.C.S.*, 1920, **117**, 1040-1045 (*oxime*)
Brink, M. *et al., CA*, 1956, **63**, 8240c (*synth*)
Tatsuo, H. *et al., J.A.C.S.*, 1974, **96**, 2246-2248 (*isol*)
Higa, T. *et al., Tetrahedron*, 1975, **31**, 2379-2381 (*isol*)
Kurata, K. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 2020-2022; 2099-2100 (*isol*)
Norte, M. *et al., Tetrahedron*, 1988, **44**, 4973-4980 (*Me ether, synth, ir, pmr*)
Sudalai, A. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 858-859 (*synth*)
Kassuhlke, K.E. *et al., Tetrahedron*, 1991, **47**, 1809-1814 (*synth*)
Itaya, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1297-1300 (*synth, ir, pmr*)

3,5-Dibromo-2-hydroxybenzoic acid D-256

3,5-Dibromosalicylic acid
[3147-55-5]



$C_7H_4Br_2O_3$ 295.915
Needles (EtOH). Mp 225° (223°) Mp 228°. pK_{a1} 2.16 (25°).

Me ester: [21702-79-4]
$C_8H_6Br_2O_3$ 309.942
Needles. Mp 149° Mp 156°. Bp_{12} 181°.

Et ester: [64831-28-3]
$C_9H_8Br_2O_3$ 323.968
Rhombic plates. Mp 101°. Bp_{16} 184°.

Amide: [17892-25-0]
$C_7H_5Br_2NO_2$ 294.93
Needles. Mp 183° dec.

Nitrile: 3,5-Dibromo-2-hydroxybenzonitrile. 2,4-Dibromo-6-cyanophenol
[40718-08-9]
$C_7H_3Br_2NO$ 276.915
Mp 167-168°.

Me ether: 3,5-Dibromo-2-methoxybenzoic acid
[13130-23-9]
$C_8H_6Br_2O_3$ 309.942
Isol. from the sponge *Didiscus* sp. Needles (EtOH aq.).
Mp 193-194°.

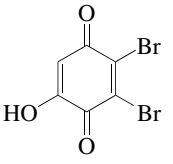
Me ether, Me ester: [15790-59-7]
$C_9H_8Br_2O_3$ 323.968
Needles. Mp 53°.

*Anilide: 3,5-Dibromo-2-hydroxy-*N*-phenylbenzamide, 9CI. 3,5-Dibromosalicylanilide, 8CI.* ***Metabromsalan, INN, USAN****. NSC 526280*
[2577-72-2]
$C_{13}H_9Br_2NO_2$ 371.028
Disinfectant, anthelmintic. Log P 4.91 (calc).
▶ CV3459525

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 230C; 374D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1146A (*nmr*)
Leulier, A. *et al., Bull. Soc. Chim. Fr.*, 1927, **41**, 1362
Musante, C. *et al., Gazz. Chim. Ital.*, 1948, **78**, 536
Berends, W. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1955, **74**, 1323
U.S. Pat., 1970, (*Dow*)3 513 196; *CA*, **73**, 35081m (*synth, use, anilide*)
Norbury, H.M. *et al., Xenobiotica*, 1981, **11**, 511 (*Metabromsalan, metab*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1120
Utkina, N.K. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1998, **47**, 2292-2294 (*isol, Me ether*)

2,3-Dibromo-5-hydroxy-1,4-benzoquinone D-257

2,3-Dibromo-5-hydroxy-2,5-cyclohexadiene-1,4-dione



$C_6H_2Br_2O_3$ 281.888

Me ether: 2,3-Dibromo-5-methoxy-1,4-benzoquinone
$C_7H_4Br_2O_3$ 295.915
Isol. from *Ptychodera flava laysanica*.

Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 22 (*occur*)

3,5-Dibromo-4-hydroxybenzyl alcohol D-258

3,5-Dibromo-4-hydroxybenzenemethanol, 9CI. 3,5-Dibromo-α, 4-dihydroxytoluene. 2,6-Dibromo-4-hydroxymethylphenol
[2316-62-3]

$C_7H_6Br_2O_2$ 281.931
Isol. from red algae and marine worms; *Thelepus setosus*, *Laurencia intermedia*, *Odonthalia corymbifera*, *Odonthalia dentata*, *Polysiphonia* spp. and *Rhodomela larix* and *Rhodomela confervoides*. Plates or leaflets (C_6H_6).
Mp 116-117°. λ_{max} 291 (EtOH) (Berdy).

α-Ac: [105960-31-4]
$C_9H_8Br_2O_3$ 323.968
Cryst. (petrol). Mp 115°.

Di-Ac: [74849-03-9]
$C_{11}H_{10}Br_2O_4$ 366.006
Mp 68-70°.

α-Me ether: 2,6-Dibromo-4-(methoxymethyl)phenol, 9CI
[71119-02-3]
$C_8H_8Br_2O_2$ 295.958
Mp 71-72°.

α-Et ether: 2,6-Dibromo-4-(ethoxymethyl)phenol, 9CI
[71119-04-5]
$C_9H_{10}Br_2O_2$ 309.985
Mp 94°.

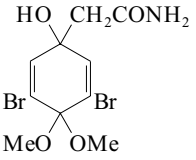
4-Benzyl ether: [249515-07-9]
$C_{14}H_{12}Br_2O_2$ 372.056
Needles (hexane). Mp 96-97°.

v. Auwers, K. *et al., Ber.*, 1899, **32**, 3373-3381 (*synth*)
Brink, M. *et al., Acta Chem. Scand.*, 1965, **19**, 255-256 (*synth*)
Craigie, J.S. *et al., Science (Washington, D.C.)*, 1967, **157**, 1058-1059 (*occur*)
Higa, T. *et al., J.A.C.S.*, 1974, **96**, 2246-2248 (*isol*)
Weinstein, B. *et al., Phytochemistry*, 1975, **14**, 2667-2670 (*isol, rev*)

Torii, S. *et al., J.O.C.*, 1979, **44**, 3305-3310 (*ethers, synth, ir, pmr*)
Sudalai, A. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 858-859 (*synth*)
Itaya, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1297-1300 (*4-benzyl ether, synth, ir, pmr*)

3,5-Dibromo-1-hydroxy-4,4-dimethoxy-2,5-cyclohexadiene-1-acetamide, 9CI D-259

[24742-01-6]



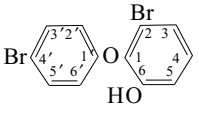
$C_{10}H_{13}Br_2NO_4$ 371.025

Related to Aplysinketal A, A-602. Isol. from the sponges *Aplysina* sp., *Verongia fistularis* and *Verongia cauliformis*. Prisms (EtOAc). Fairly sol. Et_2O, EtOAc.
Mp 191°.

Sharma, G.M. *et al., J. Antibiot., Ser. A*, 1967, **20**, 200-203 (*isol*)
Sharma, G.M. *et al., J.O.C.*, 1970, **35**, 2823-2826 (*ir, pmr, struct*)
Toscano, R.A. *et al., Acta Cryst. C*, 1992, **48**, 2235-2237 (*cryst struct*)

2,4′-Dibromo-6-hydroxydiphenyl ether D-260

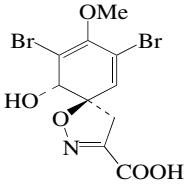
3-Bromo-2-(4-bromophenoxy)phenol, 9CI
[38926-84-0]



$C_{12}H_8Br_2O_2$ 344.002
Constit. of *Dysidea herbacea*.
Mp 95-98°. λ_{max} 295 (ϵ 1600) (MeOH) (Berdy). λ_{max} 305 (ϵ 1600) (MeOH-NaOH) (Berdy).

Sharma, G.M. *et al., Tet. Lett.*, 1972, 1715 (*synth*)

7,9-Dibromo-10-hydroxy-8-methoxy-1-oxa-2-azaspiro[4,5]deca-2,6,8-triene-3-carboxylic acid, 9CI D-261



(5*R*,6*S*)-*form*

$C_{10}H_9Br_2NO_5$ 382.993

(5*R*,6*S*)-*form* [168480-66-8]
Isol. from the sponge *Pseudoceratina* sp. Antibacterial agent. λ_{max} 224 (ϵ 19000); 285 (ϵ 9400) (MeOH).

(5*S*,6*R*)-*form*

Me ester: [179798-47-1]
[160116-56-3]
$C_{11}H_{11}Br_2NO_5$ 397.02
Alkaloid from sponges *Aplysina archeri* and *Verongula* sp.

Amide: ***Purealidin R***
[167469-52-5]
$C_{10}H_{10}Br_2N_2O_4$ 382.008
Alkaloid from the Okinawan marine sponge *Psammaplysilla purea* and from the Caribbean sponge *Verongula* sp. Oil. $[\alpha]_D^{24}$ +86 (c, 0.19 in MeOH).

Amide, N-*[4-(methoxycarbonylamino)-2-oxobutyl]:* [223580-93-6]
$C_{16}H_{19}Br_2N_3O_7$ 525.15
Alkaloid from *Aplysina cauliformis*. λ_{max} 229 (ϵ 18500); 280 (ϵ 10600) (MeOH).

Amide, N-*[4-(methoxycarbonylamino)-3-oxobutyl]:* [223580-91-4]
$C_{16}H_{19}Br_2N_3O_7$ 525.15
Alkaloid from *Aplysina cauliformis*. λ_{max} 227 (ϵ 19000); 281 (ϵ 10500) (MeOH).

(5*R,6*S**)-*form***

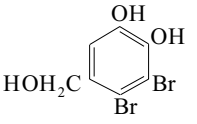
Amide, N-*(2-carboxyethyl):* ***Purpuroceratic acid A***
$C_{13}H_{14}Br_2N_2O_6$ 454.071
Alkaloid from *Pseudoceratina purpurea*. Gum. $[\alpha]_D^{20}$ -27.7 (c, 0.55 in MeOH).

Amide, N-*(3-carboxypropyl):* ***Purpuroceratic acid B***
$C_{14}H_{16}Br_2N_2O_6$ 468.098
Alkaloid from *Pseudoceratina purpurea*.

Ciminiello, P. *et al., J. Nat. Prod.*, 1994, **57**, 1564-1569 (*isol*)
Aiello, A. *et al., Biochem. Syst. Ecol.*, 1995, **23**, 377-381 (*isol*)
Kobayashi, J. *et al., Chem. Pharm. Bull.*, 1995, **43**, 403-407 (*isol, uv, cd, ir, pmr, cmr*)
Ciminiello, P. *et al., J. Nat. Prod.*, 1999, **62**, 590-593 (*Aplysina cauliformis derivs*)
Kijjoa, A. *et al., Z. Naturforsch., B*, 2005, **60**, 904-908 (*Purpuroceratic acids*)

3,4-Dibromo-5-hydroxymethyl-1,2-benzenediol D-262

2,3-Dibromo-4,5-dihydroxybenzyl alcohol. ***Lanosol***
[4950-06-5]



$C_7H_6Br_2O_3$ 297.931
Isol. from red algae *Lenormandia prolifera*, *Polysiphonia*, *Odonthalia* and *Rhodomela* spp. Glucosidase inhibitor. Cryst. (C_6H_6). Sol. bases, MeOH, Et_2O; poorly sol. H_2O.
Mp 129-130°. λ_{max} 291 (MeOH) (Berdy). λ_{max} 292 (ϵ 4073) (EtOH) (Berdy).

1,2-Disulfate ester:
$C_7H_6Br_2O_9S_2$ 458.059
Isol. as di-K salt from *Polysiphonia lanosa*.

1-Me ether: 2,3-Dibromo-4-hydroxy-5-methoxybenzenemethanol, 9CI. 2,3-Dibromo-4-hydroxymethyl-6-methoxyphenol
[1940-81-4]
$C_8H_8Br_2O_3$ 311.957
Isol. from *Rhodomela larix, Odonthalia corymbifera* and *Antithamnion plumula*. Prisms (C_6H_6). Sol. MeOH, $CHCl_3$; fairly sol. C_6H_6; poorly sol. H_2O.
Mp 129-130°.

1,2-Di-Me ether: 2,3-Dibromo-4,5-dimethoxybenzyl alcohol
$C_9H_{10}Br_2O_3$ 325.984
Isol. from *Rytiphloea tinctoria*. Cryst. (C_6H_6/hexane).
Mp 92°. Genus name incorr. given as *Rytiphlea*.

1′-Me ether: 3,4-Dibromo-5-(methoxymethyl)-1,2-benzenediol. ***Methyllanosol***
[14045-42-2]
$C_8H_8Br_2O_3$ 311.957
Constit. of *Polysiphonia lanosa* and *Rytiphloea* spp. Also from *Odonthalia washingtoniensis* and *Odonthalia floccosa*. Cryst. (C_6H_6).
Mp 129-130° (124°).

1′-Et ether: 3,4-Dibromo-5-(ethoxymethyl)-1,2-benzenediol
[54502-93-1]
$C_9H_{10}Br_2O_3$ 325.984
Constit. of *Fucus vesiculosus*, *Odonthalia dentata* and *Polysiphonia lanosa*.

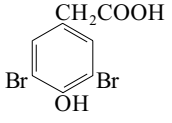
1′-Propyl ether: 3,4-Dibromo-5-(propoxymethyl)-1,2-benzenediol
[52897-62-8]

$C_{10}H_{12}Br_2O_3$ 340.011
Constit. of *Polysiphonia lanosa* and *Polysiphonia nigrescens*.

Hodgkin, J.H. *et al., Can. J. Chem.*, 1966, **44**, 74-78 (*disulfate, isol*)
Katsui, N. *et al., Tetrahedron*, 1967, **23**, 1185
Weinstein, B. *et al., Phytochemistry*, 1975, **14**, 2667 (*rev*)
Chevolot-Magueur, A.-M. *et al., Phytochemistry*, 1976, **15**, 767 (*isol*)
Saenger, P. *et al., Phytochemistry*, 1976, **15**, 1957 (*isol*)
Pedersen, M. *et al., Phytochemistry*, 1978, **17**, 291 (*isol*)
Kubo, I. *et al., Pure Appl. Chem.*, 1989, **61**, 373-375 (*Methyllanosol, isol*)
Kubo, I. *et al., J. Nat. Prod.*, 1990, **53**, 50 (*synth, deriv, pmr, cmr, ms*)
Aknin, M. *et al., Tet. Lett.*, 1992, **33**, 555 (*isol, bibl*)
Kurata, K. *et al., Phytochemistry*, 1997, **45**, 485-487 (*isol, bibl*)
Kurihara, H. *et al., J. Nat. Prod.*, 1999, **62**, 882-884 (*isol, pmr, cmr*)
Shoeib, N.A. *et al., J. Nat. Prod.*, 2004, **67**, 1445-1449 (*synth, activity*)

(3,5-Dibromo-4-hydroxyphenyl)acetic acid D-263

3,5-Dibromo-4-hydroxybenzeneacetic acid, 9CI
[24744-58-9]



$C_8H_6Br_2O_3$ 309.942
Constit. of the red alga *Halopytis incurvus*. Cryst. (H_2O).
Mp 195-196°.

Et ester: [24744-59-0]
$C_{10}H_{10}Br_2O_3$ 337.995
Cryst. (hexane). Mp 105°.

Amide: 3,5-Dibromo-4-hydroxyphenylacetamide
[17194-96-6]
$C_8H_7Br_2NO_2$ 308.957
Isol. from the sponges *Aplysina fistularis* and *Verongia archeri*. Antimicrobial agent.
Mp 190-191°.

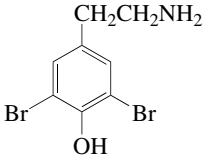
Nitrile: 3,5-Dibromo-4-hydroxybenzeneacetonitrile. 3,5-Dibromo-4-hydroxybenzyl cyanide. 2,6-Dibromo-4-(cyanomethyl)phenol
[73348-20-6]
$C_8H_5Br_2NO$ 290.942
Isol. from the sponge *Verongia aurea*. Antibacterial agent. Pale yellow solid.
Mp 176.5°.

Me ether, nitrile: 3,5-Dibromo-4-methoxybenzeneacetonitrile. 3,5-Dibromo-4-methoxybenzyl cyanide. 2,6-Dibromo-4-(cyanomethyl)anisole
[55027-78-6]
$C_9H_7Br_2NO$ 304.968
Isol. from *Verongia aurea*. Antibacterial agent.

Sharma, G.M. *et al., J.O.C.*, 1970, **35**, 2823-2826 (*synth*)
Chantraine, J.M. *et al., Phytochemistry*, 1973, **12**, 1793-1796 (*isol*)
Yamada, Y. *et al., Chem. Lett.*, 1974, 1399-1400 (*synth, amide*)
Chib, J.S. *et al., J. Pharm. Sci.*, 1978, **67**, 264-265 (*isol, amide*)
Goo, Y.M. *et al., CA*, 1980, **92**, 169100t (*nitriles*)
D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1984, **67**, 1484-1492 (*synth*)
Goo, Y.M. *et al., Arch. Pharmacal Res.*, 1985, **8**, 21-30 (*amide, isol*)
Boehlow, T.R. *et al., J.O.C.*, 2001, **66**, 3111-3118 (*nitrile, synth, ir, pmr, cmr*)

2-(3,5-Dibromo-4-hydroxyphenyl)ethylamine D-264

4-(2-Aminoethyl)-2,6-dibromophenol, 9CI. 3,5-Dibromo-4-hydroxybenzeneethanamine. 3,5-Dibromotyramine
[134755-34-3]



$C_8H_9Br_2NO$ 294.973

N,N,N-*Tri-Me: 3,5-Dibromo-4-hydroxy*-N,N,N-*trimethylbenzeneethanaminium, 9CI. 3,5-Dibromo-4-hydroxyphenethyltrimethylammonium. 3,5-Dibromo*-N,N,N-*trimethyltyramine*
[73414-57-0]
$C_{11}H_{16}Br_2NO^{\oplus}$ 338.062
Isol. from the sponge *Verongia fistularis*. Dual adrenergic agent. Needles (MeOH) (? as chloride). Poorly sol. hexane.
Mp 230° dec. (? chloride).

Me ether: (3,5-Dibromo-4-methoxyphenyl)ethylamine. 3,5-Dibromo-4-methoxybenzeneethanamine, 9CI
$C_9H_{11}Br_2NO$ 309
Alkaloid from a *Eudistoma* sp. Amorph. solid (as trifluoroacetate). λ_{max} 208 (log ϵ 4.9); 224 (log ϵ 4.3); 284 (log ϵ 3) (MeOH) (as trifluoroacetate).

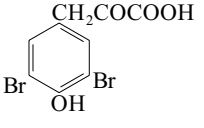
Me ether, N,N,N-*tri-Me: 3,5-Dibromo-4-methoxy*-N,N,N-*trimethylbenzeneethanaminium. 3,5-Dibromo*-N,N,N,O-*tetramethyltyramine*
[160116-58-5]
[160116-59-6]
$C_{12}H_{18}Br_2NO^{\oplus}$ 352.088
Metab. of the Caribbean sponge *Verongula* sp. and a *Pseudoceratina* sp. Amorph. solid (as trifluoroacetate). CAS no. refers to trifluoroacetate. λ_{max} 277 (ϵ 1260) (EtOH) (as trifluoroacetate).

[13062-88-9, 73414-58-1]

Benington, F. *et al., J.O.C.*, 1958, **23**, 1979-1984 (*synth*)
Hollenbeak, K.H. *et al., CA*, 1980, **92**, 180749g (*isol*)
Ciminiello, P. *et al., J. Nat. Prod.*, 1994, **57**, 1564-1569 (*N,N,N,O-tetra-Me*)
Aiello, A. *et al., Biochem. Syst. Ecol.*, 1995, **23**, 377-381 (*N,N,N,O-tetra-Me*)
Van Wagoner, R.M. *et al., J. Nat. Prod.*, 1999, **62**, 794-797 (*isol, synth, uv, pmr, cmr, Me ether*)
Fu, X. *et al., J. Nat. Prod.*, 1999, **62**, 1072-1073 (*isol, pmr, cmr, N-tri-Me*)
Schoenfeld, R.C. *et al., Bioorg. Med. Chem. Lett.*, 2002, **12**, 823-825 (*synth*)

3-(3,5-Dibromo-4-hydroxyphenyl)-2-oxopropanoic acid D-265

3,5-Dibromo-4-hydroxy-α-oxobenzenepropanoic acid. 3-(3,5-Dibromo-4-hydroxyphenyl)-2-hydroxy-2-propenoic acid. (3,5-Dibromo-4-hydroxyphenyl)pyruvic acid
[13990-07-3]

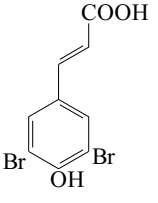


$C_9H_6Br_2O_4$ 337.952
Constit. of the alga *Halopytis incurvus*. Needles (EtOH aq.).
Mp 208° dec. Nat. prod. isol. as the α,4-di-Me ether of the enol form.

Shiba, T. *et al., J.O.C.*, 1964, **29**, 3061 (*synth*)
Chantraine, J.-M. *et al., Phytochemistry*, 1973, **12**, 1793 (*isol*)

3-(3,5-Dibromo-4-hydroxyphenyl)-2-propenoic acid D-266

3,5-Dibromo-4-hydroxycinnamic acid
[119405-33-3]



$C_9H_6Br_2O_3$ 321.953

(E)-form [56926-78-4]
Mp 244°.

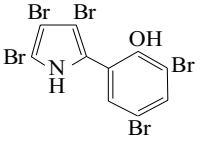
4-O-(3-Dimethylaminopropyl): 3,5-Dibromo-4-[3-(dimethylamino)propoxy]cinnamic acid
[134276-56-5]
$C_{14}H_{17}Br_2NO_3$ 407.101
Isol. from the sponge *Pseudoceratina crassa*. Cryst.
Mp 193-194° dec. λ_{max} 223 (ϵ 13700); 267 (ϵ 11000) (MeOH) (Berdy).
▶ Genotoxic.

4-O-(3-Dimethylaminopropyl), Et ester: [134276-55-4]
$C_{16}H_{21}Br_2NO_3$ 435.155
Isol. from *Pseudoceratina crassa*. Antibacterial agent. Flakes.
Mp 67°. λ_{max} 230 (ϵ 11200); 282 (ϵ 9500) (MeOH) (Berdy).
▶ Genotoxic.

Gupta, S.K. *et al., J. Indian Chem. Soc.*, 1988, **65**, 187 (*synth*)
Kassühlke, K.E. *et al., Tetrahedron*, 1991, **47**, 1809-1814 (*isol, synth, derivs*)

2-(3,5-Dibromo-2-hydroxyphenyl)-3,4,5-tribromopyrrole D-267

*2,4-Dibromo-6-(3,4,5-tribromo-1*H*-pyrrol-2-yl)phenol, 9CI. Pentabromopseudilin*
[10245-81-5]



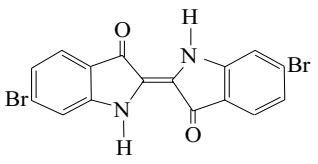
$C_{10}H_4Br_5NO$ 553.668
Pyrrole antibiotic. Isol. from the marine bacterium *Pseudomonas bromoutilis* and as the major metab. of yellow and off-white strains of *Chromobacterium*. Also from another *Chromobacterium* sp. and *Alteromonas luteo-violaceus*. Active against gram-positive bacteria. Inhibitor of esterases, aminopeptidases, elastase, urokinase and alkaline phosphatase. Cryst. (C_6H_6/hexane). Sol. Me_2CO, butanol, EtOAc, Et_2O; fairly sol. $CHCl_3$, MeOH; poorly sol. H_2O, hexane. Mp 130-170° dec. λ_{max} 286; 308 (MeOH) (Berdy). λ_{max} 284; 293; 355 (MeOH/NaOH) (Berdy).
▶ LD_{50} (mus, ivn) 25 - 75 mg/kg , LD_{50} (mus, scu) 250 - 350 mg/kg , LD_{50} (mus, ipr) 50 mg/kg.

Me ether:
$C_{11}H_6Br_5NO$ 567.695
Mp 124-125°.

Burkholder, P.R. *et al., Appl. Microbiol.*, 1966, **14**, 649 (*isol, struct*)
Hanessian, S. *et al., J.A.C.S.*, 1966, **88**, 4509 (*synth, ms*)
Lovell, F.M. *et al., J.A.C.S.*, 1966, **88**, 4510 (*cryst struct*)
ApSimon, J.W. *et al., Chem. Ind. (London)*, 1973, 275 (*synth*)
Andersen, R.J. *et al., Mar. Biol. (Berlin)*, 1974, **27**, 281 (*isol, uv, pmr, ms*)
Faulkner, D.J. *et al., Top. Antibiot. Chem.*, 1978, **2**, 9
Laatsch, H. *et al., Annalen*, 1989, 863 (*synth, bibl*)
Hanefeld, U. *et al., J.O.C.*, 1994, **59**, 3604 (*biosynth*)
Xu, Z. *et al., J.O.C.*, 1998, **63**, 5031-5041 (*synth*)

6,6′-Dibromoindigotin D-268

*6-Bromo-2-(6-bromo-1,3-dihydro-3-oxo-2*H*-indol-2-ylidene)-1,2-dihydro-3*H*-indol-3-one, 9CI. 6,6′-Dibromoindigo. Tyrian purple. C.I. Natural Violet 1*
[19201-53-7]



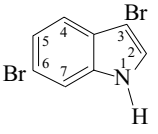
$C_{16}H_8Br_2N_2O_2$ 420.059
Major component of Tyrian Purple obt. from *Murex brandaris*, *Murex trunculus*, *Purpura aperta* and *Purpura lapillus*. Important dyestuff in ancient times, but has never been prod. commercially. Violet cryst. (1,2-dichlorobenzene).
Mp >300°.

N,N′-Di-Ac: Mp 306°.

Sachs, F. *et al., Ber.*, 1904, **37**, 1861-1874 (*synth*)
Friedländer, P. *et al., Ber.*, 1909, **42**, 765-770 (*struct*)
Baker, J.T. *et al., Tet. Lett.*, 1968, 43-46 (*biosynth*)
Süsse, P. *et al., Naturwissenschaften*, 1979, **66**, 110 (*cryst struct*)
Larsen, S. *et al., Acta Chem. Scand., Ser. A*, 1980, **34**, 171-176 (*cryst struct*)
Voss, G. *et al., Chem. Ber.*, 1989, **122**, 1199-1201 (*synth, ir, bibl*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **8**, 559 (*bibl*)
Ghireti, F. *et al., Experientia*, 1994, **50**, 802-807 (*bibl*)
Cooksey, C.J. *et al., Molecules*, 2001, **6**, 736-739 (*rev*)
Imming, P. *et al., Synth. Commun.*, 2001, **31**, 3721-3727 (*synth*)

3,6-Dibromo-1*H*-indole, 9CI D-269

[74076-56-5]



$C_8H_5Br_2N$ 274.942
Isol. from the ascidian *Distaplia regina*. Probable constit. of the hemichordates *Ptychodera flava* and *Glossobalanus* sp. Shows antibacterial activity. Oil. λ_{max} 224 (log ϵ 5.26); 282 (log ϵ 4.59); 293 (log ϵ 4.48) (hexane).

Higa, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **65**, 525 (*isol*)
Qureshi, A. *et al., Nat. Prod. Lett.*, 1999, **13**, 59-62 (*isol, pmr, cmr, activity*)

4,6-Dibromo-1*H*-indole, 9CI D-270

Glossobalol
[99910-50-6]
$C_8H_5Br_2N$ 274.942
Alkaloid from the acorn worm *Glossobalanus* sp.
Mp 60-61°.

Ac:
$C_{10}H_7Br_2NO$ 316.979
Mp 108-108.5° (102-104°).

Higa, T. *et al., Experientia*, 1985, **41**, 1487 (*isol, ir, pmr, ms, struct*)
Martin, P. *et al., Tet. Lett.*, 1987, **28**, 1645 (*synth*)
Ohta, T. *et al., Heterocycles*, 1987, **26**, 2817 (*synth*)

1,1-Dibromo-3-iodo-2-heptanone D-271

[69394-09-8]
$H_3C(CH_2)_3CHICOCHBr_2$
$C_7H_{11}Br_2IO$ 397.876

(ξ)-form
Isol. from *Bonnemaisonia hamifera*.

Jacobsen, N. *et al., Tet. Lett.*, 1978, **19**, 3065-3068 (*isol*)

3,3-Dibromo-1-iodo-2-heptanone, 9CI D-272

[54899-97-7]
$H_3CCH_2CH_2CH_2CBr_2COCH_2I$
$C_7H_{11}Br_2IO$ 397.876
Constit. of *Bonnemaisonia hamifera*.

Siuda, J.F. *et al., J.A.C.S.*, 1975, **97**, 937

Dibromoiodomethane, 9CI D-273

[593-94-2]
$CHBr_2I$
$CHBr_2I$ 299.731
Isol. from several marine algae. Plates (petrol).
Mp 22.5°. Bp_{42} 91°. Mod. stable to light in solid state, very unstable in soln.

Auger, V. *et al., C. R. Hebd. Seances Acad. Sci.*, 1908, **146**, 1038 (*synth*)
Dehmlow, E.V. *et al., Chem. Ber.*, 1982, **115**, 3894 (*synth*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Novak, I. *et al., J.O.C.*, 2002, **67**, 3510-3513 (*cmr, pmr, pe*)

1,1-Dibromo-2-iodo-1-octen-3-one, 9CI D-274

[64785-98-4]
$H_3C(CH_2)_4COCI{=}CBr_2$
$C_8H_{11}Br_2IO$ 409.887
Constit. of *Delisea fimbriata*.

Rose, A.F. *et al., Tet. Lett.*, 1977, 1847

1,1-Dibromo-3-iodo-2-propanone, 9CI D-275

1,1-Dibromo-3-iodoacetone
[59227-99-5]
$Br_2CHCOCH_2I$
$C_3H_3Br_2IO$ 341.769
Minor component of the essential oil of the edible Hawaiian red algae, *Asparagopsis taxiformis* and *Asparagopsis armata*.

Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*isol, glc, ms*)
McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367 (*isol, glc, ms*)

2,3-Dibromo-3-iodo-2-propenoic acid D-276

2,3-Dibromo-3-iodoacrylic acid
[71815-47-9]
$BrIC{=}CBrCOOH$
$C_3HBr_2IO_2$ 355.752
Constit. of the red alga *Asparagopsis taxiformis*.

Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617 (*isol*)

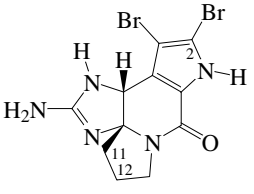
3,3-Dibromo-2-iodo-2-propenoic acid D-277

3,3-Dibromo-2-iodoacrylic acid
[71815-29-7]
$Br_2C{=}CICOOH$
$C_3HBr_2IO_2$ 355.752
Constit. of the red alga *Asparagopsis taxiformis*.

Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617 (*isol*)

Dibromoisophakellin D-278

Dibromocantharelline



(+)-*form*

$C_{11}H_{11}Br_2N_5O$ 389.049

(+)-*form* [101481-34-9]
Metab. from the New Caledonian sponge *Pseudaxinyssa cantharella*.
Cryst. + $2H_2O$ + 1MeOH (MeOH).
Mp 260°. $[\alpha]_D^{20}$ +95 (c, 1.0 in MeOH).

2-Debromo: ***Monobromoisophakellin***
$C_{11}H_{12}BrN_5O$ 310.153
Isol. from *Agelas* sp. λ_{max} 276 (log ϵ 3.84) (MeOH).

11α-Hydroxy, 12α-chloro: ***12-Chloro-11-hydroxydibromoisophakellin***
$C_{11}H_{10}Br_2ClN_5O_2$ 439.493
Isol. from the sponge *Axinella brevistyla*.
$[\alpha]_D^{23}$ +51 (c, 0.41 in MeOH). λ_{max} 207 (log ϵ 4.4); 242 (sh) (log ϵ 3.8) (MeOH).

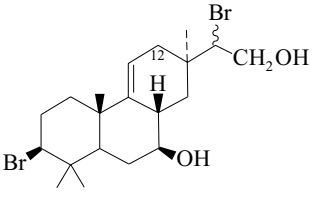
(-)-*form* [104758-96-5]
Metab. from the marine sponge *Acanthella carteri*.
Cryst. (MeOH)(as hydrochloride).
Mp 275-277° (hydrochloride). $[\alpha]_D$ -101 (c, 0.56 in MeOH).

N^1*-Me:* ***Dibromo-N^1-methylisophakellin***. N^1*-Methyldibromoisophakellin*
[373604-86-5]
$C_{12}H_{13}Br_2N_5O$ 403.076
Isol. from the sponge *Stylissa caribica*. λ_{max} 288 (log ϵ 3.92) (H_2O).

[105088-20-8]

De Nanteuil, G. *et al., Tetrahedron*, 1985, **41**, 6019-6033 (*isol, uv, ir, pmr, cmr, ms, cd, cryst struct, Dibromocantharelline*)
Fedoreyev, S.A. *et al., Tet. Lett.*, 1986, **27**, 3177-3180 (*uv, ir, pmr, cmr ms, cd, cryst struct*)
Assmann, M. *et al., J. Nat. Prod.*, 2001, **64**, 1345-1347 (*N-Me*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 2001, **64**, 1576-1578 (*Chlorohydroxydibromoisophakellin*)
Wiese, K.J. *et al., Tet. Lett.*, 2002, **43**, 5135-5136 (*synth*)
Assmann, M. *et al., Z. Naturforsch., C*, 2002, **57**, 153-156 (*Monobromoisophakellin*)

3,15-Dibromo-9(11)-isopimarene-7,16-diol D-279



$C_{20}H_{32}Br_2O_2$ 464.28

(3β,7β,15ξ)-*form* [95387-45-4]
Constit. of *Laurencia perforata*.
Cryst. (hexane/CH_2Cl_2).
Mp 106-107°. $[\alpha]_D$ +12.5 (c, 0.4 in $CHCl_3$).

Di-Ac:
$C_{24}H_{36}Br_2O_4$ 548.354
Isol. from sponge *Spongia zimocca*.

12α-Hydroxy: ***3,15-Dibromo-9(11)-isopimarene-7,12,16-triol***
[95387-47-6]
$C_{20}H_{32}Br_2O_3$ 480.279
Constit. of *Laurencia perforata*. Cryst. (hexane) (as tri-Ac).
Mp 166-168° (tri-Ac). $[\alpha]_D$ -159.5 (c, 0.68 in $CHCl_3$) (tri-Ac).

Gonzalez, A.G. *et al., J.O.C.*, 1985, **50**, 1261
Guella, G. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1992, **103**, 1019-1023 (*di-Ac*)

Dibromomethane, 9CI D-280

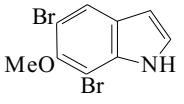
Methylene bromide. R 30B2
[74-95-3]
CH_2Br_2
CH_2Br_2 173.835
Isol. from various marine algae inc. the red alga *Asparagopsis taxiformis*. Solvent, reagent for org. synth. Liq. Spar. sol. H_2O.
d_{25}^{25} 2.48.
Fp -52.7. Bp 97°. n_D^{20} 1.5410.
▶ Fl. p. >100°. Reacn. with K metal produces shock-sensitive explosive. LD_{50} (rat, orl) 108 mg/kg. PA7350000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 71A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 106A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 102D (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 357 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 273; 1972, **3**, 189; 1974, **4**, 442-443; 1975, **5**, 398; 403; 1977, **6**, 10; 162; 274; 1979, **7**, 4; 90; 1980, **8**, 387; 1984, **11**, 157; 158; 1988, **13**, 93; 1992, **16**, 107 (*use*)
Malinowski, E.R. *et al., J. Phys. Chem.*, 1971, **75**, 3971 (*pmr*)
Kawaguchi, T. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 57 (*cryst struct*)
Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*isol*)
Goplen, T.G. *et al., Appl. Spectrosc.*, 1980, **34**, 657 (*ir*)
Hanner, A.W. *et al., Org. Mass Spectrom.*, 1982, **17**, 19 (*ms*)
Yonovich-Weiss, M. *et al., Synthesis*, 1984, 34 (*synth*)
Dostovalova, V.I. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1985, 2467; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1985, 2282 (*cmr*)
Niide, Y. *et al., J. Mol. Spectrosc.*, 1990, **139**, 11 (*Raman*)

Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **3**, 1561-1568 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0377
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 398
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DDP800

5,7-Dibromo-6-methoxy-1*H*-indole, 9CI D-281

[58933-47-4]

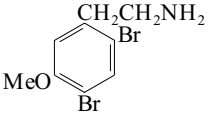


$C_9H_7Br_2NO$ 304.968
Alkaloid from the hemichordate *Ptychodera flava laysanica*.

Higa, T. *et al., Heterocycles*, 1976, **4**, 227 (*isol, pmr, struct*)

2-(2,4-Dibromo-5-methoxyphenyl)ethylamine D-282

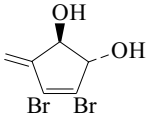
2,4-Dibromo-5-methoxybenzeneethanamine, 9CI
[121135-06-6]



$C_9H_{11}Br_2NO$ 309
First report of a naturally occurring brominated β-phenylethylamine. Isol. from the bryozoan *Amathia wilsoni*. Possible biosynthetic precursor to the Amathamide alkaloids. Oil.

Blackman, A.J. *et al., J. Nat. Prod.*, 1989, **52**, 436-438 (*isol, ir, pmr, cmr, ms, struct*)

3,4-Dibromo-5-methylene-3-cyclopentene-1,2-diol, 9CI D-283



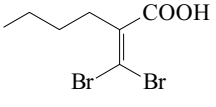
$C_6H_6Br_2O_2$ 269.92

(1R*,2S*)-form
(+)-trans-*form*
[81583-47-3]
Constit. of *Vidalia spiralis*.
Cryst. (MeOH).
Mp 112-116° dec. $[\alpha]_D^{22}$ +124 (c, 0.15 in MeOH).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 219

2-(Dibromomethylene)hexanoic acid, 9CI D-284

3,3-Dibromo-2-butylacrylic acid
[69394-16-7]

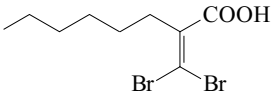


$C_7H_{10}Br_2O_2$ 285.963
Isol. from the red algae *Bonnemaisonia hamifera* and *Bonnemaisonia nootkana*.
Mp 43-44°.

Jacobsen, N. *et al., Tet. Lett.*, 1978, 3065 (*isol*)
McConnell, O.J. *et al., Phytochemistry*, 1980, **19**, 233 (*isol, synth*)
Shindo, N. *et al., CA*, 1986, **105**, 56330m (*synth*)

2-(Dibromomethylene)octanoic acid, 9CI D-285

3,3-Dibromo-2-hexylacrylic acid
[70442-40-9]

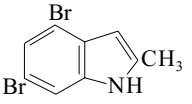


$C_9H_{14}Br_2O_2$ 314.016
Isol. from the red algae *Bonnemaisonia* spp.

McConnell, O.J. *et al., Phytochemistry*, 1980, **19**, 233 (*isol, synth*)

4,6-Dibromo-2-methyl-1*H*-indole, 9CI D-286

[99910-51-7]



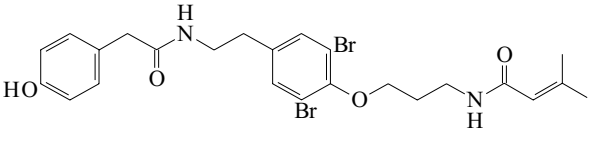
$C_9H_7Br_2N$ 288.969
Alkaloid from the acorn worm *Glossobalanus* sp.
Mp 96-96.5°.

Ac:
$C_{11}H_9Br_2NO$ 331.006
Mp 146-146.5° (141-143.5°).

Higa, T. *et al., Experientia*, 1985, **41**, 1487 (*isol, ir, pmr, ms, struct*)
Ohta, T. *et al., Heterocycles*, 1987, **26**, 2817 (*synth*)

N-[2-[3,5-Dibromo-4-[3-[(3-methyl-1-oxo-2-butenyl)amino]propoxy]phenyl]ethyl]-4-hydroxybenzeneacetamide, 9CI D-287

1,3-Dibromo-5-[2-[(4-hydroxyphenyl)acetamido]ethyl]-2-[3-(3-methyl-2-butenamido)propoxy]benzene
[160666-52-4]



$C_{24}H_{28}Br_2N_2O_4$ 568.304
Metab. from the Caribbean sponge *Iotrochota birotulata*.

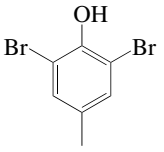
Monoiodo analogue: N-*[2-[3-Bromo-5-iodo-4-[3-[(3-methyl-1-oxo-2-butenyl)amino]propoxy]phenyl]ethyl]-4-hydroxybenzeneacetamide, 9CI*
[160666-53-5]
$C_{24}H_{28}BrIN_2O_4$ 615.305
Metab. from *Iotrochota birotulata*.

Diiodo analogue: N-*[2-[3,5-Diiodo-4-[3-[(3-methyl-1-oxo-2-butenyl)amino]propoxy]phenyl]ethyl]-4-hydroxybenzeneacetamide, 9CI*
[160666-54-6]
$C_{24}H_{28}I_2N_2O_4$ 662.305
Metab. from *Iotrochota birotulata*.

Costantino, V. *et al., J. Nat. Prod.*, 1994, **57**, 1552 (*isol, ir, pmr, cmr, struct*)

2,6-Dibromo-4-methylphenol D-288

2,6-Dibromo-p-*cresol*
[2432-14-6]



$C_7H_6Br_2O$ 265.932
Isol. from the marine polychaete *Lanice conchilega*. Needles (C_6H_6).
Mp 49° Mp 54°.

▶ GO7700000

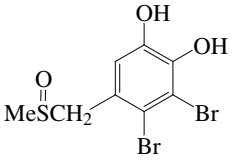
Ac: [67201-41-6]
$C_9H_8Br_2O_2$ 307.969
Mp 67°.

Benzoyl:
$C_{14}H_{10}Br_2O_2$ 370.04
Mp 94-95°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1098B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 290B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1033D (*ir*)
Zincke, Th. *et al., Annalen*, 1902, **320**, 204 (*synth*)
Baddeley, G. *et al., J.C.S.*, 1943, 525 (*synth*)
Kaemmerer, H. *et al., Spectrochim. Acta A*, 1968, **24**, 2059 (*uv*)
Weber, K. *et al., Naturwissenschaften*, 1978, **65**, 262 (*isol*)

3,4-Dibromo-5-(methylsulfonylmethyl)-1,2-benzenediol D-289

2,3-Dibromo-4,5-dihydroxybenzyl methyl sulfoxide

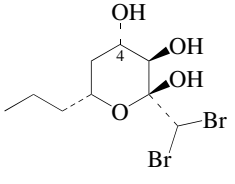


$C_8H_8Br_2O_3S$ 344.023
Isol. from the red alga *Rhodomela confervoides*. Cryst. (MeOH aq.).
Mp 168-170°.

Zhao, J. *et al., J. Nat. Prod.*, 2004, **67**, 1032-1035 (*isol, pmr, cmr, ms*)

2-(Dibromomethyl)tetrahydro-6-propyl-2*H*-pyran-2,3,4-triol D-290

2-(Dibromomethyl)-2,3,4-trihydroxy-6-propyltetrahydropyran. 1, 1-Dibromo-2,6-epoxy-2,3,4-nonanetriol



$C_9H_{16}Br_2O_4$ 348.031

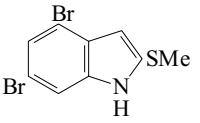
(2*R,3*R**,4*S**,6*R**)-*form***

3,4-Di-Ac: ***Pyranosylmagellanicus C***
$C_{13}H_{20}Br_2O_6$ 432.105
Constit. of the red alga *Ptilonia magellanica*. Oil. $[\alpha]_D^{25}$ +6 (c, 0.24 in CH_2Cl_2).

Lorenzo, M. *et al., Tetrahedron*, 2005, **61**, 9550-9554 (*isol, pmr, cmr, ms*)

4,6-Dibromo-2-methylthio-1*H*-indole D-291

[128351-88-2]

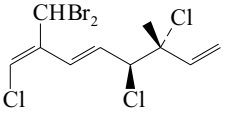


$C_9H_7Br_2NS$ 321.035
Alkaloid from the Okinawan red alga *Laurencia brongniartii*.
Cryst. (hexane/CCl_4).
Mp 59-61°.

Tanaka, J. *et al., Tetrahedron*, 1989, **45**, 7301 (*isol, ir, pmr, ms, struct*)

2-(Dibromomethyl)-1,5,6-trichloro-6-methyl-1,3,7-octatriene D-292

[65207-96-7]



$C_{10}H_{11}Br_2Cl_3$ 397.363
Constit. of *Aplysia limacina*. Oil. $[\alpha]_D$ -9.7 (c, 0.4 in $CHCl_3$).
Stereochem. revised in 1984.

Imperato, F. *et al., Experientia*, 1977, **33**, 1273-1274 (*isol*)
Crews, P. *et al., J.O.C.*, 1984, **49**, 1371-1377 (*cmr, struct*)

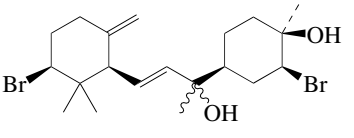
9,9-Dibromo-8-nonenoic acid D-293

[111243-21-1]
$Br_2C{=}CH(CH_2)_6COOH$
$C_9H_{14}Br_2O_2$ 314.016
Constit. of the sponge *Xestospongia* sp. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 205 (ϵ 4500); 242 (ϵ 2100) (MeOH) (Berdy).

Hirsch, S. *et al., Tetrahedron*, 1987, **43**, 3257-3261 (*isol, uv, ir, pmr, cmr, ms*)

2,14-Dibromo-8,11(18)-obtusadiene-3,7-diol D-294

Obtusadiol
[68690-92-6]

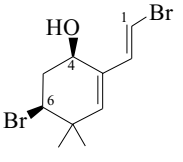


$C_{20}H_{32}Br_2O_2$ 464.28
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D^{23}$ -24.5.

Howard, B.M. *et al., Tet. Lett.*, 1978, 2453

1,6-Dibromo-1,3(8)-ochtodadien-4-ol D-295

5-Bromo-2-(2-bromoethenyl)-4,4-dimethyl-2-cyclohexen-1-ol



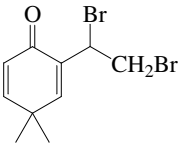
(1*E*,4*R**,6*S**)–*form*

$C_{10}H_{14}Br_2O$ 310.028

(1*E*,4*R,6*S**)-*form*** [73872-75-0]
Constit. of *Ochtodes crockeri*.
Oil. $[\alpha]_D^{20}$ -45.4 (c, 2.5 in $CHCl_3$).

(1*E*,4*S,6*S**)-*form*** [73872-76-1]
Constit. of *Ochtodes crockeri*.
Oil. $[\alpha]_D^{20}$ -71.2 (c, 3.2 in $CHCl_3$).
Paul, V.J. *et al., J.O.C.*, 1980, **45**, 3401

1,2-Dibromo-3(8),5-ochtodadien-4-one D-296
2-(1,2-Dibromoethyl)-4,4-dimethyl-2,5-cyclohexadien-1-one
[569351-30-0]



$C_{10}H_{12}Br_2O$ 308.012
Constit. of the red alga *Portieria hornemanni*. Oil. $[\alpha]_D^{24}$ +10 (c, 0.46 in CCl_4).
Kuniyoshi, M. *et al., J. Chin. Chem. Soc. (Taipei)*, 2003, **50**, 167-170 (*isol, pmr, cmr*)

18,18-Dibromo-9,17-octadecadiene-5,7-diynoic acid, 9CI D-297
$Br_2CH{=}CH(CH_2)_6CH{=}CHC{\equiv}CC{\equiv}C(CH_2)_3COOH$
$C_{18}H_{22}Br_2O_2$ 430.179

(*E*)-*form* [111216-64-9]
Isol. from the marine sponge *Xestospongia testudinaria*. λ_{max} 241 (ϵ 3000); 254 (ϵ 4900); 268 (ϵ 6900); 284 (ϵ 5700) (no solvent reported).
9,10-Dihydro: ***18,18-Dibromo-17-octadecene-5,7-diynoic acid***
$C_{18}H_{24}Br_2O_2$ 432.194
Isol. from lichens of Central Asia. λ_{max} 215 (ϵ 13200); 231 (ϵ 4800); 249 (ϵ 1800) (MeOH) (as Me ester).
Hirsh, S. *et al., Tetrahedron*, 1987, **43**, 3257-3261 (*isol, struct, uv, ir, pmr, cmr*)
Rezanka, T. *et al., Phytochemistry*, 1999, **51**, 963-968 (*9,10-dihydro acid*)

18,18-Dibromo-5,17-octadecadien-7-ynoic acid, 9CI D-298
$Br_2C{=}CH(CH_2)_8C{\equiv}CCH{=}CHCH_2CH_2CH_2COOH$
$C_{18}H_{26}Br_2O_2$ 434.21

(*Z*)-*form* [162259-39-4]
Constit. of the marine sponge *Xestospongia* sp.
Me ester: [162259-41-8]
$C_{19}H_{28}Br_2O_2$ 448.237
From *Xestospongia* sp.
Li, Y. *et al., J. Chem. Res., Synop.*, 1995, 126-127 (*isol*)

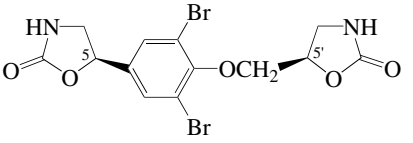
2,4-Dibromo-5-oxo-2-decenoic acid D-299
$H_3C(CH_2)_4COCHBrCH{=}CBrCOOH$
$C_{10}H_{14}Br_2O_3$ 342.027

(2ξ,4ξ)-*form*
Me ester:
$C_{11}H_{16}Br_2O_3$ 356.054
Isol. from an unidentified fungus on the red alga *Gracillaria verrucosa*. Yellow oil. $[\alpha]_D$ -10 (c, 0.2 in $CHCl_3$). λ_{max} 203 (log ϵ 3.8); 248 (log ϵ 3.3) (MeOH).
Li, X. *et al., Bull. Korean Chem. Soc.*, 2004, **25**, 607-608 (*isol, pmr, cmr, ms*)

2,4-Dibromo-5-oxo-3-decenoic acid D-300
$H_3C(CH_2)_4COCBr{=}CHCBrCOOH$
$C_{10}H_{14}Br_2O_3$ 342.027

(2ξ,3ξ)-*form*
Me ester:
$C_{11}H_{16}Br_2O_3$ 356.054
Isol. from an unidentified fungus on the red alga *Gracillaria verrucosa*. Yellow oil. $[\alpha]_D$ -40 (c, 0.2 in $CHCl_3$). λ_{max} 203 (log ϵ 3.7); 257 (log ϵ 3.5) (MeOH).
Li, X. *et al., Bull. Korean Chem. Soc.*, 2004, **25**, 607-608 (*isol, pmr, cmr, ms*)

5-[3,5-Dibromo-4-[(2-oxo-5-oxazolidinyl)methoxy]-phenyl]-2-oxazolidinone, 9CI D-301
[54448-72-5]



(5*R*,5'*R*)-*form*

$C_{13}H_{12}Br_2N_2O_5$ 436.056

(5*R*,5′*R*)-*form* [120442-03-7]
Isol. from sponge *Aplysina aerophoba*.
Mp 220-222°. $[\alpha]_D$ -33 (c,1.1 in MeOH).

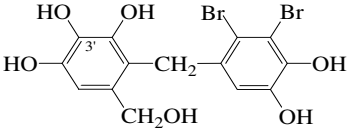
(5*R*,5′*S*)-*form*
Isol. from the sponges *Aplysina lacunosa* and *Verongula rigida* and ascidian *Clavelina oblonga*.
Mp 220-222°. $[\alpha]_D$ -6.5 (c, 0.44 in MeOH). $[\alpha]_D^{24}$ -9.2 (c, 0.25 in MeOH).

(5*S*,5′*R*)-*form*
Isol. from the sponges *Aplysina fistularis* (*Verongia fistularis*) forma *fulva*, *Aplysina lacunosa* and *Aplysina cauliformis.*
Mp 226-227° (222-225°). $[\alpha]_D^{20}$ +7.1 (c, 0.35 in MeOH).
2-Ac: [474670-22-9]
$C_{15}H_{14}Br_2N_2O_6$ 478.093
Isol. from *Suberea* aff. *praetensa*.
2,2′-Di-Ac: [474670-23-0]
$C_{17}H_{16}Br_2N_2O_7$ 520.131
Isol. from *Suberea* aff. *praetensa*.

(5*RS*,5′*SR*)-*form*
Isol. from the sponges *Aplysina cauliformis* and *Aplysina fistularis.*
Mp 247-249°.

(5ξ,5′ξ)-*form*
O-*Ac:*
$C_{15}H_{14}Br_2N_2O_6$ 478.093
Isol. from *Suberea* aff. *praetensa* sponge. Derived from a hydroxyoxazolidine tautomer.
O,O-*Di-Ac:*
$C_{17}H_{16}Br_2N_2O_7$ 520.131
Isol. from a *Suberea* sponge. Derived from the bis(hydroxyoxazolidine) tautomer.
Borders, D.B. *et al., Tet. Lett.*, 1974, 2709-2712 (*isol, uv, ir, pmr, cmr, ms, struct*)
Gopichand, Y. *et al., Tet. Lett.*, 1979, 3921-3924 (*isol*)
Makarieva, T.N. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1981, **68**, 481-484 (*occur*)
Norte, M. *et al., Tetrahedron*, 1988, **44**, 4973 (*5R,5′R-form, isol, cryst struct, abs config*)
Kijjoa, A. *et al., Z. Naturforsch., C*, 2002, **57**, 732-738 (*Suberea acetates*)
Kossuga, M.H. *et al., J. Nat. Prod.*, 2004, **67**, 1879-1881 (*Clavelina oblonga constit, isol, cmr*)
Rogers, E.W. *et al., J. Nat. Prod.*, 2005, **68**, 891-896 (*stereochem*)

2,3-Dibromo-2′,3′,4,4′,5-pentahydroxy-6′-(hydroxymethyl)diphenylmethane D-302
2-(2,3-Dibromo-4,5-dihydroxybenzyl)-3,4,5-trihydroxybenzyl alcohol



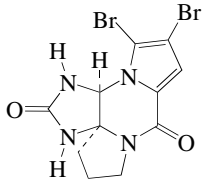
$C_{14}H_{12}Br_2O_6$ 436.053

3′-Me ether: 2-(2,3-Dibromo-4,5-dihydroxybenzyl)-3,5-dihydroxy-4-methoxybenzyl alcohol. 2,3-Dibromo-2′,4,4′,5-tetrahydroxy-6′-hydroxymethyl-3′-methoxydiphenylmethane
$C_{15}H_{14}Br_2O_6$ 450.08
Constit. of the brown alga *Leathesia nana*. Brown powder (Me_2CO).
Mp 114-116°.

Xu, X. *et al., J. Nat. Prod.*, 2004, **67**, 1661-1666 (*isol, pmr, cmr, ms*)

Dibromophakellstatin D-303

[185750-71-4]



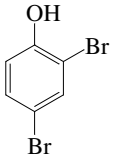
Absolute Configuration

$C_{11}H_{10}Br_2N_4O_2$ 390.034
Alkaloid from the Indian ocean sponge *Phakellia mauritiana*. Antineoplastic agent. Cryst. (toluene/MeOH).
Mp 245° (dec.).

Pettit, G.R. *et al., J. Nat. Prod.*, 1997, **60**, 180-183 (*isol, pmr, cmr, ms, cryst struct*)
Wiese, K.J. *et al., Tet. Lett.*, 2002, **43**, 5135-5136 (*synth*)
Poullennec, K.G. *et al., J.A.C.S.*, 2003, **125**, 6344-6345 (*synth*)
Cheung, R. *et al., Org. Lett.*, 2004, **6**, 3881-3884 (*synth*)
Jacquot, D.E.N. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 2295-2298 (*synth*)
Feldman, K.S. *et al., Org. Lett.*, 2005, **7**, 929-931 (*synth*)

2,4-Dibromophenol, 9CI, 8CI D-304

[615-58-7]



$C_6H_4Br_2O$ 251.905
Isol. from the acorn worms *Balanoglossus carnosus* and *Ptychodera* sp. Commonly found in marine algae, molluscs and crustaceans.
Mp 40°. Bp_{11} 154°. pK_a 7.79 (25°).
▶ LD_{50} (mus, orl) 282 mg/kg. SK8010000

Ac: [36914-79-1]
$C_8H_6Br_2O_2$ 293.942
Mp 36°.

Benzoyl:
$C_{13}H_8Br_2O_2$ 356.013
Mp 97.5°.

Me ether: 2,4-Dibromo-1-methoxybenzene. 2,4-Dibromoanisole
[21702-84-1]
$C_7H_6Br_2O$ 265.932
Constit. of the red alga *Polysiphonia sphaerocarpa*.
Mp 61.5°. Bp 272°.

Et ether: 2,4-Dibromo-1-ethoxybenzene. 2,4-Dibromophenetole
[38751-57-4]
$C_8H_8Br_2O$ 279.959
Mp 53.5°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1090B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 197A; 276A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 978C; 1026C (*ir*)
Hashimoto, T. *et al., Yakugaku Zasshi*, 1960, **80**, 1399; *CA*, **55**, 5393 (*synth*)
Kaemmerer, H. *et al., Spectrochim. Acta A*, 1968, **24**, 2059 (*uv*)
Rowbotham, J.B. *et al., Can. J. Chem.*, 1974, **52**, 3037 (*pmr*)
Tashiro, M. *et al., Org. Prep. Proced. Int.*, 1974, **6**, 107 (*synth*)
Higa, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **65**, 525-530 (*isol*)
Kajigaeshi, S. *et al., J.C.S. Perkin 1*, 1990, 897 (*Me ether, synth*)
Boyle, J.L. *et al., J. Food Sci.*, 1992, **57**, 918-922 (*occur*)
Whitfield, F.B. *et al., J. Agric. Food Chem.*, 1997, **45**, 4398-4405; 1999, **47**, 2367-2373 (*occur*)
Flodin, C. *et al., Phytochemistry*, 2000, **53**, 77-80 (*isol*)

2,6-Dibromophenol, 9CI, 8CI D-305

[608-33-3]

$C_6H_4Br_2O$ 251.905
Constit. of the marine hemichordate *Balanoglossus biminiensis*. Widespread in marine algae, fish, molluscs and crustaceans, such as *Barantolla lepte, Marphysa sanguinea, Glycera americana, Lumbrineris latreilli, Nephtys australiensis, Ceratonereis aequisetis, Australonuphis teres, Scoloplos normalis, Penaeus plebejus, Penaeus latisulcatus, Penaeus merguiensis, Platycephalus caeruleopunctatus, Nemadactylus douglasii, Polysiphonia sphaerocarpa, Ulva lactuca, Ptychoderma flava* and *Capitella* sp. Important flavour component of marine fish, molluscs and crustaceans. Needles (H_2O). Sol. EtOH, Et_2O.
Mp 56-57°. Bp_{21} 162°. pK_a 6.67 (25°). Sublimes. λ_{max} 279 (ε 2180); 286 (ε 2130) (EtOH) (Berdy). λ_{max} 305 (EtOH/NaOH) (Berdy).

Ac: [28165-72-2]
$C_8H_6Br_2O_2$ 293.942
Mp 46°.

Benzoyl:
$C_{13}H_8Br_2O_2$ 356.013
Mp 68°.

Me ether: 1,3-Dibromo-2-methoxybenzene. 2,6-Dibromoanisole
[38603-09-7]
$C_7H_6Br_2O$ 265.932
Mp 13°. Bp_{34} 143-145°.

Et ether: 1,3-Dibromo-2-ethoxybenzene. 2,6-Dibromophenetole
$C_8H_8Br_2O$ 279.959
Mp 40.5°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1083C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 261A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1016D (*ir*)
Pope, F.G. *et al., J.C.S.*, 1912, **101**, 1823-1829 (*synth*)
Ashworth, R.B. *et al., Science (Washington, D.C.)*, 1967, **155**, 1558 (*isol*)
Kaemmerer, H. *et al., Spectrochim. Acta A*, 1968, **24**, 2059-2069 (*uv*)
Dwivedi, B.K. *et al., Indian J. Pure Appl. Phys.*, 1974, **12**, 597 (*ir*)
Tashiro, M. *et al., Org. Prep. Proced. Int.*, 1975, **7**, 189-192 (*synth*)
Boyle, J.L. *et al., J. Food Sci.*, 1992, **57**, 918-922 (*occur*)
Whitfield, F.B. *et al., J. Agric. Food Chem.*, 1997, **45**, 4398-4405; 1999, **47**, 2367-2373; 4756-4762 (*occur*)

1,1-Dibromo-2-propanol D-306

[62872-25-7]
$H_3CCH(OH)CHBr_2$
$C_3H_6Br_2O$ 217.888

(ξ)-form
Isol. from the alga *Asparagopsis taxiformis*.
Woolard, F.X. *et al., Tetrahedron*, 1976, **32**, 2843 (*isol, ms*)

1,3-Dibromo-2-propanol, 9CI D-307

Glycerol 1,3-dibromohydrin. α-Dibromohydrin
[96-21-9]
$BrCH_2CH(OH)CH_2Br$
$C_3H_6Br_2O$ 217.888
Isol. from the marine alga *Asparagopsis taxiformis*. d_4^{25} 2.12.
Bp 219° part. dec. Bp_{38} 124°. n_D^{25} 1.5495.
▶ Fl. p. >107°. UB0200000

4-Nitrobenzoyl: Mp 77-78°.

Me ether: 1,3-Dibromo-2-methoxypropane
$C_4H_8Br_2O$ 231.915
Bp_{13} 83°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 278C (*nmr*)
Carré, P. *et al., Bull. Soc. Chim. Fr.*, 1910, **7**, 836 (*synth*)
Org. Synth., Coll. Vol., 2, 1943, 308 (*synth*)

Camps, F. *et al., Synthesis*, 1987, 511 (*synth*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DDR800

1,1-Dibromo-2-propanone, 9CI D-308

1,1-Dibromoacetone
[867-54-9]
$H_3CCOCHBr_2$

$C_3H_4Br_2O$ 215.872
Minor component of the essential oil of the edible Hawaiian red alga *Asparagopsis taxiformis* and of *Falkenbergia rufolanosa*. Liq. Bp_{13} 55-57°. n_D^{25} 1.5237. pK_a 11.9 (25°, H_2O).

Hughes, E.D. *et al., J.C.S.*, 1931, 3318 (*synth*)
Rappe, C. *et al., Ark. Kemi*, 1964, **21**, 503; *CA*, **59**, 431b (*synth, pmr, ir*)
Takahashi, K. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 963 (*pmr*)
Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*isol, glc*)
Combaut, G. *et al., Phytochemistry*, 1978, **17**, 1661 (*isol, glc*)
Geigert, J. *et al., J. Biol. Chem.*, 1983, **258**, 2273 (*glc, ms*)
Guthrie, J.P. *et al., J.A.C.S.*, 1984, **106**, 1351 (*pKa*)
Bostroem, G.O. *et al., J. Mol. Struct.*, 1987, **158**, 23 (*conformn*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)

1,3-Dibromo-2-propanone, 9CI, 8CI D-309

1,3-Dibromoacetone
[816-39-7]
$BrCH_2COCH_2Br$

$C_3H_4Br_2O$ 215.872
Constit. of the marine algae *Asparagopsis armata, Asparagopsis taxiformis* and *Falkenbergia rufolanosa*. Needles (petrol). Sol. Et_2O, CS_2.
Mp 27-28°. $Bp_{21.5}$ 97-98° (lit. gives a pressure range). Dec. on dist. at ordinary press.

Rappe, C. *et al., Acta Chem. Scand.*, 1962, **16**, 2467 (*synth*)
Husain, J.S. *et al., Biochem. J.*, 1968, **108**, 855 (*synth, uv*)
Fenical, W. *et al., Tet. Lett.*, 1974, 4463 (*isol*)
Hoffmann, H.M.R. *et al., Org. Mass Spectrom.*, 1976, **11**, 1077 (*ms*)
Codomier, L. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1977, **284**, 1163; 1978, **286**, 603 (*isol*)
Bostroem, G.O. *et al., J. Mol. Struct.*, 1987, **158**, 23 (*conformn*)
Menger, F.M. *et al., J.O.C.*, 1987, **52**, 3451 (*synth, ir, pmr*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **3**, 1540-1543 (*use*)

3,3-Dibromo-2-propenal, 9CI D-310

3,3-Dibromoacrolein, 8CI
[18328-08-0]
$Br_2C{=}CHCHO$

$C_3H_2Br_2O$ 213.856
Minor component of the essential oil of the alga *Asparagopsis taxiformis*. Liq. d_4^{26} 2.21. Bp_{30} 80-81.5° Bp_{17} 70-70.5°. n_D^{26} 1.5862. Dec. on standing at r.t. Stored with hydroquinone in a sealed tube at 0°.

Oxime:
$C_3H_3Br_2NO$ 228.871
Solid. Mp 77.5-79.5°.

Hydrazone: [60345-08-6]
Solid (petrol/EtOAc). Mp 131°.

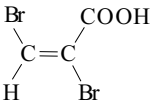
2,4-Dinitrophenylhydrazone:
Solid. Mp 180-182°.

Di-Et acetal: 1,1-Dibromo-3,3-diethoxypropene
[18484-50-9]
$C_7H_{12}Br_2O_2$ 287.979
Liq. d_4^{19} 1.58. $Bp_{1.7}$ 69.5-70°. n_D^{19} 1.4927.

Levas, M. *et al., Bull. Soc. Chim. Fr.*, 1959, 1800 (*synth*)
Raulet, C. *et al., Bull. Soc. Chim. Fr.*, 1963, 2147 (*synth*)
Gorgues, A. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1967, **265**, 1130 (*acetal*)
Burreson, B.J. *et al., Tet. Lett.*, 1975, 473 (*isol, pmr*)
Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*isol, glc*)
Freche, P. *et al., Tetrahedron*, 1977, **33**, 2069 (*synth, pmr, ir, hydrazone*)

2,3-Dibromo-2-propenoic acid, 9CI D-311

2,3-Dibromoacrylic acid
[24767-86-0]



(E)–form

$C_3H_2Br_2O_2$ 229.856

(E)-form [1578-72-9]
Mp 73-74.5°.

Et ester: [26631-69-6]
$C_5H_6Br_2O_2$ 257.909
Occurs in *Asparagopsis taxiformis* and *Asparagopsis armata*.
Bp_{11} 81-85°.

(Z)-form [24557-10-6]
Mp 84-86°.

Me ester: [26631-70-9]
$C_4H_4Br_2O_2$ 243.882
Bp_7 73-76°.

Et ester: [26631-66-3]
Occurs in *Asparagopsis taxiformis* and *Asparagopsis armata*.
Bp_2 69-71°.

Benzyl ester: [55052-02-3]
$C_{10}H_8Br_2O_2$ 319.98
$Bp_{0.1}$ 121-131°.

N,N-Diethylamide:
$C_7H_{11}Br_2NO$ 284.978
$Bp_{0.6}$ 95-97°.

Rappe, C. *et al., Ark. Kemi*, 1965, **24**, 303-313 (*synth, pmr*)
Kishida, Y. *et al., Chem. Pharm. Bull.*, 1969, **17**, 2424-2435 (*synth, ir, pmr*)
Andersson, K. *et al., Chem. Scr.*, 1972, **2**, 113-116 (*synth*)
Alexander, J. *et al., J.C.S. Perkin 1*, 1974, 2092-2095 (*benzyl ester, synth, ir, pmr*)
McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367-374 (*ir, ms*)
Org. Synth., Coll. Vol., 9, 1998, 117-120 (*Z-form, Et ester, synth, ir, pmr, cmr*)

3,3-Dibromo-2-propenoic acid, 9CI D-312

3,3-Dibromoacrylic acid
[1578-21-8]
$Br_2C{=}CHCOOH$

$C_3H_2Br_2O_2$ 229.856
Constit. of the red alga *Asparagopsis taxiformis*.
Mp 86.5-87°.

Et ester: [66656-18-6]
$C_5H_6Br_2O_2$ 257.909
Bp 212-214°.

Bromide:
C_3HBr_3O 292.752
Bp_{10} 85-86°.

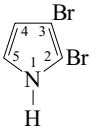
Chloride: [92925-46-7]
C_3HBr_2ClO 248.301
Bp_{12} 78-81° (lit. gives a pressure range).

[92925-53-6]

Raulet, C. *et al., Bull. Soc. Chim. Fr.*, 1963, 2147 (*synth*)
Rappe, C. *et al., Ark. Kemi*, 1965, **24**, 95 (*synth, nmr*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617 (*nmr, synth, isol*)
Stack, D.P. *et al., Synthesis*, 1984, 435 (*chloride*)

2,3-Dibromo-1*H*-pyrrole, 9CI D-313

[69624-10-8]

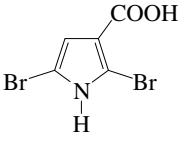


$C_4H_3Br_2N$ 224.882
Metab. from a marine sponge *Agelas* sp. Extremely unstable.

Audebert, P. *et al., Synth. Met.*, 1986, **15**, 9 (*ms, pmr*)
Tada, H. *et al., Chem. Lett.*, 1988, 803 (*isol, ir, pmr, cmr, ms*)

2,5-Dibromo-1*H*-pyrrole-3-carboxylic acid D-314

[270084-77-0]

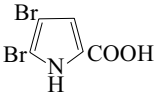


$C_5H_3Br_2NO_2$ 268.892
Isol. from *Spongia oblique*.

Xu, S.-H. *et al., Youji Huaxue*, 2000, **20**, 248-250; *CA*, **132**, 345562a (*isol*)

4,5-Dibromo-1*H*-pyrrole-2-carboxylic acid, 9CI D-315

[34649-21-3]



$C_5H_3Br_2NO_2$ 268.892
Constit. of the sponges *Agelas oroides*, *Agelas clathrodes*, *Agelas conifera* and *Agelas flabelliformis*. Possesses potent *in vitro* immunosuppressive activity. Feeding deterrent.
Mp 148° subl.

Me ester: ***Methyl 4,5-dibromo-1H-pyrrole-2-carboxylate, 9CI***
[937-16-6]
$C_6H_5Br_2NO_2$ 282.919
Constit. of *Agelas oroides*, *Phakellia fusca* and a *Lissodendoryx* sp.
Mp 161° (155°).

Amide: ***4,5-Dibromo-1H-pyrrole-2-carboxamide, 9CI***
[34649-20-2]
$C_5H_4Br_2N_2O$ 267.907
Constit. of *Acanthella carteri*, *Agelas mauritiana*, *Agelas oroides*, *Phakellia fusca* and *Pseudoceratina purpurea*. Larval metamorphosis-promoting compd. Feeding deterrent for ascidians.
Mp 164-166°. λ_{max} 233 (ϵ 6200); 273 (ϵ 11800) (MeOH) (Berdy). λ_{max} 296 (ϵ 18800) (MeOH/NaOH) (Berdy).

(Methoxymethyl)amide: ***4,5-Dibromo-N^2-methoxymethyl-1H-pyrrole-2-carboxamide***
[219782-98-6]
$C_7H_8Br_2N_2O_2$ 311.96
Isol. from the sponge *Homaxinella* sp.

Nitrile: ***4,5-Dibromo-1H-pyrrole-2-carbonitrile, 9CI***. *5-Cyano-2, 3-dibromopyrrole*
[34649-19-9]
$C_5H_2Br_2N_2$ 249.892
Constit. of *Agelas oroides*.
Mp 172-173°.

N-*Me:* ***4,5-Dibromo-1-methyl-1H-pyrrole-2-carboxylic acid, 9CI***
[66067-06-9]
$C_6H_5Br_2NO_2$ 282.919
Constit. of an unidentified orange marine sponge collected in the Marshall Islands. Cryst. ($CHCl_3$).
Mp 153°.

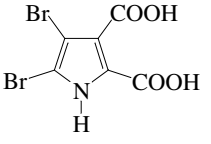
N-*Me, Me ester:* [1198-71-6]
$C_7H_7Br_2NO_2$ 296.946
Isol. from sponge *Agelas mauritiana*.
Mp 87-90°. Poss. artifact.

N-*Et:* ***4,5-Dibromo-1-ethyl-1H-pyrrole-2-carboxylic acid***
[150314-24-2]
$C_7H_7Br_2NO_2$ 296.946
Isol. from a sponge *Axinella* sp. Cryst.
Mp 141-143°. λ_{max} 205 (ϵ 10600); 239 (ϵ 8500); 275 (ϵ 12300) (MeOH).

N-*2-Propenyl:* ***1-Allyl-4,5-dibromo-1H-pyrrole-2-carboxylic acid***
[150314-25-3]
$C_8H_7Br_2NO_2$ 308.957
Isol. from a sponge *Axinella* sp. Amorph. cream-coloured solid.
Mp 128-129°. λ_{max} 205 (ϵ 12800); 238 (ϵ 10600); 273 (ϵ 14000) (MeOH).

Rinkes, I.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1941, **60**, 303-308 (*ester, synth*)
Anderson, H.J. *et al., Can. J. Chem.*, 1965, **43**, 409-414 (*ester, synth*)
Hodge, P. *et al., J.C.S.*, 1965, 459-470 (*synth, uv, ir*)
Forenza, S. *et al., Chem. Comm.*, 1971, 1129-1130 (*Agelas oroides constits*)
Chevolot, L. *et al., Heterocycles*, 1977, **7**, 891-894 (*amide*)
Schmitz, F.J. *et al., J. Nat. Prod.*, 1985, **48**, 47-53 (*ester, isol, ir, pmr, cmr, ms*)
Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1985, 578; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 547-548 (*isol*)
Fathi-Afshar, R. *et al., Can. J. Chem.*, 1988, **66**, 45-50 (*N-Me Me ester, isol, pmr, cmr*)
Gunasekera, S.P. *et al., J. Nat. Prod.*, 1989, **52**, 757-761 (*isol*)
Barrow, R.A. *et al., Nat. Prod. Lett.*, 1993, **1**, 243-250 (*isol, Axinella derivs*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 1996, **59**, 501-503 (*amide, isol*)
Ponasik, J.A. *et al., Tet. Lett.*, 1996, **37**, 6041-6044 (*synth*)
Tsukamoto, S. *et al., Tetrahedron*, 1996, **52**, 8181-8186 (*amide, isol*)
Umeyama, A. *et al., J. Nat. Prod.*, 1998, **61**, 1433-1434 (*methoxymethylamide*)
Koenig, G.M. *et al., Planta Med.*, 1998, **64**, 443-447 (*isol, pmr, cmr*)

4,5-Dibromo-1*H*-pyrrole-2,3-dicarboxylic acid D-316



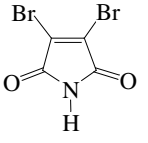
$C_6H_3Br_2NO_4$ 312.902

3-Nitrile, Me ester: 2,3-Dibromo-4-cyano-5-methoxycarbonylpyrrole
[866410-40-4]
$C_7H_4Br_2N_2O_2$ 307.929
Constit. of the sponge *Phakellia fusca*.

Xu, S. *et al., Tianran Chanwu Yanjiu Yu Kaifa*, 2003, **15**, 393-395; *CA*, **143**, 363646n (*isol*)

3,4-Dibromo-1*H*-pyrrole-2,5-dione, 9CI D-317

Dibromomaleimide
[1122-10-7]



$C_4HBr_2NO_2$ 254.865
Alkaloid from the sponge *Axinella brevistyla*. Antifungal and cytotoxic agent. Yellow needles (xylene or $CHCl_3$).
Mp 230° (226°). λ_{max} 236 (log ϵ 4.1); 243 (log ϵ 4.1); 251 (sh) (log ϵ 3.9); 303 (log ϵ 3.1) (MeOH).

N-*Me: 3,4-Dibromo-1-methyl-1*H-*pyrrole-2,5-dione. 2,3-Dibromo-N-methylmaleimide*
[3005-27-4]
$C_5H_3Br_2NO_2$ 268.892
Pale yellow needles (H_2O). Mp 121° (114-116°).

N-*Et:*
$C_6H_5Br_2NO_2$ 282.919
Cryst. (EtOH). Mp 93-94°.

N-*Butyl:* [181864-30-2]
$C_8H_9Br_2NO_2$ 310.973
Cryst.

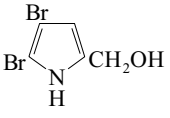
N-*Benzyl:* [91026-00-5]
$C_{11}H_7Br_2NO_2$ 344.99
Mp 117-117.5° (101-103°).

N-*Ph: 3,4-Dibromo-1-phenyl-1*H-*pyrrole-2,5-dione. 2,3-Dibromo-N-phenylmaleimide*
[65833-14-9]
$C_{10}H_5Br_2NO_2$ 330.963
Yellow solid. Mp 166-168°.

Khotinsky, E. *et al., Ber.*, 1904, **37**, 2798-2802 (*N-Me*)
Ruggli, P. *et al., Helv. Chim. Acta*, 1920, **3**, 493-514 (*synth*)
Elvidge, J.A. *et al., J.C.S.*, 1957, 2466-2472 (*synth*)
Martin, E.L. *et al., J.O.C.*, 1961, **26**, 2032-2037 (*N-Ph*)
Scharf, H.D. *et al., Chem. Ber.*, 1965, **98**, 764-780 (*N-Me, synth, ir, uv*)
Joyce, R.P. *et al., J.O.C.*, 1987, **52**, 1177-1185 (*N-benzyl*)
Chen, W. *et al., Acta Cryst. C*, 1997, **53**, 631-633 (*N-butyl, cryst struct*)
Choi, D.-S. *et al., J.O.C.*, 1998, **63**, 2646-2655 (*N-benzyl, N-Ph*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 2001, **64**, 1576-1578 (*isol, uv, ir, pmr, cmr*)

4,5-Dibromo-1*H*-pyrrole-2-methanol D-318

2,3-Dibromo-5-hydroxymethylpyrrole



$C_5H_5Br_2NO$ 254.909

*Me ether: 2,3-Dibromo-5-(methoxymethyl)-1*H-*pyrrole, 9CI*
[115502-60-8]
$C_6H_7Br_2NO$ 268.935
Metab. from a marine sponge *Agelas* sp. Extremely unstable.
Tada, H. *et al., Chem. Lett.*, 1988, 803 (*isol, pmr, cmr, ms, struct*)

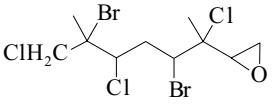
14,14-Dibromo-4,6,13-tetradecatrienoic acid D-319

$Br_2C{=}CH(CH_2)_5CH{=}CHCH{=}CHCH_2CH_2COOH$
$C_{14}H_{20}Br_2O_2$ 380.119

(4Z,6E)-form
Isol. from *Xestospongia* sp., an association of sponge cells and bacteria.
Me ester: [165128-32-5]
Oil.
Brantley, S.E. *et al., Tetrahedron*, 1995, **51**, 7667 (*isol, uv, ir, pmr, cmr, ms*)

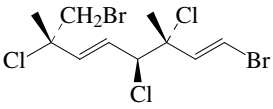
(2,5-Dibromo-1,4,6-trichloro-1,5-dimethylhexyl) oxirane, 9CI D-320

2,5-Dibromo-1,3,6-trichloro-2,6-dimethyl-7,8-epoxyoctane
[96300-30-0]



$C_{10}H_{15}Br_2Cl_3O$ 417.394
Constit. of *Plocamium cartilagineum*. Oil.
Blunt, J.W. *et al., Aust. J. Chem.*, 1985, **38**, 319

1,8-Dibromo-3,4,7-trichloro-3,7-dimethyl-1,5-octadiene D-321



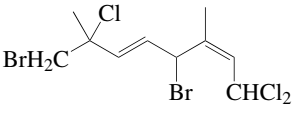
(1E,3R,4S,5E,7S)-form

$C_{10}H_{13}Br_2Cl_3$ 399.379

(1E,3R,4S,5E,7S)-form [73245-53-1]
Constit. of *Plocamium* spp. and *Aplysia californica*. Shows antifungal props. Toxic to brine shrimp. Cryst.
Mp 48.5-49°. $[\alpha]_D$ -46.3 (c, 1.03 in $CHCl_3$).

(1E,3ξ,4ξ,5E,7ξ)-form [58967-06-9]
Constit. of *Aplysia californica*.
Needles (MeOH).
Mp 20°.
Ireland, C. *et al., J.O.C.*, 1976, **41**, 2461-2465 (*isol, pmr, ms*)
Stierle, D.B. *et al., Tetrahedron*, 1979, **35**, 2855-2859 (*cryst struct, abs config*)

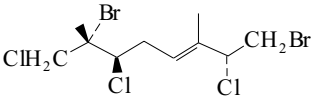
4,8-Dibromo-1,1,7-trichloro-3,7-dimethyl-2,5-octadiene D-322



$C_{10}H_{13}Br_2Cl_3$ 399.379

(2Z,4ξ,5E,7ξ)-form
Plocoralide C
[861959-27-5]
Constit. of *Plocamium corallorhiza*.
Oil. $[\alpha]_D$ -43 (c, 0.03 in $CHCl_3$).
Knott, M.G. *et al., Phytochemistry*, 2005, **66**, 1108-1112 (*Plocoralide C*)

1,7-Dibromo-2,6,8-trichloro-3,7-dimethyl-3-octene D-323

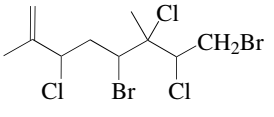


$C_{10}H_{15}Br_2Cl_3$ 401.395

(2R,3E,6R,7S)-form [96300-27-5]
Constit. of *Plocamium cartilagineum*.
Oil.
Blunt, J.W. *et al., Aust. J. Chem.*, 1985, **38**, 319

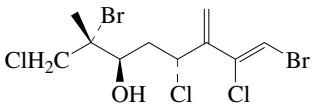
5,8-Dibromo-3,6,7-trichloro-2,6-dimethyl-1-octene D-324

[221171-36-4]



$C_{10}H_{15}Br_2Cl_3$ 401.395
Constit. of *Plocamium costatum*. Oil. $[\alpha]_D^{22}$ -33.1 (c, 0.13 in $CHCl_3$).
König, G.M. *et al., J. Nat. Prod.*, 1999, **62**, 383-385 (*isol, pmr, cmr*)

2,8-Dibromo-1,5,7-trichloro-2-methyl-6-methylene-7-octen-3-ol D-325

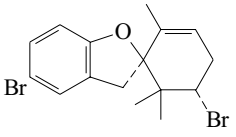


$C_{10}H_{13}Br_2Cl_3O$ 415.378

(2R,3R,5R,7Z)-form [723302-05-4]
Constit. of *Plocamium cartilagineum*.
Oil. $[\alpha]_D^{25}$ +12 (c, 0.57 in $CHCl_3$).
Díaz-Marrero, A.R. *et al., Tetrahedron*, 2004, **60**, 5049-5052 (*isol, pmr, cmr*)

5,5′-Dibromo-2′,6′,6′-trimethylspiro[benzofuran-2(3*H*),1′-cyclohex-2′-ene] D-326

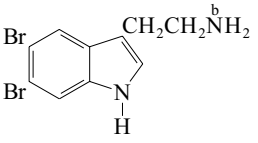
[132244-41-8]



$C_{16}H_{18}Br_2O$ 386.126
Constit. of a *Cacospongia* sp. Oil. $[\alpha]_D$ +18.3 (c, 0.224 in $CHCl_3$).
Bali, D.K.L. *et al., Aust. J. Chem.*, 1990, **43**, 2009 (*isol, pmr, cmr*)

5,6-Dibromotryptamine D-327

*5,6-Dibromo-1*H*-indole-3-ethanamine, 9CI. 3-(2-Aminoethyl)-5, 6-dibromoindole*
[41115-69-9]

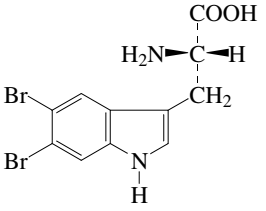


$C_{10}H_{10}Br_2N_2$ 318.01
Alkaloid from the Caribbean sponge *Polyfibrospongia maynardii*. Shows *in vitro* but not *in vivo* activity against gram-negative as well as gram-positive bacteria.
Mp 110-120°. λ_{max} 232 (ϵ 29200); 297 (ϵ 3700); 307 (ϵ 3300) (MeOH) (Berdy).

N^b-*Me:* ***5,6-Dibromo-N^b-methyltryptamine****. 5,6-Dibromo-*N*-methyl-1*H*-indole-3-ethanamine, 9CI*
[41115-68-8]
$C_{11}H_{12}Br_2N_2$ 332.037
Isol. from *Polyfibrospongia maynardii*. Shows *in vitro* but not *in vivo* activity against gram-negative as well as gram-positive bacteria.
Mp 132-134°. λ_{max} 232 (ϵ 29200); 297 (ϵ 3700); 307 (ϵ 3300) (MeOH) (Berdy).

N^b,N^b-*Di-Me:* ***5,6-Dibromo-N^b,N^b-dimethyltryptamine****. 5,6-Dibromo-*N,N*-dimethyl-1*H*-indole-3-ethanamine, 9CI*
[72853-80-6]
$C_{12}H_{14}Br_2N_2$ 346.064
Constit. of the marine sponges *Smenospongia echina*, *Smenospongia aurea* and *Verongula gigantea*. Shows antimicrobial props. Cryst. (MeOH aq.). Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 113-115°. λ_{max} 230 (ϵ 40100); 285 (ϵ 4900); 300 (ϵ 3300) (MeOH) (Derep). λ_{max} 207 (ϵ 9600); 232 (ϵ 30800); 291 (ϵ 6300) (EtOH) (Berdy).
Van Lear, G.E. *et al., Tet. Lett.*, 1973, 299-300 (*uv, pmr, ms, N^b-Me, struct*)
Djura, P. *et al., J.O.C.*, 1980, **45**, 1435-1441 (*5,6-Dibromo-*N^b,N^b*-dimethyltryptamine*)
Tymiak, A.A. *et al., Tetrahedron*, 1985, **41**, 1039-1047 (*5,6-Dibromo-N^b, N^b-dimethyltryptamine*)

5,6-Dibromotryptophan D-328

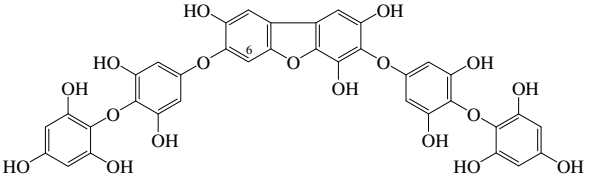


$C_{11}H_{10}Br_2N_2O_2$ 362.02

(S)-form
L-form
N^a-*Me: 5,6-Dibromo-*N*-methyl-L-tryptophan*. ***5,6-Dibromoabrine***
[488827-93-6]
$C_{12}H_{12}Br_2N_2O_2$ 376.047
Constit. of the sponge *Smenospongia* sp. Light brown powder. $[\alpha]_D^{22}$ -31 (c, 0.04 in MeOH). $[\alpha]_D^{22}$ +43.5 (c, 0.05 in 1*M* HCl). λ_{max} 228 (log ϵ 3.69); 290 (log ϵ 2.97) (MeOH).
Tasdemir, D. *et al., Zh. Neorg. Khim.*, 2002, **57**, 914-922 (*isol, uv, pmr, cmr, ms*)

Dicaval A D-329

[370553-48-3]



$C_{36}H_{24}O_{18}$ 744.575
Constit. of *Ecklonia cava*. Antioxidant.

6-Hydroxy: ***Dicaval B***
[370553-49-4]
$C_{36}H_{24}O_{19}$ 760.574
Constit. of *Ecklonia cava*. Antioxidant.
Japan. Pat., 2001, 01 302 655; *CA*, **135**, 335120c

Dichloroacetic acid, 9CI D-330

Dichloroethanoic acid
[79-43-6]
$Cl_2CHCOOH$
$C_2H_2Cl_2O_2$ 128.942
Constit. of the red alga *Asparagopsis taxiformis*. Has fungicidal props. Corrosive liq. Misc. H_2O, EtOH. d_4^{20} 1.56.
Mp 5-6° (11°). Bp 194° Bp_{20} 102°. n_D^{22} 1.4659.
▶ Fl. p. >66°. Corrosive and irritating to all tissues. LD_{50} (rbt, skn) 510 mg/kg. AG6125000

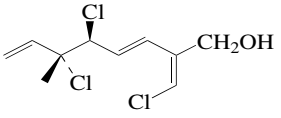
Amide: Dichloroacetamide
[683-72-7]
$C_2H_3Cl_2NO$ 127.957
Constit. of the red alga *Marginisporum aberrans*. Preservative. Shows antimicrobial props. Cryst.
Mp 98°. Bp_{745} 234°. Steam-volatile, subl.
▶ AB6475000

[2156-56-1, 13425-80-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 508B; 652C; 713C; 724B; 751D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 792A; 1007C; 1223A; 1366C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 591C; 702D; 766B (*ir*)

Doughty, H.W. *et al., J.A.C.S.*, 1931, **53**, 1594 (*synth, bibl*)
Org. Synth., Coll. Vol., 2, 1943, 181 (*synth*)
Org. Synth., Coll. Vol., 3, 1955, 260 (*amide*)
Fritz, H. *et al., Org. Magn. Reson.*, 1977, **9**, 108 (*cmr*)
Ohta, K. *et al., Phytochemistry*, 1977, **16**, 1085-1086 (*amide, isol*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617-620 (*isol*)
Pellegata, R. *et al., Synthesis*, 1985, 517 (*amide*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 169 (*rev*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1992, **16**, 115 (*use*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 409; 410
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DEL000; DEN000; DEN400; DEM800; DEM825

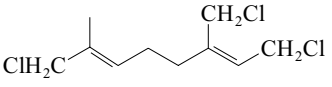
5,6-Dichloro-2-(chloromethylene)-6-methyl-3,7-octadien-1-ol D-331



$C_{10}H_{13}Cl_3O$ 255.57

(2*E*,3*E*,5*S*,6*R*)-*form* [58967-08-1]
Ac: 2-(Acetoxymethyl)-1,5,6-trichloro-6-methyl-1,3,7-octatriene [58967-07-0]
$C_{12}H_{15}Cl_3O_2$ 297.607
Constit. of the sea hare *Aplysia californica*. λ_{max} 259 (CCl_4).
Ireland, C. *et al., J.O.C.*, 1976, **41**, 2461 (*isol, uv, ir, pmr, ms*)

1,8-Dichloro-6-chloromethyl-2-methyl-2,6-octadiene, 9CI D-332

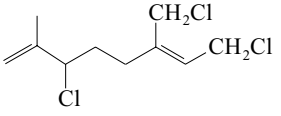


$C_{10}H_{15}Cl_3$ 241.587

(2*E*,6*Z*)-*form* [112642-59-8]
Constit. of *Chondrococcus hornemanni* and *Portieria hornemanni*. Oil.
Coll, J.C. *et al., Aust. J. Chem.*, 1987, **40**, 1893 (*isol, struct*)
Wright, A.D. *et al., J. Nat. Prod.*, 1990, **53**, 845-861 (*isol*)

3,8-Dichloro-6-chloromethyl-2-methyl-1,6-octadiene, 9CI D-333

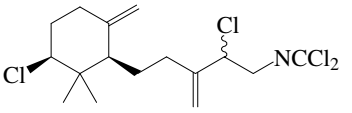
[112642-62-3]



$C_{10}H_{15}Cl_3$ 241.587
Constit. of *Chondrococcus hornemanni*. Oil. $[\alpha]_D$ -33.7 (c, 0.002 in $CHCl_3$).
Coll, J.C. *et al., Aust. J. Chem.*, 1987, **40**, 1893

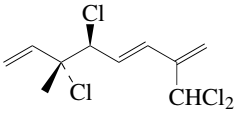
2,10-Dichloro-6,11-cyclo-3(15),7(14)-farnesadien-1-yl carbonimidic dichloride D-334

2-Chloro-5-(3-chloro-2,2-dimethyl-6-methylenecyclohexyl)-3-methylenepentyl carbonimidic dichloride
[321657-93-6]



$C_{16}H_{23}Cl_4N$ 371.175
Constit. of *Stylotella aurantium*. Oil. $[\alpha]_D^{25}$ +4.5 (c, 0.2 in $CHCl_3$). λ_{max} 205 (log ϵ 3.6) (MeOH).
Musman, M. *et al., J. Nat. Prod.*, 2001, **64**, 111-113 (*isol, pmr, cmr*)

5,6-Dichloro-2-(dichloromethyl)-6-methyl-1,3,7-octatriene D-335

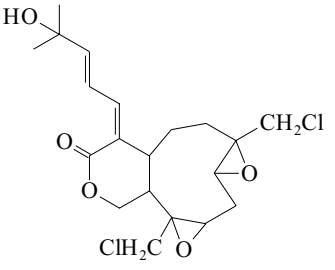


$C_{10}H_{12}Cl_4$ 274.016

(3*E*,5*S*,6*R*)-*form* [57804-28-1]
Constit. of the red alga *Plocamium cartilagineum*.
$[\alpha]_D^{25}$ -5.7 (c, 0.2 in $CHCl_3$). λ_{max} 233 (pentane).
Mynderse, J.S. *et al., Tetrahedron*, 1975, **31**, 1963-1967 (*isol, uv, pmr, ms*)

19,20-Dichloro-1,9:6,7-diepoxy-14-hydroxy-10,12-xenicadien-17,18-olide D-336

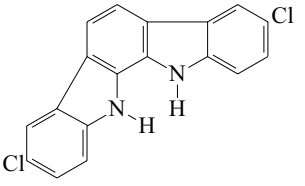
18,19-Dichloro-7,8:10,11-diepoxyisoxeniolide A



$C_{20}H_{26}Cl_2O_5$ 417.328
Constit. of *Xenia membranacea*. Amorph.
Almourabit, A. *et al., J. Nat. Prod.*, 1990, **53**, 894 (*isol, pmr*)

3,8-Dichloro-11,12-dihydroindolo[2,3-*a*]carbazole D-337

Tjipanazole D
[139083-25-3]



$C_{18}H_{10}Cl_2N_2$ 325.196
Alkaloid from blue-green alga *Tolypothrix tjipanasensis* and *Fischerella ambiguum*. λ_{max} 259 (ϵ 63100); 268 (sh) (ϵ 54100); 291 (ϵ 25500); 331 (ϵ 31000); 345 (sh) (ϵ 7300); 366 (ϵ 4030) (MeOH) (Derep).

N-*β*-D-*Xylopyranosyl:* ***Tjipanazole B***
[139083-21-9]
$C_{23}H_{18}Cl_2N_2O_4$ 457.312
Alkaloid from *Tolypothrix tjipanasensis*.
$[\alpha]_D$ -4.9 (c, 1.03 in $CHCl_3$). $[\alpha]_D$ +10.5 (c, 0.95 in $CHCl_3$/MeOH 1:1). λ_{max} 261 (ϵ 61000); 294 (ϵ 23200); 333 (ϵ 31300); 354 (ϵ 7340); 371 (ϵ 4800) (MeOH) (Derep). λ_{max} 259 (ϵ 59400); 292 (ϵ 24800); 330 (ϵ 30400); 349 (ϵ 8140); 366 (ϵ 4850) (MeOH) (Berdy).

N-*(6-Deoxy-β-*D-*gulopyranosyl):* ***Tjipanazole A1***
[139083-13-9]
$C_{24}H_{20}Cl_2N_2O_4$ 471.338
Major alkaloid from the blue-green alga *Tolypothrix tjipanasensis*. Exhibits antifungal activity. $[\alpha]_D$ +9.1 (c, 1.0 in $CHCl_3$). λ_{max} 261 (ϵ 61000); 294 (ϵ 23200); 333 (ϵ 31300); 354 (ϵ 7340); 371 (ϵ 4800) (MeOH) (Derep).

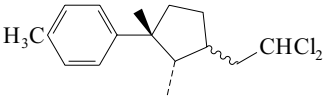
N-*α-*L-*Rhamnopyranosyl:* ***Tjipanazole A2***
[139083-14-0]
$C_{24}H_{20}Cl_2N_2O_4$ 471.338
From *Tolypothrix tjipanasensis*. Exhibits antifungal activity. $[\alpha]_D$ +25.12 (c, 1.0 in $CHCl_3$). λ_{max} 261 (ϵ 61000); 294 (ϵ 23200); 333 (ϵ 31300); 354 (ϵ 7340); 371 (ϵ 4800) (MeOH) (Derep).

N-*β-*D-*Glucopyranosyl:* ***Tjipanazole E***
[139083-22-0]
$C_{24}H_{20}Cl_2N_2O_5$ 487.338
Minor alkaloid from *Tolypothrix tjipanasensis*.
$[\alpha]_D$ +63.8 (c, 1.0 in $CHCl_3$/MeOH 1:1). λ_{max} 261 (ϵ 61000); 294 (ϵ 23200); 333 (ϵ 31300); 354 (ϵ 7340); 371 (ϵ 4800) (MeOH) (Derep). λ_{max} 259 (ϵ 54400); 293 (ϵ 21700); 332 (ϵ 26900); 350 (ϵ 7360); 368 (ϵ 4460) (MeOH) (Berdy).

Bonjouklian, R. *et al., Tetrahedron*, 1991, **47**, 7739 (*isol, uv, pmr, cmr, struct*)
Kuethe, J.T. *et al., Org. Lett.*, 2003, **5**, 3721-3723 (*synth*)

Dichlorohomolaurane D-338

[121451-08-9]

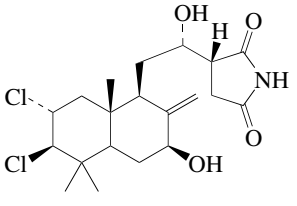


$C_{16}H_{22}Cl_2$ 285.255
Metab. of *Aplysia dactylomela*. Cryst.
Mp 125-127°.

Rao, C.B. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 322 (*isol, pmr*)

Dichlorolissoclimide D-339

[138935-82-7]



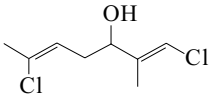
$C_{20}H_{29}Cl_2NO_4$ 418.359
Constit. of tunicate *Lissoclinum voeltzkowi*. Tyrosine metabolite and 5-aminolevulinic acid dehydrase inhibitor. Immunosuppressant.
Mp 210°. $[\alpha]_D^{20}$ -20. $[\alpha]_D^{20}$ +30 (c, 0.2 in MeOH). No comment made on conflicting optical rotations. λ_{max} 242 (ϵ 76) (EtOH).

7-Ac: ***Haterumaimide A***
[335155-25-4]
$C_{22}H_{31}Cl_2NO_5$ 460.396
Isol. from a *Lissoclinum* sp. Cytotoxic agent. $[\alpha]_D^{29}$ +31.3 (c, 0.13 in MeOH).

3-Dechloro: ***Chlorolissoclimide***
[148717-91-3]
$C_{20}H_{30}ClNO_4$ 383.914
Constit. of *Lissoclinum voeltzkowi*. Highly cytotoxic. Glass.

Malochet-Grivois, C. *et al., Tet. Lett.*, 1991, **32**, 6701-6702 (*isol, pmr, cmr*)
Biard, J.-F. *et al., Nat. Prod. Lett.*, 1994, **4**, 43-50 (*Chlorolissoclimide*)
Toupet, L. *et al., J. Nat. Prod.*, 1996, **59**, 1203-1204 (*cryst struct*)
Uddin, M.J. *et al., Heterocycles*, 2001, **54**, 1039-1048 (*Haterumaimide A*)

1,6-Dichloro-2-methyl-1,5-heptadien-3-ol D-340



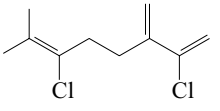
$C_8H_{12}Cl_2O$ 195.088

(1E,5Z)-form [70389-85-4]
Constit. of *Plocamium cruciferum*.
Oil. $[\alpha]_D^{28}$ -9.8 (c, 0.01 in $CHCl_3$).

Bates, P. *et al., Aust. J. Chem.*, 1979, **32**, 2545-2554 (*isol, pmr, cmr, ms*)

2,6-Dichloro-7-methyl-3-methylene-1,6-octadiene D-341

3,7-Dichloromyrcene
[57461-73-1]

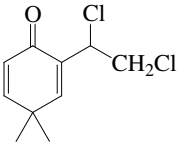


$C_{10}H_{14}Cl_2$ 205.126
Constit. of *Chondrococcus hornemanni*. Oil.

Burreson, B.J. *et al., Tet. Lett.*, 1975, 2155

1,2-Dichloro-3(8),5-ochtodadien-4-one D-342

2-(1,2-Dichloroethyl)-4,4-dimethyl-2,5-cyclohexadien-1-one
[569351-31-1]



$C_{10}H_{12}Cl_2O$ 219.11
Constit. of the red alga *Portieria hornemanni*. Oil. $[\alpha]_D^{23}$ -9.6 (c, 0.1 in $CHCl_3$).

Kuniyoshi, M. *et al., J. Chin. Chem. Soc. (Taipei)*, 2003, **50**, 167-170 (*isol, pmr, cmr*)

1,15-Dichloro-1,14-pentadecadiene-3,12-diyn-8-amine D-343

8-Amino-1,15-dichloro-1,14-pentadecadiene-3,12-diyne
$ClCH{=}CHC{\equiv}C(CH_2)_3CH(NH_2)(CH_2)_3C{\equiv}CCH{=}CHCl$
$C_{15}H_{19}Cl_2N$ 284.227

(1E,14E)-form

N-*Ac: 8-Acetamido-1,15-dichloro-1,14-pentadecadiene-3,12-diyne.* ***Taveuniamide H***
$C_{17}H_{21}Cl_2NO$ 326.264
Isol. from a mixed assemblage of *Lyngbya majuscula* and *Schizothrix* sp. λ_{max} 238 (ϵ 10300) (EtOH).

1-Chloro, N-*Ac: 8-Acetamido-1,1,15-trichloro-1,14-pentadecadiene-3,12-diyne.* ***Taveuniamide I***
$C_{17}H_{20}Cl_3NO$ 360.709
Isol. from a mixt. of *Lyngbya majuscula* and *Schizothrix* sp. $[\alpha]_D^{25}$ -2 (c, 0.4 in $CHCl_3$). λ_{max} 242 (ϵ 37500) (EtOH).

1-Chloro, 1,2,3,3,4,4-hexahydro, N-*Ac: 8-Acetamido-1,15,15-trichloro-1-pentadecen-3-yne.* ***Taveuniamide F***
$C_{17}H_{26}Cl_3NO$ 366.757
Isol. from a mixt. of *Lyngbya majuscula* and *Schizothrix* sp. $[\alpha]_D^{25}$ -5.2 (c, 0.4 in $CHCl_3$). λ_{max} 238 (ϵ 9100) (EtOH).

1,15-Dichloro, N-*Ac: 8-Acetamido-1,1,15,15-tetrachloro-1,14-pentadecadiene-3,12-diyne.* ***Taveuniamide J***
$C_{17}H_{19}Cl_4NO$ 395.154
Isol. from a mixt. of *Lyngbya majuscula* and *Schizothrix* sp.
λ_{max} 244 (ϵ 37700) (EtOH).

1,15-Dichloro, 1,2-dihydro, N-*Ac: 8-Acetamido-1,1,15,15-tetrachloro-1-pentadecen-3,12-diyne.* ***Taveuniamide G***
$C_{17}H_{21}Cl_4NO$ 397.17
Isol. from a mixt. of *Lyngbya majuscula* and *Schizothrix* sp.
$[\alpha]_D^{25}$ +0.3 (c, 0.04 in $CHCl_3$). λ_{max} 244 (ϵ 21100) (EtOH).

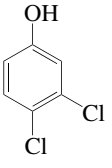
(1E,14Z)-form

3Z,4-Dihydro, N-*Ac: 8-Acetamido-1,15-dichloro-1,3,14-pentadecatrien-12-yne.* ***Taveuniamide K***
$C_{17}H_{23}Cl_2NO$ 328.28
Isol. from a mixt. of *Lyngbya majuscula* and *Schizothrix* sp.
$[\alpha]_D^{25}$ +2.4 (c, 0.1 in $CHCl_3$). λ_{max} 242 (ϵ 18200) (EtOH).

Williamson, R.T. *et al., Tetrahedron*, 2004, **60**, 7025-7033 (*isol, pmr, cmr*)

3,4-Dichlorophenol D-344

[95-77-2]
[25167-81-1]



$C_6H_4Cl_2O$ 163.002
Constit. of the marine acorn worm *Ptychodera bahamensis.*
Needles (C_6H_6/petrol).
Mp 68°. Bp_{767} 253.5°. pK_a 8.58 (25°, H_2O).

▶ SK8800000

Benzoyl:
$C_{13}H_8Cl_2O_2$ 267.11
Cryst. (EtOH). Mp 96°.

Me ether: 1,2-Dichloro-4-methoxybenzene. 3,4-Dichloroanisole
[36404-30-5]
$C_7H_6Cl_2O$ 177.029
Mp -8°.

[17847-51-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1087A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 274C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1025A (*ir*)
Holleman, A.F. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1918, **37**, 96 (*synth*)
Azouz, W.M. *et al., Biochem. J.*, 1955, **59**, 410 (*deriv*)
Bavoux, C. *et al., Acta Cryst. B*, 1980, **36**, 741 (*cryst struct*)
Corgiat, J.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1993, **106**, 83-86 (*Ptychodera bahamensis constit*)

3,5-Dichlorophenol D-345

[591-35-5]
[25167-81-1]

$C_6H_4Cl_2O$ 163.002
Constit. of the marine acorn worm *Ptychodera bahamensis.*
Mp 68°. Bp 233-234° Bp_8 122-124°. pK_a 8.19 (25°).

▶ SK8820000

Ac: [61925-86-8]
$C_8H_6Cl_2O_2$ 205.04
Needles (EtOH aq.). Mp 38°.

Benzoyl:
$C_{13}H_8Cl_2O_2$ 267.11
Needles (EtOH aq.). Mp 55°.

Me ether: 1,3-Dichloro-5-methoxybenzene. 3,5-Dichloroanisole
[33719-74-3]
$C_7H_6Cl_2O$ 177.029
Cryst. (EtOH or petrol). Mp 39° (68°).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1049C; 1085A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 200C; 263C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 981A; 1018C (*ir*)
Blanksma, J.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1908, **27**, 25 (*synth*)
Bavoux, C. *et al., Acta Cryst. B*, 1973, **29**, 2603 (*cryst struct*)
Sanyal, N.K. *et al., Indian J. Pure Appl. Phys.*, 1973, **11**, 913 (*uv, ir*)
Bisanz, T. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1973, **47**, 2279 (*pmr*)
Emsley, J.W. *et al., J.C.S. Perkin 2*, 1978, 928 (*conformn*)
Corgiat, J.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1993, **106**, 83-86 (*isol*)

1,3-Dichloro-2-propanol, 9CI D-346

Glycerol 1,3-dichlorohydrin. α,γ-Dichlorohydrin
[96-23-1]
$ClCH_2CH(OH)CH_2Cl$
$C_3H_6Cl_2O$ 128.985
Isol. from Antarctic krill and the fungus *Caldariomyces fumago.*
Solv. for hard resins and nitrocellulose; binder for water colours. Reagent for Vitamin A detn. Liq. Sol. H_2O, Et_2O. d_4^{17} 1.35 d_4^{20} 1.37. Bp 174-175°. n_D^{17} 1.4802.

▶ Fl. p. 74° (oc). Eye, skin and respiratory tract irritant. LD_{50} (rat, orl) 110 mg/kg. LD_{50} (rbt, skn) 800 mg/kg. UB1400000

Phenylurethane: Mp 73°.

Ac: [3674-10-0]
$C_5H_8Cl_2O_2$ 171.022
Bp_{15} 81°.

Chloromethyl ether:
$C_4H_7Cl_3O$ 177.457
Oil. Bp 70°.

Benzyl ether:
$C_{10}H_{12}Cl_2O$ 219.11
Liq. $Bp_{0.05}$ 99-100°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 176D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 278B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 258D (*ir*)
Hill, A.J. *et al., J.A.C.S.*, 1922, **44**, 2582-2595 (*synth*)
Fairbourne, A. *et al., J.C.S.*, 1930, 369-382 (*synth*)
Org. Synth., Coll. Vol., 1, 1932, 292-294 (*synth, bibl*)
Oliver, L.K. *et al., Clin. Chem. (Winston-Salem, N.C.)*, 1976, **22**, 1541 (*use*)
Kubota, K. *et al., CA*, 1981, **94**, 63937x (*isol*)
Franssen, M.C.R. *et al., Phytochemistry*, 1988, **27**, 1093-1096 (*isol, ms*)
Janicki, S. *et al., J.O.C.*, 1998, **63**, 3694-3700 (*chloromethyl ether*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 433
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, DGG400

1,3-Dichloropropanone, 9CI D-347

1,3-Dichloroacetone
[534-07-6]
$ClCH_2COCH_2Cl$
$C_3H_4Cl_2O$ 126.969
Constit. of the red alga *Asparagopsis armata.* Cryst. Sol. H_2O.
Mp 45°. Bp 173°.

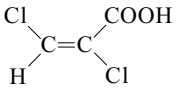
▶ Flammable, fl. p. 46°. LC_{50} (rat, ihl) 29 mg m^{-3} (2h exposure). UC1430000

2,4-Dinitrophenylhydrazone:
Cryst. Mp 132-133°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 417A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 650C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 505A (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 211 (*synth*)
Sorensen, A.M. *et al., Acta Cryst. B*, 1974, **30**, 1366 (*cryst, struct*)
Nollet, A.J.H. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1975, **94**, 59 (*synth*)
McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367-374 (*isol*)
L'abbé, G. *et al., J.C.S. Perkin 1*, 1991, 607 (*semicarbazone, synth, ir, pmr*)
O'Hagan, D. *et al., J. Labelled Compd. Radiopharm.*, 1994, **34**, 871-879 (*synth, ir, pmr, cmr*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **3**, 1653-1654 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BIK250

2,3-Dichloro-2-propenoic acid, 9CI D-348

2,3-Dichloroacrylic acid, 8CI
[13167-36-7]



(*E*)–*form*

$C_3H_2Cl_2O_2$ 140.953
Constit. of the red alga *Asparagopsis taxiformis.*

(*E*)-*form* [6795-91-1]
Cryst. Mp 60.5°.

Me ester: [3533-70-8]
$C_4H_4Cl_2O_2$ 154.98
Liq. Bp_{15} 63°.

(*Z*)-*form* [3533-68-4]
Cryst. Mp 86°.

Zincke, Th. *et al., Ber.*, 1891, **24**, 918 (*synth*)
Roedig, A. *et al., Annalen*, 1971, **754**, 35 (*synth*)
Roedig, A. *et al., Annalen*, 1979, 194 (*synth, ester*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617 (*isol*)
Voegeli, U. *et al., Org. Magn. Reson.*, 1980, **13**, 200 (*cmr*)

3,3-Dichloro-2-propenoic acid, 9CI D-349

3,3-Dichloroacrylic acid, 8CI
[1561-20-2]
$Cl_2C{=}CHCOOH$
$C_3H_2Cl_2O_2$ 140.953
Constit. of the red alga *Asparagopsis taxiformis.* Prisms ($CHCl_3$). Mp 76-77° (84-86°).

Et ester: [35245-99-9]
$C_5H_6Cl_2O_2$ 169.007
Liq. Bp 173-175° Bp_{16} 63-64°.

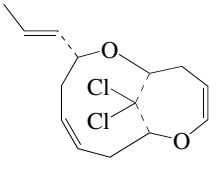
Amide: [2520-01-6]
$C_3H_3Cl_2NO$ 139.968
Needles. Mp 113°.

Chloride: [20618-08-0]
C_3HCl_3O 159.398
Bp 145-147°.

Straus, F. *et al., Ber.*, 1930, **63**, 1877 (*synth*)
Rappe, C. *et al., Ark. Kemi*, 1965, **24**, 303 (*synth*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617 (*isol*)
Stack, D.P. *et al., Synthesis*, 1984, 435 (*chloride*)

13,13-Dichloro-12-(2-propenyl)-2,7-methano-1, 6-dioxacyclododeca-4,9-diene D-350

5,5-Dichloro-1,6:4,11-diepoxy-1,8,12-tetradecatriene

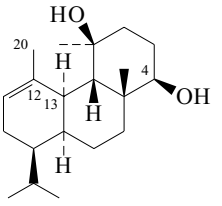


$C_{14}H_{18}Cl_2O_2$ 289.2
Isol. from *Aplysia punctata.*

Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 98 (*occur*)

α-Dictalediol D-351

[92484-29-2]



$C_{20}H_{34}O_2$ 306.487

4-Ac: ***α-Dictalediol acetate****. 4-Acetoxy-11-dictalen-1-ol*
$C_{22}H_{36}O_3$ 348.525
Constit. of a *Dictyota* sp. Cryst. Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 156-158°. $[\alpha]_D$ -1.8 (c, 0.4 in $CHCl_3$).

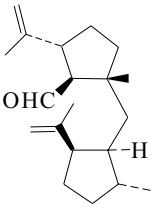
$\Delta^{12(20)}$ Isomer, 4-Ac: ***β-Dictalediol acetate****. β-Dictalediol monoacetate*
$C_{22}H_{36}O_3$ 348.525
Constit. of a *Dictyota* sp. Cryst.
Mp 136-138°. $[\alpha]_D$ -0.5 (c, 1.2 in $CHCl_3$).

Δ^{12} Isomer, 4-Ac: 4-Acetoxy-12-dictalen-1-ol
$C_{22}H_{36}O_3$ 348.525
Constit. of a *Dictyota* sp. Oil. $[\alpha]_D$ -0.3 (c, 1.82 in $CHCl_3$).

González, A.G. *et al., Chem. Comm.*, 1984, 669 (*isol, pmr, cryst struct*)
Clardy, J. *et al., Tet. Lett.*, 1987, **28**, 6699 (*β-Dictalediol monoacetate*)
Gallardo, A. *et al., Rev. Latinoam. Quim.*, 1988, **19**, 86 (*isol, pmr, cmr*)

Dictymal D-352

[114804-63-6]

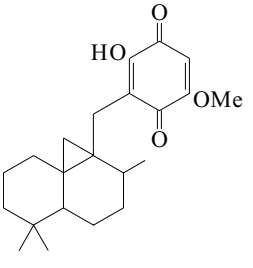


$C_{20}H_{32}O$ 288.472
Constit. of brown alga *Dictyota dichotoma*. Oil. $[\alpha]_D^{18}$ +16.4 (c, 0.88 in $CHCl_3$).

Segawa, M. *et al., Tet. Lett.*, 1987, **28**, 3703

Dictyoceratidaquinone D-353

[127506-68-7]

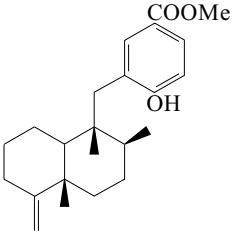


$C_{22}H_{30}O_4$ 358.477
Constit. of a Dictyoceratid sponge. Active against *Staphylococus aureus.* Yellow cryst. (hexane).
Mp 159-161°. $[\alpha]_D^{25}$ -12.8 (c, 0.21 in $CHCl_3$). Descr. in the lit. as isol. from *Dityoceratida* sp. , but Dictyoceratida is an order, not a genus. λ_{max} 215 (ϵ 8965); 286 (ϵ 16206); 425 (ϵ 344) (MeOH) (Berdy). λ_{max} 218 (ϵ 21034); 288 (ϵ 12931); 522 (ϵ 1379) (MeOH-NaOH) (Berdy).

Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1990, **26**, 47; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 37 (*isol, pmr, cmr*)
Popov, A.M. *et al., Pharm. Chem. J. (Engl. Transl.)*, 1999, **33**, 71-73 (*isol, activity*)

Dictyoceratin C D-354

Dictyoceratin
[123062-43-1]



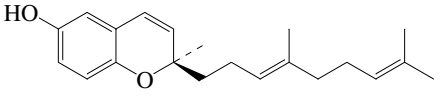
$C_{23}H_{32}O_3$ 356.504
Metab. of *Dactylospongia* sp. and *Petrosaspongia metachromia*. Solid. $[\alpha]_D^{23}$ +16.7 (c, 0.03 in $CHCl_3$). λ_{max} 261 (ϵ 11490) (MeOH) (Berdy). λ_{max} 311 (ϵ 25940) (MeOH/NaOH) (Berdy).

O-*(3-Methyl-2-butenyl)*: ***17-Isoprenyldictyoceratin C***
[777091-13-1]
$C_{28}H_{40}O_3$ 424.622
Constit. of a *Spongia* sp. Oil. $[\alpha]_D$ +8 (c, 0.08 in $CHCl_3$). λ_{max} 263 (log ϵ 4.26) ($CHCl_3$).

Kushlan, D.M. *et al., Tetrahedron*, 1989, **45**, 3307
Kwak, J.H. *et al., J. Nat. Prod.*, 2000, **63**, 1153-1156 (*isol, pmr, cmr*)
Cao, S. *et al., J. Nat. Prod.*, 2004, **67**, 1716-1718 (*17-Isoprenyldictyoceratin C*)

Dictyochromenol D-355

*2-(4,8-Dimethyl-3,7-nonadienyl)-2-methyl-2*H*-1-benzopyran-6-ol, 9CI*
[93398-32-4]



(R)-form

$C_{21}H_{28}O_2$ 312.451

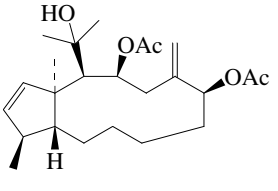
(R)-form
Oil. $[\alpha]_D^{29}$ -94.4 (c, 0.55 in $CHCl_3$).

(±)-form
Constit. of *Dictyopteris undulata*. Piscicide. Oil. λ_{max} 260 (ϵ 3700); 330 (ϵ 3000) (MeOH) (Berdy).

Dave, M.-N. *et al., Heterocycles*, 1984, **22**, 2301-2307 (*isol, pmr*)
Aoki, K. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 1915-1924 (*synth, abs config*)

Dictyocrenulol D-356

[639476-59-8]

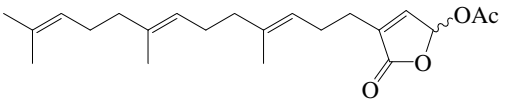


$C_{24}H_{38}O_5$ 406.561
Constit. of *Dictyota crenulata*. Oil. $[\alpha]_D^{25}$ -61.7 (c, 0.25 in $CHCl_3$).

Soto, H. *et al., Z. Naturforsch., C*, 2003, **58**, 795-798 (*isol, pmr, cmr*)

Dictyodendrillolide D-357

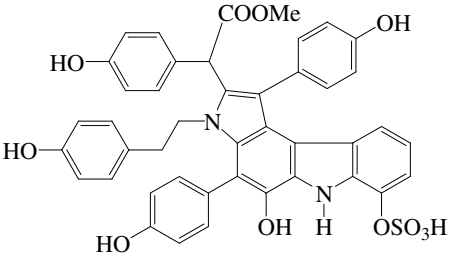
1-Acetoxy-2,6,10,14-phytatetraen-20,1-olide
[117585-47-4]



$C_{22}H_{32}O_4$ 360.492
Constit. of a *Dictyodendrilla* sp. Oil. $[\alpha]_D^{23}$ +21.9 (c, 0.43 in $CHCl_3$).

Cambie, R.C. *et al., J. Nat. Prod.*, 1988, **51**, 1014-1016 (*Dictyodendrillolide*)

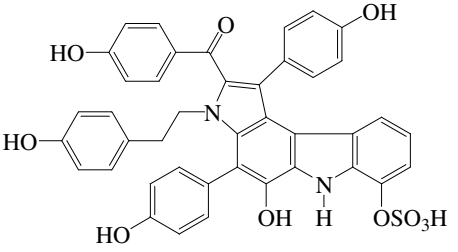
Dictyodendrin A D-358



$C_{43}H_{34}N_2O_{11}S$ 786.814
Alkaloid from the sponge *Dictyodendrilla verongiformis*. Telomerase inhibitor. Amorph. red solid (as Na salt). $[\alpha]_D^{19}$ -4.6 (c, 0.01 in MeOH/0.3*M* $NaClO_4$) (Na salt). λ_{max} 208 (ϵ 55200); 227 (ϵ 56600); 328 (ϵ 18500); 480 (ϵ 3950) (MeOH).

Warabi, K. *et al., J.O.C.*, 2003, **68**, 2765-2770 (*isol, pmr, cmr, ms*)

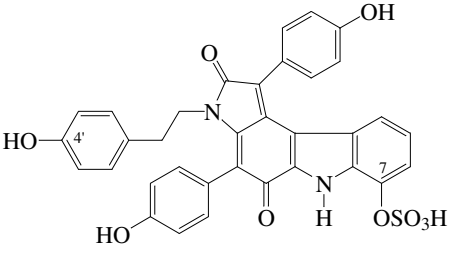
Dictyodendrin B D-359



$C_{41}H_{30}N_2O_{10}S$ 742.761
Alkaloid from the sponge *Dictyodendrilla verongiformis*. Telomerase inhibitor. Amorph. yellow solid (as Na salt). λ_{max} 228 (ϵ 34700); 305 (sh); 397 (ϵ 9010) (MeOH) (Na salt).

Warabi, K. *et al., J.O.C.*, 2003, **68**, 2765-2770 (*isol, pmr, cmr, ms*)
Fürstner, A. *et al., J.A.C.S.*, 2006, **128**, 8087-8094 (*synth*)

Dictyodendrin C D-360



$C_{34}H_{24}N_2O_9S$ 636.638

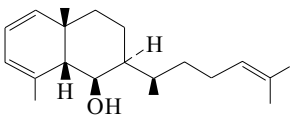
Alkaloid from the sponge *Dictyodendrilla verongiformis*. Telomerase inhibitor. Greenish-yellow solid (as Na salt). λ_{max} 238 (ϵ 18300); 277 (ϵ 10500); 302 (ϵ 8600); 415 (ϵ 6540) (MeOH) (Na salt).

7-O-*Desulfo, 4′*-O-*sulfate:* ***Dictyodendrin D***
$C_{34}H_{24}N_2O_9S$ 636.638
Alkaloid from *Dictyodendrilla verongiformis*. Telomerase inhibitor. Greenish-yellow solid (as Na salt). λ_{max} 243 (ϵ 12500); 276 (ϵ 6610); 305 (ϵ 6230); 353 (ϵ 5520); 416 (ϵ 4960) (MeOH) (Na salt).

Warabi, K. *et al., J.O.C.*, 2003, **68**, 2765-2770 (*isol, pmr, cmr, ms*)
Fürstner, A. *et al., J.A.C.S.*, 2006, **128**, 8087-8094 (*synth*)

Dictyolene D-361

[63250-22-6]

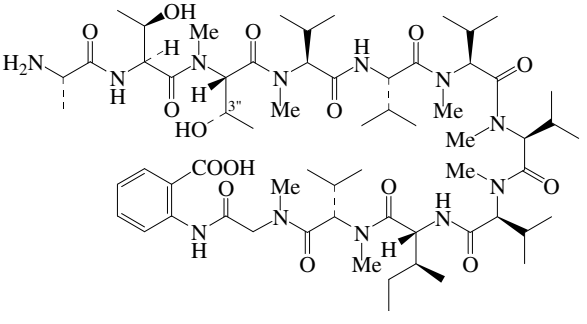


$C_{20}H_{32}O$ 288.472
Constit. of *Dictyota acutiloba*. Oil. λ_{max} 208 (ϵ 4300); 268 (ϵ 4000) (EtOH) (Derep).

Sun, H.H. *et al., J.A.C.S.*, 1977, **99**, 3516 (*isol*)
Marshall, J.A. *et al., J.A.C.S.*, 1978, **100**, 1627 (*synth*)
Greene, A.E. *et al., Tet. Lett.*, 1979, 63 (*synth*)
Banerjee, A.K. *et al., Tetrahedron*, 1993, **49**, 4761 (*synth, rev*)

Dictyonamide A D-362

[366015-39-6]

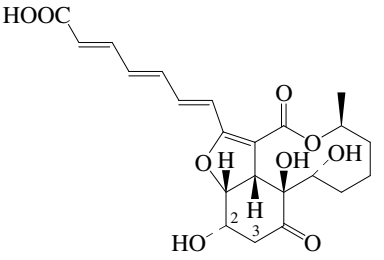


$C_{63}H_{108}N_{12}O_{15}$ 1273.618
Isol. from a marine fungus (KO63) separated from the red alga *Ceratodictyon spongiosum*. Amorph. solid. $[\alpha]_D^{22}$ -169 (c, 1 in MeOH). λ_{max} 208 (ϵ 21900); 296 (ϵ 2600) (MeOH).

3′′-O-*β*-*D*-*Fructofuranoside:* ***Dictyonamide B***
[366015-40-9]
$C_{69}H_{118}N_{12}O_{20}$ 1435.76
Isol. from a marine fungus from *Ceratodictyon spongiosum*. Amorph. solid. $[\alpha]_D^{22}$ -132 (c, 1 in MeOH). λ_{max} 209 (ϵ 19200); 296 (ϵ 1500) (MeOH).

Komatsu, K. *et al., J.O.C.*, 2001, **66**, 6189-6192

Dictyosphaeric acid B D-363



Relative Configuration

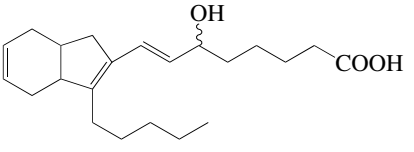
$C_{22}H_{26}O_9$ 434.442
Prod. by a *Penicillium* sp. isol. from the alga *Dictyosphaeria versluyii*. Amorph. yellow solid. $[\alpha]_D^{25}$ +76 (c, 0.02 in MeOH). λ_{max} 214 (log ϵ 3.81); 280 (sh) (log ϵ 3.82); 346 (log ϵ 4.13) (MeOH).

2-Deoxy, 2,3-didehydro: ***Dictyosphaeric acid A***
$C_{22}H_{24}O_8$ 416.427
Prod. by a *Penicillium* sp. isol. from *Dictyosphaeria versluyii*. Amorph. yellow solid. $[\alpha]_D^{25}$ +126 (c, 0.21 in MeOH). λ_{max} 214 (log ϵ 3.74); 336 (log ϵ 4.09) (MeOH).

Bugni, T.S. *et al., J. Nat. Prod.*, 2004, **67**, 1396-1399 (*isol, pmr, cmr*)

Dictyosphaerin D-364

[183995-83-7]

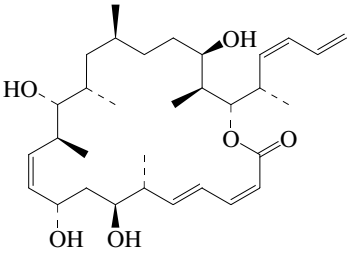


$C_{22}H_{34}O_3$ 346.509
Isol. from the marine alga *Dictyosphaeria sericea*. Unstable oil. $[\alpha]_D$ -50 (c, 1 in $CHCl_3$). λ_{max} 203 (ϵ 13500); 241 (ϵ 10000) (EtOH).

Rochfort, S.J. *et al., J. Nat. Prod.*, 1996, **59**, 1154 (*isol, uv, ir, pmr, cmr, ms*)

Dictyostatin D-365

[156312-07-1]



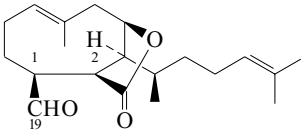
Absolute Configuration

$C_{32}H_{52}O_6$ 532.759
Macrocyclic lactone antibiotic. Isol. from a marine *Spongia* sp. Potent inducer of tubulin polymerisation. Cytotoxic agent. Amorph. solid. Sol. MeOH, $CHCl_3$.
Mp 87-88°. $[\alpha]_D^{22}$ -20 (c, 0.1 in MeOH). λ_{max} 223 (ϵ 19950); 263 (ϵ 15850) (MeOH) (Berdy).

Pettit, G.R. *et al., Chem. Comm.*, 1994, 1111-1112 (*isol, pmr, cmr*)
Paterson, I. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 4629-4633 (*synth, abs config*)
Shin, Y. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 4634-4637 (*synth, abs cofig*)
Isbrucker, R.A. *et al., Biochem. Pharmacol.*, 2004, **66**, 75-82 (*activity*)
O'Neil, G.W. *et al., J.A.C.S.*, 2006, **128**, 5340-5341 (*synth*)
Fukui, Y. *et al., Org. Lett.*, 2006, **8**, 301-304 (*synth*)

Dictyotalide A D-366

[116436-88-5]

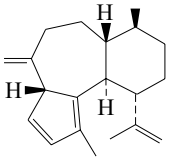


$C_{20}H_{30}O_3$ 318.455
Constit. of *Dictyota dichotoma*. Algicide. Oil. Sol. MeOH, hexane; poorly sol. H_2O. $[\alpha]_D$ -102 (c, 0.71 in $CHCl_3$).

1,2-Didehydro, 19-alcohol, 19-Ac: ***Dictyotalide B***
[116406-17-8]
$C_{22}H_{32}O_4$ 360.492
Constit. of *Dictyota dichotoma*. Oil. Sol. MeOH, hexane; poorly sol. H_2O. $[\alpha]_D$ +50.3 (c, 0.59 in $CHCl_3$).
Ishitsuka, M.O. *et al., J.O.C.*, 1988, **53**, 5010 (*isol, pmr, cmr*)

Dictyotetraene D-367

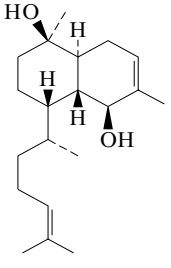
[97343-99-2]



$C_{20}H_{28}$ 268.441
Constit. of a *Dictyota* sp. Oil.
Demattè, B. *et al., Chem. Comm.*, 1985, 391; 1008

Dictyotin A D-368

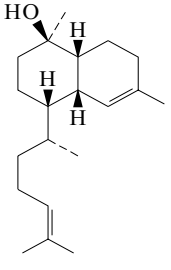
[121923-97-5]



$C_{20}H_{34}O_2$ 306.487
Metab. of *Dictyota dichotoma*. Oil. $[\alpha]_D^{20}$ -4.6 (c, 0.13 in $CHCl_3$).
Ishitsuka, M.O. *et al., Phytochemistry*, 1990, **29**, 2605 (*isol, pmr, cmr, ms*)

Dictyotin B D-369

[121923-98-6]



$C_{20}H_{34}O$ 290.488
Metab. of *Dictyota dichotoma*. Oil. $[\alpha]_D^{20}$ -30 (c, 0.19 in $CHCl_3$).

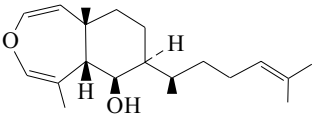
Me ether: ***Methoxydictydiene***
$C_{21}H_{36}O$ 304.515
Constit. of *Pachydictyon coriaceum* and *Dictyota dichotoma*. Oil. $[\alpha]_D^{20}$ -48 (c, 0.59 in $CHCl_3$). Struct. revised in 1990.

10-Epimer: ***Dictyotin C***
[121923-99-7]
$C_{20}H_{34}O$ 290.488
Metab. of *Dictyota dichotoma*.
$[\alpha]_D^{20}$ +5 (c, 0.61 in $CHCl_3$).

Me ether, 1,10-diepimer: ***Dictyotin D methyl ether***
$C_{21}H_{36}O$ 304.515
Constit. of *Pachydictyon coriaceum*. Oil. $[\alpha]_D^{20}$ -77 (c, 0.59 in $CHCl_3$).
Ishitsuka, M.O. *et al., Phytochemistry*, 1990, **29**, 2605 (*isol, pmr, cmr, ms*)

Dictyoxepin D-370

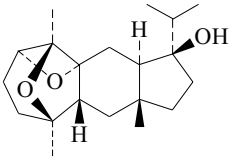
9,11-Epoxy-17-loben-3-ol
[63250-21-5]



$C_{20}H_{32}O_2$ 304.472
Constit. of *Dictyota acutiloba*. Algicide.
Sun, H.H. *et al., J.A.C.S.*, 1977, **99**, 3516

Dictyoxetane D-371

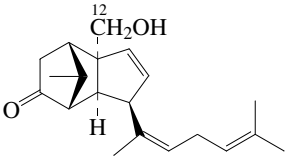
[97732-59-7]



$C_{20}H_{32}O_3$ 320.471
Constit. of *Dictyota dichotoma*. Cryst.
Mp 87-90°. $[\alpha]_D$ +35 (c, 3 in $CHCl_3$).
Pullaiah, K.C. *et al., J.O.C.*, 1985, **50**, 3665 (*isol, cryst struct*)

Dictyterpenoid B D-372

[403805-74-3]

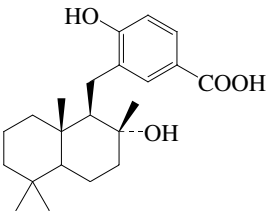


$C_{20}H_{28}O_2$ 300.44
Constit. of *Dilophus okamurae*. Oil. $[\alpha]_D^{16}$ +27 (c, 0.58 in $CHCl_3$).

12-Aldehyde: ***Dictyterpenoid A***
[403805-72-1]
$C_{20}H_{26}O_2$ 298.424
Constit. of *Dilophus okamurae*. Oil. $[\alpha]_D^{24}$ +58 (c, 0.23 in $CHCl_3$).
Suzuki, M. *et al., J. Nat. Prod.*, 2002, **65**, 121-125 (*isol, pmr, cmr*)

Dictyvaric acid D-373

[752211-90-8]



$C_{22}H_{32}O_4$ 360.492
Constit. of *Dictyopteris divaricata*. Cryst. (MeOH).
Mp 256-258°. $[\alpha]_D^{20}$ +29 (c, 0.1 in $CHCl_3$).

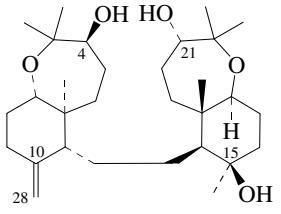
Song, F.H. *et al., Chin. Chem. Lett.*, 2004, **15**, 316-318 (*isol, pmr, cmr*)

Dicynthaurin D-374

Peptide consisting of two 30-residue monomers linked by a disulfide bond. Isol. from haemocytes of a tunicate *Halocynthia aurantium*. Shows antimicrobial activity.

Lee, I.H. *et al., Biochim. Biophys. Acta*, 2001, **1527**, 141-148 (*isol, struct*)

Dideacetylraspacionin D-375



$C_{30}H_{52}O_5$ 492.738

15-Ac: [158042-10-5]
$C_{32}H_{54}O_6$ 534.775
Constit. of *Raspaciona aculeata*. Amorph. powder. $[\alpha]_D^{25}$ -49.1 (c, 0.25 in $CHCl_3$).

15,21-Di-Ac: ***Raspacionin***
[132210-64-1]
$C_{34}H_{56}O_7$ 576.812
Constit. of sponge *Raspaciona aculeata*. Allelochemical, larvicide. Prisms (heptane).
Mp 188-189°. $[\alpha]_D$ +31.4 (c, 1.5. in $CHCl_3$).

21-Ketone: [452934-96-2]
$C_{30}H_{50}O_5$ 490.722
Constit. of *Raspaciona aculeata*. Oil. $[\alpha]_D$ -9.8 (c, 0.12 in $CHCl_3$).

21-Ketone, 15-Ac: ***21-Oxoraspacionin***
[452934-95-1]
$C_{32}H_{52}O_6$ 532.759
Constit. of *Raspaciona aculeata*. Oil. $[\alpha]_D$ -21.9 (c, 0.12 in $CHCl_3$).

4,21-Diketone, 15-Ac: ***4,21-Dioxoraspacionin***
[452934-97-3]
$C_{32}H_{50}O_6$ 530.743
Constit. of *Raspaciona aculeata*. Oil. $[\alpha]_D$ +8.4 (c, 0.12 in $CHCl_3$).

10,28-Dihydro, 10α-hydroxy, 4,21-diketone, 10-Ac: [158111-15-0]
$C_{32}H_{52}O_7$ 548.759
Constit. of *Raspaciona aculeata*. Amorph. powder. $[\alpha]_D^{25}$ -5.9 (c, 0.28 in $CHCl_3$).

10,28-Dihydro, 10β-hydroxy, 10,15-di-Ac: [158042-11-6]
$C_{34}H_{58}O_8$ 594.827
Constit. of *Raspaciona aculeata*. Amorph. powder. $[\alpha]_D^{25}$ -27.7 (c, 0.26 in $CHCl_3$).

10,28-Dihydro, 10β-hydroxy, 4,10,15-tri-Ac: [452935-02-3]
$C_{36}H_{60}O_9$ 636.865
Constit. of *Raspaciona aculeata*. Oil. $[\alpha]_D$ -15.88 (c, 0.12 in $CHCl_3$).

10,28-Dihydro, 10β-hydroxy, 4,10,21-tri-Ac: [158042-15-0]
$C_{36}H_{60}O_9$ 636.865
Constit. of *Raspaciona aculeata*. Amorph. powder. $[\alpha]_D^{25}$ -35.1 (c, 0.05 in $CHCl_3$).

10,28-Dihydro, 10β-hydroxy, 10,15,21-tri-Ac: [452935-01-2]
$C_{36}H_{60}O_9$ 636.865
Constit. of *Raspaciona aculeata*. Oil. $[\alpha]_D$ -10.6 (c, 0.12 in $CHCl_3$).

10,28-Dihydro, 10β-hydroxy, 4,10,15,21-tetra-Ac: [452935-00-1]
$C_{38}H_{62}O_{10}$ 678.902
Constit. of *Raspaciona aculeata*. Oil. $[\alpha]_D$ -19.2 (c, 0.12 in $CHCl_3$).

10,28-Dihydro, 10β-hydroxy, 4-ketone, 10-Ac: [158042-13-8]
$C_{32}H_{54}O_7$ 550.774
Constit. of *Raspaciona aculeata*. Amorph. powder. $[\alpha]_D^{25}$ -9.5 (c, 0.36 in $CHCl_3$).

10,28-Dihydro, 10β-hydroxy, 4-ketone, 10,15-di-Ac: [158042-12-7]
$C_{34}H_{56}O_8$ 592.812
Constit. of *Raspaciona aculeata*. Amorph. powder. $[\alpha]_D^{25}$ -38.5 (c, 0.37 in $CHCl_3$).

10,28-Dihydro, 10β-hydroxy, 4-ketone, 10,21-di-Ac: [158042-14-9]
$C_{34}H_{56}O_8$ 592.812
Constit. of *Raspaciona aculeata*. Amorph. powder. $[\alpha]_D^{25}$ -18.2 (c, 0.50 in $CHCl_3$).

10,28-Dihydro, 10β-hydroxy, 21-ketone, 4,10,15-tri-Ac: [452934-99-5]
$C_{36}H_{58}O_9$ 634.849
Constit. of *Raspaciona aculeata*. Oil. $[\alpha]_D$ -4.4 (c, 0.12 in $CHCl_3$).

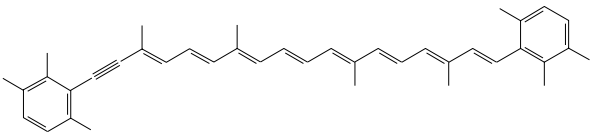
10,28-Dihydro, 10β-hydroxy, 4,21-diketone, 10-Ac: [158042-16-1]
$C_{32}H_{52}O_7$ 548.759
Constit. of *Raspaciona aculeata*. Amorph. powder. $[\alpha]_D^{25}$ -36.1 (c, 1 in $CHCl_3$).

10,28-Dihydro, 10β-hydroxy, 4,21-diketone, 10,15-di-Ac: [452934-98-4]
$C_{34}H_{54}O_8$ 590.796
Constit. of *Raspaciona aculeata*. Oil. $[\alpha]_D$ +3.6 (c, 0.12 in $CHCl_3$).

Cimino, G. *et al., J. Nat. Prod.*, 1993, **56**, 1622-1626; 1994, **57**, 784-790 (*isol, pmr, cmr, abs config, cryst struct*)
Ciavatta, M.L. *et al., Tetrahedron*, 2002, **58**, 4943-4948 (*isol, pmr, cmr*)

7,8-Didehydro-ϕ,ϕ-carotene D-376

7,8-Didehydroisorenieratene
[43161-29-1]

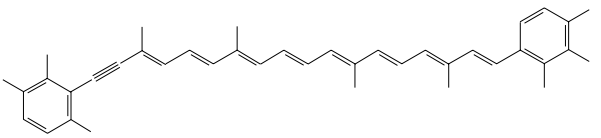


$C_{40}H_{46}$ 526.803
Constit. of *Reniera japonica*. Red needles (CH_2Cl_2/MeOH).
Mp 196°. λ_{max} 431; 456; 485 (hexane).

Hamasaki, T. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 1884 (*occur, uv, ir, pmr, ms*)
Ike, T. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 350 (*synth*)

7,8-Didehydro-ϕ,χ-carotene D-377

7,8-Didehydrorenieratene
[43161-28-0]

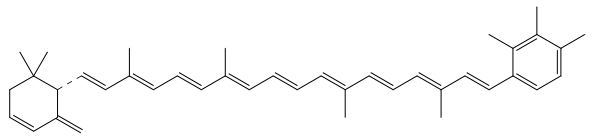


$C_{40}H_{46}$ 526.803
Constit. of *Reniera japonica*. Purplish-red needles (CH_2Cl_2/MeOH).
Mp 205-206°. λ_{max} 437; 485; 496 (hexane).

Hamasaki, T. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 1884 (*occur, uv, ir, pmr, ms*)
Ike, T. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 350 (*synth*)

3,4-Didehydro-γ,χ-carotene D-378

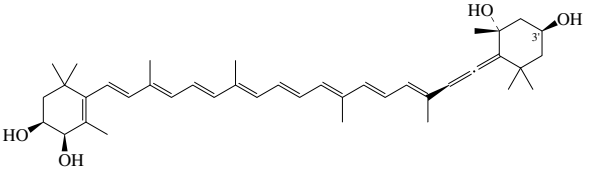
3,18-Didehydro-ϵ,χ-carotene



$C_{40}H_{50}$ 530.835

(6*S*)-*form* [115419-65-3]
Constit. of *Microciona prolifera*.
Sliwka, H.-R. *et al., Acta Chem. Scand., Ser. B*, 1987, **41**, 245-252 (*isol, pmr*)

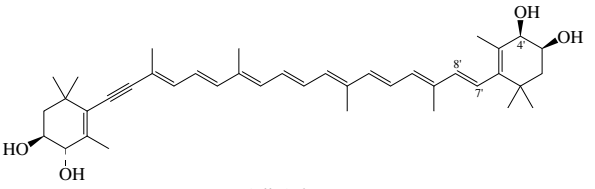
6′,7′-Didehydro-β,β-carotene-3,3′,4,5′-tetrol D-379



$C_{40}H_{56}O_4$ 600.88

(3*S*,3′*S*,4*R*,5′*R*,6′*R*)-*form*
Corbiculaxanthin
[866025-61-8]
Constit. of the corbicula clam *Corbicula japonica* (Shijimi) from brackish water. λ_{max} 220; 235; 280; 330; 350; 420; 443; 472 (Et_2O).
3′-Ac: [865866-06-4]
$C_{42}H_{58}O_5$ 642.917
Constit. of the corbicula clam, *Corbicula japonica* (Shijimi).
λ_{max} 220; 235; 280; 330; 350; 420; 443; 472 (Et_2O).
Maoka, T. *et al., J. Nat. Prod.*, 2005, **68**, 1341-1344 (*Corbiculaxanthin, 3′-Ac*)

7,8-Didehydro-β,β-carotene-3,3′,4,4′-tetrol D-380



(*all-S*)-*form*

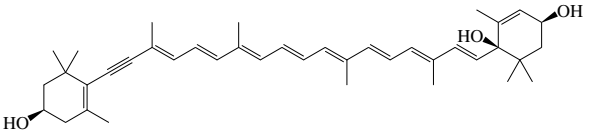
$C_{40}H_{54}O_4$ 598.864

(3*S*,3′*S*,4*R*,4′*R*)-*form*
4′-Ketone: 7′,8′-Didehydro-3,3′,4′-trihydroxy-β,β-caroten-4-one. ***4′R-Hydroxy-4-ketodiatoxanthin***
[253264-75-4]
$C_{40}H_{52}O_4$ 596.848
Constit. of the goldfish *Carassius auratus*.
7′,8′-Didehydro, 4-ketone: 7,7′,8,8′-Tetradehydro-3,3′,4′-trihydroxy-β,β-caroten-4-one. ***4′R-Hydroxy-4-ketoalloxanthin***
[253264-74-3]
$C_{40}H_{50}O_4$ 594.833
Constit. of *Carassius auratus*.

(3*S*,3′*S*,4*S*,4′*S*)-*form* [124508-52-7]
Constit. of *Asterina amurensis* and *Asterina pectinifera*.
4′-Ketone: ***4′S-Hydroxy-4-ketodiatoxanthin***
[124417-90-9]
$C_{40}H_{52}O_4$ 596.848
Constit. of *Asterina amurensis* and *Asterina pectinifera*.
7′,8′-Didehydro: 7,7′,8,8′-Tetradehydro-β,β-carotene-3,3′,4,4′-tetrol. ***4′S,4′S-Dihydroxyalloxanthin***
[124508-53-8]
$C_{40}H_{52}O_4$ 596.848
Constit. of *Asterina amurensis* and *Asterina pectinifera*.
7′,8′-Didehydro, 4-ketone: ***4′S-Hydroxy-4-ketoalloxanthin***
[124417-91-0]
$C_{40}H_{50}O_4$ 594.833
Constit. of *Asterina amurensis* and *Asterina pectinifera*.
Maoka, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **93**, 829-834 (*Asterina constits*)
Ohkubo, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1999, **124**, 333-340 (*Carassius constits*)

7,8-Didehydro-β,ϵ-carotene-3,3′,6′-triol D-381

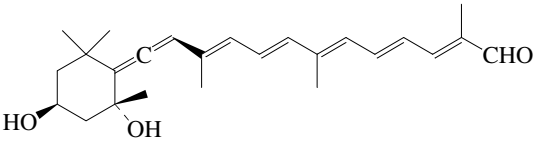
7,8-Didehydrodeepoxysalmoxanthin



$C_{40}H_{54}O_3$ 582.865

(3*R*,3′*S*,6′*R*)-*form*
Gobiusxanthin
[280774-92-7]
Constit. of the common freshwater goby (*Rhinogobius brunneus*) and a minor constit. of an *Oncorhynchus* sp. λ_{max} 420; 445; 475 (Et_2O).
Tsushima, M. *et al., J. Nat. Prod.*, 2000, **63**, 960-964 (*isol, pmr, cmr, cd, abs config*)
Matsuno, T. *et al., J. Nat. Prod.*, 2001, **64**, 507-510 (*cd*)

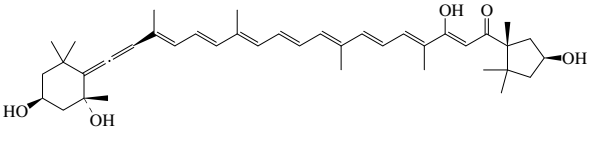
6,7-Didehydro-5,6-dihydro-3,5-dihydroxy-12′-apo-β,ψ-carotenal D-382



$C_{25}H_{34}O_3$ 382.542

(3*S*,5*R*,6*R*)-*form*
3-Ac: ***Apo-12-fucoxanthinal***
[22488-58-0]
$C_{27}H_{36}O_4$ 424.579
Constit. of *Phaeodactylum tricornutum*. λ_{max} 407 (log ϵ 4.2) (MeOH).
Shaw, B.A. *et al., Mar. Biol. (Berlin)*, 1995, **124**, 467-472 (*isol, pmr*)

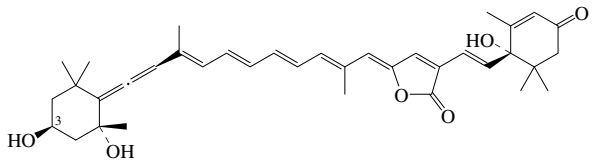
6,7-Didehydro-5,6-dihydro-3,3′,5,8′-tetrahydroxy-β,κ-caroten-6′-one D-383



$C_{40}H_{56}O_5$ 616.879

(3*S*,3′*S*,5*R*,5′*R*,6*R*)-*form* [256505-54-1]
Constit. of the oyster *Crassostrea gigas*.
Red amorph. solid. λ_{max} 468 (Et_2O).
Maoka, T. *et al., J. Nat. Prod.*, 2001, **64**, 578-581 (*isol, pmr*)

6,7-Didehydro-5,6-dihydro-3,5,6′-trihydroxy-13,14,20-trinor-3′-oxo-β,ϵ-caroten-19′,11′-olide **D-384**

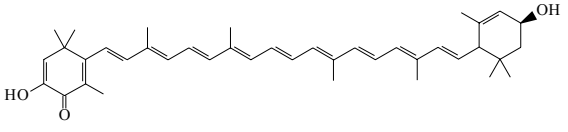


$C_{37}H_{46}O_6$ 586.767

(3S,5R,6R,6′S)-form

3-Ac: [256505-50-7]
$C_{39}H_{48}O_7$ 628.804
Constit. of the oyster *Crassostrea gigas.* Red amorph. solid. λ_{max} 457 (Et_2O).
Maoka, T. *et al., J. Nat. Prod.*, 2001, **64**, 578-581 (*isol, pmr, cmr*)

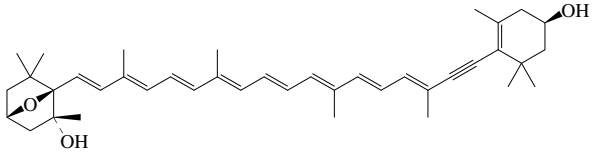
2,3-Didehydro-3,3′-dihydroxy-β,ϵ-caroten-4-one **D-385**
2,3-Didehydrofritschiellaxanthin. *α-Doradecin*
[68437-16-1]



$C_{40}H_{52}O_3$ 580.849
Constit. of Akategani estuarine crab *Sesarma haematocheir*, green algae and goldfish. λ_{max} 454; 470 (no solvent reported).

Katayama, T. *et al., Int. J. Biochem.*, 1970, **1**, 438 (*isol*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1978, **61**, 1962 (*synth*)
Matsuno, T. *et al., Nippon Suisan Gakkaishi*, 1982, **48**, 653 (*occur*)
Burczyk, J. *et al., Phytochemistry*, 1986, **26**, 121 (*occur, ir, ms, pmr*)

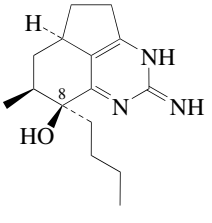
7′,8′-Didehydro-3,6-epoxy-5,6-dihydro-β,β-carotene-3′,5-diol **D-386**



$C_{40}H_{54}O_3$ 582.865

(3S,3′R,5R,6R)-form [256505-52-9]
Constit. of the oyster *Crassostrea gigas.*
Orange amorph. solid. λ_{max} 446; 476 (Et_2O).
Maoka, T. *et al., J. Nat. Prod.*, 2001, **64**, 578-581 (*isol, pmr*)

1,3*a*-Didehydro-8-hydroxyptilocaulin **D-387**
[191353-14-7]

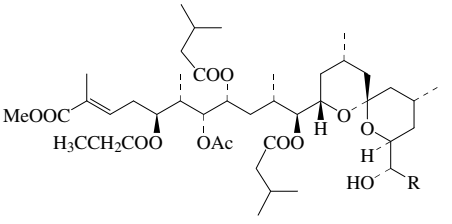


$C_{15}H_{23}N_3O$ 261.366
The name is not an accurate representation of the struct (cf. Ptilocaulin, P-696). Alkaloid from the sponges *Batzella* sp. and *Monanchora unguifera*. Antiplasmodial agent. Oil. $[\alpha]_D$ +39.3 (c, 0.28 in MeOH). λ_{max} 239; 246; 309 (MeOH).

8-Epimer:
$C_{15}H_{23}N_3O$ 261.366
Alkaloid from *Monanchora unguifera*. Antiplasmodial agent. Isol. as a mixt. with its 8-epimer.

Patil, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 704-707 (*isol, pmr, cmr*)
Hua, H.-M. *et al., Bioorg. Med. Chem.*, 2004, **12**, 6461-6464 (*isol, pmr, cmr*)

Didemnaketal A **D-388**
[135257-49-7]



Absolute Configuration

R = -$COCH_3$

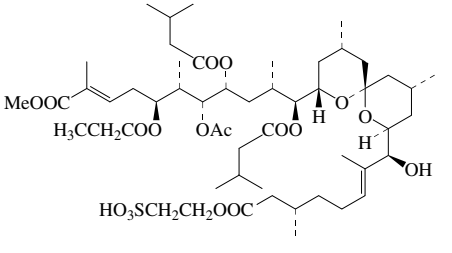
$C_{44}H_{72}O_{14}$ 825.044
Shown to be an artifact of long storage of Didemnaketal C, D-390. Isol. from the ascidian *Didemnum* sp. Poss. artifact. HIV-1 protease inhibitor. Oil. $[\alpha]_D$ -11 (c, 0.8 in $CHCl_3$). Log P 7.11 (uncertain value) (calc). λ_{max} 214 (ϵ 10000) (EtOH) (Derep).

Potts, B.C.M. *et al., J.A.C.S.*, 1991, **113**, 6321-6322 (*isol, struct*)
Pika, J. *et al., Nat. Prod. Lett.*, 1995, **7**, 291-296
Salomon, C.E. *et al., Org. Lett.*, 2002, **4**, 1699-1702 (*abs config*)

Didemnaketal B **D-389**
[135257-48-6]
As Didemnaketal A, D-388 with
R = –$C(CH_3)$=$CHCH_2CH_2CH(CH_3)CH_2COOMe$ (*E,S-*)
$C_{52}H_{86}O_{15}$ 951.242
Isol. from the ascidian *Didemnum* sp. HIV-1 protease inhibitor. Oil. Log P 9.5 (uncertain value) (calc). λ_{max} 215 (ϵ 10000) (EtOH) (Derep).

Potts, B.C.M. *et al., J.A.C.S.*, 1991, **113**, 6321-6322 (*isol, struct*)
Pika, J. *et al., Nat. Prod. Lett.*, 1995, **7**, 291-296 (*synth*)
Salomon, C.E. *et al., Org. Lett.*, 2002, **4**, 1699-1702 (*abs config*)

Didemnaketal C **D-390**
[181712-48-1]



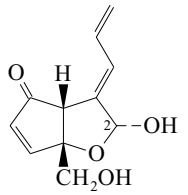
Absolute Configuration

$C_{53}H_{88}O_{18}S$ 1045.333
Isol. from the ascidian *Didemnum* sp. Oil. $[\alpha]_D$ +48 (c, 0.067 in CH_2Cl_2). Isol. as Na salt, to which CAS no. refers. λ_{max} 213 (MeCN).

Pika, J. *et al., Nat. Prod. Lett.*, 1995, **7**, 291-296 (*isol, struct, pmr, cmr*)
Salomon, C.E. *et al., Org. Lett.*, 2002, **4**, 1699-1702 (*abs config*)

Didemnenone A D-391

2,3,3a,6a-Tetrahydro-2-hydroxy-6a-(hydroxymethyl)-3-(2-propenylidene)-4H-cyclopenta[b]furan-4-one, 9CI
[110935-52-9]



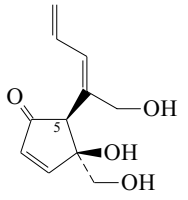
$C_{11}H_{12}O_4$ 208.213
Isol. from the didemnid tunicate *Trididemnum cyanophorum*. Cytotoxic. Could not be separated from its stereoisomer Didemnenone B. λ_{max} 243 (MeCN/NaOH) (Derep). λ_{max} 238 (ε 13000) (MeCN) (Derep). λ_{max} 238 (ε 19000) (MeCN) (Berdy). λ_{max} 243 (MeCN/MeOH) (Berdy).

2-Epimer: ***Didemnenone B***
[111056-70-3]
$C_{11}H_{12}O_4$ 208.213
From *Trididemnum cyanophorum*. Cytotoxic. λ_{max} 243 (MeCN/NaOH) (Derep). λ_{max} 238 (ε 13000) (MeCN) (Derep).

Lindquist, N. *et al., J.A.C.S.*, 1988, **110**, 1308 (*isol, struct*)
Forsyth, C.J. *et al., J.A.C.S.*, 1988, **110**, 5911-5912 (*synth, abs config*)
Sugahara, T. *et al., J.C.S. Perkin 1*, 1990, 1824 (*synth*)
Goeres, M. *et al., J.C.S. Perkin 1*, 1994, 3525 (*synth*)

Didemnenone C D-392

4-Hydroxy-4-(hydroxymethyl)-5-[1-(hydroxymethyl)-1,3-butadienyl]-2-cyclopenten-1-one, 9CI
[110935-53-0]



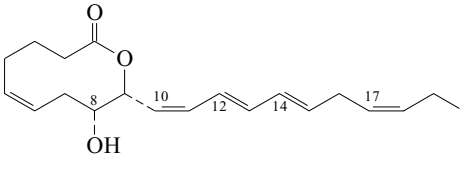
$C_{11}H_{14}O_4$ 210.229
Isol. from the didemnid tunicate *Didemnum voeltzkowi*. Cytotoxic agent. $[\alpha]_D$ -25.3 (c, 0.08 in MeOH). λ_{max} 231 (ε 16000) (MeOH) (Derep).

5-Epimer: ***Didemnenone D***
[111056-71-4]
$C_{11}H_{14}O_4$ 210.229
From *Didemnum voeltzkowi*. Cytotoxic agent. $[\alpha]_D$ -12.6 (c, 0.15 in MeOH). λ_{max} 231 (ε 16000) (MeOH) (Derep).

Lindquist, N. *et al., J.A.C.S.*, 1988, **110**, 1308 (*isol, struct*)
Goeres, M. *et al., J.C.S. Perkin 1*, 1994, 3525 (*synth*)
Sugahara, T. *et al., Chem. Pharm. Bull.*, 1995, **43**, 147 (*synth*)

Didemnilactone D-393

[137855-87-9]



$C_{20}H_{28}O_3$ 316.439
Constit. of the tunicate *Didemnum moseleyi*. Binds to Leukotriene B_4 receptor. Oil. $[\alpha]_D^{22}$ -190 (c, 0.18 in MeOH). λ_{max} 261 (ε 24900); 271 (ε 30500); 279 (ε 25400) (MeOH) (Berdy).

(14Z)-Isomer: ***Didemnilactone B***
[157810-80-5]
$C_{20}H_{28}O_3$ 316.439
From *Didemnum moseleyi*. Binds to Leukotriene B receptor. Lipoxygenase inhibitor. Oil. $[\alpha]_D^{25}$ -378 (c, 0.005 in MeOH). λ_{max} 267 (ε 36400); 274 (ε 44900); 284 (ε 36100) (MeOH) (Berdy).

17,18-Dihydro: ***Neodidemnilactone***
[137855-88-0]
$C_{20}H_{30}O_3$ 318.455
From *Didemnum moseleyi*. Binds to Leukotriene B_4 receptor. Lipoxygenase inhibitor. Oil. $[\alpha]_D^{22}$ -200 (c, 0.17 in MeOH). λ_{max} 261 (ε 22900); 271 (ε 29100); 279 (ε 24000) (MeOH) (Berdy).

(10E,14Z)-Isomer, 17,18-dihydro: ***Ascidiatrienolide C***
[122799-23-9]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Didemnum candidum*.
$[\alpha]_D$ -10.6 (c, 11.3 in $CHCl_3$). λ_{max} 262 (ε 28700); 271 (ε 35100); 281 (ε 27400) (MeOH) (Derep).

(10E,12Z,14Z)-Isomer, 8-epimer, 17,18-dihydro: ***Ascidiatrienolide B***
[122799-22-8]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Didemnum candidum*.
$[\alpha]_D$ -4.1 (c, 3.4 in $CHCl_3$). λ_{max} 262 (ε 28700); 271 (ε 35100); 281 (ε 27400) (MeOH) (Derep).

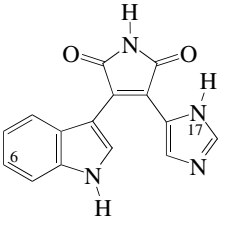
(10E,12Z,14Z)-Isomer, 17,18-dihydro: ***Ascidiatrienolide A***
[122752-22-1]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Didemnum candidum*. Phospholipase A_2 inhibitor. $[\alpha]_D$ -14.8 (c, 4.5 in $CHCl_3$). Struct. revised in 1993. λ_{max} 262 (ε 28700); 271 (ε 35100); 281 (ε 27400) (MeOH) (Derep).

[157543-71-0, 157543-73-2]

Lindquist, N. *et al., Tet. Lett.*, 1989, **30**, 2735 (*Ascidiatrienolides*)
Congreve, M.S. *et al., J.A.C.S.*, 1993, **115**, 5815 (*Ascidiatrienolide A*)
Niwa, H. *et al., Tetrahedron*, 1994, **50**, 7385 (*isol, pmr, cmr*)
Fürstner, A. *et al., Adv. Synth. Catal.*, 2002, **344**, 657-665 (*Ascidiatrienolide A, synth*)

Didemnimide A D-394

3-(1H-Imidazol-4-yl)-4-(1H-indol-3-yl)-1H-pyrrole-2,5-dione, 9CI
[186143-93-1]



$C_{15}H_{10}N_4O_2$ 278.27
Alkaloid from the Caribbean mangrove ascidian *Didemnum conchyliatum*. Potent fish feeding deterrent. Irregular orange needles (MeCN aq.).
Mp 234-235°. λ_{max} 430 (ε 3000) (MeCN).

N^{15}-*Me:* ***Didemnimide E***
[219828-98-5]
$C_{16}H_{12}N_4O_2$ 292.296
From *Didemnum granulatum*. Amorph. orange solid.

N^{17}-*Me:* ***Didemnimide C***
[186144-21-8]
$C_{16}H_{12}N_4O_2$ 292.296
From *Didemnum conchyliatum*. Potent fish feeding deterrent. Dark orange needles (MeCN aq.).
Mp >300°. λ_{max} 420 (ε 5700) (MeCN).

6-Bromo: ***Didemnimide B***
[186144-09-2]
$C_{15}H_9BrN_4O_2$ 357.166

From *Didemnum conchyliatum*. Potent fish feeding deterrent. Fine light orange needles (MeCN aq.).
Mp >300°. λ_{max} 420 (ϵ 4300) (MeCN).

6-Bromo, N^{17}-Me: ***Didemnimide D***
[186144-28-5]
$C_{16}H_{11}BrN_4O_2$ 371.193
From *Didemnum conchyliatum*. Potent fish feeding deterrent. Small dark orange needles (MeCN aq.). Mp >250° dec. More active than other Didemnimides. λ_{max} 416 (ϵ 4500) (MeCN).

Vervoort, H.C. *et al., J.O.C.*, 1997, **62**, 1486-1490 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Berlinck, R.G.S *et al., J.O.C.*, 1998, **63**, 9850-9856 (*Didemnimide E*)
Terpin, A. *et al., Tetrahedron*, 1998, **54**, 1745-1752 (*Didemnimide C, synth*)
Piers, E. *et al., J.O.C.*, 2000, **65**, 530-535 (*Didemnimide C, synth*)

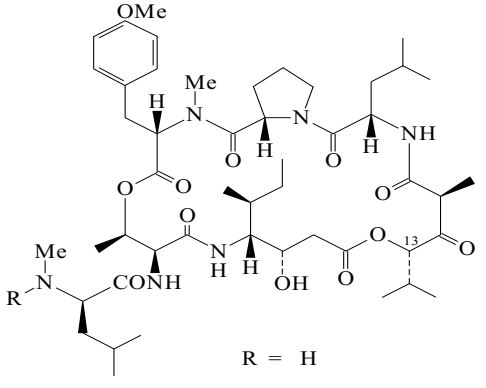
Didemnin X D-395

[133761-90-7]
As Didemnin D, D-401 with
R = Gln-Gln-Gln-$COCH_2CH(OH)(CH_2)_6CH_3$(*R*-)
$C_{82}H_{131}N_{13}O_{23}$ 1667.01
Depsipeptide antibiotic. Isol. from *Tridemnum solidum*. Cytotoxic agent. Amorph. powder.
Mp 156-158°. $[\alpha]_D^{20}$ -88.6 (c, 6 in $CHCl_3$). λ_{max} 204 (ϵ 52500); 224 (sh) (ϵ 32360); 277 (ϵ 1580) (MeOH).

Sakai, R. *et al., J.A.C.S.*, 1995, **117**, 3734-3748; 8885 (*isol, uv, ir, pmr, cmr*)

Didemnin A D-396

[77327-04-9]



$C_{49}H_{78}N_6O_{12}$ 943.188
Depsipeptide antibiotic. Isol. from *Tridemnum* sp. Antiviral and antitumour agent. Sol. $CHCl_3$, MeOH; fairly sol. toluene; poorly sol. hexane, H_2O. $[\alpha]_D$ -149.1 ($CHCl_3$). Species also forms Nordidemnin A, Nordidemnin B and Nordidemnin C (lower homologues). λ_{max} 225 (ϵ 6610); 277 (ϵ 1290); 283 (ϵ 1900) (MeOH) (Derep). λ_{max} 275 (MeOH) (Berdy).

13-Epimer: ***Epididemnin A_1***
[161754-25-2]
$C_{49}H_{78}N_6O_{12}$ 943.188
Isol. from *Tridemnum solidum*. Weak cytotoxic agent. Powder.
Mp 130-132°. $[\alpha]_D^{23}$ -100 (c, 0.1 in $CHCl_3$). λ_{max} 206 (ϵ 49300); 229 (ϵ 31000) (MeOH) (Berdy).

Rinehart, K.L. *et al., J.A.C.S.*, 1981, **103**, 1857-1859 (*struct*)
Rinehart, K.L. *et al., Science (Washington, D.C.)*, 1981, **212**, 933-935 (*isol*)
Crampton, S.L. *et al., Cancer Res.*, 1984, **44**, 1796-1801 (*props*)
Rinehart, K.L. *et al., J.A.C.S.*, 1987, **109**, 6846-6848 (*synth*)
Kessler, H. *et al., Helv. Chim. Acta*, 1989, **72**, 530-555 (*pmr, cryst struct*)
Hamada, Y. *et al., J.A.C.S.*, 1989, **111**, 669-673 (*synth*)
Schmidt, U. *et al., Synthesis*, 1991, 294-300 (*synth*)
Li, W.R. *et al., Stud. Nat. Prod. Chem.*, 1992, **10**, 241 (*rev*)
Sakai, R. *et al., J.A.C.S.*, 1995, **117**, 3734-3748 (*isol, pmr, cmr*)
Jou, G. *et al., J.O.C.*, 1997, **62**, 354-366 (*synth*)
Vera, M.D. *et al., Med. Res. Rev.*, 2002, **22**, 102-145 (*rev*)

[*Hap*^{2}]Didemnin B D-397

[244170-11-4]
As Didemnin B, D-399 with
R = H
$C_{54}H_{83}N_7O_{15}$ 1070.288
Prod. by *Tridemnum cyanophorum*. Cytotoxic agent. Amorph-solid. λ_{max} 228 (ϵ 5250); 278 (ϵ 1888); 284 (ϵ 1888) (MeOH).

Banaigs, B. *et al., Tetrahedron*, 1999, **55**, 9559-9574

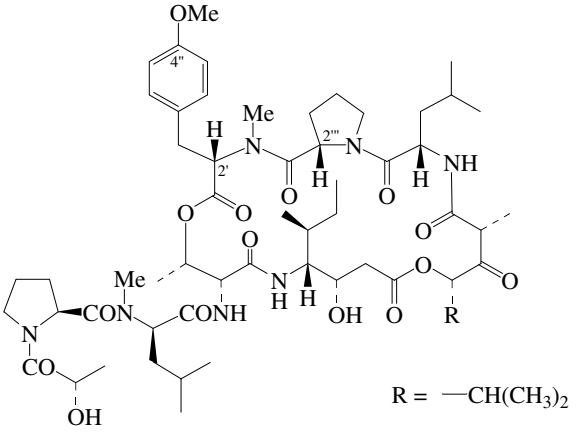
[*Hysp*^{2}]Didemnin B D-398

[244170-12-5]
As Didemnin B, D-399 with
R = $CH(CH_3)CH_2CH_3$
$C_{58}H_{91}N_7O_{15}$ 1126.395
Isol. from *Tridemnum cyanophorum*. Cytotoxic agent. Amorph. solid. λ_{max} 227 (ϵ 13800); 275 (ϵ 7010) (MeOH).

Banaigs, B. *et al., Tetrahedron*, 1999, **55**, 9559-9574

Didemnin B D-399

NSC 325319
[77327-05-0]



$C_{57}H_{89}N_7O_{15}$ 1112.368
Depsipeptide antibiotic. Isol. from *Tridemnum solidum* and *Tridemnum cyanophorum* (Didemnidae). Antiviral and antitumour agent. Sol. MeOH, $CHCl_3$; fairly sol. toluene; poorly sol. hexane, H_2O. $[\alpha]_D$ -91.9 ($CHCl_3$). Nordidemnin B (lower homologue) has also been isol. λ_{max} 225 (ϵ 6600); 277 (ϵ 2190); 283 (ϵ 1900) (MeOH).

▶ YP2834100

2‴-Epimer: ***[D-Pro^4]Didemnin B***
[173241-15-1]
$C_{57}H_{89}N_7O_{15}$ 1112.368
Isol. from *Tridemnum cyanophorum*. Cytotoxic agent. Amorph. solid. Sol. MeOH, Et_2O, $CHCl_3$, EtOAc; poorly sol. H_2O. λ_{max} 226 (ϵ 10900); 284 (ϵ 3600) (MeOH) (Berdy).

$N^{2'}$,$O^{4''}$-Di-de-Me: ***Didemnin N.*** *[Tyr^5]Didemnin B*
[155608-52-9]
$C_{55}H_{85}N_7O_{15}$ 1084.314
Isol. from *Tridemnum cyanophorum* and *Tridemnum solidum*. Cytotoxic agent. Amorph. solid.
Mp 150-152°. $[\alpha]_D^{24}$ -49 (c, 1.6 in $CHCl_3$).

Rinehart, K.L. *et al., J.A.C.S.*, 1981, **103**, 1857-1859 (*struct*)
Rinehart, K.L. *et al., Science (Washington, D.C.)*, 1981, **212**, 933-935 (*isol*)
Crampton, S.L. *et al., Cancer Res.*, 1984, **44**, 1796-1801 (*props*)
Rinehart, K.L. *et al., J.A.C.S.*, 1987, **109**, 6846-6848 (*synth*)
Hamada, Y. *et al., J.A.C.S.*, 1989, **111**, 669-673 (*synth*)
Banaigs, B. *et al., Tetrahedron*, 1989, **45**, 181-190; 1999, **55**, 9559-9574 (*struct, isol*)
Schmidt, U. *et al., Synthesis*, 1991, 294-300 (*synth*)
Li, W.R. *et al., Stud. Nat. Prod. Chem.*, 1992, **10**, 241 (*rev*)
Sakai, R. *et al., J.A.C.S.*, 1995, **117**, 3734-3748 (*Didemnin N*)

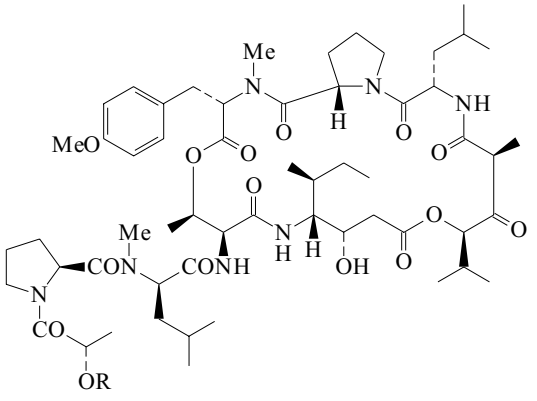
Abou-Mansour, E. *et al., Tetrahedron*, 1995, **51**, 12591-12600 (*D-ProDidemnin B, Didemnin N*)
Vera, M.D. *et al., Med. Res. Rev.*, 2002, **22**, 102-145 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, DHA300

Didemnin C D-400

[77327-06-1]
As Didemnin A, D-396 with
R = $H_3CCH(OH)CO$–
$C_{52}H_{82}N_6O_{14}$ 1015.252
Depsipeptide antibiotic. Isol. from *Tridemnum* spp. Antiviral and antitumour agent. Sol. $CHCl_3$, MeOH; fairly sol. toluene; poorly sol. H_2O, hexane. $[\alpha]_D$ -118.9 ($CHCl_3$). Species also forms Nordidemnin C (lower homologue). λ_{max} 225 (ϵ 6610); 277 (ϵ 1290); 283 (ϵ 1900) (MeOH).
Rinehart, K.L. *et al., J.A.C.S.*, 1981, **103**, 1857-1859; 1987, **109**, 6846-6848 (*struct, synth*)
Rinehart, K.L. *et al., Science (Washington, D.C.)*, 1981, **212**, 933-935 (*isol*)
Schmidt, U. *et al., Synthesis*, 1991, 294-300 (*synth*)
Li, W.R. *et al., Stud. Nat. Prod. Chem.*, 1992, **10**, 241 (*rev*)

Didemnin D D-401

[97230-30-3]



R = Gln–Gln–Gln–5–oxoPro–H

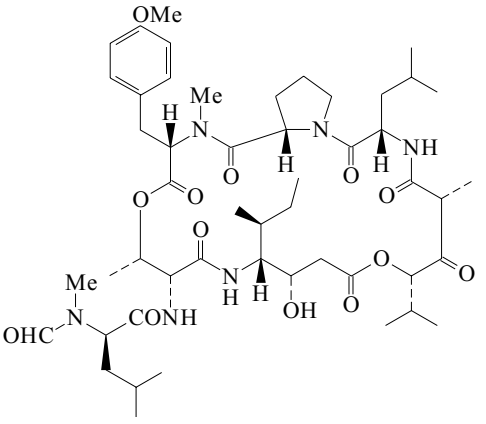
$C_{77}H_{118}N_{14}O_{23}$ 1607.859
Depsipeptide antibiotic. Isol. from *Tridemnum solidum*. Cytotoxic agent. Sol. MeOH, dioxan, $CHCl_3$; fairly sol. toluene; poorly sol. H_2O. λ_{max} 225 (ϵ 6600); 277 (ϵ 2200) (MeOH) (Derep).
Sakai, R. *et al., J.A.C.S.*, 1995, **117**, 3734-3748; 8885 (*isol, struct*)

Didemnin E D-402

[97230-31-4]
As Didemnin D, D-401 with
R = Gln-Gln-5-oxoPro-H
$C_{72}H_{110}N_{12}O_{21}$ 1479.729
Depsipeptide antibiotic. Isol. from *Tridemnum solidum*. Sol. MeOH, $CHCl_3$, dioxan; fairly sol. toluene; poorly sol. H_2O. λ_{max} 225 (ϵ 6600); 277 (ϵ 2200) (MeOH) (Derep).
Sakai, R. *et al., J.A.C.S.*, 1995, **117**, 3734-3748; 8885 (*isol, struct*)

Didemnin G D-403

[311345-48-9]



$C_{50}H_{78}N_6O_{13}$ 971.199
Depsipeptide antibiotic. Isol. from *Tridemnum solidum*.
Sakai, R. *et al., J.A.C.S.*, 1995, **117**, 3734-3748; 8885 (*isol, struct*)

Didemnin M D-404

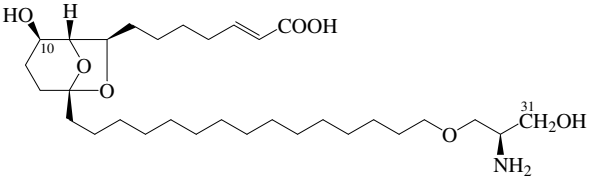
Didemnin H
[155569-80-5]
As Didemnin D, D-401 with
R = Gln-5-oxoPro-H
$C_{67}H_{102}N_{10}O_{19}$ 1351.598
Depsipeptide antibiotic. Two groups of researchers have assigned different code letters. Constit. of *Trididemnum cyanophorum*. Immunosuppressant and cytotoxic agent. Powder.
Mp 158-160°. $[\alpha]_D^{25}$ -68.4 (c, 1.1 in $CHCl_3$). λ_{max} 225 (ϵ 6600); 277 (ϵ 2200) (MeOH) (Derep). λ_{max} 204 (ϵ 57540); 224 (ϵ 24000) (MeOH).
Boulanger, A. *et al., Tet. Lett.*, 1994, **35**, 4345-4348 (*pmr, cmr*)
Sakai, R. *et al., J.A.C.S.*, 1995, **117**, 3734-3748; 8885 (*isol, uv, ir, pmr, cmr*)

Didemnin Y D-405

[133761-91-8]
As Didemnin D, D-401 with
R = Gln-Gln-Gln-Gln-$COCH_2CH(OH)(CH_2)_6CH_3$(*R*-)
$C_{87}H_{139}N_{15}O_{25}$ 1795.141
Depsipeptide antibiotic. Isol. from *Trididemnum solidum*. Cytotoxic agent.
Mp 230-240° dec. $[\alpha]_D^{20}$ -65 (c, 1 in $CHCl_3$). λ_{max} 204 (ϵ 47860); 224 (sh) (ϵ 24000); 277 (ϵ 1580) (MeOH).
Sakai, R. *et al., J.A.C.S.*, 1995, **117**, 3734-3748; 8885 (*isol, uv, ir, pmr, cmr*)

Didemniserinolipid C D-406

[242147-19-9]



Absolute Configuration

$C_{31}H_{57}NO_7$ 555.794
The abs. config. was determined for Didemniserinolipid B. Isol. from the tunicate *Didemnum* sp. Amorph. solid. $[\alpha]_D^{24}$ +32.3 (c, 0.07 in MeOH).

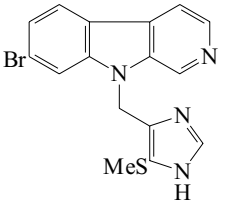
31-O-*Sulfate, Et ester:* ***Didemniserinolipid B***
[242147-18-8]
$C_{33}H_{61}NO_{10}S$ 663.912
Isol. from *Didemnum* sp. Amorph. solid (as Na salt). $[\alpha]_D^{24}$ +10.3 (c, 0.22 in $CHCl_3$) (Na salt). Struct. revised in 2002. Not prev. recognised as a sulfate. λ_{max} 206 (log ϵ 4.1) (MeOH) (Na salt).

O^{10}-*Ac:* ***Didemniserinolipid A***
[242147-17-7]
$C_{33}H_{59}NO_8$ 597.831
Isol. from *Didemnum* sp. Amorph. solid. $[\alpha]_D^{24}$ +12.5 (c, 0.08 in MeOH). λ_{max} 201 (log ϵ 4.39); 215 (log ϵ 3.96) (MeOH).

Gonzalez, N. *et al., J.O.C.*, 1999, **64**, 5705-5707 (*isol, struct*)
Kiyota, H. *et al., Org. Lett.*, 2002, **4**, 3223-3226 (*synth, abs config*)

Didemnoline A D-407

*7-Bromo-9-[[4-(methylthio)-1*H*-imidazol-3-yl]methyl]-9*H*-pyrido[3,4-*b*]indole, 9CI*
[168434-22-8]



$C_{16}H_{13}BrN_4S$ 373.275
Alkaloid from the marine ascidian *Didemnum* sp. Exhibits moderate cytotoxicity toward human epidermoid carcinoma (KB) cells. Also shows antimicrobial activity. λ_{max} 240 (ϵ 38700); 290 (ϵ 13500); 358 (ϵ 5000) (MeOH) (Berdy).

S-*Oxide:* ***Didemnoline C***
[168434-23-9]
$C_{16}H_{13}BrN_4OS$ 389.275
From *Didemnum* sp. Cytotoxic. Shows antimicrobial activity. $[\alpha]_D^{25}$ +97.2 (c, 0.1 in DMSO). Isol. as a *ca.* 10:1 insep. mixt. with Didemnoline D. λ_{max} 239 (ϵ 37200); 290 (ϵ 14000); 358 (ϵ 4000) (MeOH) (Berdy). λ_{max} 243; 277 (ϵ 34000); 288 (ϵ 2400); 342; 352 (ϵ 4000) (EtOH) (Berdy).

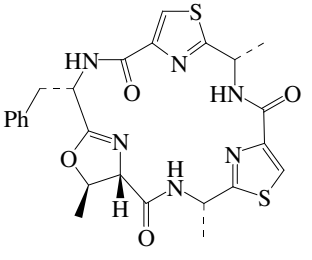
Debromo: ***Didemnoline B***
[168434-24-0]
$C_{16}H_{14}N_4S$ 294.379
From *Didemnum* sp. Moderately cytotoxic. λ_{max} 240 (ϵ 36800); 290 (ϵ 13500); 358 (ϵ 5000) (MeOH) (Berdy). λ_{max} 216 (ϵ 33000); 238 (ϵ 39800); 290 (ϵ 14100); 358 (ϵ 4900) (EtOH) (Berdy).

Debromo, S-*oxide:* ***Didemnoline D***
[168434-25-1]
$C_{16}H_{14}N_4OS$ 310.379
From *Didemnum* sp. Not obt. pure.

Schumacher, R.W. *et al., Tetrahedron*, 1995, **51**, 10125 (*isol, uv, ir, pmr, cmr, ms, struct*)
Schumacher, R.W. *et al., Tetrahedron*, 1999, **55**, 935-942 (*synth*)

Didmolamide A D-408

[528815-53-4]



Absolute Configuration

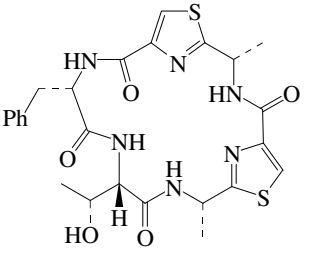
$C_{25}H_{26}N_6O_4S_2$ 538.65
Isol. from the ascidian *Didemnum molle*. Oil. $[\alpha]_D^{25}$ -35.7 (c, 0.6 in MeOH).

Stereoisomer (?): ***Banyascyclamide A***
[501903-99-7]
$C_{25}H_{26}N_6O_4S_2$ 538.65
Isol. from *Nostoc* sp. TAU strain IL-235. Amorph. solid. $[\alpha]_D^{25}$ -19.3 (c, 0.12 in MeOH). Stereochem. partly determined. May be identical with Didmolamide A. λ_{max} 218 (ϵ 17300); 238 (ϵ 17900) (MeOH).

Ploutno, A. *et al., Tetrahedron*, 2002, **58**, 9949-9957 (*Banyascyclamide A*)
Rudi, A. *et al., J. Nat. Prod.*, 2003, **66**, 575-577 (*Didmolamide A*)
You, S.-L. *et al., Tet. Lett.*, 2005, **46**, 2567-2570 (*synth*)

Didmolamide B D-409

[528815-55-6]



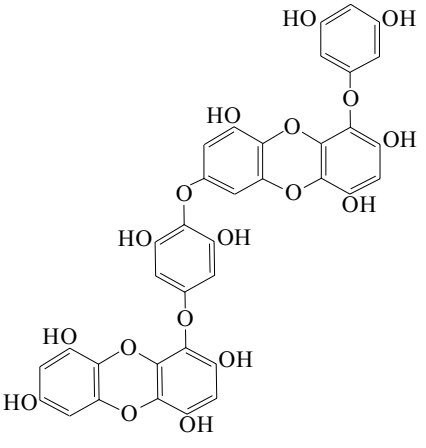
Absolute Configuration

$C_{25}H_{28}N_6O_5S_2$ 556.665
Isol. from the ascidian *Didemnum molle*. Oil. $[\alpha]_D^{25}$ -216 (c, 0.11 in MeOH).

Rudi, A. *et al., J. Nat. Prod.*, 2003, **66**, 575-577 (*isol, pmr, cmr, ms*)
You, S.-L. *et al., Tet. Lett.*, 2005, **46**, 2567-2570 (*synth*)

Dieckol D-410

*4‴-*O*-7-Bieckol*
[88095-77-6]

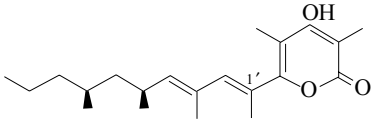


$C_{36}H_{22}O_{18}$ 742.559
Constit.of the brown algae *Ecklonia kurome* and *Eisenia bicyclis*. Inhibitor of α_2-Macroglobulin, glycation and α-amylase. Cryst. Mp 300°. λ_{max} 235 (ϵ 34000); 292 (ϵ 3500) (MeOH) (Berdy).

Fukuyama, Y. *et al., Chem. Lett.*, 1985, 739-742 (*isol*)
Glombitza, K.-W. *et al., Phytochemistry*, 1985, **24**, 543-551 (*isol, pmr, cmr*)
Kang, H.S. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1012-1014 (*isol, pmr, cmr*)
Okada, Y. *et al., J. Nat. Prod.*, 2004, **67**, 103-105 (*isol, pmr, cmr*)

Diemenensin A D-411

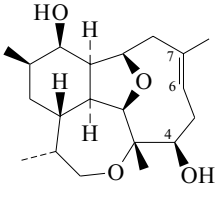
4-Hydroxy-3,5-dimethyl-6-(1,3,5,7-tetramethyl-1,3-decadienyl)-2H-pyran-2-one, 9CI
[87590-55-4]



$C_{21}H_{32}O_3$ 332.482
Prod. by *Siphonaria diemenensis*. Antimicrobial agent active against *Staphylococcus aureus* and *Bacillus subtilis*. Oil. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D$ +77.3 (c, 4.7 in MeOH). λ_{max} 246 (ϵ 8920); 305 (ϵ 13500) (pentane) (Derep). λ_{max} 247 (ϵ 8920); 307 (ϵ 13500) (pentane) (Berdy).

1′Z-Isomer: ***Diemenensin B***
[87590-56-5]
$C_{21}H_{32}O_3$ 332.482
Prod. by *Siphonaria diemenensis*. Antimicrobial agent. Oil. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D$ +32.4 (c, 1.15 in MeOH). Isom. to Diemenensin A on standing. λ_{max} 246 (ϵ 8920); 305 (ϵ 13500) (pentane) (Derep). λ_{max} 224 (ϵ 8710); 301 (ϵ 6470) (pentane) (Berdy).
Hochlowski, J.E. *et al., Tet. Lett.*, 1983, **24**, 1917-1920 (*isol, pmr, cmr*)

2,9:3,16-Diepoxy-6-asbestinene-4,11-diol D-412



(4β,6*E*,11β)–*form*

$C_{20}H_{32}O_4$ 336.47

(4β,6*E*,11β)-*form* [74145-74-7]
Cryst. (C_6H_6/hexane). Mp 156-158°.

11-Butanoyl: ***Asbestinin 3***
[74145-72-5]
$C_{24}H_{38}O_5$ 406.561
Isol. from *Briareum asbestinum*. Cryst. (Et_2O/hexane). Mp 156-158°. $[\alpha]_D^{20}$ -39.4 (c, 3.4 in $CHCl_3$).

11-Butanoyl, 4-Ac: ***Asbestinin 1***
[74219-41-3]
$C_{26}H_{40}O_6$ 448.598
Isol. from *Briareum asbestinum*. Acetylcholine antagonist. Ichthyotoxic agent. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ -26.3 (c, 3.3 in $CHCl_3$).

4-Octanoyl, 11-Ac: ***Asbestinin 6***
[146471-82-1]
$C_{30}H_{48}O_6$ 504.706
Constit. of *Briareum asbestinum*. Cytotoxic agent. Oil. $[\alpha]_D^{25}$ -75.9 (c, 4.08 in $CHCl_3$). Struct. revised in 1994.

11-Ketone, 4-octanoyl: ***Asbestinin 8***
[146471-84-3]
$C_{28}H_{44}O_5$ 460.653
Constit. of *Briareum asbestinum*. Cytotoxic agent. Oil. $[\alpha]_D^{25}$ -49 (c, 3.9 in $CHCl_3$).

(4β,6*Z*,11β)-*form*

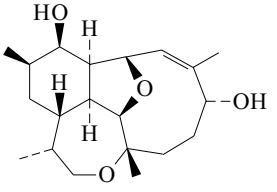
Di-Ac: ***Asbestinin 12***
$C_{24}H_{36}O_6$ 420.545
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{25}$ -24.66 (c, 2.9 in $CHCl_3$).

11-Butanoyl, 4-Ac: ***Asbestinin 2***
[74145-73-6]
$C_{26}H_{40}O_6$ 448.598
Constit. of *Briareum asbestinum*. Cryst. (hexane). Mp 184-186°. $[\alpha]_D^{20}$ -48.2 (c, 1.7 in $CHCl_3$).

4-Octanoyl, 11-Ac: ***Asbestinin 11***
$C_{30}H_{48}O_6$ 504.706
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{26}$ -14.08 (c, 6.2 in $CHCl_3$).

6β,7β-Epoxide, 11-butanoyl, 4-Ac: ***Asbestinin epoxide***
[75961-66-9]
$C_{26}H_{40}O_7$ 464.598
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{25}$ -21 (c, 0.3 in MeOH).
Stierle, D.B. *et al., J.A.C.S.*, 1980, **102**, 5088-5092 (*Asbestinins 1-5*)
Selover, S.J. *et al., J.O.C.*, 1981, **46**, 964-970 (*Asbestinin 2 epoxide, cryst struct*)
Rodriguéz, A.D. *et al., Tetrahedron*, 1993, **49**, 319 (*Asbestinins 6-10, activity*)
Rodriguéz, A.D. *et al., J. Nat. Prod.*, 1994, **57**, 1638 (*Asbestinin 6, activity*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)

2,9:3,16-Diepoxy-7-asbestinene-6,11-diol D-413

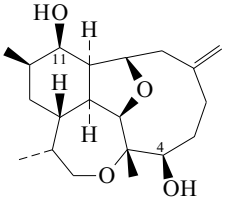


$C_{20}H_{32}O_4$ 336.47

(6α,7*Z*,11β)-*form*

Di-Ac: ***11-Acetoxy-4-deoxyasbestinin E***
[163564-81-6]
$C_{24}H_{36}O_6$ 420.545
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{24}$ +19.73 (c, 1.3 in $CHCl_3$).
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1994, **57**, 1638 (*isol, pmr, cmr*)

2,9:3,16-Diepoxy-7(19)-asbestinene-4,11-diol D-414



$C_{20}H_{32}O_4$ 336.47

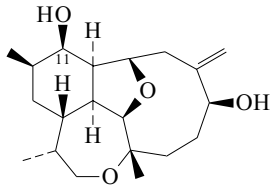
(4β,11β)-*form*

11-Ac: ***Asbestinin 20***
[163564-76-9]
$C_{22}H_{34}O_5$ 378.508
Constit. of *Briareum asbestinum*. Amorph. powder. $[\alpha]_D^{25}$ -16.74 (c, 5.2 in $CHCl_3$).

4-Ketone, 11-Ac: ***Asbestinin 10***
[146471-86-5]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Briareum asbestinum*. Cytotoxic agent. Oil. $[\alpha]_D^{25}$ -81.5 (c, 0.76 in $CHCl_3$).

4-Ketone, 11-butanoyl: ***Asbestinin 9***
[146471-85-4]
$C_{24}H_{36}O_5$ 404.545
Constit. of *Briareum asbestinum*. Cytotoxic agent. Oil. $[\alpha]_D^{27}$ -78 (c, 2 in $CHCl_3$).
Bernardelli, P. *et al., Heterocycles*, 1988, **49**, 531-556 (*rev*)
Rodriguez, A.D. *et al., Tetrahedron*, 1993, **49**, 319 (*Asbestinin 9, Asbestinin 10, activity*)
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1994, **57**, 1638 (*Asbestinin 20*)

2,9:3,16-Diepoxy-7(19)-asbestinene-6,11-diol D-415



$C_{20}H_{32}O_4$ 336.47

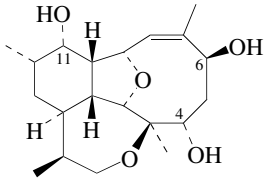
(6β,11β)-*form*

11-Ac: ***11-Acetoxy-4-deacetoxyasbestinin F***
[163564-79-2]
$C_{22}H_{34}O_5$ 378.508
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{25}$ -15.2 (c, 4.8 in $CHCl_3$).

11-Butanoyl: ***4-Deoxyasbestinin G***
[163564-80-5]
$C_{24}H_{38}O_5$ 406.561
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{25}$ -26.57 (c, 7.3 in $CHCl_3$).

Rodriguez, A.D. *et al., J. Nat. Prod.*, 1994, **57**, 1638 (*isol, pmr, cmr*)

2,9:3,16-Diepoxy-7-asbestinene-4,6,11-triol D-416



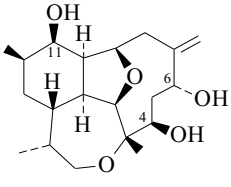
$C_{20}H_{32}O_5$ 352.47

(4α,6β,7*Z*,11α)-*form*

4-Octanoyl, 11-Ac: ***Asbestinin 18***
[163564-74-7]
$C_{30}H_{48}O_7$ 520.705
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{24}$ -0.88 (c, 2.3 in $CHCl_3$).

Rodriguez, A.D. *et al., J. Nat. Prod.*, 1994, **57**, 1638-1655 (*isol, pmr, cmr*)

2,9:3,16-Diepoxy-7(19)-asbestinene-4,6,11-triol D-417



(4β,6α,11β)–*form*

$C_{20}H_{32}O_5$ 352.47

(4β,6α,11β)-*form*

4,11-Di-Ac: ***Asbestinin 17***
$C_{24}H_{36}O_7$ 436.544
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{26}$ -18.58 (c, 16.2 in $CHCl_3$).

11-Butanoyl, 4-Ac: ***Asbestinin 5***
[74145-70-3]
$C_{26}H_{40}O_7$ 464.598
Constit. of *Briareum asbestinum*. Acetylcholine and histamine antagonist. Ichthyotoxic agent. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ -18 (c, 2.3 in $CHCl_3$).

11-Butanoyl, 4,6-di-Ac: [75961-67-0]
$C_{28}H_{42}O_8$ 506.635
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{25}$ -12 (c, 0.2 in MeOH).

4-Hexanoyl, 11-Ac: ***Asbestinin 14***
$C_{28}H_{44}O_7$ 492.651
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{25}$ +2.94 (c, 4 in $CHCl_3$).

4-Octanoyl, 11-Ac: ***Asbestinin 13***
$C_{30}H_{48}O_7$ 520.705
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{26}$ -14.59 (c, 3.7 in $CHCl_3$).

6-Ketone, 4,11-di-Ac: ***Asbestinin 19***
$C_{24}H_{34}O_7$ 434.528
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{30}$ -48.32 (c, 1.36 in $CHCl_3$).

6-Ketone, 11-butanoyl, 4-Ac: ***Asbestinin 4***
[74145-71-4]
$C_{26}H_{38}O_7$ 462.582
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{20}$ -60 (c, 2.5 in $CHCl_3$). λ_{max} 218 (ε) (MeOH) (Derep).

6-Ketone, 4-octanoyl, 11-Ac: ***Asbestinin 16***
$C_{30}H_{46}O_7$ 518.689
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{28}$ -42.38 (c, 3.8 in $CHCl_3$).

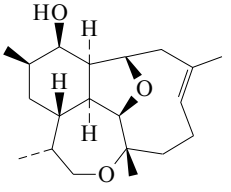
(4β,6β,11β)-*form*

4,11-Di-Ac: ***Asbestinin 15***
$C_{24}H_{36}O_7$ 436.544
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{26}$ -4.04 (c, 2.7 in $CHCl_3$).

4-Octanoyl, 11-Ac: ***Asbestinin 7***
[146471-83-2]
$C_{30}H_{48}O_7$ 520.705
Constit. of *Briareum asbestinum*. Cytotoxic agent. Oil. $[\alpha]_D^{25}$ +5 (c, 3.2 in $CHCl_3$). Struct. revised in 1994.

Stierle, D.B. *et al., J.A.C.S.*, 1980, **102**, 5088-5092 (*Asbestinin 5, isol, activity*)
Selover, S.J. *et al., J.O.C.*, 1981, **46**, 964 (*Asbestinin 5, isol, activity*)
Rodríguez, A.D. *et al., Tetrahedron*, 1993, **49**, 319 (*Asbestinin 7, activity*)
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1994, **57**, 1638 (*Asbestinins 13-17*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)

2,9:3,16-Diepoxy-6-asbestinen-11-ol D-418



(6*E*,11β)–*form*

$C_{20}H_{32}O_3$ 320.471

(6*E*,11β)-*form*

Ac: 11-Acetyl-4-deacetoxy-11-deacylasbestinin 1. ***11-Acetoxy-4-deoxyasbestinin B***
[137767-98-7]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Briareum asbestinum*. Cytotoxic agent; active against *Klebsiella pneumoniae.* Cryst.
Mp 150-152°. $[\alpha]_D^{29}$ -8.9 (c, 0.34 in $CHCl_3$). The trivial name given is confusing.

Butanoyl: ***4-Deoxyasbestinin A***
[137767-97-6]
$C_{24}H_{38}O_4$ 390.562
Constit. of *Briareum asbestinum*. Cytotoxic agent; active against *Klebsiella pneumoniae.* Oil. $[\alpha]_D^{29}$ -6.6 (c, 1.6 in $CHCl_3$).

(6*Z*,11β)-*form*

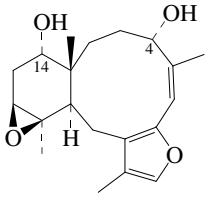
Ac: 11-Acetyl-4-deacetoxy-11-deacylasbestinin 2. ***11-Acetoxy-4-deoxyasbestinin D***
[137419-52-4]
$C_{22}H_{34}O_4$ 362.508

Constit. of *Briareum asbestinum*. Cytotoxic agent; active against *Klebsiella pneumoniae*. Oil. $[\alpha]_D^{29}$ -2.29 (c, 1.3 in $CHCl_3$).

Butanoyl: ***4-Deoxyasbestinin C***
[137419-51-3]
$C_{24}H_{38}O_4$ 390.562
Constit. of *Briareum asbestinum*. Cytotoxic agent; active against *Klebsiella pneumoniae*. Oil. $[\alpha]_D^{29}$ -1.2 (c, 0.84 in $CHCl_3$).

Morales, J.J. *et al., J. Nat. Prod.*, 1991, **54**, 1368 (*isol, pnr, cmr*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)
Crimmins, M.T. *et al., J.A.C.S.*, 2005, **127**, 17200-17201 (*synth*)

7,18:11,12-Diepoxy-5,7,17-briaratriene-4,14-diol D-419



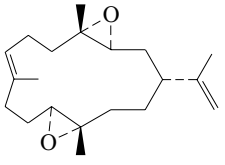
$C_{20}H_{28}O_4$ 332.439

Di-Ac: [126394-96-5]
$C_{24}H_{32}O_6$ 416.513
Constit. of a *Pachyclavularia* sp.

4-Deoxy, 14-Ac: [126394-98-7]
$C_{22}H_{30}O_4$ 358.477
Constit. of a *Pachyclavularia* sp.

Uchio, Y. *et al., Tennen Yuki Kagobutsu*, 1989, **31**, 548-553; *CA*, **112**, 175870s

3,4:11,12-Diepoxy-7,15-cembradiene D-420

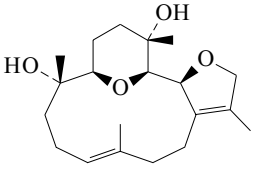


$C_{20}H_{32}O_2$ 304.472

(1R,3S,4S,7E,11S,12S)-form
3,4:11,12-Diepoxycembrene A
[62824-09-3]
Constit. of *Sinularia flexibilis*.
Cryst. (MeOH).
Mp 66-68°. $[\alpha]_D$ +63 (c, 0.5 in pentane).

Herin, M. *et al., Bull. Soc. Chim. Belg.*, 1976, **85**, 707

2,16:3,7-Diepoxy-1(15),11-cembradiene-4,8-diol D-421

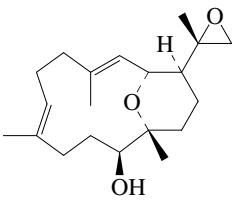


$C_{20}H_{32}O_4$ 336.47

(2S,3S,4S,7R,8S,11E)-form
Sarcodiol
[175033-27-9]
Constit. of a *Sarcophyton* sp.
Cryst.
Mp 133-135°. $[\alpha]_D$ +48.4 (c, 0.55 in $CHCl_3$).

Miyaoka, H. *et al., Chem. Lett.*, 1996, 239 (*isol, pnr, cmr, cryst struct*)

2,12:15,16-Diepoxy-3,7-cembradien-11-ol D-422



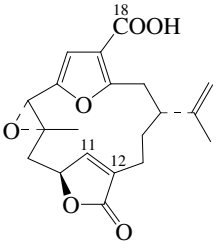
$C_{20}H_{32}O_3$ 320.471

(1S,2R,3E,7E,11S,12R)-form [824957-43-9]
Constit. of a *Eunicea* sp.
Oil. $[\alpha]_D^{20}$ +35.2 (c, 1.2 in $CHCl_3$).

11-Ac: [824957-42-8]
$C_{22}H_{34}O_4$ 362.508
Constit. of a *Eunicea* sp. Cryst.
Mp 85.5-85.8°. $[\alpha]_D^{20}$ +70.5 (c, 1.2 in $CHCl_3$).

Wei, X. *et al., Tetrahedron*, 2004, **60**, 11813-11819 (*isol, pmr, cmr, cryst struct*)

3,6:7,8-Diepoxy-3,5,11,15-cembratetraen-20,10-olid-18-oic acid D-423



$C_{20}H_{22}O_6$ 358.39

(1R,7S,8R,10S)-form

Me ester: ***Pukalide***
[58772-81-9]
$C_{21}H_{24}O_6$ 372.417
Constit. of *Sinularia abrupta*, *Sinularia polydactyla*, *Sinularia erecta*, *Tochuina tetraquetra* and *Leptogorgia virgulata*. Icthyotoxin, antifouling agent. Cryst. (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 204-206°. $[\alpha]_D$ +44 (c, 1.1 in $CHCl_3$). λ_{max} 248 (ϵ 5200) (EtOH) (Derep).
► LD_{50} (mus, scu) 8 mg/kg.

11,12-Epoxide: 3,6:7.8:11,12-Triepoxy-3,5,15-cembratrien-20,10-olid-18-oic acid
$C_{20}H_{22}O_7$ 374.39

11α,12α-Epoxide, Me ester: ***11,12-Epoxypukalide***
[95925-22-7]
$C_{21}H_{24}O_7$ 388.416
Constit. of *Leptogorgia setacea* and *Phyllogorgia dilatata*. Shows icthyodeterrent activity. Cryst. ($CHCl_3$/pentane). $[\alpha]_D$ -5.33 (c, 0.6 in MeOH). λ_{max} 238 (ϵ 5420) (EtOH) (Derep).

18-Aldehyde: 3,6:7,8-Diepoxy-18-oxo-3,5,11,15-cembratetraen-20,10-olide. ***Pukalide aldehyde***
[134455-97-3]
$C_{20}H_{22}O_5$ 342.391
Constit. of *Leptogorgia alba*. Cryst.

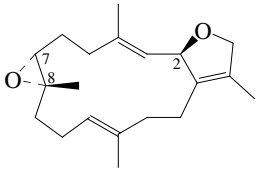
18-Aldehyde, 11α,12α-epoxide: ***Leptolide***
[852468-86-1]
$C_{20}H_{22}O_6$ 358.39
Constit. of *Leptogorgia alba*. Red glass. $[\alpha]_D^{25}$ +10.4 (c, 1.9 in $CHCl_3$). λ_{max} 234 (log ϵ 3.34); 262 (log ϵ 3.38); 292 (log ϵ 3.36) (EtOH).

Missakian, M.G. *et al., Tetrahedron*, 1975, **31**, 2513-2515 (*Pukalide*)

Ksebati, M.B. *et al., J. Nat. Prod.*, 1984, **47**, 1009-1012 (*11,12-Epoxypukalide*)
Gerhart, D.J. *et al., J. Chem. Ecol.*, 1988, **14**, 1905-1917; 1993, **19**, 2697-2704 (*Pukalide*)
Martins, D.L. *et al., J. Braz. Chem. Soc.*, 1998, **9**, 586-590; *CA*, **130**, 279449z (*11,12-Epoxypukalide, isol, activity*)
Gutiérrez, M. *et al., J. Nat. Prod.*, 2005, **68**, 614-616 (*Leptolide, Pukalide aldehyde, cryst struct, abs config*)

2,16:7,8-Diepoxy-1(15),3,11-cembratriene D-424

Sarcophytoxide
[70748-49-1]



(2*R*,3*E*,7*R*,8*R*,11*E*)-*form*

$C_{20}H_{30}O_2$ 302.456

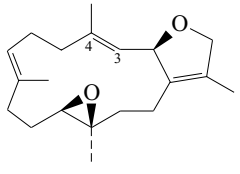
(2*R*,3*E*,7*R*,8*R*,11*E*)-*form* [111900-27-7]
Constit. of *Sarcophyton birklandi*, *Ovula ovum* and *Sarcophyton ehrenbergi*.
Mp 79-81°. $[\alpha]_D$ -191 (c, 0.4 in $CHCl_3$).

(2*R*,3*E*,7*S*,8*S*,11*E*)-*form*
Constit. of *Lobophytum pauciflorum* and of a *Sarcophyton* sp. Ichthyotoxin. Cryst.
Mp 52-56°. $[\alpha]_D$ -64 (c, 0.6 in $CHCl_3$). CAS no. not found 8-12CI.

(2*S*,3*E*,7*S*,8*S*11*E*)-*form*
Deoxosarcophine
[74841-41-1]
[84984-71-4]
Constit. of *Sarcophyton trocheliophorum*, *Sarcophyton glaucum* and *Lobophytum crassum*. Algicide. Facilitator of neuromuscular transmission, calcium antagonist. Cryst. or oil.
Mp 72-73°. $[\alpha]_D$ +157 (c, 1 in MeOH). $[\alpha]_D$ +135 (c, 0.93 in $CHCl_3$) (+129). λ_{max} 222 (ϵ 10000) (MeOH).

Kashman, Y. *et al., Tetrahedron*, 1974, **30**, 3615-3620 (*2S,7S,8S-form*)
Tursch, B. *et al., Pure Appl. Chem.*, 1976, **48**, 1-6 (*Sarcophyton trocheliophorum*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1978, **31**, 2707-2712; 1980, **33**, 879-884 (*2R,7R,8R-form*)
Frincke, J.M. *et al., Tet. Lett.*, 1980, **21**, 735-738 (*(+)-form, (-)-form*)
Kobayashi, J. *et al., Experientia*, 1983, **39**, 67-69 (*2S,7S,8S-form, cryst struct*)
Bowden, B.F. *et al., J. Nat. Prod.*, 1987, **50**, 650-659 (*2R,7S,8S-form, bibl*)
Nishitani, K. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2514 (*synth*)

2,16:11,12-Diepoxy-1(15),3,7-cembratriene D-425



(2*R*,3*E*,7*E*,11*R*,12*R*)–*form*

$C_{20}H_{30}O_2$ 302.456

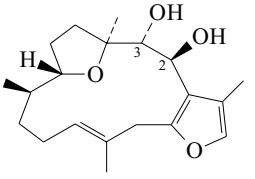
(2*R*,3*E*,7*E*,11*R*,12*R*)-*form*
Isosarcophytoxide
[70645-61-3]
Constit. of *Sarcophyton* spp. Shows weak antimycobacterial activity. Calcium antagonist. Cryst. (petrol).
Mp 67-69°. $[\alpha]_D$ -166.1 (c, 0.15 in $CHCl_3$).
3,4-Epoxide: ***2,16:3,4:11,12-Triepoxy-1(15),7-cembradiene***
[70645-59-9]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Sarcophyton* spp. Oil. $[\alpha]_D$ -46.7 (c, 0.09 in $CHCl_3$).

(2*R*,3*E*,7*E*,11*S*,12*S*)-*form*
Constit. of *Sarcophyton trocheliophorum*.
Oil. $[\alpha]_D^{24}$ +160 (c, 0.22 in $CHCl_3$).

(2*S*,3*E*,7*E*,11*R*,12*R*)-*form* [111900-29-9]
Constit. of *Sarcophyton birklandi* and *Sarcophyton glaucum*.
Cryst.
Mp 70-71°. $[\alpha]_D$ -64 (c, 0.6 in $CHCl_3$). $[\alpha]_D$ +210 ($CHCl_3$).

Bowden, B.F. *et al., Aust. J. Chem.*, 1979, **32**, 653-659 (*isol, struct*)
Bowden, B.F. *et al., J. Nat. Prod.*, 1987, **50**, 650-659 (*isol, cryst struct*)
Wu, Y.-C. *et al., J. Chin. Chem. Soc. (Taipei)*, 1992, **39**, 355-357 (*isol, pmr, cmr*)
König, G.M. *et al., J. Nat. Prod.*, 1998, **61**, 494-496 (*cmr*)
Koenig, G.M. *et al., Planta Med.*, 2000, **66**, 337-342 (*activity*)

4,7:14,16-Diepoxy-1(14),11,15-cembratriene-2,3-diol D-426

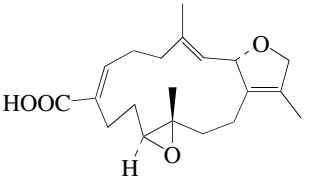


$C_{20}H_{30}O_4$ 334.455

(2*S*,3*R*,4*S*,7*S*,8*R*,11*E*)-*form*
Pachyclavularadiol
[73112-63-7]
Constit. of *Pachyclavularia violacea*.
Cryst. (MeCN).
Mp 132-134°. $[\alpha]_D$ +161 (c, 0.6 in $CHCl_3$).
2-Ac: [73112-64-8]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Pachyclavularia violacea*. Cryst. (pentane).
Mp 107-109°. $[\alpha]_D$ +137 (c, 0.03 in $CHCl_3$).
2,3-Di-Ac: [73112-65-9]
$C_{24}H_{34}O_6$ 418.529
Constit. of *Pachyclavularia violacea*. Oil. $[\alpha]_D$ -60 (c, 0.1 in $CHCl_3$).

Bowden, B.F. *et al., Aust. J. Chem.*, 1979, **32**, 2265

2,16:11,12-Diepoxy-1(15),3,7-cembratrien-19-oic acid D-427

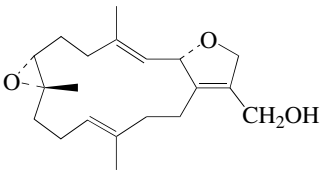


$C_{20}H_{28}O_4$ 332.439

(2*S,3*E*,7*E*,11*S**,12*S**)-*form***
Me ester: ***Lobophynin C***
[192222-21-2]
$C_{21}H_{30}O_4$ 346.466
Constit. of *Lobophytum schoedei*. Oil. $[\alpha]_D^{25}$ +109.3 (c, 0.31 in $CHCl_3$).

Yamada, K. *et al., J. Nat. Prod.*, 1997, **60**, 798-801 (*isol, pmr, cmr*)

2,16:7,8-Diepoxy-1(15),3,11-cembratrien-17-ol D-428

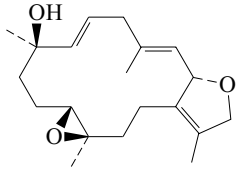


$C_{20}H_{30}O_3$ 318.455

(2*S,3*E*,7*R**,8*R**,11*E*)-*form***
Ac: ***Lobophynin B***
[192222-19-8]
$C_{22}H_{32}O_4$ 360.492
Constit. of *Lobophytum schoedei*. Oil. $[\alpha]_D^{25}$ +122.6 (c, 0.13 in $CHCl_3$).
Yamada, K. *et al., J. Nat. Prod.*, 1997, **60**, 798-801 (*isol, pmr, cmr*)

2,16:11,12-Diepoxy-1(15),3,6-cembratrien-8-ol D-429

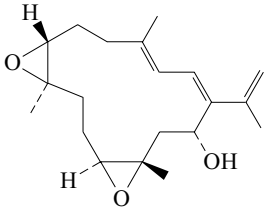
[132160-46-4]



$C_{20}H_{30}O_3$ 318.455

(2α,3*E*,6*E*,8β,11β,12β)-*form*
8-Hydroxyisosarcophytoxide-6-ene
Constit. of *Sinularia mayi*.
Oil. $[\alpha]_D$ +90.7 (c, 0.52 in $CHCl_3$).
Kusumi, T. *et al., Chem. Lett.*, 1990, 1315 (*isol, pmr*)

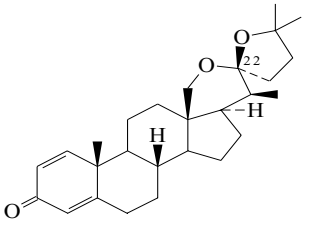
7,8:11,12-Diepoxy-1,3,15-cembratrien-14-ol D-430



$C_{20}H_{30}O_3$ 318.455

(1*E*,3*E*,7*R,8*R**,11*S**,12*S**,14*R**)-*form***
Ac: [149182-65-0]
$C_{22}H_{32}O_4$ 360.492
Constit. of *Sarcophyton tortuosum*. Oil. $[\alpha]_D$ +110 (c, 1 in CCl_4).
Leone, P.A. *et al., J. Nat. Prod.*, 1993, **56**, 521 (*isol, pmr, cmr*)

18,22:22,25-Diepoxycholesta-1,4-dien-3-one D-431



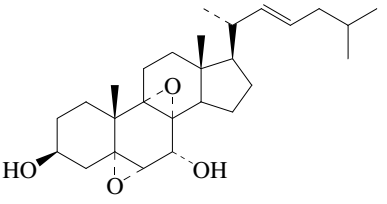
(20*R*,22*R*)–*form*

$C_{27}H_{38}O_3$ 410.595

(20*R*,22*R*)-*form*
Constit. of a *Sinularia* sp.
Oil.

(20*R*,22*S*)-*form*
Constit. of a *Sinularia* sp.
Oil.
Ciminiello, P. *et al., Experientia*, 1990, **46**, 980 (*isol, pmr, cmr*)

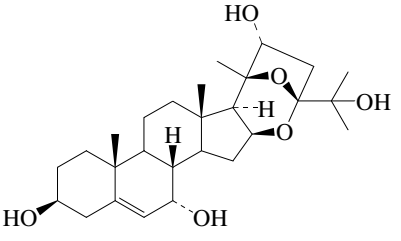
5,6:8,9-Diepoxycholest-22-ene-3,7-diol D-432



$C_{27}H_{42}O_4$ 430.626

(3β,5α,6α,7α,8α,9α,22*E*)-*form*
Homaxisterol B_1
[877373-33-6]
Constit. of a *Homaxinella* sp.
Amorph. solid.
Mansoor, T.A. *et al., J. Nat. Prod.*, 2006, **69**, 131-134 (*Homaxisterol B_1*)

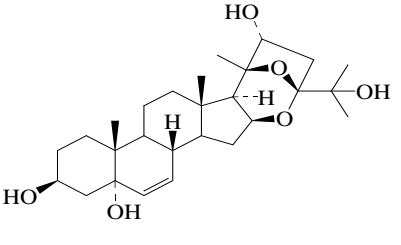
16,24:20,24-Diepoxycholest-5-ene-3,7,22,25-tetrol D-433



$C_{27}H_{42}O_6$ 462.625

(3β,7α,16β,20*R*,22*R*,24*S*)-*form*
22-Ac: ***Suberoretisteroid D***
[849920-31-6]
$C_{29}H_{44}O_7$ 504.662
Constit. of *Subergorgia reticulata*. Glass. $[\alpha]_D^{20}$ -73 (c, 0.056 in $CHCl_3$).
Zhang, W. *et al., Helv. Chim. Acta*, 2005, **88**, 87-94 (*Suberoretisteroid D*)

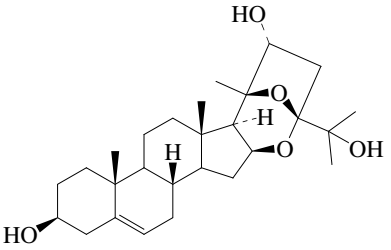
16,24:20,24-Diepoxycholest-6-ene-3,5,22,25-tetrol D-434



$C_{27}H_{42}O_6$ 462.625

(3β,5α,16β,20*R*,22*R*,24*S*)-*form*
22-Ac: ***Suberoretisteroid E***
[849920-32-7]
$C_{29}H_{44}O_7$ 504.662
Constit. of *Subergorgia reticulata*. Glass. $[\alpha]_D^{20}$ -26 (c, 0.142 in $CHCl_3$).
Zhang, W. *et al., Helv. Chim. Acta*, 2005, **88**, 87-94 (*Suberoretisteroid E*)

16,24:20,24-Diepoxycholest-5-ene-3,22,25-triol D-435



$C_{27}H_{42}O_5$ 446.626

(3β,16β,20*R*,22*R*,24*S*)-*form* [287389-67-7]
Constit. of *Gorgonella umbraculum*. Struct. revised in 2005.

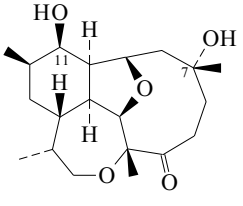
3-Ac: ***Suberoretisteroid A***
[849920-30-5]
$C_{29}H_{44}O_6$ 488.663
Constit. of *Subergorgia reticulata*. Glass. $[\alpha]_D^{20}$ -22.5 (c, 0.25 in $CHCl_3$).

22-Ac: ***Suberoretisteroid B***
[569348-54-5]
$C_{29}H_{44}O_6$ 488.663
Constit. of *Gorgonella umbraculum* and *Subergorgia reticulata*. Cryst.
Mp 160-162°. $[\alpha]_D$ -20 (c, 0.15 in $CHCl_3$). $[\alpha]_D^{20}$ -44 (c, 0.38 in $CHCl_3$).

3,22-Di-Ac: ***Suberoretisteroid C***
[287389-68-8]
$C_{31}H_{46}O_7$ 530.7
Constit. of *Subergorgia reticulata*. Glass. $[\alpha]_D^{20}$ -33 (c, 0.375 in $CHCl_3$).

Subrahmanyam, C. *et al., J. Chem. Res., Synop.*, 2000, 182-183 (*Gorgonella umbraculum constit*)
Anjaneyulu, A.S.R. *et al., Nat. Prod. Res.*, 2003, **17**, 149-152 (*22-Ac*)
Zhang, W. *et al., Acta Cryst. E*, 2005, **61**, o2884-o2886 (*Suberoretisteroid A, cryst struct*)
Zhang, W. *et al., Helv. Chim. Acta*, 2005, **88**, 87-94 (*Suberoretisteroids A-C*)

2,9:3,16-Diepoxy-7,11-dihydroxy-4-asbestinanone D-436



$C_{20}H_{32}O_5$ 352.47

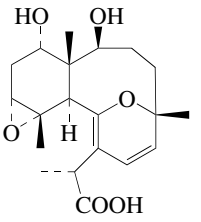
(7α,11β)-*form*

11-Ac: ***Asbestinin 21***
$C_{22}H_{34}O_6$ 394.507
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{24}$ -27.17 (c, 1.8 in $CHCl_3$).

11-Butanoyl: ***Asbestinin 22***
$C_{24}H_{38}O_6$ 422.561
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{22}$ -30.61 (c, 1.6 in $CHCl_3$).

Rodriguez, A.D. *et al., J. Nat. Prod.*, 1994, **57**, 1638 (*isol, pmr, cmr*)

5,9:11,12-Diepoxy-2,14-dihydroxy-6,8-briaradien-18-oic acid D-437



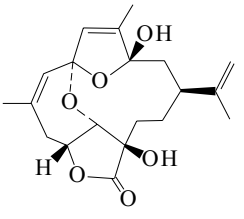
$C_{20}H_{28}O_6$ 364.438

2-Butanoyl, 14-Ac, Me ester: ***Briareolate ester C***
[153977-15-2]
$C_{27}H_{38}O_8$ 490.592
Constit. of *Briareum asbestinum*. Amorph. powder.

Dookran, R. *et al., Tetrahedron*, 1994, **50**, 1983-1992 (*isol, pmr, cmr*)

3,6:6,11-Diepoxy-3,12-dihydroxy-4,7,15-cembratrien-20,10-olide D-438

Coralloidolide B
[107748-87-8]

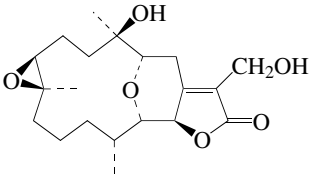


Relative configuration

$C_{20}H_{26}O_6$ 362.422
Constit. of *Alcyonium coralloides*. Amorph. powder. $[\alpha]_D^{20}$ -85.4 (c, 0.78 in EtOH).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1987, **70**, 63

3,13:7,8-Diepoxy-4,17-dihydroxy-1(15)-cembren-16,14-olide D-439

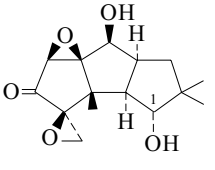


$C_{20}H_{30}O_6$ 366.453

(3*S*,4*R*,7*S*,8*R*,12*R*,13*S*,14*R*)-*form*
Eunicenolide
[200271-88-1]
Constit. of *Eunicea succinea*.
Oil. $[\alpha]_D^{25}$ +13.7 (c, 2 in $CHCl_3$). λ_{max} 229 (ϵ 8500) (MeOH).

Rodriguez, A.D. *et al., J. Nat. Prod.*, 1998, **61**, 40-45 (*isol, pmr, cmr*)

4,15:6,7-Diepoxy-1,8-dihydroxy-5-hirsutanone D-440



Absolute configuration

$C_{15}H_{20}O_5$ 280.32

(1α,4β,6β,7β,8β)-*form*

Coriolin

[33404-85-2]

Metab. of *Coriolus consors* ATCC20305. Antibiotic active against gram-positive bacteria, *Trichomonas* and Yoshida sarcoma cells. Cryst. Sol. MeOH, EtOAc; fairly sol. $CHCl_3$, H_2O, CCl_4, C_6H_6. Mp 175°. $[\alpha]_D$ -20.7 (c, 0.03 in $CHCl_3$).

▶ LD_{50} (mus, ivn) 9 mg/kg. WH0203000

1-Octanoyl: ***5-Ketocoriolin B***

[39928-65-9]

$C_{23}H_{34}O_6$ 406.518

Metab. of *Coriolus consors* ATCC20305. Immunostimulant. Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane.

1-(2-Hydroxyoctanoyl): ***Coriolin C***

[33400-90-7]

$C_{23}H_{34}O_7$ 422.517

Metab. of *Coriolus consors* ATCC20305. Sol. MeOH, Me_2CO; poorly sol. H_2O.

5β-Alcohol, 1-octanoyl: ***Coriolin B***

[33400-89-4]

$C_{23}H_{36}O_6$ 408.534

Metab. of *Coriolus consors* ATCC20305 and a fungus separated from a *Jaspis* marine sponge. Shows antitumour props. Cryst. Sol. MeOH, EtOAc, C_6H_6, Me_2CO; poorly sol. H_2O, hexane, CCl_4. Mp 198-202°. $[\alpha]_D$ +105.2 (c, 0.003 in CH_2Cl_2).

5β-Alcohol, 1-(2-hydroxyoctanoyl): ***Dihydrocoriolin C***

[49644-26-0]

$C_{23}H_{36}O_7$ 424.533

Constit. of *Coriolus consors* and a fungus separated from a *Jaspis* marine sponge. Solid.

Mp 152-155°. $[\alpha]_D$ +49.8 (c, 0.003 in MeOH).

8-Ketone, 1-octanoyl: ***Diketocoriolin B***

[77790-11-5]

$C_{23}H_{32}O_6$ 404.502

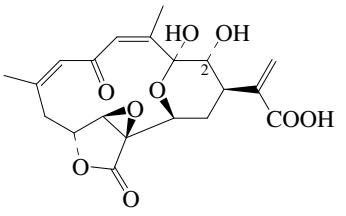
Metab. of *Coriolus consors* ATCC20305. Immunostimulant. Na/K-ATPase inhibitor. Enhances antibody formation. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.

▶ LD_{50} (mus, ipr) 40 mg/kg.

[74183-95-2, 74183-96-3]

Takahashi, S. *et al., Tet. Lett.*, 1969, 4663-4666; 1970, 1637-1639; 1971, 1955-1958 (*isol, struct, Coriolin B, Coriolin C*)
Japan. Pat., 1972, 72 39 698; *CA*, **79**, 144864p (*5-Ketocoriolin B*)
Nakamura, H. *et al., J. Antibiot.*, 1974, **27**, 301-302 (*abs config*)
Tanabe, M. *et al., Tet. Lett.*, 1974, 2271-2274 (*biosynth*)
Danishefsky, S. *et al., Tet. Lett.*, 1980, 3439-3442 (*synth, Coriolin B, Diketocoriolin B*)
Shibasaki, M. *et al., Tet. Lett.*, 1980, 3587-3590 (±*-form, synth*)
Trost, B.M. *et al., J.A.C.S.*, 1981, **103**, 7380-7381 (±*-form, synth*)
Tatsuta, K. *et al., Tetrahedron*, 1981, **37**, 4365-4369 (±*-form, synth*)
Iseki, K. *et al., Tetrahedron*, 1981, **37**, 4411-4418 (±*-form, synth*)
Mehta, G. *et al., Chem. Comm.*, 1982, 540-541 (±*-form, synth*)
Koreeda, M. *et al., J.A.C.S.*, 1983, **105**, 7203-7205 (±*-form, synth*)
Wender, P.A. *et al., Tet. Lett.*, 1983, **24**, 5325 (*synth*)
Demuth, M. *et al., Helv. Chim. Acta*, 1984, **67**, 2023-2027 (±*-form, synth*)
Ito, T. *et al., Tetrahedron*, 1984, **40**, 241-255 (±*-form, synth*)
Schuda, P.F. *et al., Tetrahedron*, 1984, **40**, 2365-2380 (±*-form, synth*)
Demuth, M. *et al., J.A.C.S.*, 1986, **108**, 4149-4154 (*synth, bibl*)
Van Hijfte, L. *et al., J.O.C.*, 1987, **52**, 4647-4667 (±*-form, synth*)
Malzer, J. *et al., Org. Synth. Highlights*, VCH, 1991, 323 (*synth, rev*)
Weinges, K. *et al., Annalen*, 1993, 1133-1140; 1994, 99-101 (*Coriolin B, synth*)
Cheng, X.-C. *et al., J.O.C.*, 1994, **59**, 6344-6348 (*Coriolin B, Dihydrocoriolin C, isol, cmr*)
Domon, K. *et al., Tet. Lett.*, 1997, **38**, 465-468 (*synth*)
Mizuno, H. *et al., J.O.C.*, 1999, **64**, 2648-2656 (*synth*)
Singh, V. *et al., Tetrahedron*, 2000, **56**, 7785-7795 (*synth*)
Mehta, G. *et al., J.C.S. Perkin 1*, 20 1, 1153-1161 (*synth*)
Paquette, L.A. *et al., J.A.C.S.*, 2002, **124**, 9199-9203 (*synth*)

3,13:11,12-Diepoxy-2,3-dihydroxy-6-oxo-4,7,15(17)-cembratrien-20,10-olid-16-oic acid D-441



$C_{20}H_{22}O_9$ 406.388

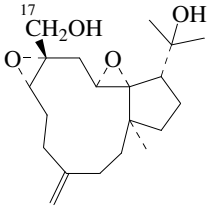
2-Ac, Me ester:

$C_{23}H_{26}O_{10}$ 462.452

Constit. of *Pseudopterogorgia bipinnata*.

Fenical, W. *et al., J. Nat. Prod.*, 1987, **50**, 1001-1008

7,8:10,11-Diepoxy-4(16)-dolabellene-17,18-diol D-442



$C_{20}H_{32}O_4$ 336.47

(7α,8α,10α,11α)-*form*

Stolonidiol

[112661-59-3]

Constit. of soft coral *Clavularia* sp. Cytotoxic and ichthyotoxic. Neurotrophic factor. Choline acetyltransferase inducer. Viscous oil. $[\alpha]_D$ -31 (c, 1.4 in $CHCl_3$).

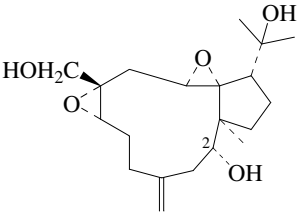
17-Ac: Stolonidiol acetate

$C_{22}H_{34}O_5$ 378.508

Constit. of *Clavularia* sp. Cytotoxic and ichthyotoxic agent. Viscous oil. $[\alpha]_D$ -26.8 (c, 0.38 in $CHCl_3$).

Mori, K. *et al., Tet. Lett.*, 1987, **28**, 5673 (*cryst struct*)
Yabe, T. *et al., J. Nat. Prod.*, 2000, **63**, 433-435 (*activity*)
Miyaoka, H. *et al., Tet. Lett.*, 2001, **42**, 9233-9266 (*synth*)

7,8:10,11-Diepoxy-4(16)-dolabellene-2,17,18-triol D-443



$C_{20}H_{32}O_5$ 352.47

(2α,7α,8α,10α,11α)-*form*

2-Ac: 2-Acetoxystolonidiol. ***Clavinflol A***

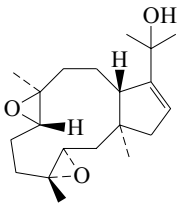
[473577-14-9]

$C_{22}H_{34}O_6$ 394.507

Constit. of *Clavularia inflata* and *Clavularia koellikeri*. Oil. $[\alpha]_D^{25}$ -101 (c, 0.98 in $CHCl_3$).

Iwashima, M. *et al., J. Nat. Prod.*, 2002, **65**, 1441-1446 (*isol, pmr, cmr*)
Shen, Y.C. *et al., J. Chin. Chem. Soc. (Taipei)*, 2003, **50**, 471-476 (*isol, pmr, cmr*)

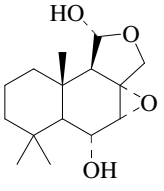
3,4:7,8-Diepoxy-12-dolabellen-18-ol D-444



$C_{20}H_{32}O_3$ 320.471

(1*R,3*R**,4*S**,7*R**,8*R**,11*R**)-*form*** [129932-80-5]
Constit. of brown algae *Dictyota pardarlis* f. *pseudohamata* A7749 and *Dictyota divaricata*. Antimalarial agent. Cryst. (C_6H_6/EtOAc).
Mp 118.5-119.5°. $[\alpha]_D^{25}$ +57.6 (c, 0.024 in $CHCl_3$).
Wright, A.D. *et al., Tetrahedron*, 1990, **46**, 3851 (*isol, struct*)
Rao, C.B. *et al., Phytochemistry*, 1991, **30**, 1971 (*isol, pmr, cmr*)

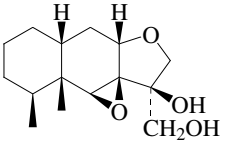
7,8:11,12-Diepoxy-6,11-drimanediol D-445



$C_{15}H_{24}O_4$ 268.352

(6α,7α,8α,11α)-*form*
Dendocarbin N
[350986-87-7]
Constit. of *Dendrodoris carbunculosa*.
Oil. $[\alpha]_D^{25}$ -40 (c, 0.03 in $CHCl_3$).
Sakio, Y. *et al., J. Nat. Prod.*, 2001, **64**, 726-731 (*isol, pmr, cmr*)

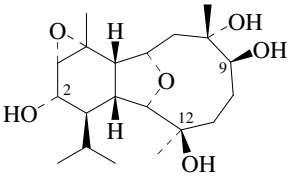
6,7:8,13-Diepoxy-11,12-eremophilanediol D-446



$C_{15}H_{24}O_4$ 268.352

(6β,7β,8α,10β,11β*OH*)-*form*
Peribysin B
Prod. by *Periconia byssoides* isol. from *Aplysia kurodai*.
Pale yellow oil. $[\alpha]_D$ +42.9 (c, 0.07 in EtOH). λ_{max} 223 (log ϵ 2.68) (EtOH).
Yamada, T. *et al., Org. Biomol. Chem.*, 2004, **2**, 2131-2135 (*isol, pmr, cmr*)

3,4:6,13-Diepoxy-2,8,9,12-eunicellanetetrol D-447

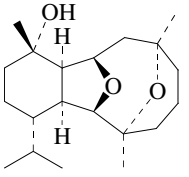


$C_{20}H_{34}O_6$ 370.485

(2α,3α,4α,6α,8α,9β,12β,13α)-*form*
2,9-Di-Ac: ***Epoxycladine B***
[845298-28-4]
$C_{24}H_{38}O_8$ 454.559
Constit. of *Cladiella kashmani*. Oil. $[\alpha]_D^{25}$ -11 (c, 0.44 in $CHCl_3$).
2,12-Di-Ac: ***Epoxycladine A***
[845298-27-3]
$C_{24}H_{38}O_8$ 454.559
Constit. of *Cladiella kashmani*. Oil. $[\alpha]_D^{25}$ -12 (c, 0.34 in $CHCl_3$).
Chill, L. *et al., J. Nat. Prod.*, 2005, **68**, 19-25 (*isol, pmr, cmr*)

6,13:8,12-Diepoxy-4-eunicellanol D-448

6,13:8,12-Diepoxy-4-cladicellanol



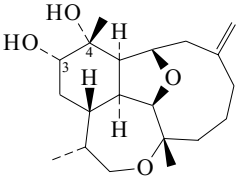
(4α,6β,8α,12α,13β)-*form*

$C_{20}H_{34}O_3$ 322.487

(4α,6β,8α,12α,13β)-*form*
Oil. $[\alpha]_D$ -11 (c, 0.6 in $CHCl_3$).
Ac: ***Polyanthellin A***
[503552-48-5]
$C_{22}H_{36}O_4$ 364.524
Constit. of *Briareum polyanthes*. Oil. $[\alpha]_D^{20}$ -9.9 (c, 1 in $CHCl_3$).

(*ent*-4α,6β,8α,12α,13β)-*form* [125239-56-7]
Constit. of a *Briareum* sp. (DD6).
Glass. $[\alpha]_D$ +19.4 (c, 0.57 in $CHCl_3$). Struct. revised in 2003.
Ac: [125239-57-8]
$C_{22}H_{36}O_4$ 364.524
Constit. of a *Briareum* sp. (DD6). Oil. $[\alpha]_D$ +8.9 (c, 0.22 in $CHCl_3$). Struct. revised in 2003.
Bowden, B.F. *et al., Aust. J. Chem.*, 1989, **42**, 1705-1726 (*isol, pmr, cmr*)
Ospina, C.A. *et al., J. Nat. Prod.*, 2003, **66**, 357-363 (*isol, pmr, cmr, cryst struct*)

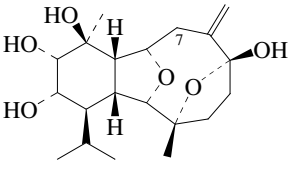
6,13:12,16-Diepoxy-8(19)-eunicellene-3,4-diol D-449



$C_{20}H_{32}O_4$ 336.47

(3α,4α,6β,12α,13β,15α)-*form*
3-Octanoyl: ***Briarellin I***
[171528-05-5]
$C_{28}H_{46}O_5$ 462.668
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{26}$ -35.2 (c, 1 in $CHCl_3$).
Rodríguez, A.D. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1853 (*isol, pmr, cmr*)

6,13:9,12-Diepoxy-8(19)-eunicellene-2,3,4,9-tetrol D-450



$C_{20}H_{32}O_6$ 368.469

(2α,3α,4β,9β*OH*)-*form*

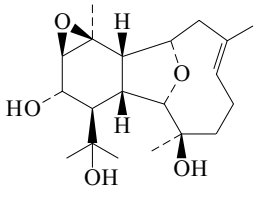
2,3,4-Tri-Ac: ***Massileunicellin A***
[251298-75-6]
$C_{26}H_{38}O_9$ 494.581
Constit. of *Eunicella cavolinii*. Amorph. powder. $[\alpha]_D^{20}$ -5 (c, 0.3 in $CHCl_3$).

Δ^7-Isomer(Z), 2,3,4-tri-Ac: ***Massileunicellin B***
[251298-76-7]
$C_{26}H_{38}O_9$ 494.581
Constit. of *Eunicella cavolinii*. Amorph. solid.

8β,19-Dihydro, 2,3,4-tri-Ac: ***Massileunicellin C***
[251298-77-8]
$C_{26}H_{40}O_9$ 496.597
Constit. of *Eunicella cavolinii*. Amorph. solid.

Mancini, I. *et al., Helv. Chim. Acta*, 1999, **82**, 1681-1689 (*isol, pmr, cmr*)

3,4:6,13-Diepoxy-8-eunicellene-2,12,15-triol D-451



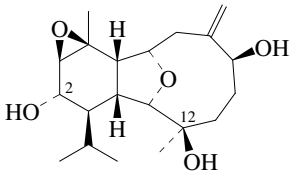
$C_{20}H_{32}O_5$ 352.47

(2α,3β,4β,6α,12β,13α)-*form*

Tri-Ac: ***Calicophirin A***
[134381-18-3]
$C_{26}H_{38}O_8$ 478.581
Constit. of a *Calicogorgia* sp. Insecticide. Oil. $[\alpha]_D^{19}$ -92.3 (c, 0.37 in $CHCl_3$).

Ochi, M. *et al., Heterocycles*, 1991, **32**, 19 (*isol, pmr, cmr, activity*)

3,4:6,13-Diepoxy-8(19)-eunicellene-2,9,12-triol D-452



$C_{20}H_{32}O_5$ 352.47

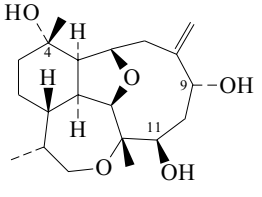
(2α,3β,4β,6α,9β,12β,13α)-*form*

12-Ac: ***Epoxycladine C***
[845298-29-5]
$C_{22}H_{34}O_6$ 394.507
Constit. of *Cladiella kashmani*. Oil. $[\alpha]_D^{25}$ -9 (c, 0.4 in $CHCl_3$).

2,12-Di-Ac: ***Epoxycladine D***
[845298-30-8]
$C_{24}H_{36}O_7$ 436.544
Constit. of *Cladiella kashmani*. Oil. $[\alpha]_D^{25}$ -21 (c, 0.27 in $CHCl_3$).

Chill, L. *et al., J. Nat. Prod.*, 2005, **68**, 19-25 (*isol, pmr, cmr*)

6,13:12,16-Diepoxy-8(19)-eunicellene-4,9,11-triol D-453



$C_{20}H_{32}O_5$ 352.47

(4α,6β,9α,11β,12α,13β,15α)-*form*

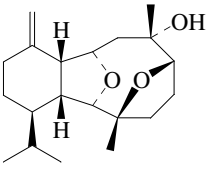
11-Octanoyl: ***Briarellin E***
[171528-02-2]
$C_{28}H_{46}O_6$ 478.668
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{28}$ -25.24 (c, 1.5 in $CHCl_3$).

9-Ketone, 11-octanoyl: ***Briarellin F***
[171528-03-3]
$C_{28}H_{44}O_6$ 476.652
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{30}$ -30.8 (c, 1.3 in $CHCl_3$).

11-Ketone, 4-octanoyl: ***Briarellin G***
[171528-04-4]
$C_{28}H_{44}O_6$ 476.652
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{30}$ +33.2 (c, 2.5 in $CHCl_3$).

Rodríguez, A.D. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1853 (*isol, pmr, cmr*)
Corminboeuf, O. *et al., J.A.C.S.*, 2003, **125**, 6650-6652 (*synth*)

6,13:9,12-Diepoxy-4(18)-eunicellen-8-ol D-454



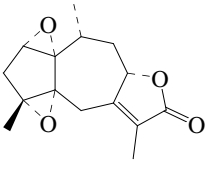
$C_{20}H_{32}O_3$ 320.471

(1β,5β,6α,8α,9β,12β,13α,14β)-*form*

Vigulariol
[369362-15-2]
Constit. of *Vigularia juncea*.
Oil. $[\alpha]_D^{27}$ +3.6 (c, 0.24 in $CHCl_3$).

Su, J.-H. *et al., Bull. Chem. Soc. Jpn.*, 2005, **78**, 877-879 (*Vigulariol*)

1,2:4,5-Diepoxy-7(11)-guaien-12,8-olide D-455



(1α,2α,4α,5α,8α,10α)-*form*

$C_{15}H_{18}O_4$ 262.305

(1α,2α,4α,5α,8α,10α)-*form*

Americanolide C
[178176-88-0]
Constit. of *Pseudopterogorgia americana*.
Oil. $[\alpha]_D^{28}$ -29 (c, 1 in $CHCl_3$).

(1α,2α,4α,5α,8α,10β)-*form*

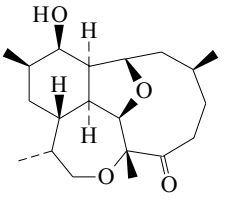
10-Epiamericanolide C
[205507-13-7]
Constit. of *Pseudopterogorgia americana*.
Oil. $[\alpha]_D^{26}$ -179.7 (c, 6.4 in $CHCl_3$). λ_{max} 218 (ε 6300) (MeOH).

(1α,2α,4α,5α,8β,10α)-*form*

8-Epiamericanolide C
[205507-15-9]
Constit. of *Pseudopterogorgia americana*.
Oil. $[\alpha]_D^{26}$ +26.3 (c, 1.5 in $CHCl_3$). λ_{max} 218 (ε 7560) (MeOH).

Rodríguez, A.D. *et al., J. Nat. Prod.*, 1996, **59**, 653-657 (*Americanolide C*)
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1998, **61**, 451-455 (*Epiamericanolides*)

2,9:3,16-Diepoxy-11-hydroxy-4-asbestinanone D-456

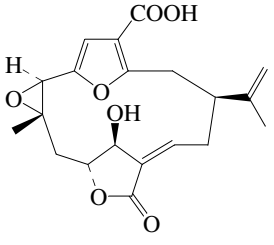


$C_{20}H_{32}O_4$ 336.47

(7β,11β)-*form*

Ac: ***Asbestinin 23***
[163564-78-1]
$C_{22}H_{34}O_5$ 378.508
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{24}$ +19.73 (c, 1.3 in $CHCl_3$).
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1994, **57**, 1638 (*isol, pmr, cmr*)

3,6:7,8-Diepoxy-11-hydroxy-3,5,12,15-cembratetraen-20,10-olid-18-oic acid D-457



$C_{20}H_{22}O_7$ 374.39

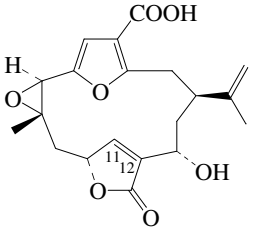
(1*S*,7*R*,8*S*,10*R*,11*S*,12*Z*)-*form*

11-Ac, Me ester: [122535-66-4]
$C_{23}H_{26}O_8$ 430.454
Constit. of *Sinularia polydactyla*. Glass. $[\alpha]_D$ -176 (c, 0.02 in $CHCl_3$). λ_{max} 204 (ϵ 9090); 246 (ϵ 3380) (EtOH).

3,4:5,6-Diepoxide: 3,4:3,6:5,6:7,8-Tetraepoxy-11-hydroxy-12,15-cembradien-20,10-olid-18-oic acid
$C_{20}H_{22}O_9$ 406.388

3ξ,4ξ:5ξ,6ξ-Diepoxide, 11-Ac, Me ester: [134455-99-5]
$C_{23}H_{26}O_{10}$ 462.452
Constit. of *Sinularia polydactyla*. Glass. $[\alpha]_D$ -132 (c, 0.0005 in $CHCl_3$). λ_{max} 210 (sh) (ϵ 12500); 220 (ϵ 12980) (EtOH).
Bowden, B.F. *et al., Aust. J. Chem.*, 1989, **42**, 757-763 (*isol, pmr, cmr*)

3,6:7,8-Diepoxy-13-hydroxy-3,5,11,15-cembratetraen-20,10-olid-18-oic acid D-458



$C_{20}H_{22}O_7$ 374.39

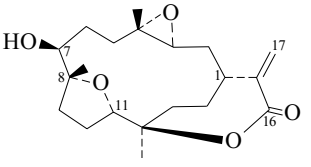
(1*S*,7*R*,8*S*,10*R*,13*S*)-*form*

13-Ac, Me ester: ***13α-Acetoxypukalide***
[122535-65-3]
$C_{23}H_{26}O_8$ 430.454
Constit. of *Sinularia polydactyla*. Cryst.
Mp 99-101.5°. $[\alpha]_D$ +22.4 (c, 0.74 in $CHCl_3$). λ_{max} 203 (ϵ 10300); 210 (sh) (ϵ 8800); 255 (ϵ 4025) (EtOH).

11β,12β-Epoxide: 3,6:7,8:11,12-Triepoxy-13-hydroxy-3,5,15-cembratrien-20,10-olid-18-oic acid
$C_{20}H_{22}O_8$ 390.389

11β,12β-Epoxide, 13-Ac, Me ester: ***13α-Acetoxy-11β,12β-epoxypukalide***
[122535-64-2]
$C_{23}H_{26}O_9$ 446.453
Constit. of *Sinularia polydactyla*. Glass. $[\alpha]_D$ -4.2 (c, 0.006 in $CHCl_3$). λ_{max} 203 (ϵ 6349); 216 (ϵ 4370); 242 (ϵ 2820) (EtOH).
Bowden, B.F. *et al., Aust. J. Chem.*, 1989, **42**, 757-763 (*isol, pmr, cmr*)
Mizobuchi, S. *et al., Fish. Sci.*, 1994, **60**, 345-346 (*isol, pmr*)

3,4:8,11-Diepoxy-7-hydroxy-15(17)-cembren-16,12-olide D-459

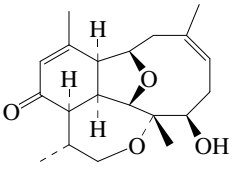


$C_{20}H_{30}O_5$ 350.454

(1*R*,3*S*,4*S*,7*S*,8*R*,11*S*,12*R*)-*form*

Ac: [87877-08-5]
$C_{22}H_{32}O_6$ 392.491
Constit. of the soft coral *Sinularia flexibilis*. Cryst. Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 149-150°. $[\alpha]_D$ +31 (c, 0.5 in MeOH).
Mori, K. *et al., Chem. Lett.*, 1983, 1515

6,13:12,16-Diepoxy-11-hydroxy-3,8-eunicelladien-2-one D-460



$C_{20}H_{28}O_4$ 332.439

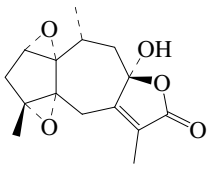
(6β,8*Z*,11β,12α,13β)-*form*

Pachyclavulariaenone D
[473882-79-0]
Cryst. Mp 94-96°. $[\alpha]_D^{29}$ +67 (c, 0.09 in $CHCl_3$). λ_{max} 229 (ϵ 11950) (EtOH aq.).

Ac: ***Pachyclavulariaenone B***
[341997-97-5]
$C_{22}H_{30}O_5$ 374.476
Constit. of *Pachyclavularia violacea*. Powder.
Mp 52-54°. $[\alpha]_D^{28}$ -1.9 (c, 2.2 in $CHCl_3$).

Butanoyl: ***Pachyclavulariaenone A***
[341997-96-4]
$C_{24}H_{34}O_5$ 402.53
Constit. of *Pachyclavularia violacea*. Oil. $[\alpha]_D^{28}$ -2.7 (c, 0.6 in $CHCl_3$).
Wang, G.-H. *et al., Tet. Lett.*, 2001, **42**, 2333-2336 (*isol, pmr, cmr*)
Wang, G.-H. *et al., J. Nat. Prod.*, 2002, **65**, 1475-1478 (*Pachyclavulariaenone D*)

1,2:4,5-Diepoxy-8-hydroxy-7(11)-guaien-12,8-olide D-461



(1α,2α,4α,5α,8α*OH*,10α)-*form*

$C_{15}H_{18}O_5$ 278.304

(1α,2α,4α,5α,8α*OH*,10α)-*form*

Me ether: ***8-Epimethoxyamericanolide A (incorr.)***
[205507-14-8]
$C_{16}H_{20}O_5$ 292.331
Constit. of *Pseudopterogorgia americana*. Oil. $[\alpha]_D^{26}$ -66.8 (c, 2.3 in $CHCl_3$). λ_{max} 214 (ϵ 7560) (MeOH).

(1α,2α,4α,5α,8β*OH*,10α)-*form*

Americanolide A
[178176-87-9]
Constit. of *Pseudopterogorgia americana*.
Semisolid.
Mp 82°. $[\alpha]_D^{28}$ -70 (c, 1 in $CHCl_3$).

Me ether: ***Methoxyamericanolide A (incorr.)***
[178176-89-1]
$C_{16}H_{20}O_5$ 292.331
Constit. of *Pseudopterogorgia americana*. Semisolid.
Mp 97°. $[\alpha]_D$ -73 (c, 1 in $CHCl_3$).

(1α,2α,4α,5α,8β*OH*,10β)-*form*

Me ether: ***10-Epimethoxyamericanolide A (incorr.)***
[205507-12-6]
$C_{16}H_{20}O_5$ 292.331
Constit. of *Pseudopterogorgia americana*. Solid ($CHCl_3$/MeOH). $[\alpha]_D^{26}$ +151.6 (c, 1.8 in $CHCl_3$). λ_{max} 214 (ϵ 8350) (MeOH).

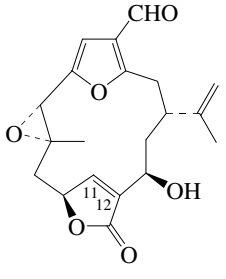
(1β,2β,3β,4β,8β*OH*,10α)-*form*

Americanolide B
[178233-21-1]
Constit. of *Pseudopterogorgia americana*.
Oil. $[\alpha]_D^{28}$ -45 (c, 1 in $CHCl_3$).

Me ether: ***Methoxyamericanolide B (incorr.)***
[178233-22-2]
$C_{16}H_{20}O_5$ 292.331
Constit. of *Pseudopterogorgia americana*. Semisolid.
Mp 96°. $[\alpha]_D^{28}$ -79 (c, 1 in $CHCl_3$). The cryst. struct. determination was unable to determine the abs. config.

Rodríguez, A.D. *et al., J. Nat. Prod.*, 1996, **59**, 653-657 (*isol, pmr, cmr*)
Richardson, P.L. *et al., Acta Cryst. C*, 1998, **54**, 66-68 (*Methoxyamericanolide B, cryst struct*)
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1998, **61**, 451-455 (*Epimethoxyamericanolides, cryst struct*)

3,6:7,8-Diepoxy-13-hydroxy-18-oxo-3,5,11,15-cembratetraen-20,10-olide D-462



$C_{20}H_{22}O_6$ 358.39

(1*R*,7*S*,8*S*,10*S*,13*R*)-*form*

Ac: ***Deepoxylophotoxin***. *Deoxylophotoxin. Deoxolophotoxin*
[134455-93-9]
$C_{22}H_{24}O_7$ 400.427
Constit. of *Lophogorgia violacea*. Called Deoxolophotoxin or Deoxylophotoxin in the lit. but Deepoxylophotoxin is more correct.

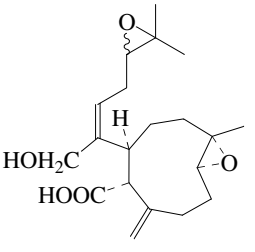
11α,12α-Epoxide, Ac: ***Lophotoxin***
[78697-56-0]
$C_{22}H_{24}O_8$ 416.427
Metab. of gorgonian corals *Lophogorgia alba, Lophogorgia cuspidata* and *Lophogorgia rigida*. Potent neuromuscular toxin. Cryst. (EtOAc/2,3,3-trimethylpentane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 164-166°. $[\alpha]_D^{27}$ +14.2 (c, 1.7 in $CHCl_3$).
► LD_{50} (mus, ipr) 8 mg/kg; LD_{50} (mus, scu) 8.9 mg/kg. XF0791000

11α,12α-Epoxide, 18-carboxylic acid, 13-Ac, Me ester: ***13-Acetoxy-11,12-epoxypukalide***. *Lopholide*
[326595-72-6]
[122535-64-2]
$C_{23}H_{26}O_9$ 446.453
Constit. of *Lophogorgia violacea* and *Leptogorgia rigida*.

18-Carboxylic acid, 13-Ac, Me ester: ***13-Acetoxypukalide***
[852459-57-5]
$C_{23}H_{26}O_8$ 430.454
Constit. of *Leptogorgia rigida*.

Fenical, W. *et al., Science (Washington, D.C.)*, 1981, **212**, 1512-1514 (*Lophotoxin, Deepoxylophotoxin, pmr, cmr*)
Jacobs, R.S. *et al., Tetrahedron*, 1985, **41**, 981-984 (*Lophotoxin, rev*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1989, **42**, 757-763 (*13-Acetoxypukalide, Lopholide*)
Abramson, S.N. *et al., J. Med. Chem.*, 1991, **34**, 1798-1804 (*activity*)
Epifanio, R. de A. *et al., J. Braz. Chem. Soc.*, 2000, **11**, 584-591 (*Deepoxylophotoxin, 13-Acetoxy-11,12-epoxypukalide*)
Gutiérrez, M. *et al., J. Nat. Prod.*, 2005, **68**, 614-616 (*Lophotoxin, cryst struct, abs config*)

6,7:13,14-Diepoxy-17-hydroxy-1(19),10-xenicadien-18-oic acid D-463



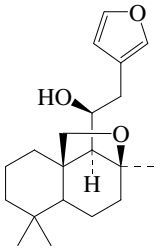
$C_{20}H_{30}O_5$ 350.454

(6α,7α,10*E*,14ξ)-*form*

Me ester, Ac: ***Xenitacin***
[479067-66-8]
$C_{23}H_{34}O_6$ 406.518
Constit. of *Xenia umbellata*. Oil. $[\alpha]_D^{25}$ +12.3 (c, 0.12 in $CHCl_3$). λ_{max} 211 (log ϵ 4.02) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1882-1885 (*isol, pmr, cmr*)

8,20:15,16-Diepoxy-13(16),14-labdadien-11-ol D-464

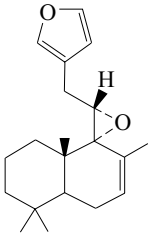


$C_{20}H_{30}O_3$ 318.455

(8β,11*S*)-*form*
Cacofuran B
[383413-08-9]
Constit. of a *Cacospongia* sp.
Cryst. (EtOAc/hexane).
Mp 141-145°. $[\alpha]_D$ -15 (c, 2 in CH_2Cl_2).

Ac: ***Cacofuran A***
[383413-07-8]
$C_{22}H_{32}O_4$ 360.492
Constit. of a *Cacospongia* sp. Glass. $[\alpha]_D$ -30 (c, 0.4 in CH_2Cl_2).
Tanaka, J. *et al., J. Nat. Prod.*, 2001, **64**, 1468-1470 (*isol, pmr, cmr, cryst struct*)

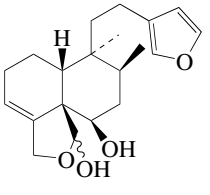
9,11:15,16-Diepoxy-7,13(16),14-labdatriene D-465



$C_{20}H_{28}O_2$ 300.44

(9α,11*S*)-*form*
Ghiselinin
[79827-31-9]
Constit. of the nudibranch *Hypselodoris ghiselinii*.
Oil. $[\alpha]_D$ +7.5 (c, 0.27 in MeOH).
Hochlowski, J.E. *et al., J.O.C.*, 1982, **47**, 88-91 (*isol, pmr, cmr*)

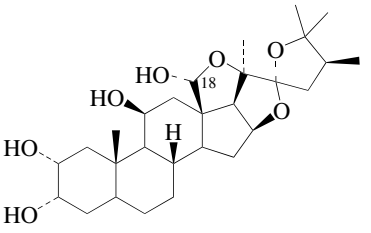
15,16:18,19-Diepoxy-3,13(16),14-labdatriene-6,19-diol D-466



$C_{20}H_{28}O_4$ 332.439

(*ent*-5α,6α,8α,19ξ)-*form*
Raspailol
[224778-76-1]
Constit. of a *Raspailia* sponge.
Oil. $[\alpha]_D$ +32.7 (c, 1.15 in MeOH). λ_{max} 206 (ε 10000) (MeOH).
West, L.M. *et al., Aust. J. Chem.*, 1998, **51**, 1097-1101 (*isol, pmr, cmr*)

18,20:22,25-Diepoxy-24-methylfurostane-2,3,11,18-tetrol D-467



$C_{28}H_{44}O_7$ 492.651

(2α,3α,5α,11β,18*R*,20*R*,22*S*,24*S*)-*form*
2,3-Di-Ac: [858950-54-6]
$C_{32}H_{48}O_9$ 576.726
Constit. of *Isis hippuris*. Powder.
Mp 273-275°. $[\alpha]_D$ -23 (c, 0.38 in $CHCl_3$).

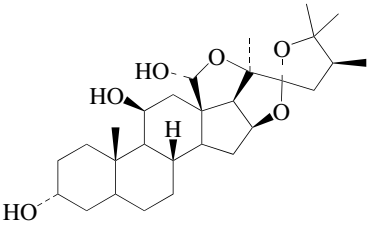
18-Ketone (lactone): ***22,25-Epoxy-2,3,11-trihydroxy-24-methyl-furostan-18,20-olide***
[858950-36-4]
$C_{28}H_{42}O_7$ 490.636
Constit. of *Isis hippuris*. Powder.
Mp 253-254°. $[\alpha]_D$ -27 (c, 0.92 in $CHCl_3$).

18-Ketone (lactone), 2-Ac: [858950-38-6]
$C_{30}H_{44}O_8$ 532.673
Constit. of *Isis hippuris*. Powder.
Mp 204-205°. $[\alpha]_D$ -17 (c, 1.28 in $CHCl_3$).

18-Ketone (lactone), 3-Ac: [858950-40-0]
$C_{30}H_{44}O_8$ 532.673
Constit. of *Isis hippuris*. Powder.
Mp 244-245°. $[\alpha]_D$ +4 (c, 1.4 in $CHCl_3$).

18-Ketone (lactone), 2,3-di-Ac: [858950-34-2]
$C_{32}H_{46}O_9$ 574.71
Constit. of *Isis hippuris*. Powder.
Mp 270-272°. $[\alpha]_D$ -8 (c, 0.32 in $CHCl_3$).
Chao, C.-H. *et al., J. Nat. Prod.*, 2005, **68**, 880-885 (*Isis hippuris constits*)

18,20:22,25-Diepoxy-24-methylfurostane-3,11,18-triol D-468

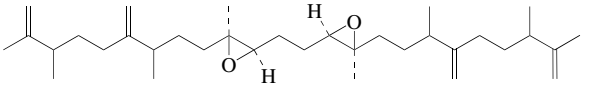


$C_{28}H_{44}O_6$ 476.652

(3α,5α,11β,18*R*,20*R*,22*S*,24*S*)-*form*
3-Ac: [858950-52-4]
$C_{30}H_{46}O_7$ 518.689
Constit. of *Isis hippuris*. Powder.
Mp 269-271°. $[\alpha]_D$ -43 (c, 0.31 in $CHCl_3$).
Chao, C.-H. *et al., J. Nat. Prod.*, 2005, **68**, 880-885 (*Isis hippuris constit*)

10,11:14,15-Diepoxy-2,3,7,10,15,18,22,23-octamethyl-6,19-dimethylene-1,23-tetracosadiene D-469

[220719-38-0]

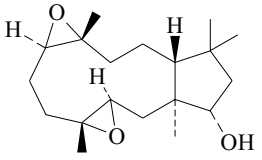


$C_{34}H_{58}O_2$ 498.831

Constit. of *Botryococcus braunii*. Oil. $[\alpha]_D^{20}$ -2 (c, 0.35 in heptane).

Metzger, P. *et al., Tetrahedron*, 1999, **55**, 167-176 (*isol, pmr, cmr*)

3,4:7,8-Diepoxy-1,4,8,12,12-pentamethylbicyclo[9.3.0]tetradecan-14-ol D-470



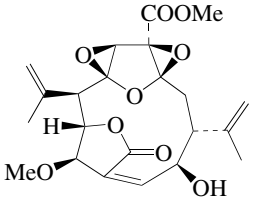
$C_{19}H_{32}O_3$ 308.46

Constit. of *Dictyota pardarlis*. Oil. $[\alpha]_D^{25}$ +40.8 (c, 0.12 in $CHCl_3$).

Wright, A.D. *et al., Helv. Chim. Acta*, 1991, **74**, 1801 (*isol, pmr, cmr*)

β,β-Diepoxypseudopterolide methanol adduct D-471

[203575-50-2]



$C_{22}H_{26}O_9$ 434.442

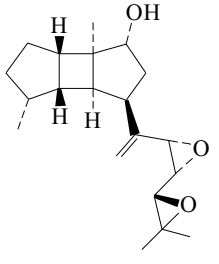
Constit. of *Pseudopterogorgia acerosa*. Yellow oil. $[\alpha]_D^{25}$ +4 (c, 3.5 in $CHCl_3$). λ_{max} 246 (ϵ 1890) ($CHCl_3$).

Rodriguez, A.D. *et al., J. Nat. Prod.*, 1998, **61**, 401-404 (*isol, pmr, cmr*)

15,16:17,18-Diepoxy-13-spaten-5-ol D-472

Spatol

[76520-52-0]



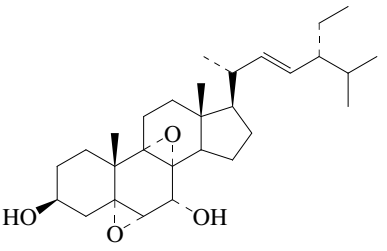
$C_{20}H_{30}O_3$ 318.455

Constit. of *Spatoglossum schmittii*. Cryst.

Mp 100-102°. $[\alpha]_D$ +45.6 (c, 1.6 in $CHCl_3$).

Gerwick, W.H. *et al., J.O.C.*, 1983, **48**, 3325 (*isol, cryst struct*)
Salomon, R.G. *et al., J.A.C.S.*, 1991, **113**, 3096 (*synth*)
Murthi, K.K. *et al., Tet. Lett.*, 1994, **35**, 517 (*synth*)
Tanaka, M. *et al., Tetrahedron*, 1994, **50**, 12843 (*synth*)

5,6:8,9-Diepoxystigmast-22-ene-3,7-diol D-473



$C_{29}H_{46}O_4$ 458.68

(3β,5α,6α,7α,8α,9α,22*E*,24*R*)-*form*

Homaxisterol B₂

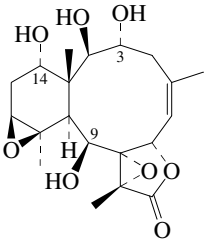
[877373-34-7]

Constit. of a *Homaxinella* sp.

Amorph. solid.

Mansoor, T.A. *et al., J. Nat. Prod.*, 2006, **69**, 131-134 (*Homaxisterol B₂*)

8,17:11,12-Diepoxy-2,3,9,14-tetrahydroxy-5-briaren-18,7-olide D-474



$C_{20}H_{28}O_8$ 396.436

(2β,3α,5*Z*,7α,8α,9β,11β,12β,14α,17α)-*form*

3,9,14-Tri-Ac: ***Brianthein C***

[383366-83-4]

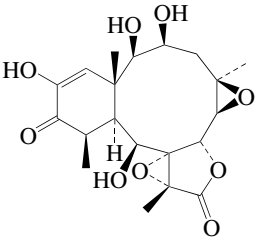
$C_{26}H_{34}O_{11}$ 522.548

Constit. of *Briareum excavatum*.

$[\alpha]_D^{20}$ +32.6 (c, 0.4 in EtOH).

Aoki, S. *et al., Tetrahedron*, 2001, **57**, 8951-8957 (*isol, pmr, cmr*)

5,6:8,17-Diepoxy-2,3,9,13-tetrahydroxy-12-oxo-13-briaren-18,7-olide D-475



$C_{20}H_{26}O_9$ 410.42

Enolised α-diketone.

(2β,3β,5β,6β,7α,8α,9β,17α)-*form*

2,3,9-Tri-Ac: ***Briaexcavatolide X***

[782496-58-6]

$C_{26}H_{32}O_{12}$ 536.532

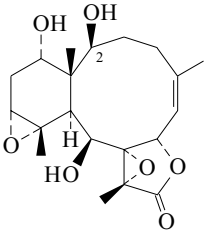
Constit. of *Briareum excavatum*. Powder.

Mp 220-221°. $[\alpha]_D^{25}$ -39 (c, 0.2 in $CHCl_3$). Struct. revised in 2006.

λ_{max} 241 (log ϵ 3.39) (MeOH).

13-Deoxy, 3-butanoyl, 2,9-di-Ac: ***Briaexcavatin C***
[899436-65-8]
$C_{28}H_{36}O_{11}$ 548.586
Constit. of *Briareum excavatum*. Powder.
Mp 79-81°. $[\alpha]_D^{25}$ -25 (c, 0.4 in $CHCl_3$).
Sung, P.-J. *et al., Tetrahedron*, 2004, **60**, 8975-8979 (*Briaexcavatolide X*)
Sung, P.-J. *et al., Tetrahedron*, 2006, **62**, 5686-5691 (*Briaexcavatin C*)

8,17:11,12-Diepoxy-2,9,14-trihydroxy-5-briaren-18,7-olide D-476

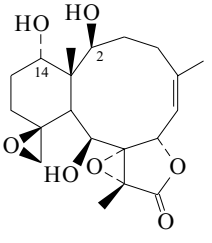


$C_{20}H_{28}O_7$ 380.437

Tri-Ac: ***Briareolide D***
[132750-56-2]
$C_{26}H_{34}O_{10}$ 506.549
Constit. of *Briareum* sp. Antiinflammatory agent. Gum.

2-Butanoyl, 9,14-di-Ac: ***Briareolide C***
[132750-55-1]
$C_{28}H_{38}O_{10}$ 534.602
Constit. of a *Briareum* sp. Antiinflammatory agent. Powder (Me_2CO/hexane).
Mp 139-140°.
Pordesimo, E.O. *et al., J.O.C.*, 1991, **56**, 2344 (*isol, pmr, cmr*)

8,17:11,20-Diepoxy-2,9,14-trihydroxy-5-briaren-18,7-olide D-477

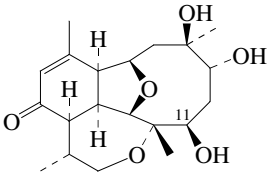


$C_{20}H_{28}O_7$ 380.437
The opposite abs. config. has been tentatively assigned; see note under 8,17-Epoxy-2,9,12,14-tetrahydroxy-5,11(20)-briaradien-18,7-olide, E-528.

2,14-Di-Ac: 2,14-Diacetoxy-8,17:11,20-diepoxy-9-hydroxy-5-briaren-18,7-olide
[126636-51-9]
$C_{24}H_{32}O_9$ 464.511
Isol. from *Junceella gemmacea*. Oil. $[\alpha]_D$ +57.1 (c, 0.16 in $CHCl_3$).

Tri-Ac: ***Umbraculolide B***
[288850-27-1]
$C_{26}H_{34}O_{10}$ 506.549
Constit. of *Gorgonella umbraculum*. Plates ($CHCl_3$).
Mp 220°. $[\alpha]_D^{27}$ +14 (c, 0.2 in $CHCl_3$).
Bowden, B.F. *et al., Aust. J. Chem.*, 1990, **43**, 151 (*isol, pmr, cmr*)
Subrahmanyam, C. *et al., Tetrahedron*, 2000, **56**, 4585-4588 (*Umbraculolide B*)

6,13:12,16-Diepoxy-8,9,11-trihydroxy-3-eunicellen-2-one D-478



$C_{20}H_{30}O_6$ 366.453

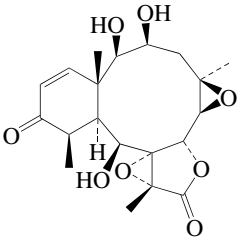
(6β,8β,9α,11β,12α,13β)-form
Pachyclavulariaenone G
[473882-82-5]
Constit. of *Pachyclavularia violacea*.
Cryst.
Mp 189-192°. $[\alpha]_D^{29}$ +14 (c, 0.43 in $CHCl_3$). λ_{max} 229 (ε 10834) (EtOH aq.).

9-Ac: ***Pachyclavulariaenone F***
[473882-81-4]
$C_{22}H_{32}O_7$ 408.491
Constit. of *Pachyclavularia violacea*. Cryst.
Mp 87-90°. $[\alpha]_D^{29}$ +41 (c, 1.74 in $CHCl_3$). λ_{max} 229 (ε 11028) (EtOH aq.).

11-Ac: ***Pachyclavulariaenone C***
[341997-98-6]
$C_{22}H_{32}O_7$ 408.491
Constit. of *Pachyclavularia violacea*. Cryst.
Mp 220-223°. $[\alpha]_D^{27}$ -82 (c, 0.5 in $CHCl_3$).

9,11-Di-Ac: ***Pachyclavulariaenone E***
[473882-80-3]
$C_{24}H_{34}O_8$ 450.528
Constit. of *Pachyclavularia violacea*. Cryst.
Mp 97-99°. $[\alpha]_D^{29}$ +31 (c, 0.33 in $CHCl_3$). λ_{max} 229 (ε 10880) (EtOH aq.).
Wang, G.-H. *et al., Tet. Lett.*, 2001, **42**, 2333-2336 (*Pachyclavulariadienone C, isol, pmr, cmr, cryst struct*)
Wang, G.H. *et al., J. Nat. Prod.*, 2002, **65**, 1475-1478 (*Pachyclavuloriaenones E,F,G, cryst struct*)

5,6:8,17-Diepoxy-2,3,9-trihydroxy-12-oxo-13-briaren-18,7-olide D-479

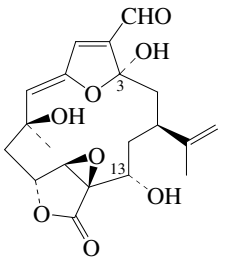


$C_{20}H_{26}O_8$ 394.421

(2β,3β,5β,6α,7α,8α,9β,17α)-form

2,3,9-Tri-Ac: ***Briaexcavatolide Y***
[782496-60-0]
$C_{26}H_{32}O_{11}$ 520.532
Constit. of *Briareum excavatum*. Powder.
Mp 119-121°. $[\alpha]_D^{25}$ -15 (c, 0.7 in $CHCl_3$). Struct. revised in 2006.
λ_{max} 226 (log ε 3.62) (MeOH).
Sung, P.-J. *et al., Tetrahedron*, 2004, **60**, 8975-8979 (*isol, pmr, cmr*)
Sung, P.-J. *et al., Tetrahedron*, 2006, **62**, 5686-5691 (*struct*)

3,6:11,12-Diepoxy-3,8,13-trihydroxy-18-oxo-4,6,15-cembratrien-20,10-olide D-480

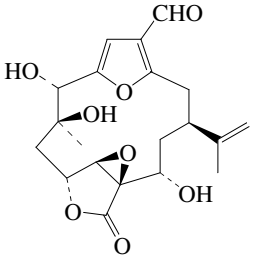


$C_{20}H_{24}O_8$ 392.405

(1*S*,3*R*,6*Z*,8*S*,11*R*,12*R*,13*S*)-*form*

3-Me ether, 13-Ac: 3-Methoxy-8-hydroxylophotoxin (incorr.)
[326595-74-8]
$C_{23}H_{28}O_9$ 448.469
Constit. of *Lophogorgia violacea*. Amorph. solid.
Mp 172-175°. $[\alpha]_D^{25}$ -190 (c, 1 in $CHCl_3$).
Epifanio, R. de A. *et al., J. Braz. Chem. Soc.*, 2000, **11**, 584-591 (*isol, pmr, cmr*)

3,6:11,12-Diepoxy-7,8,13-trihydroxy-18-oxo-3,5,15-cembratrien-20,10-olide D-481

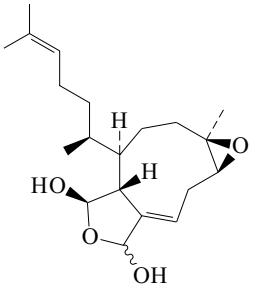


$C_{20}H_{24}O_8$ 392.405

(1*S*,7*S*,8*S*,11*R*,12*R*,13*S*)-*form*

7,13-Di-Ac: 7-Acetoxy-8-hydroxylophotoxin (incorr.)
[326595-73-7]
$C_{24}H_{28}O_{10}$ 476.479
Constit. of *Lophogorgia violacea*. Cryst. (EtOAc/hexane).
Mp 254-258°. $[\alpha]_D^{25}$ -13 (c, 1 in $CDCl_3$).
Epifanio, R. de A. *et al., J. Braz. Chem. Soc.*, 2000, **11**, 584-591 (*isol, pmr, cmr*)

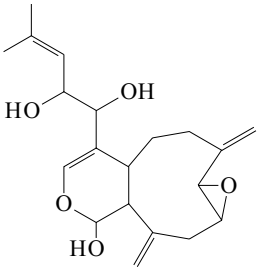
6,7:18,19-Diepoxy-1(9),13-xenicadiene-18,19-diol D-482



$C_{20}H_{32}O_4$ 336.47

Di-Me ether: ***Dictyoepoxide***
[152340-06-2]
$C_{22}H_{36}O_4$ 364.524
Constit. of a *Dictyota* sp. Vasopressin receptor antagonist. Norepinephrin inhibitor. Oil.
Patil, A.D. *et al., Phytochemistry*, 1993, **33**, 1061 (*isol, pmr, cmr*)

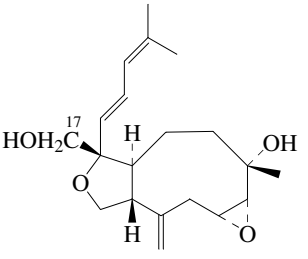
7,8:17,18-Diepoxy-1(19),6(20),10(17),13-xenicatetraene-11,12,18-triol D-483



$C_{20}H_{28}O_5$ 348.438

Tri-Ac: ***Bisdeoxyhavannahin***
$C_{26}H_{34}O_8$ 474.55
Constit. of *Xenia membranacea*. Amorph.
Almourabit, A. *et al., J. Nat. Prod.*, 1990, **53**, 894 (*isol, pmr*)

7,8:10,18-Diepoxy-1(19),11,13-xenicatriene-6,17-diol D-484



$C_{20}H_{30}O_4$ 334.455

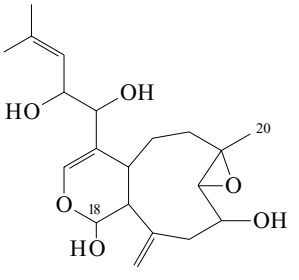
(6α,7α,8α)-*form*

Xeniaether C
[178802-76-1]
Constit. of a *Xenia* sp.
Oil. $[\alpha]_D$ -37.5 (c, 0.07 in MeOH).

17-Octadecanoyl: ***Xeniaether D***
[178802-77-2]
$C_{38}H_{64}O_5$ 600.921
Constit. of a *Xenia* sp. Oil. $[\alpha]_D$ -30 (c, 0.14 in MeOH).

17-Hexadecanoyl: ***Xeniaether E***
[178802-78-3]
$C_{36}H_{60}O_5$ 572.867
Constit. of a *Xenia* sp. Oil. $[\alpha]_D$ -43 (c, 0.03 in MeOH).
Iwagawa, T. *et al., Heterocycles*, 1996, **43**, 1271-1277 (*isol, pmr, cmr*)

6,7:17,18-Diepoxy-1(19),10(17),13-xenicatriene-8,11,12,18-tetrol D-485



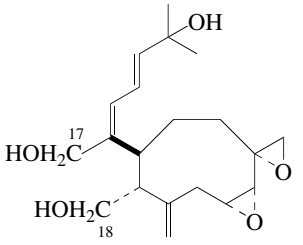
$C_{20}H_{30}O_6$ 366.453

11,12,18-Tri-Ac: ***9-Desacetyl-7,8-epoxyxenicin***
$C_{26}H_{36}O_9$ 492.565
Constit. of *Xenia membranacea*. Amorph. $[\alpha]_D$ +49 (c, 0.5 in $CHCl_3$).

20-Acetoxy, 11,12,18-tri-Ac: ***18-Acetoxy-9-deacetyl-7,8-epoxyxenicin***
$C_{28}H_{38}O_{11}$ 550.602
Constit. of *Xenia membranacea*. Amorph. $[\alpha]_D$ +29 (c, 0.5 in $CHCl_3$).

Almourabit, A. *et al., J. Nat. Prod.*, 1990, **53**, 894 (*isol, pmr, cmr*)

6,20:7,8-Diepoxy-1(19),10,12-xenicatriene-14,17,18-triol D-486

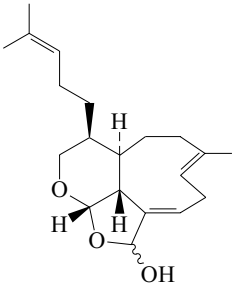


$C_{20}H_{30}O_5$ 350.454

(6α,7α,8α)-*form*

17-Octadecanoyl, 18-Ac: ***Azamilide J***
[178802-81-8]
$C_{40}H_{66}O_7$ 658.957
Constit. of a *Xenia* sp. Oil. $[\alpha]_D$ -79 (c, 0.08 in MeOH).
Iwagawa, T. *et al., Heterocycles*, 1996, **43**, 1271-1277 (*isol, pmr, cmr*)

17,18:18,19-Diepoxy-1(9),6,13-xenicatrien-19-ol D-487

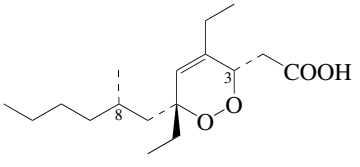


$C_{20}H_{30}O_3$ 318.455

Me ether: 17,18:18,19-Diepoxy-19-methoxy-1(9),6,13-xenicatriene
$C_{21}H_{32}O_3$ 332.482
Metab. of *Dictyota divaricata*. Oil. $[\alpha]_D^{25}$ -138.6 (c, 0.51 in $CHCl_3$).
König, G.M. *et al., Phytochemistry*, 1991, **30**, 3679 (*isol, pmr, cmr*)

4,6-Diethyl-3,6-dihydro-6-(2-methylhexyl)-1,2-dioxin-3-acetic acid D-488

4,6-Diethyl-3,6-epidioxy-8-methyl-4-dodecenoic acid



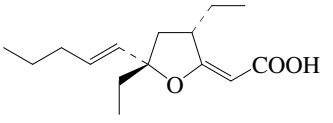
$C_{17}H_{30}O_4$ 298.422

(3*S*,6*R*,8*S*)-*form* [206443-24-5]
Isol. from the sponge *Plakortis* aff. *angulospiculatus.*
Oil. $[\alpha]_D$ -19.8 (c, 0.9 in $CHCl_3$).

Me ester: [206443-27-8]
$C_{18}H_{32}O_4$ 312.448
Isol. from *Plakortis* aff. *angulospiculatus.* Oil. $[\alpha]_D$ -21.1 (c, 0.4 in $CHCl_3$).

Et ester: [211757-32-3]
$C_{19}H_{34}O_4$ 326.475
Isol. from a *Plakortis* sp. Amorph. solid. $[\alpha]_D^{20}$ -25 (c, 0.1 in hexane). Config. not determined.
Braekman, J.C. *et al., J. Nat. Prod.*, 1998, **61**, 1038-1042 (*isol, pmr, cmr*)
Compagnone, R.S. *et al., Tetrahedron*, 1998, **54**, 3057-3068 (*isol, ir, pmr, cmr, ms*)

[3,5-Diethyldihydro-5-(1-pentenyl)-2(5*H*)-furanylidene]acetic acid D-489

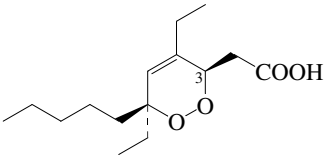


$C_{15}H_{24}O_3$ 252.353

Et ester: [68914-61-4]
$C_{17}H_{28}O_3$ 280.406
Isol. from *Chondrosia collectrix*.
$[\alpha]_D^{20}$ -116 (c, 1.4 in CCl_4). Possible artifact. λ_{max} 244 (ϵ 11500) (MeOH).
Stierle, D.B. *et al., J.O.C.*, 1979, **44**, 964-968 (*isol, pmr, cmr*)

4,6-Diethyl-3,6-dihydro-6-pentyl-1,2-dioxin-3-acetic acid D-490

4,6-Diethyl-3,6-epidioxy-4-undecenoic acid



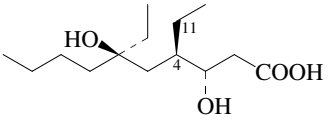
$C_{15}H_{26}O_4$ 270.368

(3*R,6*S**)-*form***

Me ester:
$C_{16}H_{28}O_4$ 284.395
Isol. from *Plakortis simplex*.
Holzworth, M. *et al., J. Nat. Prod.*, 2005, **68**, 759-761 (*isol, pmr, cmr, ms*)

4,6-Diethyl-3,6-dihydroxydecanoic acid D-491

Secoplakortide Z



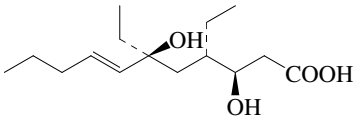
$C_{14}H_{28}O_4$ 260.373

Et ester: ***Ethyl secoplakortide Z***
[211632-57-4]
$C_{16}H_{32}O_4$ 288.426
Isol. from the sponge *Plakortis lita*. Gold oil. $[\alpha]_D^{25}$ -24.2 (c, 1.1 in CH_2Cl_2).

4,11-Didehydro, Et ester: Ethyl 6-ethyl-4-ethylidene-3,6-dihydroxydecanoate. ***Ethyl didehydrosecoplakortide Z***
[211632-61-0]
$C_{16}H_{30}O_4$ 286.411

Isol. from the sponge *Plakortis lita*.
Harrison, B. *et al., J. Nat. Prod.*, 1998, **61**, 1033-1037

4,6-Diethyl-3,6-dihydroxy-7-undecenoic acid D-492

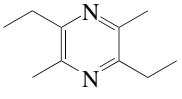


$C_{15}H_{28}O_4$ 272.384

(3*R*,4*S*,6*S*,7*E*)-*form*
Et ester: [68914-62-5]
[68964-12-5]
$C_{17}H_{32}O_4$ 300.437
Isol. from *Chondrosia collectrix*.
$[\alpha]_D^{20}$ +0.32 (c, 1.3 in CCl_4). Possible artifact.
Stierle, D.B. *et al., J.O.C.*, 1979, **44**, 964-970 (*isol, pmr, cmr*)

2,5-Diethyl-3,6-dimethylpyrazine D-493

[18903-30-5]



$C_{10}H_{16}N_2$ 164.25
Isol. from an arctic marine bacterium. Liq. Bp 214-217° Bp_2 65°.
Octahydrate: Mp 48-50°.
Asinger, F. *et al., Monatsh. Chem.*, 1959, **90**, 402-416 (*synth*)
Baltes, W. *et al., J. Agric. Food Chem.*, 1987, **35**, 340-346 (*occur, coffee, ms*)
Rizzi, G.P. *et al., J. Agric. Food Chem.*, 1988, **36**, 349-352 (*synth, ms, pmr, uv*)
Silwar, R. *et al., Z. Lebensm.-Unters. -Forsch.*, 1992, **195**, 112-119 (*occur*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol*)

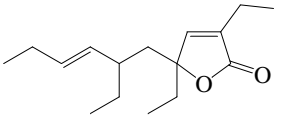
2,6-Diethyl-3,5-dimethylpyrazine D-494

[18940-74-4]

$C_{10}H_{16}N_2$ 164.25
Isol. from an arctic marine bacterium. Characterised spectroscopically.
Baltes, W. *et al., J. Agric. Food Chem.*, 1987, **35**, 340-346 (*occur, coffee, ms*)
Rizzi, G.P. *et al., J. Agric. Food Chem.*, 1988, **36**, 349-352 (*occur, ms, uv*)
Silwar, R. *et al., Z. Lebensm.-Unters. -Forsch.*, 1992, **195**, 112-119 (*occur*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol*)

3,5-Diethyl-5-(2-ethyl-3-hexenyl)-2(5*H*)-furanone D-495

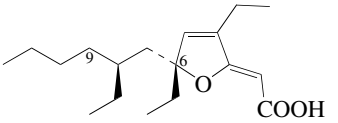
[74096-83-6]



$C_{16}H_{26}O_2$ 250.38
Constit. of *Plakortis halichondrioides*.
Stierle, D.B. *et al., J.O.C.*, 1980, **45**, 3396-3401 (*isol, pmr*)

[3,5-Diethyl-5-(2-ethylhexyl)-2(5*H*)-furanylidene]acetic acid D-496

3,6-Epoxy-4,6,8-triethyl-2,4-dodecadienoic acid

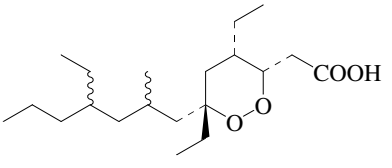


$C_{18}H_{30}O_3$ 294.433

(2*Z*,6*R*,8*S*)-*form*
Me ester: [206443-26-7]
$C_{19}H_{32}O_3$ 308.46
Isol. from the sponge *Plakortis* aff. *angulospiculatus*. Oil. $[\alpha]_D$ -78 (c, 0.2 in $CHCl_3$). λ_{max} 285 (ϵ 8900) (MeOH) (Berdy).
*9,10-Didehydro(*E-*), Me ester:* [74096-82-5]
$C_{19}H_{30}O_3$ 306.444
Isol. from the sponge *Plakortis halichondrioides*.
$[\alpha]_D$ -175 (c, 1.4 in CCl_4).
Schmidt, E.W. *et al., Tet. Lett.*, 1996, **37**, 6681-6684 (*didehydro Me ester*)
Compagnone, R.S. *et al., Tetrahedron*, 1998, **54**, 3057-3068 (*isol, ir, pmr, cmr, ms*)
Akiyama, M. *et al., Tet. Lett.*, 2005, **46**, 7483-7485 (*didehydro Me ester, synth*)

4,6-Diethyl-6-(4-ethyl-2-methylheptyl)-1,2-dioxane-3-acetic acid D-497

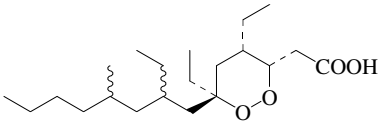
3,6-Epidioxy-4,6,10-triethyl-8-methyltridecanoic acid. ***14-Norplakortide Q***



$C_{20}H_{38}O_4$ 342.518
Isol. from the sponge *Plakortis zyggompha*. Oil (as Me ester).
$[\alpha]_D^{22}$ -128 (c, 0.1 in $CHCl_3$) (Me ester).
*11,12-Didehydro(*E-*):* ***11,12-Didehydro-14-norplakortide Q***
$C_{20}H_{36}O_4$ 340.502
Isol. from *Plakortis zyggompha*. Oil (as Me ester).
Berrué, F. *et al., Tetrahedron*, 2005, **61**, 11843-11849 (*isol, pmr, cmr*)

4,6-Diethyl-6-(2-ethyl-4-methyloctyl)-1,2-dioxane-3-acetic acid D-498

3,6-Epidioxy-4,6,8-triethyl-10-methyltetradecanoic acid
[211757-34-5]

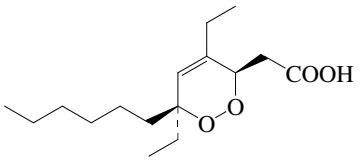


Absolute Configuration

$C_{21}H_{40}O_4$ 356.545
Isol. from *Plakortis* sp. Amorph. solid. $[\alpha]_D^{20}$ -168 (c, 1.5 in CH_2Cl_2).
Braekman, J.C. *et al., J. Nat. Prod.*, 1998, **61**, 1038-1042

4,6-Diethyl-6-hexyl-3,6-dihydro-1,2-dioxin-3-acetic acid D-499

4,6-Diethyl-3,6-epidioxy-4-dodecenoic acid



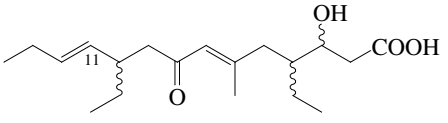
$C_{16}H_{28}O_4$ 284.395

(3*R,6*S**)-*form***

Me ester:
$C_{17}H_{30}O_4$ 298.422
Isol. from *Plakortis simplex*.

Holzworth, M. *et al., J. Nat. Prod.*, 2005, **68**, 759-761 (*isol, pmr, cmr, ms*)

4,10-Diethyl-3-hydroxy-6-methyl-8-oxo-6,11-tetradecadienoic acid D-500



$C_{19}H_{32}O_4$ 324.459

(3ξ,4ξ,6*E*,10ξ,11*E*)-*form*

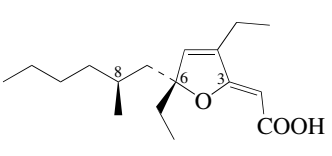
[874190-06-4 (Me ester)]
Constit. of the sponge *Plakortis simplex*.
Oil (as Me ester). $[\alpha]_D^{25}$ +25.1 (c, 1.5 in $CHCl_3$) (Me ester).
λ_{max} 235 (ϵ 18500) (MeCN) (Me ester).

11,12-Dihydro: 4,10-Diethyl-3-hydroxy-6-methyl-8-oxo-6-tetradecenoic acid
[874190-08-6 (Me ester)]
$C_{19}H_{34}O_4$ 326.475
Constit. of *Plakortis simplex*. Oil (as Me ester). $[\alpha]_D^{25}$ +23.3 (c, 0.9 in $CHCl_3$) (Me ester). λ_{max} 235 (ϵ 18500) (MeCN) (Me ester).

Campagnuolo, C. *et al., Eur. J. Org. Chem.*, 2005, 5077-5083 (*isol, pmr, cmr*)

[3,5-Diethyl-5-(2-methylhexyl)-2(5*H*)-furanylidene]acetic acid D-501

3,6-Epoxy-4,6-diethyl-8-methyl-2,4-dodecadienoic acid



$C_{17}H_{28}O_3$ 280.406

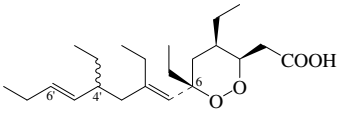
(2*Z*,6*R*,8*S*)-*form*

Me ester: [206443-25-6]
$C_{18}H_{30}O_3$ 294.433
Isol. from the sponge *Plakortis* aff. *angulospiculatus*. Oil. $[\alpha]_D$ -92 (c, 1.1 in $CHCl_3$). λ_{max} 285 (ϵ 8900) (MeOH). λ_{max} 285 (ϵ 11000); 293 (ϵ 9000) (MeOH) (Berdy).

Braekman, J.C. *et al., J. Nat. Prod.*, 1998, **61**, 1038-1042 (*isol, pmr, cmr*)
Compagnone, R.S. *et al., Tetrahedron*, 1998, **54**, 3057-3068 (*isol, ir, pmr, cmr, ms*)

6-(2,4-Diethyl-1,5-octadienyl)-4,6-diethyl-1,2-dioxane-3-acetic acid, 9CI D-502

3,6-Epidioxy-4,6,8,10-tetraethyl-7,11-tetradecadienoic acid



(1′*E*,3*R*,4*R*,4′ξ,5′*E*,6*S*)-*form*

$C_{22}H_{38}O_4$ 366.54

(1′*E*,3*R*,4*R*,4′ξ,5′*E*,6*S*)-*form* [202343-59-7]
Isol. from the sponge *Plakortis* sp.
Oil. $[\alpha]_D^{23}$ +49.8 (c, 0.2 in $CHCl_3$) (as Me ester).

5′,6′-Dihydro: ***6-(2,4-Diethyl-1-octenyl)-4,6-diethyl-1,2-dioxane-3-acetic acid***. *3,6-Epidioxy-4,6,8,10-tetraethyl-7-tetradecenoic acid* [202343-43-9]
$C_{22}H_{40}O_4$ 368.556
Isol. from a *Plakortis* sp. Oil (as Me ester). $[\alpha]_D^{23}$ +12.4 (c, 0.4 in $CHCl_3$) (Me ester).

(1′*E*,3*S*,4*R*,4′*R*,5′*E*,6*S*)-*form* [202214-86-6]
Isol. from the sponge *Plakortis* sp.
Pale yellow oil. $[\alpha]_D^{25}$ +76.2 (c, 1.6 in $CHCl_3$).

5′,6′-Dihydro: Isol. from *Plakortis* sp.
Pale yellow oil (as Me ester). $[\alpha]_D^{23}$ +55 (c, 0.56 in $CHCl_3$) (Me ester).

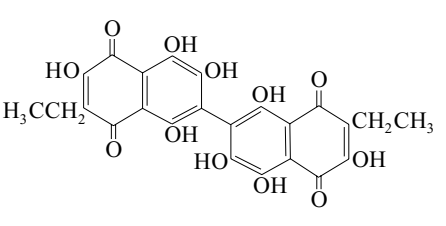
(1′*E*,3*S*,4*S*,4′*R*,5′*E*,6*R*)-*form*
Plakortide P. *Plakortide N (obsol.)*†
[552334-12-0]
Isol. from *Plakortis halichondrioides*.
Oil. $[\alpha]_D^{24}$ -275 (c, 0.52 in $CHCl_3$). Suffix letter changed from N to P to avoid duplication.

(1′*E*,3*R*,4*R*,4ξ,5′*E*,6ξ)-*form* [206554-08-7]
Isol. from *Plakortis* aff. *angulospiculatus*.
Oil. $[\alpha]_D$ +164 (c, 2.4 in $CHCl_3$).

Fontana, A. *et al., J. Nat. Prod.*, 1998, **61**, 1427-1429 (*isol, ir, pmr, cmr*)
Fontana, A. *et al., Tetrahedron*, 1998, **54**, 2041-2048 (*isol, ir, pmr, cmr*)
Compagnone, R.S. *et al., Tetrahedron*, 1998, **54**, 3057-3068 (*isol, ir, pmr, cmr, ms*)
Jiménez, M. de S. *et al., J. Nat. Prod.*, 2003, **66**, 655-661; 1404 (*Plakortide P*)

3,3′-Diethyl-2,2′,5,5′,7,7′,8,8′-octahydroxy-6,6′-bi-1,4-naphthoquinone D-503

6,6′-Bi[3-ethyl-2,7-dihydroxynaphthazarin]

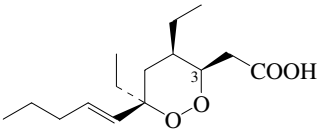


$C_{24}H_{18}O_{12}$ 498.399
Isol. from the deep sea holuthuroids *Psychropotes longicauda*, *Benthodytes typica* and *Benthodytes lingua*. Also from the lichen *Cetraria islandica* var. *polaris*. Fine raspberry-coloured cryst. (C_6H_6).
Mp 155-157°. V. small amount isolated. λ_{max} 216 (log ϵ 4.42); 238 (log ϵ 4.45); 270 (sh) (log ϵ 4.2); 318 (log ϵ 3.97); 452 (sh) (log ϵ 3.72); 514 (log ϵ 3.85); 552 (sh) (log ϵ 3.65) (MeOH).

Marshall, D.S. *et al., Ph.D. Thesis*, University of Aberdeen, 1984, (*isol, uv, pmr, ms*)
Stepanenko, L.S. *et al., Phytochemistry*, 1997, **46**, 565-568 (*isol, uv, ir, pmr, cmr, ms*)

4,6-Diethyl-6-(1-pentenyl)-1,2-dioxane-3-acetic acid D-504

3,6-Epidioxy-4,6-diethyl-7-undecenoic acid



(3*R**,4*R**,6*R**,7*E*)-*form*

$C_{15}H_{26}O_4$ 270.368

(3*R*,4*R*,6*R*,7*E*)-*form* [68914-70-5]
[77123-30-9, 77123-31-0]
Isol. from the sponge *Chondrosia collectrix*.

Me ester: [68914-69-2]
[68964-13-6]
$C_{16}H_{28}O_4$ 284.395
Isol. from the sponge *Chondrosia collectrix*.

(3*R*,4*R*,6*S*,7*E*)-*form*
Plakortide L
[397033-69-1]
Isol. from a Jamaican *Plakortis* sp.
Oil. $[\alpha]_D^{25}$ -44 (c, 0.2 in $CHCl_3$).

Me ester: ***Plakortide K***
[397033-64-6]
$C_{16}H_{28}O_4$ 284.395
Isol. from a *Plakortis* sp. Oil. $[\alpha]_D^{25}$ -116 (c, 0.5 in $CHCl_3$).

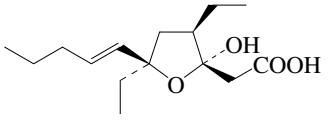
(3*R*,4*S*,6*S*,7*E*)-*form* [68964-55-6]
Isol. from *Chondrosia collectrix*.

Me ester: [68964-13-6]
Isol. from *Chondrosia collectrix*.

Stierle, D.B. *et al., J.O.C.*, 1979, **44**, 964-968 (*isol, pmr*)
Hu, J.-F. *et al., Tetrahedron*, 2001, **57**, 9379-9383; 2002, **58**, 1233 (*isol, pmr, cmr*)

3,5-Diethyltetrahydro-2-hydroxy-5-(1-pentenyl)-2-furanacetic acid, 9CI D-505

3,6-Epoxy-4,6-diethyl-3-hydroxy-7-undecenoic acid



Relative Configuration

$C_{15}H_{26}O_4$ 270.368

(2*R*,3*R*,5*R*)-*form*

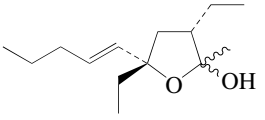
Et ester: [68914-60-3]
$C_{17}H_{30}O_4$ 298.422
Isol. from *Chondrosia collectrix*.
$[\alpha]_D^{20}$ +0.86 (c, 1.2 in CCl_4). Possible artifact.

Et ether, Et ester: [68914-58-9]
$C_{19}H_{34}O_4$ 326.475
Isol. from the sponge *Chondrosia collectrix*.
$[\alpha]_D^{20}$ +1.3 (c, 1.2 in CCl_4). C-2 config. not confirmed. Possible artifact.

Stierle, D.B. *et al., J.O.C.*, 1979, **44**, 964-970 (*isol, pmr, cmr*)

3,5-Diethyltetrahydro-2-methyl-5-(1-pentenyl)-2-furanol, 9CI D-506

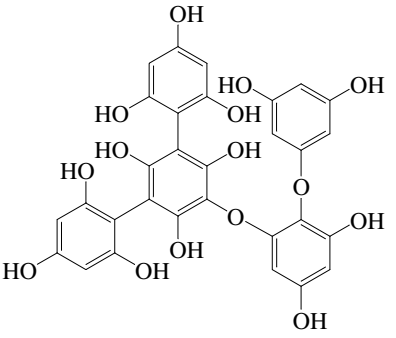
2,4-Diethyltetrahydro-5-hydroxy-5-methyl-2-(1-pentenyl)furan
[68914-59-0]



$C_{14}H_{26}O_2$ 226.358
Isol. from the sponge *Chondrosia collectrix*.
$[\alpha]_D^{20}$ +12.3 (c, 2.2 in CCl_4).

Stierle, D.B. *et al., J.O.C.*, 1979, **44**, 964-968 (*isol, pmr, cmr*)

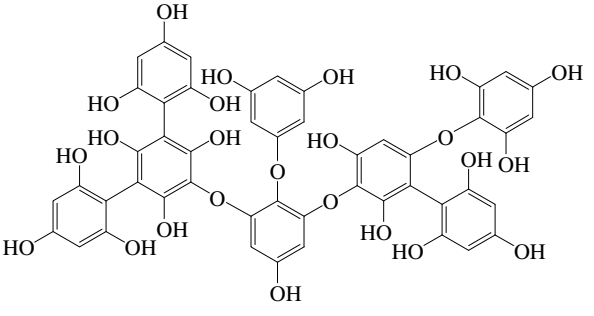
Difucodiphlorethol A D-507



$C_{30}H_{22}O_{15}$ 622.495
Isol. from brown alga *Sargassum spinuligerum*.

Glombitza, K.W. *et al., Phytochemistry*, 1997, **46**, 1417-1422 (*isol, pmr, ms*)

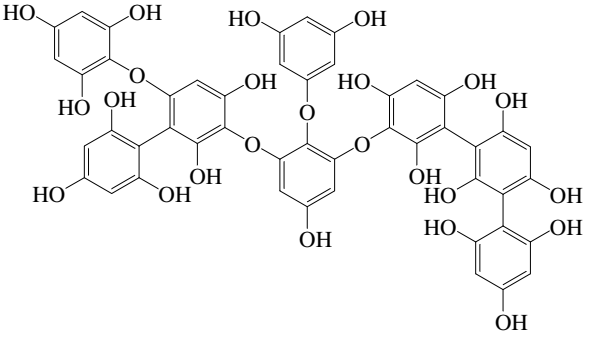
Difucofucotetraphlorethol A D-508



$C_{48}H_{34}O_{24}$ 994.782
Isol. from brown alga *Cystophora retroflexa*.

Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol, pmr, cmr, ms*)

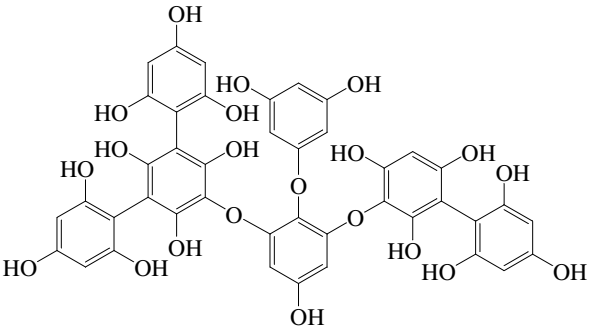
Difucofucotetraphlorethol B D-509



$C_{48}H_{34}O_{24}$ 994.782
Isol. from brown alga *Cystophora retroflexa*.

Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol, pmr, cmr, ms*)

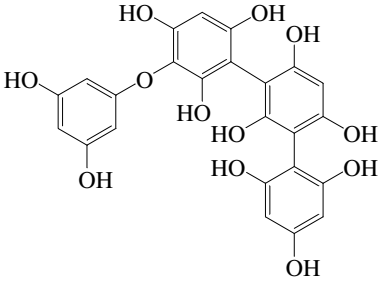
Difucofucotriphlorethol A D-510



$C_{42}H_{30}O_{21}$ 870.686
Isol. from brown alga *Cystophora retroflexa*.

Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol, pmr, cmr, ms*)

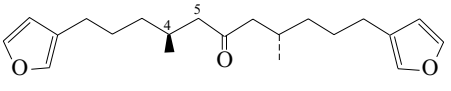
Difucophlorethol A D-511



$C_{24}H_{18}O_{12}$ 498.399
Isol. from brown algae *Himanthalia elongata*, *Cystophora retroflexa*, *Cystophora torulosa* and *Xiphophora chondrophylla*.

Glombitza, K.W. *et al., Planta Med.*, 1985, **50**, 42
Glombitza, K. *et al., Phytochemistry*, 1997, **46**, 735-740; 1999, **50**, 869-881

1,11-Di-3-furanyl-4,8-dimethyl-6-undecanone D-512



(4*S*,8*S*)–*form*

$C_{21}H_{30}O_3$ 330.466

(4*S*,8*S*)-*form*
Cacospongione A
[103000-69-7]
Constit. of *Cacospongia scalaris*.
Oil.

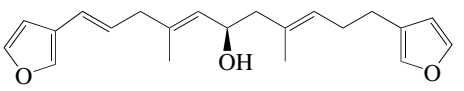
*4,5-Didehydro (*E-*):* ***Cacospongienone B***
[102856-54-2]
$C_{21}H_{28}O_3$ 328.45
From *Cacospongia scalaris*. Cytotoxic, antimicrobial and anti-inflammatory agent. Oil. λ_{max} 220 (ϵ 11400); 242 (ϵ 9000) (cyclohexane) (Derep).

*4,5-Didehydro (*Z-*):* ***Cacospongienone A***
[102856-53-1]
$C_{21}H_{28}O_3$ 328.45
Constit. of *Cacospongia scalaris*. Cytotoxic, antimicrobial and antiinflammatory agent. Oil. λ_{max} 220 (ϵ 11400); 242 (ϵ 9000) (cyclohexane) (Derep).

(4*RS*, 8*SR*)-*form*
Tetrahydrofurospongin 2
[35671-21-7]
Isol. from *Spongia officinalis* and *Hippospongia communis*.
Oil. Opt. inactive (*meso*-).

Cimino, G. *et al., Tetrahedron*, 1972, **28**, 267 (*Tetrahydrofurospongin*)
Guella, G. *et al., Helv. Chim. Acta*, 1986, **69**, 726 (*Cacospongione, Cacospongienones*)
Da Rosa, S. *et al., J. Nat. Prod.*, 1995, **58**, 1776 (*Cacospongienones A,B, isol, activity*)

1,11-Di-3-furanyl-4,8-dimethyl-1,4,8-undecatrien-6-ol, 9CI D-513



$C_{21}H_{26}O_3$ 326.435

(*R*)-*form*
Tetradehydrofurospongin I
[85404-64-4]
Constit. of *Spongia* spp.
Oil. $[\alpha]_D$ +21.8 (c, 0.78 in $CHCl_3$). Struct. revised in 1996.

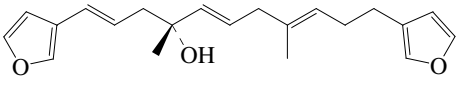
Ac:
$C_{23}H_{28}O_4$ 368.472
Constit. of *Spongia* spp. Oil. $[\alpha]_D$ +28.9 (c, 1.5 in $CHCl_3$).

(*S*)-*form*
Untenospongin B
[124666-37-1]
Constit. of a *Hippospongia* sp. NS87002. Coronary vasodilator. Oil. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D$ -20.1 (c, 1.02 in $CHCl_3$). $[\alpha]_D^{25}$ -1.5 (c, 2.7 in $CHCl_3$). λ_{max} 207 (ϵ 21800); 230 (sh) (EtOH).

Kazlauskas, R. *et al., Tet. Lett.*, 1976, 1331-1332 (*Tetradehydrofurospongin I*)
Umeyama, A. *et al., Aust. J. Chem.*, 1989, **42**, 459-462 (*Untenospongin B, isol, activity*)
Kobayashi, J. *et al., Chem. Pharm. Bull.*, 1993, **41**, 381-382 (*Untenospongin B, abs config*)
Fontana, A. *et al., J. Nat. Prod.*, 1996, **59**, 869 (*R-form, abs config, pmr, cmr*)
Rifai, S. *et al., Mar. Drugs*, 2004, **2**, 147-153 (*Utenospongin B, pmr, cmr, activity*)

1,11-Di-3-furanyl-4,8-dimethyl-1,5,8-undecatrien-4-ol D-514

Isotetradehydrofurospongin 1
[85344-76-9]

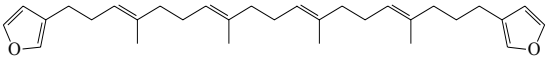


$C_{21}H_{26}O_3$ 326.435
Struct. revised in 2001. Constit. of a *Spongia* sp. Oil. $[\alpha]_D^{20}$ -10 (c, 0.4 in $CHCl_3$). λ_{max} 227 (log ϵ 4.6) (EtOH).

Capon, R.J. *et al., Experientia*, 1982, **38**, 1444-1445 (*isol*)
Capon, R.J. *et al., J. Nat. Prod.*, 2001, **64**, 638-639 (*isol, pmr, cmr, struct*)

Difurospinosulin D-515

[35890-98-3]

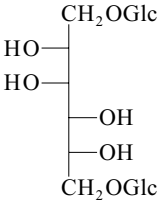


$C_{31}H_{44}O_2$ 448.687
Constit. of *Ircinia spinosula*. Oil. λ_{max} 218 (ϵ 4800) (cyclohexane) (Derep).

Cimino, G. *et al., Tetrahedron*, 1972, **28**, 1315

1,6-Di-*O*-β-D-glucopyranosyl-D-mannitol D-516

O-*β*-D-*Glucopyranosyl-(1→6)*-O-*β*-D-*glucopyranosyl-(1→1)*-D-*mannitol, 8CI*
[28976-36-5]

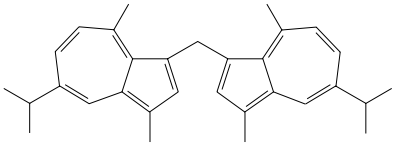


$C_{18}H_{34}O_{16}$ 506.457
Occurs in the brown algae *Fucus vesiculosus, Fucus spiralis, Pelvetia canaliculata, Laminaria cloustoni* and *Desmarestia aculeata*.
$[\alpha]_D^{20}$ -14 (c, 2.0 in H_2O).

Lindberg, B. *et al., Acta Chem. Scand.*, 1953, **7**, 1119 (*isol*)
Bouveng, H. *et al., Acta Chem. Scand.*, 1955, **9**, 168 (*isol*)
Coassini, L.L. *et al., CA*, 1970, **73**, 63240f

2,2′-Diguaiazulenylmethane D-517

1,1′-Methylenebis[3,8-dimethyl-5-(1-methylethyl)]azulene
[55544-35-9]



$C_{31}H_{36}$ 408.625
Constit. of a *Pseudothesia* sp. and *Calicogorgia granulosa*. Blue solid.
Mp 187-189°. λ_{max} 248 (ϵ 44670); 294 (ϵ 70795); 309 (ϵ 48980); 372 (ϵ 16220); 385 (ϵ 16220); 629 (ϵ 1995) (MeOH) (Berdy).

Treibs, W. *et al., Chem. Ber.*, 1959, **92**, 2152-2163 (*synth*)
Okuda, R.K. *et al., Pure Appl. Chem.*, 1982, **54**, 1907-1914 (*isol*)
Seo, Y. *et al., J. Nat. Prod.*, 1996, **59**, 985-986 (*isol, pmr, cmr*)

1,4-Diguanidinobutane D-518

N,N′′′-*1,4-Butanediylbisguanidine, 9CI*. ***Arcaine***
[544-05-8]
$HN{=}C(NH_2)NH(CH_2)_4NHC(NH_2){=}NH$
$C_6H_{16}N_6$ 172.233
Occurs in marine bivalve *Arca noae* and in *Panus tigrinus*. Also from the marine polychaete worm *Audouinia tentaculata*. Lowers blood sugar of mammals.

Sulfate: [14923-17-2]
[36587-93-6]
Needles. Mp 291° dec.

Picrate:
Needles or fine powder. Mp 251-254° dec.

Kutscher, F. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1931, **199**, 27; **203**, 132 (*isol*)
Sugino, K. *et al., Bull. Chem. Soc. Jpn.*, 1942, **17**, 126; *CA*, **41**, 4455 (*synth*)
Roche, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1965, **260**, 7023 (*isol*)
Boldt, A. *et al., Phytochemistry*, 1971, **10**, 731 (*biosynth*)
Thailambal, V.G. *et al., Acta Cryst. C*, 1985, **41**, 105 (*cryst struct*)

1,5-Diguanidinopentane D-519

N,N′-*1,5-Pentanediylbisguanidine, 9CI. 1,1′-Pentamethylenediguanidine, 8CI. Diamidinocadaverine*. ***Audouine***
[5070-04-2]
$HN{=}C(NH_2)NH(CH_2)_5NHC(NH_2){=}NH$
$C_7H_{18}N_6$ 186.259
Alkaloid in the polychaete worm *Audouinia tentaculata*. Pale-yellow oil. Sol. H_2O.

Sulfate:
Needles. Mp 317-318°.

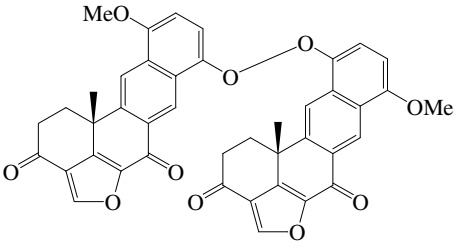
Picrate:
Yellow needles. Mp 226-227°.

[14279-79-9, 38142-20-0, 52780-74-2, 58585-48-1]

Roche, C. *et al., C. R. Hebd. Seances Acad. Sci.*, 1965, **260**, 7023
Robin, Y. *et al., Bull. Soc. Chim. Fr.*, 1967, 3965

Dihalenaquinolide A D-520

[681260-09-3]

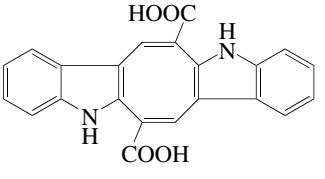


$C_{42}H_{30}O_{10}$ 694.693
Isol. from the sponge *Petrosia elastica*.
$[\alpha]_D^{25}$ +45 (c, 0.1 in $CHCl_3$). λ_{max} 229; 301 (MeOH).

Di-O-*de-Me, di-Et ether:* ***Dihalenaquinolide B***
[681260-42-4]
$C_{44}H_{34}O_{10}$ 722.747
Isol. from *Petrosia elastica*.
$[\alpha]_D^{25}$ +70.8 (c, 0.1 in $CHCl_3$). λ_{max} 228; 300 (MeOH).
Shen, Y.C. *et al., Tet. Lett.*, 2004, **45**, 2463-2466 (*isol, pmr, cmr, ms*)

5,12-Dihydrocycloocta[1,2-*b*:5,6-*b′*]diindole-6,13-dicarboxylic acid, 9CI D-521

Caulerpinic acid. *Caulerpin diacid*
[28056-19-1]



$C_{22}H_{14}N_2O_4$ 370.364
Struct. revised in 1978, formerly assigned as a dibenzophenazine.
Alkaloid from the green alga *Caulerpa racemosa*. Dark brown cryst.
Mp 256° subl.

Mono-Me ester: ***Monomethyl caulerpinate***
[137761-17-2]
$C_{23}H_{16}N_2O_4$ 384.39
Alkaloid from *Caulerpa racemosa*. Orange-yellow needles.
Mp 158-161°.

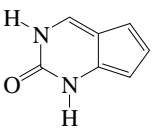
Di-Me ester: ***Caulerpin***
[26612-48-6]
$C_{24}H_{18}N_2O_4$ 398.417
Pigment from green algae *Caulerpa serrulata*, *Caulerpa racemosa*, *Caulerpa sertularioides*, *Caulerpa taxifolia*, *Caulerpa cuppresoides*, *Caulerpa scalpelliformis*, *Caloglossa leprieurii* and *Laurencia majuscula*. Plant growth regulator, phycotoxin, vermifuge. Red prisms or needles (Et_2O or Me_2CO). Fairly sol. Et_2O, Me_2CO; poorly sol. H_2O.
Mp 317°. λ_{max} 222 (ϵ 50000); 270 (ϵ 27000); 292 (ϵ 29000); 317 (ϵ 35000) (MeOH) (Berdy).
▶ LD_{50} (mus, ivn) 200 - 400 mg/kg, LD_{50} (mus, orl) 2000 - 4000 mg/kg.

N,N′-*Di-Me, di-Me ester:* [65079-49-4]
Red needles ($CHCl_3$/petrol). Mp 262-263°.

Aguilar-Santos, S. *et al., J.C.S.(C)*, 1970, 842-843 (*isol, uv, ir, pmr, ms*)

Maiti, B.C. *et al., J. Chem. Res., Synop.*, 1978, 126-127; *J. Chem. Res., Miniprint*, 1978, 1683-1693 (*isol, ur, ir, pmr, ms, struct, synth*)
Schwede, J.G. *et al., Phytochemistry*, 1987, **26**, 155-158 (*occur, Caulerpin*)
Anjaneyulu, A.S.R. *et al., Phytochemistry*, 1991, **30**, 3041-3042 (*mono Me-ester*)
Govenkar, M.B. *et al., Phytochemistry*, 2000, **54**, 979-981 (*Caulerpin, isol, cmr*)

1,3-Dihydrocyclopentapyrimidin-2-one D-522



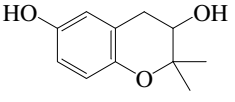
$C_7H_6N_2O$ 134.137

Tentative struct. Isol. from a sponge *Haliclona* sp. Shows antibiotic props.
Mp 260-265°. No CAS no. assigned. No further work reported to 2001.

Stempien, M.F. *et al., CA*, 1977, **86**, 95905 (*isol, struct*)

3,4-Dihydro-3,6-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran D-523

*3,4-Dihydro-2,2-dimethyl-2*H*-1-benzopyran-3,6-diol.* ***Antibiotic F 11334A$_3$****. F 11334A$_3$*



$C_{11}H_{14}O_3$ 194.23

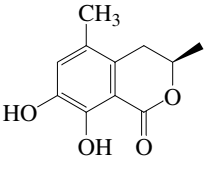
(-)-*form*

Prod. by the marine-derived *Acremonium murorum*.
Cryst.
Mp 175°. $[\alpha]_D^{23}$ -41 (c, 0.25 in MeOH) (c, 1 in MeOH). λ_{max} 218 (sh) (ε 5590); 227 (ε 5240); 297 (ε 3670) (MeOH).

Tanaka, M. *et al., J. Antibiot.*, 1999, **52**, 827-830 (*isol, struct*)
Abdel-Lateff, A. *et al., J. Nat. Prod.*, 2002, **65**, 1605-1611 (*isol, pmr, cmr*)

3,4-Dihydro-7,8-dihydroxy-3,5-dimethyl-1*H*-2-benzopyran-1-one D-524

3,4-Dihydro-7,8-dihydroxy-3,5-dimethylisocoumarin. 7-Hydroxy-5-methylmellein



(*R*)-*form*

$C_{11}H_{12}O_4$ 208.213

(*R*)-*form*

Prod. by a marine-derived *Nodulisporium* sp.

*7-Me ether: 3,4-Dihydro-8-hydroxy-7-methoxy-3,5-dimethyl-1*H*-2-benzopyran-1-one.* ***Avicennin B***
$C_{12}H_{14}O_4$ 222.24
Isol. from the endophytic fungus of *Avicennia marina*. Plates.
Mp 159-160°. $[\alpha]_D^{22}$ -53.8. λ_{max} 256 (ε 5470); 340 (ε 4500) ($CHCl_3$).

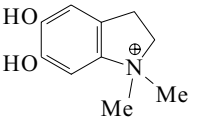
(ξ)-*form*

7-Me ether: Isol. from the fungus *Cytospora eucalypticola*.
Needles. λ_{max} 257 (log ε 3.5); 338 (log ε 3.2) (EtOH).

Lin, Y. *et al., Huaxue Tongbao*, 2001, **3**, 30
Kokubun, T. *et al., Phytochemistry*, 2003, **62**, 779-782 (*isol, pmr, cmr*)
Wang, J. *et al., Acta Cryst. E*, 2005, **61**, 784-785 (*cryst struct*)
Pontius, A. *et al., Planta Med.*, 2006, **72**, 1025-1026 (*isol*)

2,3-Dihydro-5,6-dihydroxy-1,1-dimethylindolium(1+) D-525

[113679-36-0]

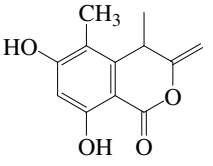


$C_{10}H_{14}NO_2^{\oplus}$ 180.226
Isol. from a deep water marine sponge *Dercitus* sp. Cryst. + $1H_2O$ (MeOH/$CHCl_3$) (as chloride). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 244° (chloride). CAS no. refers to chloride. λ_{max} 206 (ε 12200); 289 (ε 3700) (MeOH) (Berdy). λ_{max} 209 (ε 16500); 248 (ε 5800); 303 (ε 5100) (MeOH/NaOH) (Berdy).

Kohmoto, S. *et al., Experientia*, 1988, **44**, 85 (*isol, uv, ir, pmr, cmr, ms, struct*)

3,4-Dihydro-6,8-dihydroxy-4,5-dimethyl-3-methylene-1*H*-2-benzopyran-1-one D-526

6,8-Dihydroxy-4,5-dimethyl-3-methylene-1-isochromanone



$C_{12}H_{12}O_4$ 220.224

(ξ)-*form*

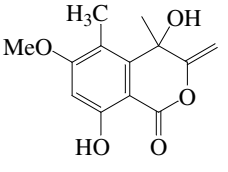
*8-*O*-α-D-Glucopyranoside:* ***Halorosellin B***
[500723-05-7]
$C_{18}H_{22}O_9$ 382.366
Prod. by *Halorosellinia oceanica* BCC 5149. Amorph. solid.
$[\alpha]_D^{30}$ +240.6 (c, 0.14 in EtOH). λ_{max} 218; 267; 315 (EtOH).

*6-Me ether, 8-*O*-α-D-glucopyranoside:* ***Halorosellin A***
[500723-04-6]
$C_{19}H_{24}O_9$ 396.393
Prod. by *Halorosellinia oceanica* BCC 5149. Amorph. solid.
$[\alpha]_D^{30}$ +203 (c, 0.07 in EtOH). λ_{max} 222; 268; 302 (EtOH).

Chinworrungsee, M. *et al., J.C.S. Perkin 1*, 2002, 2473-2476 (*isol, pmr, cmr*)

3,4-Dihydro-4,8-dihydroxy-6-methoxy-4,5-dimethyl-3-methylene-1*H*-2-benzopyran-1-one D-527

4,8-Dihydroxy-6-methoxy-4,5-dimethyl-3-methylene-1-isochromanone



$C_{13}H_{14}O_5$ 250.251

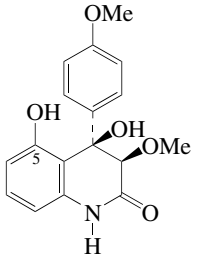
(+)-*form*

Prod. by *Halorosellinia oceanica* BCC 5149.
Needles. $[\alpha]_D$ +92.6 (c, 0.05 in EtOH). λ_{max} 218; 261; 306 (EtOH).

Chinworrungsee, M. *et al., J.C.S. Perkin 1*, 2002, 2473-2476 (*isol, pmr, cmr*)

3,4-Dihydro-4,5-dihydroxy-3-methoxy-4-(4-methoxyphenyl)-2(1*H*)-quinolinone D-528

[184046-65-9]



Relative Configuration

$C_{17}H_{17}NO_5$ 315.325

Prod. by *Penicillium* sp. NTC-47 and *Penicillium* cf. *simplicissimum*. Prisms (MeOH).

Mp 208-210°. $[\alpha]_D^{20}$ -55 (c, 0.02 in MeOH). λ_{max} 225 (ϵ 35000); 280 (ϵ 7000); 296 (ϵ 8400).

*5-Deoxy: 3,4-Dihydro-4-hydroxy-3-methoxy-4-(4-methoxyphenyl)-2(1*H*)-quinolinone*

[183854-01-5]

$C_{17}H_{17}NO_4$ 299.326

Prod. by *Penicillium* sp. NTC-47, *Penicillium* cf. *simplicissimum* and a marine-derived *Penicillium janczewski*. Needles (MeOH).

Mp 76-79°. $[\alpha]_D^{20}$ -62 (c, 0.3 in MeOH). λ_{max} 229 (ϵ 11000); 254 (ϵ 6500); 281 (ϵ 2800) (MeOH).

*5-Deoxy, O^3-de-Me: 3,4-Dihydro-3,4-dihydroxy-4-(4-methoxyphenyl)-2(1*H*)-quinolinone*

$C_{16}H_{15}NO_4$ 285.299

Prod. by a marine-derived *Penicillium janczewskii*. Amorph. solid. $[\alpha]_D^{15}$ -4.2 (c, 0.5 in MeOH).

3-Epimer, 5-deoxy, O^3-de-Me:

$C_{16}H_{15}NO_4$ 285.299

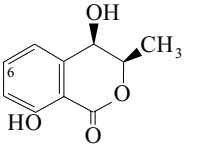
Prod. by a marine-derived *Penicillium janczewskii*. Amorph. solid. $[\alpha]_D^{15}$ -12.9 (c, 0.7 in MeOH).

Hayashi, H. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 914-916 (*isol, uv, ir, pmr, cmr*)
Kusano, M. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 2559-2568 (*isol, uv, pmr, cmr, ms*)
He, J. *et al., J. Nat. Prod.*, 2005, **68**, 1397-1399 (*isol, pmr, cmr*)

3,4-Dihydro-4,8-dihydroxy-3-methyl-1*H*-2-benzopyran-1-one, 9CI D-529

3,4-Dihydro-4,8-dihydroxy-3-methylisocoumarin. ***4-Hydroxymellein***

[33788-22-6]



(3*R*,4*R*)–*form*

$C_{10}H_{10}O_4$ 194.187

λ_{max} 244 (ϵ 7820); 312 (ϵ 4370) (MeOH) (Derep).

▶ NQ7830050

(3*R*,4*R*)-*form*

(-)-cis-*form*

[32885-83-9]

Prod. by *Aspergillus melleus*, *Aspergillus ochraceus*, *Botryosphaeria obtusa*, *Lasiodiplodia theobromae*, *Septoria nodorum* and the marine-derived *Microsphaeropsis* sp. H5-50.

Mp 123-124°. $[\alpha]_D$ -31 (MeOH). λ_{max} 244 (ϵ 7820); 312 (ϵ 4370) (MeOH) (Berdy).

*5-Chloro, 6-hydroxy: 5-Chloro-3,4-dihydro-4,6,8-trihydroxy-3-methyl-1*H*-2-benzopyran-1-one.* ***5-Chloro-4,6-dihydroxymellein***

[190957-36-9]

$C_{10}H_9ClO_5$ 244.631

Metab. of *Plectophomella* sp. Cryst. (CH_2Cl_2/MeOH).

Mp 172.5°. $[\alpha]_D$ -76.9 (c, 0.3 in $CHCl_3$). λ_{max} 320 (log ϵ 4.09) (MeOH).

(3*R*,4*S*)-*form*

(-)-trans-*form*

[70287-70-6]

Prod. by *Apiospora camptospora* and the marine-derived *Microsphaeropsis* sp. H5-50. Constit. of *Moringa oleifera* (horseradish tree) and *Septoria nodorum*.

Mp 131-132°. $[\alpha]_D$ -29 (MeOH).

6-Hydroxy: [265976-69-0]

Prod. by *Phomopsis helianthi*.

(3*S*,4*S*)-*form*

(+)-cis-*form*

[60132-20-9]

Constit. of *Aspergillus ochraceus*, *Cercospora beticola* and *Lasiodiplodia theobromae*.

Prisms.

Mp 118-119° (112-117°) Mp 131-132°. $[\alpha]_D$ +37 (MeOH).

λ_{max} 247 (ϵ 5300); 315 (ϵ 4200) (MeOH).

Di-Ac: Mp 83-85°.

(3*R*,4*R*)-*form*

*6-Hydroxy: 3,4-Dihydro-4,6,8-trihydroxy-3-methyl-1*H*-2-benzopyran-1-one.* ***4,6-Dihydroxymellein***

[62574-12-3]

$C_{10}H_{10}O_5$ 210.186

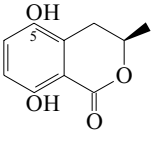
Metab. of *Cercospora scirpicola* and *Phomopsis helianthi*. Phytotoxic agent. Solid.

Mp 183-185°.

Cole, R.J. *et al., J. Agric. Food Chem.*, 1971, **19**, 909 (*isol*)
Aldridge, D.C. *et al., J.C.S.(C)*, 1971, 1623 (*isol*)
Camarda, L. *et al., Phytochemistry*, 1976, **15**, 537 (*abs config*)
Assante, G. *et al., Phytochemistry*, 1977, **16**, 243-247 (*4,6-Dihydroxymellein*)
Saluja, M.P. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 1044 (*isol*)
Abell, C. *et al., Chem. Comm.*, 1987, 586 (*biosynth*)
Devys, M. *et al., Z. Naturforsch., C*, 1992, **47**, 779 (*isol, pmr, abs config*)
Krohn, K. *et al., Phytochemistry*, 1997, **45**, 313-320 (*5-Chloro-4,6-dihydroxymellein*)
Höller, U. *et al., J. Nat. Prod.*, 1999, **62**, 114-118 (*marine isol*)
Avantaggiato, G. *et al., Nat. Toxins*, 1999, **7**, 119-127 (*4,6-Dihydroxymellein*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 133

3,4-Dihydro-5,8-dihydroxy-3-methyl-1*H*-2-benzopyran-1-one, 9CI D-530

3,4-Dihydro-5,8-dihydroxy-3-methylisocoumarin. ***5-Hydroxymellein***



$C_{10}H_{10}O_4$ 194.187

(*R*)-*form* [67549-52-4]

Prod. by *Botryosphaeria obtusa* and *Septoria nodorum*. Isol. from a marine-derived *Epicoccum* sp.

Mp 234-237°. $[\alpha]_D^{20}$ -72. λ_{max} 222 (log ϵ 4.29); 252 (log ϵ 3.84); 350 (log ϵ 3.78) (EtOH) (Berdy).

*5-Me ether: 3,4-Dihydro-8-hydroxy-5-methoxy-3-methyl-1*H*-2-benzopyran-1-one, 9CI. 3,4-Dihydroxy-8-hydroxy-5-methoxy-3-methylisocoumarin*

[67549-53-5]

$C_{11}H_{12}O_4$ 208.213

Isol. from fungi-infested trunk wood of *Macrolobium bifolium* and the heartwood of *Euphorbia fidjiana*. Cryst. (Et_2O/hexane).

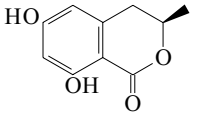
Mp 71-72°. $[\alpha]_D^{21}$ -116 ($CHCl_3$). λ_{max} 240 (sh) (log ϵ 3.68); 343 (log ϵ 3.56) (EtOH).

[77844-96-3, 87425-30-7]

De Alvarenga, M.A. *et al., Phytochemistry*, 1978, **17**, 511-516 (*isol, ir, uv, pmr, ms*)
Harwood, L.M. *et al., Chem. Comm.*, 1982, 1120 (*synth*)
Venkatasubbaiah, P. *et al., J. Nat. Prod.*, 1990, **53**, 1628-1630 (*isol*)
Cambie, R.C. *et al., Phytochemistry*, 1991, **30**, 287-292 (*5-Methoxymellein*)
Devys, M. *et al., Phytochemistry*, 1994, **35**, 825-826 (*isol, pmr*)

3,4-Dihydro-6,8-dihydroxy-3-methyl-1*H*-2-benzopyran-1-one D-531

3,4-Dihydro-6,8-dihydroxy-3-methylisocoumarin. ***6-Hydroxymellein***
[19314-92-2]



(*R*)–*form*

$C_{10}H_{10}O_4$ 194.187

(*R*)-*form* [70901-60-9]
Metab. of *Aspergillus terreus*, *Gilmaniella humicola*, *Penicillium thomii*, *Gymnoascus cetosus*, *Lachnum papyraceum* and *Pyricularia oryzae*. Phytotoxic agent. Prisms (Me_2CO/petrol).
Mp 214-217°. $[\alpha]_D^{20}$ -63 (c, 0.6 in EtOH). λ_{max} 216 (log ϵ 4.12); 269 (log ϵ 3.97); 304 (log ϵ 3.61) (EtOH) (Berdy). λ_{max} 216; 270 (ϵ 12900); 303 (ϵ 5759) (MeOH) (Derep). λ_{max} 243 (ϵ 3800); 308 (ϵ 10000) (Derep).

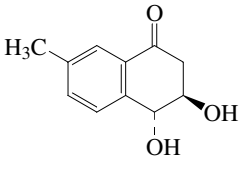
*7-Chloro, 6-Me ether: 7-Chloro-3,4-dihydro-8-hydroxy-6-methoxy-3-methyl-1*H*-2-benzopyran-1-one, 9CI*. ***7-Chloro-6-methoxymellein***. *Antibiotic LL-N313η*. *LL-N313η*
[15815-79-9]
[82263-56-7, 85163-35-5]
$C_{11}H_{11}ClO_4$ 242.658
Prod. by a marine-derived *Coniothyrium* sp. 193H77 and *Sporormia affinis*. Antifungal agent. Cryst. (EtOAc/hexane). Sol. MeOH, $CHCl_3$; poorly sol. Et_2O, H_2O, hexane.
Mp 170-171°. $[\alpha]_D^{20}$ -47 (c, 0.3 in $CHCl_3$). $[\alpha]_D^{25}$ -71.3 (c, 0.5 in MeOH). λ_{max} 224 (ϵ 25400); 272 (ϵ 12600); 305 (ϵ 6800) (MeOH). λ_{max} 224 (ϵ 29700); 272 (ϵ 25000); 340 (ϵ 6420) (MeOH/NaOH).

[6803-02-7]

McGahren, W.J. *et al., J.O.C.*, 1968, **33**, 1577-1580 (*7-Chloro-6-methoxymellein*)
Henderson, G.B. *et al., J.C.S. Perkin 1*, 1982, 1111-1115; 3037-3039 (*synth, biosynth*)
Höller, U. *et al., Dissertation*, Univ. of Braunschweig, 1999, (*7-Chloro-6-methoxymellein*)

3,4-Dihydro-3,4-dihydroxy-7-methyl-1(2*H*)-naphthalenone D-532

3,4-Dihydroxy-7-methyl-1-tetralone



(3*R**,4*R**)-*form*

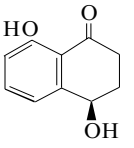
$C_{11}H_{12}O_3$ 192.214

(3*R,4*R**)-*form***
Prod. by a marine-derived *Acremonium* sp.
Powder. Isol. as a mixt. with the (3*R**,4*S**)-isomer, to which data refers. λ_{max} 251 (log ϵ 3.6); 296 (log ϵ 2.9) (MeOH).

(3*R,4*S**)-*form***
Prod. by a marine-derived *Acremonium* sp. Isol. as a mixt. with the (3*R**,4*R**)-isomer.
Abdel-Lateff, A. *et al., J. Nat. Prod.*, 2002, **65**, 1605-1611 (*isol, pmr, cmr*)

3,4-Dihydro-4,8-dihydroxy-1(2*H*)-naphthalenone, 9CI D-533

4,8-Dihydroxy-1-tetralone. ***Isosclerone***. *Regiolone*. *Antibiotic PD6*. *PD6*
[62332-73-4]



(*R*)–*form*

$C_{10}H_{10}O_3$ 178.187

(*R*)-*form*
Prod. by the fungi *Discula* sp., *Microsphaeropsis* sp. and *Phaeoacremonium aleophilum*. Isol from *Engelhardtia roxburghiana*, *Juglans mandshurica* var. *sieboldiana* and *Juglans regia*. Sol. C_6H_6, $CHCl_3$; poorly sol. hexane. $[\alpha]_D$ -68 (c, 0.05 in MeOH). Partial racemates probably isol. from *E. roxburghiana* and *J. regia*. λ_{max} 215 (ϵ 17800); 260 (ϵ 10000); 293 (ϵ 5200) (MeOH) (Berdy).

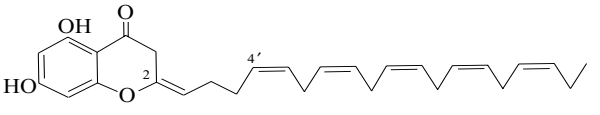
(*S*)-*form* [54712-38-8]
Metab. of *Sclerotinia sclerotiorum* and *Verticillium dahliae*. Constit. of the fruit of *Juglans mandshurica* var. *sieboldiana*. Phytotoxin. Cryst. (petrol). Sol. C_6H_6, $CHCl_3$; fairly sol. EtOAc, EtOH; poorly sol. hexane, H_2O.
Mp 74-76° (72°). $[\alpha]_D^{15}$ +19 (c, 0.34 in $CHCl_3$). λ_{max} 215 (ϵ 18200); 260 (ϵ 10000); 343 (ϵ 4265) (MeOH) (Berdy).

Dibenzoyl: Mp 125-127°.

(±)-*form* [51114-98-8]
Metabolite of *Scytalidium* sp. F-4 strain.
Cryst. (hexane).
Mp 70-72°.

Findlay, J.A. *et al., Can. J. Chem.*, 1973, **51**, 3299 (*ir, uv, pmr*)
Morita, T. *et al., Agric. Biol. Chem.*, 1974, **38**, 1501 (*uv, ord, pmr, ms*)
Stipanovic, R.D. *et al., Mycologia*, 1977, **69**, 164
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 1497; 4540 (*isol, synth*)
Talapatra, S.K. *et al., Phytochemistry*, 1988, **27**, 3929 (*isol, cd, pmr, cmr*)
Venkatasubbaiah, P. *et al., J. Nat. Prod.*, 1991, **54**, 1293 (*isol*)
Fujimoto, H. *et al., Chem. Pharm. Bull.*, 1998, **46**, 423-429 (*isol, pmr, cmr*)
Laurent, D. *et al., Tetrahedron*, 2002, **58**, 9163-9167 (*isol, pmr, cmr*)
Machida, K. *et al., Chem. Pharm. Bull.*, 2005, **53**, 934-937 (*isol, cd, ms*)
Lin, W.-Y. *et al., Planta Med.*, 2005, **71**, 171-175 (*isol*)

2,3-Dihydro-5,7-dihydroxy-2-(4,7,10,13,16-nonadecapentaenylidene)-4*H*-1-benzopyran-4-one D-534

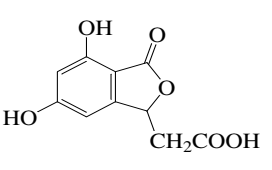


$C_{28}H_{34}O_4$ 434.574
Mp 45-46°.

(2*E*,4′*Z*,7′*Z*,10′*Z*,13′*Z*,16′*Z*)-*form* [85644-11-7]
Isol. from the brown alga *Zonaria tournefortii*.
Tringali, C. *et al., Gazz. Chim. Ital.*, 1982, **112**, 465 (*isol, struct*)

1,3-Dihydro-4,6-dihydroxy-3-oxo-1-isobenzofuranacetic acid D-535

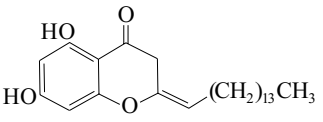
3-Carboxymethyl-5,7-dihydroxyphthalide. ***Herbaric acid***



$C_{10}H_8O_6$ 224.17

(-)-*form*
Prod. by *Cladosporium herbarum* isol. from the marine sponge *Callyspongia aerizusa*.
Amorph. brown powder. $[\alpha]_D$ -27 (c, 0.18 in MeOH).
Jadulco, R. *et al., J. Nat. Prod.*, 2002, **65**, 730-733 (*isol, pmr, cmr, ms*)

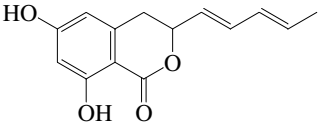
2,3-Dihydro-5,7-dihydroxy-2-pentadecylidene-4*H*-1-benzopyran-4-one D-536



$C_{24}H_{36}O_4$ 388.546

(*E*)-*form* [85644-09-3]
Isol. from the brown alga *Zonaria tournefortii*.
Mp 67-68°.
Tringali, C. *et al., Gazz. Chim. Ital.*, 1982, **112**, 465

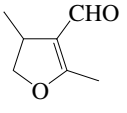
3,4-Dihydro-6,8-dihydroxy-3-(1,3-pentadienyl)-1*H*-2-benzopyran-1-one D-537
Arthrolactone



$C_{14}H_{14}O_4$ 246.262

(1′*E*,3ξ,3′*E*)-*form*
Prod. by the marine-derived *Aspergillus flavus* Gö 100/4.
Pale yellow oil.
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*isol, pmr, cmr*)

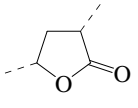
4,5-Dihydro-2,4-dimethyl-3-furancarboxaldehyde D-538
3-Formyl-4,5-dihydro-2,4-dimethylfuran



$C_7H_{10}O_2$ 126.155

(+)-*form*
Prod. by *Asteromyces cruciatus*.
Oil. $[\alpha]_D^{20}$ +38.9 (c, 0.61 in $CHCl_3$). λ_{max} 272 (log ϵ 3.41) (EtOH).
Höller, U. *et al., Eur. J. Org. Chem.*, 1999, 2949-2955 (*isol, pmr, cmr*)

Dihydro-3,5-dimethyl-2(3*H*)-furanone, 9CI D-539
α-Methyl-γ-valerolactone. 2,4-Dimethyl-γ-butyrolactone
[5145-01-7]



(3*S*,5*R*)-*form*

$C_6H_{10}O_2$ 114.144
Bp 201° Bp_{18} 80-82°.

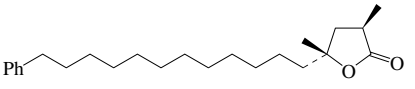
(3*S*,5*R*)-*form*
Prod. by *Asteromyces cruciatus*.
Oil. $[\alpha]_D^{20}$ +3.8 (c, 0.53 in $CHCl_3$).

(3*S*,5*S*)-*form* [127514-78-7]
Volatile light yellow oil. No opt. rotation given.

(3*RS*,5*RS*)-*form*
(±)-trans-*form*
[24405-08-1]
Liq., obt. by glc.

(3*RS*,5*SR*)-*form*
(±)-cis-*form*
[24405-07-0]
Liq., obt. by glc.
Fujita, T. *et al., Aust. J. Chem.*, 1974, **27**, 2205 (*synth*)
Pyysalo, H. *et al., Finn. Chem. Lett.*, 1975, 129 (*synth*)
Hussain, S.A.M.T. *et al., J.C.S. Perkin 1*, 1975, 1480 (*nmr, ir, synth*)
Hullot, P. *et al., Can. J. Chem.*, 1977, **55**, 266 (*synth*)
Davies, S.G. *et al., Tetrahedron*, 1990, **46**, 4847-4856 (*synth*)
Chu, K.S. *et al., J.O.C.*, 1991, **56**, 5196-5202 (*synth*)
Myers, A.G. *et al., J.O.C.*, 1996, **61**, 2428 (*S,S-form, synth*)
Höller, U. *et al., Eur. J. Org. Chem.*, 1999, 2949-2955 (*isol*)

Dihydro-3,5-dimethyl-5-(12-phenyldodecyl)-2(3*H*)-furanone D-540



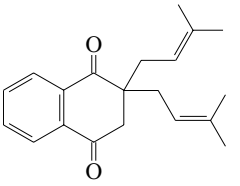
(3*R**,5*R**)-*form*

$C_{24}H_{38}O_2$ 358.563

(3*R,5*R**)-*form***
Isol. from the Palauan sponge *Plakortis nigra*.
Oil. $[\alpha]_D$ +19.3 (c, 0.05 in MeOH). λ_{max} 252 (ϵ 326); 258 (ϵ 296); 268 (ϵ 235) (MeOH).

(3*R,5*S**)-*form***
Isol. from *Plakortis nigra*.
Oil. $[\alpha]_D$ -7.1 (c, 0.13 in MeOH). λ_{max} 254 (ϵ 196); 261 (ϵ 215); 268 (ϵ 170) (MeOH).
Sandler, J.S. *et al., J. Nat. Prod.*, 2002, **65**, 1258-1261 (*isol, pmr, cmr*)

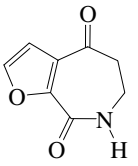
2,3-Dihydro-2,2-diprenylnaphthoquinone D-541
2,3-Dihydro-2,2-bis(3-methyl-2-butenyl)-1,4-naphthalenedione
[82214-84-4]



$C_{20}H_{24}O_2$ 296.408
Isol. from the brown alga *Landsburgia quercifolia*. Oil.

Kapoor, N.K. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 184 (*synth*)
Perry, N.B. *et al., J. Nat. Prod.*, 1991, **54**, 978 (*isol, pmr, cmr*)

6,7-Dihydro-4*H*-furo[2,3-*c*]azepine-4,8(5*H*)-dione D-542
Fuscaine
[223678-23-7]

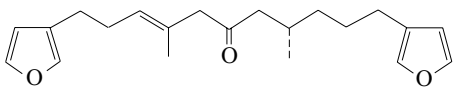


$C_8H_7NO_3$ 165.148
Isol. from the Chinese sponge *Phakellia fusca*. Cytotoxic.

Zeng, L.-M. *et al., CA*, 1999, **130**, 309248c

Dihydrofurospongin 2 D-543

[35671-22-8]



$C_{21}H_{28}O_3$ 328.45

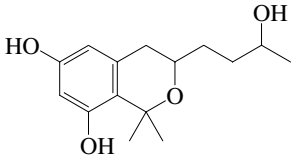
Constit. of *Spongia officinalis* and *Hippospongia communis*. Oil. $[\alpha]_D$ -0.91 ($CHCl_3$).

Cimino, G. *et al., Tetrahedron*, 1972, **28**, 267

3,4-Dihydro-3-(3-hydroxybutyl)-1,1-dimethyl-1*H*-2-benzopyran-6,8-diol D-544

6,8-Dihydroxy-3-(3-hydroxybutyl)-1,1-dimethylisochroman

[862694-08-4]

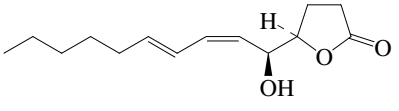


$C_{15}H_{22}O_4$ 266.336

Constit. of the stems of the mangrove *Bruguiera gymnorrhiza*. Amorph. solid. $[\alpha]_D^{20}$ -10 (c, 0.05 in MeOH). λ_{max} 282 (log ϵ 3.93) (MeOH). λ_{max} 279 (log ϵ 4.04) (MeOH/HCl). λ_{max} 293 (log ϵ 3.83) (MeOH/NaOH).

Han, L. *et al., Planta Med.*, 2005, **71**, 160-164 (*isol, uv, pmr, cmr*)

Dihydro-5-(1-hydroxy-2,4-decadienyl)-2(3*H*)-furanone D-545



$C_{14}H_{22}O_3$ 238.326

(1′*S*,2′*Z*,4′*E*,5*R*)-*form*

Isol. from *Litophyton arboreum*.

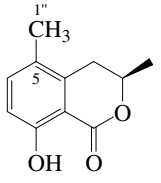
Pale yellow oil. $[\alpha]_D$ +98.3 (c, 0.24 in EtOH). λ_{max} 228 (log ϵ 4.32) (EtOH).

Rezanka, T. *et al., Tetrahedron*, 2001, **57**, 8743-8749

3,4-Dihydro-8-hydroxy-3,5-dimethyl-1*H*-2-benzopyran-1-one, 9CI D-546

3,4-Dihydro-8-hydroxy-3,5-dimethylisocoumarin. ***5-Methylmellein***. *5-Methylochracin*

[26277-19-0]



(*R*)-*form*

$C_{11}H_{12}O_3$ 192.214

(*R*)-*form* [7734-92-1]

Minor metab. of *Fusicoccum amygdali*, also obt. from wood of *Semecarpus* spp. Also from *Hypoxylon* spp., *Nummularia* spp. and mangrove fungus No. 1839. Active against phytopathogenic fungi. Cryst.

Mp 126-127°. $[\alpha]_D^{15}$ -105 (c, 0.5 in $CHCl_3$). λ_{max} 214 (log ϵ 4.34); 248 (log ϵ 3.83); 323 (log ϵ 3.23) (EtOH). λ_{max} 247 (log ϵ 3.82); 322 (log ϵ 3.63) (EtOH/$AlCl_3$).

*1′-Carboxylic acid: 3,4-Dihydro-8-hydroxy-3-methyl-1-oxo-1*H*-2-benzopyran-5-carboxylic acid*. ***5-Carboxymellein***

[69135-42-8]

$C_{11}H_{10}O_5$ 222.197

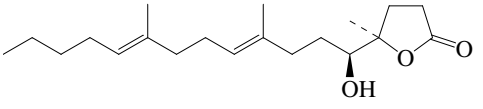
Isol. from wood fungus and from *Valsa ceratosperma*. Metab. of *Hypoxylon* spp. and mangrove fungus No. 1839.

Mp 250-252°. $[\alpha]_D^{25}$ -195 (c, 0.14 in EtOH).

[67549-51-3]

Ballio, A. *et al., Tet. Lett.*, 1966, 3723 (*isol, struct*)
De Alvarenga, M.A. *et al., Phytochemistry*, 1978, **17**, 511-516 (*isol, ir, uv, ms, Carboxymellein*)
Carpenter, R.C. *et al., Phytochemistry*, 1980, **19**, 445-447 (*isol, uv, pmr*)
Krohn, K. *et al., Phytochemistry*, 1997, **45**, 313-320 (*isol, cryst struct*)
Chen, G. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2006, **42**, 138-141 (*mangrove fungus 1839, isol*)

Dihydro-5-(1-hydroxy-4,8-dimethyl-4,8-tridecadienyl)-5-methyl-2(3*H*)-furanone D-547



$C_{20}H_{34}O_3$ 322.487

(1′*S*,4′*E*,5*R*,8′*E*)-*form*

Isol. from *Litophyton arboreum*.

Pale yellow oil. $[\alpha]_D$ +132.8 (c, 0.37 in EtOH). λ_{max} 217 (log ϵ 3.49) (EtOH).

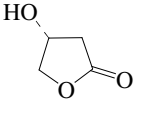
Rezanka, T. *et al., Tetrahedron*, 2001, **57**, 8743-8749

Dihydro-4-hydroxy-2(3*H*)-furanone, 9CI D-548

3-Hydroxy-4-butanolide. 3,4-Dihydroxybutanoic acid γ-lactone. 3-Hydroxy-γ-butyrolactone

[5469-16-9]

[131432-37-6]



(*R*)-*form*

$C_4H_6O_3$ 102.09

(*R*)-*form* [58081-05-3]

Acid hydrol. prod. of Oscillatoxin A, O-133.

Viscous oil. $Bp_{0.4}$ 103-105° $Bp_{0.1}$ 90-95°. $[\alpha]_D^{23}$ +86 (c, 2 in EtOH).

O-*β*-D-*Glucopyranoside:* ***Kinsenoside***

[151870-74-5]

$C_{10}H_{16}O_8$ 264.232

Constit. of *Anoectochilus koshunensis*. Oil. $[\alpha]_D^{16}$ +48.4 (c, 2.07 in EtOH).

*Me ether: Dihydro-4-methoxy-2(3*H*)-furanone*

[137008-54-9]

$C_5H_8O_3$ 116.116

Oil. $[\alpha]_D^{23}$ +34.2 (c, 0.92 in $CHCl_3$).

(*S*)-*form* [7331-52-4]

Metab. of alga *Lyngbya majuscula*. Also isol. from human and rat blood serum. Endogenous satiety substance. $Bp_{0.1}$ 120°. $[\alpha]_D$ -86.1 (c, 3.1 in EtOH).

O-*β*-D-*Glucopyranoside:* ***Goodyeroside A***

[211107-44-7]

Constit. of *Crocus sativus* (saffron) and *Goodyera* spp.

Needles (EtOH).

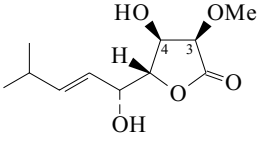
Mp 156-157°. $[\alpha]_D^{25}$ -71.2 (c, 0.55 in H_2O) (tetra-Ac).

Mori, K. *et al., Tetrahedron*, 1979, **35**, 933-940 (*synth, ir, pmr*)
Saito, S. *et al., Chem. Lett.*, 1984, 1389-1392 (*synth*)

Moore, R.E. *et al., J.O.C.*, 1984, **49**, 2484-2489 (*synth, isol*)
Ainslie, R.D. *et al., Phytochemistry*, 1986, **25**, 2654-2655 (*isol, pmr*)
Henrot, S. *et al., Synth. Commun.*, 1986, **16**, 183-190 (*synth*)
Seebach, D. *et al., Synthesis*, 1986, 37-40 (*synth*)
Tanaka, A. *et al., Synthesis*, 1987, 570-572 (*synth*)
Uchikawa, O. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 2025-2029 (*synth, ir, pmr, cmr, bibl*)
Luk, K.-C. *et al., Synthesis*, 1988, 226-227 (*synth, ir, pmr, ms*)
Sugita, Y. *et al., J.C.S. Perkin 1*, 1992, 2855-2861 (*S-form*)
Ito, A. *et al., Phytochemistry*, 1993, **33**, 1133-1137 (*synth, Kinsenoside*)
Yuasa, Y. *et al., Liebigs Ann./Recl.*, 1997, 1877-1879 (*synth, pmr, cmr, ms*)
Straubinger, M. *et al., J. Agric. Food Chem.*, 1998, **46**, 3238-3243 (*S-form glucoside*)
Masse, C.E. *et al., J.A.C.S.*, 1998, **120**, 4123-4134 (*synth, ir, pmr, cmr*)
Du, X.-M. *et al., Phytochemistry*, 1998, **49**, 1925-1928 (*Kinsenoside*)
Huang, G. *et al., Tetrahedron*, 1998, **54**, 1355-1360 (*synth, ir, pmr, cmr*)
Gao, W.-Y. *et al., Planta Med.*, 1999, **65**, 425-427 (*Goodyeroside A*)
Du, X.-M. *et al., Biol. Pharm. Bull.*, 2000, **23**, 731-734 (*Goodyeroside A*)
Ensch, C. *et al., Helv. Chim. Acta*, 2003, **86**, 233-246 (*S-form, synth, ir, pmr*)
Zhang, X. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 711-721 (*Kinsenoside, Goodyeroside A, synth*)

Dihydro-4-hydroxy-5-(1-hydroxy-4-methyl-2-pentenyl)-3-methoxy-2(3*H*)-furanone D-549

3,5-Dihydroxy-2-methoxy-8-methyl-6-nonen-1,4-olide



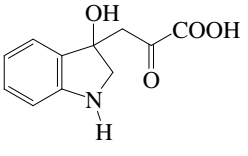
Relative configuration

$C_{11}H_{18}O_5$ 230.26
Constit. of the sponge *Jaspis* sp.

*4-Deoxy, 3,4-didehydro: 5-(1-Hydroxy-4-methyl-2-pentenyl)-3-methoxy-2(5*H*)-furanone. 5-Hydroxy-2-methoxy-8-methyl-2,6-nonadien-1,4-olide*
[118477-08-0]
$C_{11}H_{16}O_4$ 212.245
Constit. of *Jaspis* sp.
Adamczeski, M. *et al., J.A.C.S.*, 1989, **111**, 647 (*isol, pmr, cmr*)

3-(2,3-Dihydro-3-hydroxy-1*H*-indol-3-yl)-2-oxopropanoic acid D-550

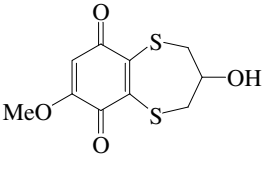
*2,3-Dihydro-3-hydroxy-α-oxo-1*H*-indole-3-propanoic acid*



$C_{11}H_{11}NO_4$ 221.212

(ξ)-*form*
Prod. by the marine-derived *Halomonas* sp. RK377.
Amorph. solid.
Liang, L. *et al., Dissertation*, Univ. of Göttingen, 2003, (*isol, pmr, cmr, ms*)

3,4-Dihydro-3-hydroxy-7-methoxy-2*H*-1,5-benzodithiepine-6,9-dione D-551

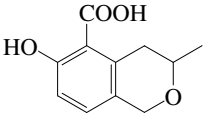


$C_{10}H_{10}O_4S_2$ 258.319

(-)-*form*
Constit. of the mangrove plant *Bruguiera sexangula* var. *rhynchopetala*.
Violet solid. $[\alpha]_D^{20}$ -45 (c, 0.08 in $CHCl_3$). λ_{max} 241 (log ϵ 3.59); 320 (log ϵ 3.49); 541 (log ϵ 2.68) ($CHCl_3$).
Bao, S. *et al., Helv. Chim. Acta*, 2005, **88**, 2757-2763 (*isol, pmr, cmr*)

3,4-Dihydro-6-hydroxy-3-methyl-1*H*-2-benzopyran-5-carboxylic acid D-552

6-Hydroxy-3-methylisochroman-5-carboxylic acid

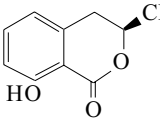


$C_{11}H_{12}O_4$ 208.213

(ξ)-*form*
Prod. by endophytic mangrove fungus No. 1839.
Brown oil. λ_{max} 220; 245; 316 (EtOH).
Chen, G. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2006, **42**, 138-141 (*isol, pmr, cmr*)

3,4-Dihydro-8-hydroxy-3-methyl-1*H*-2-benzopyran-1-one, 9CI D-553

3,4-Dihydro-8-hydroxy-3-methylisocoumarin. ***Mellein***. *Ochracin*
[17397-85-2]
[16281-42-8]



(*R*)–*form*

$C_{10}H_{10}O_3$ 178.187
Hepatitis C virus protease inhibitor. Sol. MeOH, $CHCl_3$, bases; fairly sol. H_2O; poorly sol. hexane. λ_{max} 212 (ϵ 20000); 246 (ϵ 6500); 314 (ϵ 4100) (MeOH) (Derep). λ_{max} 246 (ϵ 6480); 315 (ϵ 3990) (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 125 mg/kg. NQ7860000

(R)-form [480-33-1]
Isol. from *Aspergillus* spp. and other fungi. Shows antifungal effect. Inhibits Hepatitis C virus protease. Cryst. (hexane/Et_2O). Mp 51.5-52°. $[\alpha]_D$ -108.15 ($CHCl_3$).
Ac:
$C_{12}H_{12}O_4$ 220.224
Cryst. Mp 126-127°.
Me ether: **O-*Methylmellein***
[76985-75-6]
$C_{11}H_{12}O_3$ 192.214
Constit. of *Septoria nodorum*. Cryst.
Mp 88-89°. $[\alpha]_D^{15}$ -250.

(S)-form [62623-84-1]
Metab. of an unidentified fungus.
Mp 51.5-52°. $[\alpha]_D^{25}$ +102 (c, 1.07 in $CHCl_3$).
Me ether: ***Dictafolin A***
[193544-57-9]
Constit. of the root bark of *Dictamnus angustifolius*.
Mp 87°. $[\alpha]_D^{26}$ +257 (c, 0.5 in $CHCl_3$) (synthetic). $[\alpha]_D$ +30 (c, 0.02 in $CHCl_3$) (Dictafolin A). Struct. of Dictafolin A revised in 2006.

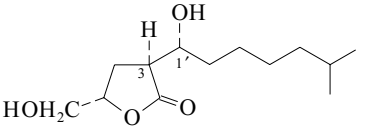
(±)-*form* [1200-93-7]
Mp 39°.

Patterson, E.L. *et al., Experientia*, 1966, **22**, 209 (*isol*)
Arakawa, H. *et al., Annalen*, 1969, **728**, 152 (*config*)
Turner, B.W. *et al., J.C.S.(C)*, 1971, 1623 (*isol*)
Narasimhan, N.S. *et al., Tetrahedron*, 1971, **27**, 617 (*synth*)
Grove, J.F. *et al., J.C.S. Perkin 1*, 1972, 2400; 1979, 2048 (*isol*)
Arai, Y. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 3311 (*synth*)

Guyot, M. *et al., Tet. Lett.*, 1973, 3433 (*synth*)
Camarda, L. *et al., Phytochemistry*, 1976, **15**, 537 (*isol*)
Devys, M. *et al., Phytochemistry*, 1980, **19**, 2221 (*Methylmellein*)
Abell, C. *et al., Chem. Comm.*, 1982, 1011; 1983, 694 (*biosynth*)
Regan, A.C. *et al., Chem. Comm.*, 1983, 764 (*synth*)
Harwood, L.M. *et al., J.C.S. Perkin 1*, 1984, 2577 (*synth*)
Claydon, N. *et al., Phytochemistry*, 1985, **24**, 937-943 (*isol*)
Mori, K. *et al., Tetrahedron*, 1985, **41**, 5295 (*synth*)
Okuno, T. *et al., Agric. Biol. Chem.*, 1986, **50**, 997 (*isol, derivs*)
Napolitano, E. *et al., Gazz. Chim. Ital.*, 1991, **121**, 455 (*synth*)
Takeuchi, N. *et al., Heterocycles*, 1992, **33**, 357 (*synth*)
Dimitriadis, C. *et al., Tetrahedron: Asymmetry*, 1997, **8**, 2153-2158 (*synth*)
Höller, U. *et al., J. Nat. Prod.*, 1999, **62**, 114-118 (*isol, activity*)
Schubert, T. *et al., Synthesis*, 1999, 2045-2048 (*Me ether*)
Dai, J.R. *et al., J. Nat. Prod.*, 2001, **64**, 125-126 (*activity*)
Donner, C.D. *et al., Molecules*, 2004, **9**, 498-512 (*synth*)
Dai, J. *et al., Eur. J. Org. Chem.*, 2006, 3498-3506 (*Dictafolin A*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 129 (*activity*)

Dihydro-5-(hydroxymethyl)-3-(1-hydroxy-6-methylheptyl)-2(3*H*)-furanone D-554

4-(Hydroxymethyl)-2-(1-hydroxy-6-methylheptyl)butanolide
[138797-47-4]



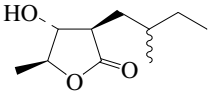
$C_{13}H_{24}O_4$ 244.33
Prod. by a marine actinomycete. Pale yellow oil. $[\alpha]_D$ +22.3 (c, 0.61 in CH_2Cl_2).

[138797-48-5]

Pathirana, C. *et al., Tet. Lett.*, 1991, **32**, 7001 (*isol, synth*)

Dihydro-4-hydroxy-5-methyl-3-(2-methylbutyl)-2(3*H*)-furanone D-555

3-Hydroxy-4-methyl-2-(2-methylbutyl)butanolide

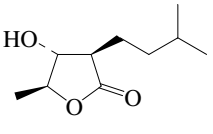


$C_{10}H_{18}O_3$ 186.25

(2′ξ,3*R*,4*R*,5*S*)-*form*
***Antibiotic MKN 004D**. MKN 004D*
Prod. by a marine *Streptomyces* strain M02750.
$[\alpha]_D^{25}$ -8.3 (c, 0.25 in MeOH).
Cho, K.W. *et al., J. Nat. Prod.*, 2001, **64**, 664-667

Dihydro-4-hydroxy-5-methyl-3-(3-methylbutyl)-2(3*H*)-furanone D-556

3-Hydroxy-4-methyl-2-(3-methylbutyl)butanolide



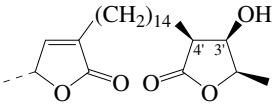
(3*R*,4*R*,5*S*)-*form*

$C_{10}H_{18}O_3$ 186.25
Struct. diagram and MF do not correspond with each other in ref.

(3*R*,4*R*,5*S*)-*form*
***Antibiotic MKN 004B**. MKN 004B*
Prod. by a marine *Streptomyces* strain M02750.
$[\alpha]_D$ -10.1 (c, 0.24 in MeOH).

(3*S*,4*R*,5*S*)-*form*
***Antibiotic MKN 004C**. MKN 004C*
Prod. by a marine *Streptomyces* strain M02750.
Gum. $[\alpha]_D^{25}$ +1.1 (c, 0.42 in MeOH).
Cho, K.W. *et al., J. Nat. Prod.*, 2001, **64**, 664-667

Dihydro-4-hydroxy-5-methyl-3-[14-(5-methyl-2-oxo-3-furanyl)tetradecyl]-2(3*H*)-furanone D-557



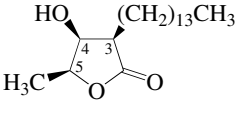
Relative Configuration

$C_{24}H_{40}O_5$ 408.577
Related to Ancepsenolide, A-483. Isol. from the gorgonian *Pterogorgia anceps*. Amorph. powder. $[\alpha]_D$ -4.7 (c, 0.3 in $CHCl_3$). λ_{max} 213 (ϵ 5200) (EtOH).

3′,4′-Didehydro:
$C_{24}H_{38}O_5$ 406.561
Isol. from *Pterogorgia anceps*. Amorph. powder. $[\alpha]_D$ -27.2 (c, 5.6 in $CHCl_3$). λ_{max} 210 (ϵ 15000) (EtOH).
Guo, Y.-W. *et al., J. Nat. Prod.*, 1999, **62**, 1194-1196 (*isol, uv, pmr, cmr*)

4,5-Dihydro-4-hydroxy-5-methyl-2-tetradecyl-2(3*H*)-furanone D-558

3-Hydroxy-4-methyl-2-tetradecyl-4-butanolide



(3*R*,4*S*,5*S*)-*form*

$C_{19}H_{36}O_3$ 312.492

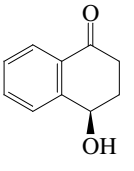
(3*R*,4*S*,5*S*)-*form*
Constit. of the fruits of *Trichilia claussenii*.
Cryst. (hexane).
Mp 93-94°. $[\alpha]_D^{22}$ -43.6 (c, 0.67 in $CHCl_3$).

(3*R,4*R**,5*R**)-*form***
Ac: [81576-10-5]
$C_{21}H_{38}O_4$ 354.529
Constit. of the gorgonian *Plexaura flava*. Oil. $[\alpha]_D^{20}$ +36.1 (c, 1.9 in CH_2Cl_2).

(3*R,4*S**,5*R**)-*form***
Ac: [81576-11-6]
Constit. of *Plexaura flava*.
Powder. $[\alpha]_D^{20}$ -36.6 (c, 1.5 in CH_2Cl_2).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 105-112 (*Ac, isol, ir, pmr, ms*)
Sibi, M.P. *et al., J.O.C.*, 1996, **61**, 7848-7855 (*synth*)
Pupo, M.T. *et al., Phytochemistry*, 1998, **48**, 307-310 (*isol, pmr, cmr, ms*)
Liu, B. *et al., Tet. Lett.*, 2001, **42**, 2533-2535 (*synth*)
Takahashi, S. *et al., Tetrahedron*, 2005, **61**, 6540-6545 (*synth*)

3,4-Dihydro-4-hydroxy-1(2*H*)-naphthalenone D-559

4-Hydroxy-1-tetralone
[21032-12-2]



(*R*)-*form*

$C_{10}H_{10}O_2$ 162.188

(*R*)-*form* [412020-55-4]
Constit. of *Engelhardtia roxburghiana* and *Juglans mandshurica* var. *sieboldiana*.
Mp 41-43°. $[\alpha]_D^{26}$ -41.5 (c, 0.17 in $CHCl_3$).

(*S*)-*form*
Constit. of the fruit of *Juglans mandshurica* var. *sieboldiana*.
Amorph. yellow powder. $[\alpha]_D^{25}$ +21 (c, 0.3 in $CHCl_3$).

O-*β*-D-*Glucopyranoside:* ***Juglanoside A***
$C_{16}H_{20}O_7$ 324.33
Constit. of the fruit of *Juglans mandshurica*. Amorph. powder. $[\alpha]_D^{25}$ -77 (c, 0.9 in MeOH). λ_{max} 247 (log ε 4.1); 285 (log ε 3.3) (MeOH).

O-*[3,4,5-Trihydroxybenzoyl-(→6)-β-D-glucopyranoside]:*
[641625-64-1]
$C_{23}H_{24}O_{11}$ 476.436
Constit. of *Juglans regia* (walnut). Protein tyrosine phosphatase inhibitor. Oil. $[\alpha]_D^{25}$ -43 (c, 0.67 in MeOH). λ_{max} 214 (log ε 4.01); 261 (log ε 3.91) (MeOH).

(±)-*form*
Prod. by the marine-derived *Microsphaeropsis* sp. H5-50.

2,4-Dinitrophenylhydrazone: Mp 194°.

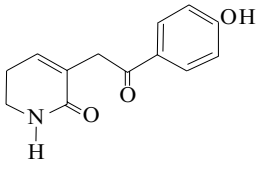
Benzoyl:
$C_{17}H_{14}O_3$ 266.296
Cryst. (cyclohexane). Mp 94-95°.

(ξ)-*form*
Constit. of *Ampelocera edentula, Ammannia baccifera* and *Juglans regia* (walnut). Fungal and bacterial metab. of naphthalene and 1-naphthol. Exhibits antileishmanial activity. Oil. λ_{max} 205 (log ε 4.35); 249 (log ε 4.04); 289 (log ε 3.2) (MeOH).

Boyland, E. *et al., J.C.S.*, 1951, 1837-1841 (*benzoyl*)
Bollag, J.M. *et al., J. Agric. Food Chem.*, 1975, **23**, 85-90 (*metab, ir, uv, pmr, ms*)
Cerniglia, C.E. *et al., Appl. Environ. Microbiol.*, 1982, **43**, 1070
Fournet, A. *et al., Planta Med.*, 1994, **60**, 8-12 (*isol, pmr, cmr*)
Höller, U. *et al., Dissertation*, Univ. of Braunschweig, 1999, (*isol, pmr, cmr*)
Joly, S. *et al., Tetrahedron: Asymmetry*, 2001, **12**, 2283-2287 (*R-form, synth, pmr, cmr*)
An, T.Y. *et al., Chin. Chem. Lett.*, 2003, **14**, 489-490 (*Juglans regia glycoside*)
Liu, L. *et al., Chem. Pharm. Bull.*, 2004, **52**, 566-569 (*cd, pmr, Juglanoside A*)
Machida, K. *et al., Chem. Pharm. Bull.*, 2005, **53**, 934-937 (*isol, cd*)
Lin, W.-Y. *et al., Planta Med.*, 2005, **71**, 171-175 (*isol*)

5,6-Dihydro-3-[2-(4-hydroxyphenyl)-2-oxoethyl]-2(1*H*)-pyridinone, 9CI D-560

[71886-38-9]

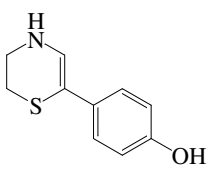


$C_{13}H_{13}NO_3$ 231.251
Isol. from an algae-infested Caribbean sponge *Halichondria melanodocia*. Cryst. ($CHCl_3$/MeOH).
Mp 235-235.5°.

Gopichand, Y. *et al., J.O.C.*, 1979, **44**, 4995 (*isol, uv, ir, pmr, ms, struct*)

3,4-Dihydro-6-(4-hydroxyphenyl)-2*H*-1,4-thiazine D-561

*4-(3,4-Dihydro-2*H*-1,4-thiazin-6-yl)phenol, 9CI*

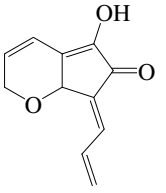


$C_{10}H_{11}NOS$ 193.269

S,S-*Dioxide: 4-(3,4-Dihydro-1,1-dioxido-2*H*-1,4-thiazin-6-yl) phenol, 9CI. 3,4-Dihydro-6-(4-hydroxyphenyl)-1,1-dioxo-2*H*-1,4-thiazine*
[154887-08-8]
$C_{10}H_{11}NO_3S$ 225.268
Alkaloid from the sponge *Anchinoe tenacior*. λ_{max} 274 (ε 8100) (MeOH).

Casapullo, A. *et al., Tet. Lett.*, 1994, **35**, 2421-2422 (*isol, uv, pmr*)

7,7*a*-Dihydro-5-hydroxy-7-(2-propenylidene)cyclopenta[*c*]pyran-6(2*H*)-one, 9CI D-562



(*E*)-*form*

$C_{11}H_{10}O_3$ 190.198

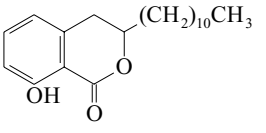
(*E*)-(ξ)-*form* [67654-92-6]
Isol. from the marine sponge *Ulosa* sp. λ_{max} 248 (ε 22000); 340 (ε 12000) (MeOH). λ_{max} 263 (ε 30000); 423 (ε 10000) (MeOH/KOH).

(*Z*)-(ξ)-*form* [67654-93-7]
Isol. from an *Ulosa* sp.

Wratten, S.J. *et al., Tet. Lett.*, 1978, 961-964 (*isol, uv, pmr*)

3,4-Dihydro-8-hydroxy-3-undecyl-1*H*-2-benzopyran-1-one D-563

3,4-Dihydro-8-hydroxy-3-undecylisocoumarin



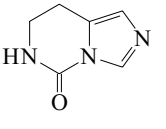
$C_{20}H_{30}O_3$ 318.455

(+)-*form* [75808-39-8]
Isol. from the alga *Caulocystis cephalornithos*.
Plates (hexane).
Mp 89-90°. $[\alpha]_D^{21}$ +37.7 (c, 1 in $CHCl_3$).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1980, **33**, 2097 (*isol*)

7,8-Dihydroimidazo[1,5-*c*]pyrimidin-5(6*H*)-one, 9CI D-564

5,6,7,8-Tetrahydro-5-oxoimidazo[1,5-c]pyrimidine. 5,6,7,8-Tetrahydroimidazo[1,5-c]pyrimidin-5-one
[14509-66-1]



$C_6H_7N_3O$ 137.141
Metab. from the Caribbean sponge *Aplysina fistularis* f. *fulva*.
Cryst. (EtOH).
Mp 220-222°.

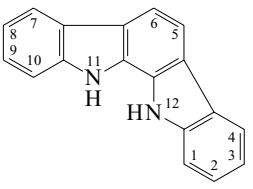
Methiodide: [51720-37-7]
Cryst. Mp 228-230° dec.

Mechoulam, R. *et al., Tetrahedron*, 1967, **23**, 239 (*synth, pmr, ir, use*)
Durant, C.G. *et al., J. Med. Chem.*, 1976, **19**, 923 (*synth*)
Jairam, R. *et al., J.O.C.*, 1992, **57**, 4136 (*synth*)
Ciminiello, P. *et al., J. Nat. Prod.*, 1994, **57**, 705 (*isol, pmr, cmr*)

11,12-Dihydroindolo[2,3-*a*]carbazole, 9CI D-565

Indolo[2,3-a]carbazole

[60511-85-5]



$C_{18}H_{12}N_2$ 256.306

Residue present in a number of microbial and marine alkaloids. Cryst. (EtOH).

Mp 370°.

N-*Me:*

$C_{19}H_{14}N_2$ 270.333

Prisms (EtOH). Mp 244-245°.

N,N′-*Di-Me:*

$C_{20}H_{16}N_2$ 284.36

Needles (Me_2CO aq.). Mp 209°.

N-*(6-Deoxy-β-D-gulopyranosyl):* ***Tjipanazole G1***

$C_{24}H_{22}N_2O_4$ 402.449

Minor alkaloid from the blue-green alga *Tolypothrix tjipanasensis*. Protein kinase C activator. Exhibits antifungal activity. $[\alpha]_D$ +9.1 (c, 1.0 in $CHCl_3$). λ_{max} 256 (ε 35400); 270 (ε 32800); 287 (ε 18800); 324 (ε 20000); 343 (ε 5800); 359 (ε 4080) (MeOH) (Derep).

N-*α-L-Rhamnopyranosyl:* ***Tjipanazole G2***

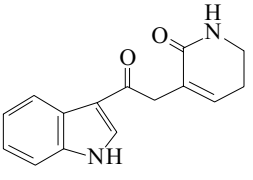
$C_{24}H_{22}N_2O_4$ 402.449

Minor constit. of *Tolypothrix tjipanasensis*. λ_{max} 256 (ε 35400); 270 (ε 32800); 287 (ε 18800); 324 (ε 20000); 343 (ε 5800); 359 (ε 4080) (MeOH) (Derep).

Mann, F.G. *et al., J.C.S.*, 1958, 1525 (*synth, derivs*)
Hünig, S. *et al., Annalen*, 1976, 1090 (*uv*)
Bonjouklian, R. *et al., Tetrahedron*, 1991, **47**, 7739 (*Tjipanazoles*)

5,6-Dihydro-3-[2-(1*H*-indol-3-yl)-2-oxoethyl]-2(1*H*)-pyridinone, 9CI D-566

[71886-40-3]



$C_{15}H_{14}N_2O_2$ 254.288

Isol. from an algae-infested Caribbean sponge *Halichondria melanodocia*. Cryst. ($MeOH/CHCl_3$).

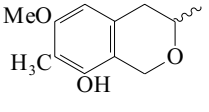
Mp 194-194.5°.

Gopichand, Y. *et al., J.O.C.*, 1979, **44**, 4995 (*isol, uv, ir, pmr, ms, struct*)

3,4-Dihydro-6-methoxy-3,7-dimethyl-1*H*-2-benzopyran-8-ol, 9CI D-567

8-Hydroxy-6-methoxy-3,7-dimethylisochroman

[70080-82-9]



$C_{12}H_{16}O_3$ 208.257

Prod. by *Penicillium corylophilum* and *Penicillium steckii*. Mycotoxin. Plant growth regulator.

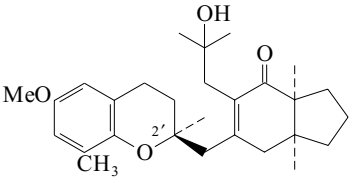
Mp 122°.

▶ NQ7185000

Cox, R.H. *et al., J. Agric. Food Chem.*, 1979, **27**, 999-1001 (*isol*)
Cutler, H.G. *et al., Agric. Biol. Chem.*, 1989, **53**, 1975 (*isol*)
Malmstrom, J. *et al., Phytochemistry*, 2000, **54**, 301-309 (*occur*)

6-[(3,4-Dihydro-6-methoxy-2,8-dimethyl-2*H*-1-benzopyran-2-yl)methyl]-1,2,3,3*a*,7,7*a*-hexahydro-5-(2-hydroxy-2-methylpropyl)-3*a*,7*a*-dimethyl-4*H*-inden-4-one, 9CI D-568

[148270-16-0]



$C_{28}H_{40}O_4$ 440.622

Metab. of *Cystoseira baccata*. Oil. $[\alpha]_D^{20}$ +2.06 (c, 2.9 in $CHCl_3$).

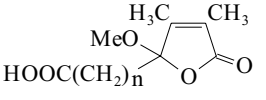
2′-Epimer: [148347-78-8]

$C_{28}H_{40}O_4$ 440.622

Metab. of *Cystoseira baccata*. Oil. $[\alpha]_D^{20}$ +28.9 (c, 2.7 in $CHCl_3$).

Valls, R. *et al., Phytochemistry*, 1993, **32**, 961 (*isol, pmr, cmr, ms*)

2,5-Dihydro-2-methoxy-3,4-dimethyl-5-oxo-2-furannonanoic acid D-569



n = 8

$C_{16}H_{26}O_5$ 298.378

(±)-*form*

Me ester: [75239-73-5]

$C_{17}H_{28}O_5$ 312.405

Constit. of the red alga *Ahnfeltia paradoxa*.

Nomura, Y. *et al., Chem. Lett.*, 1980, 955 (*isol, ms*)

2,5-Dihydro-2-methoxy-3,4-dimethyl-5-oxo-2-furanundecanoic acid D-570

As 2,5-Dihydro-2-methoxy-3,4-dimethyl-5-oxo-2-furannonanoic acid, D-569 with

n = 10

$C_{18}H_{30}O_5$ 326.432

(±)-*form*

Me ester: [75239-71-3]

$C_{19}H_{32}O_5$ 340.459

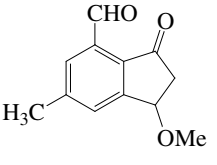
Constit. of the red alga *Coeloseira pacifica*. Cryst.

Mp 54-55°. λ_{max} 211 (ε 9400) (MeOH).

Nomura, Y. *et al., Chem. Lett.*, 1980, 955 (*isol, pmr, cmr*)

2,3-Dihydro-1-methoxy-6-methyl-3-oxo-1*H*-indene-4-carboxaldehyde D-571

7-Formyl-3-methoxy-5-methyl-1-indanone



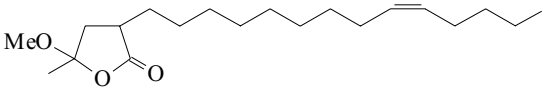
$C_{12}H_{12}O_3$ 204.225

Isol. from *Lyngbya majuscula*. Antitumour agent. Oil. $[\alpha]_D$ +1.3 (c, 1.1 in MeOH). Prob. a partial racemate. λ_{max} 214 (log ϵ 4.2); 250 (log ϵ 3.9) (MeOH).

Nagle, D.G. *et al., J. Nat. Prod.*, 2000, **63**, 1431-1433

Dihydro-5-methoxy-5-methyl-3-(9-tetradecenyl)-2(3*H*)-furanone D-572

[156992-91-5]



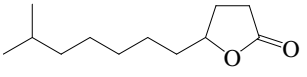
$C_{20}H_{36}O_3$ 324.503

Constit. of the sea pen *Virgularia* sp. Oil. $[\alpha]_D$ +3.2 (c, 1.1 in $CHCl_3$).

Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 55 (*isol, ir, pmr, cmr*)

Dihydro-5-(6-methylheptyl)-2(3*H*)-furanone D-573

10-Methyl-4-undecanolide



$C_{12}H_{22}O_2$ 198.305

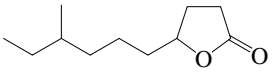
(ξ)-*form*

Prod. by the marine *Streptomyces* sp. strain GWS-BW-H5.

Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 837-865 (*isol, ms*)

Dihydro-5-(4-methylhexyl)-2(3*H*)-furanone D-574

8-Methyl-4-decanolide



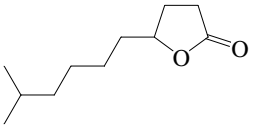
$C_{11}H_{20}O_2$ 184.278

Prod. by the marine *Streptomyces* sp. B6007.

Stritzke, K. *et al., J. Nat. Prod.*, 2004, **67**, 395-401 (*isol, ms*)

Dihydro-5-(5-methylhexyl)-2(3*H*)-furanone D-575

9-Methyl-4-decanolide



$C_{11}H_{20}O_2$ 184.278

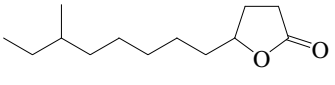
(ξ)-*form*

Prod. by a marine bacterium.

Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol*)

Dihydro-5-(6-methyloctyl)-2(3*H*)-furanone D-576

10-Methyl-4-dodecanolide



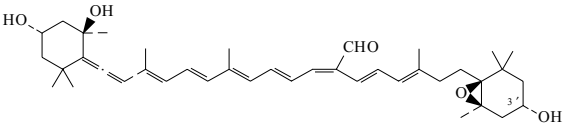
$C_{13}H_{24}O_2$ 212.331

(ξ)-*form*

Prod. by the marine *Streptomyces* strain GWS-BW-H5.

Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 837-865 (*isol, ms*)

7′,8′-Dihydroneoxanthin-20′-al D-577



$C_{40}H_{56}O_5$ 616.879

(13′*E*)-*form*

*3′-O-[β-D-Galactopyranosyl-(1→4)-β-D-glucopyranoside]: **Carotenoid P 457**. P 457*

[55068-71-8]

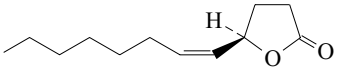
$C_{52}H_{76}O_{15}$ 941.163

Isol. from the dinoflagellates *Amphidinium carterae*, *Gymnodinium splendens*, *Gymnodinium dorsum*, *Glenodinium* sp., and the marine dinoflagellate *Thoracosphaera heimii*. λ_{max} 424; 452; 480 (MeOH).

Johansen, J.E. *et al., Phytochemistry*, 1974, **13**, 2261-2271 (*occur*)
Bjoernland, T. *et al., Biochem. Syst. Ecol.*, 1990, **18**, 307-316 (*Thoracosphaera heimii constit*)
Aakermann, T. *et al., Acta Chem. Scand.*, 1993, **47**, 1207-1213 (*isol, pmr, cmr, ms, struct*)
Englert, G. *et al., J. Nat. Prod.*, 1995, **58**, 1675-1682; 1997, **60**, 536 (*isol, uv, ir, pmr, cmr, cd*)

Dihydro-5-(1-octenyl)-2(3*H*)-furanone D-578

5-Dodecen-4-olide



$C_{12}H_{20}O_2$ 196.289

(*R,Z*)-*form*

Buibuilactone

[139477-52-4]

Isol. from the beetle *Anomala cuprea* Also prod. by a marine bacterium. Sex pheromone. $Bp_{0.2}$ 115°. $[\alpha]_D^{24}$ -80.9 (c, 0.99 in $CHCl_3$). $[\alpha]_D^{24}$ -61.8 (c, 1 in hexane).

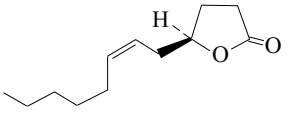
[139477-53-5]

Leal, W.S. *et al., Naturwissenschaften*, 1991, **78**, 521 (*isol, struct*)
Fukusaki, E. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1160 (*synth*)
Koseki, K. *et al., Tetrahedron*, 1993, **49**, 5961 (*synth*)
Dickschat, J.S. *et al., J. Chem. Ecol.*, 2005, **31**, 925-947 (*marine isol*)

Dihydro-5-(2-octenyl)-2(3*H*)-furanone, 9CI D-579

5-(2-Octenyl)tetrahydrofuran-2-one. 6-Dodecen-4-olide

[15456-69-6]



(*R*,Z)–*form*

$C_{12}H_{20}O_2$ 196.289

Isol. from butterfat and from the tarsal organs of deer. Also prod. by *Sporobolomyces odorus* and a marine bacterium. Intermed. in synth. of 5,12-Dihydroxy-6,8,10,14-eicosatetraenoic acid, D-677.

(*R,Z*)-*form* [63357-99-3]

$[\alpha]_D^{20}$ -16.1 (c, 0.3 in MeOH).

(*S,Z*)-*form* [63357-98-2]

$[\alpha]_D^{20}$ +15 (c, 0.1 in MeOH).

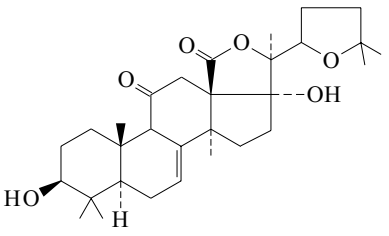
[18679-18-0, 60551-23-7, 127127-84-8]

Brownlee, R.G. *et al., Nature (London)*, 1969, **221**, 284 (*isol*)
Sucrow, W. *et al., Chem. Ber.*, 1975, **108**, 3518 (*synth*)
Meuller-Schwarze, D. *et al., J. Chem. Ecol.*, 1976, **2**, 389; 1978, **4**, 247

Burger, B.V. *et al., Z. Naturforsch., C*, 1977, **32**, 49 (*synth*)
Ravid, U. *et al., Tetrahedron*, 1978, **34**, 1449 (*synth*)
Dormán, G. *et al., J.C.S. Perkin 1*, 1989, 1543 (*use*)
Lee, S.-L. *et al., J. Ferment. Bioeng.*, 1994, **78**, 114 (*isol*)
Dickschat, J.S. *et al., J. Chem. Ecol.*, 2005, **31**, 925-947 (*marine isol*)

9,11-Dihydro-22,25-oxido-11-oxoholothurinogenin D-580

*22,25-Epoxy-3β,17α-dihydroxy-11-oxolanost-7-ene-18,20*S*-lactone*
[112570-87-3]

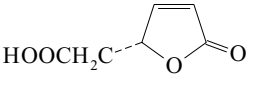


$C_{30}H_{44}O_6$ 500.674
Aglycone from *Holothuria atra* and *Holothuria scabra*. Cryst. (MeOH).
Mp 280-282°. $[\alpha]_D$ +16.6.

Sarma, N.S. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 715

2,5-Dihydro-5-oxo-2-furanacetic acid, 9CI, 8CI D-581

5-(Carboxymethyl)-2,5-dihydro-2-furanone. ***Muconolactone***
[6666-46-2]



(R)–form

$C_6H_6O_4$ 142.111
λ_{max} 201 (ϵ 7540) (MeOH).

(*R*)-*form* [32486-24-1]
Me ester: [104532-57-2]
$C_7H_8O_4$ 156.138
Isol. from *Plakortis lita* and *Plakortis simplex*. Oil. $[\alpha]_D$ -96.1 (c, 1.05 in $CHCl_3$). Genus name erroneously given in the paper as Plakorta.

(*S*)-*form* [1124-48-7]
Cryst. (EtOAc/C_6H_6). Mp 76-77.5°. $[\alpha]_D$ +57 (c,0.51 in EtOH).
Me ester: [112789-73-8]
Isol. from *Xestospongia* sp. Cytotoxic.
Mp 44.5-46.5°. $[\alpha]_D$ +96 (c, 1.05 in $CHCl_3$). λ_{max} 205 (MeOH).
Chloride:
$C_6H_5ClO_3$ 160.556
Bp_7 53-54°.
Anilide:
$C_{12}H_{11}NO_3$ 217.224
Mp 84°.

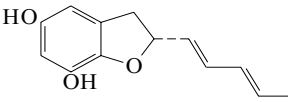
(±)-*form* [118544-79-9]
Needles (CH_2Cl_2/hexane). Mp 112°.
Et ester: [118864-32-7]
$C_8H_{10}O_4$ 170.165
$Bp_{0.046}$ 94-96°.
Chloride:
Liq. Bp_2 125°.

[54911-84-1, 85195-89-7, 85195-91-1]

Jaroszwski, J.W. *et al., J.O.C.*, 1982, **47**, 3974 (*synth, ir, pmr*)
Janda, M. *et al., Coll. Czech. Chem. Comm.*, 1983, **48**, 96 (*synth, derivs, pmr*)
Quiñoà, E. *et al., J.O.C.*, 1986, **51**, 4260-4264 (*isol, pmr, cmr, ms, ir, uv*)
Hizuka, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 1550 (*synth, ir, pmr, ms*)
Murayama, T. *et al., Experientia*, 1989, **45**, 898 (*isol*)
Bloch, R. *et al., Tetrahedron*, 1989, **45**, 3731 (*Me ester, synth*)
De Guzman, F.S. *et al., J. Nat. Prod.*, 1990, **53**, 926-931 (*isol, pmr, cmr, ms*)
Ribbons, D.W. *et al., Tetrahedron*, 1994, **50**, 3587-3594 (*synth, abs config*)
Cain, R.B. *et al., J. Chem. Res., Synop.*, 1996, 526 (*uv, cd*)
Gawronski, J.K. *et al., J.O.C.*, 1996, **61**, 1513-1515 (*uv, cd*)

2,3-Dihydro-2-(1,3-pentadienyl)-5,7-benzofurandiol, 9CI D-582

Asperfuran. *Arthrographol*
[138331-36-9]



$C_{13}H_{14}O_3$ 218.252

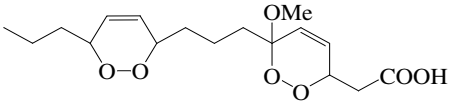
(*R*)-*form* [129277-10-7]
Metab. of *Arthrographis pinicola*, *Aspergillus oryzae* and the marine-derived *Aspergillus flavus* Go 100/4. Possesses antifungal props.
Needles (EtOAc/cyclohexane).
Mp 130° Mp 122°. $[\alpha]_D^{20}$ -20.9 (c, 0.21 in Me_2CO). λ_{max} 227 (ϵ 32300); 295 (ϵ 3720) (MeOH).

[127818-09-1, 129257-93-8]

Ayer, W.A. *et al., Can. J. Microbiol.*, 1990, **36**, 83-85 (*isol, struct*)
Pfefferle, W. *et al., J. Antibiot.*, 1990, **43**, 648-654 (*isol, struct*)
Ayer, W.A. *et al., Can. J. Chem.*, 1991, **69**, 1909 (*synth*)
Miyake, M. *et al., Chem. Lett.*, 1993, 1683 (*synth*)
Miyake, M. *et al., Heterocycles*, 1996, **43**, 665 (*synth*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

6-[3-(3,6-Dihydro-6-propyl-1,2-dioxin-3-yl)propyl]-3,6-dihydro-6-methoxy-1,2-dioxin-3-acetic acid, 9CI D-583

6-Methoxy-3,6:10,13-diperoxy-4,11-hexadecadienoic acid
[154702-57-5]



$C_{17}H_{26}O_7$ 342.388
Isol. from the sponge *Plakortis simplex*.

Me ester: [154702-58-6]
$C_{18}H_{28}O_7$ 356.415
Isol. from *Plakortis simplex*.

Rudi, A. *et al., J. Nat. Prod.*, 1993, **56**, 2178-2182 (*isol*)

3,4-Dihydro-2*H*-pyrrole, 9CI D-584

1-Pyrroline. FEMA 3898
[5724-81-2]

C_4H_7N 69.106
Male sex pheromone of Mediterranean fruit fly *Ceratitis capitata*. Present in clam and squid. Primary odour constit. of sperm. Stable in dil. soln., trimerises readily.

N-*Oxide:* [24423-88-9]
C_4H_7NO 85.105
Cyclic nitrone used in intramol. 1,3-dipolar cycloadditions.
$Bp_{0.1}$ 74-76°.

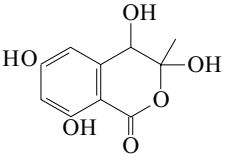
Trimer: See Dodecahydrotripyrrolo[1,2-*a*:1′,2′-*c*:1″,2″-*e*][1,3,5]triazine in *The Combined Chemical Dictionary.*

Amoore, J.E. *et al., J. Chem. Ecol.*, 1975, **1**, 299
Poisel, H. *et al., Monatsh. Chem.*, 1978, **109**, 925 (*synth, pmr*)
Baker, R. *et al., Chem. Comm.*, 1985, 824
Bock, H. *et al., Chem. Ber.*, 1987, **120**, 1961 (*synth, pe, bibl*)
Guillemin, J.-C. *et al., Tetrahedron*, 1988, **44**, 4447 (*synth, pmr*)
Murahashi, S. *et al., J.O.C.*, 1990, **55**, 1736-1744 (*N-oxide, synth, ir, pmr*)

Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 4389-4390 (*N-oxide, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 1568

3,4-Dihydro-3,4,6,8-tetrahydroxy-3-methyl-1*H*-2-benzopyran-1-one D-585

3,4-Dihydro-3,4,6,8-tetrahydroxy-3-methylisocoumarin. 3,4,6-Trihydroxymellein
[108354-31-0]

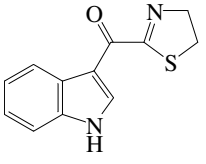


$C_{10}H_{10}O_6$ 226.185
Prod. by *Ceratocystis minor* and a fungus isol. from a marine sediment. Prisms (MeOH aq.).
Mp 208-212° (204-206°). Racemic. Isolates may be different diastereoisomers. λ_{max} 216 (ϵ 13240); 224 (sh) (ϵ 11130); 264 (ϵ 6780); 301 (ϵ 4620) (MeOH).

Ayer, W.A. *et al., Can. J. Chem.*, 1987, **65**, 765 (*isol, uv, ir, pmr, cmr*)
Cui, C.-B. *et al., J. Antibiot.*, 1996, **49**, 216 (*isol, uv, ir, pmr, cmr*)
Nomoto, S. *et al., Liebigs Ann./Recl.*, 1997, 721 (*synth, ir, pmr, cmr*)

3-(4,5-Dihydro-2-thiazolecarbonyl)-1*H*-indole D-586

*(4,5-Dihydro-2-thiazolyl)-1*H*-indole-3-ylmethanone, 9CI*
[244295-62-3]

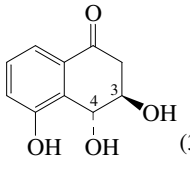


$C_{12}H_{10}N_2OS$ 230.29
Prod. by *Paracoccus* sp. Uv absorbent.

Japan. Pat., 1999, 99 269 175; *CA*, **131**, 242087z

3,4-Dihydro-3,4,5-trihydroxy-1(2*H*)-naphthalenone, 9CI D-587

3,4,5-Trihydroxy-1-tetralone



(3*R*,4*R*)-*form*

$C_{10}H_{10}O_4$ 194.187

(3*R*,4*R*)-*form*
Antibiotic PD3. *PD3*
[88899-01-8]
Prod. by *Penicillium diversum* var. *aureum*. Cytotoxic agent. Cryst. (Me_2CO). Sol. MeOH, C_6H_6, EtOAc; poorly sol. H_2O.
Mp 199-200° dec. $[\alpha]_D^{22}$ -14.2 (c, 2.5 in MeOH).

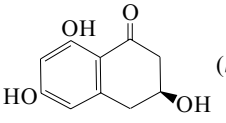
*5-Me ether: 3,4-Dihydro-3,4-dihydroxy-5-methoxy-1(2*H*)-naphthalenone. 3,4-Dihydroxy-5-methoxytetralone*
[103763-59-3]
$C_{11}H_{12}O_4$ 208.213
Mp 172-174°.

(3*S*,4*S*)-*form*
4,5-O-Ethylidene: ***Humicolone***
$C_{12}H_{12}O_4$ 220.224
Prod. by marine-derived *Humicola grisea*. Cytotoxic. $[\alpha]_D^{20}$ +8.1 (c, 0.3 in MeOH). λ_{max} 207 (ϵ 96000); 253 (ϵ 12000); 310 (ϵ 3700) (MeOH).

Japan. Pat., 1985, 85 62 989; *CA*, **103**, 176976 (*isol*)
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 1497 (*isol, pmr, cmr, struct*)
Laurent, D. *et al., Tetrahedron*, 2002, **58**, 9163-9167 (*Humicolone*)

3,4-Dihydro-3,6,8-trihydroxy-1(2*H*)-naphthalenone, 9CI D-588

3,6,8-Trihydroxy-1-tetralone. ***Scytalone***



(*S*)–*form*

$C_{10}H_{10}O_4$ 194.187
Metab. of *Scytalidium* spp. and *Phialophora lagerbergii*. Also isol. from various fungal sources. Intermed. in melanin biosynth.

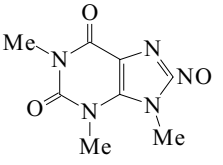
(*S*)-*form* [59872-10-5]
Prod. by *Verticillium dahliae* and a marine-derived *Alternaria* sp. Stamm 6588. Sol. MeOH, Et_2O; poorly sol. H_2O, hexane.
Mp 164.5-168.5°. $[\alpha]_D^{25}$ +32 (c, 0.25 in 95% EtOH). λ_{max} 232 (ϵ 8170); 283 (ϵ 12640); 317 (ϵ 4850) (MeOH) (Berdy). λ_{max} 222 (ϵ 15130); 232 (ϵ 6460); 284 (ϵ 12900); 322 (ϵ 6760) (EtOH) (Berdy). λ_{max} 210 (ϵ 21400); 253 (ϵ 5370); 334 (ϵ 31620) (EtOH-NaOH) (Berdy).

(±)-*form* [144068-45-1]
Metab. of *Lachnellula* sp.
Cryst. (Et_2O/C_6H_6 or H_2O).
Mp 185-190° (172-174°).
Tri-Ac: Mp 120-123°.
6-Me ether: Mp 76-84°.
[49598-85-8]

Findlay, J.A. *et al., Can. J. Chem.*, 1973, **51**, 1617; 3299 (*isol, pmr, ir, uv*)
Bycroft, B.W. *et al., Chem. Comm.*, 1974, 443 (*synth*)
Aldbridge, D.C. *et al., J.C.S. Perkin 1*, 1974, 1540 (*isol, ir, pmr*)
Bell, A.A. *et al., Tetrahedron*, 1976, **32**, 1353 (*biosynth, uv, pmr, ms, isol*)
Seto, H. *et al., Tet. Lett.*, 1977, 487 (*biosynth, cmr*)
Sankawa, U. *et al., Chem. Pharm. Bull.*, 1981, **29**, 3536 (*biosynth*)
Fabrice, V. *et al., Tetrahedron*, 1990, **46**, 2827 (*isol, cd, bibl*)
Viviani, F. *et al., New J. Chem.*, 1992, **16**, 81 (*synth*)
Semar, M. *et al., Z. Naturforsch., C*, 1996, **51**, 500 (*isol*)

3,9-Dihydro-1,3,9-trimethyl-8-nitroso-1*H*-purine-2,6-dione, 9CI D-589

1,3,9-Trimethyl-8-nitrosoisoxanthine
[153534-80-6]



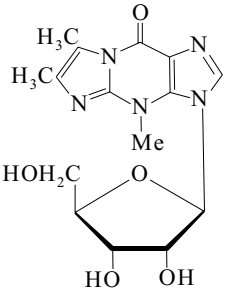
$C_8H_9N_5O_3$ 223.191
The first isoxanthine (isocaffeine) deriv. from a natural source. Isol. from the sea cucumber *Cucumaria frondosa*. Powder.
Mp 273° dec.

Yayli, N. *et al., J. Nat. Prod.*, 1994, **57**, 84-89 (*isol, uv, ir, pmr, cmr, struct*)

3,4-Dihydro-4,6,7-trimethyl-3-β-D-ribofuranosyl-9*H*-imidazo[1,2-*a*]purin-9-one, 9CI D-590

MimG

[108274-04-0]



$C_{15}H_{19}N_5O_5$ 349.346

Isol. from *Sulfolobus solfataricus, Thermoproteus neutrophilus* and *Pyrodictium occultum*. No phys. props. reported.

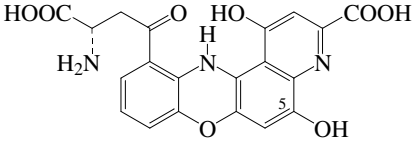
McCloskey, J.A. *et al., Nucleic Acids Res.*, 1987, **15**, 683 (*isol, struct*)

Dihydroxanthommatin D-591

*α-Amino-3-carboxy-1,5-dihydroxy-γ-oxo-12*H*-pyrido[3,2-*a*]phenoxazine-11-butanoic acid, 9CI*

[25705-16-2]

[81624-03-5]



$C_{20}H_{15}N_3O_8$ 425.354

(S)-form

Found in eyes and skin of *Loligo vulgaris, Sepia officinalis* and other molluscs, also in heads of flies *Musca domestica* and bees *Apis mellifera*, and in lepidopteran wings and excreta.

Red cryst. Mp >350°.

5-O-*Sulfate:* ***Ommatin D***

[28991-26-6]

$C_{20}H_{15}N_3O_{11}S$ 505.418

Occurs in lepidopteran wings and excreta. Isol. from the secretions of the butterfly *Vanessa urticae*. Red-brown powder.

5-O-*β-D-Glucopyranoside:* ***Rhodommatin***

$C_{26}H_{25}N_3O_{13}$ 587.496

Occurs in lepidopteran wings and excreta. Isol. from the secretions of *Vanessa urticae*. Red cryst. Mp >350°.

[121727-27-3]

Butenandt, A. *et al., Annalen*, 1957, **607**, 207-214 (*Ommatin D*)

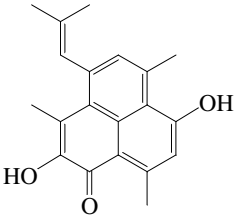
Butenandt, A. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1960, **321**, 258-275 (*Ommatin D, Rhodommatin*)

Bolognese, A. *et al., J. Het. Chem.*, 1988, **25**, 1247-1250

5,10-Dihydroxy-1,3,5,7,10,12,14-amphilectaheptaen-9-one D-592

Elisabatin C

[325691-46-1]



$C_{20}H_{20}O_3$ 308.376

Constit. of *Pseudopterogorgia elisabethae*. Red needles.

Mp 227-228°. λ_{max} 210 (ε 17000); 256 (ε 11000); 430 (ε 5500); 458 (ε 4700) (MeOH).

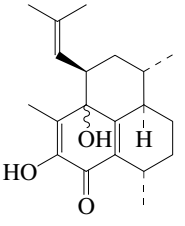
Rodríguez, A.D. *et al., Tetrahedron*, 2000, **56**, 9015-9023 (*isol, pmr, cmr*)

Baran, P. *et al., J. Chem. Crystallogr.*, 2003, **33**, 711-718 (*cryst struct*)

10,12-Dihydroxy-8(13),10,14-amphilectatrien-9-one D-593

Elisabethol

[433300-34-6]



$C_{20}H_{28}O_3$ 316.439

Constit. of *Pseudopterogorgia elisabethae*. λ_{max} 240 (MeOH).

12-Hydroperoxide: 12-Hydroperoxy-10-hydroxy-8(13),10,14-epiamphilectatrien-9-one

12-Hydroperoxide, 10-Ac:

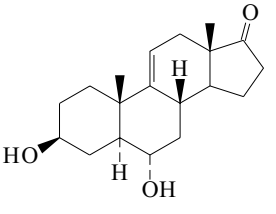
$C_{22}H_{30}O_5$ 374.476

Constit. of *Pseudopterogorgia* sp. Yellow oil. $[\alpha]_D$ -11.3 (c, 0.006 in MeOH).

Harvis, C.A. *et al., Tet. Lett.*, 1988, **29**, 4361 (*hydroperoxide Ac*)

Ata, A. *et al., Tetrahedron*, 2003, **59**, 4215-4222 (*Elisabethol*)

3,6-Dihydroxyandrost-9(11)-en-17-one D-594



$C_{19}H_{28}O_3$ 304.428

(3β,5α,6α)-*form*

6-O-*[4*-O-*Sulfo-6-deoxy-β-D-glucopyranoside], 3-sulfate:* ***Latespinoside D***

[178200-93-6]

$C_{25}H_{38}O_{13}S_2$ 610.699

Constit. of *Astropecten latespinosus*. Amorph. powder.

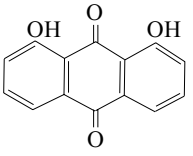
Mp 210-215°. $[\alpha]_D$ +50.2 (c, 1.5 in MeOH).

Higuchi, R. *et al., Annalen*, 1996, 837-840 (*Latespinoside D*)

1,8-Dihydroxyanthraquinone, 8CI D-595

1,8-Dihydroxy-9,10-anthracenedione, 9CI. Chrysazin. ***Dantron, INN****. Danthron, BAN. Istizin. Danivac. Dorbane. Many other names*

[117-10-2]



$C_{14}H_8O_4$ 240.215

Occurs in roots of *Rheum palmatum* (Turkey rhubarb), leaves and stems of *Xyris semifuscata*, tissue culture of *Cinchona ledgeriana* and leaves of *Pyrrhalta luteola*. Isol. from *Watersipora subtorquata*. Used in photometric detn. of B; fluorimetric detn. of Mg (λ_{max} 600 nm). Cathartic. Square orange plates (Me_2CO), metastable fine fibres by rapid cryst. Sol. EtOH, alkalis; insol. H_2O.

Mp 193°. pK_{a1} 8.3; pK_{a2} 12.46 (25°). Log P 1.92 (calc). It has been suggested that the 1,10-dioxo tautomer is present in the crystal state but there is no spectroscopic evidence for this.

▶ Can discolour urine when used therapeutically. Exp. carcinogen. Possible human carcinogen (IARC 2B). CB6650000

Di-Ac: [1963-82-2]

$C_{18}H_{12}O_6$ 324.289

Yellow needles. Mp 231-232°.

▶ CB6690000

Mono-Me ether: 1-Hydroxy-8-methoxyanthraquinone

[5539-66-2]

$C_{15}H_{10}O_4$ 254.242

Orange-red needles (EtOH). Mp 197-198°.

Di-Me ether: 1,8-Dimethoxyanthraquinone

[6407-55-2]

$C_{16}H_{12}O_4$ 268.268

Yellow cryst. Mp 219°.

Mono-Et ether: 1-Ethoxy-8-hydroxyanthraquinone

$C_{16}H_{12}O_4$ 268.268

Cryst. (EtOH). Mp 179-180°.

Di-Et ether: 1,8-Diethoxyanthraquinone

$C_{18}H_{16}O_4$ 296.322

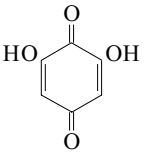
Cryst. (AcOH). Mp 166-169°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 91B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 87D (*ir*)
Naylor, C.A. *et al., J.A.C.S.*, 1931, **53**, 4112
Aoyama, S. *et al., Yakugaku Zasshi*, 1932, **52**, 17
Lish, P.M. *et al., J. Am. Pharm. Assoc.*, 1958, **47**, 371 (*pharmacol*)
Kido, H. *et al., Anal. Chim. Acta*, 1960, **23**, 116 (*ir*)
Beynon, J.H. *et al., Appl. Spectrosc.*, 1960, **14**, 156 (*ms*)
Ruggieri, R. *et al., Anal. Chim. Acta*, 1961, **25**, 145 (*use*)
Prakesh, A. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1965, **122**, 272 (*cryst struct*)
Fairbairn, J.W. *et al., J. Pharm. Pharmacol.*, 1970, **22**, 584 (*pharmacol*)
Idris, K.A. *et al., Egypt. J. Chem.*, 1973, 67 (*uv*)
Morley, J.O. *et al., J.C.S. Perkin 2*, 1973, 1626 (*pmr*)
Fournier, G. *et al., Phytochemistry*, 1975, **14**, 2099 (*isol*)
Breimer, D.D. *et al., Pharmacology*, 1976, **14**, 30 (*metab*)
Case, M.T. *et al., Drug Chem. Toxicol.*, 1978, **1**, 89 (*tox*)
Berger, Y. *et al., Org. Magn. Reson.*, 1978, **11**, 375 (*cmr*)
Cameron, A.W. *et al., Aust. J. Chem.*, 1982, **35**, 2095 (*synth*)
Howard, D.F. *et al., Naturwissenschaften*, 1982, **69**, 91 (*isol*)
Roman Ceba, M. *et al., Mikrochim. Acta*, 1983, **2**, 85 (*detn, Mg*)
Mueller, K. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1984, **317**, 120 (*synth*)
Gattuso, J.M. *et al., Drug Saf.*, 1984, **10**, 47 (*rev*)
Khanapure, S.P. *et al., J.O.C.*, 1987, **52**, 5685 (*deriv, synth, pmr, ir*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 2970 (*synonyms*)
IARC Monog., 1990, **50**, 265 (*rev, tox*)
Grunwell, J.R. *et al., J.O.C.*, 1991, **56**, 91 (*synth, pmr*)
Kahr, B. *et al., Angew. Chem., Int. Ed.*, 1992, **31**, 1 (*tautom*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1215
Jeong, S.-J. *et al., J. Nat. Prod.*, 2002, **65**, 1344-1345 (*sol, Watersipora*)
Kampmann, B. *et al., J.O.C.*, 2002, **67**, 3878-3883 (*Et ethers, synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DMH400

2,6-Dihydroxy-1,4-benzoquinone D-596

2,6-Dihydroxy-2,5-cyclohexadiene-1,4-dione, 9CI

[35069-70-6]



$C_6H_4O_4$ 140.095

Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 286 (ϵ 15100); 287 (ϵ 22200); 376 (ϵ 1020); 385 (ϵ 600) (MeOH) (Berdy). λ_{max} 283 (ϵ 14500); 287 (ϵ 19050); 375 (ϵ 560); 377 (ϵ 602) ($CHCl_3$) (Berdy). λ_{max} 287 (ϵ 19200); 377 (ϵ 630) (EtOH) (Berdy).

Di-Me ether: 2,6-Dimethoxy-1,4-benzoquinone

[530-55-2]

$C_8H_8O_4$ 168.149

Widespread in wood and woody tissues, prob. as degradn. prod. of lignin. Isol. esp. from the Simaroubaceae, e.g. *Picrasma, Ailanthus* spp. Also prod. by the marine fungus *Dendryphiella salina* grown on waste sulfite liquor. Constit. of bark of *Phyllostachys heterocycla* var. *pubescens* (moso bamboo) and isol. from the mangrove plant *Bruguiera sexangula* var. *rhynchopetala*. Shows antibacterial props. Yellow cryst. (AcOH).

Mp 252°. λ_{max} 288 (ϵ 12600) (MeOH) (Derep).

▶ Causes dermatitis. Mutagenic props. DK4750000

Di-Me ether, 4-oxime: [22867-29-4]

$C_8H_9NO_4$ 183.163

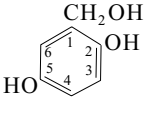
Yellow plates (H_2O). Mp 218.8° dec.

Polonsky, J. *et al., Bull. Soc. Chim. Fr.*, 1959, 1157; 1962, 1715 (*isol, deriv*)
Horner, L. *et al., Chem. Ber.*, 1961, **94**, 1291 (*synth*)
Bolker, H.I. *et al., Can. J. Chem.*, 1969, **47**, 2109 (*deriv*)
Schmalle, H. *et al., Naturwissenschaften*, 1977, **64**, 534 (*cryst struct, deriv*)
Org. Synth., 1977, **57**, 78 (*synth*)
Nishina, A. *et al., J. Agric. Food Chem.*, 1991, **39**, 266 (*isol, deriv*)
Frick, E. *et al., Nat. Prod. Lett.*, 1996, **9**, 153-159 (*synth*)
Omura, K. *et al., Synthesis*, 1998, 1145-1148 (*synth*)
Villemin, D. *et al., Synth. Commun.*, 2002, **32**, 1501-1515 (*di-Me ether, synth*)
Bao, S. *et al., Helv. Chim. Acta*, 2005, **88**, 2757-2763 (*Bruguiera, isol*)

2,5-Dihydroxybenzyl alcohol, 8CI D-597

2,5-Dihydroxybenzenemethanol, 9CI. α,2,5-Trihydroxytoluene. 2-(Hydroxymethyl)-1,4-benzenediol. Gentisyl alcohol. Salirepol. Gentisin alcohol

[495-08-9]

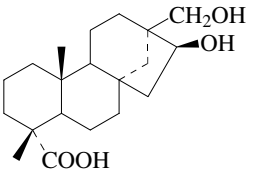


$C_7H_8O_3$ 140.138

Metab. of *Phoma* spp., *Penicillium roqueforti*, *Phyllosticta* sp. and a marine *Aspergillus varians*. Phytotoxic. Red-brown cryst. (Et_2O/petrol). Sol. H_2O, Et_2O, EtOH; fairly sol. C_6H_6, $CHCl_3$; poorly sol. hexane. Mp 104-105°. Readily oxidised.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1141B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 363B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1067B (*ir*)
Biellmann, J.F. *et al., Bull. Soc. Chim. Fr.*, 1971, 1676 (*synth*)
Burton, G. *et al., Can. J. Chem.*, 1980, **58**, 1839 (*cmr*)
Casiraghi, G. *et al., Synthesis*, 1980, 124 (*synth*)
Smetanina, O.F. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 243-244 (*marine isol*)

16,17-Dihydroxy-18-beyeranoic acid D-598



$C_{20}H_{32}O_4$ 336.47

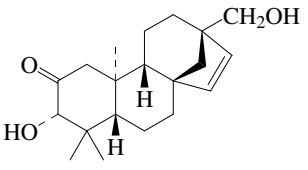
16β-*form*

Me ester: ***Ceriopsin B***
[478175-19-8]
$C_{21}H_{34}O_4$ 350.497
Constit. of *Ceriops decandra*. Cryst. (MeOH).
Mp 164-166°. $[\alpha]_D^{25}$ -37.5 (c, 0.8 in $CHCl_3$).

16-Ketone: 17-Hydroxy-16-oxo-18-beyeranoic acid
$C_{20}H_{30}O_4$ 334.455

16-Ketone, Me ester: ***Ceriopsin A***
[478175-18-7]
$C_{21}H_{32}O_4$ 348.481
Constit. of *Ceriops decandra*. Cryst. (MeOH).
Mp 135-139°. $[\alpha]_D^{25}$ -47 (c, 0.6 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., Phytochemistry*, 2002, **60**, 777-782 (*isol, pmr, cmr*)

3,17-Dihydroxy-15-beyeren-2-one D-599



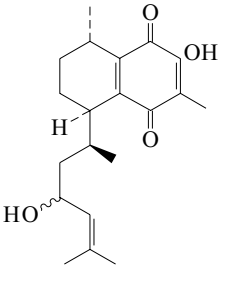
$C_{20}H_{30}O_3$ 318.455

(*ent*-3β)-*form*

Di-Ac: ***Rhizophorin D***
[480427-82-5]
$C_{24}H_{34}O_5$ 402.53
Constit. of *Rhizophora mucronata*. Cryst. (MeOH).
Mp 165-168°. $[\alpha]_D^{25}$ -45.1 (c, 1.75 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., J. Asian Nat. Prod. Res.*, 2002, **4**, 53-61 (*isol, pmr, cmr*)

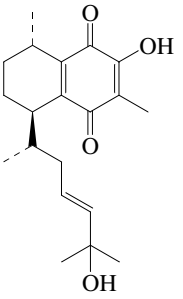
3,14-Dihydroxy-1(6),3,15-bifloratriene-2,5-dione D-600

[118169-36-1]



$C_{20}H_{28}O_4$ 332.439
Constit. of *Pseudopterogorgia* sp. Orange oil.
Harvis, C.A. *et al., Tet. Lett.*, 1988, **29**, 4361 (*struct*)

3,16-Dihydroxy-1(6),3,14-bifloratriene-2,5-dione D-601

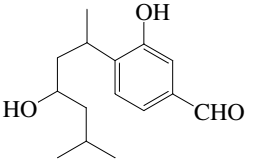


$C_{20}H_{28}O_4$ 332.439

(10α,14*E*)-*form* [325691-48-3]
Constit. of *Pseudopterogorgia elisabethae*.
Orange oil. $[\alpha]_D^{25}$ +220 (c, 0.25 in $CHCl_3$). λ_{max} 206 (ϵ 16000); 282 (ϵ 12000); 326 (ϵ 1800) (MeOH).
Rodríguez, A.D. *et al., Tetrahedron*, 2000, **56**, 9015-9023 (*isol, pmr, cmr*)

1,9-Dihydroxy-1,3,5-bisabolatrien-15-al D-602

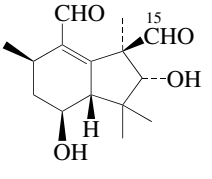
Parahigginin
[227598-37-0]



$C_{15}H_{22}O_3$ 250.337
Constit. of the sponge *Parahigginsia* sp.

9-Ac: 9-Acetoxy-1-hydroxy-1,3,5-bisabolatrien-15-al. ***Parahigginol B***
[224176-18-5]
$C_{17}H_{24}O_4$ 292.374
Constit. of a *Parahigginsia* sp. Oil. $[\alpha]_D$ -11.4 (c, 0.58 in $CHCl_3$). λ_{max} 224 (log ϵ 4); 265 (log ϵ 3.8); 316 (log ϵ 3.4) (MeOH).
J. Chin. Chem. Soc. (Taipei), 1999, **46**, 201-204 (*isol, pmr, cmr*)
Chen, C.-Y. *et al., J. Nat. Prod.*, 1999, **62**, 573-576 (*Parahigginol B*)

4,7-Dihydroxy-1(9)-botryene-10,15-dial D-603



$C_{15}H_{22}O_4$ 266.336

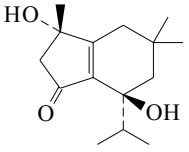
(4β,7α)-*form*

Di-Ac: ***Hymendial***
[196796-11-9]
$C_{19}H_{26}O_6$ 350.411
Metab. of *Hymenoscyphus epiphyllus*. Cryst.
Mp 144-147°. $[\alpha]_D^{22}$ +157 (c, 1.1 in $CHCl_3$). λ_{max} 249 (ϵ 7500) (MeOH).

15-Alcohol: 4,7,15-Trihydroxy-1(9)-botryen-10-al. 7-Hydroxydeacetylbotryenalol
[850715-18-3]
$C_{15}H_{24}O_4$ 268.352
Metab. of a *Geniculosporium* sp. isol. from a *Polysiphonia* sp. Cryst. (MeOH).
Mp 200-201°. $[\alpha]_D^{25}$ +78.3 (c, 0.02 in MeOH).

Thines, E. *et al., Z. Naturforsch., C*, 1997, **52**, 413-420 (*Hymendial*)
Krohn, K. *et al., J. Nat. Prod.*, 2005, **68**, 400-405 (*Geniculosporium metab*)

5,9-Dihydroxy-1(6)-brasilen-7-one D-604



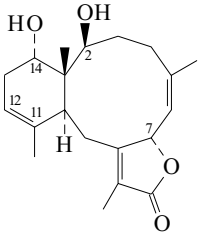
(5β,9α)–*form*

$C_{15}H_{24}O_3$ 252.353

(5β,9α)-*form*
Metab. of *Laurencia obtusa*.
Cryst. (Et_2O/cyclohexane).
Mp 126-128°. $[\alpha]_D^{25}$ +7.1 (c, 3 in EtOH).

(5β,9β)-*form*
Metab. of *Laurencia obtusa*.
Cryst. (CH_2Cl_2/Et_2O).
Mp 130-132°. $[\alpha]_D^{25}$ +1.1 (c, 1.5 in MeOH).
Caccamese, S. *et al., J. Nat. Prod.*, 1990, **53**, 1287 (*isol, pmr, cmr, cryst struct*)
Amico, V. *et al., Phytochemistry*, 1991, **30**, 1921 (*isol, pmr, cmr*)

2,14-Dihydroxy-5,8(17),11-briaratrien-18,7-olide D-605



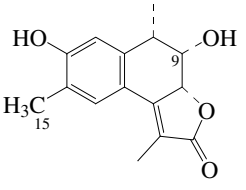
(2β,5*Z*,7α,14α)–*form*

$C_{20}H_{28}O_4$ 332.439

(2β,5*Z*,7α,14α)-*form*
2,14-Di-Ac: ***Brianthein W***
[91178-23-3]
$C_{24}H_{32}O_6$ 416.513
Constit. of *Briareum polyanthes*. Cryst. (Me_2CO/2,3,3-trimethylpentane).
Mp 205-209°. λ_{max} 228 (ϵ 7500) (EtOH) (Derep).
2-Propanoyl, 14-Ac: ***Funicolide A***
[171370-66-4]
$C_{25}H_{34}O_6$ 430.54
Constit. of *Funiculina quadrangularis*.
$[\alpha]_D^{20}$ +33.2 (c, 0.6 in EtOH).
2-Butanoyl, 14-Ac: ***Funicolide D***
[171370-68-6]
$C_{26}H_{36}O_6$ 444.567
Constit. of *Funiculina quadrangularis*.
$[\alpha]_D^{20}$ +33.2 (c, 0.25 in EtOH).
2-(3-Methyl-2-butenoyl), 14-Ac: ***Malayenolide C***
[225662-11-3]
$C_{27}H_{36}O_6$ 456.578
Constit. of *Veretillum malayense*. Amorph. solid. $[\alpha]_D$ +69.9 (c, 1.5 in $CHCl_3$). λ_{max} 222 (ϵ 25900) (EtOH).
2-Benzoyl, 14-Ac: ***Malayenolide A***
[225662-09-9]
$C_{29}H_{34}O_6$ 478.584
Constit. of *Veretillum malayense*. Amorph. solid. $[\alpha]_D$ +158 (c, 1.05 in $CHCl_3$). λ_{max} 228 (ϵ 21950) (EtOH).
11β,12β-Epoxide: 11,12-Epoxy-2,14-dihydroxy-5,8(17)-briaradien-18,7-olide
$C_{20}H_{28}O_5$ 348.438
11β,12β-Epoxide, 2-butanoyl, 14-Ac: ***14-Acetoxy-2-butanoyloxy-11,12-epoxy-5,8(17)-briaradien-18,7-olide***
[112781-24-5]
$C_{26}H_{36}O_7$ 460.566
Isol. from *Briareum steckei*. Plates (CH_2Cl_2/hexane).
Mp 158-160°. $[\alpha]_D$ +55.2 (c, 0.27 in $CHCl_3$).
11β,12β-Epoxide, 2-(3-methyl-2-butenoyl), 14-Ac: ***Malayenolide D***
[225662-12-4]
$C_{27}H_{36}O_7$ 472.577
Constit. of *Veretillum malayense*. Amorph. solid. $[\alpha]_D$ +29 (c, 0.69 in $CHCl_3$). λ_{max} 220 (ϵ 26200) (EtOH).
11β,12β-Epoxide, 2-benzoyl, 14-Ac: ***Malayenolide B***
[225662-10-2]
$C_{29}H_{34}O_7$ 494.583
Constit. of *Veretillum malayense*. Amorph. solid. $[\alpha]_D$ +85 (c, 0.6 in $CHCl_3$). λ_{max} 226 (ϵ 21850) (EtOH).

(2β,5*Z*,7β,14α)-*form*
2-Propanoyl, 14-Ac: ***7-Epifunicolide A***
[171485-64-6]
$C_{25}H_{34}O_6$ 430.54
Constit. of *Funiculina quadrangularis*.
$[\alpha]_D^{20}$ -43.3 (c, 0.14 in EtOH).
Cardellina, J.H. *et al., J.O.C.*, 1984, **49**, 3398
Bowden, B.F. *et al., Aust. J. Chem.*, 1987, **40**, 2085
Guerriero, A. *et al., Helv. Chim. Acta*, 1995, **78**, 1465 (*Funicolides*)
Sheu, J.-H. *et al., J. Nat. Prod.*, 1996, **59**, 935 (*isol, pmr, cmr*)
Fu, X. *et al., J. Nat. Prod.*, 1999, **62**, 584-586 (*Malayenolides*)

3,9-Dihydroxy-1,3,5,7(11)-cadinatetraen-12,8-olide D-606



(8α,9α,10α)-*form*

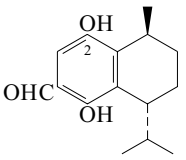
$C_{15}H_{16}O_4$ 260.289

(8α,9α,10α)-*form*
3-Me ether: 9-Hydroxy-3-methoxy-1,3,5,7(11)-cadinatetraen-12,8-olide. ***Vallapin***
$C_{16}H_{18}O_4$ 274.316
Constit. of *Heritiera littoralis*. Cryst.
Mp 269°. $[\alpha]_D^{25}$ -289.5. λ_{max} 216 (ϵ 11970); 239 (ϵ 12310); 286 (ϵ 16800); 310 (ϵ 17222) (cyclohexane).

(8α,9β,10α)-*form*
3-Me ether: ***Heritianin***
[133442-99-6]
$C_{16}H_{18}O_4$ 274.316
Constit. of *Heritiera littoralis*.
15-Hydroxy: 3,9,15-Trihydroxy-1,3,5,7(11)-cadinatetraen-12,8-olide
15-Hydroxy, 3-Me ether: ***9,15-Dihydroxy-3-methoxy-1,3,5,7(11)-cadinatetraen-12,8-olide. Vallapianin***
[133362-70-6]
$C_{16}H_{18}O_5$ 290.315
Constit. of *Heritiera littoralis*. Powder (Et_2O).
Mp 182°. $[\alpha]_D^{25}$ +225. λ_{max} 218 (ϵ 12111); 239 (ϵ 13277); 283 (ϵ 15722); 296 (ϵ 16444); 302 (ϵ 16777) (EtOH).
Miles, H.D. *et al., J. Nat. Prod.*, 1991, **54**, 286-289 (*isol, pmr, cmr, cryst struct*)

2,5-Dihydroxy-1,3,5-cadinatrien-15-al D-607

2,5-Dihydroxy-15-calamenenal



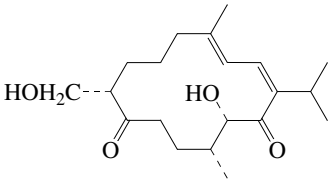
$C_{15}H_{20}O_3$ 248.321

Different numbering systems used in the lit.

(7α,10β)-*form*

2-Me ether: ***5-Hydroxy-2-methoxy-1,3,5-cadinatrien-15-al****. 5-Hydroxy-2-methoxy-15-calamenen-15-al*
[143705-32-2]
$C_{16}H_{22}O_3$ 262.348
Constit. of *Parerythropodium fulvum fulvum*. Oil. $[\alpha]_D$ +104 (c, 0.5 in CCl_4).
Green, D. *et al., J. Nat. Prod.*, 1992, **55**, 1186-1196 (*isol, pmr, cmr*)

13,19-Dihydroxy-1,3-cembradiene-9,14-dione D-608



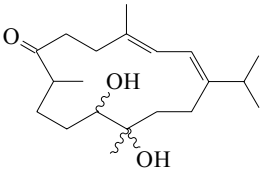
$C_{20}H_{32}O_4$ 336.47

(1*E*,3*Z*,8*S*,12*R*,13*S*)-*form*
7,8-Dihydroflabellatene A
[745819-66-3]
Constit. of *Gyrophyllum sibogae*.
Cryst.
Mp 175-176°. $[\alpha]_D^{25}$ +84.6 (c, 0.1 in $CHCl_3$). λ_{max} 298 (log ϵ 4.3) (MeOH).

3β,4β-Epoxide: 3,4-Epoxy-13,19-dihydroxy-1-cembrene-9,14-dione. ***7,8-Dihydroflabellatene B***
[745819-67-4]
$C_{20}H_{32}O_5$ 352.47
Constit. of *Gyrophyllum sibogae*. Oil. $[\alpha]_D^{25}$ +77 (c, 0.0013 in $CHCl_3$). λ_{max} 281 (log ϵ 2.31) (MeOH).
Reyes, F. *et al., J. Nat. Prod.*, 2004, **67**, 1190-1192 (*Gyrophyllum sibogae constits, pmr, cmr, cryst struct*)

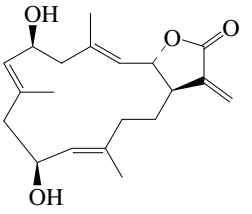
11,12-Dihydroxy-1,3-cembradien-7-one D-609

[147217-22-9]



$C_{20}H_{34}O_3$ 322.487
Constit. of a *Eunicea* sponge. Cryst. (MeOH).
Mp 156-157°. $[\alpha]_D$ +11.3 (c, 0.7 in $CHCl_3$).
Shin, J. *et al., Tetrahedron*, 1993, **49**, 515 (*isol, pmr, cmr*)

6,10-Dihydroxy-3,7,11,15(17)-cembratetraen-16,2-olide D-610



$C_{20}H_{28}O_4$ 332.439

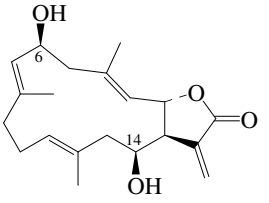
(1*R*,2*S*,3*E*,6*S*,7*E*,10*S*,11*E*)-*form*

6-Ac: [314739-99-6]
$C_{22}H_{30}O_5$ 374.476
Constit. of *Clavularia koellikeri*. Oil. $[\alpha]_D^{25}$ -25.8 (c, 0.12 in $CHCl_3$). λ_{max} 213 (log ϵ 3.52) (EtOH).

10-Ac: [314740-00-6]
$C_{22}H_{30}O_5$ 374.476
Constit. of *Clavularia koellikeri*. Oil. $[\alpha]_D^{25}$ -44 (c, 0.15 in $CHCl_3$). λ_{max} 219 (log ϵ 3.48) (EtOH).

Di-Ac: ***Claviolide***
[475111-81-0]
$C_{24}H_{32}O_6$ 416.513
Constit. of *Clavularia violacea*. Oil. $[\alpha]_D^{25}$ -33.8 (c, 0.05 in $CHCl_3$). λ_{max} 210 (log ϵ 4.12) (MeOH).
Iwashima, M. *et al., J. Nat. Prod.*, 2000, **63**, 1647-1652 (*isol, pmr, cmr*)
Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1535-1539 (*Claviolide*)

6,14-Dihydroxy-3,7,11,15(17)-cembratetraen-16,2-olide D-611



$C_{20}H_{28}O_4$ 332.439

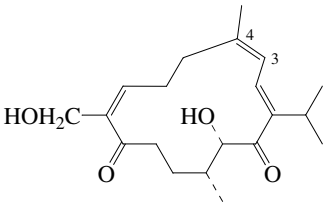
(1*S*,2*S*,3*E*,6*S*,7*E*,11*E*,14*S*)-*form*
Kericembrenolide E
[104992-90-7]
Constit. of *Clavularia koellikeri*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{21}$ -53 ($CHCl_3$).

6-Ac: ***Kericembrenolide D***
[104992-91-8]
$C_{22}H_{30}O_5$ 374.476
Constit. of *Clavularia koellikeri*. Cytotoxic agent. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{22}$ -71 ($CHCl_3$).

14-Ac: [314739-98-5]
$C_{22}H_{30}O_5$ 374.476
Constit. of *Clavularia koellikeri*. Oil. $[\alpha]_D^{25}$ -35.6 (c, 0.18 in $CHCl_3$). λ_{max} 215 (log ϵ 3.44) (EtOH).

Di-Ac: ***Kericembrenolide C***
[104992-92-9]
$C_{24}H_{32}O_6$ 416.513
Constit. of *Clavularia koellikeri*. Cytotoxic agent. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{22}$ -56 ($CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 2306 (*Kericembrenolides*)
Iwashima, M. *et al., J. Nat. Prod.*, 2000, **63**, 1647-1652 (*14-Ac*)

13,19-Dihydroxy-1,3,7-cembratriene-9,14-dione D-612

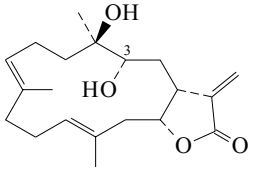


$C_{20}H_{30}O_4$ 334.455

(1*E*,3*Z*,7*Z*,12*R*,13*S*)-*form*
Flabellatene A
[222173-72-0]
Constit. of *Lissodendoryx flabellata*.
Yellow oil. $[\alpha]_D$ -12.7 (c, 0.3 in $CHCl_3$). λ_{max} 205 (ϵ 2920); 224 (ϵ 2680); 293 (ϵ 4080) ($CHCl_3$).

3β,4β-Epoxide: 3,4-Epoxy-13,19-dihydroxy-1,7-cembradiene-9, 14-dione. ***Flabellatene B***
[222173-73-1]
$C_{20}H_{30}O_5$ 350.454
Constit. of *Lissodendoryx flabellata*. Yellow oil. $[\alpha]_D$ +5.2 (c, 0.2 in $CHCl_3$). λ_{max} 236 (ϵ 7210) ($CHCl_3$).
Fontana, A. *et al., Tetrahedron*, 1999, **55**, 1143-1152 (*isol, pmr, cmr*)

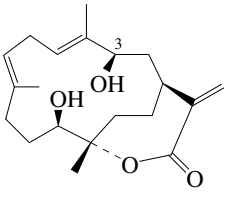
3,4-Dihydroxy-7,11,15(17)-cembratrien-16,14-olide D-613



$C_{20}H_{30}O_4$ 334.455

3-Ac: ***Stylelide***
[80375-67-3]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Styela plicata*. Oil.
Wasylyk, J.M. *et al., J. Nat. Prod.*, 1989, **52**, 1360-1362 (*isol, pmr, cmr*)

3,11-Dihydroxy-4,7,15(17)-cembratrien-16,12-olide D-614

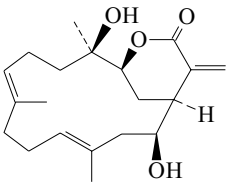


$C_{20}H_{30}O_4$ 334.455

(1*S*,3*R*,4*E*,7*E*,11*R*,12*S*)-*form*
Sandensolide
[182211-01-4]
Constit. of the corals *Sinularia flexibilis* and *Sinularia sandensis.*
Needles (Me_2CO/hexane).
Mp 188-190°. $[\alpha]_D^{27}$ +55.5 (c, 0.90 in $CHCl_3$).

3-Ac: ***3*-O-*Acetylsandensolide***
$C_{22}H_{32}O_5$ 376.492
Constit. of *Sinularia flexibilis.* Needles (Me_2CO/hexane).
Mp 163-165°. $[\alpha]_D^{27}$ +36.5 (c, 0.85 in $CHCl_3$). λ_{max} 217 ($CHCl_3$).
Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 1997, **60**, 9-12 (*isol, pmr, cmr*)

4,14-Dihydroxy-7,11,15(17)-cembratrien-16,3-olide D-615

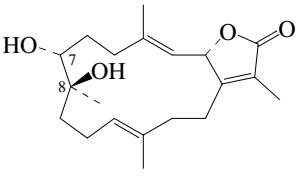


$C_{20}H_{30}O_4$ 334.455

(1*S*,3*S*,4*R*,7*E*,11*E*,14*S*)-*form*
Crassin
[28068-69-1]

14-Ac: ***Crassin acetate***
$C_{22}H_{32}O_5$ 376.492
Constit. of *Pseudoplexaura porosa* and other *Pseudoplexaura* spp. Cryst.
Mp 138-140°. $[\alpha]_D$ +70.4. λ_{max} 215 (ϵ 5000) (MeOH) (Berdy).
Hossain, M.B. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1969, **88**, 1413 (*cryst struct*)
Weinheimer, A.J. *et al., J. Nat. Prod.*, 1975, **38**, 378 (*isol*)
McMurry, J.E. *et al., J.A.C.S.*, 1990, **112**, 6942 (*synth*)
Dauben, W.G. *et al., Tet. Lett.*, 1990, **31**, 2393 (*synth*)

7,8-Dihydroxy-1(15),3,11-cembratrien-16,2-olide D-616



(2*S*,3*E*,7*R*,8*S*,11*E*)-*form*

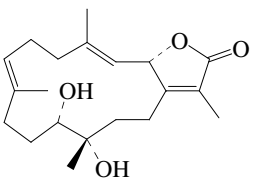
$C_{20}H_{30}O_4$ 334.455

(2*S*,3*E*,7*R*,8*S*,11*E*)-*form*
7,8-Dihydroxydeepoxysarcophine
[214900-61-5]
Constit. of *Sinularia polydactyla*.
$[\alpha]_D^{25}$ +2 (c, 0.22 in $CHCl_3$).

(2*S*,3*E*,7*S*,8*R*,11*E*)-*form*
Sarcophytonin D
[99647-44-6]
[137822-14-1]
Constit. of *Sarcophyton trocheliophorum*.
Cryst.
Mp 143-145°. $[\alpha]_D^{25}$ +106 (c, 0.024 in $CHCl_3$). λ_{max} 210 (log ϵ 4.1) (MeOH).

8-Me ether: 7-Hydroxy-8-methoxy-1(15),3,11-cembratrien-16, 2-olide
[878665-07-7]
$C_{21}H_{32}O_4$ 348.481
Constit. of *Sarcophyton trocheliophorum*.
$[\alpha]_D^{24}$ -23 (c, 0.53 in $CHCl_3$).
Duh, C.-Y. *et al., J. Nat. Prod.*, 1996, **59**, 595-598 (*Sarcophyton constits*)
Grote, D. *et al., Nat. Prod. Res.*, 2006, **20**, 285-291 (*Sinularia constit*)

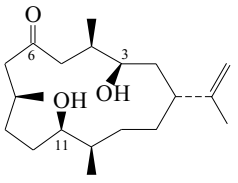
11,12-Dihydroxy-1(15),3,7-cembratrien-16,2-olide D-617



$C_{20}H_{30}O_4$ 334.455

(2*S*,3*E*,7*E*,11*S*,12*S*)-*form*
Sarcophydiol
[702668-89-1]
Constit. of a *Sarcophyton* sp.
Ma, X.-Q. *et al., Gaodeng Xuexiao Huaxue Xuebao*, 2004, **25**, 479-481; *CA*, **141**, 36335g (*isol, pmr, cmr*)

3,11-Dihydroxy-15-cembren-6-one D-618



$C_{20}H_{36}O_3$ 324.503

(1*R*,3*R*,4*R*,8*S*,11*R*,12*R*)-*form*
Dihydroplexaurolone
[119979-75-8]
Metab. of *Plexaura* sp.
Prisms (Me_2CO/hexane).
Mp 125-126°. $[\alpha]_D$ +42 (c, 0.12 in $CHCl_3$).

11-Ketone: 3-Hydroxy-15-cembrene-6,11-dione. ***Plexaurolone***
[75248-46-3]
$C_{20}H_{34}O_3$ 322.487
Metab. of *Plexaura* sp. Cryst. (Me_2CO/petrol).
Mp 110-111°.

3,11-Diketone: 15-Cembrene-3,6,11-trione. ***Dehydroplexaurolone***
[119979-76-9]
$C_{20}H_{32}O_3$ 320.471
Metab. of *Plexaura* sp. Needles (Me_2CO/petrol).
Mp 93-95°. $[\alpha]_D$ +48 (c, 0.27 in $CHCl_3$).

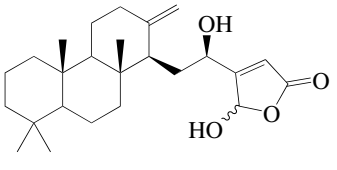
(1ξ,3ξ,4ξ,8ξ,11ξ,12ξ)-*form*

Di-Ac: ***3,11-Diacetoxy-15-cembren-16-one***
[106001-38-1]
$C_{24}H_{40}O_5$ 408.577
Isol. from mollusc *Planaxis sulcatus*. Needles ($CHCl_3$).
Mp 145°. $[\alpha]_D^{22}$ -40.

3,11-Diketone: ***Isodehydroplexaurolone***
[120053-65-8]
$C_{20}H_{32}O_3$ 320.471
Metab. of *Planaxis* sp. Cubes (Me_2CO/petrol).
Mp 196-199°. $[\alpha]_D$ -11 (c, 0.09 in $CHCl_3$). Stereoisomeric at C-4 and/or C-12 with dehydroplexaurolone.
Ealick, S.E. *et al., Acta Cryst. B*, 1980, **36**, 1901 (*cryst struct*)
Linz, G.S. *et al., Tet. Lett.*, 1986, **27**, 4833-4836 (*isol, Planaxis*)
Chan, W.R. *et al., Tetrahedron*, 1989, **45**, 103 (*cryst struct*)

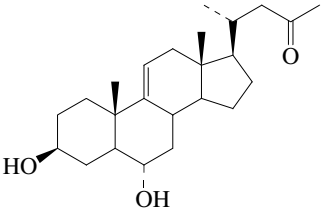
16,25-Dihydroxy-13(24),17-cheilanthadien-19,25-olide D-619

[334491-27-9]



$C_{25}H_{38}O_4$ 402.573
Constit. of an *Ircinia* sponge. Amorph. solid. $[\alpha]_D^{25}$ -118.7 (c, 0.44 in $CHCl_3$). λ_{max} 202 (log ϵ 4) (EtOH).
Buchanan, M.S. *et al., J. Nat. Prod.*, 2001, **64**, 300-303 (*isol, pmr, cmr*)
Basabe, P. *et al., J.O.C.*, 2005, **70**, 9480-9485 (*synth, abs config*)

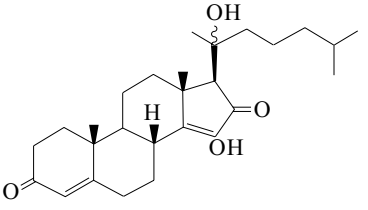
3,6-Dihydroxychol-9(11)-en-23-one D-620



$C_{24}H_{38}O_3$ 374.562

(3β,5α,6α)-*form* [61515-26-2]
Isol. from hydrolysates of the starfish *Marthasterias glacialis* saponins.
Cryst. (MeOH aq.).
Mp 201-205°.
Smith, D.S.H. *et al., J.C.S. Perkin 1*, 1973, 1745-1754 (*isol*)
De Simone, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1979, **64**, 25-32 (*isol, pmr, cmr*)

15,20-Dihydroxycholesta-4,14-diene-3,16-dione, 9CI D-621



$C_{27}H_{40}O_4$ 428.611

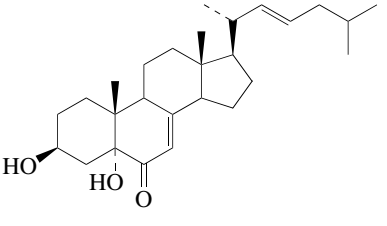
20ξ-*form* [79801-09-5]
Constit. of *Leptogorgia sarmentosa*.
Cryst. (Et_2O/petrol).
Mp 167-171°. $[\alpha]_D^{25}$ +46 (c, 0.5 in $CHCl_3$).
Cimino, G. *et al., Tet. Lett.*, 1981, 3013

18,20-Dihydroxycholesta-1,4-diene-3,16-dione D-622

$C_{27}H_{40}O_4$ 428.611

20*S*-*form*
Constit. of *Antipathes subpinnata*.
Oil.
Aiello, A. *et al., J. Nat. Prod.*, 1992, **55**, 321 (*isol, pmr, cmr*)

3,5-Dihydroxycholesta-7,22-dien-6-one D-623



$C_{27}H_{42}O_3$ 414.627

(3β,5α,22*E*)-*form* [135529-69-0]
Constit. of *Oscarella lobularis*.

22,23-Dihydro: 3,5-Dihydroxycholest-7-en-6-one
[38623-96-0]
$C_{27}H_{44}O_3$ 416.643
Constit. of *Oscarella lobularis*. Oil. λ_{max} 248 (ϵ 12000) (MeOH).
Aiello, A. *et al., Steroids*, 1991, **56**, 337-340 (*isol, pmr*)

3,6-Dihydroxycholesta-7,25-dien-24-one D-624

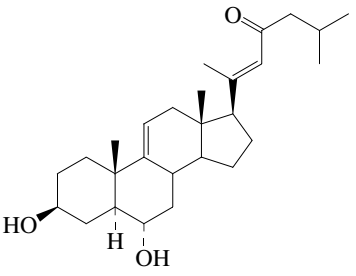
$C_{27}H_{42}O_3$ 414.627

(3β,5α,6α)-*form*

Constit. of *Spongionella gracilis*.

Madaio, A. *et al., J. Nat. Prod.*, 1989, **52**, 952 (*isol, pmr*)

3,6-Dihydroxycholesta-9(11),20(22)-dien-23-one D-625



(3β,5α,6α,20*E*)-*form*

$C_{27}H_{42}O_3$ 414.627

(3β,5α,6α,20*E*)-*form* [72983-07-4]

From *Astropecten aurantiacus* and *Marthasterias glacialis*.

(3β,5α,6α,20ξ)-*form* [37717-05-8]

Constit. of the starfishes *Acanthaster planci, Asterias vulgaris, Asterias rubens* and *Astropecten* spp.

Mp 117-119°. λ_{max} 248 (ϵ 14750) (EtOH).

3-O-*Sulfate:* [891828-15-2]

$C_{27}H_{42}O_6S$ 494.691

Constit. of *Asterias amurensis*.

$[\alpha]_D$ +7.2 (c, 0.5 in MeOH).

6-O-*(6-Deoxy-β-D-glucopyranoside):* [50676-98-7]

$C_{33}H_{52}O_7$ 560.77

Isol. from *Acanthaster planci*. Cryst. (MeOH) (as tetra-Ac).

Mp 222-224° (tetra-Ac). $[\alpha]_D^{21}$ -14.5 (c, 1.4 in $CHCl_3$) (tetra-Ac).

Sheikh, Y.M. *et al., J.A.C.S.*, 1972, **94**, 3278-3280 (*3β,5α,6α-form, isol*)

Habermehl, G. *et al., Z. Naturforsch., C*, 1973, **28**, 225-226 (*3β,5α,6α-form, isol*)

Fleming, W.J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 267-272 (*isol*)

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1978, **26**, 1852-1863 (*3β,5α, 6α-form, isol*)

De Simone, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1979, **64**, 25-32 (*20E-form, isol*)

Itakura, Y. *et al., Annalen*, 1983, 56-68 (*3β,5α,6α-form, isol*)

Findlay, J.A. *et al., J. Nat. Prod.*, 1983, **46**, 876-880 (*glucoside, isol*)

Liu, H.-W. *et al., J. Chin. Pharm. Sci.*, 2006, **15**, 1-5; *CA*, **145**, 59465w (*3-sulfate*)

3,6-Dihydroxycholesta-9(11),24-dien-23-one D-626

$C_{27}H_{42}O_3$ 414.627

(3β,5α,6α)-*form*

Marthasterone

[36564-29-1]

Aglycone from spiny starfish *Marthasterias glacialis*, also present as glycosides in starfish *Asterias amurensis*. Isol. from *A. amurensis* as Asterosaponin A and Asterosaponin B. These were inhomogeneous glycoside mixtures containing Marthasterone and Cholest-9(11)-ene-3,6,23-triol, C-618 which do not appear to have been further separated or fully characterised.

3-Sulfate: [250686-87-4]

$C_{27}H_{42}O_6S$ 494.691

Constit. of *Asterias rathbuni* and *Lysastrosoma anthosticta*.

Amorph. powder. $[\alpha]_D$ +4.2 (c, 0.65 in MeOH).

6-O-*β-D-Glucopyranoside: Marthasterone glucoside*

[60492-18-4]

$C_{33}H_{52}O_8$ 576.769

Constit. of *Marthasterias glacialis*. Cryst. (as penta-Ac).

Mp 250-253° (penta-Ac).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[β-D-quinovopyranosyl-(1→2)]-β-D-quinovopyranosyl-(1→3)-β-D-glucopyranoside], 3-sulfate:* ***Marthasteroside B***

[89383-07-3]

$C_{57}H_{92}O_{27}S$ 1241.404

Constit. of *Coscinasterias tenuispina*, *Marthasterias glacialis*, *Luidia clathrata* and *Luidia maculata*. Molluscicide. Sol. MeOH.

$[\alpha]_D$ +9 (MeOH). CAS number refers to Na salt.

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-quinovopyranosyl-(1→4)-[β-D-quinovopyranosyl-(1→2)]-β-D-quinovopyranosyl-(1→3)-β-D-glucopyranoside], 3-sulfate:* ***Luidiaglycoside C***

[89365-98-0]

$C_{57}H_{92}O_{27}S$ 1241.404

Constit. of *Luidia maculata*.

$[\alpha]_D$ +13 (MeOH).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-[β-D-quinovopyranosyl-(1→2)]-β-D-quinovopyranosyl-(1→3)-β-D-glucopyranoside], 3-sulfate:* ***Nipoglycoside B***

[154093-04-6]

$C_{57}H_{92}O_{28}S$ 1257.403

Constit. of *Distolasterias nipon*.

$[\alpha]_D$ -1.5 (MeOH).

Ikegami, S. *et al., Agric. Biol. Chem.*, 1972, **36**, 2449-2452; 1973, **37**, 367-370 (*Asterosaponins*)

Smith, D.S.H. *et al., J.C.S. Perkin 1*, 1973, 1745-1754 (*Marthasterone*)

Nicholson, S.H. *et al., J.C.S. Perkin 1*, 1976, 1357-1360 (*Marthasterone glucoside*)

Krebs, H.C. *et al., Annalen*, 1984, 296-305 (*Luidiaglycoside C*)

Bruno, I. *et al., J.C.S. Perkin 1*, 1984, 1875-1883 (*Marthasteroside B*)

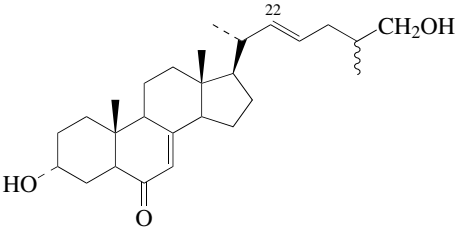
Riccio, R. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 869-893 (*Marthasteroside B*)

Iorizzi, M. *et al., J. Nat. Prod.*, 1993, **56**, 1786-1798 (*Nipoglycoside B*)

Ivanchina, N.V. *et al., J. Nat. Prod.*, 2001, **64**, 945-947 (*3-sulfate*)

Levina, E.V. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2001, **50**, 313-315 (*3-sulfate*)

3,26-Dihydroxycholesta-7,22-dien-6-one D-627



$C_{27}H_{42}O_3$ 414.627

(3α,5α,22*E*,25ξ)-*form*

26-Sulfate: ***Asterasterol C***

[193008-27-4]

$C_{27}H_{42}O_6S$ 494.691

Constit. of an Antarctic starfish (Asteriidae).

$[\alpha]_D$ +8.3 (MeOH).

22,23-Dihydro, 26-sulfate: 3,26-Dihydroxycholest-7-ene-6-one 26-sulfate. ***Asterasterol B***

[193008-26-3]

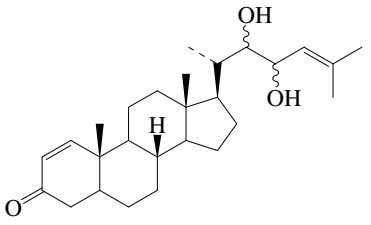
$C_{27}H_{44}O_6S$ 496.707

Constit. of an Antarctic starfish (Asteriidae).

$[\alpha]_D$ +12.5 (MeOH).

De Marino, S. *et al., Tetrahedron*, 1997, **53**, 8625-8628 (*isol, pmr, cmr*)

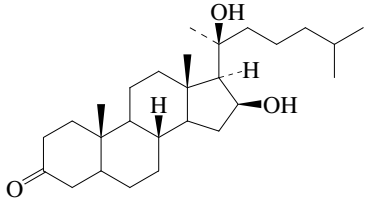
22,23-Dihydroxycholesta-1,24-dien-3-one D-628



$C_{27}H_{42}O_3$ 414.627

(5α,22ξ,23ξ)-*form* [250147-54-7]
Constit. of *Alcyonium gracillimum* and a *Scleronephthya* sp.
Cryst.
Mp 106-109°. $[\alpha]_D^{22}$ -40.9 (c, 0.13 in $CHCl_3$). λ_{max} 229 (ϵ 15000) (MeOH).
Tomono, Y. *et al., J. Nat. Prod.*, 1999, **62**, 1538-1541 (*isol, pmr, cmr*)
Yan, X.-H. *et al., Youji Huaxue*, 2004, **24**, 1233-1238; *CA*, **142**, 71702 (*isol, pmr, cmr*)

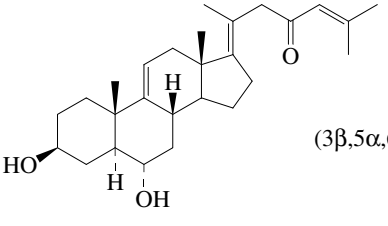
16,20-Dihydroxycholestan-3-one D-629



$C_{27}H_{46}O_3$ 418.659

(16β,20*S*)-*form* [257904-94-2]
Constit. of *Leptogorgia sarmentosa*.
Solid. $[\alpha]_D$ +14.4 (c, 0.16 in $CHCl_3$).
16-Ketone: ***20-Hydroxycholestane-3,16-dione***
[257904-93-1]
$C_{27}H_{44}O_3$ 416.643
Constit. of *Leptogorgia sarmentosa*. Wax. $[\alpha]_D$ -47.3 (c, 0.11 in $CHCl_3$).
Garrido, L. *et al., Steroids*, 2000, **65**, 85-88 (*isol, pmr, cmr*)

3,6-Dihydroxycholesta-9(11),17(20),24-trien-23-one D-630



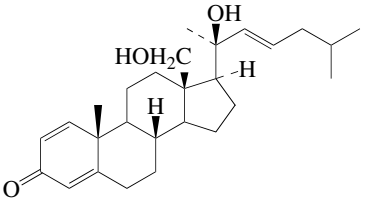
(3β,5α,6α,17(20)*E*)-*form*

$C_{27}H_{40}O_3$ 412.611

(3β,5α,6α,17(20)*E*)-*form* [72920-16-2]
Minor aglycone of the starfish *Astropecten aurantiacus.*
6-O-(4-O-Sulfo-6-deoxy-β-D-glucopyranoside), 3-sulfate: ***Latespinoside C***
[178200-92-5]
$C_{33}H_{50}O_{13}S_2$ 718.882
Constit. of *Astropecten latespinosus.* Amorph. powder.
Mp 178-181°. $[\alpha]_D$ +29 (c, 0.86 in MeOH). λ_{max} 234 (log ϵ 3.95) (MeOH).
*6-O-[β-D-Fucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-*xylo*-hexopyranosid-4-uloside 4-hydrate], 3-O-sulfate:* ***Co-Aris II***
[110325-44-5]
$C_{57}H_{90}O_{27}S$ 1239.388
Constit. of *Asterias amurensis.* Powder.
Mp 192-200°.
24,25-Dihydro: ***3,6-Dihydroxycholesta-9(11),17(20)-dien-23-one***
[72920-15-1]
$C_{27}H_{42}O_3$ 414.627
Aglycone of the starfish *Astropecten aurantiacus.*

(3β,5α,6α,17(20)*Z*)-*form* [72920-17-3]
Aglycone of the starfish *Astropecten aurantiacus.*
24,25-Dihydro: [72983-77-8]
Aglycone of the starfish *Astropecten aurantiacus.*
De Simone, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1979, **64**, 25-32 (*isol, pmr, cmr, dihydro*)
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1829-1832 (*Co-Aris II*)
Higuchi, R. *et al., Annalen*, 1996, 837-840 (*Latespinoside C*)

18,20-Dihydroxycholesta-1,4,22-trien-3-one D-631



$C_{27}H_{40}O_3$ 412.611

20*S*-*form* [137575-99-6]
Constit. of *Antipathes subpinnata.*
Aiello, A. *et al., Steroids*, 1991, **56**, 513-517 (*isol, pmr, cmr*)

3,6-Dihydroxycholest-9(11)-en-23-one D-632

$C_{27}H_{44}O_3$ 416.643

(3β,5α,6α)-*form*
Dihydromarthasterone
[34218-94-5]
Isol. from hydrolysates of the starfish *Marthasterias glacialis* and *Stichaster striatus.*
Cryst. (Me_2CO/hexane).
Mp 167-169°.
3-Sulfate: [367923-38-4]
$C_{27}H_{44}O_6S$ 496.707
Constit. of *Lysastrosoma anthosticta.* Amorph. solid. $[\alpha]_D^{20}$ +9.5 (c, 1.2 in MeOH).
*6-O-[β-D-Fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→4)-β-D-glucopyranoside], 3-*O*-sulfate:* ***Santiagoside***
[144207-69-2]
$C_{51}H_{84}O_{23}S$ 1097.277
Constit. of *Neosmilaster georgianus.* Glass (as Na salt). $[\alpha]_D^{20}$ -50 (c, 0.145 in MeOH).
*6-O-[β-D-Fucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-β-D-glucopyranoside], 3-*O*-sulfate:* ***Marthasteroside C***
[89383-08-4]
$C_{57}H_{94}O_{27}S$ 1243.419
Constit. of *Coscinasterias tenuispina* and *Marthasterias glacialis.*
$[\alpha]_D$ +13.3 (MeOH). CAS no. refers to Na salt.
*6-O-[β-D-Fucopyranosyl-(1→2)-6-deoxy-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-β-D-glucopyranoside], 3-*O*-sulfate:* ***Luidiaglycoside D***
[89365-99-1]
$C_{57}H_{94}O_{27}S$ 1243.419
Constit. of *Luidia maculata.*
$[\alpha]_D$ +14.5 (MeOH).

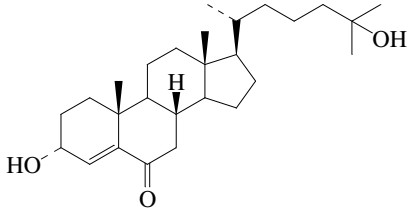
6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-β-D-glucopyranoside], 3*-O-*sulfate:* ***Nipoglycoside C***
[154073-59-3]
$C_{57}H_{94}O_{27}S$ 1243.419
Constit. of *Distolasterias nipon*.
$[\alpha]_D$ 0 (MeOH).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-*xylo*-hexopyranosid-4-uloside 4′-hydrate], 3*-O-*sulfate:* ***Ruberoside D***
[270249-50-8]
$C_{57}H_{94}O_{27}S$ 1243.419
Constit. of *Asterias rubens*.

6-O-*[β-D-Galactopyranosyl-(1→3)-β-D-fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Anasteroside A***
[402490-50-0]
$C_{62}H_{102}O_{32}S$ 1391.535
Constit. of *Anasterias minuta*. Amorph. powder.
Mp 222-224°. $[\alpha]_D^{20}$ +13.6 (c, 0.3 in DMSO).

Smith, D.S.H. *et al., J.C.S. Perkin 1*, 1973, 1745-1754 (*Dihydromarthasterone*)
Krebs, H.C. *et al., Annalen*, 1984, 296-305 (*Luidiaglycoside D*)
Neira, C. *et al., J. Nat. Prod.*, 1984, **47**, 182-183 (*Dihydromarthasterone*)
Bruno, I. *et al., J.C.S. Perkin 1*, 1984, 1875-1883 (*Marthasteroside C*)
Vazquez, M.J. *et al., Tetrahedron*, 1992, **48**, 6739 (*Santiagoside*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1993, **56**, 1786-1798 (*Nipoglycoside C*)
Sandvoss, M. *et al., Eur. J. Org. Chem.*, 2000, 1253-1262 (*Ruberoside D*)
Levina, E.V. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2001, **50**, 313-315 (*3-sulfate*)
Chludil, H.D. *et al., J. Nat. Prod.*, 2002, **65**, 153-157 (*Anasteroside A*)

3,25-Dihydroxycholest-4-en-6-one D-633



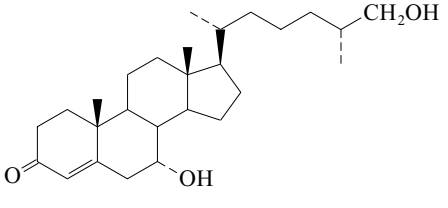
$C_{27}H_{44}O_3$ 416.643

3α-form

3-Ac:
$C_{29}H_{46}O_4$ 458.68
Constit. of *Dasystenella acanthina*. Amorph. powder. $[\alpha]_D^{25}$ +76.5 (c, 0.06 in $CHCl_3$). λ_{max} 232 (ε 6740) (MeOH).

Mellado, G.G. *et al., Steroids*, 2004, **69**, 291-299 (*isol, pmr, cmr*)

7,26-Dihydroxycholest-4-en-3-one D-634



$C_{27}H_{44}O_3$ 416.643

(7α,25R)-form [192187-67-0]
Cryst. (CH_2Cl_2/hexane). Mp 168-169°. λ_{max} 242 (log ε 4.2) (MeOH).

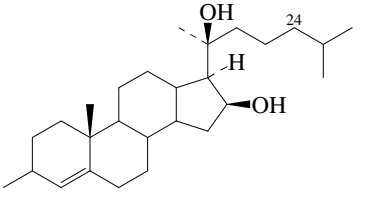
7-O-*[2-(Acetylamino)-2-deoxy-β-D-glucopyranosyl]:* ***Pavoninin 2***
[94426-00-3]
$C_{35}H_{57}NO_8$ 619.837
Ichthyotoxic, haemolytic and shark-repelling factor of *Pardachirus pavoninus*.
$[\alpha]_D^{29}$ +31 (c, 1.6 in EtOH).

7-O-*[2-(Acetylamino)-2-deoxy-β-D-glucopyranosyl], 26-Ac:* ***Pavoninin 1***
[94426-01-4]
$C_{37}H_{59}NO_9$ 661.874
Ichthyotoxic, haemolytic, and shark-repelling factor of the sole *Pardachirus pavoninus*.
$[\alpha]_D^{20}$ +19 (c, 1.1 in $CHCl_3$). λ_{max} 244 (ε 12600) (MeOH) (Berdy).

Ac:
Cryst. (Et_2O/hexane). Mp 128-129°. λ_{max} 242 (log ε 4.2) (MeOH).

Tachibana, K. *et al., Tetrahedron*, 1985, **41**, 1027-1037 (*Pavoninins 1-2*)
Ohnishi, Y. *et al., Bioorg. Med. Chem.*, 1997, **5**, 2251-2265 (*Pavoninin 1, synth*)
Kim, H.S. *et al., Tetrahedron*, 1997, **53**, 8129-8136 (*synth*)

16,20-Dihydroxycholest-4-en-3-one D-635



(16β,20*S*)-*form*

$C_{27}H_{44}O_3$ 416.643

(16β,20S)-form

16-Ac: ***Nanjiol C***
[473739-40-1]
$C_{29}H_{46}O_4$ 458.68
Constit. of *Nephthea bayeri*. Oil. $[\alpha]_D^{25}$ +73.8 (c, 0.69 in $CHCl_3$). λ_{max} 241 (log ε 4.07) (MeOH).

24,25-Didehydro: 16,20-Dihydroxycholesta-4,24-dien-3-one
$C_{27}H_{42}O_3$ 414.627

24,25-Didehydro, 16-Ac: ***Nanjiol E***
[862587-18-6]
$C_{29}H_{44}O_4$ 456.664
Constit. of *Nephthea bayeri*.
$[\alpha]_D^{25}$ +66 (c, 0.2 in $CHCl_3$). λ_{max} 241 (log ε 4.18) (MeOH).

(16α,20ξ)-form

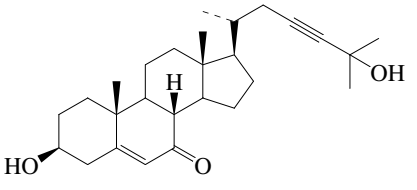
16-Epiguggulsterol III
[84709-26-2]
Constit. of *Leptogorgia sarmentosa*.

(16β,20ξ)-form

Guggulsterol III
[39025-27-9]
Constit. of *Commiphora mukul* and *Leptogorgia sarmentosa*.
Cryst. (Me_2CO).
Mp 181-183°. $[\alpha]_D$ +75.3 (c, 0.2 in $CHCl_3$).

Patil, V.D. *et al., Tetrahedron*, 1972, **28**, 2341
Benvegnu, R. *et al., Experientia*, 1982, **38**, 1443 (*isol*)
Shao, Z.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1675-1677 (*Nanjiol C*)
Yan, X.H. *et al., Chin. Chem. Lett.*, 2005, **16**, 356-358 (*Nanjiol E*)

3,25-Dihydroxycholest-5-en-23-yn-7-one D-636



$C_{27}H_{40}O_3$ 412.611

3β-*form*

Gelliusterol D

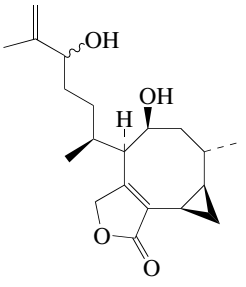
[351198-09-9]

Constit. of a *Gellius* sponge.

$[\alpha]_D$ -6.7 (c, 0.11 in MeOH). λ_{max} 236 (ϵ 23656) (MeOH).

Gallimore, W.A. *et al., J. Nat. Prod.*, 2001, **64**, 741-744 (*isol, pmr, cmr*)

4,13-Dihydroxy-1,14-crenuladien-19,18-olide D-637



$C_{20}H_{30}O_4$ 334.455

(4β,13ξ)-*form*

4-Ac: 13-Hydroxyacetoxycrenulide (incorr.)

[206988-63-8]

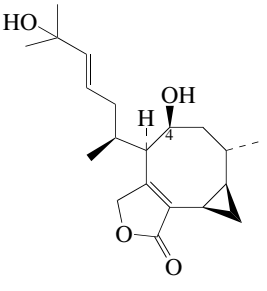
$C_{22}H_{32}O_5$ 376.492

Constit. of a *Dictyota* sp. Oil. $[\alpha]_D^{25}$ +17.3 (c, 0.33 in $CHCl_3$).

λ_{max} 224 (ϵ 6450) (no solvent reported).

Zarraga, O.,M. *et al., Bol. Soc. Chil. Quim.*, 1997, 73-79; *CA*, **128**, 319147s (*isol, pmr, cmr*)

4,14-Dihydroxy-1,12-crenuladien-19,18-olide D-638



$C_{20}H_{30}O_4$ 334.455

(4β,12*E*)-*form*

4-Ac: 14-Hydroxyacetoxycrenulide (incorr.)

[206988-62-7]

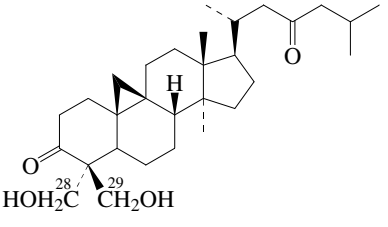
$C_{22}H_{32}O_5$ 376.492

Constit. of a *Dictyota* sp. Oil. $[\alpha]_D^{25}$ +19.6 (c, 0.27 in $CHCl_3$).

λ_{max} 227 (ϵ 6720) (no solvent reported).

Zarraga, O.,M. *et al., Bol. Soc. Chil. Quim.*, 1997, 73-79; *CA*, **128**, 319147s (*isol, pmr, cmr*)

28,29-Dihydroxycycloartane-3,23-dione D-639



$C_{30}H_{48}O_4$ 472.707

*28-*O*-Sulfate:* ***Capisterone B***

[760202-17-3]

$C_{30}H_{48}O_7S$ 552.771

Metab. of *Penicillus capitatus*. Amorph. solid. $[\alpha]_D^{25}$ +0.19 (c, 0.052 in MeOH).

*29-Ac, 28-*O*-sulfate:* ***Capisterone A***

[760202-16-2]

$C_{32}H_{50}O_8S$ 594.808

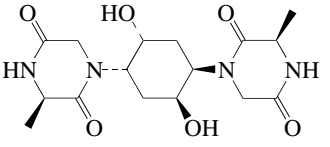
Metab. of *Penicillus capitatus*. Amorph. solid. $[\alpha]_D^{25}$ -9.6 (c, 0.019 in MeOH).

Puglisi, M.P. *et al., Tetrahedron*, 2004, **60**, 7035-7039 (*Capisterones A and B*)

Li, X.-C. *et al., J. Nat. Prod.*, 2006, **69**, 542-546 (*Capisterones A and B*)

1,1′-(2,5-Dihydroxy-1,4-cyclohexanediyl)bis [3-methyl-2,5-piperazinedione], 9CI D-640

[174881-49-3]



$C_{16}H_{24}N_4O_6$ 368.389

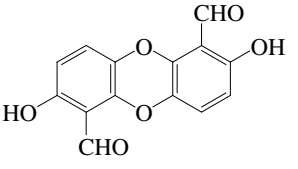
Dimeric dipeptide. Isol. from the starfish *Pentaceraster regulus*. Mp 223-225°. $[\alpha]_D$ -0.23 (c, 0.6 in Py).

Anjaneyulu, A.S.R. *et al., J. Chem. Res., Synop.*, 1996, 50-51 (*isol, ir, pmr, cmr, ms*)

2,7-Dihydroxydibenzo[*b,e*]dioxin-1,6-dicarboxaldehyde, 9CI D-641

Aplidioxin B

[217483-60-8]



$C_{14}H_8O_6$ 272.214

Isol. from the ascidian *Aplidiopsis ocellata*. Yellow powder.

*2-Me ether: 2-Hydroxy-7-methoxydibenzo[*b,e*]dioxin-1,6-dicarboxaldehyde, 9CI.* ***Aplidioxin A***

[217483-55-1]

$C_{15}H_{10}O_6$ 286.24

Isol. from *Aplidiopsis ocellata*. Yellow cryst. (C_6H_6). Subl. 198°.

Wolf, D. *et al., J. Nat. Prod.*, 1999, **62**, 167-169 (*isol, ir, pmr, cmr, cryst struct*)

3′,7-Dihydroxy-4′,5-dimethoxyflavone D-642

Luteolin 4′,5-dimethyl ether

[72629-61-9]

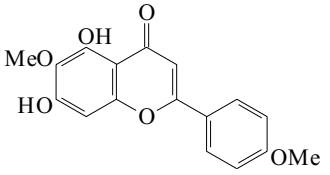
$C_{17}H_{14}O_6$ 314.294

Isol. from *Phyllospadix japonica*.

Takagi, M. *et al., Agric. Biol. Chem.*, 1979, **43**, 2417-2418 (*isol*)

5,7-Dihydroxy-4′,6-dimethoxyflavone D-643

*5,7-Dihydroxy-6-methoxy-2-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, 9CI*. ***Pectolinarigenin***. *Hortensin*
[520-12-7]



$C_{17}H_{14}O_6$ 314.294
Constit. of *Olearia paniculata*, *Eupatorium semiserratum, Millingtonia hortensis* and many other plants. Yellow needles (EtOH or Me_2CO aq.).
Mp 218.5° (215-216°). Struct. of Hortensin has been revised twice in 1992 and 1995. Originally thought to be 3,4′,6,7-Tetrahydroxyflavone and then 4′,5-Dihydroxy-6,7-dimethoxyflavone.

7-O-*α-L-Rhamnopyranoside:* [34413-70-2]
$C_{23}H_{24}O_{10}$ 460.437
Isol. from *Kickxia ramosissima*.

7-O-*β-D-Glucopyranoside:* ***Linaroside***
[53452-12-3]
$C_{23}H_{24}O_{11}$ 476.436
Constit. of *Acanthus* sp., *Arnica* sp., *Centaurea* sp., *Linaria* spp., *Lantana camara* and *Oncidium excavatum*. Shows nematocidal activity. Light yellow needles (MeOH). Mp 266-268°.

7-O-*(6*-O-*Acetyl-β-D-glucopyranoside):* ***Lantanoside***†
$C_{25}H_{26}O_{12}$ 518.473
Constit. of *Lantana camara*. Shows nematocidal activity. Needles (MeOH). Mp 210-212°. λ_{max} 268; 318 (MeOH).

7-O-*β-D-Galacturonopyranoside:* [146367-95-5]
$C_{23}H_{22}O_{12}$ 490.42
Constit. of *Monoclea forsteri* and *Monoclea gottschei*. Cryst. (MeOH aq.).

7-O-*β-D-Glucuronopyranoside:* ***Comanthoside B***
[70938-60-2]
$C_{23}H_{22}O_{12}$ 490.42
Isol. from *Comanthosphace japonica*. Fine yellow needles (MeOH). Mp 209-211°.

7-O-*β-D-Glucuronopyranoside, Me ester:* ***Comanthoside A***
[70938-59-9]
$C_{24}H_{24}O_{12}$ 504.446
Isol. from *Comanthosphace japonica*. Pale yellow needles (MeOH). Mp 252-255°.

7-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-galactopyranoside]: Pectolinarigenin 7-robinobioside*
[142925-51-7]
$C_{29}H_{34}O_{15}$ 622.579
Constit. of *Kickxia aegyptiaca*.

7-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: Pectolinarigenin 7-rutinoside.* ***Pectolinarin***. *Pectolinaroside. Neolinarin*
[28978-02-1]
$C_{29}H_{34}O_{15}$ 622.579
Isol. from *Cirsium* spp., *Kickxia elatine, Linaria* spp. and *Duranta plumieri*. Cytotoxic. Light-yellow amorph. solid or needles (EtOH). Mp 254-255° dec. $[\alpha]_D$ -98.5 (AcOH). Neolinarin was the name given to the cryst. form of Pectolinarin which was later considered identical to the amorph. material (Zemplén *et al*, 1942). λ_{max} 275; 330 (MeOH) (Berdy).

7-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 5-Ac:* ***5-O-Acetylpectolinarin***
$C_{31}H_{36}O_{16}$ 664.616
Constit. of *Linaria vulgaris*. Component of Liu Chuan Yu. Cryst. (petrol/Et_2O). Mp 134-138°. $[\alpha]_D^{18}$ -68.5.

7-O-*[2*-O-*Acetyl-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Isolinariin A***
[145613-81-6]
$C_{31}H_{36}O_{16}$ 664.616
Constit. of *Linaria japonica*. Pale yellow powder + $2H_2O$. $[\alpha]_D^{20}$ -105.4 (c, 0.72 in Py).

7-O-*[3*-O-*Acetyl-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Isolinariin B***
[145613-82-7]
$C_{31}H_{36}O_{16}$ 664.616
Constit. of *Linaria japonica*. Pale yellow needles + $2\frac{1}{2}H_2O$ (MeOH aq.). Mp 146-150°. $[\alpha]_D$ -113.5 (c, 0.74 in Py).

7-O-*[4*-O-*Acetyl-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Linariin***
[53755-56-9]
$C_{31}H_{36}O_{16}$ 664.616
Constit. of *Kickxia ramosissima* and *Linaria* spp. Pale yellow needles (MeOH). Mp 252-254°. $[\alpha]_D^{20}$ -87.8 (c, 0.74 in Py).

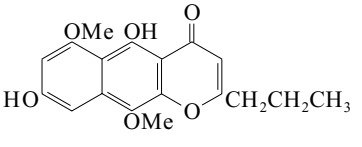
7-O-*[2,3,4-Tri*-O-*acetyl-α-L-rhamnopyranosyl-(1→6)-2,3,4-tri*-O-*acetyl-β-D-glucopyranoside]: Hexaacetylpectolinarin*
[12691-48-4]
$C_{41}H_{46}O_{21}$ 874.802
Constit. of *Linaria vulgaris* and *Linaria sessilis*. Mp 242-244°.

Di-Ac:
Needles. Mp 151°.

Robinson, R. *et al., J.C.S.*, 1930, 829 (*synth*)
Merz, K.W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1936, **274**, 126 (*isol*)
Zemplén, G. *et al., Ber.*, 1942, **75**, 489
Kupchan, S.M. *et al., Tetrahedron*, 1969, **25**, 1603 (*isol, uv*)
Farkas, L. *et al., Tet. Lett.*, 1970, 187 (*synth*)
Morita, N. *et al., Phytochemistry*, 1973, **12**, 421 (*Pectolinarin*)
Smirnova, L.P. *et al., Khim. Prir. Soedin.*, 1974, **10**, 249; 313; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 259; 320 (*Linariin, Linaroside*)
Morita, N. *et al., Yakugaku Zasshi*, 1974, **94**, 913 (*Linariin*)
Arisawa, M. *et al., Chem. Pharm. Bull.*, 1976, **27**, 1252 (*Comanthosides*)
Lin, C.N. *et al., Chem. Pharm. Bull.*, 1978, **26**, 2036 (*Pectolinarin*)
Goudard, M. *et al., Phytochemistry*, 1978, **17**, 145 (*ms*)
Williams, C.A. *et al., Phytochemistry*, 1979, **18**, 803 (*7-glucoside*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Horie, T. *et al., Yakugaku Zasshi*, 1985, **105**, 232 (*synth*)
Sing, M. *et al., Pharmazie*, 1987, **42**, 490 (*7-rhamnoside*)
Otsuka, H. *et al., J. Nat. Prod.*, 1992, **55**, 1252 (*isol, derivs*)
Kraut, L. *et al., Z. Naturforsch., C*, 1992, **47**, 794 (*7-galacturonoside*)
Mahoto, S.B. *et al., Tetrahedron*, 1994, **50**, 9439 (*Linaroside*)
Hase, T. *et al., Phytochemistry*, 1995, **40**, 287 (*Hortensin, pmr, cmr*)
Begum, S. *et al., J. Nat. Prod.*, 2000, **63**, 765-767 (*Lantanoside, Linaroside, pmr, activity*)
Tundis, R. *et al., Bioorg. Med. Chem. Lett.*, 2005, **15**, 4757-4760 (*isol, activity*)

5,8-Dihydroxy-6,10-dimethoxy-2-propyl-4*H*-naphtho[2,3-*b*]pyran-4-one D-644

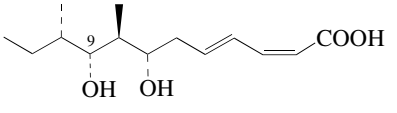
[111397-47-8]



$C_{18}H_{18}O_6$ 330.337
Constit. of the crinoid *Comanthus parvicirrus*. Orange-red needles (Me_2CO/EtOH).
Mp 214-214.5°.

Sakuma, Y. *et al., Aust. J. Chem.*, 1987, **40**, 1613-1616

7,9-Dihydroxy-8,10-dimethyl-2,4-dodecadienoic acid D-645



$C_{14}H_{24}O_4$ 256.341

(2*Z*,4*E*,7*S*,8*S*,9*R*,10*S*)-*form*

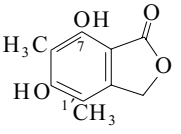
7-O-*(*E-*Cinnamoyl), amide:* ***Basiliskamide B***
[474410-87-2]
$C_{23}H_{31}NO_4$ 385.502
Prod. by a marine *Bacillus laterosporus*. Solid. $[\alpha]_D^{25}$ -12 (MeOH). λ_{max} 262 (ϵ 43000) (MeOH).

9-O-*(*E-*Cinnamoyl), amide:* ***Basiliskamide A***. *Antibiotic TAN 1771B. TAN 1771B*
[170034-41-0]
[474410-77-0]
$C_{23}H_{31}NO_4$ 385.502
Prod. by a *Bacillus* sp. and a marine *Bacillus laterosporus*. Antifungal agent. Solid. $[\alpha]_D^{25}$ -78 (MeOH). λ_{max} 204 (ϵ 19400); 216 (ϵ 22700); 222 (ϵ 21600); 262 (ϵ 40000) (MeOH) (Berdy).

Japan. Pat., 1995, 206 797; *CA*, **123**, 306561u (*TAN 1771B*)
Barsby, T. *et al., J. Nat. Prod.*, 2002, **65**, 1447-1451 (*Basiliskamides*)
Lipomi, D.J. *et al., Org. Lett.*, 2004, **6**, 3533-3536 (*synth*)

5,7-Dihydroxy-4,6-dimethyl-1(3*H*)-isobenzofuranone D-646

5,7-Dihydroxy-4,6-dimethylphthalide
[98567-35-2]



$C_{10}H_{10}O_4$ 194.187
Prod. by *Aspergillus duricaulis*. Cryst. ($CHCl_3$).
Mp 193-194°. λ_{max} 216 (log ϵ 4.3); 261 (log ϵ 3.9); 299 (log ϵ 3.4) (MeOH).

*5-Me ether: 7-Hydroxy-5-methoxy-4,6-dimethyl-1(3*H*)-isobenzofuranone. 7-Hydroxy-5-methoxy-4,6-dimethylphthalide*
[194241-08-2]
$C_{11}H_{12}O_4$ 208.213
Prod. by *Hansfordia* sp. I85-94 and the marine-derived *Monochaetia* sp. 193A20. Antifungal agent. Solid. λ_{max} 214 (ϵ 27100); 249 (ϵ 6600); 303 (ϵ 3000) (MeOH).

*5-Me ether, 7-*O-*(4-*O-*methyl-β-*D*-glucopyranoside):* [194241-09-3]
$C_{18}H_{24}O_9$ 384.382
Prod. by *Hansfordia* sp. I85-94. Cryst.
Mp 170-175°. $[\alpha]_D$ -8 (c, 0.7 in $CHCl_3$). λ_{max} 213 (ϵ 23800); 250 (ϵ 5700); 292 (ϵ 1900) (MeOH).

*7-Me ether: 5-Hydroxy-7-methoxy-4,6-dimethyl-1(3*H*)-isobenzofuranone. 5-Hydroxy-7-methoxy-4,6-dimethylphthalide*
[98567-37-4]
$C_{11}H_{12}O_4$ 208.213
Prod. by *Aspergillus duricaulis* and *Penicillium citreo-viride*. Cryst. (EtOAc).
Mp 214° (202.5-203.5°). λ_{max} 216 (log ϵ 4.4); 262 (log ϵ 4.1) (MeOH).

*Di-Me ether: 5,7-Dimethoxy-4,6-dimethyl-1(3*H*)-isobenzofuranone. 5,7-Dimethoxy-4,6-dimethylphthalide*
[98580-12-2]
$C_{12}H_{14}O_4$ 222.24
Prod. by the marine-derived *Monochaetia* sp. 193A20. Antifungal agent. Solid.
Mp 98-100° dec. λ_{max} 212 (log ϵ 4.4); 248 (log ϵ 3.9); 292 (log ϵ 3.3) (MeOH).

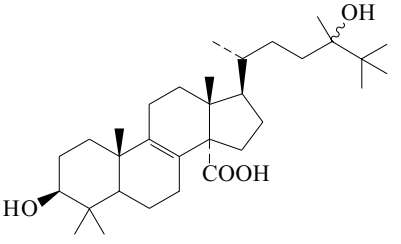
*1′-Hydroxy, 7-Me ether: 5-Hydroxy-4-(hydroxymethyl)-7-methoxy-6-methyl-1(3*H*)-isobenzofuranone*
[98567-38-5]
$C_{11}H_{12}O_5$ 224.213
From *Aspergillus duricaulis*. Cryst.
Mp 153-155°.

*1′-Methoxy: 5,7-Dihydroxy-4-(methoxymethyl)-6-methyl-1(3*H*)-isobenzofuranone*
[98567-36-3]
$C_{11}H_{12}O_5$ 224.213
From *Aspergillus duricaulis*.

*1′-Methoxy, 7-Me ether: 5-Hydroxy-7-methoxy-4-(methoxymethyl)-6-methyl-1(3*H*)-isobenzofuranone*
[98567-39-6]
$C_{12}H_{14}O_5$ 238.24
From *Aspergillus duricaulis*. Needles.
Mp 111-112°.

Achenbach, H. *et al., Annalen*, 1985, 1596-1628 (*isol, uv, pmr, cmr, ms*)
Lai, S. *et al., Chem. Lett.*, 1990, 589 (*7-Me ether*)
Schneider, G. *et al., Nat. Prod. Lett.*, 1997, **10**, 133-138 (*Hansfordia derivs*)
Höller, U. *et al., Mycol. Res.*, 2000, **104**, 1354-1365 (*Monochaeta phthalides*)

3,24-Dihydroxy-24,25-dimethyllanost-8-en-30-oic acid D-647



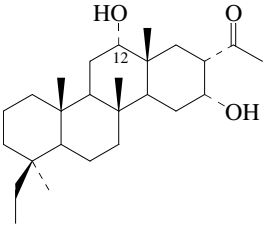
$C_{32}H_{54}O_4$ 502.776

(3β,24ξ)-*form*

3-O-*[2-Acetamido-2-deoxy-β-*D*-glucopyranosyl-(1→2)-β-*D*-galactopyranoside], 30*-O-α-*L*-xylopyranosyl ester:* ***Eryloside E***
[157566-49-9]
$C_{51}H_{85}NO_{18}$ 1000.228
Constit. of *Erylus goffrilleri*. Immunosuppressive agent. $[\alpha]_D$ -23.4 (c, 0.44 in MeOH).

Gulavita, N.K. *et al., Tet. Lett.*, 1994, **35**, 4299 (*isol, pmr, cmr*)

12,16-Dihydroxy-20,24-dimethyl-25-nor-24-scalaranone D-648



(12α,16α)-*form*

$C_{26}H_{44}O_3$ 404.632

(12α,16α)-*form*

Di-Ac:
$C_{30}H_{48}O_5$ 488.706
Isol. from *Carteriospongia foliascens*. Needles (CH_2Cl_2/MeOH).
Mp 256-258°.

(12α,16β)-*form*

12-Ac: [99617-39-7]
$C_{28}H_{46}O_4$ 446.669
Constit. of sponge *Carteriospongia foliascens*. Oil. $[\alpha]_D$ +36 (c, 0.77 in $CHCl_3$).

16-(3-Hydroxybutanoyl), 12-Ac: [221163-29-7]
$C_{32}H_{52}O_6$ 532.759
Constit. of *Strepsichordaia lendenfeldi*. Oil. $[\alpha]_D^{25}$ +26.5 (c, 1.62 in $CHCl_3$).

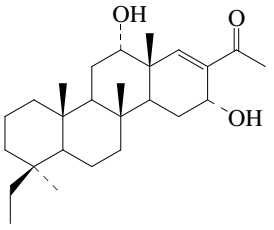
12-Ketone: 16-Hydroxy-20,24-dimethyl-25-nor-12,24-scalaranedione

12-Ketone, 16-Ac: [757223-05-5]
$C_{28}H_{44}O_4$ 444.653

Constit. of *Phyllospongia madagascarensis*. Amorph. solid. $[\alpha]_D^{25}$ 0 (c, 0.03 in $CHCl_3$).

Braekman, J.C. *et al., Tetrahedron*, 1985, **41**, 4603 (*12-Ac*)
Quinn, R.J. *et al., Aust. J. Chem.*, 1989, **42**, 751-755 (*di-Ac*)
Jahn, T. *et al., J. Nat. Prod.*, 1999, **62**, 375-377 (*diester*)
Ponomarenko, L.P. *et al., J. Nat. Prod.*, 2004, **67**, 1507-1510 (*Phyllospongia madagascarensis constit*)

12,16-Dihydroxy-20,24-dimethyl-25-nor-17-scalaren-24-one D-649



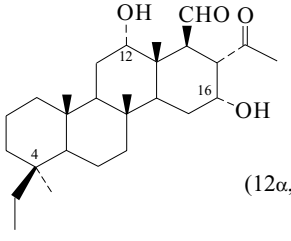
$C_{26}H_{42}O_3$ 402.616

(12α,16α)-*form*

12-(3-Acetoxybutanoyl): ***Phyllofenone C***
[306997-44-4]
$C_{32}H_{50}O_6$ 530.743
Constit. of *Strepsichordaia aliena*. Amorph. solid. $[\alpha]_D$ +16 (c, 0.4 in CH_2Cl_2).

Jiménez, J.I. *et al., J. Nat. Prod.*, 2000, **63**, 1388-1392 (*isol, pmr, cmr*)

12,16-Dihydroxy-20,24-dimethyl-24-oxo-25-scalaranal D-650



(12α,16α)–*form*

$C_{27}H_{44}O_4$ 432.642
C-14 config. not indicated for Scalarherbacin B, prob. the same as for the other compds. in this entry.

(12α,16α)-*form*

16-Ac: ***Scalarherbacin B***
[73723-40-7]
$C_{29}H_{46}O_5$ 474.679
Isol. from sponge *Dysidea herbacea*.

Di-Ac: ***Scalarherbacin B acetate***
$C_{31}H_{48}O_6$ 516.717
Isol. from *Dysidea herbacea*.

(12α,16β)-*form*

12-Ac: ***12α-Acetoxy-16β-hydroxy-20,24-dimethyl-24-oxo-25-scalaranal***
[99617-38-6]
$C_{29}H_{46}O_5$ 474.679
Constit. of sponge *Carteriospongia foliascens* and a *Phyllospongia* sp. Ichthyotoxin. Oil. $[\alpha]_D$ +95.6 (c, 0.27 in $CHCl_3$).

12,16-Di-Ac:
$C_{31}H_{48}O_6$ 516.717
Constit. of *Strepsichordaia lendenfeldi*. Oil. $[\alpha]_D$ +88.1 (c, 0.24 in $CHCl_3$).

16-Propanoyl, 12-Ac:
$C_{32}H_{50}O_6$ 530.743
Constit. of *Strepsichordaia lendenfeldi*. Oil. $[\alpha]_D$ +96 (c, 0.33 in $CHCl_3$).

16-(3R-Hydroxybutanoyl), 12-Ac:
$C_{33}H_{52}O_7$ 560.77
Constit. of *Strepsichordaia lendenfeldi*. Oil. $[\alpha]_D$ +61.3 (c, 1.08 in $CHCl_3$).

16-(3-Hydroxypentanoyl), 12-Ac:
$C_{34}H_{54}O_7$ 574.796
Constit. of *Strepsichordaia lendenfeldi*. Oil. $[\alpha]_D$ +60.3 (c, 0.46 in $CHCl_3$).

(12β,16α)-*form*

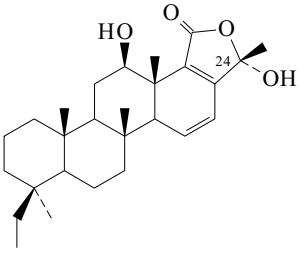
16-O-(3-Hydroxypentanoyl): ***Foliaspongin***
[78570-09-9]
$C_{32}H_{52}O_6$ 532.759
Isol. from *Phyllospongia foliascens*. Shows antiinflammatory props. Cryst. (MeOH). Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 186-189°. $[\alpha]_D$ +44 ($CHCl_3$).

12-Ketone, 16-O-(3-hydroxypentanoyl): ***Dehydrofoliaspongin***
[125990-21-8]
$C_{32}H_{50}O_6$ 530.743
Constit. of *Phyllospongia foliascens*. Glass. $[\alpha]_D$ +39 (c, 3.7 in $CHCl_3$).

12-Ketone, 16-O-(3S-hydroxy-4-methylpentanoyl): ***Phyllofoliaspongin***
[125990-20-7]
$C_{33}H_{52}O_6$ 544.77
Constit. of *Phyllospongia foliascens*. Vasodilator, platelet aggregation inhibitor. Glass. $[\alpha]_D^{20}$ +40 (c, 0.9 in $CHCl_3$).

Kashman, Y. *et al., Tet. Lett.*, 1979, 3879
Kikuchi, H. *et al., Chem. Pharm. Bull.*, 1981, **29**, 1492-1494; 1983, **31**, 552-556 (*Foliaspongin*)
Braekman, J.C. *et al., Tetrahedron*, 1985, **41**, 4603-4613 (*Carteriospongia foliascens constits*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2078 (*Phyllofoliaspongin, Dihydrofoliaspongin*)
Bowden, B.F. *et al., J. Nat. Prod.*, 1992, **55**, 1234-1240 (*Strepsichordaia lendenfeldi constits*)
Roy, M.C. *et al., J. Nat. Prod.*, 2002, **65**, 1838-1842 (*Phyllospongia constit*)

12,24-Dihydroxy-20,24-dimethyl-15,17-scaladien-25,24-olide D-651



(12β,24α)–*form*

$C_{27}H_{40}O_4$ 428.611

(12β,24α)-*form*

12-(3-Hydroxypentanoyl): ***Phyllactone E***
[145680-53-1]
$C_{32}H_{48}O_6$ 528.728
Constit. of *Phyllospongia foliascens*.

12-(3-Hydroxy-4-methylpentanoyl): ***Phyllactone G***
[152186-80-6]
$C_{33}H_{50}O_6$ 542.754
Isol. from the sponge *Phyllospongia foliascens*. Isol. as a mixt. with Phyllactone F.

(12β,24β)-*form*

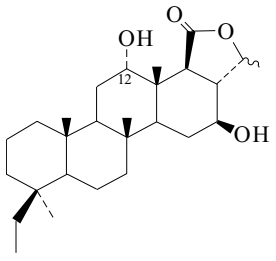
12-(3-Hydroxypentanoyl): ***Phyllactone D***
[145613-56-5]
$C_{32}H_{48}O_6$ 528.728
Constit. of *Phyllospongia foliascens*.

12-(3-Hydroxy-4-methylpentanoyl): ***Phyllactone F***
[152110-15-1]
$C_{33}H_{50}O_6$ 542.754

Isol. from the sponge *Phyllospongia foliascens*. Isol. as a mixt with Phyllactone G.

Fu, X. *et al., J. Nat. Prod.*, 1992, **55**, 1607; 1993, **56**, 1985-1988 (*isol, pmr, cmr*)

12,16-Dihydroxy-20,24-dimethyl-25,24-scalarano-lide D-652

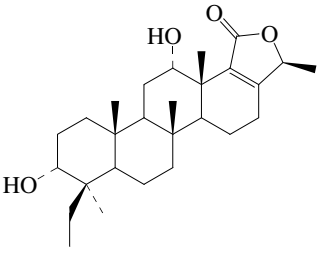


$C_{27}H_{44}O_4$ 432.642

(12α,16β)-*form*

12-Ac: ***12α-Acetoxy-16β-hydroxy-20,24-dimethyl-25,24-scalaranolide***
[99631-23-9]
$C_{29}H_{46}O_5$ 474.679
Constit. of sponge *Carteriospongia foliascens*. Oil (as diacetate). $[\alpha]_D$ +67 (di-Ac).
Braekman, J.C. *et al., Tetrahedron*, 1985, **41**, 4603

3,12-Dihydroxy-20,24-dimethyl-17-scalaren-25,24-olide D-653



$C_{27}H_{42}O_4$ 430.626

(3α,12α,24*S*)-*form*

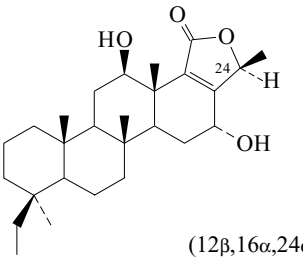
3-Ac: ***Phyllolactone C***
[356566-82-0]
$C_{29}H_{44}O_5$ 472.664
Constit. of *Phyllospongia lamellosa*. Powder. $[\alpha]_D^{20}$ +8.6 (c, 0.14 in MeOH). λ_{max} 216 (ϵ 8425) (MeOH).

3-Propanoyl: ***Phyllolactone B***
[356566-81-9]
$C_{30}H_{46}O_5$ 486.69
Constit. of *Phyllospongia lamellosa*. Powder. $[\alpha]_D^{20}$ +10.6 (c, 0.09 in MeOH). λ_{max} 203 (ϵ 6179) (MeOH).

3-Propanoyl, 12-Ac: ***Phyllolactone D***
[356566-83-1]
$C_{32}H_{48}O_6$ 528.728
Constit. of *Phyllospongia lamellosa*. Amorph. solid. $[\alpha]_D^{20}$ +7.2 (c, 0.08 in MeOH). λ_{max} 215 (ϵ 5500) (MeOH).

3-Butanoyl: ***Phyllolactone A***
[356566-80-8]
$C_{31}H_{48}O_5$ 500.717
Constit. of *Phyllospongia lamellosa*. Powder. $[\alpha]_D^{20}$ +9.5 (c, 0.254 in MeOH). λ_{max} 215 (ϵ 5100) (MeOH).
Chang, L.C. *et al., Tetrahedron*, 2001, **57**, 5731-5738 (*isol, pmr, cmr*)

12,16-Dihydroxy-20,24-dimethyl-17-scalaren-25,24-olide D-654



(12β,16α,24α*H*)–*form*

$C_{27}H_{42}O_4$ 430.626

(12β,16α,24α*H*)-*form*

12-(3-Hydroxypentanoyl): ***Phyllactone B***
[145680-52-0]
$C_{32}H_{50}O_6$ 530.743
Constit. of *Phyllospongia foliascens*. Needles (Me_2CO). Mp 179-180°. $[\alpha]_D$ +27 (c, 0.98 in $CHCl_3$). λ_{max} 216 (ϵ 8494) (MeOH) (Berdy).

12-(3-Acetoxypentanoyl), 16-Ac: ***Phyllactone C***
[145613-55-4]
$C_{36}H_{54}O_8$ 614.818
Constit. of *Phyllospongia foliascens*. Gum. $[\alpha]_D$ +29 (c, 0.22 in $CHCl_3$).

(12β,16α,24β*H*)-*form*

12-(3-Hydroxypentanoyl): ***Phyllactone A***
[145613-54-3]
$C_{32}H_{50}O_6$ 530.743
Constit. of *Phyllospongia foliascens*. Needles (Me_2CO). Mp 193-194°. $[\alpha]_D$ +11 (c, 1.13 in $CHCl_3$). λ_{max} 211 (ϵ 7028) (MeOH) (Berdy).

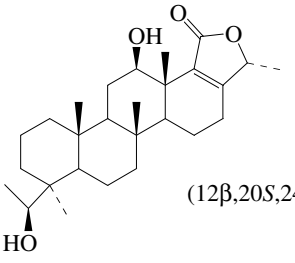
(12ξ,16ξ,24ξ)-*form*

Phyllactone H
Constit. of a *Phyllospongia* sp.
Mp 272-274°. Stereochem. not clear from the paper. Mp. refers to a mixt. with Phyllactone I.

24-Epimer: ***Phyllactone I***
$C_{27}H_{42}O_4$ 430.626
Constit. of a *Phyllospongia* sp.

Fu, X. *et al., J. Nat. Prod.*, 1992, **55**, 1607-1613 (*Phyllactones A-C*)
Wang, Y.Q. *et al., CA*, 1996, **126**, 184024k (*Phyllactone H, Phyllactone I*)

12,20-Dihydroxy-20,24-dimethyl-17-scalaren-25,24-olide D-655



(12β,20*S*,24*R*)-*form*

$C_{27}H_{42}O_4$ 430.626

(12β,20*S*,24*R*)-*form*

12-(3-Hydroxybutanoyl), 20-Ac: ***Honulactone D***
[306971-09-5]
$C_{33}H_{50}O_7$ 558.754
Constit. of *Strepsichordaia aliena*. Cryst. $[\alpha]_D$ +62 (c, 0.25 in CH_2Cl_2).

12-(3-Hydroxypentanoyl), 20-Ac: ***Honulactone J***
[306971-15-3]
$C_{34}H_{52}O_7$ 572.781
Constit. of *Strepsichordaia aliena*. Cryst. $[\alpha]_D$ +80.7 (c, 0.67 in CH_2Cl_2).

12-(3-Hydroxybutanoyl), 20-propanoyl: ***Honulactone L***
[306971-17-5]
$C_{34}H_{52}O_7$ 572.781
Constit. of *Strepsichordaia aliena*. Cryst. $[\alpha]_D$ +90.1 (c, 0.77 in CH_2Cl_2).

(12β,20*S*,24*S*)-*form*

20-Ac: [85735-14-4]
$C_{29}H_{44}O_5$ 472.664
Constit. of a *Carteriospongia* sp. Cryst. (Et_2O/petrol). Mp 252-254°. $[\alpha]_D$ +20 (c, 3.3 in $CHCl_3$).

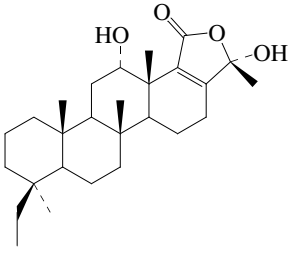
12-(3-Hydroxybutanoyl), 20-Ac: ***Honulactone C***
[306971-08-4]
$C_{33}H_{50}O_7$ 558.754
Constit. of *Strepsichordaia aliena*. Cryst. $[\alpha]_D$ +71.2 (c, 0.57 in CH_2Cl_2).

12-(3-Hydroxypentanoyl), 20-Ac: ***Honulactone I***
[306971-14-2]
$C_{34}H_{52}O_7$ 572.781
Constit. of *Strepsichordaia aliena*. Cryst. $[\alpha]_D$ +83.4 (c, 0.96 in CH_2Cl_2).

12-(3-Hydroxybutanoyl), 20-propanoyl: ***Honulactone K***
[306971-16-4]
$C_{34}H_{52}O_7$ 572.781
Constit. of *Strepsichordaia aliena*. Cryst. $[\alpha]_D$ +90.1 (c, 0.77 in CH_2Cl_2).

Croft, K.D. *et al., J.C.S. Perkin 1*, 1983, 155-159 (*20-Ac*)
Jiménez, J.I. *et al., J.O.C.*, 2000, **65**, 6837-6840 (*Honulactones, cryst struct*)

12,24-Dihydroxy-20,24-dimethyl-17-scalaren-25,24-olide D-656

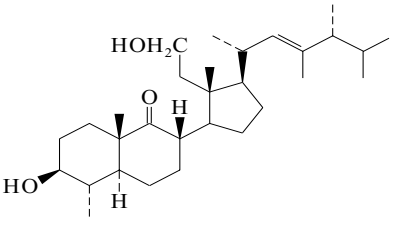


$C_{27}H_{42}O_4$ 430.626

(12α,24α)-*form*
Phyllolactone E
[356566-84-2]
Constit. of *Phyllospongia lamellosa*.
Oil. $[\alpha]_D^{20}$ +3 (c, 0.02 in MeOH). λ_{max} 214 (ϵ 6050) (MeOH).
Chang, L.C. *et al., Tetrahedron*, 2001, **57**, 5731-5738 (*isol, pmr, cmr*)

3,11-Dihydroxy-4,23-dimethyl-9,11-secoergost-22-en-9-one D-657

3,11-Dihydroxy-4,23,24-trimethyl-9,11-secocholest-22-en-9-one

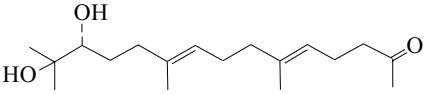


$C_{30}H_{52}O_3$ 460.739

(3β,4α,5α,22*E*,24*R*)-*form* [161236-63-1]
Constit. of a *Pseudopterogorgia* sp.
Powder. $[\alpha]_D$ -11.5 (c, 1.7 in MeOH).
He, H. *et al., Tetrahedron*, 1995, **51**, 51 (*isol, pmr, cmr*)

14,15-Dihydroxy-1,2-dinor-6,10-phytadien-3-one D-658

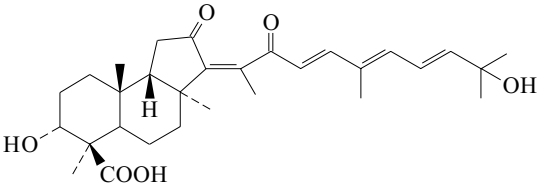
13,14-Dihydroxy-6,10,14-trimethyl-5,9-pentadecadien-2-one



$C_{18}H_{32}O_3$ 296.449

(6*E*,10*E*,14*R*)-*form* [81373-96-8]
Isol. from *Cystophora moniliformis*.
Viscous oil. $[\alpha]_D^{20}$ -9.7 (c, 1 in CH_2Cl_2).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 171

3,25-Dihydroxy-12,15-dioxo-13,16,20(22),23-isomalabaricatetraen-29-oic acid D-659

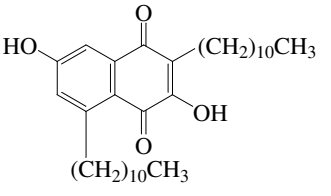


$C_{30}H_{42}O_6$ 498.658

(3α,13*Z*,16*E*,20(22)*E*,23*E*)-*form*
3-Ac: ***Globostellatic acid A***
[175669-10-0]
$C_{32}H_{44}O_7$ 540.695
Constit. of *Stelletta globostellata*. Yellow amorph. solid. $[\alpha]_D^{23}$ -45.7 (c, 0.35 in MeOH). λ_{max} 222 (ϵ 24000); 326 (ϵ 56000) (MeOH). λ_{max} 226 (ϵ 24000); 326 (ϵ 56000) (MeOH) (Berdy).
Ryu, G. *et al., J. Nat. Prod.*, 1996, **59**, 512 (*isol, pmr, cmr*)

3,7-Dihydroxy-2,5-diundecyl-1,4-naphthoquinone D-660

3,7-Dihydroxy-2,5-diundecyl-1,4-naphthalenedione



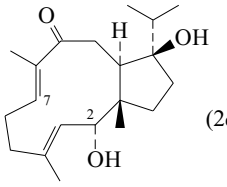
$C_{32}H_{50}O_4$ 498.745
Constit. of the mangrove plant *Aegiceras corniculatum*. Yellow powder.
Mp 75-77°. λ_{max} 222 (log ϵ 4.02); 272 (log ϵ 3.87); 302 (log ϵ 3.65); 346 (log ϵ 3.53) (MeOH).
Xu, M. *et al., J. Nat. Prod.*, 2004, **67**, 762-766 (*isol, pmr, cmr, ms*)

4,11-Dihydroxy-2-dodecenoic acid D-661

Secopatulolide C
$H_3CCH(OH)(CH_2)_6CH(OH)CH{=}CHCOOH$
$C_{12}H_{22}O_4$ 230.303
Open-chain form of Patulolide C.

(-)-(*E*)-*form*
Isol. from a fungus obt. from a marine sponge.
Oil. $[\alpha]_D$ -10 (c, 0.09 in MeOH).
Smith, C.J. *et al., J. Nat. Prod.*, 2000, **63**, 142-145

2,12-Dihydroxy-3,7-dolabelladien-9-one D-662



(2α,3*E*,7*E*)–*form*

$C_{20}H_{32}O_3$ 320.471

(2α,3*E*,7*E*)-*form*

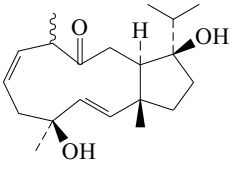
2-Ac: ***2-Acetoxy-12-hydroxy-3,7-dolabelladien-9-one***
$C_{22}H_{34}O_4$ 362.508
Constit. of *Dictyota pardalis* f. *pseudohamata*. Cryst. ($CHCl_3$/petrol).
Mp 173-174°. $[\alpha]_D$ -73.2 (c, 3.58 in $CHCl_3$). $[\alpha]_D^{25}$ +52 (c, 0.04 in $CHCl_3$).

(2α,3*E*,7*Z*)-*form*

2-Ac:
$C_{22}H_{34}O_4$ 362.508
Constit. of *Dictyota pardalis* f. *pseudohamata*. Oil. $[\alpha]_D^{25}$ +80 (c, 0.43 in $CHCl_3$).

Rao, C.B. *et al., J.O.C.*, 1986, **51**, 2736
König, G.M. *et al., Tetrahedron*, 1994, **50**, 8011 (*derivs*)

4,12-Dihydroxy-2,6-dolabelladien-9-one D-663



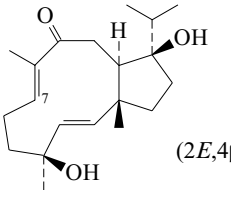
$C_{20}H_{32}O_3$ 320.471

(2*E*,4β,6*Z*,8ξ)-*form* [102977-76-4]
Constit. of *Dictyota dichotoma*.
Oil. $[\alpha]_D$ +13.3 (c, 0.03 in $CHCl_3$).

8-Epimer: [103064-45-5]
$C_{20}H_{32}O_3$ 320.471
From *Dictyota dichotoma*. Oil. $[\alpha]_D$ -52.3 (c, 0.3 in $CHCl_3$).

Rao, C.B. *et al., J.O.C.*, 1986, **51**, 2736-2742

4,12-Dihydroxy-2,7-dolabelladien-9-one D-664



(2*E*,4β,7*E*)–*form*

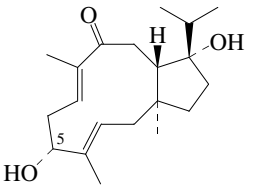
$C_{20}H_{32}O_3$ 320.471

(2*E*,4β,7*E*)-*form*
Constit. of *Dictyota dichotoma*.
Cryst. (EtOAc/petrol).
Mp 212-213°. $[\alpha]_D$ -6.5 (c, 0.12 in MeOH). λ_{max} 250 (ϵ 2020) (MeOH) (Derep).

(2*E*,4β,7*Z*)-*form*
From *Dictyota dichotoma*.
Cryst. ($CHCl_3$/petrol).
Mp 153-155°. $[\alpha]_D$ -99.3 (c, 3.28 in $CHCl_3$). λ_{max} 228 (ϵ 2400) (MeOH) (Derep).

Rao, C.B. *et al., J.O.C.*, 1986, **51**, 2736

5,12-Dihydroxy-3,7-dolabelladien-9-one D-665



(3*E*,5α,7*E*,12α)-*form*

$C_{20}H_{32}O_3$ 320.471

(3*E*,5α,7*E*,12α)-*form*

5-Ac: [159001-97-5]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Dictyota bartayresiana* and *Dictyota pardalis* f. *pseudohamata*. Cryst.
Mp 166-168°. $[\alpha]_D$ -60 (c, 1.17 in $CHCl_3$).

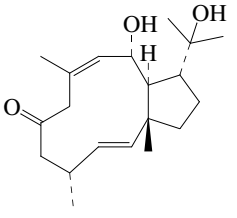
(3*E*,5α,7*Z*,12α)-*form*

5-Ac: [159001-98-6]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Dictyota bartayresiana* and *Dictyota pardalis* f. *pseudohamata*. Oil. $[\alpha]_D$ +53.3 (c, 1.3 in $CHCl_3$).

[156790-24-8, 156857-37-3]

König, G.M. *et al., J. Nat. Prod.*, 1994, **57**, 1529-1538 (*Dictyota pardalis constits*)
Rao, C.B. *et al., Phytochemistry*, 1994, **37**, 509-513 (*Dictyota bartayresiana constits*)

10,18-Dihydroxy-2,8-dolabelladien-6-one D-666



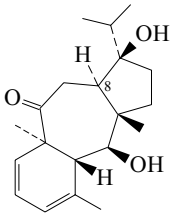
$C_{20}H_{32}O_3$ 320.471

(2*E*,8*Z*,10α)-*form*

Di-Ac: [216770-36-4]
$C_{24}H_{36}O_5$ 404.545
Constit. of a *Dysidea* sp. Oil. $[\alpha]_D$ -13.8 (c, 0.65 in $CHCl_3$).

Lu, Q. *et al., J. Nat. Prod.*, 1998, **61**, 1096-1100 (*isol, pmr, cmr*)

9,13-Dihydroxy-1,3-dolastadien-6-one D-667



(5α,8α,9β,12β,13β,14β)–*form*

$C_{20}H_{30}O_3$ 318.455

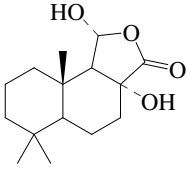
(5α,8α,9β,12β,13β,14β)-*form*

13-Ac: [160550-95-8]
$C_{22}H_{32}O_4$ 360.492
Constit. of *Dictyota pardalis* f. *pseudohamata*. Oil. $[\alpha]_D^{25}$ +40 (c, 0.21 in $CHCl_3$).

(5α,8β,9β,12β,13β,14β)-*form*

13-Ac: [160488-99-3]
$C_{22}H_{32}O_4$ 360.492
Constit. of *Dictyota pardalis* f. *pseudohamata*. Oil. $[\alpha]_D^{25}$ -107 (c, 0.31 in $CHCl_3$).
König, G.M. *et al., J. Nat. Prod.*, 1994, **57**, 1529 (*isol, pmr, cmr*)

8,11-Dihydroxy-12,11-drimanolide D-668

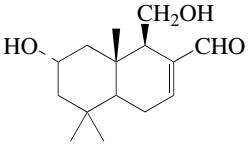


$C_{15}H_{24}O_4$ 268.352

(8α,11α)-*form*

Dendocarbin D
[350986-77-5]
Constit. of *Dendrodoris carbunculosa*.
Oil. $[\alpha]_D^{25}$ +15 (c, 0.02 in $CHCl_3$).
Sakio, Y. *et al., J. Nat. Prod.*, 2001, **64**, 726-731 (*isol, pmr, cmr*)

2,11-Dihydroxy-7-drimen-12-al D-669

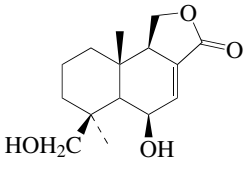


$C_{15}H_{24}O_3$ 252.353

2α-*form*

Di-Ac: ***Hodgsonal***
[212710-95-7]
$C_{19}H_{28}O_5$ 336.427
Constit. of *Bathydoris hodgsoni*. Oil. $[\alpha]_D$ -6.4 (c, 1.2 in $CHCl_3$). λ_{max} 224 (ε 9200) (MeOH).
Iken, K. *et al., Tet. Lett.*, 1998, **39**, 5635-5638 (*isol, pmr, cmr*)

6,14-Dihydroxy-7-drimen-12,11-olide D-670

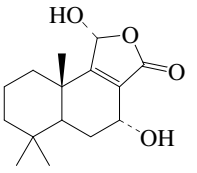


$C_{15}H_{22}O_4$ 266.336

6β-*form*

6-(4-Nitrobenzoyl): ***14-Hydroxy-6β-(4-nitrobenzoyloxy)cinnamolide***
[204716-04-1]
$C_{22}H_{25}NO_7$ 415.442
Metab. of *Aspergillus versicolor* isol. from *Penicillus capitatus*. Pale yellow solid.
Mp 99-104°. $[\alpha]_D$ -76 (c, 0.54 in MeOH). λ_{max} 256 (ε 8200) (MeOH).
Belofsky, G.N. *et al., Tetrahedron*, 1998, **54**, 1715-1724 (*isol, pmr, cmr*)

7,11-Dihydroxy-8-drimen-12,11-olide D-671



(7α,11α)-*form*

$C_{15}H_{22}O_4$ 266.336

(7α,11α)-*form*

Dendocarbin M
[350986-86-6]
Constit. of *Dendrodoris carbunculosa*. λ_{max} 210 (ε 13000) (MeOH).

11-Et ether: 11-Ethoxy-7-hydroxy-8-drimen-12,11-olide. ***Dendocarbin K***
[350986-84-4]
$C_{17}H_{26}O_4$ 294.39
Constit. of *Dendrodoris carbunculosa*. Oil. $[\alpha]_D^{25}$ -57 (c, 0.04 in $CHCl_3$). λ_{max} 216 (ε 9000) (MeOH).

(7α,11β)-*form*

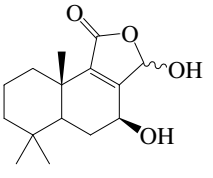
Dendocarbin L
[350986-85-5]
Constit. of *Dendrodoris carbunculosa*. λ_{max} 210 (ε 13000) (MeOH).

11-Et ether: ***Dendocarbin J***
[350986-83-3]
$C_{17}H_{26}O_4$ 294.39
Constit. of *Dendrodoris carbunculosa*. Oil. $[\alpha]_D^{25}$ +17 (c, 0.06 in $CHCl_3$).

(7β,11α)-*form*

7,11-Dihydroxyconfertifolin. ***Fuegin***
[6750-10-3]
Constit. of *Drimys winteri*.
Cryst. (CH_2Cl_2/petrol).
Mp 170-172°. $[\alpha]_D$ +76 (c, 1.12 in $CHCl_3$).
Appel, H.H. *et al., Tetrahedron*, 1963, **19**, 635 (*isol*)
Nakano, T. *et al., Tetrahedron*, 1999, **55**, 1561-1568 (*synth*)
Sakio, Y. *et al., J. Nat. Prod.*, 2001, **64**, 726-731 (*isol, pmr, cmr*)

7,12-Dihydroxy-8-drimen-11,12-olide D-672

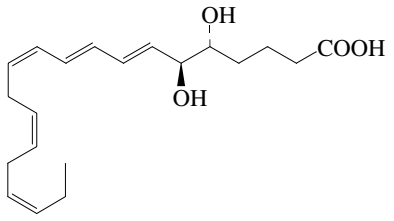


$C_{15}H_{22}O_4$ 266.336

(7β,12ξ)-*form*

12-Et ether: 12-Ethoxy-7-hydroxy-8-drimen-11,12-olide. ***Dendocarbin I***
[350986-82-2]
$C_{17}H_{26}O_4$ 294.39
Constit. of *Dendrodoris carbunculosa*. Oil. $[\alpha]_D^{25}$ -47 (c, 0.02 in $CHCl_3$).
Sakio, Y. *et al., J. Nat. Prod.*, 2001, **64**, 726-731 (*isol, pmr, cmr*)

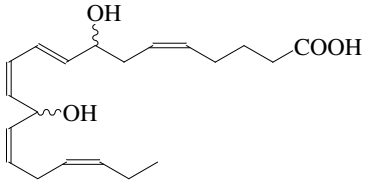
5,6-Dihydroxy-7,9,11,14,17-eicosapentaenoic acid D-673



$C_{20}H_{30}O_4$ 334.455

(5*R,6*S**,7*E*,9*E*,11*Z*,14*Z*,17*Z*)-*form***
Constit. of the red alga *Rhodymenia pertusa*.
Jiang, Z.D. *et al., Phytochemistry*, 2000, **53**, 129-133

8,13-Dihydroxy-5,9,11,14,17-eicosapentaenoic acid D-674

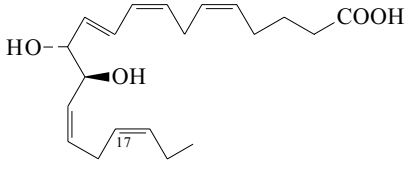


$C_{20}H_{30}O_4$ 334.455

(5*Z*,8ξ,9*E*,11*Z*,13ξ,14*Z*,17*Z*)-*form*
Barnacle muscle stimulatory factor. BMSF
[886847-35-4]
Isol. from barnacles (*Balanus balanus*). Increases body muscular activity in barnacles.
Maskrey, B.H. *et al., J. Exp. Biol.*, 2006, **209**, 558-566 (*isol, ms*)

12,13-Dihydroxy-5,8,10,14,17-eicosapentaenoic acid D-675

[135378-18-6]



$C_{20}H_{30}O_4$ 334.455

(5*Z*,8*Z*,10*E*,12*R*,13*S*,14*Z*,17*Z*)-*form*
Constit. of the red algae *Farlowia mollis* and *Gracilariopsis lemaneiformis*.
$[\alpha]_D$ +12.6 (c, 0.22 in CCl_4) (as di-Ac, Me ester). Config. revised in 1990.

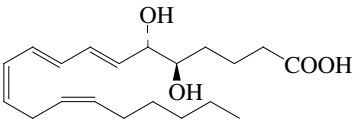
17,18-Dihydro: 12,13-Dihydroxy-5,8,10,14-eicosatetraenoic acid
[131938-74-4]
$C_{20}H_{32}O_4$ 336.47
Constit. of *Farlowia mollis* and *Gracilariopsis lemaneiformis*. Config. revised in 1990. Isol. as di-Ac, Me ester.

[121979-37-1, 121979-38-2, 128478-67-1]

Solem, M.L. *et al., Lipids*, 1989, **24**, 256 (*isol*)
Lumin, S. *et al., Tet. Lett.*, 1990, **31**, 2971 (*isol, pmr*)
Jiang, Z.-D. *et al., Phytochemistry*, 1991, **30**, 1187 (*isol, struct*)

5,6-Dihydroxy-7,9,11,14-eicosatetraenoic acid D-676

5,6-DiHETE



(5*R*,6*S*,7*E*,9*E*,11*Z*,14*Z*)-*form*

$C_{20}H_{32}O_4$ 336.47

(5*R*,6*S*,7*E*,9*E*,11*Z*,14*Z*)-*form*
Constit. of the red alga *Rhodymenia pertusa*.

Me ester:
$C_{21}H_{34}O_4$ 350.497
$[\alpha]_D^{23}$ -1.4 (c, 0.29 in MeOH). λ_{max} 260 (log ϵ 4.26); 271 (log ϵ 4.21); 286 (log ϵ 4.14) (MeOH).

(5*S*,6*R*,7*E*,9*E*,11*Z*,14*Z*)-*form*
Metab. of arachidonic acid derived from Leukotriene A_4.

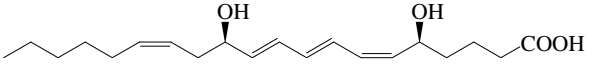
Me ester:
Oil. $[\alpha]_D^{20}$ +0.91 (c, 0.44 in $CHCl_3$). Other diastereoisomers also prepd.

(5*S*,6*S*,7*E*,9*E*,11*Z*,14*Z*)-*form* [82948-87-6]
$[\alpha]_D^{22}$ -65 (c, 0.05 in EtOH).

Cristol, J.P. *et al., Res. Commun. Chem. Pathol. Pharmacol.*, 1988, **59**, 423
Nicolaou, K.C. *et al., Angew. Chem., Int. Ed.*, 1989, **28**, 587 (*synth, ir, uv, pmr*)
Muller, A. *et al., Prostaglandins*, 1989, **38**, 635 (*synth, biochem*)
Kugel, C. *et al., Tet. Lett.*, 1989, **30**, 4947 (*synth, pmr, ms*)
Jiang, Z.D. *et al., Phytochemistry*, 2000, **53**, 129-133 (*isol, pmr, cmr*)

5,12-Dihydroxy-6,8,10,14-eicosatetraenoic acid D-677

[73151-67-4]



(5*S*,6*Z*,8*E*,10*E*,12*R*,14*Z*)-*form*

$C_{20}H_{32}O_4$ 336.47
Leukotriene receptor agonist.

(5*S*,6*Z*,8*E*,10*E*,12*R*,14*Z*)-*form*
Leukotriene B_4. LTB_4
[71160-24-2]
Powerful chemotactic substance for macrophages and neutrophils, involved in tissue response to inflammation. Oil. $[\alpha]_D^{25}$ +12.6 (c, 0.46 in $CDCl_3$).

Me ester: [83058-42-8]
$[\alpha]_D^{20}$ +6.5 (c, 1.8 in CCl_4). λ_{max} 260; 270; 282 (MeOH).

Methylamide: 5,12-Dihydroxy-N,N-*dimethyl-6,8,10,14-eicosatetraenamide*
[127745-49-7]
$C_{21}H_{35}NO_3$ 349.512
Inhibits neutrophil degranulation induced by LTB_4.

Dimethylamide:
$C_{22}H_{37}NO_3$ 363.539
Inhibitor of LTB_4 binding. Oxygen- and light-sensitive. λ_{max} 270 (ϵ 50000) (no solvent reported).

(3-Aminopropyl)amide: N-*(3-Aminopropyl)-5,12-dihydroxy-6,8,10,14-eicosatetraenamide. LTB_4-APA*
[89596-43-0]
$C_{23}H_{40}N_2O_3$ 392.581
Affinity label for the LTB_4 receptor. Selectively binds to high affinity leucocyte LTB_4 receptors and induces receptor desensitisation.

5,12-Di-Ac:
$C_{24}H_{36}O_6$ 420.545
Selective, competitive and reversible inhibitor of LTB_4.

δ-Lactone: Tetrahydro-6-(7-hydroxy-1,3,5,9-pentadecatetraenyl)-2H-pyran-2-one. Leukotriene B_4 δ-lactone
[85082-09-3]
$C_{20}H_{30}O_3$ 318.455
Useful intermed. giving LTB_4 covalently bound to a variety of ligands.

19-Hydroxy: 5,12,19-Trihydroxy-6,8,10,14-eicosatetraenoic acid
[81994-54-9]
$C_{20}H_{32}O_5$ 352.47
LTB_4 metab. λ_{max} 260; 271; 281 (MeOH).

20-Hydroxy: 5,12,20-Trihydroxy-6,8,10,14-eicosatetraenoic acid
[79516-82-8]
$C_{20}H_{32}O_5$ 352.47
Primary metab. of LTB_4.

14,15-Didehydro: 5,12-Dihydroxy-6,8,10-eicosatrien-14-ynoic acid
[114616-11-4]
$C_{20}H_{30}O_4$ 334.455
Precursor of tritiated LTB_4. Inhibits LTB_4.

6,7,14,15-Tetradehydro: 5,12-Dihydroxy-8,10-eicosadiene-6,14-diynoic acid
[90108-38-6]
$C_{20}H_{28}O_4$ 332.439
Deuteration or tritiation intermed. LTB_4 antagonist. No phys. props. reported.

12-Oxo: 5-Hydroxy-12-oxo-6,8,10,14-eicosatetraenoic acid. 12-Oxo-LTB_4
[136696-10-1]
$C_{20}H_{30}O_4$ 334.455
Biosynth. from LTB_4. Formed from LTB_4 by polymorphonuclear leucocytes.

20-Oxo: 5-Hydroxy-20-oxo-6,8,10,14-eicosatetraenoic acid
$C_{20}H_{30}O_5$ 350.454
LTB_4 metab.

(5*S*,6*E*,8*Z*,10*E*,12*S*,14*Z*)-*form*
(5S,12S)-DiHETE. Leukotriene B_x. LTB_x
Metab. of arachidonic acid found in human leucocytes. Has weak chemotactic activity. Cryst.
Mp 101-103°. Biosynth. markedly diff. from LTB_4.

(5*S*,6*E*,8*E*,10*E*,12*R*,14*Z*)-*form*
6-trans-*Leukotriene B_4. (5S,12R)-DiHETE*
[71652-82-9]
LTB_4 metab. Biosynth. from LTA_4 and cysteinyl leukotrienes.

(5*S*,6*Z*,8*E*,10*E*,12*S*,14*Z*)-*form*
12-epi-*Leukotriene B_4*
[83709-73-3]
Leukotriene metab. Less active than LTB_4.

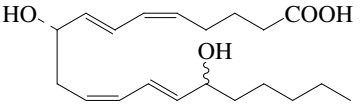
(5*S*,6*E*,8*E*,10*E*,12*S*,14*Z*)-*form*
6-trans-*12*-epi-*Leukotriene B_4*
[71548-19-1]
Leukotriene metab.

(5*RS*,12*S*,6*E*,8*E*,10*E*,14*Z*)-*form*
Constit. of the red alga *Murrayella periclados*.

[79056-01-2, 82978-32-3, 82978-33-4, 98056-93-0, 98056-94-1, 98103-85-6, 98167-17-0]

Borgeat, P. *et al., J. Biol. Chem.*, 1979, **254**, 2643 (*struct*)
Goetzl, J.E. *et al., J. Exp. Med.*, 1981, **153**, 482 (*di-Ac*)
Ford-Hutchinson, A.W. *et al., Prostaglandins*, 1981, **21**, 143; 1983, **25**, 29 (*biochem*)
Corey, E.J. *et al., Tet. Lett.*, 1981, **22**, 1077; 1587; 3339 (*synth, uv, bibl*)
Showell, H.J. *et al., Biochem. Biophys. Res. Commun.*, 1982, **106**, 741 (*synth, biochem*)
Zamboni, R. *et al., Tet. Lett.*, 1982, **23**, 2631; 4751 (*synth, bibl*)
Lee, C.W. *et al., J. Biol. Chem.*, 1983, **258**, 15004 (*biosynth*)
Young, R.N. *et al., Prostaglandins*, 1983, **26**, 605 (*biochem*)
Mills, L.S. *et al., Tet. Lett.*, 1983, **24**, 409 (*synth*)
Fuganti, C. *et al., Tet. Lett.*, 1983, **24**, 5285 (*synth*)
Green, R.H. *et al., Tetrahedron*, 1983, **39**, 1687 (*rev*)
Nicolaou, K.C. *et al., J.A.C.S.*, 1984, **106**, 3548 (*synth*)
Sugiura, M. *et al., J.A.C.S.*, 1984, **106**, 4021 (*conformn*)
Adams, J. *et al., Tet. Lett.*, 1984, **25**, 1227 (*synth*)
Han, C.-O. *et al., J.O.C.*, 1986, **51**, 1253 (*synth, uv, pmr*)
Nicolaou, K.C. *et al., Tet. Lett.*, 1986, **27**, 1881 (*synth, bibl*)
Le Merrer, Y. *et al., Tet. Lett.*, 1986, **27**, 4161 (*synth*)
Leblanc, Y. *et al., Prostaglandins*, 1987, **33**, 617 (*synth*)
Kitamura, S. *et al., Eur. J. Biochem.*, 1988, **176**, 725 (*synth*)
Guindon, Y. *et al., J.O.C.*, 1988, **53**, 267 (*synth, pmr, uv*)
Tsai, B.S. *et al., Prostaglandins*, 1989, **37**, 287 (*synth, biochem, ir, uv, pmr*)
Avignon-Tropis, M. *et al., Tet. Lett.*, 1989, **30**, 6335 (*synth*)
Kiel, D. *et al., Adv. Prostaglandin, Thromboxane, Leukotriene Res.*, 1990, **21A**, 403 (*rev*)
Le Merrer, Y. *et al., Bull. Soc. Chim. Fr.*, 1990, 798 (*synth, uv, pmr*)
Kobayashi, Y. *et al., J.O.C.*, 1990, **55**, 5324 (*synth, ir, pmr*)
Shimazaki, T. *et al., J. Biol. Chem.*, 1991, **266**, 20899
Babudri, F. *et al., J.O.C.*, 1991, **56**, 6245 (*synth, pmr*)
Kerdesky, F.A.J. *et al., J.O.C.*, 1993, **58**, 3516 (*synth, pmr, ir, uv*)
Bernart, M.W. *et al., Phytochemistry*, 1994, **36**, 1233 (*isol*)
Khanapure, S.P. *et al., J.O.C.*, 1995, **60**, 1806 (*12-Oxo-LTB_4, synth, pmr, cmr*)
Benkouider, A. *et al., J. Chem. Res., Synop.*, 1999, 104-105 (*synth*)
Rodriguez, A. *et al., Tetrahedron*, 2001, **57**, 25-37 (*synth, uv, pmr, cmr*)

9,15-Dihydroxy-5,7,11,13-eicosatetraenoic acid D-678

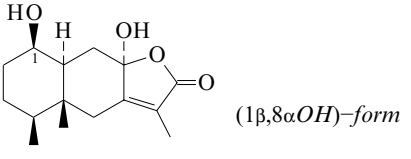


$C_{20}H_{32}O_4$ 336.47

(5*Z*,7*E*,9*S*,11*Z*,13*E*,15ξ)-*form* [189082-75-5]
Me ester: [189082-76-6]
$C_{21}H_{34}O_4$ 350.497
Isol. from the red alga *Polyneura latissima*. Oil. $[\alpha]_D^{23}$ -7.5 (c, 0.05 in MeOH). λ_{max} 204 (ϵ 18000); 232 (ϵ 47700); 238 (ϵ 49600) (MeOH).

Jiang, Z.-D. *et al., Lipids*, 1997, **32**, 231-235 (*isol, pmr, cmr, ms*)

1,8-Dihydroxy-7(11)-eremophilen-12,8-olide D-679



(1β,8α*OH*)–*form*

$C_{15}H_{22}O_4$ 266.336

(1β,8α*OH*)-*form*
1-Ac: ***Palmosalide B***
[128255-37-8]
$C_{17}H_{24}O_5$ 308.374
Constit. of *Coelogorgia palmosa*. Oil. $[\alpha]_D$ +52.8 (c, 1.5 in $CHCl_3$).

1-Ketone: ***(-)-Istanbulin A***
[115473-65-9]
$C_{15}H_{20}O_4$ 264.321
Constit. of the leaves of *Sarcandra glabra*. Cryst.
Mp 245°. $[\alpha]_D^{17}$ -110 (c, 0.6 in MeOH).

(1α,8β*OH*,10β)-*form*
1-Angeloyl:
$C_{20}H_{28}O_5$ 348.438
Constit. of *Senecio almeydae, Senecio cachinalensis* and *Senecio viravira*. Gum. $[\alpha]_D^{24}$ -18 (c, 0.45 in $CHCl_3$).

1-Tigloyl:
$C_{20}H_{28}O_5$ 348.438
Constit. of *Senecio almeydae*. Gum.

8-Me ether, 1-Ac: [324077-41-0]
$C_{18}H_{26}O_5$ 322.4
Constit. of *Senecio miser*. Cryst.

Mp 143-145°. $[\alpha]_D^{25}$ +20 (c, 0.02 in $CHCl_3$). λ_{max} 231 (log ϵ 3.46) ($CHCl_3$).

8-Me ether, 1-angeloyl: [135377-72-9]
$C_{21}H_{30}O_5$ 362.465
Constit. of *Senecio cachinalensis* and *Senecio poepigii*. Gum.
$[\alpha]_D$ +12.5 (c, 0.072 in $CHCl_3$).

(4α,5α,8β*OH*,10β)-*form*

1-Ketone: ent-*8α-Hydroxy-1-oxo-7(11)-eremophilen-12,8-olide.*
Istanbulin A
[35481-83-5]
$C_{15}H_{20}O_4$ 264.321
Isol. from *Smyrnium olusatrum* (alexanders). Cryst.
Mp 246°. $[\alpha]_D^{20}$ +81.5 (MeOH). λ_{max} 285 (ϵ 158) (MeOH) (Berdy).
λ_{max} 221 (log ϵ 4.16); 285 (log ϵ 2.2) (EtOH).

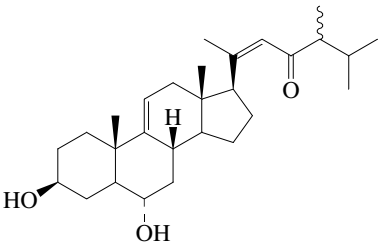
(4α,5α,8α*OH*,10α)-*form*

1-Ketone: ***8,10-Diepiistanbulin A***
$C_{15}H_{20}O_4$ 264.321
Constit. of *Senecio bracteolatus*. Oil. $[\alpha]_D$ -64 (c, 0.68 in $CHCl_3$).

Ulubelen, A. *et al., Tet. Lett.*, 1971, **12**, 4455-4456 (*Istanbulin A*)
Budešinský, M. *et al., Coll. Czech. Chem. Comm.*, 1984, **49**, 1311-1317 (*abs config, Istanbulin A*)
Bohlmann, F. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 707-736 (*8,10-Diepiistanbulin A*)
Wang, A. *et al., Yaoxue Xuebao*, 1988, **23**, 64-66 (*(-)-Istanbulin A*)
Weimer, D.F. *et al., Tet. Lett.*, 1990, **31**, 1973-1976 (*Palmosalide B*)
Dupré, S. *et al., Phytochemistry*, 1991, **30**, 1211-1220 (*isol, pmr*)
Reina, M. *et al., J. Nat. Prod.*, 2001, **64**, 6-11 (*8-Me ether-1-Ac, cryst struct*)
Reina, M. *et al., Nat. Prod. Res.*, 2006, **20**, 13-19 (*Senecio poepigii constit*)

3,6-Dihydroxyergosta-9(11),20(22)-dien-23-one D-680

3,6-Dihydroxy-24-methylcholesta-9(11),20(22)-dien-23-one

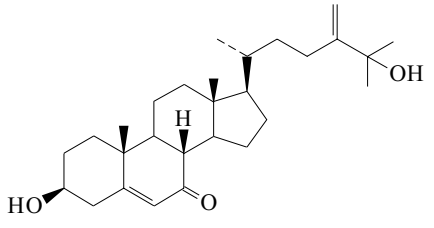


$C_{28}H_{44}O_3$ 428.654

(3β,5α,6α,20(22)*E*,24ξ)-*form* [218799-17-8]
Constit. of *Asterias amurensis*.
Cryst.
Mp 127-128°. $[\alpha]_D^{20}$ -13.2 (c, 0.19 in $CHCl_3$). λ_{max} 248 (EtOH).

Gorshkov, B.A. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1998, **120**, 235-239 (*isol, pmr*)

3,25-Dihydroxyergosta-5,24(28)-dien-7-one D-681



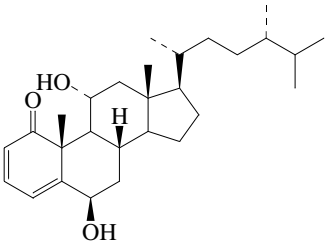
$C_{28}H_{44}O_3$ 428.654

3β-*form* [147641-74-5]
Constit. of *Stelodoryx chlorophylla*.
$[\alpha]_D$ -31.9 (c, 0.3 in $CHCl_3$).

De Riccardis, F. *et al., J. Nat. Prod.*, 1993, **56**, 282 (*isol, pmr, cmr, ms*)

6,11-Dihydroxyergosta-2,4-dien-1-one D-682

6,11-Dihydroxy-24-methylcholesta-2,4-dien-1-one



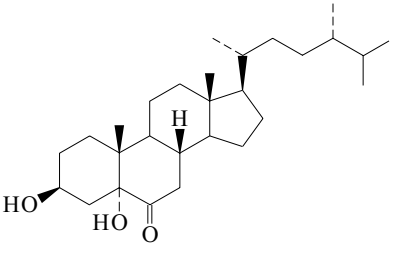
$C_{28}H_{44}O_3$ 428.654

(6β,11α,24*S*)-*form*
Stoloniferone E
[475111-78-5]
Constit. of *Clavularia viridis*.
Amorph. solid. $[\alpha]_D^{25}$ +10 (c, 0.05 in $CHCl_3$). λ_{max} 222 (log ϵ 3.79); 280 (log ϵ 4.01) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1535-1539 (*isol, pmr, cmr*)

3,5-Dihydroxyergostan-6-one D-683

3,5-Dihydroxy-24-methylcholestan-6-one



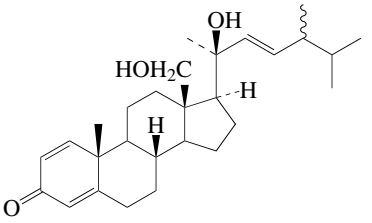
$C_{28}H_{48}O_3$ 432.685

(3β,5α,24*S*)-*form* [133883-20-2]
Constit. of *Sclerophytum* spp.
Cryst.
Mp 251-253°. $[\alpha]_D^{29}$ -32 (c, 0.24 in $CHCl_3$).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 297 (*isol, pmr, cmr*)

18,20-Dihydroxyergosta-1,4,22-trien-3-one D-684

18,20-Dihydroxy-24-methylcholesta-1,4,22-trien-3-one

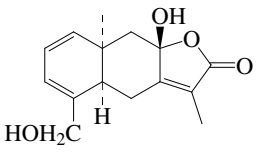


$C_{28}H_{42}O_3$ 426.638

(20*S*,22*E*,24ξ)-*form* [137576-00-2]
Constit. of *Antipathes subpinnata*.

Aiello, A. *et al., Steroids*, 1991, **56**, 513 (*isol, pmr, cmr*)

8,15-Dihydroxy-1,3,7(11)-eudesmatrien-12,8-olide D-685

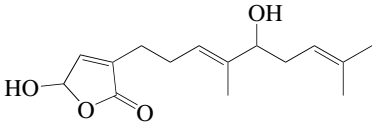


$C_{15}H_{18}O_4$ 262.305

(5α,8β*OH*,10α)-*form*

15-Ac: ***Tubipolide C***
[385793-34-0]
$C_{17}H_{20}O_5$ 304.342
Constit. of *Tubipora musica*. Oil. $[\alpha]_D^{25}$ -79.7 (c, 0.05 in $CHCl_3$). λ_{max} 236 (log ϵ 4.28); 268 (log ϵ 3.13) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 2001, **64**, 1430-1433 (*isol, pmr, cmr*)

1,8-Dihydroxy-2,6,10-farnesatrien-15,1-olide D-686

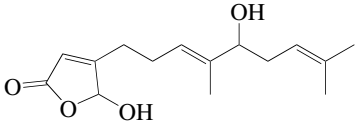


$C_{15}H_{22}O_4$ 266.336

1-Me ether: [209163-43-9]
$C_{16}H_{24}O_4$ 280.363
Constit. of *Ritterella rete*. Yellow oil. $[\alpha]_D$ -20 (c, 0.1 in MeOH). λ_{max} 232 (log ϵ 2.8); 278 (log ϵ 2.4) ($CHCl_3$).
Lenis, L.A. *et al., Tetrahedron*, 1998, **54**, 5385-5406 (*isol, pmr, cmr*)

8,15-Dihydroxy-2,6,10-farnesatrien-1,15-olide D-687

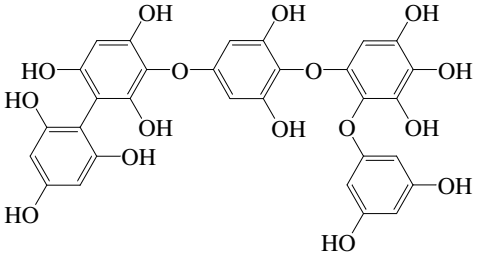
[209163-42-8]



$C_{15}H_{22}O_4$ 266.336
Constit. of *Ritterella rete*. Yellow oil. $[\alpha]_D$ -5.4 (c, 0.22 in MeOH). λ_{max} 280 (log ϵ 2.1) (no solvent reported).
Lenis, L.A. *et al., Tetrahedron*, 1998, **54**, 5385-5406 (*isol, pmr, cmr*)

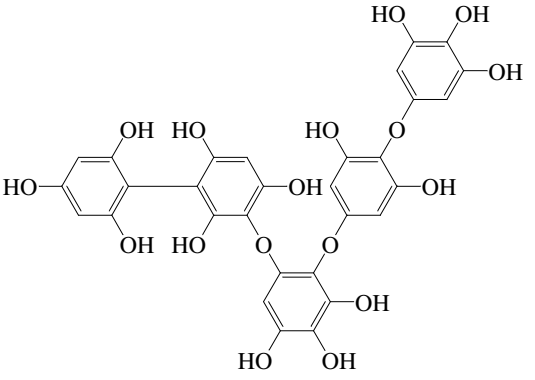
Dihydroxyfucotriphlorethol A D-688

[189216-27-1]



$C_{30}H_{22}O_{16}$ 638.494
Isol. from *Cystophora torulosa*, *Sargassum spinuligerum* and *Carpophyllum angustifolium*. Isol. as per-Ac, to which CAS no. refers.
Glombitza, K.W. *et al., Nat. Toxins*, 1997, **5**, 58-63 (*isol, struct*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

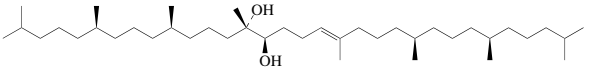
Dihydroxyfucotriphlorethol B D-689



$C_{30}H_{22}O_{17}$ 654.494
Apparently different skeleton from Fucotriphlorethol B′F-109. Isol. from brown algae *Sargassum spinuligerum* and *Carpophyllum angustifolium*.
Glombitza, K.W. *et al., Phytochemistry*, 1997, **46**, 1417-1422 (*isol, struct*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

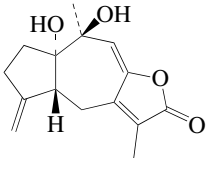
Dihydroxyglycopaene D-690

[188413-80-1]



$C_{40}H_{80}O_2$ 593.071
Constit. of *Botryococcus braunii*. Oil. $[\alpha]_D$ -2.5 (c, 5.6 in heptane).
Delahais, V. *et al., Phytochemistry*, 1997, **44**, 671-678 (*isol, pmr, cmr*)

1,10-Dihydroxy-4(15),7(11),8-guaiatrien-12,8-olide D-691



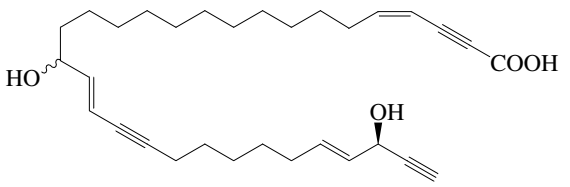
(1α,5β,10β)-*form*

$C_{15}H_{18}O_4$ 262.305

(1α,5β,10β)-*form*
Menverin C
[838862-37-6]
Constit. of *Menella verrucosa*.
Oil. $[\alpha]_D^{20}$ -152 (c, 0.375 in $CHCl_3$). λ_{max} 276 (log ϵ 4.35) (MeOH).

(1β,5β,10β)-*form*
Menverin D
[838862-38-7]
Constit. of *Menella verrucosa*.
Oil. λ_{max} 273 (log ϵ 4.06) (MeOH).
Zhang, W. *et al., Helv. Chim. Acta*, 2004, **87**, 2919-2925 (*Menverins C and D*)

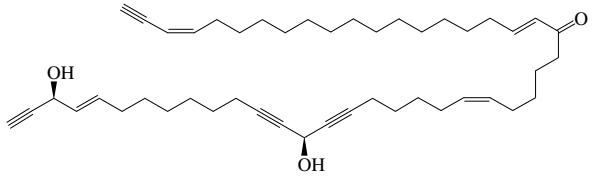
17,29-Dihydroxy-4,18,27-hentriacontatriene-2,20,30-triynoic acid D-692



$C_{31}H_{44}O_4$ 480.686

(4*Z*,17ξ,18*E*,27*E*,29*R*)-*form*
Corticatic acid D
Isol. from the sponge *Petrosia corticata*.
Oil. $[\alpha]_D^{20}$ -19.7 (c, 0.07 in $CHCl_3$). λ_{max} 244 (ϵ 13000); 259 (ϵ 7990) (MeOH).
Nishimura, S. *et al., J. Nat. Prod.*, 2002, **65**, 1353-1356 (*isol*)

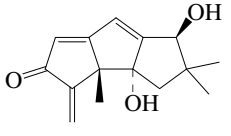
33,44-Dihydroxy-3,18,25,42-hexatetracontatetraene-1,31,34,45-tetrayn-20-one D-693
Petrotetrayndiol C



$C_{46}H_{68}O_3$ 669.041

(3*Z*,18*E*,25*Z*,33*S*,42*E*,44*S*)-*form* [246239-78-1]
Constit. of a sponge *Petrosia* sp. Cytotoxic agent. Oil.
Lim, Y.J. *et al., J. Nat. Prod.*, 1999, **62**, 1215-1217; 2001, **64**, 46-53 (*isol,pmr,cmr*)

2,10-Dihydroxy-4(15),6,8-hirsutatrien-5-one D-694



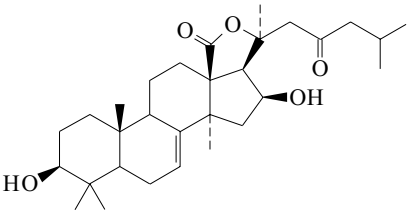
(2α,10β)-*form*

$C_{15}H_{18}O_3$ 246.305

(2α,10β)-*form*
Hirsutanol A
[210897-86-2]
Metab. of an unidentified fungus isolated from a *Haliclona* sponge. Nitric oxide synthase and cyclooxygenase-2 expression inhibitor. $[\alpha]_D^{25}$ -23.5 (c, 0.97 in MeOH). λ_{max} 218 (ϵ 2920); 306 (ϵ 4276) (MeOH).
4α,15-Dihydro: 2,10-Dihydroxy-6,8-hirsutadien-5-one. ***Hirsutanol C***
[210897-92-0]
$C_{15}H_{20}O_3$ 248.321
Metab. of an unidentified fungus isolated from a *Haliclona* sponge.
$[\alpha]_D^{25}$ +20.6 (c, 0.31 in MeOH). λ_{max} 206 (ϵ 896); 282 (ϵ 1658) (MeOH).

(2β,10β)-*form*
Hirsutanol B
[210897-89-5]
Metab. of an unidentified fungus isolated from a *Haliclona* sponge.
Wang, G.-Y.-S. *et al., Tetrahedron*, 1998, **54**, 7335-7342 (*isol, pmr, cmr*)

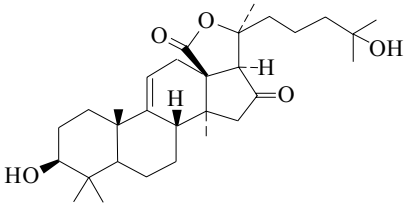
3,16-Dihydroxyholost-7-en-23-one D-695



$C_{30}H_{46}O_5$ 486.69

(3β,16β)-*form*
*16-Ac, 3-*O*-[3-*O*-methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfato-β-D-xylopyranoside]:* ***Cucumarioside A_o-1***
[168433-95-2]
$C_{60}H_{94}O_{30}S$ 1327.451
Constit. of *Cucumaria japonica*.
*16-Ac, 3-*O*-[3-*O*-methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Cucumarioside A_2-5***
[583028-05-1]
$C_{61}H_{96}O_{31}S$ 1357.477
Constit. of *Cucumaria conicospermium*. Cryst.
Mp 207-209°. $[\alpha]_D^{20}$ -44 (c, 0.1 in Py).
Drozdova, O.A. *et al., Khim. Prir. Soedin.*, 1993, **29**, 200; *Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 200
Avilov, S.A. *et al., J. Nat. Prod.*, 2003, **66**, 910-916 (*Cucumarioside A_2-5*)

3,25-Dihydroxyholost-9(11)-en-16-one D-696



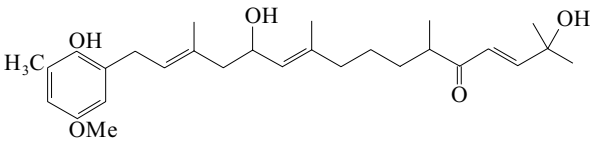
$C_{30}H_{46}O_5$ 486.69

3β-*form*
Stichopogenin A_4. Holotoxinogenin
[23519-00-8]
Constit. of *Stychopus japonicus.*
Cryst. (Me_2CO aq.).
Mp 238-240°. $[\alpha]_D^{20}$ -97.6 (c, 0.25 in $CHCl_3$).
25-Me ether: [53586-51-9]
$C_{31}H_{48}O_5$ 500.717
Aglycone from *Stychopus japonicus.* Cryst. ($CHCl_3$).
Mp 236-238°.
Elyakov, G.B. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1975, **52**, 321-323 (*biosynth*)
Tan, W.L. *et al., J.O.C.*, 1975, **40**, 466-470 (*struct*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1976, **24**, 266-274 (*isol, struct*)

2,12-Dihydroxy-16-(2-hydroxy-5-methoxy-3-methylphenyl)-2,6,10,14-tetramethyl-3,10,14-hexadecatrien-5-one, 9CI D-697

2-(5,15-Dihydroxy-3,7,11,15-tetramethyl-12-oxo-2,6,13-hexadecatrienyl)-4-methoxy-6-methylphenol

[83644-04-6]



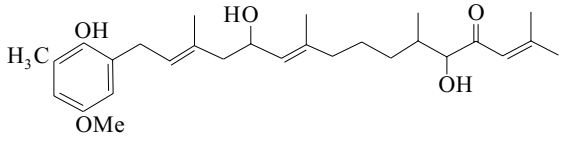
$C_{28}H_{42}O_5$ 458.637

Constit. of brown alga *Cystoseira elegans*. Light-yellow oil. $[\alpha]_D$ +5.7 (c, 9.5 in MeOH).

Banaigs, B. *et al., Tet. Lett.*, 1982, **23**, 3271

5,12-Dihydroxy-16-(2-hydroxy-5-methoxy-3-methylphenyl)-2,6,10,14-tetramethyl-2,10,14-hexadecatrien-4-one, 9CI D-698

[89926-70-5]



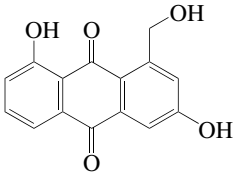
$C_{28}H_{42}O_5$ 458.637

Constit. of *Cystoseira elegans*. Oil. $[\alpha]_D$ +3.2 (c, 1.86 in MeOH).

Banaigs, B. *et al., Phytochemistry*, 1983, **22**, 2865

3,8-Dihydroxy-1-hydroxymethylanthraquinone D-699

3,8-Dihydroxy-1-hydroxymethyl-9,10-anthracenedione. ***ω-Hydroxyaloesaponarin II***



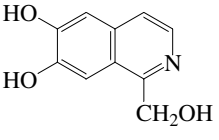
$C_{15}H_{10}O_5$ 270.241

Prod. by recombinant host *Streptomyces lividans* K4-114 and the marine-derived *Streptomyces* sp. B1108.

Kalaitzis, J.A. *et al., J. Nat. Prod.*, 2004, **67**, 1419-1422 (*isol, pmr, cmr*)
Laatsch, H. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

6,7-Dihydroxy-1-hydroxymethylisoquinoline D-700

1-Hydroxymethyl-6,7-isoquinolinediol



$C_{10}H_9NO_3$ 191.186

7-Me ether: 6-Hydroxy-7-methoxy-1-isoquinolinemethanol. 6-Hydroxy-1-hydroxymethyl-7-methoxyisoquinoline

[367947-68-0]

$C_{11}H_{11}NO_3$ 205.213

Alkaloid from the sponge *Haliclona* sp. Needles (EtOH). Mp 202-204°. λ_{max} 239 (log ϵ 4.35); 253 (sh) (log ϵ 3.87); 258 (log ϵ 3.73); 279 (log ϵ 3.56); 325 (log ϵ 3.32); 363 (log ϵ 3.31) (MeOH).

6,7-Di-Me ether, N-*oxide: 1-Hydroxymethyl-6,7-dimethoxyisoquinoline* N-*oxide*

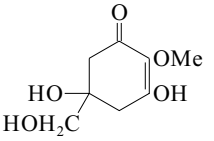
$C_{12}H_{13}NO_4$ 235.239

Alkaloid from the seeds of *Calycotome villosa* ssp. *intermedia*. Mp 209-211°. λ_{max} 217; 259; 304; 338; 352 (MeOH).

Rashid, M.A. *et al., J. Nat. Prod.*, 2001, **64**, 1249-1250 (*7-Me ether, isol*)
Saito, N. *et al., Chem. Pharm. Bull.*, 2004, **52**, 282-286 (*7-Me ether, synth, pmr, cmr, ms*)
El Antri, A. *et al., Fitoterapia*, 2004, **75**, 774-778 (*6,7-di-Me ether N-oxide*)

3,5-Dihydroxy-5-(hydroxymethyl)-2-methoxy-2-cyclohexen-1-one, 9CI D-701

[65318-54-9]



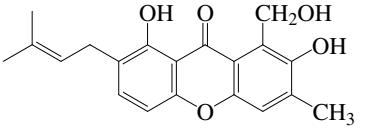
$C_8H_{12}O_5$ 188.18

Isol. from fish eggs, *Sphaerechinus granularis, Paracentrotus lividus* and *Palythoa tuberculosa*. Identified in the caprophores of *Helvella leucomelaneae* and in extracts of *Trichothecium roseum*. Syrup. λ_{max} 268 nm (ϵ 15700) ($H^{\oplus}$), 292 (25100) ($OH^{\ominus}$).

Ito, S. *et al., Tet. Lett.*, 1977, 2429 (*isol*)
Chioccara, F. *et al., Bull. Soc. Chim. Belg.*, 1980, **89**, 1101 (*isol, uv, pmr, ms*)
Lemoyne, F. *et al., Z. Naturforsch., C*, 1985, **40**, 612 (*isol, hplc, uv, pmr, cmr, ms*)
Chioccara, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **85**, 459 (*isol*)

2,8-Dihydroxy-1-hydroxymethyl-3-methyl-7-prenylxanthone D-702

*2,8-Dihydroxy-1-(hydroxymethyl)-3-methyl-7-(3-methyl-2-butenyl)-9*H-*xanthen-9-one*



$C_{20}H_{20}O_5$ 340.375

*2-*O-*(3-Methyl-2-butenyl): 8-Hydroxy-1-hydroxymethyl-3-methyl-7-prenyl-2-prenyloxyxanthone.* ***Isoemericellin***

$C_{25}H_{28}O_5$ 408.493

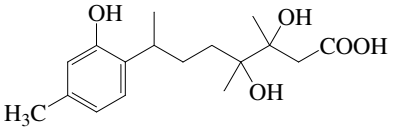
Isol. from *Emericella variecolor* derived from the sponge *Haliclona valliculata*. Yellow needles.

Mp 112°. λ_{max} 203; 236; 270; 295; 384 (EtOH).

Bringmann, G. *et al., Phytochemistry*, 2003, **63**, 437-443 (*isol, pmr, cmr, ms*)

3,4-Dihydroxy-7-(2-hydroxy-4-methylphenyl)-3,4-dimethyloctanoic acid D-703

*2,5-Dideoxy-4-*C*-[3-(2-hydroxy-4-methylphenyl)butyl]-3-*C*-methylpentonic acid, 9CI*



$C_{17}H_{26}O_5$ 310.389

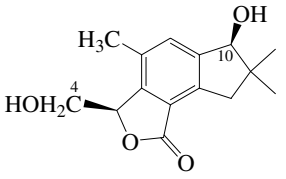
Et ester: [811860-52-3]

$C_{19}H_{30}O_5$ 338.443

Constit. of the marine sponge *Didiscus* sp.

Hoang, T.H. *et al., CA*, 2005, **142**, 71700q (*isol*)

4,10-Dihydroxy-2,6,8-illudalatrien-15,5-olide D-704

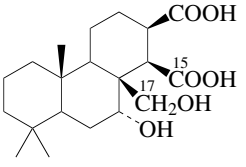


$C_{15}H_{18}O_4$ 262.305

(5*R*,10*S*)-*form*

4-Nitrate ester: ***Alcyopterosin M***
[288851-39-8]
$C_{15}H_{17}NO_6$ 307.302
Constit. of *Alcyonium paessleri*. Oil. $[\alpha]_D^{25}$ -23.16 (c, 0.79 in $CHCl_3$). λ_{max} 234 (log ϵ 3.65); 238 (log ϵ 3.64); 296 (log ϵ 3.35) (CH_2Cl_2).
Palermo, J.A. *et al., J.O.C.*, 2000, **65**, 4482-4486 (*isol, pmr, cmr*)

7,17-Dihydroxy-15,16-isocopalanedioic acid D-705



$C_{20}H_{32}O_6$ 368.469

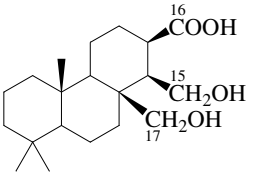
7α-*form*

15→17 Lactone, 7-Ac, Me ester: Methyl 7α-acetoxy-15,17-isocopalanolid-16-oate. ***7α-Acetoxydendrillol 3****. Aplyroseol 9*
[178180-04-6]
$C_{23}H_{34}O_6$ 406.518
Constit. of *Chromodoris obsoleta* and *Aplysilla rosea*. Needles or gum.
Mp 60-63°. $[\alpha]_D^{28}$ -6.4 (c, 0.31 in $CHCl_3$).

15→17-Lactone, 7-butanoyl, Me ester: ***Aplyroseol 8***
[200437-54-3]
$C_{25}H_{38}O_6$ 434.572
Constit. of *Aplysilla rosea*. Gum.

Miyamoto, T. *et al., Tetrahedron*, 1996, **52**, 8187-8198 (*isol, pmr, cmr*)
Taylor, W.C. *et al., Aust. J. Chem.*, 1997, **50**, 895-902 (*Aplyroseols*)

15,17-Dihydroxyisocopalan-16-oic acid D-706

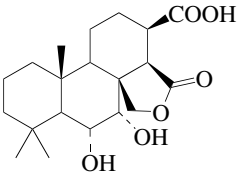


$C_{20}H_{34}O_4$ 338.486

16→17-Lactone, 15-Ac: ***Aplyroseol 14***
[200437-64-5]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Aplysilla rosea*. Solid.
Mp 146-148°. Struct. revised in 2003.

Taylor, W.C. *et al., Aust. J. Chem.*, 1997, **50**, 895-902 (*isol, pmr, cmr*)
Arnó, M. *et al., J.O.C.*, 2003, **68**, 1242-1251 (*synth, struct*)

6,7-Dihydroxy-15,17-isocopalanolid-16-oic acid D-707



$C_{20}H_{30}O_6$ 366.453

(6α,7α)-*form*

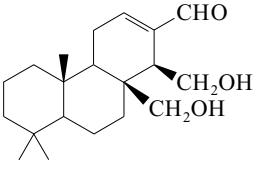
6-Butanoyl, Me ester: ***Aplyroseol 10***
[200437-56-5]
$C_{25}H_{38}O_7$ 450.571
Constit. of *Aplysilla rosea*. Glass.

6-Butanoyl, 7-Ac, Me ester: ***Aplyroseol 11***
[200437-58-7]
$C_{27}H_{40}O_8$ 492.608
Constit. of *Aplysilla rosea*. Glass.

7-Butanoyl, 6-Ac, Me ester: ***Aplyroseol 12***
[200437-60-1]
$C_{27}H_{40}O_8$ 492.608
Constit. of *Aplysilla rosea*. Needles.

Taylor, W.C. *et al., Aust. J. Chem.*, 1997, **50**, 895-902 (*isol, pmr, cmr*)

15,17-Dihydroxy-12-isocopalen-16-al D-708

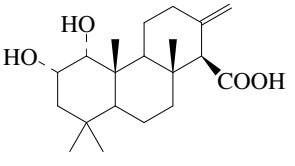


$C_{20}H_{32}O_3$ 320.471

Di-Ac: ***15,17-Diacetoxy-12-isocopalen-16-al***
[157924-85-1]
$C_{24}H_{36}O_5$ 404.545
Constit. of *Spongia zimocca*.
$[\alpha]_D^{25}$ -3.8 (c, 1.4 in $CHCl_3$).

Zubía, E. *et al., J. Nat. Prod.*, 1994, **57**, 725 (*isol, pmr, cmr*)

1,2-Dihydroxy-13(16)-isocopalen-15-oic acid D-709



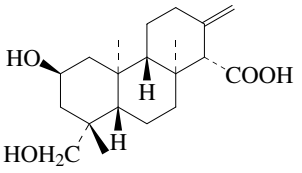
$C_{20}H_{32}O_4$ 336.47

(1α,2α)-*form*

Me ester: ***Coelodiol***
[883725-47-1]
$C_{21}H_{34}O_4$ 350.497
Constit. of *Coelocarteria* cf. *singaporensis*. Amorph. solid. $[\alpha]_D$ +4 (c, 0.2 in $CHCl_3$).

Fattorusso, E. *et al., Tet. Lett.*, 2006, **47**, 2197-2200 (*Coelodiol*)

2,19-Dihydroxy-13(16)-isocopalen-15-oic acid D-710

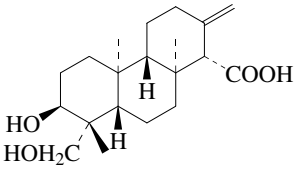


$C_{20}H_{32}O_4$ 336.47

(*ent*-2α)-*form*

2,19-Di-Ac, (1,3-dihydroxy-2-propyl) ester: ***Austrodorin A***
[252854-60-7]
$C_{27}H_{42}O_8$ 494.624
Constit. of *Austrodoris kerguelenensis.*
$[\alpha]_D$ +22.9 (c, 0.18 in $CHCl_3$).
Gavagnin, M. *et al., Tet. Lett.*, 1999, **40**, 8471-8475 (*isol, pmr, cmr*)
Gavagnin, M. *et al., Tetrahedron*, 2003, **59**, 5579-5583 (*isol, stereochem*)

3,19-Dihydroxy-13(16)-isocopalen-15-oic acid D-711

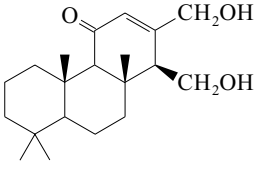


$C_{20}H_{32}O_4$ 336.47

(*ent*-3α)-*form*

3,19-Di-Ac, (1,3-dihydroxy-2-propyl) ester: ***Austrodorin B***
[252854-61-8]
$C_{27}H_{42}O_8$ 494.624
Constit. of *Austrodoris kerguelenensis.*
$[\alpha]_D$ +20.7 (c, 0.1 in $CHCl_3$).
Gavagnin, M. *et al., Tet. Lett.*, 1999, **40**, 8471-8475 (*isol, pmr, cmr*)

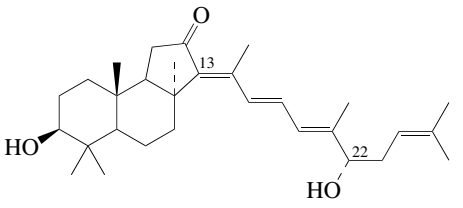
15,16-Dihydroxy-12-isocopalen-11-one D-712



$C_{20}H_{32}O_3$ 320.471

Di-Ac: 15,16-Diacetoxy-12-isocopalen-11-one
[157924-86-2]
$C_{24}H_{36}O_5$ 404.545
Constit. of *Spongia zimocca*.
$[\alpha]_D^{25}$ -54.2 (c, 0.36 in $CHCl_3$).
Zubía, E. *et al., J. Nat. Prod.*, 1994, **57**, 725 (*isol, pmr, cmr*)

3,22-Dihydroxy-13,15,17(20),24-isomalabaricatetraen-12-one D-713



(3β,13*E*,15*E*,17(20)*E*,22*S*)-*form*

$C_{30}H_{46}O_3$ 454.692

(3β,13*E*,15*E*,17(20)*E*,22*S*)-*form*

3-Ac: ***Stelliferin B***
[134176-95-7]
$C_{32}H_{48}O_4$ 496.729
Constit. of the sponge *Jaspis stellifera*. Oil. $[\alpha]_D^{23}$ -166 (c, 0.6 in C_6H_6). λ_{max} 345 (26000) (EtOH).

Di-Ac: ***Stelliferin F***
[134128-18-0]
$C_{34}H_{50}O_5$ 538.766
Constit. of *Jaspis stellifera*. Oil. $[\alpha]_D^{23}$ -377 (c, 0.005 in C_6H_6). λ_{max} 338 (ϵ 24000) (EtOH). λ_{max} 338 (ϵ 24100) (EtOH) (Berdy).

(3β,13*Z*,15*E*,17(20)*E*,22*S*)-*form*

3-Ac: ***Stelliferin A***
[134128-15-7]
$C_{32}H_{48}O_4$ 496.729
Constit. of *Jaspis stellifera* and *Stelletta globostellata*. Oil. $[\alpha]_D^{22}$ -126.6 (c, 0.5 in C_6H_6). λ_{max} 343 (ϵ 25000) (MeOH). λ_{max} 345 (ϵ 23000) (EtOH) (Berdy).

Di-Ac: ***Stelliferin E***
[134128-17-9]
$C_{34}H_{50}O_5$ 538.766
Constit. of *Jaspis stellifera*. Oil. $[\alpha]_D^{23}$ -409 (c, 0.1 in C_6H_6). λ_{max} 338 (ϵ 24000) (EtOH).

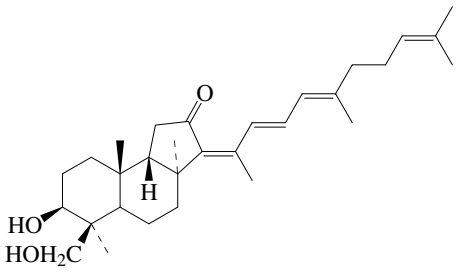
22-Deoxy: 3-Hydroxy-13,15,17(20),24-isomalabaricatetraen-12-one. ***Stelliferin D***
[134131-18-3]
$C_{30}H_{46}O_2$ 438.692
Constit. of *Jaspis stellifera* and *Stelletta globostellata*. Oil. $[\alpha]_D^{23}$ +201 (c, 0.3 in C_6H_6). λ_{max} 350 (ϵ 20000) (EtOH).

22-Ketone, 3-Ac: 3-Acetoxy-13,15,17(20),24-isomalabaricatetraene-12,22-dione. ***Stelliferin C***
[134128-16-8]
$C_{32}H_{46}O_4$ 494.713
Constit. of *Jaspis stellifera*. Oil. $[\alpha]_D^{23}$ -15.2 (c, 0.35 in C_6H_6). λ_{max} 357 (22000); 360 (sh) (EtOH).

(3α,13*Z*,15*E*,17(20)*E*,22ξ)-*form*

*3-Ac, 22-*O*-α-D-ribopyranoside:* ***Stelliferin riboside***
[351444-64-9]
$C_{37}H_{56}O_8$ 628.845
Constit. of *Geodia globostellifera*. Yellow oil. $[\alpha]_D$ -119 (c, 0.02 in MeOH). λ_{max} 338 (ϵ 47640) (EtOH).
Tsuda, M. *et al., Tetrahedron*, 1991, **47**, 2181-2194 (*isol, uv, ir, pmr, cmr, ms*)
Oku, N. *et al., J. Nat. Prod.*, 2000, **63**, 205-209 (*Stellata globostellata constits*)
Tabudravu, J.N. *et al., J. Nat. Prod.*, 2001, **64**, 813-815 (*Stelliferin riboside*)

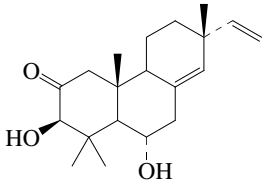
3,29-Dihydroxy-13,15,17(20),24-isomalabaricatetraen-12-one D-714



$C_{30}H_{46}O_3$ 454.692

(3β,13*Z*,15*E*,17(20)*E*)-*form*
29-Hydroxystelliferin D
[260436-27-9]
Constit. of *Stelletta globostellata*.
Yellow solid. $[\alpha]_D^{25}$ -34 (c, 0.2 in MeOH). λ_{max} 239 (log ϵ 3.88); 353 (log ϵ 4.46) (MeOH).
Oku, N. *et al., J. Prod. Nat.*, 2000, **63**, 205-209 (*isol, pmr, cmr*)

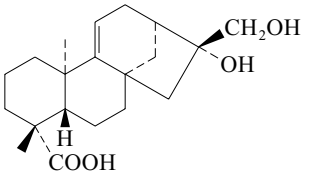
3,6-Dihydroxy-8(14),15-isopimaradien-2-one D-715



$C_{20}H_{30}O_3$ 318.455

(3β,6α)-*form*
Di-Ac: ***Rhizophorin E***
[480427-83-6]
$C_{24}H_{34}O_5$ 402.53
Constit. of *Rhizophora mucronata*. Oil. $[\alpha]_D^{25}$ -26.4 (c, 1.7 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., J. Asian Nat. Prod. Res.*, 2002, **4**, 53-61 (*isol, pmr, cmr*)

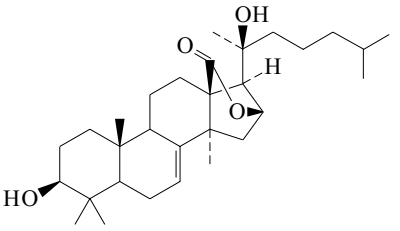
16,17-Dihydroxy-9(11)-kauren-19-oic acid D-716



$C_{20}H_{30}O_4$ 334.455

(*ent*-16β*OH*)-*form* [55483-24-4]
Constit. of roasted coffee. Isol. from *Ichthyothere terminalis*. Cryst. (Me_2CO). Mp 184-185°. $[\alpha]_D^{20}$ +32.2 (EtOH).
19-Aldehyde: ***16,17-Dihydroxy-9(11)-kauren-19-al***
[765315-59-1]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Bruguiera gymnorrhiza*. Amorph. solid. $[\alpha]_D^{20}$ +4.8 (c, 0.3 in $CHCl_3$).
Obermann, H. *et al., Chem. Ber.*, 1975, **108**, 1093
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 2317
Han, L. *et al., J. Nat. Prod.*, 2004, **67**, 1620-1623 (*aldehyde*)

3,20-Dihydroxy-7-lanosten-18,16-olide D-717

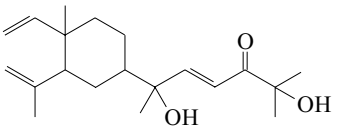


$C_{30}H_{48}O_4$ 472.707

(3β,16β,20*S*)-*form*
20-Ac: ***Onekotanogenin***
[113269-42-4]
$C_{32}H_{50}O_5$ 514.744
Constit. of *Psolus fabricii*. Cryst.
Mp 113-115°. $[\alpha]_D^{20}$ -84.3 (c, 0.3 in $CHCl_3$).
Kalinin, V.I. *et al., Khim. Prir. Soedin.*, 1987, **23**, 674; *Chem. Nat. Compd. (Engl. Transl.)*, 560 (*isol, pmr, cmr*)

13,18-Dihydroxy-8,10,15-lobatrien-17-one D-718

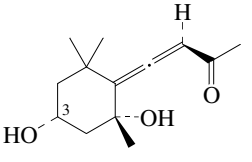
[130170-07-9]



$C_{20}H_{32}O_3$ 320.471
Constit. of a *Sclerophytum* sp. Oil. $[\alpha]_D^{30}$ +16.6 (c, 1.2 in $CHCl_3$).
Rao, C.B. *et al., Indian J. Chem., Sect. B*, 1990, **29**, 681 (*isol, pmr*)

3,5-Dihydroxy-6,7-megastigmadien-9-one D-719

4-(2,4-Dihydroxy-2,6,6-trimethylcyclohexylidene)-3-buten-2-one, 9CI. 2,6,6-Trimethyl-1-(3-oxo-1-butenylidene)-2,4-cyclohexanediol



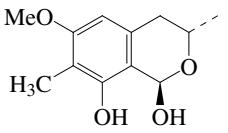
(3*R*,5*R*,7R_{ax})-*form*

$C_{13}H_{20}O_3$ 224.299

(3*S*,5*R*,7R_{ax})-*form*
Grasshopper ketone
[41703-38-2]
Isol. from the grasshopper *Romalea microptera*.
Needles (Me_2CO/C_6H_6).
Mp 134-136°. $[\alpha]_D^{25}$ -63 (c, 1.15 in MeOH).
3-Ac: ***Apo-9′-fucoxanthinone***
[26289-05-4]
$C_{15}H_{22}O_4$ 266.336
Isol. from *Padina tetrastromatica* and dinoflagellate *Amphidinium* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{19}$ -284 (c, 0.1 in MeOH). λ_{max} 231 (ϵ 2800); 280 (ϵ 700) (MeOH).
Doi, Y. *et al., J. Nat. Prod.*, 1995, **58**, 1097-1099 (*Apo-9′-fucoxanthinone*)
Parameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 463-467 (*Apo-9′-fucoxanthinone*)

1,8-Dihydroxy-6-methoxy-3,7-dimethylisochroman D-720

*3,4-Dihydro-6-methoxy-3,7-dimethyl-1*H*-2-benzopyran-1,8-diol*



$C_{12}H_{16}O_4$ 224.256

(1*R,3*S**)-*form***

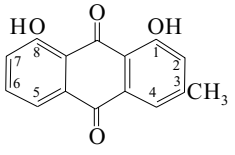
Prod. by the marine-derived *Penicillium steckii*. $[\alpha]_D^{20}$ -6.3 (c, 0.083 in MeOH). λ_{max} 224 (sh) (log ϵ 3.9); 282 (log ϵ 3.45) (MeOH).

Malmstrom, J. *et al., Phytochemistry*, 2000, **54**, 301-309 (*isol, pmr, cmr*)

1,8-Dihydroxy-3-methylanthraquinone D-721

1,8-Dihydroxy-3-methyl-9,10-anthracenedione, 9CI. ***Chrysophanol****. 3-Methylchrysazin. Rheic acid. Chrysophanic acid. Archinin. Rumicin*

[481-74-3]



$C_{15}H_{10}O_4$ 254.242

Constit. of *Cassia*, *Rumex*, *Rheum*, *Asphodelus*, *Muehlenbeckia* spp., *Monilinia fructicola* and others. V. widely distributed in plants and also found in the marine annelid *Urechis unicinctus*. Antimicrobial, cathartic agent. Golden-yellow plates (C_6H_6). Mp 200-201° (196°). pK_a 8.91 (20°, H_2O). Log P 2.42 (calc). λ_{max} 223 (ϵ 36000); 253 (ϵ 20000); 274 (ϵ 10000); 285 (ϵ 11000); 405 (sh) (ϵ); 427 (ϵ 11000); 450 (sh) (ϵ) (MeOH) (Derep).

▶ CB6725000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 88A (*ir*)
King, F.E. *et al., J.C.S.*, 1952, 4580 (*synth*)
Bloom, H. *et al., J.C.S.*, 1959, 178 (*ir*)
Banville, J. *et al., Can. J. Chem.*, 1974, **52**, 80 (*synth, uv, pmr*)
Harris, T.M. *et al., J.A.C.S.*, 1976, **98**, 6065 (*synth*)
Kraus, G.A. *et al., J.O.C.*, 1983, **48**, 3439 (*synth*)
Kelly, T.R. *et al., J.O.C.*, 1983, **48**, 3573 (*isol*)
Anderson, J.A. *et al., Phytochemistry*, 1986, **25**, 103 (*biosynth*)
Ahmed, S.A. *et al., Chem. Comm.*, 1987, 883 (*synth*)
Danielsen, K. *et al., Magn. Reson. Chem.*, 1992, **30**, 359 (*pmr, cmr*)
Schmidt, R.R. *et al., Synthesis*, 1994, 255 (*synth, pmr*)
Chang, S. *et al., J. Korean Chem. Soc.*, 1998, **42**, 64-68; *CA*, **129**, 2852 (*isol, Urechis*)

3,8-Dihydroxy-1-methylanthraquinone D-722

3,8-Dihydroxy-1-methyl-9,10-anthracenedione, 9CI.
Aloesaponarin II

[53254-94-7]

$C_{15}H_{10}O_4$ 254.242

Obt. from stems of *Aloe saponaria*. Orange needles. Mp 269-270° (250-254° dec.). λ_{max} 300; 380; 475 (MeOH/KOH) (Derep). λ_{max} 270 (sh); 280 (ϵ 5010); 390 (sh); 410 (ϵ 1260); 430 (sh) (MeOH) (Derep).

3-Me ether: 8-Hydroxy-3-methoxy-1-methylanthraquinone
[69964-33-6]
$C_{16}H_{12}O_4$ 268.268
Cryst. (Me_2CO). Mp 179-180°.

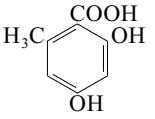
*3-*O*-(2,6-Dideoxy-β-*D*-*arabino*-hexopyranoside):* ***Halawanone C***
$C_{21}H_{20}O_7$ 384.385
Prod. by a marine-derived *Streptomyces* sp.

Yagi, A. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1159; 1977, **25**, 1764; 1771 (*isol*)
Roberge, G. *et al., Synthesis*, 1979, 148 (*synth, ir, uv, pmr*)
Franck, B. *et al., Tet. Lett.*, 1980, **21**, 1185 (*synth*)
Cameron, D.W. *et al., Aust. J. Chem.*, 1981, **34**, 2401 (*synth*)
Ford, P.W. *et al., J. Nat. Prod.*, 1998, **61**, 1232-1236 (*Halawanone C*)

2,4-Dihydroxy-6-methylbenzoic acid, 9CI D-723

*6-Methyl-β-resorcylic acid, 8CI. 4,6-Dihydroxy-*o*-toluic acid.* ***Orsellinic acid****. Orsellic acid. Orcinol-2-carboxylic acid*

[480-64-8]



$C_8H_8O_4$ 168.149

Residue present in lichen acids. Isol. from cultures of *Penicillium* spp., *Hypoxylon* spp. and other microorganisms such as the marine-derived *Chaetomium* sp. Gö 100/9. Needles + $1H_2O$ (AcOH aq.). Mp 176° dec. pK_a 2.1 (25°).

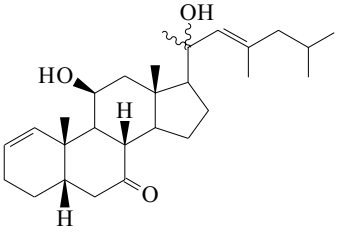
*(2-Oxo-3*E*-pentenyl) ester:* ***Globosumone A***
[856240-54-5]
$C_{13}H_{14}O_5$ 250.251
Isol. from *Chaetomium globosum* and the marine-derived *Chaetomium* sp. Gö 100/9. Cytotoxic. Mp 148-149°. λ_{max} 219 (log ϵ 5.32); 265 (log ϵ 5.01); 299 (log ϵ 4.58) (MeOH).

*(4*S*-Hydroxy-2-oxopentyl) ester:* ***Globosumone B***
[856240-56-7]
$C_{13}H_{16}O_6$ 268.266
Isol. from *Chaetomium globosum* and the marine-derived *Chaetomium* sp. Gö 100/9. Cytotoxic. Mp 168-170°. $[\alpha]_D^{25}$ +4.9 (c, 0.05 in MeOH). λ_{max} 217 (log ϵ 4.72); 265 (log ϵ 4.52); 301 (log ϵ 4.08) (MeOH).

*(3*R*,4*S*-Dihydroxy-2-oxopentyl) ester:* ***Globosumone C***
[856240-58-9]
$C_{13}H_{16}O_7$ 284.265
Isol. from *Chaetomium globosum*. Mp 162-165°. $[\alpha]_D^{25}$ -19 (c, 0.08 in MeOH). λ_{max} 218 (log ϵ 4.41); 265 (log ϵ 4.18); 301 (log ϵ 3.76) (MeOH).

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1258B (*nmr*)
Pettersson, G. *et al., Acta Chem. Scand.*, 1965, **19**, 414-420 (*biosynth*)
Harris, T.M. *et al., J.A.C.S.*, 1966, **88**, 2053-2054 (*synth*)
Huneck, S. *et al., Tetrahedron*, 1968, **24**, 2707-2755 (*ms*)
Aberhart, D.J. *et al., J.C.S.(C)*, 1969, 704-707 (*ms, uv*)
Kato, T. *et al., Chem. Pharm. Bull.*, 1972, **20**, 1574-1578 (*synth, pmr, ir*)
Hase, T.A. *et al., Acta Chem. Scand., Ser. B*, 1978, **32**, 701-702 (*synth*)
Evans, G.E. *et al., J.C.S. Perkin 1*, 1988, 755-761 (*synth, uv, ir, pmr, ms*)
Spencer, J.B. *et al., Chem. Comm.*, 1992, 646-648 (*biosynth*)
Woodward, S. *et al., J. Gen. Microbiol.*, 1993, **139**, 153-159 (*isol, props*)
Bashyal, B.P. *et al., J. Nat. Prod.*, 2005, **68**, 724-728 (*Globosumones A-C*)

11,20-Dihydroxy-23-methylcholesta-1,22-dien-7-one, 9CI D-724



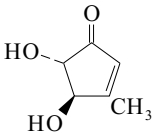
$C_{28}H_{44}O_3$ 428.654

(5β,7β,20ξ,22*E*)-*form* [132194-32-2]

Constit. of *Hypnea musciformis*. Cryst.

Babu, M. *et al., Phytochemistry*, 1990, **29**, 3965 (*isol, pmr*)

4,5-Dihydroxy-3-methyl-2-cyclopenten-1-one D-725



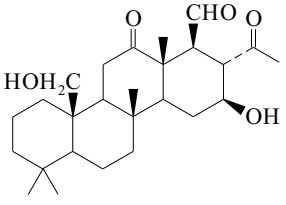
$C_6H_8O_3$ 128.127
λ_{max} 220 (ϵ 3900) (EtOH) (Derep).

(4*R*,5*S*)-*form* [137493-41-5]
Constit. of *Grateloupia filicina*. Oil. $[\alpha]_D^{20}$ -46 (c, 0.96 in $CHCl_3$).

[137493-40-4]

Ohira, S. *et al., Agric. Biol. Chem.*, 1991, **55**, 2437-2438 (*isol, pmr, cmr, synth, abs config*)

16,22-Dihydroxy-24-methyl-12,24-dioxo-25-scalaranal D-726

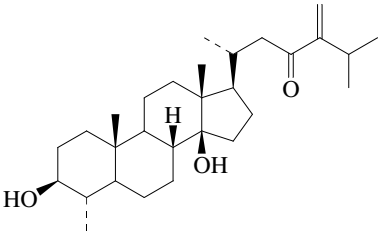


$C_{26}H_{40}O_5$ 432.599

16β-*form*
Di-Ac: [75605-87-7]
$C_{30}H_{44}O_7$ 516.673
Constit. of a *Phyllospongia* sp. Needles (Et_2O).
Mp 107.2-108.6°. $[\alpha]_D^{21}$ +132.2 (c, 1.15 in $CHCl_3$).
Kazlauskas, R. *et al., Aust. J. Chem.*, 1980, **33**, 1783 (*isol, pmr*)

3,14-Dihydroxy-4-methylergost-24(28)-en-23-one D-727

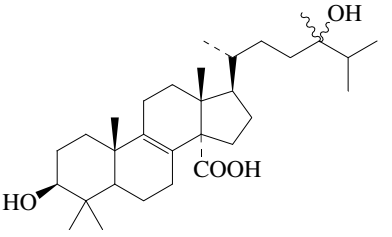
3,14-Dihydroxy-4-methyl-24-methylenecholestan-23-one



$C_{29}H_{48}O_3$ 444.696

(3β,4α,14β)-*form* [623167-71-5]
Constit. of *Nephthea chabroli*.
Cryst.
Mp 150-151°. $[\alpha]_D^{25}$ +66.2 (c, 0.09 in MeOH).
Zhang, W. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1009-1011 (*isol, pmr, cmr*)

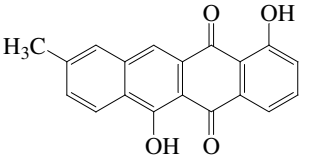
3,24-Dihydroxy-24-methyllanost-8-en-30-oic acid D-728



$C_{31}H_{52}O_4$ 488.749

(3β,24ξ)-*form* [403847-97-2]
Constit. of *Erylus formosus*.
$[\alpha]_D^{20}$ -61.6 (c, 0.13 in $CDCl_3$). λ_{max} 242 (log ϵ 3.1) ($CDCl_3$).
Kubanek, J. *et al., Nat. Prod. Lett.*, 2001, **15**, 275-285 (*isol, pmr, cmr*)

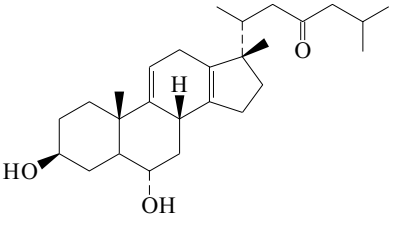
1,6-Dihydroxy-9-methyl-5,12-naphthacenedione D-729



$C_{19}H_{12}O_4$ 304.301
Prod. by the marine-derived *Streptomyces* sp. Mei 6-1,2.

1-Deoxy, 4-hydroxy: 1,11-Dihydroxy-8-methyl-5,12-naphthacenedione
$C_{19}H_{12}O_4$ 304.301
Prod. by the marine-derived *Streptomyces* sp. Mei 6-1,2.
Laatsch, H. *et al., Dissertation*, Univ. of Göttingen, 2005

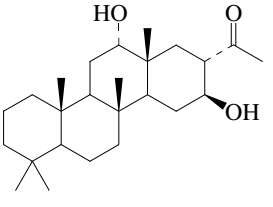
3,6-Dihydroxy-17-methyl-18-norcholesta-9(11),13-dien-23-one D-730



$C_{27}H_{42}O_3$ 414.627

(3β,5α,6α,17βMe)-*form*
Calcarigenin
[71801-49-5]
Artifact produced from hydrolysis of the extracts of *Astropecten aurantiacus* and *Patiriella calcar.*
Oil. $[\alpha]_D$ -2.8 ($CHCl_3$).
De Simone, F. *et al., Tet. Lett.*, 1979, 959

12,16-Dihydroxy-24-methyl-25-nor-24-scalaranone D-731

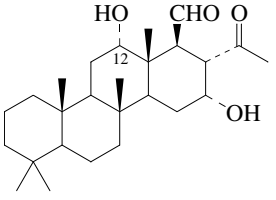


$C_{25}H_{42}O_3$ 390.605

(12α,16β)-*form*

12-Ac: [478364-22-6]
$C_{27}H_{44}O_4$ 432.642
Constit. of a *Phyllospongia* sp. Glass. $[\alpha]_D^{23}$ +41 (c, 1.24 in $CHCl_3$).
Roy, M.C. *et al., J. Nat. Prod.*, 2002, **65**, 1838-1842 (*isol, pmr, cmr*)

12,16-Dihydroxy-24-methyl-24-oxo-25-scalaranal D-732



(12α,16α)-*form*

$C_{26}H_{42}O_4$ 418.615

(12α,16α)-*form*

16-Ac: ***Scalarherbacin A***
[73723-38-3]
$C_{28}H_{44}O_5$ 460.653
Constit. of *Dysidea herbacea*.

Di-Ac: ***Scalarherbacin A acetate***
$C_{30}H_{46}O_6$ 502.69
Constit. of *Dysidea herbacea*.

(12α,16β)-*form*

12-Ac: [478364-18-0]
$C_{28}H_{44}O_5$ 460.653
Constit. of a *Phyllospongia* sp. Cryst. (MeOH aq.).
Mp 185-187°. $[\alpha]_D^{23}$ +138 (c, 0.83 in $CHCl_3$).

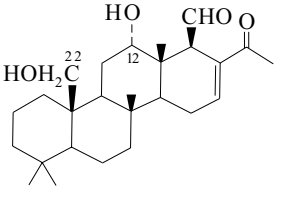
Di-Ac: [478364-24-8]
Constit. of a *Phyllospongia* sp.
Glass. $[\alpha]_D^{23}$ +108 (c, 0.64 in $CHCl_3$).

(12β,16β)-*form*

Constit. of a *Phyllospongia* sp.
Amorph. powder. $[\alpha]_D^{21}$ +82.4 (c, 1 in Py).

12-Ketone, Ac: ***16-Acetoxy-24-methyl-12,24-dioxo-25-scalaranal***
[116331-46-5]
$C_{28}H_{42}O_5$ 458.637
Constit. of *Carteriospongia flabellifera*. Cryst.
Mp 227-229°. $[\alpha]_D$ +135 (c, 0.74 in $CHCl_3$).
Kashman, Y. *et al., Tet. Lett.*, 1979, 3879 (*isol*)
Kazlauskas, R. *et al., Aust. J. Chem.*, 1980, **33**, 1783 (*isol, pmr*)
Schmitz, F.J. *et al., J. Nat. Prod.*, 1988, **51**, 745 (*isol*)
Roy, M.C. *et al., J. Nat. Prod.*, 2002, **65**, 1838-1842 (*Phyllospongia constits*)

12,22-Dihydroxy-24-methyl-24-oxo-16-scalaren-25-al D-733



$C_{26}H_{40}O_4$ 416.6

12α-*form*

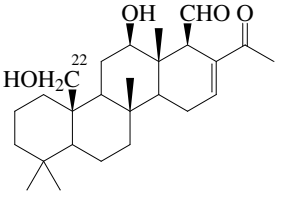
12-Ac: [81575-77-1]
$C_{28}H_{42}O_5$ 458.637
Constit. of a *Lendenfeldia* sp., *Halichondria* sp. and other sponges.
Platelet aggregation inhibitor. Unstable foam. Sol. $CHCl_3$, MeOH; poorly sol. H_2O. λ_{max} 231 (ϵ 11000) (MeOH) (Derep).

22-Aldehyde, 12-Ac: ***12-Acetoxy-24-methyl-24-oxo-16-scalarene-22,25-dial***
[107551-74-6]
$C_{28}H_{40}O_5$ 456.621
Isol. from *Halichondria* spp. and a Dictyoceratid sponge.
Antimicrobial. Amorph.

22-Carboxylic acid: ***12-Hydroxy-24-methyl-24,25-dioxo-16-scalaren-22-oic acid***
[107551-75-7]
$C_{26}H_{38}O_5$ 430.583
Isol. from *Halichondria* spp. and a Dictyoceratid sponge. Amorph. solid. λ_{max} 231 (ϵ 11000) (MeOH) (Derep).

22-Carboxylic acid, 12-ketone: ***24-Methyl-12,24,25-trioxo-16-scalaren-22-oic acid***
[81575-76-0]
$C_{26}H_{36}O_5$ 428.567
Isol. from a *Lendenfeldia* sp. and *Halichondria* sp. Platelet aggregation inhibitor. Antifouling agent. Cryst. (Et_2O/petrol). Sol. $CHCl_3$, MeOH; poorly sol. H_2O.
Mp 251-252°. $[\alpha]_D^{21}$ +33.5 (c, 1 in $CHCl_3$). λ_{max} 231 (ϵ 10800) (MeOH) (Derep).
Kazlauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 51-59 (*12-Ac, 22-carboxylic acid 12-ketone*)
Nakagawa, M. *et al., Tet. Lett.*, 1987, **28**, 431-434 (*22-aldehyde 12-Ac, 22-carboxylic acid*)

12,22-Dihydroxy-24-methyl-24-oxo-16-scalaren-25-al D-734



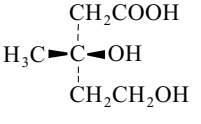
$C_{26}H_{40}O_4$ 416.6

12β-*form*

22-Ac: [264254-86-6]
$C_{28}H_{42}O_5$ 458.637
Constit. of *Glossodoris sedna* and *Glossodoris dalli*. Oil. $[\alpha]_D$ -12.2 (c, 0.1 in $CHCl_3$). λ_{max} 204; 229; 273 (EtOH).
Fontana, A. *et al., J. Nat. Prod.*, 2000, **63**, 527-530 (*isol, pmr, cmr*)

3,5-Dihydroxy-3-methylpentanoic acid D-735

Mevalonic acid. *Hiochic acid*
[150-97-0]



(*R*)–*form*

$C_6H_{12}O_4$ 148.158

(*R*)-*form* [17817-88-8]
Intermed. in biosynth. of terpenoids and steroids.
Oil.

5-Phosphate: 5-Phosphomevalonic acid
[73566-35-5]
$C_6H_{13}O_7P$ 228.138
Isol. from various plants and microorganisms. Active form of mevalonic acid.
Mp 152-154° (as tris-cyclohexylammonium salt).

5-Diphosphate: [1492-08-6]
$C_6H_{14}O_{10}P_2$ 308.118
Intermed. in terpene biosynth. Oil.

5-Diphosphate, dibrucine salt:
Cryst. + $6H_2O$ (Me_2CO aq.). Mp 173-175°.

Di-Ac:
$C_{10}H_{16}O_6$ 232.233
Yellow oil. $[\alpha]_D$ -3.6 (c, 1 in EtOH).

*δ-Lactone: Tetrahydro-4-hydroxy-4-methyl-2*H*-pyran-2-one, 9CI.* ***Mevalonolactone****. Divalonic acid*
[19115-49-2]
[503-48-0]
$C_6H_{10}O_3$ 130.143
Isol. from a marine-derived *Trichoderma harzianum* OUPS-N115. In equilibrium with mevalonic acid, well incorporated into terpenes and steroids. Active against *Enterobacter agglomerans* and *Fusarium avenaceum*. Cryst.
Mp 28°. $Bp_{0.005}$ 100-108°. $[\alpha]_D$ -23.7 (c, 4 in EtOH) (>99% ee).

(*S*)-*form*
Oil.

Nitrile: 4-Cyano-3-methyl-1,3-butanediol. Mevalononitrile. 3,5-Dihydroxy-3-methylpentanenitrile
[176589-60-9]
$C_6H_{11}NO_2$ 129.158
Viscous oil. $[\alpha]_D^{24}$ +1.62 (c, 1.63 in $CHCl_3$) (93% ee).

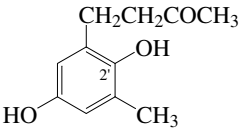
δ-Lactone: [19022-60-7]
Cryst. Mp 28°. $[\alpha]_D^{26}$ +22.8 (c, 10 in EtOH).

(±)-*form* [690-72-2]

δ-Lactone: [674-26-0]
Prod. by *Lactobacillus plantarum*. Active against *Enterobacter agglomerans* and *Fusarium avenaceum*.
Mp 27-28°. $Bp_{0.1}$ 110°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1153B (*nmr*)
Eberle, M. *et al., Helv. Chim. Acta*, 1960, **43**, 1508-1513 (*abs config*)
Dugan, R.E. *et al., Anal. Biochem.*, 1968, **22**, 249-259 (*lactone, glc*)
Cornforth, J.W. *et al., Biochem. Soc. Symp.*, 1970, **29**, 5-15 (*rev*)
Hanson, J.R. *et al., Adv. Steroid Biochem. Pharmacol.*, 1971, **1**, 51-72 (*biosynth*)
Johnson, R.N. *et al., Aust. J. Chem.*, 1971, **24**, 1659-1666 (*lactone, pmr*)
Cornforth, J.W. *et al., Chem. Soc. Rev.*, 1973, **2**, 1-20 (*rev*)
Ellison, R.A. *et al., Synthesis*, 1974, 719 (*(±)-form lactone, synth*)
Huang, F. *et al., J.A.C.S.*, 1975, **97**, 4144-4145 (*R-form, S-form, synth*)
Linares, A. *et al., Biochem. Biophys. Res. Commun.*, 1977, **77**, 974 (*enzymic synth*)
Knotz, J. *et al., Plant Physiol.*, 1977, **60**, 81-85 (*biosynth*)
Hanson, J.R. *et al., Compr. Org. Chem.*, 1979, **5**, 989-1023 (*rev*)
Lewer, P. *et al., J.C.S. Perkin 1*, 1983, 1417-1420 (*(±)-form lactone, synth*)
Pérez, L.M. *et al., Phytochemistry*, 1983, **22**, 431-433 (*biochem*)
Takano, S. *et al., Chem. Comm.*, 1984, 82-83 (*R-form lactone, S-form lactone, synth*)
Bardshiri, E. *et al., J.C.S. Perkin 1*, 1984, 1765-1767 (*(±)-form lactone, synth*)
Bonadies, F. *et al., Tet. Lett.*, 1984, **25**, 5431-5434 (*R-form lactone, S-form lactone, synth*)
Frye, S.V. *et al., J.O.C.*, 1985, **50**, 3402-3404 (*R-form lactone, S-form lactone, synth*)
Mori, K. *et al., Tetrahedron*, 1985, **41**, 557-559 (*R-form lactone, synth*)
Schneider, J.A. *et al., J.O.C.*, 1986, **51**, 1077-1079 (*R-form lactone, S-form lactone, synth*)
Ferraboschi, P. *et al., J.C.S. Perkin 1*, 1987, 2301-2303 (*(±)-form lactone, synth, pmr*)
Sargsyan, M.S. *et al., Khim. Prir. Soedin.*, 1990, **26**, 31-32; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 24-25 (*(±)-form, synth*)
Sugai, T. *et al., Tetrahedron*, 1990, **46**, 3463-3468 (*R-form lactone, synth, pmr*)
Mash, E.A. *et al., J.O.C.*, 1991, **56**, 885-888 (*R-form lactone, synth ir, pmr, cmr*)
Bolitt, V. *et al., J.O.C.*, 1991, **56**, 4238-4240 (*S-form lactone, synth*)
Ray, N.C. *et al., Tetrahedron*, 1992, **48**, 9427-9432 (*R-form lactone, synth*)
Ferraboschi, P. *et al., Synlett*, 1994, 754-756 (*R-form, S-form, lactones, synth*)
Davis, F.A. *et al., J.O.C.*, 1995, **60**, 6148-6153 (*R-form lactone, synth*)
Lakner, F.J. *et al., J.O.C.*, 1996, **61**, 3923-3925 (*R-form, nitrile, lactone, synth, pmr, cmr, ir*)
Kishida, M. *et al., J.C.S. Perkin 1*, 1997, 891-895 (*R-form lactone, synth, pmr, cmr*)
Shimizu, M. *et al., Tetrahedron: Asymmetry*, 1997, **8**, 2519-2522 (*synth*)
Amagata, T. *et al., J. Antibiot.*, 1998, **51**, 33-40 (*lactone, isol*)
Eguchs, T. *et al., J.A.C.S.*, 1998, **120**, 5427-5433 (*lactone*)
Orru, R.V.A. *et al., Synthesis*, 1998, 1259-1263 (*lactone, synth*)
Niku-Paavola, M.-L. *et al., J. Appl. Microbiol.*, 1999, **86**, 29-35 (*isol, activity*)
Buckley, S.L.J. *et al., ARKIVOC*, 2002, **viii**, 46-56 (*lactine, synth*)
Eguchi, T. *et al., Tetrahedron*, 2003, **59**, 6035-6038 (*lactone, synth*)

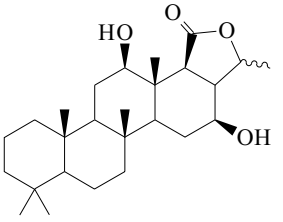
4-(2,5-Dihydroxy-3-methylphenyl)-2-butanone D-736



$C_{11}H_{14}O_3$ 194.23

2′-Me ether: 4-(5-Hydroxy-2-methoxy-3-methylphenyl)-2-butanone
[220676-91-5]
$C_{12}H_{16}O_3$ 208.257
Constit. of *Cystoseira abies*. Oil. λ_{max} 220 (ϵ 8357); 280 (ϵ 2300) (EtOH).
Fernández, J.J. *et al., Nat. Prod. Lett.*, 1998, **12**, 285-291 (*isol, pmr, cmr*)

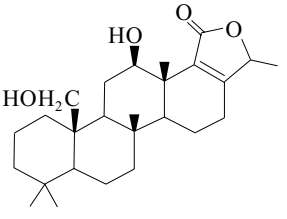
12,16-Dihydroxy-24-methyl-25,24-scalaranolide D-737



$C_{26}H_{42}O_4$ 418.615

(12β,16β)-*form* [135048-59-8]
Metab. of *Phyllospongia dendyi*.
Cryst. ($CHCl_3$/petrol).
Mp 282-285°. $[\alpha]_D^{25}$ +11 (c, 0.13 in $CHCl_3$).
Rao, C.B. *et al., J. Nat. Prod.*, 1991, **54**, 364-371 (*isol, pmr, cmr*)

12,22-Dihydroxy-24-methyl-17-scalaren-25,24-olide D-738

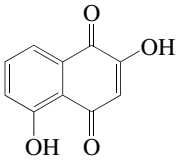


$C_{26}H_{40}O_4$ 416.6

12β-*form*
22-Hydroxy-24-methylscalarolide
[85337-13-9]
Constit. of *Chromodoris sedna*.
Cryst.
Mp 278-279°.
Hochlowski, J.E. *et al., J.O.C.*, 1983, **48**, 1738-1740 (*isol*)

2,5-Dihydroxy-1,4-naphthoquinone, 8CI D-739

2,5-Dihydroxy-1,4-naphthalenedione, 9CI. ***2-Hydroxyjuglone***
[4923-55-1]



$C_{10}H_6O_4$ 190.155
Prod. by *Verticillium dahliae* and the marine-derived *Alternaria* sp. Stamm 6588. Gelation inhibitor for uncured polyester resin. Orange-brown needles (AcOH).
Mp 216-219° dec. λ_{max} 284; 429 ($CHCl_3$) (Berdy). λ_{max} 282; 411 (MeOH-HCl) (Berdy). λ_{max} 261; 386; 410 (ϵ 2300); 470 (EtOH-NaOH) (Berdy).

▶ QL7960000

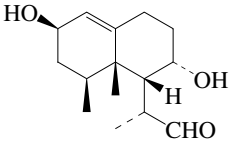
Di-Ac:
$C_{14}H_{10}O_6$ 274.229
Yellow needles (petrol). Mp 152°.

2-Me ether: 5-Hydroxy-2-methoxy-1,4-naphthoquinone
[15127-94-3]
$C_{11}H_8O_4$ 204.182
Constit. of *Juglans mandshurica* and *Platycarya strobilacea*. Cytotoxic agent. Yellow cryst. (MeOH).
Mp 164°. λ_{max} 242 (ϵ 12600); 282 (ϵ 12800); 407 (ϵ 4440); 420 (ϵ 4440) (EtOH) (Berdy).

5-Me ether: 2-Hydroxy-5-methoxy-1,4-naphthoquinone
[71186-96-4]
$C_{11}H_8O_4$ 204.182
Yellow needles. Mp 174-176°.

MacLeod, J.W. *et al., J.O.C.*, 1960, **25**, 36 (*synth*)
Bowie, J.H. *et al., J.A.C.S.*, 1965, **87**, 5094 (*ms*)
Piette, L.H. *et al., J. Phys. Chem.*, 1967, **71**, 29 (*epr, nmr*)
Singh, I. *et al., Tetrahedron*, 1968, **24**, 6053 (*uv*)
Singh, H. *et al., Tetrahedron*, 1969, **25**, 5301 (*synth*)
U.S. Pat., 1970, 3 553 293; *CA*, **74**, 64869 (*use*)
Stipanovic, R.D. *et al., Mycologia*, 1977, **69**, 164 (*isol*)
Kondo, A. *et al., CA*, 1979, **91**, 71707a; 137167h (*2-Me ether, isol*)
Barre, G. *et al., Tet. Lett.*, 1986, **27**, 6197 (*cmr, pmr*)
Kopanski, L. *et al., Annalen*, 1987, 793 (*synth, deriv, uv, ir, pmr, ms*)
Khanna, R.N. *et al., Synth. Commun.*, 1989, **19**, 3151-3157 (*synth*)
Kim, S.-H. *et al., J. Nat. Prod.*, 1998, **61**, 643-645 (*5-Hydroxy-2-methoxynaphthoquinone*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

2,7-Dihydroxy-1(10)-nardosinen-12-al D-740



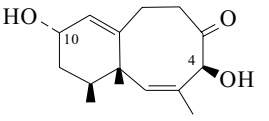
$C_{15}H_{24}O_3$ 252.353

(2β,7α,11R)-form

7-Ac: [77160-92-0]
$C_{17}H_{26}O_4$ 294.39
Constit. of *Lemnalia africana*. Cryst.
Mp 146-148°. $[\alpha]_D$ -127.1 (c, 0.11 in $CHCl_3$).

Bowden, B.F. *et al., Aust. J. Chem.*, 1980, **33**, 2737-2747 (*isol, pmr, cmr*)

4,10-Dihydroxy-2,8-neolemnadien-5-one D-741



$C_{15}H_{22}O_3$ 250.337

(4β,10α)-form

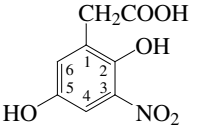
4-Ac: ***4-Acetoxy-10-hydroxy-2,8-neolemnadien-5-one***
$C_{17}H_{24}O_4$ 292.374
Constit. of *Lemnalia africana*. Cryst.
Mp 111-112°. $[\alpha]_D$ +440 (c, 1.16 in $CHCl_3$).

Di-Ac: ***4,10-Diacetoxy-2,8-neolemnadien-5-one***
$C_{19}H_{26}O_5$ 334.411
Constit. of *Lemnalia africana*. Oil. $[\alpha]_D$ +222 (c, 1.1 in $CHCl_3$).

Izac, R.R. *et al., Tetrahedron*, 1981, **37**, 2569

(2,5-Dihydroxy-3-nitrophenyl)acetic acid D-742

2,5-Dihydroxy-3-nitrobenzeneacetic acid

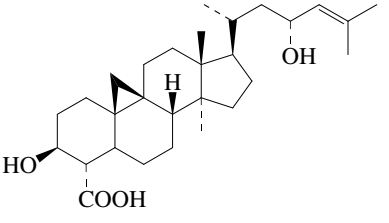


$C_8H_7NO_6$ 213.146

Me ester: [145772-52-7]
$C_9H_9NO_6$ 227.173
Prod. by *Pseudomonas syringae* pv. *papulans* and the marine-derived *Flavobacterium* sp. T436. Plant growth regulator. λ_{max} 280 (log ϵ 2.46); 400 (log ϵ 1.9) (MeOH).

Evidente, A. *et al., Phytochemistry*, 1992, **31**, 4105-4107 (*Me ester, isol*)
Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*Me ester, isol*)

3,23-Dihydroxy-29-norcycloart-24-en-28-oic acid D-743



$C_{29}H_{46}O_4$ 458.68

(3β,23R)-form

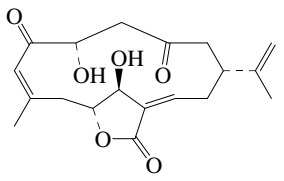
3-O-Sulfate, 28-Me ester: [260559-95-3]
$C_{30}H_{48}O_7S$ 552.771
Constit. of *Tricleocarpa fragilis*. Amorph. solid. $[\alpha]_D^{28}$ +38 (c, 0.8 in MeOH). λ_{max} 200 (MeOH).

23-Ketone: 3-Hydroxy-29-nor-23-oxocycloart-24-en-28-oic acid
$C_{29}H_{44}O_4$ 456.664

23-Ketone, 3-O-sulfate, 28-Me ester: [260559-96-4]
$C_{30}H_{46}O_7S$ 550.755
Constit. of *Tricleocarpa fragilis*. Amorph. solid. $[\alpha]_D^{28}$ +40 (c, 0.03 in MeOH). λ_{max} 239 (MeOH).

Horgen, F.D. *et al., J. Nat. Prod.*, 2000, **63**, 210-216 (*isol, pmr, cmr*)

5,11-Dihydroxy-18-nor-3,6-dioxo-7,12,15-cembratrien-20,10-olide D-744



(1*R*,5*S*,7*Z*,10*R*,11*S*,12*Z*)-*form*

$C_{19}H_{24}O_6$ 348.395

(1*R*,5*S*,7*Z*,10*R*,11*S*,12*Z*)-*form*

5-Et ether: ***1-Epileptocladolide A***
[605659-48-1]
$C_{21}H_{28}O_6$ 376.449
Constit. of *Sinularia leptoclados* and *Sinularia parva*. Oil. $[\alpha]_D^{29}$ -55 (c, 0.4 in $CHCl_3$).

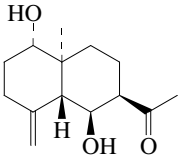
(1*S*,5*S*,7*E*,10*R*,11*S*,12*Z*)-*form*

5-Et ether: ***7E-Leptocladolide A***
[605659-49-2]
$C_{21}H_{28}O_6$ 376.449
Constit. of *Sinularia leptoclados* and *Sinularia parva*. Oil. $[\alpha]_D^{29}$ -63.5 (c, 0.52 in $CHCl_3$).

(1*S*,5*S*,7*Z*,10*R*,11*S*,12*Z*)-*form*

5-Et ether: ***Leptocladolide A***
[605659-47-0]
$C_{21}H_{28}O_6$ 376.449
Constit. of *Sinularia leptoclados* and *Sinularia parva*. Oil. $[\alpha]_D^{25}$ -33.3 (c, 0.24 in $CHCl_3$).
Ahmed, A.F. *et al., Tetrahedron*, 2003, **59**, 7337-7344 (*isol, pmr, cmr*)

1,6-Dihydroxy-13-nor-4(15)-eudesmen-11-one D-745

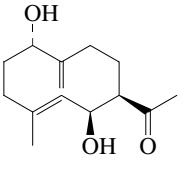


$C_{14}H_{22}O_3$ 238.326

(1α,5β,6β,10α)-*form*

*6-O-(4-Hydroxy-4-methyl-2*E*-pentenoyl):* [865668-56-0]
$C_{20}H_{30}O_5$ 350.454
Constit. of a *Eunicea* sp. Oil. $[\alpha]_D^{25}$ +32 (c, 1.1 in $CHCl_3$). λ_{max} 204 (ε 14000) (MeOH).
Garzón, S.P. *et al., J. Nat. Prod.*, 2005, **68**, 1354-1359 (*Eunicea constit*)

1,6-Dihydroxy-13-nor-4,10(14)-germacradien-11-one D-746



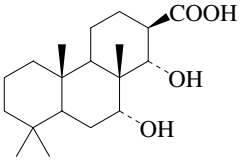
$C_{14}H_{22}O_3$ 238.326

(1α,4*E*,6β)-*form*

*6-O-(4-Hydroxy-4-methyl-2*E*-pentenoyl):* [865668-57-1]
$C_{20}H_{30}O_5$ 350.454
Constit. of a *Eunicea* sp. Oil. $[\alpha]_D^{25}$ +77.6 (c, 1.2 in $CHCl_3$). λ_{max} 206 (ε 11800) (MeOH).

1-Ketone: 6-Hydroxy-13-nor-4,10(14)-germacradiene-1,11-dione
$C_{14}H_{20}O_3$ 236.31
*1-Ketone, 6-O-(4-hydroxy-4-methyl-2*E*-pentenoyl):* [865668-58-2]
$C_{20}H_{28}O_5$ 348.438
Constit. of a *Eunicea* sp. Oil. $[\alpha]_D^{25}$ +12.3 (c, 1.0 in $CHCl_3$). λ_{max} 206 (ε 13400) (MeOH).
Garzón, S.P. *et al., J. Nat. Prod.*, 2005, **68**, 1354-1359 (*Eunicea constits*)

7,14-Dihydroxy-15-nor-16-isocopalanoic acid D-747



(7α,14α)-*form*

$C_{19}H_{32}O_4$ 324.459

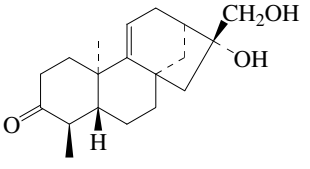
(7α,14α)-*form*

7-Ac, Me ester: ***Aplyroseol 17***
[200437-70-3]
$C_{22}H_{36}O_5$ 380.523
Constit. of *Aplysilla rosea*. Gum.

(7α,14β)-*form*

7-Ac, Me ester: ***Aplyroseol 18***
[200437-72-5]
$C_{22}H_{36}O_5$ 380.523
Constit. of *Aplysilla rosea*. Cryst.
Taylor, W.C. *et al., Aust. J. Chem.*, 1997, **50**, 895-902 (*isol, pmr, cmr*)

16,17-Dihydroxy-19-nor-9(11)-kauren-3-one D-748

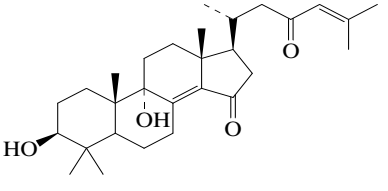


$C_{19}H_{28}O_3$ 304.428

(*ent*-16β)-*form* [873222-60-7]
Constit. of *Bruguiera sexangula* var. *rhynchopetala*.
Amorph. solid. $[\alpha]_D^{20}$ +52.3 (c, 0.15 in $CHCl_3$).
Bao, S. *et al., Helv. Chim. Acta*, 2005, **88**, 2757-2763 (*Bruguiera sexangula constit*)

3,9-Dihydroxy-30-norlanosta-8(14),24-diene-15,23-dione D-749

3,9-Dihydroxy-4,4-dimethylcholesta-8(14),24-diene-15,23-dione



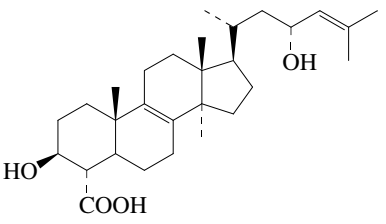
$C_{29}H_{44}O_4$ 456.664

(3β,9α)-*form*

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]: ***Sarasinoside L***
[865369-07-9]
$C_{62}H_{98}N_2O_{28}$ 1319.453

Constit. of *Melophlus sarassinorum*. Yellow amorph. solid. $[\alpha]_D^{20}$ -10.2 (c, 0.5 in MeOH). λ_{max} 249 (MeOH).
Dai, H.-F. *et al., J. Nat. Prod.*, 2005, **68**, 1231-1237 (*Sarasinoside L*)

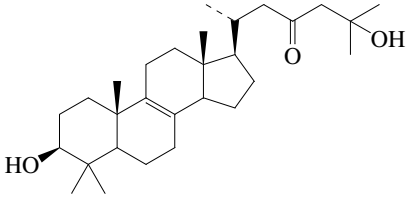
3,23-Dihydroxy-29-norlanosta-8,24-dien-28-oic acid D-750



$C_{29}H_{46}O_4$ 458.68

(3β,23*R*)-*form*
3-O-*Sulfate, 28-Me ester:* [260560-41-6]
$C_{30}H_{48}O_7S$ 552.771
Constit. of *Tricleocarpa fragilis*. Amorph. solid. $[\alpha]_D^{23}$ +53.5 (c, 0.11 in MeOH). λ_{max} 210 (MeOH).
23-Ketone: 3-Hydroxy-29-nor-23-oxolanosta-8,24-dien-28-oic acid
$C_{29}H_{44}O_4$ 456.664
23-Ketone, 3-O-*sulfate, 28-Me ester:* [260560-42-7]
$C_{30}H_{46}O_7S$ 550.755
Constit. of *Tricleocarpa fragilis*. Amorph. solid. $[\alpha]_D^{28}$ +36 (c, 0.1 in MeOH). λ_{max} 239 (MeOH).
Horgen, F.D. *et al., J. Nat. Prod.*, 2000, **63**, 210-216 (*isol, pmr, cmr*)

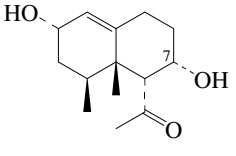
3,25-Dihydroxy-30-norlanost-8-en-23-one D-751
3,25-Dihydroxy-4,4-dimethylcholest-8-en-23-one



$C_{29}H_{48}O_3$ 444.696

3β-*form*
3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Sarasinoside J***
[865369-05-7]
$C_{62}H_{102}N_2O_{27}$ 1307.485
Constit. of *Melophlus sarassinorum*. Yellow amorph. solid. $[\alpha]_D^{20}$ -9.8 (c, 0.05 in MeOH). λ_{max} 202 (MeOH).
Dai, H.-F. *et al., J. Nat. Prod.*, 2005, **68**, 1231-1237 (*Sarasinoside J*)

2,7-Dihydroxy-13-nor-1(10)-nardosinen-11-one D-752



(2α,7α)-*form*

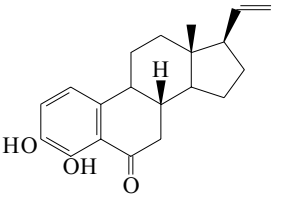
$C_{14}H_{22}O_3$ 238.326

(2α,7α)-*form*
Laevinol B
[874384-35-7]
Constit. of *Lemnalia laevis*.
$[\alpha]_D^{25}$ -132 (c, 0.2 in $CHCl_3$).
7-Formyl: ***Laevinol A***
[874384-34-6]
$C_{15}H_{22}O_4$ 266.336
Constit. of *Lemnalia laevis*.
$[\alpha]_D^{25}$ -173 (c, 0.4 in $CHCl_3$).
7-Ketone: 2-Hydroxy-13-nor-1(10)-nardosinene-7,11-dione. ***Laevinol E***
[874384-38-0]
$C_{14}H_{20}O_3$ 236.31
Constit. of *Lemnalia laevis*.
$[\alpha]_D^{25}$ -145 (c, 0.1 in $CHCl_3$).

(2α,7β)-*form*
Laevinol C
[874384-36-8]
Constit. of *Lemnalia laevis*.
$[\alpha]_D^{25}$ -98 (c, 0.1 in $CHCl_3$).

(2β,7α)-*form*
Laevinol D
[874384-37-9]
Constit. of *Lemnalia laevis*.
$[\alpha]_D^{25}$ -136 (c, 0.3 in $CHCl_3$).
7-Formyl: [77160-97-5]
$C_{15}H_{22}O_4$ 266.336
Constit. of *Lemnalia africana*.
Bowden, B.F. *et al., Aust. J. Chem.*, 1980, **33**, 2737-2747 (*Lemnalia africana constit*)
El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 1749-1753 (*Laevinols A-E*)

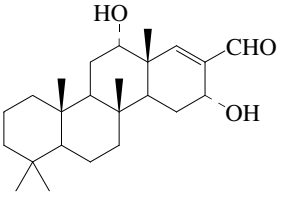
3,4-Dihydroxy-19-norpregna-1,3,5(10),20-tetraen-6-one D-753



$C_{20}H_{24}O_3$ 312.408

3-O-*[4-Acetyl-6-deoxy-β-L-altropyranoside]:* ***Hapaioside***
[159397-70-3]
$C_{28}H_{36}O_8$ 500.588
Constit. of *Cribrochalina olemda*. Amorph. solid. $[\alpha]_D^{20}$ -34.8 (c, 0.028 in MeOH).
Yeung, B.K.S. *et al., Tetrahedron*, 1994, **50**, 12593 (*isol, pmr, cmr*)

12,16-Dihydroxy-25-nor-17-scalaren-24-al D-754
[186803-31-6]



(12α,16α)-*form*

$C_{24}H_{38}O_3$ 374.562

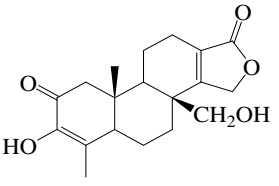
(12α,16α)-*form*
12-Ac: ***Norscalaral B***
$C_{26}H_{40}O_4$ 416.6
Constit. of *Cacospongia scalaris*. Amorph. powder. $[\alpha]_D$ +5.2 (c, 0.4 in $CHCl_3$). λ_{max} 222 (ε 6252) (MeOH).

(12α,16β)-*form*

12-Ac: ***Norscalaral A***
[186803-30-5]
$C_{26}H_{40}O_4$ 416.6
Constit. of *Cacospongia scalaris*. Amorph. powder. $[\alpha]_D$ +48.5 (c, 0.2 in $CHCl_3$). λ_{max} 225 (ϵ 4913) (MeOH).
Rueda, A. *et al., J.O.C.*, 1997, **62**, 1481-1485 (*isol, pmr, cmr*)

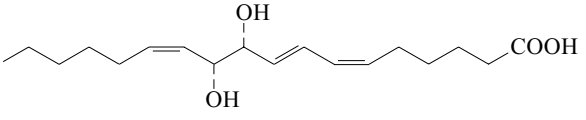
3,17-Dihydroxy-19-nor-3,13-spongiadiene-2,16-dione D-755

Zimoclactone B
[384828-98-2]



$C_{19}H_{24}O_5$ 332.396
Constit. of *Spongia zimocca* ssp. *irregularia*. Cryst. (EtOH). Mp 274-275°. $[\alpha]_D^{25}$ -11 (c, 0.011 in EtOH).
Zeng, L.-M. *et al., Huaxue Xuebao*, 2001, **59**, 1675-1679 (*isol, pmr, cmr, cryst struct*)

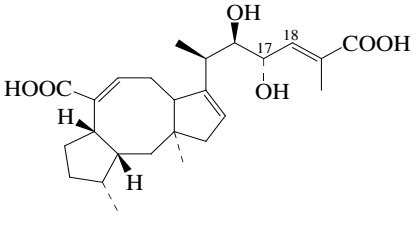
10,11-Dihydroxy-6,8,12-octadecatrienoic acid D-756



$C_{18}H_{30}O_4$ 310.433

(6*Z*,8*E*,10*R,11*R**,12*Z*)-*form*** [121979-39-3]
Isol. from the red alga *Farlowia mollis*.
Oil (as di-Ac, Me ester). λ_{max} 234 (log ϵ 4.224) (no solvent reported) (di-Ac, Me ester).
Solem, M.L. *et al., Lipids*, 1989, **24**, 256 (*isol, uv*)

16,17-Dihydroxy-7,13,18-ophiobolatriene-21,24-dioic acid D-757

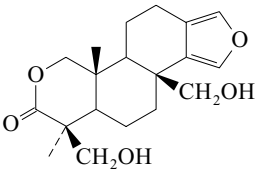


$C_{25}H_{36}O_6$ 432.556

(16*R*,17*S*,18*E*)-*form*
Halorosellinic acid
[373623-06-4]
Isol. from the marine fungus *Halorosellinia oceanica*.
Cryst. $[\alpha]_D^{29}$ +20.67 (c, 0.59 in MeOH). λ_{max} 207 (MeOH).
17-Deoxy: 16-Hydroxy-7,13,18-ophiobolatriene-21,24-dioic acid. ***17-Dehydroxyhalorosellinic acid***
$C_{25}H_{36}O_5$ 416.556
Constit. of *Halorosellinia oceanica*. Cryst. $[\alpha]_D^{28}$ +42.42 (c, 0.066 in MeOH). λ_{max} 210 (MeOH).
Chinworrungsee, M. *et al., Bioorg. Med. Chem. Lett.*, 2001, **11**, 1965-1969 (*Halorosellinic acid*)
Chinworrungsee, M. *et al., J.C.S. Perkin 1*, 2002, 2473-2476 (*17-deoxy*)

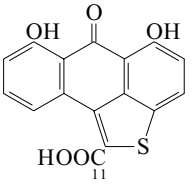
17,19-Dihydroxy-2-oxa-13(16),14-spongiadien-3-one D-758

[130574-79-7]



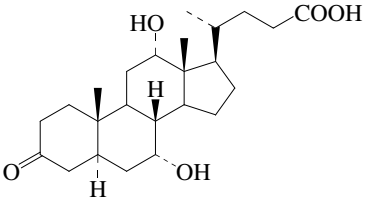
$C_{19}H_{26}O_5$ 334.411
Constit. of a *Spongia* sp. Gum.
Gunasekera, S.P. *et al., J.O.C.*, 1991, **56**, 1250 (*isol, pmr, cmr*)

5,7-Dihydroxy-6-oxo-6*H*-anthra[1,9-*bc*]thiophene-1-carboxylic acid D-759



$C_{16}H_8O_5S$ 312.302
Me ester: [138685-33-3]
$C_{17}H_{10}O_5S$ 326.329
Constit. of the bryozoan *Dakaira subovoidea*. Hypolipaemic agent.
Mp 230-235°.
*11-Alcohol: 5,7-Dihydroxy-1-(hydroxymethyl)-6*H*-anthra[1,9-bc]thiophen-6-one, 9CI*
[138685-32-2]
$C_{16}H_{10}O_4S$ 298.319
Constit. of *Dakaira subovoidea*. Hypolipaemic. Antioxidant.
Mp 260°. λ_{max} 220 (ϵ 24700); 231 (ϵ 23100); 285 (ϵ 8400); 327 (ϵ 4500); 366 (ϵ 4500); 420 (ϵ 9000); 434 (ϵ 4800) (EtOH) (Berdy).
Shindo, T. *et al., Experientia*, 1993, **49**, 177 (*isol, struct*)
Kelly, T.R. *et al., Org. Lett.*, 2000, **2**, 2351-2352 (*synth*)

7,12-Dihydroxy-3-oxocholan-24-oic acid D-760



(5α,7α,12α)-*form*

$C_{24}H_{38}O_5$ 406.561

(5α,7α,12α)-*form*
3-Ketoallocholic acid
[16265-24-0]
Pheromone of sea lamprey (*Petromyzon marinus*).
Me ester: [14772-92-0]
Cryst. (Me_2CO aq.). Mp 156-157° (150-152°). $[\alpha]_D^{23}$ +43 (c, 2 in MeOH).
Me ester, oxime: [15073-84-4]
Needles. Mp 205-206°. $[\alpha]_D^{25}$ +58.7 (c, 0.91 in MeOH).
Di-Ac, Me ester: [15111-23-6]
Mp 132-133°. $[\alpha]_D$ +45 (c,0.98 in $CHCl_3$).

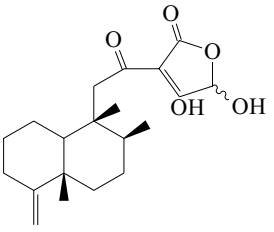
(5β,7α,12α)-*form* [2304-89-4]
Cryst. (EtOAc). Mp 218-220°. $[\alpha]_D$ +41 (MeOH).

Me ester: [14772-99-7]
Mp 181-183°.

Di-Ac, Me ester: Mp 203° (200-201°).

Shaw, R. *et al., J. Chromatogr.*, 1980, **202**, 347 (*hplc*)
Dayal, B. *et al., Steroids*, 1980, **35**, 81 (*cd*)
Iida, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 1934 (*ester*)
Tohma, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 2890 (*ester*)
Riva, S. *et al., J.O.C.*, 1986, **51**, 2902; 1988, **53**, 88
Zhu, X. *et al., Can. J. Chem.*, 1987, **65**, 2447 (*ester*)
Kirk, D.N. *et al., J.C.S. Perkin 2*, 1990, 1567 (*pmr*)
Yun, S.-S. *et al., Steroids*, 2003, **68**, 297-304 (*3-Ketoallocholic acid*)

14,15-Dihydroxy-12-oxo-4(18),13-clerodadien-16,15-olide D-761



$C_{20}H_{28}O_5$ 348.438

15ξ-*form*

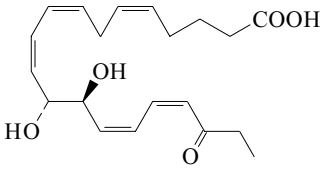
14-Me ether: 15-Hydroxy-14-methoxy-12-oxo-4(18),13-clerodadien-16,15-olide. ***Smenotronic acid***
[228575-24-4]
$C_{21}H_{30}O_5$ 362.465
Constit. of a *Smenospongia* sp. Solid. λ_{max} 224 (ϵ 18200) (no solvent reported).

15-Me ether: 14-Hydroxy-15-methoxy-12-oxo-4(18),13-clerodadien-16,15-olide. ***Dactyltronic acid***
$C_{21}H_{30}O_5$ 362.465
Constit. of *Dactylospongia elegans*. Solid. $[\alpha]_D^{25}$ -4 (c, 3.5 in $CHCl_3$). λ_{max} 294 (EtOH) (Berdy).

[158243-19-7, 158243-20-0]

López, M.D. *et al., J. Nat. Prod.*, 1994, **57**, 992 (*Dactyltronic acid*)
Bourguet-Kondracki, M.-L. *et al., Tet. Lett.*, 1999, **40**, 3149-3150 (*Smenotronic acid*)

12,13-Dihydroxy-18-oxo-5,8,10,14,16-eicosapentaenoic acid D-762

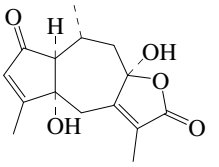


$C_{20}H_{28}O_5$ 348.438

(5*Z*,8*Z*,10*Z*,12*R,13*S**,14*Z*,16*Z*)-*form***

Di-Ac, Me ester: [135405-21-9]
$C_{25}H_{34}O_7$ 446.539
Constit. of the red alga *Gracilariopsis lemaneiformis*.
$[\alpha]_D^{23}$ -2.4 (c, 0.12 in MeOH). λ_{max} 236 (ϵ 23000) (MeOH).
Jiang, Z.D. *et al., Phytochemistry*, 1991, **30**, 1187 (*isol*)

5,8-Dihydroxy-2-oxo-3,7(11)-guaiadien-12,8-olide D-763



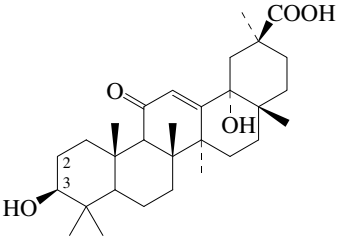
$C_{15}H_{18}O_5$ 278.304

(1α,5α,8α,10α)-*form*

Americanolide I

8-Me ether: ***Methoxyamericanolide I***
[205507-17-1]
$C_{16}H_{20}O_5$ 292.331
Constit. of *Pseudopterogorgia americana*. Oil. $[\alpha]_D^{26}$ -150 (c, 0.2 in $CHCl_3$). λ_{max} 218 (ϵ 14400) (MeOH).
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1998, **61**, 451-455 (*isol, pmr, cmr*)

3,18-Dihydroxy-11-oxo-12-oleanen-30-oic acid D-764



(3β,18α)-*form*

$C_{30}H_{46}O_5$ 486.69

(3β,18α)-*form*

18α-Hydroxyglycyrrhetic acid
[17991-67-2]
Constit. of *Glycyrrhiza uralensis* (Chinese licorice) and *Glycyrrhiza glabra* (licorice).
Cryst. ($CHCl_3$/petrol).
Mp 252-255° dec. $[\alpha]_D^{20}$ +60 (c, 0.17 in Me_2CO).

(3β,18β)-*form*

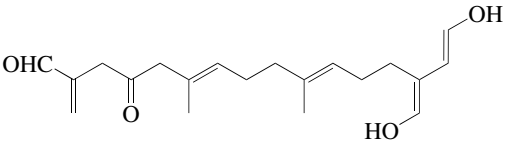
30→18 Lactone, 3-Ac: 3β-Acetoxy-11-oxo-12-oleanen-30,18β-olide. ***Echinolactone A***
[67463-79-0]
$C_{32}H_{46}O_5$ 510.712
Constit. of *Echinopora lamellosa*. Cryst. (MeOH).
Mp 245°.

30→18 Lactone, 3-ketone, 2,2-dibromo: 2,2-Dibromo-3,11-dioxo-12-oleanen-30,18β-olide. ***Echinolactone B***
[94354-98-0]
$C_{30}H_{40}Br_2O_4$ 624.452
Isol. from *Echinopora lamellosa*. Cryst. (MeOH).
Mp 225°.

Canonica, L. *et al., Gazz. Chim. Ital.*, 1967, **97**, 769 (*18α-Hydroxyglycyrrhetic acid*)
Sanduja, R. *et al., Chem. Comm.*, 1984, 1091

1,20-Dihydroxy-13-oxo-1,3(20),6,10,15(17)-phytapentaen-16-al D-765

13-Oxo-6,10,15(17)-phytatriene-1,16,20-trial



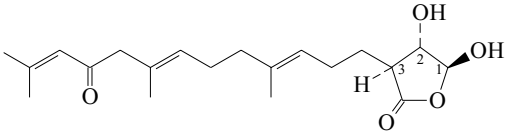
$C_{20}H_{28}O_4$ 332.439

Enolised dialdehyde function at C-1/C-20, notional parent of isolated di-Ac.

(all-*E*)-*form*

Di-Ac: 1,20-Diacetoxy-13-oxo-1,3(20),6,10,15(17)-phytapentaen-16-al
[99695-00-8]
$C_{24}H_{32}O_6$ 416.513
Constit. of the alga *Chlorodesmis fastigiata*. λ_{max} 249 (ϵ 15800) (MeOH).
Paul, V.J. *et al., Phytochemistry*, 1985, **24**, 2239-2243 (*isol, pmr, cmr*)

1,2-Dihydroxy-13-oxo-6,10,14-phytatrien-20,1-olide D-766



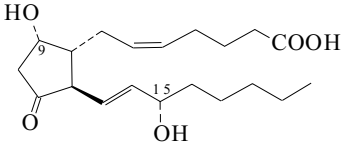
(1β,2α,3α*H*,6*E*,10*E*)–*form*

$C_{20}H_{30}O_5$ 350.454

(1β,2α,3α*H*,6*E*,10*E*)-*form* [136624-29-8]
Constit. of *Bifurcaria bifurcata*.

(1β,2α,3β*H*,6*E*,10*E*)-*form* [136734-93-5]
Constit. of *Bifurcaria bifurcata*.
Hougaard, L. *et al., Tet. Lett.*, 1991, **32**, 3577 (*isol, pmr, cmr*)

9,15-Dihydroxy-11-oxo-5,13-prostadienoic acid D-767



(5*Z*,9*S*,13*E*,15*S*)–*form*

$C_{20}H_{32}O_5$ 352.47Log P 1.77 (calc).

(5*Z*,9*S*,13*E*,15*S*)-*form*

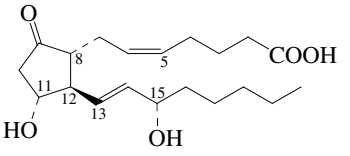
Prostaglandin D_2. *PGD_2*
[41598-07-6] Metab. of PGH_2. Found in human tissues, isol. from *Plexaura homomalla*. Bronchoconstrictor, inhibits platelet aggregation. Cryst.
Mp 68°.
▶ Exp. reprod. effects (low dose). UK7930000

13,14-Dihydro, 15-ketone: 9-Hydroxy-11,15-dioxo-5-prostenoic acid
[59894-07-4]
$C_{20}H_{32}O_5$ 352.47
PGD_2 metab.

[118594-01-7, 118594-29-9, 118594-30-2, 118594-31-3]

Hayashi, M. *et al., J.O.C.*, 1973, **38**, 2115 (*synth, ir, pmr*)
Jones, R.L. *et al., Br. J. Pharmacol.*, 1976, **56**, 339p (*biochem*)
Anderson, N.H. *et al., Prostaglandins*, 1977, **14**, 61 (*synth*)
Watanabe, T. *et al., Arch. Biochem. Biophys.*, 1982, **216**, 372 (*biosynth*)
Stehle, R.G. *et al., Methods Enzymol.*, 1982, **86**, 436 (*rev*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 8094
Bundy, G.L. *et al., J. Med. Chem.*, 1983, **26**, 790 (*synth, pharmacol*)
Collington, E.W. *et al., Tet. Lett.*, 1983, **24**, 3125 (*synth*)
Cepa, S.R. *et al., Prostaglandins*, 1984, **27**, 645 (*ms*)
Suzuki, M. *et al., Tet. Lett.*, 1984, **25**, 1383 (*synth*)
Whittle, B.J.R. *et al., Adv. Exp. Med. Biol.*, 1985, **192**, 109 (*rev, props*)
Cainelli, G. *et al., Tetrahedron*, 1985, **41**, 1385 (*synth*)
Ogawa, Y. *et al., J.O.C.*, 1986, **51**, 1625 (*synth*)
Eur. Pat., 1988, 281 239; *CA*, **110**, 75151y (*synth, pmr*)
Giles, H. *et al., Prostaglandins*, 1988, **35**, 277 (*rev*)
Therapeutic Applications of Prostaglandins, (eds. Vane, J.R. *et al*), E. Arnold, 1993, (*pharmacol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, POC275

11,15-Dihydroxy-9-oxo-5,13-prostadienoic acid, 9CI D-768



(5*Z*,8*R*,11*R*,12*R*,13*E*,15*S*)-form

$C_{20}H_{32}O_5$ 352.47Log P 1.77 (calc).

(5*Z*,8*R*,11*R*,12*R*,13*E*,15*R*)-*form*

15-Epiprostaglandin E_2
[38873-82-4]
[31660-13-6 ((±)-form), 31687-35-1 (Me ester)]
Isol. from *Plexaura homomalla*.
Oil (as Me ester).

15-Ac, Me ester:
$C_{23}H_{36}O_6$ 408.534
Isol. from the coral *Plexaura homomalla*.

(5*Z*,8*R*,11*R*,12*R*,13*E*,15*S*)-*form*

Prostaglandin E_2. *PGE_2*. *Dinoprostone, BAN, INN, JAN, USAN. Dinopron EM. Enzaprost E. Medullin. Minprostin E_2. Prostarmon E. Prostenon. Prostin E_2. U 12062*
[363-24-6]
Present in mammalian tissues, also in invertebrates such as *Modiolus demissus*, *Gracilaria verrucosa*, *Gracilaria chorda*, in which it arises by a different biosynthetic route. Occurs in *Gracilaria lichenoides*, *Gracilaria asiatica*, *Phascolosoma japonica*, *Haliotis ovina*, *Crenomytilus grayanus*, *Stichopus japonicus*, *Distolasterias nippon*, *Halocynthia auranticum* and *Seriola quinqueradiata*. Most common and biologically active of mammalian prostaglandins. Oxytocic, abortifacient and vasodilator. Luteolytic agent. Cryst.
Mp 66-68°. $[\alpha]_D^{26}$ -61 (c, 1 in THF).
▶ Adverse gastrointestinal and cardiovascular effects reported when used therapeutically. Human and exp. reprod. effects (low doses). Exp. teratogen. LD_{50} (rat, orl) 500 mg/kg. UK8000000

Me ester: [31753-17-0]
Oil.

15-Ac, Me ester:
$C_{23}H_{36}O_6$ 408.534
Isol. from *Plexaura homomalla*.

1,15-Lactone: [62410-93-9]
$C_{20}H_{30}O_4$ 334.455
Isol. from the nudibranch *Tethys fimbria*. Cryst. (Et_2O/pentane). Mp 76.5-77.5°. $[\alpha]_D^{20}$ -185 (c, 0.15 in $CHCl_3$).

1,15-Lactone, 11-Ac: [62410-96-2]
$C_{22}H_{32}O_5$ 376.492
Isol. from *Tethys fimbria*.

(5*E*,8*R*,11*R*,12*R*,13*E*,15*S*)-*form*

(5E)-Prostaglandin E_2
[36150-00-2]
Plates (Et_2O/hexane). Mp 76-77°. $[\alpha]_D$ -66 (c, 0.983 in EtOH) (c, 0.903 in $CHCl_3$).
▶ Exp. teratogen.

(5*Z*,8*R*,11*S*,12*R*,13*E*,15*S*)-*form*

11-Epiprostaglandin E_2. 11-epi-*PGE_2*
[38310-90-6]
Oil. $[\alpha]_D^{25}$ -26 (c, 0.0076 in EtOH).

(5*Z*,8*S*,11*R*,12*R*,13*E*,15*S*)-*form*

8-Epiprostaglandin E_2. 8-Isoprostaglandin E_2

[27415-25-4]

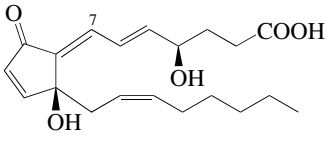
[31660-17-0 ((±)-form)]

Cryst. powder.

[38873-84-6]

Bergström, S. *et al., Biochim. Biophys. Acta*, 1964, **90**, 207 (*biosynth*)
Corey, E.J. *et al., J.A.C.S.*, 1969, **91**, 5675-5677 (*E_2, synth*)
Corey, E.J. *et al., Tet. Lett.*, 1970, 307 (*synth*)
Light, R.J. *et al., Eur. J. Biochem.*, 1972, **28**, 232-240 (*15-Epi-E_2, isol*)
Bundy, G.L. *et al., J.A.C.S.*, 1972, **94**, 2124 (*synth*)
Horton, E.W. *et al., Proc. R. Soc. London, B*, 1972, **182**, 411 (*rev*)
Floyd, D.M. *et al., Tet. Lett.*, 1972, 3269-3272 (*synth*)
Von Euler, U.S. *et al., Arch. Int. Pharmacodyn. Ther.*, 1973, **202**, 295 (*rev, pharmacol*)
Heather, J.B. *et al., Tet. Lett.*, 1973, 2313 (*synth*)
Sih, C.J. *et al., J.A.C.S.*, 1975, **97**, 865 (*synth*)
Uekama, K. *et al., Chem. Lett.*, 1977, 1389 (*cd*)
Schneider, W.P. *et al., J.A.C.S.*, 1977, **99**, 1222 (*synth, ms*)
Andersen, N.H. *et al., Prostaglandins*, 1977, **14**, 61-101 (*synth*)
Van Dyk, J.M. *et al., Drugs of Today (Barcelona)*, 1978, **14**, 74 (*rev*)
Chen, S.-M.L. *et al., J.O.C.*, 1978, **43**, 3450 (*synth, ir, pmr, cmr, ms*)
Nakamura, N. *et al., Tet. Lett.*, 1978, 1549 (*synth, pmr*)
Newton, R.F. *et al., J.C.S. Perkin 1*, 1979, 2789-2792 (*synth*)
De Titta, G.T. *et al., Acta Cryst. B*, 1980, **36**, 638-645 (*cryst struct, conformn*)
Freas, W. *et al., J. Exp. Biol.*, 1980, **84**, 169-185 (*E_2, isol*)
Howard, C. *et al., J.C.S. Perkin 1*, 1981, 2049 (*Me ester, synth, ir, pmr*)
Stehle, R.G. *et al., Methods Enzymol.*, 1982, **86**, 436-458 (*rev*)
Donaldson, R.E. *et al., J.O.C.*, 1983, **48**, 2167 (*synth*)
Tanaka, T. *et al., Tet. Lett.*, 1985, **26**, 5575 (*synth*)
Suzuki, M. *et al., J.A.C.S.*, 1988, **110**, 4718-4726 (*synth*)
Johnson, C.R. *et al., J.A.C.S.*, 1988, **110**, 4726 (*synth, pmr, cmr*)
Cimino, G. *et al., Tet. Lett.*, 1989, **30**, 3589 (*isol, derivs*)
Murray, C.K. *et al., J.A.C.S.*, 1990, **112**, 5660 (*synth*)
Therapeutic Applications of Prostaglandins, (eds., Vane, J. R. *et al*), E. Arnold, 1993, (*pharmacol*)
Nicolaou, K.C. *et al., Classics in Total Synthesis, Targets, Strategies, Methods*, VCH, 1996, 65 (*bibl, synth*)
Karotchenko, O.D. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1999, **35**, 612-615 (*marine, occur*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1414
Furstner, A. *et al., Angew. Chem., Int. Ed.*, 2000, **39**, 1234-1236 (*1,15-lactone*)
Taber, D.F. *et al., Tetrahedron*, 2000, **56**, 5991-5994 (*synth*)
Hua, Y. *et al., CA*, 2001, **134**, 126145 (*Gracilaria asiatica constit*)
Schneider, C. *et al., Lipids*, 2002, **37**, 217-221 (*15-Ac Me ester*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, DVJ200

4,12-Dihydroxy-9-oxo-5,7,10,14-prostatetraenoic acid D-769



(4*R*,5*E*,7*E*,12*S*,14*Z*)-*form*

$C_{20}H_{28}O_5$ 348.438

(4*R*,5*E*,7*E*,12*S*,14*Z*)-*form*

[184175-58-4]

Isol. from the soft coral *Clavularia viridis*.

Solid. $[\alpha]_D^{25}$ -92.3 (c, 0.2 in MeOH). λ_{max} 233 (log ϵ 4.03); 301 (log ϵ 4.01) (MeOH).

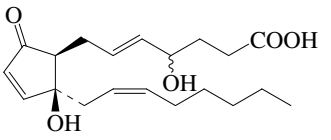
(4*R*,5*E*,7*Z*,12*S*,14*Z*)-*form* [184175-59-5]

Isol. from *Clavularia viridis*.

Solid. $[\alpha]_D^{26}$ -83.2 (c, 0.1 in MeOH). λ_{max} 233 (log ϵ 4.14); 305 (log ϵ 4.11) (EtOH).

Watanabe, K. *et al., J. Nat. Prod.*, 1996, **59**, 980 (*isol, uv, ir, cd, pmr, cmr, ms*)

4,12-Dihydroxy-9-oxo-5,10,14-prostatrienoic acid D-770



$C_{20}H_{30}O_5$ 350.454

(4ξ,5*E*,8*S*,12*S*,14*Z*)-*form*

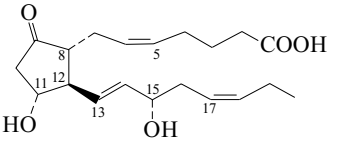
Di-Ac, Me ester:

$C_{25}H_{36}O_7$ 448.555

Isol. from *Clavularia viridis*. Viscous oil. $[\alpha]_D^{25}$ +22.8 (c, 0.08 in $CHCl_3$). Config. not confirmed. λ_{max} 208 (ϵ 8900) (MeOH).

Watanabe, K. *et al., Chem. Pharm. Bull.*, 2003, **51**, 909-913 (*isol, pmr, cmr*)

11,15-Dihydroxy-9-oxo-5,13,17-prostatrienoic acid, 9CI D-771



$C_{20}H_{30}O_5$ 350.454

(5*Z*,8*R*,11*R*,12*R*,13*E*,15*S*,17*Z*)-*form*

Prostaglandin E_3. PGE_3

[802-31-3]

Constit. of sheep prostate gland and human menstrual fluid.

Cryst. (hexane/Et_2O).

Mp 84.5-85.5°. $[\alpha]_D^{24}$ -50 (c, 1 in THF).

1,15-Lactone: [123314-22-7]

$C_{20}H_{28}O_4$ 332.439

Constit. of the nudibranch *Tethys fimbria*.

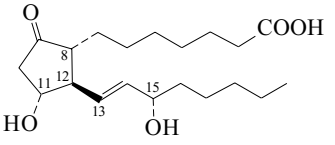
1,15-Lactone, 11-Ac: [123314-21-6]

$C_{22}H_{30}O_5$ 374.476

Constit. of *Tethys fimbria*.

Bergström, S. *et al., Ark. Kemi*, 1963, **19**, 563 (*isol, ms*)
Samuelsson, B. *et al., J.A.C.S.*, 1963, **85**, 1878 (*struct, pmr*)
Axen, U. *et al., Chem. Comm.*, 1970, 602 (*synth*)
Corey, E.J. *et al., J.A.C.S.*, 1971, **93**, 1490 (*synth*)
Cimino, G. *et al., Tet. Lett.*, 1989, **30**, 3589-3592 (*isol, derivs*)
Okamoto, S. *et al., Tet. Lett.*, 1989, **30**, 4379 (*synth*)

11,15-Dihydroxy-9-oxo-13-prostenoic acid, 9CI D-772



(8*R*,11*R*,12*R*,13*E*,15*S*)–*form*

$C_{20}H_{34}O_5$ 354.486

Log P 2.26 (calc).

Approved for clinical use in several European countries (1999)

(8*R*,11*R*,12*R*,13*E*,15*S*)-*form*

(8α,11α,15α)-form. Prostaglandin E_1. PGE_1. ***Alprostadil, BAN, INN, USAN****. Alprox-TD. Caverject. Femprox. Minprog. Muse. Prostin VR. Prostivas. U 10136*

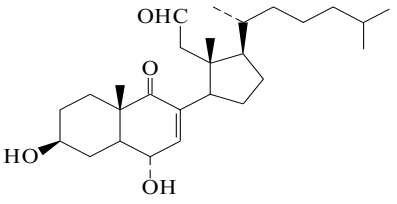
[745-65-3]

Constit. of sheep's prostate and calf thymus glands. Occurs in semen and human blood serum. Isol. from the gorgonian *Plexaura homomalla*. Vasodilator and inhibitor of platelet aggregation. Cryst. (EtOAc).

Mp 114-116.5°. $[\alpha]_D^{24}$ -53.2 (c, 0.977 in THF).
▶ LD_{50} (rat, orl) 228 mg/kg. Human and exp. reprod. effects. Exp. teratogen (low doses). GY4569800

Miyares Cao, C.M. *et al., Rev. Cubana Farm.*, 1974, **8**, 97-126 (*Pleaxaura homomalla constit*)

3,6-Dihydroxy-9-oxo-9,11-secocholest-7-en-11-al D-773

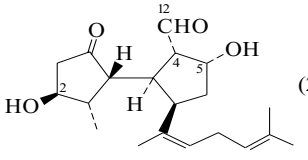


$C_{27}H_{44}O_4$ 432.642

(3β,6α)-*form* [137888-09-6]
Constit. of *Spongia officinalis*.
Amorph. powder. $[\alpha]_D$ +5 (c, 0.2 in $CHCl_3$).

Migliuolo, A. *et al., Tetrahedron*, 1991, **47**, 7937 (*isol, pmr, cmr, synth*)

2,5-Dihydroxy-10-oxo-4,10-seco-13(15),17-spatadien-12-al D-774



(2*S*,4*S*,5*R*,13(15)*Z*)–*form*

$C_{20}H_{30}O_4$ 334.455

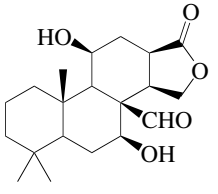
(2*S*,4*S*,5*R*,13(15)*Z*)-*form*
2-Ac: [81575-05-5]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Dilophus marginatus*. Oil. $[\alpha]_D^{20}$ +125 (c, 1.2 in $CHCl_3$).
2,5-Di-Ac: ***Dilkamural***
[245511-34-6]
$C_{24}H_{34}O_6$ 418.529
Constit. of *Dilophus okamurae*. Oil. $[\alpha]_D^{27}$ +32 (c, 0.3 in $CHCl_3$).

(2*S*,4*S*,5*S*,13(15)*Z*)-*form*
5-Ac: [81575-06-6]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Dilophus marginatus*. Oil. $[\alpha]_D^{20}$ +65 (c, 0.5 in CCl_4).

(2*S*,4ξ,5ξ,13(15)*Z*)-*form*
12-Alcohol, 2,5-di-Ac: ***2,5-Diacetoxy-12-hydroxy-4,10-seco-13(15),17-spatadien-10-one***
[81575-08-8]
$C_{24}H_{36}O_6$ 420.545
Isol. from *Dilophus marginatus*. Viscous oil. $[\alpha]_D^{20}$ +158 (c, 1.1 in CCl_4).

Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 129-144 (*Dilophus marginatus constits*)
Ninomiya, M. *et al., J.O.C.*, 1999, **64**, 5436-5440 (*Dilkamural*)

7,11-Dihydroxy-16-oxo-17-spongianal D-775

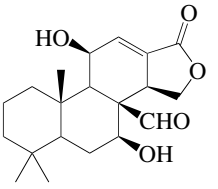


$C_{20}H_{30}O_5$ 350.454

(7β,11β)-*form*
Di-Ac: [189457-14-5]
$C_{24}H_{34}O_7$ 434.528
Constit. of *Chromodoris hamiltoni*. Oil. $[\alpha]_D^{21}$ +38 (c, 0.19 in $CHCl_3$).

McPhail, K. *et al., Tetrahedron*, 1997, **53**, 4655-4660 (*isol, pmr, cmr*)

7,11-Dihydroxy-16-oxo-12-spongien-17-al D-776

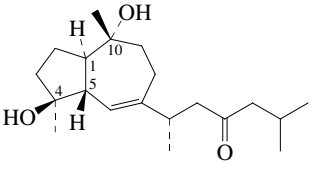


$C_{20}H_{28}O_5$ 348.438

(7β,11β)-*form*
Di-Ac: [189457-26-9]
$C_{24}H_{32}O_7$ 432.513
Constit. of *Chromodoris hamiltoni*. Oil. $[\alpha]_D^{21}$ +97 (c, 0.18 in $CHCl_3$).

McPhail, K. *et al., Tetrahedron*, 1997, **53**, 4655-4660 (*isol, pmr, cmr*)

4,10-Dihydroxy-7-pachydictyen-13-one D-777



(1α,4β,5β,10α,11*S*)-*form*

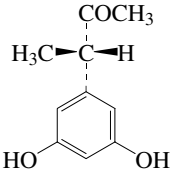
$C_{20}H_{34}O_3$ 322.487

(1α,4β,5β,10α,11*S*)-*form*
Hydratoxeniolone
[107168-61-6]
Constit. of a *Xenia* sp.
Oil. $[\alpha]_D^{22}$ +8 (c, 0.3 in $CHCl_3$).

(1β,4α,5α,10β,11*S*)-*form*
Hydratoisoxeniolone
[107168-62-7]
Constit. of a *Xenia* sp.
Oil. $[\alpha]_D^{22}$ -4.7 (c, 1.2 in $CHCl_3$).

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4641-4652 (*isol, pmr, cmr*)

3-(3,5-Dihydroxyphenyl)-2-butanone D-778



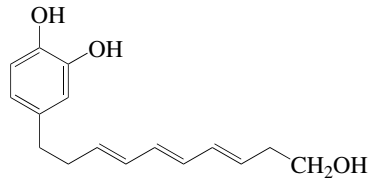
$C_{10}H_{12}O_3$ 180.203

(*S*)-*form* [218166-80-4]
Prod. by a *Coniothyrium* sp. from the sponge *Ectyoplasia ferox*. Oil. $[\alpha]_D^{20}$ +124 (c, 0.12 in $CHCl_3$). λ_{max} 217 (ε 27900); 280 (ε 1170) (EtOH).

Höller, U. *et al., J. Nat. Prod.*, 1999, **62**, 114-118 (*isol, uv, ir, pmr, cmr, ms*)

10-(3,4-Dihydroxyphenyl)-3,5,7-decatrien-1-ol D-779

4-(10-Hydroxy-3,5,7-decatrienyl)-1,2-benzenediol



$C_{16}H_{20}O_3$ 260.332

(*all-E*)-*form*

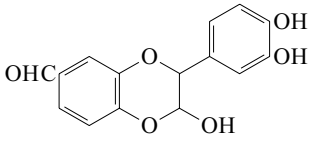
1,3′-Di-Ac: [206666-59-3]
$C_{20}H_{24}O_5$ 344.407
Alarm pheromone of marine mollusc *Haminoea callidegenita*.

1,4′-Di-Ac: [206666-58-2]
$C_{20}H_{24}O_5$ 344.407
Alarm pheromone of *Haminoea callidegenita*.

Tri-Ac: [206666-57-1]
$C_{22}H_{26}O_6$ 386.444
Alarm pheromone of *Haminoea callidegenita*.

Spinella, A. *et al., Tet. Lett.*, 1998, **39**, 2005-2008 (*isol, pmr, cmr*)
Izzo, I. *et al., Tet. Lett.*, 2000, **41**, 3975-3978 (*synth*)

3-(3,4-Dihydroxyphenyl)-2,3-dihydro-2-hydroxy-1,4-benzodioxin-6-carboxaldehyde D-780

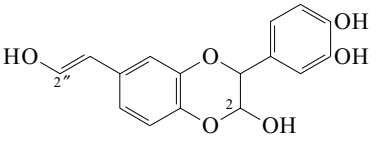


$C_{15}H_{12}O_6$ 288.256

2-Sulfate: [160014-88-0]
$C_{15}H_{12}O_9S$ 368.32
Isol. from the sponge *Jaspis* sp. Inducer of larval metamorphosis in ascidians, e.g. *Halocynthia roretzi*. Racemic. λ_{max} 228 (ϵ 13400); 271 (ϵ 7700) (MeOH) (Berdy).

Tsukamoto, S. *et al., Tetrahedron*, 1994, **50**, 13583

3-(3,4-Dihydroxyphenyl)-2,3-dihydro-6-(2-hydroxyethenyl)-1,4-benzodioxin-2-ol D-781

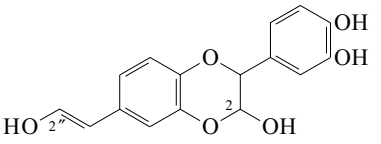


$C_{16}H_{14}O_6$ 302.283
Enol.

2,2′′-Di-O-sulfate: [160014-86-8]
$C_{16}H_{14}O_{12}S_2$ 462.411
Isol. from the sponge *Jaspis* sp. Inducer of larval metamorphosis in ascidians, e.g. *Halocynthia roretzi*. Racemic. λ_{max} 261 (ϵ 13800) (MeOH) (Berdy).

Tsukamoto, S. *et al., Tetrahedron*, 1994, **50**, 13583

3-(3,4-Dihydroxyphenyl)-2,3-dihydro-7-(2-hydroxyethenyl)-1,4-benzodioxin-2-ol D-782



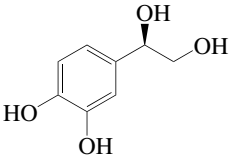
$C_{16}H_{14}O_6$ 302.283
Enol.

2,2′′-Di-O-sulfate: [160014-87-9]
$C_{16}H_{14}O_{12}S_2$ 462.411
Isol. from the sponge *Jaspis* sp. Inducer of larval metamorphosis in ascidians, e.g. *Halocynthia roretzi*. Racemic. λ_{max} 215 (ϵ 17200); 263 (ϵ 7700) (MeOH) (Berdy).

Tsukamoto, S. *et al., Tetrahedron*, 1994, **50**, 13583

1-(3,4-Dihydroxyphenyl)-1,2-ethanediol, 8CI D-783

4-(1,2-Dihydroxyethyl)-1,2-benzenediol, 9CI. 3,4-Dihydroxyphenylglycol
[3343-19-9]



(*R*)-*form*

$C_8H_{10}O_4$ 170.165

(ξ)-*form*

Constit. of the fruit of *Olea europeae* (olives).

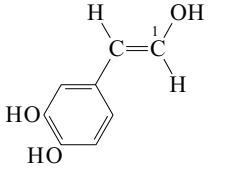
2-Et ether, 1-O-[α-L-rhamnopyranosyl-(1→3)-[3,4-dihydroxy-E-cinnamoyl-(→4)]-β-D-glucopyranoside]: ***Ilicifolioside A****. β-Ethoxyacteoside*
[599205-57-9]
$C_{31}H_{40}O_{16}$ 668.647
Constit. of the aerial parts of *Acanthus ilicifolius*. Amorph. powder. $[\alpha]_D^{25}$ -72 (c, 0.8 in MeOH).

[55254-51-8, 64998-12-5, 64998-13-6, 326491-80-9]

Benigni, J.D. *et al., J. Med. Chem.*, 1963, **6**, 607 (*synth*)
Bianchi, G. *et al., Phytochemistry*, 1994, **35**, 1335 (*isol*)
Wu, J. *et al., Phytochemistry*, 2003, **63**, 491-495 (*isol, pmr, cmr, Ilicifolioside A*)

2-(3,4-Dihydroxyphenyl)ethenol D-784

2-(3,4-Dihydroxyphenyl)vinyl alcohol. 3,4-Dihydroxystyryl alcohol



(*E*)−*form*

$C_8H_8O_3$ 152.149
Enol-form of 3,4-Dihydroxyphenylacetaldehyde.

(*E*)-*form*

1-O-Sulfate: 3,4-Dihydroxystyryl sulfate. ***Jaspisin***
[158080-67-2]
$C_8H_8O_6S$ 232.214
Isol. from the marine sponge *Jaspis* sp. Sea urchin gamete inhibitor. Endoproteinase inhibitor. Inhibits the fertilisation of *Asterina pectinifera*. Viscous oil (as Na salt). λ_{max} 204; 260 (ϵ 25704); 300 (ϵ 9900) (MeOH) (Berdy). λ_{max} 211 (ϵ 19600); 258 (ϵ 10300); 298 (ϵ 3400) (pH 4.5 buffer) (Berdy). λ_{max} 208 (ϵ 42655);

243 (ϵ 19054); 298 (ϵ 14454); 350 (ϵ 12882) (MeOH/NaOH) (Berdy).

1-O-*Sulfate, salt with* N,N-*dimethylguanidine (1:1):* ***(E)-Narain*** [158080-68-3]
Isol. from a *Jaspis* sp. Induces metamorphosis of the larvae of *Halocynthia roretzi*. Induces metamorphosis in ascidian larvae. λ_{max} 213 (ϵ 14200); 262 (ϵ 7800); 305 (ϵ 3000) (no solvent reported) (Derep). λ_{max} 207 (ϵ 16800); 260 (ϵ 8800); 299 (ϵ 3500) (MeOH) (Derep).

1-O-*(3,4-Dihydroxy*-E-*cinnamoyl):* [99816-39-4]
$C_{17}H_{14}O_6$ 314.294
Isol. from the callus cultures of *Lavandula angustifolia* (lavender). Associated with chelate formation. Oil.

1-Me ether: 4-(2-Methoxyethenyl)-1,2-benzenediol
[112750-53-5]
$C_9H_{10}O_3$ 166.176
Oil.

Tri-Me ether: 1,2-Dimethoxy-4-(2-methoxyethenyl)benzene, 9CI
[136114-02-8]
$C_{11}H_{14}O_3$ 194.23
Oil. $Bp_{0.1}$ 104°.

(Z)-form

1-O-*Sulfate:* ***Isojaspisin***
[158080-69-4]
$C_8H_8O_6S$ 232.214
Isol. from a *Jaspis* sp. Inhibits hatching of sea urchin embryos. Viscous oil (as Na salt). λ_{max} 212 (ϵ 18000); 257 (ϵ 12700); 296 (ϵ 3400) (H_2O at pH 4.5) (Derep).

1-O-*Sulfate, salt with* N,N-*dimethylguanidine (1:1):* ***(Z)-Narain*** [158080-70-7]
Isol. from a *Jaspis* sp. Induces metamorphosis in ascidian larvae. λ_{max} 207 (ϵ 16800); 260 (ϵ 8800); 299 (ϵ 3500) (MeOH) (Derep). λ_{max} 212 (ϵ 14200); 261 (ϵ 7800); 305 (ϵ 3000) (MeOH) (Berdy).

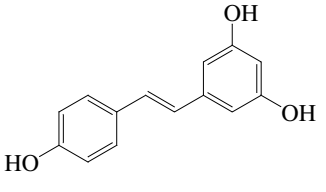
1-O-*(3,4-Dihydroxy*-E-*cinnamoyl):* ***Nepetoidin B*** [55486-06-1]
Isol. from *Perilla frutescens* (perilla), *Plectranthus caninus* and the callus cultures of *Lavandula angustifolia* (lavender). Constit. of many of the Lamiaceae.
Yellow cryst.
Mp 183-185° (dec.). λ_{max} 213 (ϵ 20900); 250 (ϵ 15900); 340 (ϵ 19100) (EtOH) (Berdy).

[157961-35-8, 157961-40-5, 158080-70-7]

Kunz, H. *et al., Chem. Ber.*, 1983, **116**, 220 (*deriv*)
Banthorpe, D.V. *et al., Phytochemistry*, 1985, **24**, 2677-2680 (*caffeoyl derivs*)
Nakanishi, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1772-1774 (*caffeoyl derivs*)
Comins, D.L. *et al., Tet. Lett.*, 1991, **32**, 2995 (*deriv*)
Ohta, S. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1752 (*Jaspisin*)
Ikegami, S. *et al., J. Biol. Chem.*, 1994, **269**, 23262 (*Jaspisin*)
Cerda-Garcia-Rojas, C.M. *et al., J. Nat. Prod.*, 1994, **57**, 1758 (*isol*)
Ohta, S. *et al., Tet. Lett.*, 1994, **35**, 4579 (*Isojaspisin*)
Tsukamoto, S. *et al., Tet. Lett.*, 1994, **35**, 5873 (*Narain*)
Grayer, R.J. *et al., Phytochemistry*, 2003, **64**, 519-528 (*Nepetoidin B, occur*)

1-(3,5-Dihydroxyphenyl)-2-(4-hydroxyphenyl)ethylene D-785

5-[2-(4-Hydroxyphenyl)ethenyl]-1,3-benzenediol, 9CI. 3,4′,5-Stilbenetriol, 8CI. 3,4′,5-Trihydroxystilbene. ***Resveratrol***
[36469-58-6]



(*E*)-*form*

$C_{14}H_{12}O_3$ 228.247

(E)-form [501-36-0]
Phytoalexin from *Veratrum grandiflorum* (roots), *Pinus sibirica* (bark), *Vitis vinifera* and *Arachis hypogaea*. Also from *Polygonum* and *Nothofagus* spp., *Cudrania javanensis*, *Eucalyptus* spp. and other plants in the Leguminosae , Liliaceae , Myrtaceae, Gramineae and other families. Fungicide, bactericide. Resveratrol in red wines has been postulated to be associated with beneficial health effects. Shows tyrosinase inhibitory activity. Nutriceutical with a positive influence on blood lipid profile. Inhibits cell adhesion molecules (ICAM-1 and VCAM-1). Cryst. (MeOH aq.). Sol. EtOH, Me_2CO; poorly sol. H_2O.
Mp 265-267°. λ_{max} 218 (ϵ 21400); 227 (sh) (ϵ 14800); 307 (ϵ 27500); 320 (ϵ 26900) (EtOH).

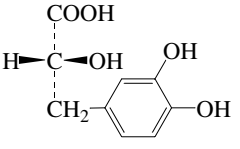
Tri-Ac: ***Triacetylresveratrol****. Resveratrol triacetate*
[42206-94-0]
$C_{20}H_{18}O_6$ 354.359
Isol. from the sponge *Kirkpatrickia variolosa*. Cryst. ($CHCl_3$/MeOH).
Mp 130° (118.5-119.5°). λ_{max} 300 (ϵ 25120); 312 (ϵ 24550); 326 (ϵ 14450) (EtOH).

[33626-08-3, 54443-64-0]

Jayatilake, G.S. *et al., J. Nat. Prod.*, 1995, **58**, 1958 (*isol, triacetate, pmr, cmr*)
Commodari, F. *et al., Magn. Reson. Chem.*, 2005, **43**, 567-572 (*pmr, cmr, cryst struct*)
Farina, A. *et al., Nat. Prod. Res.*, 2006, **20**, 247-252 (*synth*)

3-(3,4-Dihydroxyphenyl)-2-hydroxypropanoic acid D-786

α,3,4-Trihydroxybenzenepropanoic acid, 9CI. 3-(3,4-Dihydroxyphenyl)lactic acid. Danshensu
[23028-17-3]



(*R*)-*form*

$C_9H_{10}O_5$ 198.175

(R)-form [76822-21-4]
Constit. of Coptidis Rhizoma (root of *Coptis chinensis*) and *Salvia miltiorrhiza*. Coronary vasodilator. Prisms ($EtOAc/C_6H_6$).
Mp 84-87°. $[\alpha]_D^{18}$ +10.8 (c, 3.7 in MeOH).

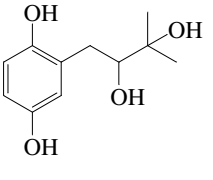
2-O-*Sulfate: 3-(3,4-Dihydroxyphenyl)-2-(sulfooxy)propanoic acid.* ***Tichocarpol B***
$C_9H_{10}O_8S$ 278.239
Isol. from the red alga *Tichocarpus crinitus*. Amorph. solid. $[\alpha]_D^{28}$ +5.9 (c, 0.34 in H_2O).

[42085-50-7, 67810-33-7, 67920-52-9, 69339-96-4, 81075-52-7]

Ishii, T. *et al., J. Nat. Prod.*, 2004, **67**, 1764-1766 (*Tichocarpol B*)

1-(2,5-Dihydroxyphenyl)-3-methyl-2,3-butanediol D-787

2-(2,3-Dihydroxy-3-methylbutyl)-1,4-benzenediol, 9CI. ***Antibiotic F 11334A1****. F 11334A1*

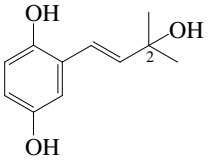


$C_{11}H_{16}O_4$ 212.245

(+)-form
Prod. by the marine-derived *Acremonium murorum*. Inhibitor of membrane-bound neutral sphingomyelinase. Powder. $[\alpha]_D^{23}$ +36 (c, 0.2 in MeOH). λ_{max} 216 (sh) (ϵ 4580); 226 (sh) (ϵ 3690); 293 (ϵ 3050) (MeOH).

Tanaka, M. *et al., J. Antibiot.*, 1999, **52**, 827-830 (*isol, struct*)
Abdel-Lateff, A. *et al., J. Nat. Prod.*, 2002, **65**, 1605-1611 (*isol, pmr, cmr*)

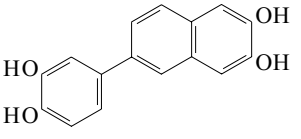
4-(2,5-Dihydroxyphenyl)-2-methyl-3-buten-2-ol D-788
2-(3-Hydroxy-3-methyl-1-butenyl)-1,4-benzenediol. ***Antibiotic F 11334B$_1$.*** *F 11334B$_1$*



$C_{11}H_{14}O_3$ 194.23
Prod. by the marine-derived *Acremonium murorum*. Inhibitor of membrane-bound neutral sphingomyelinase. Powder. λ_{max} 248 (sh) (ϵ 8500); 322 (ϵ 3840) (MeOH).

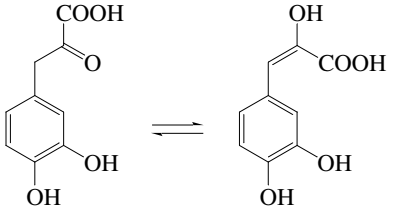
2-Me ether: 2-(3-Methoxy-3-methyl-1-butenyl)-1,4-benzenediol. ***Antibiotic F 11334B$_2$.*** *F 11334B$_2$*
$C_{12}H_{16}O_3$ 208.257
Prod. by *Acremonium murorum*. Inhibitor of membrane-bound neutral sphingomyelinase. Powder. λ_{max} 249 (sh) (ϵ 9860); 325 (ϵ 4490) (MeOH).
Tanaka, M. *et al., J. Antibiot.*, 1999, **52**, 827-830

6-(3,4-Dihydroxyphenyl)-2,3-naphthalenediol D-789
[160014-89-1]



$C_{16}H_{12}O_4$ 268.268
Isol. from the sponge *Jaspis* sp. Artifact.
Tsukamoto, S. *et al., Tetrahedron*, 1994, **50**, 13583 (*isol, ir, pmr, cmr*)

3-(3,4-Dihydroxyphenyl)-2-oxopropanoic acid D-790
3,4-Dihydroxy-α-oxobenzenepropanoic acid, 9CI. (3,4-Dihydroxyphenyl)pyruvic acid, 8CI. 3-(3,4-Dihydroxyphenyl)-2-hydroxy-2-propenoic acid
[4228-66-4]

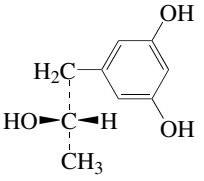


$C_9H_8O_5$ 196.159
Enol-form predominates. Cryst. (H_2O). Mp 190°.

(E)-enol-form
Me ester: [214534-57-3]
$C_{10}H_{10}O_5$ 210.186
Constit. of the alga *Caulerpa taxifolia*.

(Z)-enol-form
Me ester: [214534-55-1]
Constit. of *Caulerpa taxifolia*.
Billek, G. *et al., Monatsh. Chem.*, 1961, **92**, 343-351 (*synth*)
Harley-Mason, J. *et al., Tetrahedron*, 1963, **19**, 65-76 (*synth*)
Haavaldsen, R. *et al., Acta Chem. Scand.*, 1967, **21**, 1095-1097 (*synth*)
Mancini, I. *et al., Helv. Chim. Acta*, 1998, **81**, 1681-1691 (*Me ester, isol, pmr, cmr*)

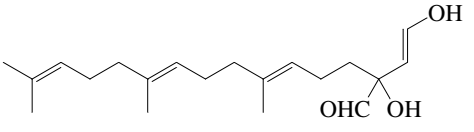
1-(3,5-Dihydroxyphenyl)-2-propanol D-791
5-(2-Hydroxypropyl)-1,3-benzenediol. ***Orcinotriol***



$C_9H_{12}O_3$ 168.192

(S)-form [205648-56-2]
Metab. of the sponge-derived yeast *Aureobasidium pullulans*. $[\alpha]_D^{25}$ +6 (c, 1.1 in MeOH). λ_{max} 208 (ϵ 17000); 276 (ϵ 5900) (MeOH).
Shigemori, H. *et al., J. Nat. Prod.*, 1998, **61**, 696-698 (*isol, uv, ir, pmr, cmr*)

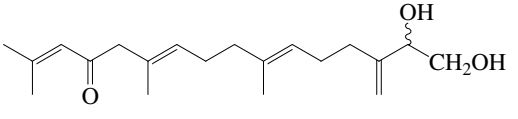
1,3-Dihydroxy-1,6,10,14-phytatetraen-20-al D-792



$C_{20}H_{32}O_3$ 320.471

(1E,3ξ,6E,10E)-form
Di-Ac: [849475-55-4]
$C_{24}H_{36}O_5$ 404.545
Constit. of *Caulerpa brownii*.
Handley, J.T. *et al., Aust. J. Chem.*, 2005, **58**, 39-46 (*isol, pmr, cmr*)

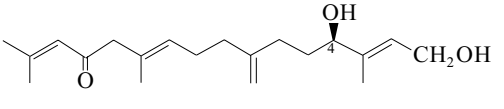
1,2-Dihydroxy-3(20),6,10,14-phytatetraen-13-one D-793
15,16-Dihydroxy-2,6,10-trimethyl-14-methylene-2,6,10-hexadecatrien-4-one



$C_{20}H_{32}O_3$ 320.471

(2ξ,6E,10E)-form [869481-98-1]
Constit. of *Bifurcaria bifurcata*.
Oil. $[\alpha]_D^{25}$ +3 (c, 0.52 in $CHCl_3$).
Ortalo-Magné, A. *et al., Phytochemistry*, 2005, **66**, 2316-2323 (*Bifurcaria bifurcata constit*)

1,4-Dihydroxy-2,7(19),10,14-phytatetraen-13-one D-794
13,16-Dihydroxy-2,6,14-trimethyl-10-methylene-2,6,14-hexadecatrien-4-one

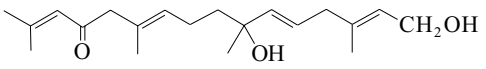


$C_{20}H_{32}O_3$ 320.471

(2E,4R,10E)-form
Constit. of *Cystoseira crinita*.
Oil. $[\alpha]_D$ +96.5 (c, 1 in EtOH).
4-Ketone: 1-Hydroxy-2,7(19),10,14-phytatetraene-4,13-dione. 16-Hydroxy-2,6,14-trimethyl-10-methylene-2,6,14-hexadecatriene-4,13-dione
$C_{20}H_{30}O_3$ 318.455
Constit. of *Cystoseira crinita*. Oil.
Amico, V. *et al., Phytochemistry*, 1981, **20**, 1085

1,7-Dihydroxy-2,5,10,14-phytatetraen-13-one D-795

10,16-Dihydroxy-2,6,10,14-tetramethyl-2,6,11,14-hexadecatetraen-4-one, 9CI

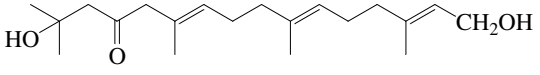


$C_{20}H_{32}O_3$ 320.471

(2*E*,5*E*,7ξ,10*E*)-*form* [79404-60-7]
Constit. of *Cystoseira crinita*.
Oil. $[\alpha]_D$ -16.1 (c, 1 in EtOH).
Amico, V. *et al., Phytochemistry*, 1981, **20**, 1085

1,15-Dihydroxy-2,6,10-phytatrien-13-one D-796

2,16-Dihydroxy-2,6,10,14-tetramethyl-6,10,14-hexadecatrien-4-one

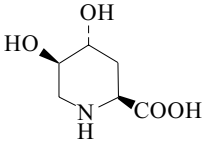


$C_{20}H_{34}O_3$ 322.487

(2*E*,6*E*,10*E*)-*form* [869304-89-2]
Constit. of *Bifurcaria bifurcata*.
Oil.
Ortalo-Magné, A. *et al., Phytochemistry*, 2005, **66**, 2316-2323 (*Bifurcaria bifurcata constit*)

4,5-Dihydroxy-2-piperidinecarboxylic acid D-797

4,5-Dihydroxypipecolic acid



(2*S*,4*R*,5*R*)–*form*

$C_6H_{11}NO_4$ 161.157

(2*S*,4*R*,5*R*)-*form* [59246-13-8]
Isol. from *Julbernardia paniculata*, *Julbernardia globifera* (Leguminosae) and *Brachystegia speciformis.*

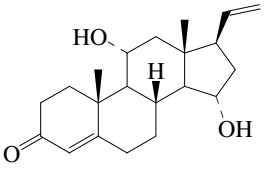
4-Sulfate: 4,5-Dihydroxypipecolic acid 4-sulfate. ***Cribronic acid***
[552866-14-5]
$C_6H_{11}NO_7S$ 241.221
Isol. from the sponge *Cribrochalina olemda*. Glutamate receptor agonist. Fine needles (MeOH aq.). $[\alpha]_D^{18}$ -16.3 (c, 0.24 in H_2O).

(2*S*,4*R*,5*S*)-*form* [59284-78-5]
Constit. of *Calliandra haematocephala* and *Derris elliptica* (Leguminosae).
Mp 239-243° dec. $[\alpha]_D^{20}$ -22.9 (c, 2 in H_2O).

(2*S*,4*S*,5*S*)-*form* [59246-14-9]
From *Calliandra haematocephala, Derris elliptica*, *Isoberlinia tomentosa* and *Isoberlinia angolensis* (Leguminosae).
Cubes (as hydrochloride).
Mp 195-196° (hydrochloride). $[\alpha]_D^{20}$ +24.4 (c, 0.64 in 2*M* HCl) (hydrochloride).

(2ξ,4ξ,5ξ)-*form*
N-*Me: 4,5-Dihydroxy-1-methyl-2-piperidinecarboxylic acid.*
***Glabrin*†**
[35024-30-7]
$C_7H_{13}NO_4$ 175.184
Isol. from seeds of *Pongamia glabra* (Leguminosae). Cryst. ($EtOH/H_2O/Et_2O$).
Mp 290-292° dec. $[\alpha]_D^{20}$ -54.82 (5*M* HCl).
[35024-31-8, 38146-56-4, 63357-05-1, 114297-04-0, 126641-66-5, 126643-94-5]
Kumar, P.S.J. *et al., Tet. Lett.*, 1971, 4451-4454 (*Glabrin*)
Evrard, G. *et al., Cryst. Struct. Commun.*, 1972, **1**, 215-217; 1974, **3**, 61-63 (*cryst struct*)
Marlier, M. *et al., Phytochemistry*, 1972, **11**, 2597-2599; 1976, **15**, 183-185 (*Calliandra haematocephala, Derris elliptica constits*)
Shewry, P.R. *et al., Phytochemistry*, 1976, **15**, 1981-1983 (*2S,4R,5R-form, isol, bibl*)
Bashyal, B.P. *et al., Tetrahedron*, 1987, **43**, 415-422; 423-430 (*synth, ir, pmr, ms*)
Thieme, M. *et al., Synthesis*, 2000, 2051-2059 (*synth, pmr*)
Sakai, R. *et al., J. Nat. Prod.*, 2003, **66**, 784-787 (*Cribronic acid*)

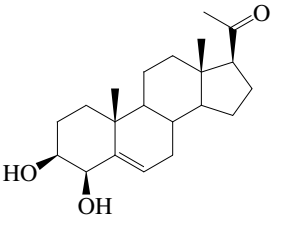
11,15-Dihydroxypregna-4,20-dien-3-one D-798



$C_{21}H_{30}O_3$ 330.466

(11α,15α)-*form*
Di-Ac: [719285-02-6]
$C_{25}H_{34}O_5$ 414.541
Constit. of *Subergorgia mollis.* Cryst.
Mp 100-102°. $[\alpha]_D^{27}$ +61.4 (c, 0.44 in $CHCl_3$). λ_{max} 243 (log ϵ 4.08) (MeOH).
Wu, S.-L. *et al., J. Chin. Chem. Soc. (Taipei)*, 2004, **51**, 205-208; *CA*, **141**, 103421x (*isol, pmr, cmr*)

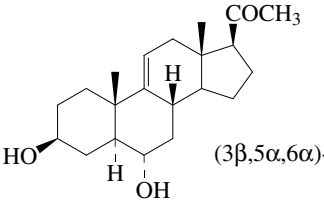
3,4-Dihydroxypregn-5-en-20-one D-799



$C_{21}H_{32}O_3$ 332.482

(3β,4β)-*form*
3-O-*Sulfate:* [122143-90-2]
$C_{21}H_{32}O_6S$ 412.546
Isol. from sponge *Stylopus australis.* Needles (EtOAc/MeOH).
Mp 120-121°. $[\alpha]_D^{25}$ -100 (c, 0.1 in MeOH).
Prinsep, M.R. *et al., J. Nat. Prod.*, 1989, **52**, 657-659

3,6-Dihydroxypregn-9(11)-en-20-one, 9CI D-800



(3β,5α,6α)-*form*

$C_{21}H_{32}O_3$ 332.482

(3β,5α,6α)-*form*
Asterosapogenin I. *Asterone*
[37717-02-5]
Isol. from *Asterias amurensis* and *Acanthaster planci.*
Mp 162-163° Mp 193-196°. $[\alpha]_D^{23}$ +65.2 ($CHCl_3$).

3-O-*Sulfate:* ***3-O-Sulfoasterone***
[290824-47-4]
$C_{21}H_{32}O_6S$ 412.546
Constit. of *Aphelasterias japonica*. Amorph. powder. $[\alpha]_D$ +34.5 (c, 0.32 in MeOH).

3-O-*Sulfate, salt with:* [514828-14-9]
$C_{31}H_{45}NO_8S$ 591.764
Constit. of *Lethasterias nanimensis chelifera*. Amorph. solid. $[\alpha]_D^{25}$ +36.7 (c, 0.3 in MeOH).

6-O-*(6-Deoxy-β-D-glucopyranoside), 3*-O-*sulfate:* ***Forbeside E3***
[129602-19-3]
$C_{27}H_{42}O_{10}S$ 558.689
Isol. from the starfish *Asterias forbesi* and *Aphelasterias japonica*. Shows hemolytic activity. Powder (as Na salt).
Mp 206° (Na salt). $[\alpha]_D^{28}$ -3.5 (c, 0.004 in H_2O). $[\alpha]_D$ +20.9 (c, 0.33 in MeOH).

6-O-*(6-Deoxy-4*-O-*sulfo-β-D-glucopyranoside), 3*-O-*sulfate:* ***Cheliferoside L1***
[143572-73-0]
$C_{27}H_{42}O_{13}S_2$ 638.753
Constit. of *Aphelasterias japonica* and *Lethasterias nanimensis chelifera*. Amorph. powder or cryst. (as di-Na salt).
Mp 159-161° (di-Na salt). $[\alpha]_D$ +21.9 (c, 0.23 in MeOH). CAS no. refers to di-Na salt.

6-O-*[β-D-Galactopyranosyl-(1→3)-β-D-fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Anasteroside B***
[402490-53-3]
$C_{56}H_{90}O_{32}S$ 1307.374
Constit. of *Anasterias minuta*. Amorph. powder.
Mp 228-231°. $[\alpha]_D^{20}$ -8.9 (c, 0.3 in DMSO).

6-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside]:* [73036-18-7]
$C_{50}H_{80}O_{24}$ 1065.168
Mp 275-276.5°. $[\alpha]_D$ +28.5 ($CHCl_3$/MeOH 1:1). Degradn. prod. of, 6-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-[6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate.*

3-O-*[β-D-Fucopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 6*-O-*sulfate:* [865092-63-3]
$C_{49}H_{78}O_{26}S$ 1115.206
Constit. of *Culcita novaeguineae*. Amorph. powder.
Mp 203-204°. $[\alpha]_D^{20}$ +8 (c, 0.15 in MeOH).

6-O-*[β-D-Fucopyranosyl-(1→4)-β-D-fucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Asterosaponin A***
[37217-57-5]
$C_{45}H_{72}O_{22}S$ 997.117
Saponin from the starfish *Asterias amurensis*.

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate:* [161996-22-1]
$C_{49}H_{78}O_{26}S$ 1115.206
Constit. of *Oreaster reticulatus*.

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Novaeguinoside A***
[105404-81-7]
$C_{50}H_{80}O_{26}S$ 1129.232
Constit. of *Culcita novaeguineae*. Powder.
Mp 213-215°. $[\alpha]_D^{20}$ +6 (c, 0.1 in MeOH).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* [72471-58-0]
$C_{50}H_{80}O_{27}S$ 1145.232
Isol. from starfish *Acanthaster planci*. Also in *Luidia maculata* and *Astropecten latespinosus*. Needles (as Na salt).
Mp 214-216° (Na salt). $[\alpha]_D^{23}$ +8 (c, 0.55 in H_2O) (Na salt).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Pectinioside D***
[113322-01-3]
$C_{51}H_{82}O_{27}S$ 1159.259
Constit. of *Asterina pectinifera*. Amorph. powder.
Mp 230-235° dec. $[\alpha]_D$ +15.6 (c, 0.41 in MeOH).

(3β,5α,6α,17β*H*)-*form*
Isoasterone

3-O-*Sulfate, salt with:* [514828-16-1]
$C_{31}H_{45}NO_8S$ 591.764
Constit. of *Lethasterias nanimensis chelifera*. Amorph. solid. $[\alpha]_D^{25}$ -6.7 (c, 0.1 in MeOH).

Yasumoto, T. *et al., Agric. Biol. Chem.*, 1965, **29**, 804-808 (*Asterosaponin A, props*)
Sheikh, Y.M. *et al., J.A.C.S.*, 1972, **94**, 3278-3280 (*Asterosapogenin I, isol, pmr, cd*)
Ikegami, S. *et al., Tet. Lett.*, 1972, 1601-1604 (*Asterosapogenin I, isol, struct*)
ApSimon, J.W. *et al., Can. J. Chem.*, 1973, **51**, 850-855; 1974, **52**, 4113-4116 (*Asterosapogenin I, isol, synth*)
Ikegami, S. *et al., Tetrahedron*, 1973, **29**, 1807-1810 (*Asterosaponin A*)
Smith, D.S.H. *et al., J.C.S. Perkin 1*, 1975, 1751-1753 (*Asterosapogenin I, synth, pmr*)
Ikegami, S. *et al., Tet. Lett.*, 1979, 1769-1772 (*Glycoside B_2 degradation product*)
Komori, T. *et al., Annalen*, 1983, 24-36 (*Acanthaster planci saponin*)
Noguchi, Y. *et al., Annalen*, 1987, 341-348 (*Asterone, cmr*)
Dubois, M.A. *et al., Annalen*, 1988, 495-500 (*Pectinioside D*)
Findlay, J.A. *et al., J. Nat. Prod.*, 1990, **53**, 710-712 (*Forbeside E3*)
Kicha, A.A. *et al., Khim. Prir. Soedin.*, 1991, 520-523; *Chem. Nat. Compd. (Engl. Transl.)*, 1991, **27**, 452-454 (*Cheliferoside L1*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1995, **58**, 10-26 (*Oreaster reticulatus saponin*)
Ivanchina, N.V. *et al., J. Nat. Prod.*, 2000, **63**, 1178-1181 (*Aphelasterias japonica constits, activity*)
Chludil, H.D. *et al., J. Nat. Prod.*, 2002, **65**, 153-157 (*Anasteroside B*)
Kicha, A.A. *et al., Tet. Lett.*, 2003, **44**, 1935-1937 (*Lethasterias salts*)
Tang, H.F. *et al., Chin. Chem. Lett.*, 2005, **16**, 619-622 (*Novaeguinoside A*)
Tang, H.-F. *et al., Planta Med.*, 2005, **71**, 458-463 (*Culcita novaeguineae constit*)

3,17-Dihydroxypregn-5-en-20-one D-801

$C_{21}H_{32}O_3$ 332.482

(3β,17αOH)-*form*
17α-Hydroxypregnenolone
[387-79-1]
A mammalian hormone; also found in ovaries of crayfish *Astacus leptodactylus*.
Cryst. (AcOH).
Mp 273° (225-227°). $[\alpha]_D$ -62 ($CHCl_3$).
▶ TU5548000

[1887-95-2, 2643-02-9, 26040-00-6, 39946-45-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1052A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 577C (*nmr*)
Wilson, H. *et al., Anal. Biochem.*, 1960, **1**, 402 (*uv*)
Fritsch, W. *et al., Chem. Ber.*, 1963, **96**, 68 (*synth, 3β-form*)
Jankowski, K. *et al., Can. J. Chem.*, 1969, **47**, 751; 1968, **46**, 1835 (*pmr*)
Brooks, C.J.W. *et al., Steroids*, 1970, **15**, 283 (*ms*)
Nambara, T. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1937; 1973, **21**, 565 (*synth, ir, pmr*)
Ollivier, F. *et al., Gen. Comp. Endocrinol.*, 1986, **61**, 214-228 (*occur, crayfish*)

2,3-Dihydroxy-1-propanesulfonic acid, 9CI D-802

[10296-76-1]
$HOCH_2CH(OH)CH_2SO_3H$
$C_3H_8O_5S$ 156.159

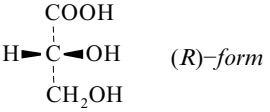
(±)-*form*
Isol. from *Navicula pelliculosa*.

Ba salt:
Cryst. (H_2O).

Friese, H. *et al., Ber.*, 1938, **71**, 1303 (*synth*)
Manecke, G. *et al., Angew. Chem.*, 1958, **70**, 503 (*synth*)
Busby, W.F. *et al., Biochim. Biophys. Acta*, 1966, **121**, 160 (*isol*)
Edmonds, J.S. *et al., J.C.S. Perkin 1*, 1983, 2375 (*cmr, pmr*)

2,3-Dihydroxypropanoic acid, 9CI D-803

Glyceric acid. Glyceronic acid
[473-81-4]



(*R*)–*form*

$C_3H_6O_4$ 106.078

(R)-form
D-form
[6000-40-4]
Isol. from various plants, e.g. *Vicia faba* and cress. Intermed. in plant metabolic cycles. Thick gum. Dec. on dist. Laevorotatory.

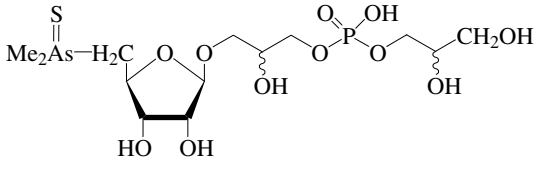
2-O-α-D-Mannopyranoside: ***Digeneaside***
[68005-65-2]
$C_9H_{16}O_9$ 268.22
Isol. from red algae *Alsidium*, *Chondria*, *Laurencia*, *Polysiphonia*, *Halopytis*, *Vidalia* and *Digenea* spp.
Mp 255-270° dec. (as Na salt). $[\alpha]_D^{18}$ +106 (c, 1 in H_2O).

[115136-20-4]

Karrer, P. *et al., Helv. Chim. Acta*, 1924, **7**, 931 (*synth*)
Brewster, P. *et al., Nature (London)*, 1950, **166**, 178 (*abs config*)
Sallach, *et al., J.A.C.S.*, 1952, **74**, 2415 (*synth, bibl*)
Bouveng, H. *et al., Acta Chem. Scand.*, 1955, **9**, 807 (*Digeneaside*)
Biochem. Prep., 1966, **11**, 50 (*synth*)
Barton, D.H.R. *et al., J.C.S.(C)*, 1967, 128 (*synth*)
Kirst, G.O. *et al., Phytochemistry*, 1980, **19**, 1107 (*Digeneaside*)

3-[[(2,3-Dihydroxypropoxy)hydroxyphosphinyl]oxy]-2-hydroxypropyl 5-deoxy-5-(dimethylarsinothioyl)-β-D-ribofuranoside D-804

[761458-56-4]

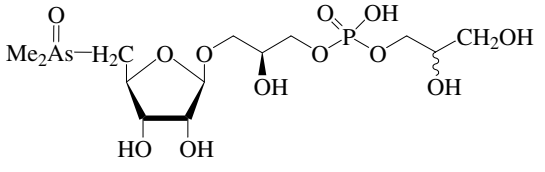


$C_{13}H_{28}AsO_{11}PS$ 498.319
Isol. from canned commercial sea- and freshwater mussels.

Schmeisser, E. *et al., Chem. Comm.*, 2004, 1824-1825
Soeroes, C. *et al., J. Environ. Monit.*, 2005, **7**, 688-692

3-[[(2,3-Dihydroxypropoxy)hydroxyphosphinyl]oxy]-2-hydroxypropyl 5-deoxy-5-(dimethylarsinoyl)-β-D-ribofuranoside, 9CI D-805

[88216-76-6]



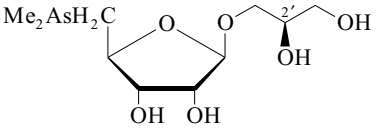
$C_{13}H_{28}AsO_{12}P$ 482.252
Isol. from edible seaweeds *Hizikia fusiforme*, *Sphaerotrichia divaricata*, *Undaria pinnatifida* and *Sargassum latifolia* and from freshwater mussels.

2′,3′-Dihexadecanoyl: [115921-38-5]
$C_{45}H_{88}AsO_{14}P$ 959.077
Isol. from the brown alga *Undaria pinnatifida*.

Morita, M. *et al., Chemosphere*, 1988, **17**, 1147-1152

2,3-Dihydroxypropyl [5-deoxy-5-(dimethylarsino)] ribofuranoside D-806

3-[[5-Deoxy-5-(dimethylarsinoyl)ribofuranosyl]oxy]-1,2-propanediol



$C_{10}H_{21}AsO_6$ 312.194
Where known, the nat. compds. have the β-D-ribo, 2′*R*-config. illus.

As-*Oxide: 2′,3′-Dihydroxypropyl [5-deoxy-5-(demethylarsinyl)]-ribofuranoside*
[103476-61-5]
$C_{10}H_{21}AsO_7$ 328.193
Isol. from brown algae *Laminaria japonica* and *Ecklonia radiata*, giant clam *Tridacna maxima* and various freshwater mussels *Anodonta anatina*, *Dreissena polymorpha*, *Unio pictorum* and *Unio tumidas*. Oil. $[\alpha]_D^{20}$ -2.6 (c, 5.5 in MeOH).

As-*Oxide,* $O^{3'}$*-sulfate:* [88216-77-7]
$C_{10}H_{21}AsO_{10}S$ 408.258
Isol. from kidney of giant clam *Tridacna maxima* and brown algae *Sargassum lacerifolium* and *Hizikia fusiforme*. Cryst.
Mp 163-175°.

As-*Sulfide: 2,3-Dihydroxypropyl 5-deoxy-5-(dimethylarsinothioyl) ribofuranoside*
[761458-55-3]
$C_{10}H_{21}AsO_6S$ 344.26
Isol. from various freshwater mussels *Anodonta anatina*, *Dreissena polymorpha*, *Unio pictorum* and *Unio tumidas*. 2′-Config. not certain.

As-*Sulfide,* $O^{3'}$*-sulfate:* [865197-06-4]
$C_{10}H_{21}AsO_9S_2$ 424.324
Isol. from the gonads and muscles of giant scallop *Pecten maximus*. $O^{2'}$-Config. not determined.

2,3:2′,3′-Diisopropylidene: [103411-73-0]
Oil. $Bp_{0.05}$ 150°. $[\alpha]_D^{19}$ +30.

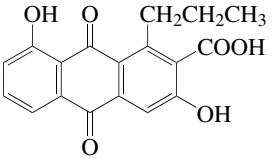
2,3:2′,3′-Diisopropylidene, As-*oxide:* [103411-74-1]
Oil. $[\alpha]_D^{20}$ -7.7.

[77939-93-6]

Edmonds, J.S. *et al., J.C.S. Perkin 1*, 1982, 2989-2993; 1983, 2375-2382; 1987, 577-580 (*oxide, oxide sulfate, isol, cmr, pmr*)
Shibata, Y. *et al., Agric. Biol. Chem.*, 1987, **51**, 391-398 (*oxide, isol, pmr, cmr, hplc*)
McAdam, D.P. *et al., Aust. J. Chem.*, 1987, **40**, 1901-1908 (*oxide, oxide sulfate*)
Francesconi, K.A. *et al., J.C.S. Perkin 1*, 1991, 2707-2716 (*Sargassum lacerifolium constit*)
Edmonds, J.S. *et al., Nat. Prod. Rep.*, 1993, **10**, 421-428 (*oxide, isol, rev*)
Stick, R.V. *et al., Aust. J. Chem.*, 2001, **54**, 181-183 (*oxide, synth*)
Kahn, M. *et al., Environ. Chem.*, 2005, **2**, 171-176 (*As-sulfide O-sulfate*)

3,8-Dihydroxy-1-propylanthraquinone-2-carboxylic acid D-807

9,10-Dihydro-3,8-dihydroxy-9,10-dioxo-1-propyl-2-anthracenecarboxylic acid. ***Antibiotic K 1115A****. K 1115A*
[208525-17-1]

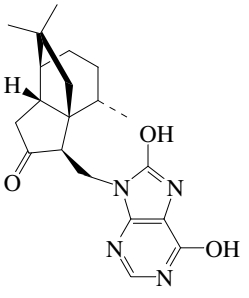


$C_{18}H_{14}O_6$ 326.305
Prod. by *Streptomyces griseorubiginosus* Mer-K1115 and the marine-derived *Streptomyces* sp. FX-58. Binding inhibitor of activator protein-1. Orange rods (MeOH). Sol. DMSO, MeOH; fairly sol. EtOAc, Me_2CO, H_2O. Mp 255-258°. λ_{max} 220 (ϵ 20900); 282 (ϵ 29200); 411 (ϵ 7600) (MeOH) (Berdy). λ_{max} 252 (ϵ 20900); 321 (ϵ 27000); 388 (ϵ 4800); 501 (ϵ 6400) (MeOH/NaOH) (Berdy).

Goto, M. *et al., J. Antibiot.*, 1998, **51**, 539-544; 545-552 (*isol, uv, ir, pmr, cmr, activity*)
Uno, H. *et al., Chem. Lett.*, 2000, 1014-1015 (*synth*)
Huang, Y.-F. *et al., J. Asian Nat. Prod. Res.*, 2006, **8**, 495-498 (*marine isol*)

6-(6,8-Dihydroxy-9-purinyl)suberosanone D-808

[864514-59-0]

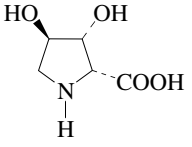


$C_{20}H_{26}N_4O_3$ 370.45
Isol. from *Subergorgia suberosa*. Powder. $[\alpha]_D^{20}$ +28 (c, 0.2 in $CHCl_3$). λ_{max} 212; 264 (MeOH).

Qi, S.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1288-1289 (*isol, pmr, cmr*)

3,4-Dihydroxy-2-pyrrolidinecarboxylic acid D-809

3,4-Dihydroxyproline, 9CI



(2R,3R,4R)-form

$C_5H_9NO_4$ 147.13

(2R,3R,4R)-form [302593-22-2]
Cryst. (MeOH aq.). Mp 242° dec. $[\alpha]_D^{20}$ +46.2 (c, 1.0 in H_2O).

(2R,3S,4R)-form [105118-17-0]
Cryst. (EtOH aq. or Me_2CO aq.). $[\alpha]_D^{20}$ -7.4 (c, 0.5 in H_2O). Dec. at 247°.

(2S,3R,4R)-form [74644-88-5]
Found in toxic peptides of *Amanita virosa*. Potent and specific β-D-glucuronidase inhibitor. $[\alpha]_D^{19}$ -12.6 (c, 0.53 in H_2O).

(2S,3R,4S)-form [95341-64-3]
Constit. of the adhesive protein of *Mytilus edulis*.
$[\alpha]_D^{20}$ +7.5 (c, 0.5 in H_2O).

(2S,3S,4R)-form [95341-65-4]
Cryst. Mp 220° dec. $[\alpha]_D^{20}$ -56.8 (c, 0.16 in H_2O).

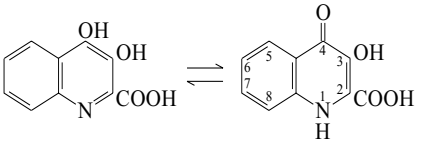
(2S,3S,4S)-form [23161-63-9]
Constit. of the cell walls of *Navicula pelliculosa*, *Navicula incerta*, *Nitzschia angularis*, *Nitzschia thermalis*, *Nitzschia alba*, *Cylindrotheca fusiformis*, *Cyclotella cryptica* and *Phaeodactylum tricornutum*. $[\alpha]_D^{22}$ -63 (c, 0.8 in H_2O).

(2ξ,3ξ,4ξ)-form [63121-50-6]
Constit. of *Aspergillus tamarii*.

Hudson, C.B. *et al., Aust. J. Chem.*, 1968, **21**, 769-782 (*synth*)
Nakajima, T. *et al., Science (Washington, D.C.)*, 1969, **164**, 1400-1401 (*2S,3S,4S-form, isol, struct, occur*)
Karle, I.L. *et al., Science (Washington, D.C.)*, 1969, **164**, 1401-1402 (*2S,3S,4S-form, ms, cryst struct*)
Adams, E. *et al., Annu. Rev. Biochem.*, 1980, **49**, 1005-1061 (*rev*)
Buku, A. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1980, **77**, 2370-2371 (*2S,3R,4R-form, occur*)
Kahl, J.-U. *et al., Annalen*, 1981, 1445-1450 (*synth*)
Lindblad, W.J. *et al., J. Chromatogr.*, 1984, **315**, 447-450 (*synth*)
Razak, A.A. *et al., CA*, 1985, **103**, 19499 (*2ξ,3ξ,4ξ-form, occur*)
Ohfune, Y. *et al., Tet. Lett.*, 1985, **26**, 5307-5308 (*synth*)
Rule, C.J. *et al., Tet. Lett.*, 1985, **26**, 5379-5380 (*glucuronidase inhibitor*)
Baird, P.D. *et al., J.C.S. Perkin 1*, 1987, 1785-1791 (*synth, bibl*)
Austin, G.N. *et al., Tetrahedron*, 1987, **43**, 3095-3108 (*synth, ir, pmr, cmr, ms*)
Moss, W.O. *et al., Chem. Comm.*, 1990, 51-53 (*synth*)
Arakawa, Y. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2219-2224 (*synth*)
Bols, M. *et al., Acta Chem. Scand.*, 1992, **46**, 298-300 (*synth*)
Taylor, S.W. *et al., J.A.C.S.*, 1994, **116**, 10803-10804 (*2S,3R,4S-form, occur*)
Zanardi, F. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 1167-1180 (*synth, pmr, cmr*)
Weir, C.A. *et al., J.O.C.*, 1999, **64**, 1554-1558 (*synth, pmr, cmr*)
Kim, J.H. *et al., Synlett*, 1999, 614-616 (*synth, pmr, cmr*)
Lee, B.W. *et al., Synthesis*, 2000, 1305-1309 (*2R,3R,4R-form, synth, pmr, cmr*)
El-Ashry, E.H. *et al., Carbohydr. Res.*, 2003, **338**, 2265-2290 (*rev, synth*)
Taylor, C.M. *et al., Tetrahedron*, 2005, **61**, 9611-9617 (*synth*)
Davis, F.A. *et al., Tet. Lett.*, 2006, **47**, 2743-2746 (*2R,3S,4R-form, synth*)

3,4-Dihydroxy-2-quinolinecarboxylic acid D-810

1,4-Dihydro-3-hydroxy-4-oxo-2-quinolinecarboxylic acid. 3,4-Dihydroxyquinaldinic acid. 3-Hydroxy-4(1H)-quinolinone-2-carboxylic acid
[33925-79-0]



$C_{10}H_7NO_4$ 205.17
Constit. of the Mediterranean sponge *Aplysinaaerophoba*.
Mp 261-262° (253-254°) dec. λ_{max} 247 (ϵ 29100); 256 (ϵ 28800); 300 (ϵ 1740); 321 (ϵ 2110); 365 (ϵ 8580); 382 (ϵ 7580) (MeOH).

Coppini, D. *et al., Gazz. Chim. Ital.*, 1950, **80**, 36 (*synth*)
Fattorusso, E. *et al., Gazz. Chim. Ital.*, 1971, **101**, 104 (*isol, uv, ir, struct*)

4,8-Dihydroxy-2-quinolinecarboxylic acid D-811

1,4-Dihydro-8-hydroxy-4-oxo-2-quinolinecarboxylic acid. 4,8-Dihydroxyquinaldinic acid. ***Xanthurenic acid****. Xanthuric acid*
[59-00-7]

$C_{10}H_7NO_4$ 205.17
Metab. of tryptophan. Present in human urine as metab. of Kynurenine, K-111 in cases of vitamin B_6 deficiency. Occurs as a moulting inhibitor in crustaceans. Constit. of *Trididemnum* sp. Yellow cryst. (H_2O). Mp 286° (297°). Forms a monohydrate.

▶ UZ9275000

8-O-β-D-Glucopyranoside: ***Cardinalic acid***†
[97451-32-6]
$C_{16}H_{17}NO_9$ 367.312
Tryptophan metab. of *Drosophila melanogaster*.

Me ester: [5934-38-3]

$C_{11}H_9NO_4$ 219.196
Yellow cryst. (MeOH). Mp 262°.

Dibenzoyl, Me ester:
$C_{25}H_{17}NO_6$ 427.412
Mp 171°.

4-Me ether: 8-Hydroxy-4-methoxy-2-quinolinecarboxylic acid, 9CI.
Quinolobactin
[28027-14-7]
$C_{11}H_9NO_4$ 219.196
Alkaloid from *Pseudomonas fluorescens*. Siderophore.
Mp 248°. λ_{max} 211 (log ϵ 4.48); 249 (log ϵ 4.56); 315 (log ϵ 3.45); 348 (log ϵ 3.57) (MeOH).

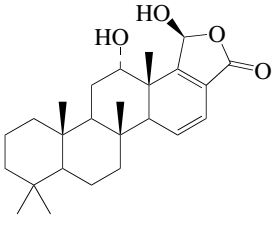
8-Me ether: 4-Hydroxy-8-methoxy-2-quinolinecarboxylic acid
[2929-14-8]
$C_{11}H_9NO_4$ 219.196
Metab. of tryptophan. Possible endogenous carcinogen in man.
Mp 240-241°.
▶ Exp. carcinogen. UZ9550000

[121691-37-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 870D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 449B (*nmr*)
Mebane, A.D. *et al., J.A.C.S.*, 1951, **73**, 3520
Furst, A. *et al., J.O.C.*, 1951, **16**, 412
Price, J.M. *et al., J. Biol. Chem.*, 1956, **223**, 699 (*isol, synth, deriv*)
Neuenhaus, W. *et al., Z. Naturforsch., B*, 1980, **35**, 1569-1571 (*Quinolobactin*)
Suzuki, M. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2340
Ferre, J. *et al., J. Biol. Chem.*, 1985, **260**, 7509; 1990, **265**, 7407 (*Cardinalic acid*)
de Silva, E.D. *et al., Tet. Lett.*, 1992, **33**, 2917-2920 (*Trididemnum, isol*)
Okabe, N. *et al., Acta Cryst. C*, 1996, **52**, 663 (*cryst struct*)
Mossialos, D. *et al., Appl. Environ. Microbiol.*, 2000, **66**, 487-492 (*Quinolobactin*)
Moon, B. *et al., Tetrahedron*, 2000, **56**, 9057-9062 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DNC200; HLT500

12,25-Dihydroxy-15,17-scalaradien-24,25-olide D-812

12,19-Dihydroxy-15,17-scalaradien-20,19-olide

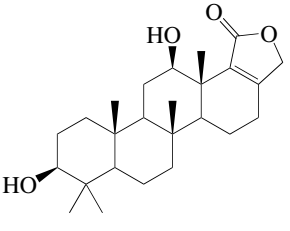


$C_{25}H_{36}O_4$ 400.557

(12α,25β)-*form*

12-Ac: [185801-42-7]
$C_{27}H_{38}O_5$ 442.594
Constit. of *Spongia matamata*. Needles.
Mp 126-128°. $[\alpha]_D$ +84.5 (c, 0.73 in $CHCl_3$). λ_{max} 226 (ϵ 5100); 282 (ϵ 2400) (CH_2Cl_2).
Lu, Q. *et al., J. Nat. Prod.*, 1997, **60**, 195-198 (*isol, pmr, cmr*)

3,12-Dihydroxy-17-scalaren-25,24-olide D-813



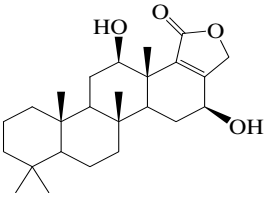
$C_{25}H_{38}O_4$ 402.573

(3β,12β)-*form*

Sesterstatin 1
[199165-87-2]
Constit. of *Hyrtios erecta*.
Amorph. powder. Sol. MeOH, CH_2Cl_2, MeCN, H_2O.
Mp 297-298°. $[\alpha]_D^{22}$ +16.3 (c, 0.12 in $CHCl_3$). λ_{max} 217 (ϵ 1550) (MeOH).

3-Ac: ***3-Acetylsesterstatin 1***
[393828-32-5]
$C_{27}H_{40}O_5$ 444.61
Constit. of *Hyrtios erecta*. Amorph. solid. $[\alpha]_D$ +82.7 (c, 1.85 in CH_2Cl_2). λ_{max} 217 (log ϵ 2.71) (MeOH).
Pettit, G.R. *et al., J. Nat. Prod.*, 1998, **61**, 13-16 (*Sesterstatin 1*)
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2002, **65**, 2-6 (*3-Acetylsesterstatin 1*)

12,16-Dihydroxy-17-scalaren-25,24-olide D-814



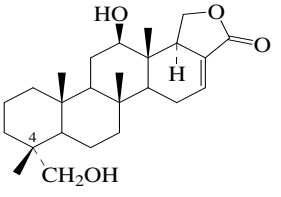
$C_{25}H_{38}O_4$ 402.573

(12β,16β)-*form*

16-Hydroxyscalarolide
[301842-57-9]
Constit. of *Hyrtios erectus*.
Needles.
Mp 300-303°. $[\alpha]_D^{25}$ -25 (c, 0.16 in $CHCl_3$). λ_{max} 208 (log ϵ 3.85) (MeOH).

16-Ac: ***Sesterstatin 7***. *16-Acetoxyscalarolide*
[301842-59-1]
$C_{27}H_{40}O_5$ 444.61
Constit. of *Hyrtios erecta*. Amorph. solid. $[\alpha]_D$ -19.5 (c, 1.15 in CH_2Cl_2).
Miyaoka, H. *et al., J. Nat. Prod.*, 2000, **63**, 1369-1372 (*isol, pmr, cmr*)
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2005, **68**, 1782-1784; 2006, **69**, 172 (*Sesterstatin 7*)

12,19-Dihydroxy-16-scalaren-24,25-olide D-815



$C_{25}H_{38}O_4$ 402.573

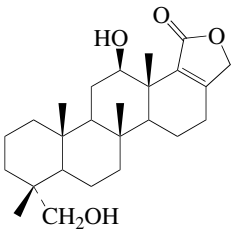
12β-*form*

Di-Ac: ***Hyrtiosin B***†
[862200-48-4]
$C_{29}H_{42}O_6$ 486.647
Constit. of *Hyrtios erecta*. Amorph. powder. $[\alpha]_D^{20}$ +7 (c, 0.16 in $CHCl_3$).

4-Epimer: 12,20-Dihydroxy-16-scalaren-24,25-olide
$C_{25}H_{38}O_4$ 402.573

4-Epimer, di-Ac: ***Hyrtiosin A***†
[862200-47-3]
$C_{29}H_{42}O_6$ 486.647
Constit. of *Hyrtios erecta*. Amorph. powder. $[\alpha]_D^{20}$ +5 (c, 0.17 in $CHCl_3$).
Yu, Z.-G. *et al., Helv. Chim. Acta*, 2005, **88**, 1004-1009 (*Hyrtiosins*)

12,19-Dihydroxy-17-scalaren-25,24-olide D-816



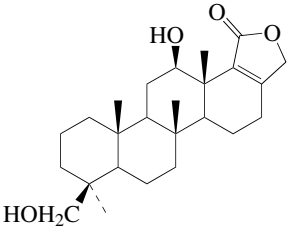
$C_{25}H_{38}O_4$ 402.573

12β-*form*

Sesterstatin 3
[199165-89-4]
Constit. of *Hyrtios erecta*.
Amorph. powder. Sol. MeOH, MeCN, H_2O, CH_2Cl_2.
Mp 293-294°. $[\alpha]_D^{22}$ +27.2 (c, 0.22 in $CHCl_3$). λ_{max} 217 (ϵ 8680) (MeOH).

19-Ac: ***19-Acetylsesterstatin 3***
[393828-33-6]
$C_{27}H_{40}O_5$ 444.61
Constit. of *Hyrtios erecta*. Amorph. solid. $[\alpha]_D$ +39 (c, 1.05 in CH_2Cl_2). λ_{max} 219 (log ϵ 2.46) (MeOH).
Pettit, G.R. *et al., J. Nat. Prod.*, 1998, **61**, 13-16 (*Sesterstatin 3*)
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2002, **65**, 2-6 (*19-Acetylsesterstatin 3*)

12,20-Dihydroxy-17-scalaren-25,24-olide D-817

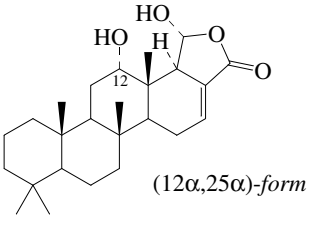


$C_{25}H_{38}O_4$ 402.573

12β-*form*

Sesterstatin 2
[199165-88-3]
Constit. of *Hyrtios erecta*.
Amorph. powder. Sol. MeOH, CH_2Cl_2, MeCN, H_2O. $[\alpha]_D^{22}$ +13.8 (c, 0.09 in $CHCl_3$). λ_{max} 216 (ϵ 8030) (MeOH).
Pettit, G.R. *et al., J. Nat. Prod.*, 1998, **61**, 13-16 (*isol, pmr, cmr*)

12,25-Dihydroxy-16-scalaren-24,25-olide D-818



(12α,25α)-*form*

$C_{25}H_{38}O_4$ 402.573

(12α,25α)-*form*

Constit. of a *Hyrtios* sp. NGF synthesis stimulator, shows antidementia props. Cryst. (MeOH).
Mp 194°. $[\alpha]_D^{16}$ +15.4 (c, 0.35 in $CHCl_3$). λ_{max} 221 (ϵ 7900) (MeOH) (Berdy).

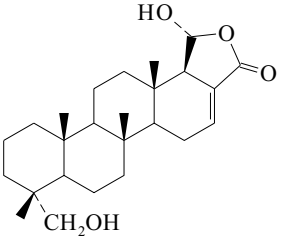
12-Ac: ***Scalarin***
[41410-58-6]
$C_{27}H_{40}O_5$ 444.61
Constit. of *Cacospongia scalaris* and *Spongia virgultosa*. Cryst. (petrol). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 133-135°. $[\alpha]_D$ +43.2 (c, 1.5 in $CHCl_3$). λ_{max} 220 (ϵ 8500) (MeOH) (Berdy).

(12β,25α)-*form*

12-Deacetyl-12-episcalarin
[508193-31-5]
Constit. of a *Spongia* sp.
$[\alpha]_D^{25}$ -17.3 (c, 0.2 in $CHCl_3$). λ_{max} 204 (log ϵ 3.8) (MeOH).

12-Ac: ***12-Episcalarin***
[64825-79-2]
$C_{27}H_{40}O_5$ 444.61
From *Spongia nitens*, *Spongia agaricina*, *Hyrtios erecta* and *Chromodoris funerea*. Cryst. (EtOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 236-238°. $[\alpha]_D$ -57 (c, 1 in $CHCl_3$). λ_{max} 222 (ϵ 784) (MeOH) (Berdy).
Fattorusso, E. *et al., Tetrahedron*, 1972, **28**, 5993-5997 (*isol*)
Cimino, G. *et al., J.C.S. Perkin 1*, 1977, 1587
Kernan, M.R. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1988, **89**, 275 (*12-Episcalarin, isol*)
Doi, Y. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2190 (*isol, pmr, cmr*)
Cambie, R.C. *et al., Acta Cryst. C*, 1999, **55**, 112-114 (*Scalarin, cryst struct*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 2003, **66**, 438-440 (*12-Deacetyl-12-episcalarin*)

19,25-Dihydroxy-16-scalaren-24,25-olide D-819



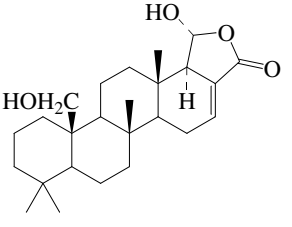
$C_{25}H_{38}O_4$ 402.573

25α-*form*

19-Ac: [175413-21-5]
$C_{27}H_{40}O_5$ 444.61
Constit. of *Hyrtios* cf. *erectus*. Amorph. solid. $[\alpha]_D^{23}$ -2.3 (c, 0.66 in $CHCl_3$). λ_{max} 218 (ϵ 3300) (MeOH) (Berdy).

Di-Ac: ***Hyrtiosin C***
[862200-49-5]
$C_{29}H_{42}O_6$ 486.647
Constit. of *Hyrtios erecta*. Amorph. powder.
Ryu, G. *et al., J. Nat. Prod.*, 1996, **59**, 515-517 (*19-Ac*)
Yu, Z.-G. *et al., Helv. Chim. Acta*, 2005, **88**, 1004-1009 (*Hyrtiosin C*)

22,25-Dihydroxy-16-scalaren-24,25-olide D-820



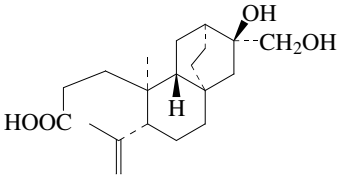
$C_{25}H_{38}O_4$ 402.573

25α-*form*

22-Ac: [782491-79-6]
$C_{27}H_{40}O_5$ 444.61
Constit. of a *Smenospongia* sp. Amorph. solid. $[\alpha]_D^{25}$ -33.1 (c, 0.23 in MeOH). λ_{max} 220 (log ϵ 3.8) (MeOH).

Di-Ac: [782491-78-5]
$C_{29}H_{42}O_6$ 486.647
Constit. of a *Smenospongia* sp. Amorph. solid. $[\alpha]_D^{25}$ -22.9 (c, 0.11 in MeOH). λ_{max} 221 (log ϵ 3.79) (MeOH).
Rho, J.-R. *et al., J. Nat. Prod.*, 2004, **67**, 1748-1751 (*isol, pmr, cmr*)

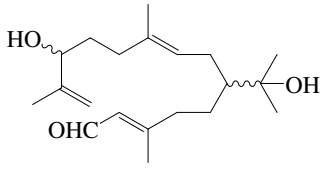
16,17-Dihydroxy-3,4-seco-4(18)-atisen-3-oic acid D-821



$C_{20}H_{32}O_4$ 336.47

(*ent*-16α)-*form*
Agallochaol C
[862255-95-6]
Constit. of *Excoecaria agallocha*. Oil. $[\alpha]_D^{20}$ -34 (c, 0.5 in $CHCl_3$).
Wang, J.-D. *et al., Helv. Chim. Acta*, 2005, **88**, 979-985 (*Agallochaol C*)

7,15-Dihydroxy-9,10-seco-3,8,11-cembratrien-10-al D-822



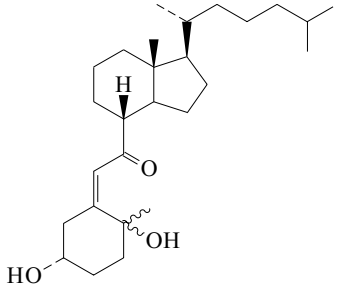
(3*E*,11*E*)-*form*

$C_{20}H_{34}O_3$ 322.487

(3*E*,11*E*)-*form*
15-Ac: [544444-75-9]
$C_{22}H_{36}O_4$ 364.524
Constit. of a *Nephthea* sp.

(3*E*,11*Z*)-*form*
15-Ac: [544444-76-0]
Constit. of a *Nephthea* sp.
Gross, H. *et al., Org. Biomol. Chem.*, 2003, **1**, 944-949 (*isol, pmr, cmr*)

3,10-Dihydroxy-9,10-secocholest-5-en-7-one, 9CI D-823



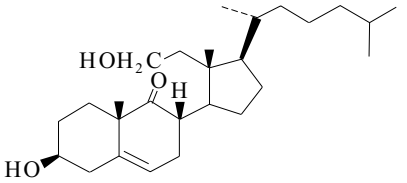
$C_{27}H_{46}O_3$ 418.659

(3*S*,5*Z*,10ξ)-*form*
Ketone 250
[35454-94-5]
Isol. from various fish liver oils and the aerial parts of many plants. Mp 73°.

2,4-Dinitrophenylhydrazone: Mp 150°.

Semicarbazone: Mp 195°.
Baron, C. *et al., Ann. Chim. (Paris)*, 1956, **1**, 897 (*synth*)
Raoul, Y. *et al., Bull. Soc. Chim. Biol.*, 1956, **38**, 885; 1963, **45**, 145 (*isol, props, synth*)
Fuerst, W. *et al., Zentralbl. Pharm., Pharmakother. Laboratoriumsdiagn.*, 1977, **116**, 21 (*isol*)

3,11-Dihydroxy-9,11-secocholest-5-en-9-one D-824

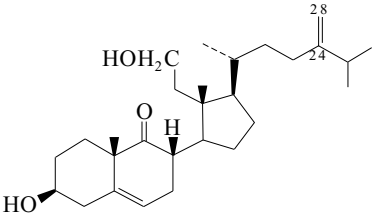


$C_{27}H_{46}O_3$ 418.659

3β-*form* [85650-23-3]
Constit. of *Sinularia* spp. Cryst. (C_6H_6/hexane). Mp 112-113°.
Bonini, C. *et al., J.O.C.*, 1983, **48**, 2108

3,11-Dihydroxy-9,11-secoergosta-5,24(28)-dien-9-one D-825

3,11-Dihydroxy-24-methylene-9,11-secocholest-5-en-9-one



$C_{28}H_{46}O_3$ 430.67

3β-*form* [81419-47-8]
Constit. of a *Sinularia* sp. Cryst. (EtOAc/hexane). Mp 118-120°. $[\alpha]_D^{24}$ -27 (c, 0.9 in $CHCl_3$).

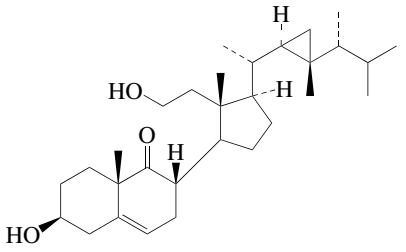
24,28S-Dihydro: 3,11-Dihydroxy-24-methyl-9,11-secocholest-5-en-9-one
$C_{28}H_{48}O_3$ 432.685
Constit. of a *Sinularia* spp. Cryst. (EtOAc/petrol). Mp 134-135°. $[\alpha]_D^{24}$ -45 (c, 0.83 in $CHCl_3$).

11-Ac: [85650-24-4]
$C_{30}H_{48}O_4$ 472.707
From a *Sinularia* sp.

24S,28-Dihydro, 11-Ac: [85650-25-5]
$C_{30}H_{50}O_4$ 474.723
From a *Sinularia* sp.

(3β,8α*H*)-*form* [85700-73-8]
Constit. of a *Sinularia* sp.
Kazlauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 69
Bonini, C. *et al., J.O.C.*, 1983, **48**, 2108 (*isol*)

3,11-Dihydroxy-9,11-secogorgost-5-en-9-one D-826



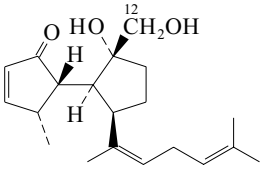
$C_{30}H_{50}O_3$ 458.723

(3β,24*R*)-*form*
Secogorgosterol
[34290-98-7]
Constit. of the gorgonians *Pseudopterogorgia americana* and *Pseudopterogorgia hummelinkii*. Gum.

5α,6α-Epoxide: 5,6-Epoxy-3,11-dihydroxy-9,11-secogorgost-5-en-9-one. ***5,6-Epoxysecogorgosterol***
[34712-18-0]
$C_{30}H_{50}O_4$ 474.723
Constit. of the gorgonian *Pseudopterogorgia americana*.

Green, D. *et al., J. Nat. Prod.*, 1992, **55**, 1186-1196 (*isol, pmr, cmr*)
Schultz, L.W. *et al., Acta Cryst. C*, 1995, **51**, 415-419 (*isol, cryst struct*)
He, H. *et al., Tetrahedron*, 1995, **51**, 51-58 (*isol, cmr*)
Naz, S. *et al., Tet. Lett.*, 2000, **41**, 6035-6040 (*isol, pmr, cmr*)

4,12-Dihydroxy-4,10-seco-2,13(15),17-spatatrien-10-one D-827

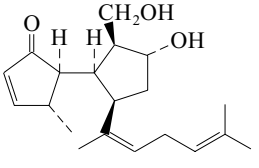


$C_{20}H_{30}O_3$ 318.455

12-Ac: [140671-32-5]
$C_{22}H_{32}O_4$ 360.492
Constit. of *Dictyota fenestrata*. Oil. $[\alpha]_D$ -61 (c, 0.54 in $CHCl_3$).

Van Altena, I.A. *et al., Aust. J. Chem.*, 1992, **45**, 541 (*isol, pmr, cmr*)

5,12-Dihydroxy-4,10-seco-2,13(15),17-spatatrien-10-one D-828

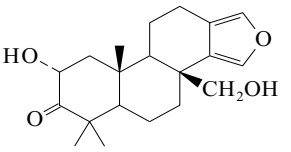


$C_{20}H_{30}O_3$ 318.455

(4*S*,5*R*,13(15)*Z*)-*form*
Di-Ac: ***Dilophus enone***
[121961-78-2]
$C_{24}H_{34}O_5$ 402.53
Constit. of alga *Dilophus okamurai*. Antifeedant. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -46 (c, 1.30 in $CHCl_3$). λ_{max} 205 (ε 17000) (MeOH) (Berdy).

Kurata, K. *et al., Tet. Lett.*, 1989, **30**, 1567

2,17-Dihydroxy-13(16),14-spongiadien-3-one D-829



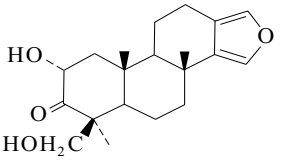
$C_{20}H_{28}O_4$ 332.439

2α-*form* [157799-20-7]
Constit. of a *Spongia* sp. Oil.

2β-*form* [157799-21-8]
Constit. of a *Spongia* sp. Oil.

Searle, P.A. *et al., Tetrahedron*, 1994, **50**, 9893 (*isol, pmr, cmr*)

2,19-Dihydroxy-13(16),14-spongiadien-3-one D-830

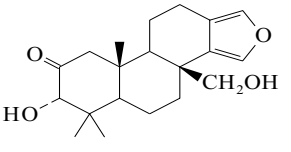


$C_{20}H_{28}O_4$ 332.439

2α-*form*
Isospongiadiol
[111139-69-6]
Constit. of sponge *Spongia* sp. and *Hyatella intestinalis*. Shows cytotoxic and antiviral props. Cryst. (MeOH aq.).
Mp 181-183°. $[\alpha]_D^{20}$ -50 (c, 3.0 in CH_2Cl_2).

Kohmoto, S. *et al., Chem. Lett.*, 1987, 1687
Cambie, R.C. *et al., J. Nat. Prod.*, 1988, **51**, 293
Zoretic, P.A. *et al., J.O.C.*, 1996, **61**, 1806 (*synth*)
Ribeiro, A.A. *et al., Magn. Reson. Chem.*, 1998, **36**, 325-335 (*pmr, cmr*)

3,17-Dihydroxy-13(16),14-spongiadien-2-one D-831



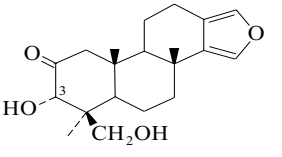
$C_{20}H_{28}O_4$ 332.439

3α-*form* [157799-19-4]
Constit. of a *Spongia* sp.
Solid. $[\alpha]_D$ +64.5 (c, 1.7 in $CHCl_3$).

3β-*form* [157799-18-3]
Constit. of a *Spongia* sp.
Solid (EtOAc/hexane).
Mp 165-167.5°. $[\alpha]_D$ -8.1 (c, 1.7 in $CHCl_3$).

Searle, P.A. *et al., Tetrahedron*, 1994, **50**, 9893 (*isol, pmr, cmr*)

3,19-Dihydroxy-13(16),14-spongiadien-2-one D-832



$C_{20}H_{28}O_4$ 332.439
λ_{max} 240 (ε 1470) ($CHCl_3$) (Derep).

3α-*form*

Spongiadiol

[71302-28-8]

Constit. of *Spongia* spp.

Cryst. (EtOAc).

Mp 181-183°. $[\alpha]_D^{21}$ +73.6 (c, 1 in $CHCl_3$).

Di-Ac: [71302-24-4]

$C_{24}H_{32}O_6$ 416.513

Constit. of *Spongia* spp. Cryst. (MeOH).

Mp 131.5-133°. $[\alpha]_D^{25}$ +14.5 (c, 1 in $CHCl_3$).

3β-*form*

Epispongiadiol

[71302-26-6]

Constit. of *Spongia* spp. and *Hyatella intestinalis*.

Cryst. (EtOAc).

Mp 157-158.5°. $[\alpha]_D^{21}$ +18.7 (c, 1 in $CHCl_3$).

3-Ac:

$C_{22}H_{30}O_5$ 374.476

Constit. of *Hyatella intestinalis*. Cryst. (Me_2CO/hexane).

Mp 216-218°. $[\alpha]_D$ +34 (c, 0.15 in $CHCl_3$).

Di-Ac: [71302-30-2]

Constit. of *Spongia* spp. and *Hyatella intestinalis*.

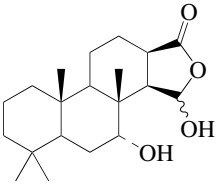
Cryst. (MeOH).

Mp 195-198°. $[\alpha]_D^{21}$ +45.2 (c, 1 in $CHCl_3$).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1979, **32**, 867 (*isol, struct*)

Cambie, R.C. *et al., J. Nat. Prod.*, 1988, **51**, 293 (*isol, deriv*)

7,15-Dihydroxy-16-spongianone D-833



$C_{20}H_{32}O_4$ 336.47

(7α,15ξ)-*form*

7-Ac: ***Aplyroseol 15***

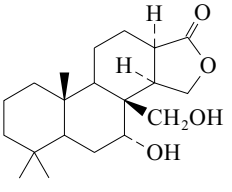
[200437-66-7]

$C_{22}H_{34}O_5$ 378.508

Constit. of *Aplysilla rosea*. Gum.

Taylor, W.C. *et al., Aust. J. Chem.*, 1997, **50**, 895-902 (*isol, pmr, cmr*)

7,17-Dihydroxy-16-spongianone D-834



$C_{20}H_{32}O_4$ 336.47

7α-*form*

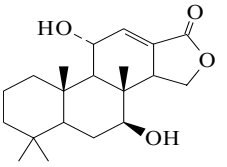
Di-Ac: [106009-72-7]

$C_{24}H_{36}O_6$ 420.545

Isol. from *Aplysilla rosea*. Glass.

Karuso, P. *et al., Aust. J. Chem.*, 1986, **39**, 1629

7,11-Dihydroxy-12-spongien-16-one D-835



$C_{20}H_{30}O_4$ 334.455

(7β,11α)-*form*

Constit. of *Spongia officinalis*. Isol. as crystalline mixt. with 11β-isomer, Mp 60°.

(7β,11β)-*form*

Constit. of *Spongia officinalis*.

Cryst. (Me_2CO).

Mp 60°. Occurs as inseparable mixt. with 7β,11α-form.

Di-Ac: ***Dorisenone D***

[178180-01-3]

$C_{24}H_{34}O_6$ 418.529

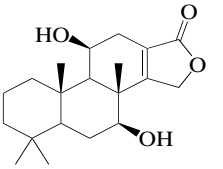
Constit. of *Chromodoris obsoleta*. Needles (MeOH).

Mp 202-204°. $[\alpha]_D^{27}$ +102 (c, 0.84 in $CHCl_3$). λ_{max} 214 (ϵ 9700) (MeOH) (Berdy).

González, A.G. *et al., Tetrahedron*, 1984, **40**, 4109-4113 (*Spongia officinalis constits*)

Miyamoto, T. *et al., Tetrahedron*, 1996, **52**, 8187-8198 (*Dorisenone D*)

7,11-Dihydroxy-13-spongien-16-one D-836



$C_{20}H_{30}O_4$ 334.455

(7β,11β)-*form*

Di-Ac: ***Dorisenone C***

[178180-00-2]

$C_{24}H_{34}O_6$ 418.529

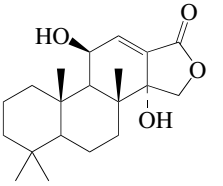
Constit. of *Chromodoris obsoleta*. Amorph. solid.

Mp 187-190°. $[\alpha]_D^{27}$ +35.5 (c, 0.2 in $CHCl_3$). λ_{max} 212 (ϵ 9000) (hexane). λ_{max} 212 (ϵ 9000) (MeOH) (Berdy).

Miyamoto, T. *et al., Tetrahedron*, 1996, **52**, 8187-8198 (*isol, pmr, cmr*)

Abad, A. *et al., Tetrahedron*, 2005, **61**, 1961-1970 (*synth*)

11,14-Dihydroxy-12-spongien-16-one D-837



$C_{20}H_{30}O_4$ 334.455

(11β,14α)-*form*

11-Ac: ***Dorisenone B***

[178179-99-2]

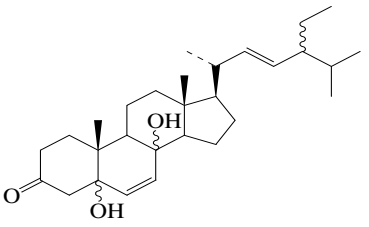
$C_{22}H_{32}O_5$ 376.492

Constit. of *Chromodoris obsoleta*. Needles (MeOH).

Mp 248-250°. $[\alpha]_D^{27}$ +230.4 (c, 0.33 in $CHCl_3$). λ_{max} 213 (ϵ 7000) (EtOH). λ_{max} 213 (ϵ 7000) (MeOH) (Berdy).

Miyamoto, T. *et al., Tetrahedron*, 1996, **52**, 8187-8198 (*isol, pmr, cmr*)

5,8-Dihydroxystigmasta-6,22-dien-3-one D-838

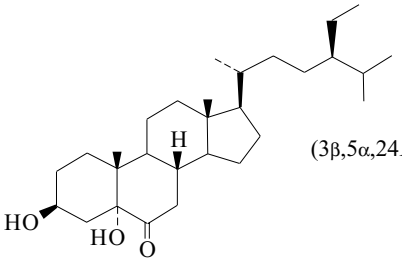


$C_{29}H_{46}O_3$ 442.681

(5ξ,8ξ,22*E*,24ξ)-*form* [870535-12-9]
Constit. of *Laurencia cartilaginea*.
Yang, X.-Y. *et al., Guangpu Shiyanshi*, 2005, **22**, 12-16; *CA*, **144**, 19295p

3,5-Dihydroxystigmastan-6-one D-839

3,5-Dihydroxy-24-ethylcholestan-6-one



(3β,5α,24*R*)–*form*

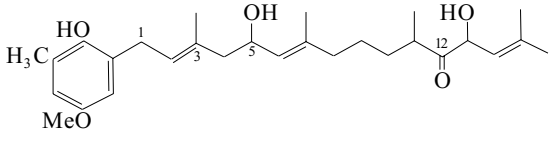
$C_{29}H_{50}O_3$ 446.712

(3β,5α,24*R*)-*form* [55051-78-0]
Constit. of *Podocarpus lambertius* and *Plenasium banksiifolium* (preferred genus name *Osmunda*). Cryst. Mp 246-248°. $[\alpha]_D^{22}$ -14.4 (c, 0.01 in MeOH).

(3β,5α,24*S*)-*form*
Constit. of *Spirastrella inconstans*. Cryst. (MeOH). Mp 253-254°. $[\alpha]_D$ +1.34 (c, 0.258 in MeOH).
Campello, J. de P. *et al., Phytochemistry*, 1975, **14**, 243 (*isol*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 1980, **28**, 3137 (*isol*)
Dawidar, A.M. *et al., Z. Naturforsch., B*, 1980, **35**, 102 (*synth*)
Habib, N.S. *et al., Sci. Pharm.*, 1981, **49**, 258 (*synth*)
Das, B. *et al., J. Nat. Prod.*, 1992, **55**, 1310 (*isol, pmr, cmr*)

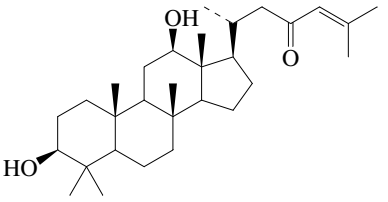
2-(5,13-Dihydroxy-3,7,11,15-tetramethyl-12-oxo-2,6,14-hexadecatrienyl)-4-methoxy-6-methylphenol D-840

4,12-Dihydroxy-16-(2-hydroxy-5-methoxy-3-methylphenyl)-2,6,10,14-tetramethyl-2,10,14-hexadecatrien-5-one



$C_{28}H_{42}O_5$ 458.637
Metab. of marine alga *Cystoseira elegans*. Oil. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D$ -96 (c, 9.96 in MeOH). λ_{max} 214 (ϵ 11500); 288 (ϵ 3100) (MeOH) (Berdy).
Banaigs, B. *et al., Tetrahedron*, 1983, **39**, 629

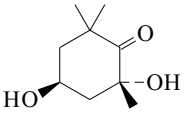
3,12-Dihydroxy-4,4,8-trimethylcholest-24-en-23-one D-841



$C_{30}H_{50}O_3$ 458.723

(3β,8β,12β)-*form*
Solid.
3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Sarasinoside D***
[147769-47-9]
$C_{62}H_{102}N_2O_{26}$ 1291.486
Constit. of *Asteropus sarasinosum*. Protein kinase C inhibitor. Cryst. Sol. MeOH, butanol; fairly sol. $CHCl_3$; poorly sol. H_2O. Mp 207-211°. $[\alpha]_D^{20}$ -12.7 (MeOH).
Espada, A. *et al., Tetrahedron*, 1992, **48**, 8685-8696 (*isol, pmr, cmr*)

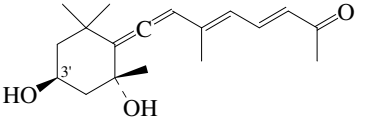
2,4-Dihydroxy-2,6,6-trimethylcyclohexanone D-842



$C_9H_{16}O_3$ 172.224

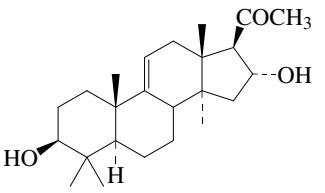
(2*R*,4*S*)-*form*
4-Ac: [176300-88-2]
$C_{11}H_{18}O_4$ 214.261
Constit. of *Padina tetrastromatica*.
Parameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 463-467 (*isol, pmr, cmr*)

8-(2,4-Dihydroxy-2,6,6-trimethylcyclohexylidene)-6-methyl-3,5,7-octatrien-2-one D-843



$C_{18}H_{26}O_3$ 290.402
Carotenoid numbering shown.
3′-Ac: ***Apo-13′-fucoxanthinone***
[183182-96-9]
$C_{20}H_{28}O_4$ 332.439
Constit. of *Phaeodactylum tricornutum*. λ_{max} 329 (log ϵ 4.19) (MeOH).
Shaw, B.A. *et al., Mar. Biol. (Berlin)*, 1995, **124**, 467-472 (*isol, pmr*)

3,16-Dihydroxy-4,4,14-trimethylpregn-9(11)-en-20-one D-844



$C_{24}H_{38}O_3$ 374.562

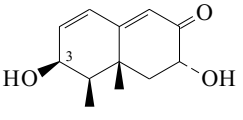
(3β,5α,16α)-*form*

16-Ac, 3-O-[3-O-methyl-β-D-glucopyranosyl-(1→3)-6-O-sulfo-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranoside]: ***Kuriloside C***
[139307-92-9]
$C_{50}H_{80}O_{25}S$ 1113.233
Isol. from the holothurian *Duasmodactyla kurilensis*.
Mp 210° dec. (as Na salt). $[\alpha]_D^{20}$ -38 (c, 0.1 in Py) (Na salt). CAS no. refers to Na salt.

16-Ac, 3-O-[3-O-methyl-β-D-glucopyranosyl-(1→3)-6-O-sulfo-β-D-glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranoside]: ***Kuriloside A***
[139307-91-8]
$C_{56}H_{90}O_{30}S$ 1275.375
Isol. from the holothurian *Duasmodactyla kurilensis*.
Mp 215° dec. (as Na salt). $[\alpha]_D^{20}$ -13 (c, 0.1 in Py) (Na salt). CAS no. refers to Na salt.

Avilov, S.A. *et al., Khim. Prir. Soedin.*, 1991, **27**, 221-226; *Chem. Nat. Compd. (Engl. Transl.)*, 1991, **27**, 188-192

3,7-Dihydroxy-11,12,13-trinor-1,9-eremophiladien-8-one D-845



$C_{12}H_{16}O_3$ 208.257

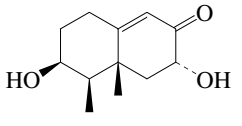
(3β,7α)-*form*

3-(7-Carboxy-6-methyl-2,4-heptadienoyl): ***Dendryphiellin A1***
[133562-49-9]
$C_{21}H_{26}O_6$ 374.433
Constit. of *Dendryphiella salina*. Oil. $[\alpha]_D^{20}$ +444.8 (c, 0.17 in EtOH).

Guerriero, A. *et al., Helv. Chim. Acta*, 1990, **73**, 2090 (*isol, pmr, cmr*)

3,7-Dihydroxy-11,12,13-trinor-9-eremophilen-8-one D-846

*3,7-Dihydroxy-4*a*,5-dimethyl-4,4*a*,5,6,7,8-hexahydro-2(3*H*)-naphthalenone*



$C_{12}H_{18}O_3$ 210.272

(3β,7α)-*form*

*3-O-(8-Hydroxy-6*R*-methyl-2*E*,4*E*-octadienoyl):* ***Dendryphiellin A***
[113592-81-7]
$C_{21}H_{28}O_5$ 360.449
Metab. of *Dendryphiella salina*. Oil. $[\alpha]_D^{20}$ +571.1 (c, 0.31 in EtOH). λ_{max} 272 (ε 37100) (EtOH) (Berdy).

*3-O-(6*R*-Methyl-2*E*,4*E*-octadienoyl):* ***Dendryphiellin C***
[121661-41-4]
$C_{21}H_{28}O_4$ 344.45
Metab. of *Dendryphiella salina*. Oil. $[\alpha]_D^{20}$ +506.9 (c, 0.41 in MeOH).

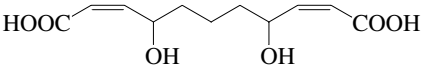
*3-O-(6*R*-Ethyl-7-hydroxy-2*E*,4*E*-heptadienoyl):* ***Dendryphiellin D***
[121678-87-3]
$C_{21}H_{28}O_5$ 360.449
Metab. of *Dendryphiella salina*. Oil. $[\alpha]_D^{20}$ +349.1 (c, 0.092 in EtOH).

*3-O-(6*R*-Hydroxy-6-methyl-2*E*,4*E*-octadienoyl):* ***Dendryphiellin B***
[121678-86-2]
$C_{21}H_{28}O_5$ 360.449
Metab. of *Dendryphiella salina*. Oil. $[\alpha]_D^{20}$ +280 (c, 0.05 in EtOH).

Guerriero, A. *et al., Helv. Chim. Acta*, 1988, **71**, 57; 1989, **72**, 438 (*isol, pmr, cmr, uv, cd*)
Akao, H. *et al., Tetrahedron*, 1999, **55**, 7757-7770 (*synth*)

4,8-Dihydroxy-2,9-undecadienedioic acid D-847

3,7-Dihydroxy-1,8-nonadiene-1,9-dicarboxylic acid



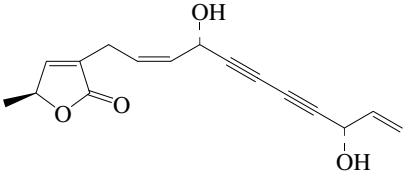
$C_{11}H_{16}O_6$ 244.244

(2*Z*,4ξ,8ξ,9*Z*)-*form*

Diamide: 4,8-Dihydroxy-2,9-undecadienediamide
[382138-86-5]
$C_{11}H_{18}N_2O_4$ 242.274
Isol. from an unidentified marine actinomycete.

Smelcerovic, A.A. *et al., Hem. Ind.*, 2001, **55**, 399-401 (*isol*)

3-(4,9-Dihydroxy-2,10-undecadiene-5,7-diynyl)-5-methyl-2(5*H*)-furanone D-848



$C_{16}H_{16}O_4$ 272.3

(4′*S*,5*S*,9′*S*)-*form*

Isol. from *Sarcophyton tracheliophorum*.
Pale yellow oil. $[\alpha]_D$ +47.1 (c, 0.11 in EtOH). λ_{max} 220 (log ε 3.15); 235 (log ε 2.97); 245 (log ε 2.1); 260 (log ε 2.71) (EtOH).

Rezanka, T. *et al., Tetrahedron*, 2001, **57**, 8743-8749

6,11-Dihydroxy-2,8-undecadienoic acid D-849

$HOCH_2CH_2CH{=}CHCH_2CH(OH)CH_2CH_2CH{=}CHCOOH$
$C_{11}H_{18}O_4$ 214.261

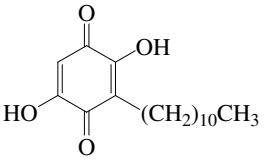
(2*Z*,8*E*)-*form*

1,11-Lactone, 6-O-(6-O-acetyl-β-D-glucopyranoside): ***Litorine***
$C_{19}H_{28}O_9$ 400.425
Isol. from the mollusc *Littorina aspera*. Cryst. Sol. EtOAc. λ_{max} 225 (MeOH). λ_{max} 227 ($CHCl_3$) (Berdy).

Perez Gutierrez, R.M. *et al., Drugs Exp. Clin. Res.*, 1987, **13**, 191-194

2,5-Dihydroxy-3-undecyl-1,4-benzoquinone D-850

2,5-Dihydroxy-3-undecyl-2,5-cyclohexadiene-1,4-dione, 9CI. ***Embelin****. Embelic acid. Embeliaquinone*
[550-24-3]



$C_{17}H_{26}O_4$ 294.39
Constit. of *Embelia ribes*, *Embelia tsjersium-cottam*, *Embelia barbeyana*, *Embelia robusta*, *Embelia kilimandscharica*, *Ardisia humilis*, *Rapanea umbellata*, *Connarus ritchiei*, , *Myrsine africana*, *Myrsine semiserrata*, *Myrsine capitellata* and *Rapanea neurophylla*. Used as a 1% soln. in EtOH for photometric detn. of Al, Be, Ba, Ca, Mg, Sr, Th, U. Anthelminthic, potent oral contraceptive. Antiinflammatory, analgesic. Inhibitor of reverse transcriptase. Antitumour agent. potent inhibitor of XAIP (x-linked inhibitor of apoptosis). Orange cryst. (MeOH or hexane/EtOH). Insol. H_2O. Mp 145-146°. Log P 5.14 (calc). λ_{max} 292 (ϵ 16200); 424 (ϵ 280) (95% EtOH) (Derep). λ_{max} 292 (ϵ 17400); 426 (ϵ 340) (MeOH) (Berdy).

▶ Exp. reprod. effects (male and female). DK4230000

Di-Ac:
Yellow cryst. (MeOH aq.). Mp 54° Mp 59°.

5-Me ether: 2-Hydroxy-5-methoxy-3-undecyl-1,4-benzoquinone. ***5-O-Methylembelin***
[56005-10-8]
$C_{18}H_{28}O_4$ 308.417
Constit. of *Aegiceras corniculatum* and *Myrsine africana* (cape myrtle). Piscicide. Orange cryst.
Mp 95-96°. λ_{max} 285 (ϵ 398) (95% EtOH) (Derep).

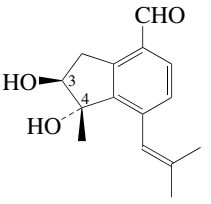
5-Me ether, 2-Ac: ***2-O-Acetyl-5-O-methylembelin***
$C_{20}H_{30}O_5$ 350.454
Constit. of *Aegiceras corniculatum*.

Di-Me ether:
Cryst. (MeOH aq.). Mp 58°.

5-Et ether: 5-Ethoxy-2-hydroxy-3-undecyl-1,4-benzoquinone. ***5-O-Ethylembelin***
$C_{19}H_{30}O_4$ 322.444
Constit. of the mangrove plant *Aegiceras corniculatum*. Orange cryst.
Mp 59-60°. λ_{max} 220 (log ϵ 3.62); 289 (log ϵ 3.68) (MeOH).

Merian, M. *et al., Helv. Chim. Acta*, 1948, **31**, 2237 (*isol*)
Fieser, L.F. *et al., J.A.C.S.*, 1948, **70**, 71 (*synth*)
Rao, C.B. *et al., Fresenius' Z. Anal. Chem.*, 1960, **175**, 114; 1961, **178**, 277; 1963, **198**, 183 (*detn, Th, U, Al, Be, Ba, Ca, Mg, Sr*)
Natori, S. *et al., Chem. Pharm. Bull.*, 1964, **12**, 236 (*ir, uv*)
Dallacker, F. *et al., Chem. Ber.*, 1972, **105**, 614 (*synth*)
Desai, H.K. *et al., Indian J. Chem., Sect. B*, 1975, **13**, 97; 1977, **15**, 291 (*isol*)
Joshi, B.S. *et al., J.C.S. Perkin 1*, 1975, 327 (*isol, ms, pmr*)
Thappa, R.K. *et al., Indian J. Pharm.*, 1976, **38**, 17 (*synth, pharmacol*)
Gupta, O.P. *et al., Indian J. Physiol. Pharmacol.*, 1977, **21**, 31 (*pharmacol*)
Gomez, E. *et al., J. Nat. Prod.*, 1989, **52**, 649 (*5-O-Methylembelin*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 42
Pfeifer, J. *et al., Annalen*, 1995, 131 (*synth, deriv, ir, pmr, cmr*)
Poigny, S. *et al., Tetrahedron*, 1998, **54**, 14791-14802 (*synth*)
Miles, D.H. *et al., Tetrahedron*, 2001, **57**, 5769-5772 (*5-O-Methylembelin*)
Nikolovska-Coleska, Z. *et al., J. Med. Chem.*, 2004, **27**, 2430-2440 (*pharmacol*)
Xu, M. *et al., J. Nat. Prod.*, 2004, **67**, 762-766 (*Aegiceras corniculatum constits*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EAJ600

3,4-Dihydroxy-1(10),5,7(11),8-valerenatetraen-14-al D-851



$C_{15}H_{18}O_3$ 246.305

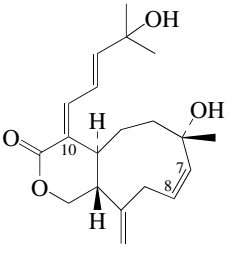
(3β,4α)-*form*

3-Ac: ***Caulerpal A***
[896100-44-0]
$C_{17}H_{20}O_4$ 288.343
Constit. of *Caulerpa taxifolia*. Oil. $[\alpha]_D^{24}$ +6 (c, 0.12 in $CHCl_3$). λ_{max} 202 (ϵ 60256); 266 (ϵ 6455) (MeOH).

4-Me ether: 3-Hydroxy-4-methoxy-1(10),5,7(11),8-valerenatetraen-14-al
[896100-45-1]
$C_{16}H_{20}O_3$ 260.332
Constit. of *Caulerpa taxifolia*. Oil. $[\alpha]_D^{24}$ -6 (c, 0.29 in $CHCl_3$). λ_{max} 202 (ϵ 69183); 266 (ϵ 6854) (MeOH).

Mao, S.-C. *et al., Bioorg. Med. Chem. Lett.*, 2006, **16**, 2947-2950 (*Caulerpals A and B*)

6,14-Dihydroxy-1(19),7,10,12-xenicatetraen-17,18-olide D-852



(6α,7*Z*,10*E*)-*form*

$C_{20}H_{28}O_4$ 332.439

(6α,7*Z*,10*E*)-*form*

Xeniatine A
[167172-85-2]
Constit. of *Xenia* spp.
Needles.
Mp 150-151°. $[\alpha]_D^{27}$ +462 (c, 0.08 in MeOH).

7α,8α-Epoxide: ***Xeniatine A epoxide***
[169337-62-6]
$C_{20}H_{28}O_5$ 348.438
Constit. of *Xenia* spp. Oil. $[\alpha]_D^{27}$ -16.3 (c, 0.07 in MeOH).

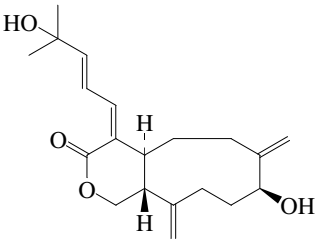
(6α,7*Z*,10*Z*)-*form*

Isoxeniatine A
[169869-81-2]
Constit. of *Xenia* spp.
Amorph. $[\alpha]_D^{27}$ +300 (c, 0.13 in MeOH).

7α,8α-Epoxide: ***Isoxeniatine C***
[183071-69-4]
$C_{20}H_{28}O_5$ 348.438
Constit. of *Xenia* spp. Oil. $[\alpha]_D$ -28 (c, 0.05 in MeOH). λ_{max} 273 (ϵ 12800) (no solvent reported).

Iwagawa, T. *et al., Chem. Lett.*, 1995, 695-696 (*isol, pmr, cmr*)
Iwagawa, T. *et al., Tetrahedron*, 1995, **51**, 11111-11118; 1996, **52**, 13121-13128 (*isol, pmr, cmr*)

7,14-Dihydroxy-1(19),6(20),10,12-xenicatetraen-17,18-olide D-853



$C_{20}H_{28}O_4$ 332.439

(7β,10*Z*)-*form*

Xeniolide F

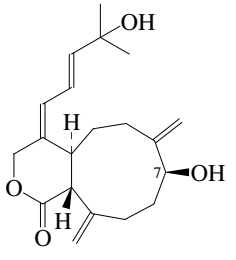
[437710-61-7]

Constit. of a *Xenia* soft coral.

Amorph. solid. $[\alpha]_D^{25}$ +91.6 (c, 0.23 in CH_2Cl_2). λ_{max} 207 (log ϵ 4.23); 267 (log ϵ 4.35) (MeOH).

Anta, C. *et al., J. Nat. Prod.*, 2002, **65**, 766-768 (*isol, pmr, cmr*)

7,14-Dihydroxy-1(19),6(20),10,12-xenicatetraen-18,17-olide D-854



(7β,10*E*,12*E*)-*form*

$C_{20}H_{28}O_4$ 332.439

(7β,10*E*,12*E*)-*form*

Blumiolide B

[866403-77-2]

Constit. of *Xenia blumi*.

Oil. $[\alpha]_D^{25}$ +33 (c, 0.4 in $CHCl_3$). λ_{max} 225 (log ϵ 3.8) (MeOH).

(7ξ,10*E*,12*E*)-*form*

7-Hydroperoxide: ***Xeniolide G***

[479067-62-4]

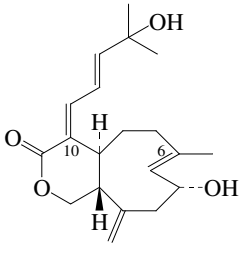
$C_{20}H_{28}O_5$ 348.438

Constit. of *Xenia umbellata*. Oil. $[\alpha]_D^{25}$ +27.5 (c, 0.4 in $CHCl_3$). λ_{max} 222 (log ϵ 3.88) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1882-1885 (*Xeniolide G*)

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 1336-1340 (*Blumiolide B*)

8,14-Dihydroxy-1(19),6,10,12-xenicatetraen-17,18-olide D-855



(6*E*,10*E*)-*form*

$C_{20}H_{28}O_4$ 332.439

(6*E*,10*E*)-*form*

Xeniolide A

[70389-63-8]

Isol. from *Xenia macrospiculata*.

Viscous oil. $[\alpha]_D^{25}$ -6 (c, 2.9 in $CHCl_3$). λ_{max} 268 (ϵ 15500) (MeOH) (Derep).

(6*E*,10*Z*)-*form*

Isoxeniolide A

[71117-53-8]

Constit. of *Xenia novae-britanniae.*

Cryst. (CH_2Cl_2).

Mp 171-172°. $[\alpha]_D$ +50 (c, 0.66 in MeOH).

6β,7β-Epoxide: ***6,7-Epoxyisoxeniolide A***

[71093-24-8]

$C_{20}H_{28}O_5$ 348.438

Constit. of *Xenia novae-britanniae.* Cryst. (CH_2Cl_2).

Mp 234-236°. $[\alpha]_D$ +119 (c, 0.27 in 1:1 $CHCl_3$/MeOH).

(6*Z*,10*Z*)-*form*

8-Ketone: 14-Hydroxy-8-oxo-1(19),6,10,12-xenicatetraen-17,18-olide. ***Blumiolide C***

[866403-78-3]

$C_{20}H_{26}O_4$ 330.423

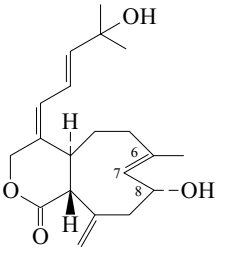
Constit. of *Xenia blumi*. Oil. $[\alpha]_D^{25}$ +66 (c, 0.4 in $CHCl_3$). λ_{max} 256 (log ϵ 4.2) (MeOH).

Kashman, Y. *et al., Tet. Lett.*, 1978, 4833-4836 (*Xeniolide A*)

Braekman, J.C. *et al., Bull. Soc. Chim. Belg.*, 1979, **88**, 71-77 (*Isoxeniolide A, 6,7-Epoxyisoxeniolide A*)

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 1336-1340 (*Blumiolide C*)

8,14-Dihydroxy-1(19),6,10,12-xenicatetraen-18,17-olide D-856



$C_{20}H_{28}O_4$ 332.439

8α-*form*

Xeniolide B

[70389-64-9]

Constit. of *Xenia macrospiculata*.

Unstable oil. $[\alpha]_D^{25}$ -4 (c, 0.3 in $CHCl_3$). λ_{max} 242 (ϵ 15900) (MeOH) (Derep).

8-Ac: [74175-97-6]

$C_{22}H_{30}O_5$ 374.476

Constit. of *Xenia* spp. Oil.

6,7-Epoxide: 6,7-Epoxy-8,14-dihydroxy-1(19),10,12-xenicatrien-19,18-olide. ***6,7-Epoxyxeniolide B***

[74175-98-7]

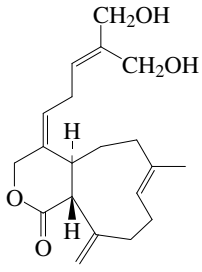
$C_{20}H_{28}O_5$ 348.438

Constit. of *Xenia* spp. Oil.

Kashman, Y. *et al., Tet. Lett.*, 1978, **19**, 4833-1836 (*Xeniolide B*)

Kashman, Y. *et al., J.O.C.*, 1980, **45**, 3814-3824 (*8-Ac, 6,7-epoxide*)

15,16-Dihydroxy-1(19),6,10,13-xenicatetraen-18,17-olide D-857



$C_{20}H_{28}O_4$ 332.439

(6*E*,10*E*)-*form*

Xeniadiol

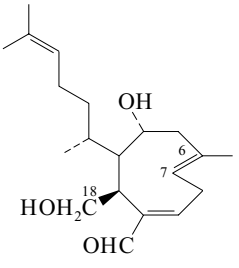
[251343-62-1]

Constit. of a *Xenia* sp.

Oil. $[\alpha]_D^{27}$ -5 (c, 0.6 in $CHCl_3$).

Miyaoka, H. *et al., Tetrahedron*, 1999, **55**, 12977-12982 (*isol, pmr, cmr*)

4,18-Dihydroxy-1(9),6,13-xenicatrien-19-al D-858



$C_{20}H_{32}O_3$ 320.471

Abs. config. of these xenicanes from brown algae confirmed (1990) as being opposite to those isol. from soft corals.

18-Ac: ***Fukurinolal****. Hydroxyacetyldictyolal*

[84164-85-2]

$C_{22}H_{34}O_4$ 362.508

Constit. of brown seaweed *Dilophus okamurai* and *Dictyota dichotoma*. Cryst.

Mp 79-80°. $[\alpha]_D^{18}$ -189 (c, 0.20 in $CHCl_3$).

18-Aldehyde: 4-Hydroxy-1(19),6,13-xenicatriene-18,19-dial. ***Hydroxydictyodial***

[89482-11-1]

$C_{20}H_{30}O_3$ 318.455

From *Dictyota crenulata*. Cryst. or oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 79-81°. $[\alpha]_D^{25}$ -121 (c, 0.33 in EtOH). $[\alpha]_D$ -256 (c, 2.41 in $CHCl_3$). λ_{max} 228 (ϵ 5000) (MeOH) (Berdy).

18-Aldehyde, 4-Ac: ***4-Acetoxydictyodial****. 4-Acetyldictyodial (incorr.)*

[760996-47-2]

$C_{22}H_{32}O_4$ 360.492

Constit. of *Dictyota linearis*. Oil. $[\alpha]_D^{20}$ -163.6 (c, 0.3 in CH_2Cl_2).

*6*R*,7*R*-Epoxide, 18-Ac:* ***6,7-Epoxyfukurinolal***

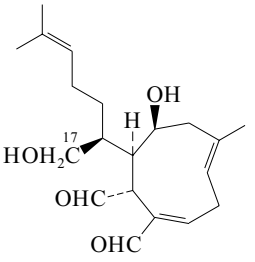
$C_{22}H_{34}O_5$ 378.508

Isol. from *Dictyota* sp. Cryst.

Mp 53-54°. $[\alpha]_D$ -80.7 (c, 0.29 in $CHCl_3$).

Enoki, N. *et al., Chem. Lett.*, 1982, 1749-1752 (*Hydroxyacetyldictyolal*)
Ochi, M. *et al., Chem. Lett.*, 1982, 1927-1930 (*Fukurinolal*)
Tanaka, J. *et al., Chem. Lett.*, 1984, 231 (*Hydroxydictyodial*)
Norte, M. *et al., Tetrahedron*, 1990, **46**, 6125 (*isol, abs config, epoxide*)
Siamopoulou, P. *et al., Phytochemistry*, 2004, **65**, 2025-2030 (*4-Acetoxydictyodial*)

4,17-Dihydroxy-1(9),6,13-xenicatriene-18,19-dial D-859



$C_{20}H_{30}O_4$ 334.455

(1(9)*E*,4*S*,6*E*,10*S*)-*form*

17-Ac: 17-Acetoxy-4-hydroxy-1(9),6,13-xenicatriene-18,19-dial

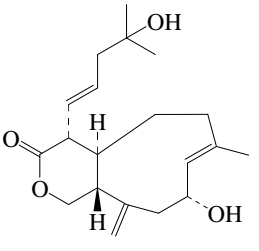
[133585-91-8]

$C_{22}H_{32}O_5$ 376.492

Constit. of *Dictyota divaricata*. Oil. $[\alpha]_D^{25}$ -128.8 (c, 0.08 in $CHCl_3$).

König, G.M. *et al., Tetrahedron*, 1991, **47**, 1399-1410 (*Dictyota divaricata constit*)

8,14-Dihydroxy-1(19),6,11-xenicatrien-17,18-olide D-860



$C_{20}H_{30}O_4$ 334.455

(6*E*,8α,11*E*)-*form*

Dihydroxeniolide A

[663154-57-2]

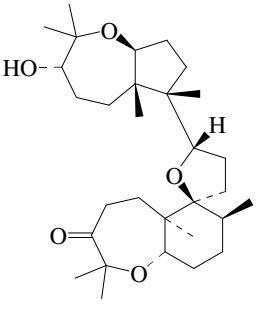
Constit. of a *Xenia* sp.

Oil. $[\alpha]_D^{25}$ -31.2 (c, 1.21 in $CHCl_3$).

Miyaoka, H. *et al., Heterocycles*, 2003, **61**, 189-196 (*isol, pmr, cmr, abs config*)

22-Dihydroyardenone D-861

[233607-63-1]



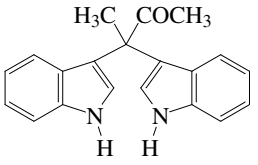
$C_{30}H_{50}O_5$ 490.722

Constit. of *Ptilocaulis spiculifer*. Oil. $[\alpha]_D$ +3.3 (c, 0.1 in MeOH).

Rudi, A. *et al., Tetrahedron*, 1999, **55**, 5555-5566 (*isol, pmr, cmr*)

3,3-Di-1*H*-indol-3-yl-2-butanone D-862

[28926-40-1]

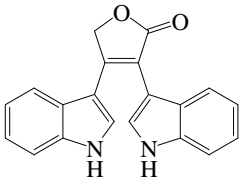


$C_{20}H_{18}N_2O$ 302.375
Isol. from the marine bacterium *Vibrio parahaemolyticus* Bio249. Pale yellow solid.
Mp 197° (synthetic). λ_{max} 274 (sh) (log ϵ 2.91); 281 (log ϵ 2.94); 289 (log ϵ 2.89) (MeOH).

Zhungietu, G.I. *et al., CA*, 1970, **73**, 25230u (*synth*)
Veluri, R. *et al., J. Nat. Prod.*, 2003, **66**, 1520-1523 (*isol, pmr, cmr, ms*)

3,4-Di-1*H*-indol-3-yl-2(5*H*)-furanone, 9CI D-863

[244295-63-4]

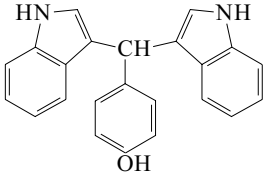


$C_{20}H_{14}N_2O_2$ 314.343
Prod. by *Paracoccus* sp. UV absorbent.

Japan. Pat., 1999, 99 269 175; *CA*, **131**, 242087s

4-[(Di-1*H*-indol-3-yl)methyl]phenol, 9CI D-864

7,7-Bis(3-indolyl)-p-*cresol. 4-Hydroxyphenyldi-3-indolylmethane*
[151358-47-3]



$C_{23}H_{18}N_2O$ 338.408
Isol. from a strain of the bacterium *Vibrio* sp. obtained from a marine sponge *Hyatella* sp. Exhibits antimicrobial activity. Gum. λ_{max} 224 (ϵ 52500); 282 (ϵ 11500) (MeOH) (Derep).

Oclarit, J.M. *et al., Nat. Prod. Lett.*, 1994, **4**, 309-312 (*isol, pmr, cmr, uv, ir*)

Diiodoacetic acid D-865

[598-89-0]
$I_2CHCOOH$
$C_2H_2I_2O_2$ 311.846
Constit. of *Asparagopsis taxiformis*. Pale-yellow needles ($CHCl_3$). Mod. sol. H_2O.
Mp 110-111°.

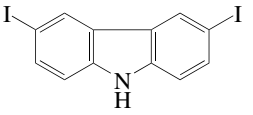
Amide: Diiodoacetamide
[5875-23-0]
$C_2H_3I_2NO$ 310.861
Constit. of *Asparagopsis taxiformis*. Cryst. (H_2O).
Mp 201-202° dec. (softens at 198°).

[82665-91-6]

Clarke, L. *et al., J.A.C.S.*, 1914, **36**, 1899-1908 (*synth*)
Cobb, R.L. *et al., J.O.C.*, 1958, **23**, 1368-1405 (*synth*)
Woolard, F.X. *et al., Tetrahedron*, 1976, **32**, 2843-2846 (*amide, isol*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617-620 (*isol*)

3,6-Diiodo-9*H*-carbazole D-866

[57103-02-3]



$C_{12}H_7I_2N$ 419.003
Alkaloid from the cyanobacterium *Kyrtuthrix maculans*. Leaflets (EtOH).
Mp 202-204°.

N-*Ac:*
$C_{14}H_9I_2NO$ 461.04
Needles (EtOH or C_6H_6). Mp 224-225°.

N-*Me:* [90338-06-0]
$C_{13}H_9I_2N$ 433.03
Needles (hexane) or rods (Me_2CO). Mp 187° (181-182°).

N-*Benzoyl:* [96853-15-5]
$C_{19}H_{13}I_2N$ 509.127
Needles (hexane). Mp 169-172°.

N-*Ph:* [57103-21-6]
$C_{18}H_{11}I_2N$ 495.101
Needles (hexane). Mp 179-180°.

Tucker, S.H. *et al., J.C.S.*, 1926, 546-553; 1927, 1214-1221 (*synth*)
Ambrose, J.F. *et al., J. Electrochem. Soc.*, 1975, **122**, 876-894 (*synth, 9-Ph*)
Beginn, C. *et al., Macromol. Chem. Phys.*, 1994, **195**, 2353-2370 (*synth, pmr, cmr*)
Lee, S.-C. *et al., Phytochemistry*, 1999, **52**, 537-540 (*isol, pmr, cmr, ms*)
Bonesi, S.M. *et al., J. Het. Chem.*, 2001, **38**, 77-87 (*synth, ir, pmr, cmr, ms*)
Monge, M.E. *et al., J. Het. Chem.*, 2002, **39**, 933-941 (*9-Me, 9-Ph, 9-benzyl*)
Filimonov, V.D. *et al., Zh. Org. Khim.*, 2003, **39**, 924-929; *Russ. J. Org. Chem. (Engl. Transl.)*, 2003, **39**, 875-880 (*synth, ms*)

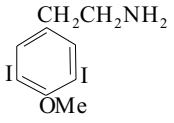
Diiodomethane, 9CI D-867

Methylene iodide
[75-11-6]
CH_2I_2
CH_2I_2 267.836
Isol. from various marine algae. Liq. Spar. sol. H_2O. d_{15}^{15} 3.33. Mp 6°. Bp 181° part. dec. Bp_{70} 106-107°. n_D^{20} 1.7405 (1.7425). Polymorphic, with 3 phases in crystalline state.
▶ Violent reaction with copper-zinc alloys. LD_{50} (rat, ipr) 403 mg/kg. PA8575000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 71D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 106B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 103B (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 358 (*synth*)
Malinowski, E.R. *et al., J. Phys. Chem.*, 1971, **75**, 3971 (*pmr*)
Kawaguchi, T. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 57 (*cryst struct*)
Altabev, N. *et al., Chem. Ind. (London)*, 1973, 331 (*synth*)
Ford, T.A. *et al., J. Mol. Spectrosc.*, 1975, **58**, 185 (*ir, Raman*)
Dostovalova, V.I. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1987, 2719; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1987, 2521 (*cmr*)
Torrie, B.H. *et al., J. Raman Spectrosc.*, 1987, **18**, 215 (*Raman*)
Torrie, B.H. *et al., Mol. Phys.*, 1989, **68**, 835 (*cryst struct*)
Abraham, M.H. *et al., J.C.S. Perkin 2*, 1993, 299 (*props*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **3**, 1899-1903 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0382
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DNF800

3,5-Diiodo-4-methoxyphenylethylamine D-868

3,5-Diiodo-4-methoxybenzenethanamine
[89631-86-7]



$C_9H_{11}I_2NO$ 403.001
Metab. of an unidentified didemnid tunicate. Isol. from the ascidian *Didemnum rubeum*. Mildly cytotoxic, antifungal. Cryst. (petrol). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 55-57°.

Hydrochloride:
Cryst. ($CHCl_3$). Mp 213-215°.

Jatzkewitz, H. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1951, **287**, 43-46 (*synth*)
Sesin, D.F. *et al., Tet. Lett.*, 1984, **25**, 403-404 (*isol, pmr, cmr, synth*)
Ford, P.W. *et al., J. Nat. Prod.*, 1997, **60**, 1051-1053 (*isol*)

1,3-Diiodo-2-propanol D-869

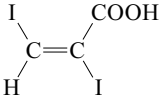
Glycerol 1,3-diiodohydrin. α-Diiodohydrin. Iotone. Iothion
[534-08-7]
$ICH_2CH(OH)CH_2I$
$C_3H_6I_2O$ 311.889
Isol. from *Asparagopsis taxiformis*. Yellow cryst. d^{15} 2.4.
Fp -20. $Bp_{0.004}$ 70°.
▶ LD_{50} (mus, orl) 325 mg/kg. UB1950000

4-Nitrobenzoyl:
Cryst. Mp 81-82°.

Fairbourne, A. *et al., J.C.S.*, 1932, 1976 (*synth*)
Lusignani, G. *et al., Boll. Chim. Farm.*, 1939, **78**, 557; *CA*, **34**, 2322 (*synth*)
de Haas, G.H. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1965, **84**, 436 (*synth*)
Woolard, F.X. *et al., Tetrahedron*, 1976, **32**, 2843 (*isol*)

2,3-Diiodo-2-propenoic acid, 9CI D-870

2,3-Diiodoacrylic acid
[24767-87-1]



(*E*)–*form*

$C_3H_2I_2O_2$ 323.857
Minor component of the aq. extract of Hawaiian red alga *Asparagopsis taxiformis*.

(*E*)-*form* [14092-48-9]
Cryst. (cyclohexane). Mp 103.5-105.5°.

Me ester: [71264-45-4]
$C_4H_4I_2O_2$ 337.883
Cryst. (CCl_4). Mp 37.5-38.5°.

Et ester: [71264-46-5]
$C_5H_6I_2O_2$ 351.91
Bp_3 67°.

(*Z*)-*form* [14173-06-9]
Needles (CCl_4). Mp 109-111.5°.

Me ester: [14092-47-8]
Liq. Mp 2-3°.

Kai, F. *et al., Chem. Pharm. Bull.*, 1966, **14**, 1122 (*synth, Me ester, ir, pmr*)
Hollins, R.A. *et al., J.O.C.*, 1979, **44**, 3931 (*synth, pmr, cmr*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617 (*isol, synth, glc, ms*)
Voegeli, V. *et al., Org. Magn. Reson.*, 1980, **13**, 200 (*cmr*)
Pagni, R.M. *et al., J.O.C.*, 1988, **53**, 4477 (*synth*)
Doad, G.J.S. *et al., J. Chem. Res., Synop.*, 1989, 313 (*Et ester, synth*)
Hénaff, N. *et al., J.C.S. Perkin 1*, 2000, 395-400 (*Z-form, Me ester, synth*)

3,3-Diiodo-2-propenoic acid, 9CI D-871

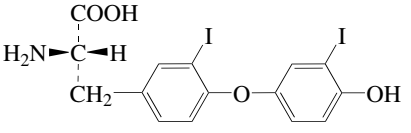
3,3-Diiodoacrylic acid, 8CI
[59110-13-3]
$I_2C{=}CHCOOH$
$C_3H_2I_2O_2$ 323.857
Minor component of the aqueous extract of Hawaiian red alga *Asparagopsis taxiformis*. Prisms (H_2O).
Mp 133°.

Octyl ester: [136354-84-2]
Liq. Bp 78-83°.

Homolka, B. *et al., Ber.*, 1885, **18**, 2282 (*synth*)
Masuda, E. *et al., Yakugaku Zasshi*, 1934, **54**, 1091 (*synth*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617 (*isol, synth, glc, ms*)
Sugimoto, J. *et al., Chem. Lett.*, 1991, 1319 (*synth, ir, pmr, ester*)

3,3′-Diiodothyronine D-872

O-*(4-Hydroxy-3-iodophenyl)-3-iodotyrosine, 9CI. 3-[4-(4-Hydroxy-3-iodophenoxy)-3-iodophenyl]alanine, 8CI*
[4604-41-5]
[70-40-6]

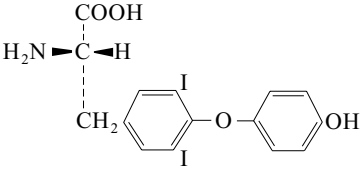


$C_{15}H_{13}I_2NO_4$ 525.081
Constit. of blood in mammals. Cryst. + $2H_2O$ (MeOH aq.).
Mp 198-199° (as dihydrate).

Gemmill, C.L. *et al., J.A.C.S.*, 1956, **78**, 2434-2436 (*synth*)
Gavin, L.A. *et al., J. Clin. Invest.*, 1978, **61**, 1276-1285 (*formn*)
Michel, R. *et al., Rev. Fr. Endocrinol. Clin., Nutr. Metab.*, 1984, **25**, 95-106 (*formn*)

3,5-Diiodothyronine D-873

O-*(4-Hydroxyphenyl)-3,5-diiodotyrosine, 9CI. β-[4-(*p*-Hydroxyphenoxy)-3,5-diiodophenyl]alanine*
[534-51-0]



(*S*)–*form*

$C_{15}H_{13}I_2NO_4$ 525.081

(*R*)-*form*
D-form
Mp 265° dec. $[\alpha]_D^{20}$ -27.1 (c, 1 in 0.35*M* EtOH/HCl).
N-*Ac:*
$C_{17}H_{15}I_2NO_5$ 567.118
Mp 143-145°. $[\alpha]_D^{19}$ -30.5 (c, 6 in dioxan).
Et ester:
$C_{17}H_{17}I_2NO_4$ 553.135
Mp 132-136°. $[\alpha]_D^{19}$ -43.4 (c, 0.99 in dioxan).

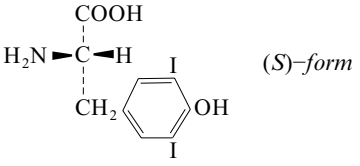
(*S*)-*form*
L-form
[1041-01-6]
Occurs in proteins of marine algae.
Mp 255° dec.
Me ether: O-*(4-Methoxyphenyl)-3,5-diiodotyrosine*
$C_{16}H_{15}I_2NO_4$ 539.108
Mp 241° dec. $[\alpha]_D^{26}$ +19.4 (EtOH/HCl). $[\alpha]_D^{22}$ -6.7 (EtOH/NaOH).

[5563-89-3]

Elks, J. *et al., J.C.S.*, 1952, 2366 (*synth*)
Cody, V. *et al., Acta Cryst. B*, 1972, **28**, 2244 (*cryst struct*)

3,5-Diiodotyrosine, 9CI D-874

2-Amino-3-(4-hydroxy-2,5-diiodophenyl)propanoic acid. Iodogorgoic acid. Agontan. Apothyrin. Cemiod. Dityrin. Flaianina. Itir. Normotiroides. Diiodogorgoic acid. Diiodogorgonic acid
[66-02-4]



(*S*)–*form*

$C_9H_9I_2NO_3$ 432.984
Thyroid inhibitor. Used to treat Graves' disease and other disorders. Log P -0.29 (uncertain value) (calc). ^{125}I and ^{131}I labelled cpds. are used as radioactive agents.

▶YP2505000

(*R*)-*form*
D-form
[16711-71-0]
Needles (AcOH aq.). Mp 194° dec. $[\alpha]_D$ +2.75 (*M* HCl).
Anhydride: Mp 204° dec.

(*S*)-*form*
L-form
[300-39-0]
Constit. of Thyroglobulin from the thyroid gland; intermed. in thyroxin biosynth. Found in skeletal proteins of corals, sponges and other marine organisms, such as *Heterochordaria abietina, Undaria pinnatifida*, *Sargassum thunbergii*, *Polysiphonia urceolata*, *Dendrodoa grossularia* and *Porphyra umbilicalis*.
Needles (H_2O or EtOH aq.).
Mp 199-200° dec. (215° dec.). $[\alpha]_D^{28}$ +2.3 (c, 5.016 in 1.1*M* HCl). $[\alpha]_D^{28}$ -2.27 (25% NH_4OH). Pharmacol. active isomer.
Hydrochloride:
Needles (MeOH/Et_2O). Mp 211° dec. Darkens at 208°.
Me ester:
$C_{10}H_{11}I_2NO_3$ 447.011
Plates (EtOH). Mp 192° dec. Darkens at 186.5°.
N-tert-*Butyloxycarbonyl:*
Cryst. (EtOAc/petrol). Mp 187-189°. $[\alpha]_D^{24}$ -10.2 (c, 2 in DMF).

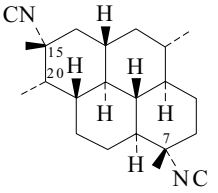
(±)-*form* [620-59-7]
Needles (EtOH aq.), plates (H_2O). Mp 195° (200°) dec. pK_{a1} 2.12; pK_{a2} 6.48; pK_{a2} 7.82 (25°).

[14679-68-6]

Block, P. *et al., J.A.C.S.*, 1943, **65**, 1430 (*synth*)
Tong, W. *et al., J. Biol. Chem.*, 1954, **207**, 59 (*metab*)
Srinivasan, M. *et al., J. Sci. Ind. Res., Sect. B*, 1954, **13**, 184; *CA*, **49**, 6879g (*synth*)
Amaral, A.D. *et al., CA*, 1972, **77**, 111749 (*occur*)
Cody, V. *et al., J. Appl. Crystallogr.*, 1972, **5**, 140 (*cryst struct*)
Ito, K. *et al., CA*, 1977, **86**, 3897 (*occur*)
Pitt-Rivers, R. *et al., Horm. Proteins Pept.*, 1978, **6**, 391 (*rev*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 9005

7,15-Diisocyanoisocycloamphilectane D-875

7,15-Diisocyanoadociane
[74799-55-6]

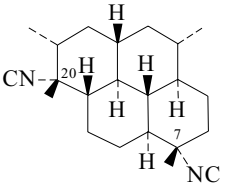


$C_{22}H_{32}N_2$ 324.508
Constit. of *Adocia* spp. Cryst. Poorly sol. hexane.
Mp 123-124°. $[\alpha]_D^{20}$ +45.8 (c, 0.7 in $CHCl_3$).

Kazlauskas, R. *et al., Tet. Lett.*, 1980, **21**, 315-318 (*cryst struct, rel config*)
Garson, M.J. *et al., Chem. Comm.*, 1986, 35-36 (*biosynth*)

7,20-Diisocyanoisocycloamphilectane D-876

7,20-Diisocyanoadociane
[60197-58-2]



$C_{22}H_{32}N_2$ 324.508
Isol. from a sponge *Adocia* sp., from the Great Barrier reef and *Cymbastela hooperi*. Potent *in vitro* antimalarial activity. Shows antimycobacterial and cytotoxic activities. Cryst. (hexane).
Mp 109-110°. $[\alpha]_D^{22}$ +47.4 (c, 0.7 in CH_2Cl_2).

7-Isothiocyanate: ***20-Isocyano-7-isothiocyanatoisocycloamphilectane***
[175861-78-6]
$C_{22}H_{32}N_2S$ 356.574
Constit. of *Cymbastela hooperi*. Shows antimycobacterial, antimalarial and cytotoxic activities. Oil. $[\alpha]_D^{25}$ +23.3 (c, 0.15 in $CHCl_3$). Has - NCS replacing - NC at C-7. λ_{max} 247 (ϵ 1250) (MeOH) (Berdy).

7-Isocyanate: ***7-Isocyanato-20-isocyanoisocycloamphilectane***
[175861-79-7]
$C_{22}H_{32}N_2O$ 340.508
Constit. of *Cymbastela hooperi*. Oil. $[\alpha]_D^{25}$ +36.1 (c, 0.75 in $CHCl_3$). Has - NCO replacing - NC at C-7.

20-Isocyanate: ***20-Isocyanato-7-isocyanoisocycloamphilectane***. *20-Isocyanato-7-isocyanoadociane*
[175861-80-0]
$C_{22}H_{32}N_2O$ 340.508
Isol. from the tropical marine sponge *Cymbastela hooperi*. Shows potent *in vitro* antimalarial activity. Oil. $[\alpha]_D^{25}$ +37 (c, 0.58 in $CHCl_3$). Has - NCO replacing - NC at C-20.

[175861-77-5]

Baker, J.T. *et al., J.A.C.S.*, 1976, **98**, 4010 (*isol, cryst struct, pmr*)
Corey, E.J. *et al., J.A.C.S.*, 1987, **109**, 287-289 (*synth*)
Fookes, C.J.R. *et al., J.C.S. Perkin 1*, 1988, 1003 (*cryst struct, biosynth*)
Koenig, G.M. *et al., Magn. Reson. Chem.*, 1995, **33**, 694 (*pmr, cmr*)
Koenig, G.M. *et al., J.O.C.*, 1996, **61**, 3259-3267 (*isol, ir, pmr, cmr, uv, ms, bibl, activity*)
Koenig, G.M. *et al., Planta Med.*, 2000, **66**, 337-342 (*activity*)
Simpson, J.S. *et al., Org. Biomol. Chem.*, 2004, **2**, 939-948 (*biosynth*)
Fairweather, K.A. *et al., Org. Lett.*, 2006, **8**, 3395-3398 (*synth*)

1,12-Diisothiocyanato-1,11-dodecadiene D-877

$SCNCH{=}CH(CH_2)_8CH{=}CHNCS$
$C_{14}H_{20}N_2S_2$ 280.457

(*Z,Z*)-*form* [111602-96-1]
Constit. of the marine sponge *Pseudaxinyssa* sp.
1,2-Dihydro: 1,12-Diisothiocyanato-1-dodecene
[111603-05-5]
$C_{14}H_{22}N_2S_2$ 282.473
Constit. of *Pseudaxinyssa* sp.
Karuso, P. *et al., Tet. Lett.*, 1987, **28**, 4633; 1988, **29**, 2506 (*isol*)

1,20-Diisothiocyanato-1-eicosene D-878

$SCN(CH_2)_{18}CH{=}CHNCS$
$C_{22}H_{38}N_2S_2$ 394.688

(*Z*)-*form* [111603-12-4]
Constit. of the marine sponge *Pseudaxinyssa* sp.
Karuso, P. *et al., Tet. Lett.*, 1987, **28**, 4633; 1988, **29**, 2506 (*isol*)

1,17-Diisothiocyanato-1,16-heptadecadiene D-879

$SCNCH{=}CH(CH_2)_{13}CH{=}CHNCS$
$C_{19}H_{30}N_2S_2$ 350.591

(*Z,Z*)-*form* [111603-01-1]
Constit. of the marine sponge *Pseudaxinyssa* sp.
1,2-Dihydro: 1,17-Diisothiocyanato-1-heptadecene
[111603-10-2]
$C_{19}H_{32}N_2S_2$ 352.607
Constit. of *Pseudaxinyssa* sp.
Karuso, P. *et al., Tet. Lett.*, 1987, **28**, 4633; 1988, **29**, 2506 (*isol*)

1,16-Diisothiocyanato-1,15-hexadecadiene D-880

$SCNCH{=}CH(CH_2)_{12}CH{=}CHNCS$
$C_{18}H_{28}N_2S_2$ 336.565

(*Z,Z*)-*form* [111603-00-0]
Constit. of the marine sponge *Pseudaxinyssa* sp.
1,2-Dihydro: 1,16-Diisothiocyanato-1-hexadecene
[111603-09-9]
$C_{18}H_{30}N_2S_2$ 338.58
Constit. of *Pseudaxinyssa* sp.
Karuso, P. *et al., Tet. Lett.*, 1987, **28**, 4633; 1988, **29**, 2506 (*isol*)

1,19-Diisothiocyanato-1,18-nonadecadiene D-881

$SCNCH{=}CH(CH_2)_{15}CH{=}CHNCS$
$C_{21}H_{34}N_2S_2$ 378.645

(*Z,Z*)-*form*
Constit. of the marine sponge *Pseudaxinyssa* sp.
1,2-Dihydro: 1,19-Diisothiocyanato-1-nonadecene
[111603-11-3]
$C_{21}H_{36}N_2S_2$ 380.661
Constit. of *Pseudaxinyssa* sp.
Karuso, P. *et al., Tet. Lett.*, 1987, **28**, 4633; 1988, **29**, 2506 (*isol*)

1,18-Diisothiocyanato-1,17-octadecadiene D-882

$SCNCH{=}CH(CH_2)_{14}CH{=}CHNCS$
$C_{20}H_{32}N_2S_2$ 364.618

(*Z,Z*)-*form* [111603-02-2]
Constit. of the marine sponge *Pseudaxinyssa* sp. λ_{max} 221 (ϵ 70000); 265 (ϵ 12200) (hexane) (Derep). λ_{max} 205 (ϵ 12200); 221 (ϵ 70000) (hexane) (Berdy).
1,2-Dihydro: 1,18-Diisothiocyanato-1-octadecene
[111603-03-3]
$C_{20}H_{34}N_2S_2$ 366.634
Constit. of *Pseudaxinyssa* sp. λ_{max} 212 (ϵ 69500); 262 (sh) (ϵ 12300); 270 (ϵ 13400) (hexane) (Derep). λ_{max} 212 (ϵ 69500); 270 (ϵ 13400) (hexane) (Berdy).
Karuso, P. *et al., Tet. Lett.*, 1987, **28**, 4633; 1988, **29**, 2506 (*isol, uv, ir, pmr, cmr*)

1,15-Diisothiocyanato-1,14-pentadecadiene D-883

$SCNCH{=}CH(CH_2)_{11}CH{=}CHNCS$
$C_{17}H_{26}N_2S_2$ 322.538

(*Z,Z*)-*form* [111602-99-4]
Constit. of the marine sponge *Pseudaxinyssa* sp.
1,2-Dihydro: 1,15-Diisothiocyanato-1-pentadecene
[111603-08-8]
$C_{17}H_{28}N_2S_2$ 324.554
Constit. of *Pseudaxinyssa* sp.
Karuso, P. *et al., Tet. Lett.*, 1987, **28**, 4633; 1988, **29**, 2506 (*isol*)

1,14-Diisothiocyanato-1,13-tetradecadiene D-884

$SCNCH{=}CH(CH_2)_{10}CH{=}CHNCS$
$C_{16}H_{24}N_2S_2$ 308.511

(*Z,Z*)-*form* [111602-98-3]
Constit. of the marine sponge *Pseudaxinyssa* sp.
1,2-Dihydro: 1,14-Diisothiocyanato-1-tetradecene
[111603-07-7]
$C_{16}H_{26}N_2S_2$ 310.527
Constit. of *Pseudaxinyssa* sp.
Karuso, T. *et al., Tet. Lett.*, 1987, **28**, 4633; 1988, **29**, 2506 (*isol*)

1,13-Diisothiocyanato-1,12-tridecadiene D-885

$SCNCH{=}CH(CH_2)_9CH{=}CHNCS$
$C_{15}H_{22}N_2S_2$ 294.484

(*Z,Z*)-*form* [111602-97-2]
Constit. of the marine sponge *Pseudaxinyssa* sp.
1,2-Dihydro: 1,13-Diisothiocyanato-1-tridecene
[111603-06-6]
$C_{15}H_{24}N_2S_2$ 296.5
Constit. of *Pseudaxinyssa* sp.
Karuso, P. *et al., Tet. Lett.*, 1987, **28**, 4633; 1988, **29**, 2506 (*isol*)

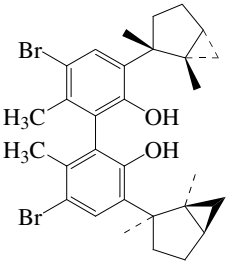
1,11-Diisothiocyanato-1-undecene D-886

$SCN(CH_2)_9CH{=}CHNCS$
$C_{13}H_{20}N_2S_2$ 268.446

(*Z*)-*form* [111603-04-4]
Constit. of the marine sponge *Pseudaxinyssa* sp.
Karuso, P. *et al., Tet. Lett.*, 1987, **28**, 4633; 1988, **29**, 2506 (*isol*)

8,8′-Dilaurinterol D-887

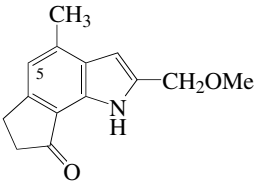
[874193-61-0]



$C_{30}H_{36}Br_2O_2$ 588.421
Error in struct. diag. in ref. Constit. of *Laurencia microcladia*. Oil. $[\alpha]_D^{20}$ -28.8 (c, 0.06 in CH_2Cl_2). λ_{max} 236 (log ϵ 3.3); 289 (log ϵ 3) (hexane).
Kladi, M. *et al., Tetrahedron*, 2006, **62**, 182-189 (*Laurencia obtusa constit*)

Dilemmaone A D-888

[205990-55-2]



$C_{14}H_{15}NO_2$ 229.278
Alkaloid probably from the sponge *Ectyonancora flabellata*. Off-white solid.
Mp 146-148°. Genus name freq. spelt Ectyonanchora. λ_{max} 250 (ϵ 8060); 310 (ϵ 4100) ($CHCl_3$).

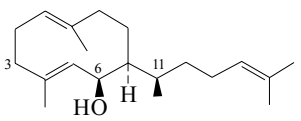
O-*De-Me:* ***Dilemmaone B***
[205990-56-3]
$C_{13}H_{13}NO_2$ 215.251
Alkaloid probably from *Ectyonancora flabellata*. Buff solid.
Mp 168-170°. λ_{max} 250 (ϵ 8420); 310 (ϵ 4230) ($CHCl_3$).

5-Hydroxy: ***Dilemmaone C***
[205990-57-4]
$C_{14}H_{15}NO_3$ 245.277
Alkaloid probably from *Ectyonancora flabellata*. Pale yellow solid.
Mp 187-190°. λ_{max} 250 (ϵ 7950); 310 (ϵ 12330) ($CHCl_3$).

Beukes, D.R. *et al., J. Nat. Prod.*, 1998, **61**, 699-701 (*isol, uv, ir, pmr, cmr, ms*)

Dilophol D-889

[62853-97-8]



Absolute configuration

$C_{20}H_{34}O$ 290.488
Constit. of algae *Dilophus ligulatus* and *Dictyota dichotoma*.
$[\alpha]_D$ -4.3.

Ac: ***Acetyldilophol***
$C_{22}H_{36}O_2$ 332.525
Constit. of brown alga *Pachydictyon coriaceum*.
$[\alpha]_D$ -30.9 (c, 0.57 in $CHCl_3$).

3β-Hydroxy: ***3-Hydroxydilophol***
$C_{20}H_{34}O_2$ 306.487
Metab. of *Dictyota divaricata*. Oil. $[\alpha]_D^{25}$ -27.3 (c, 0.02 in $CHCl_3$).

3β-Hydroxy, 6-Ac: ***3-Hydroxyacetyldilophol***
$C_{22}H_{36}O_3$ 348.525
Constit. of *Pachydictyon coriaceum*.
$[\alpha]_D$ -7.2 (c, 0.64 in $CHCl_3$).

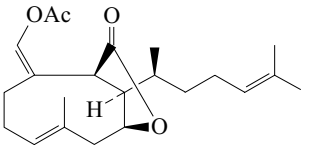
3β-Hydroxy, di-Ac: ***3-Acetoxyacetyldilophol***
$C_{24}H_{38}O_4$ 390.562
Constit. of *Dictyota dichotoma*. Cryst. (hexane).
Mp 73-74°. $[\alpha]_D^{25}$ +7.9 (c, 2.2 in $CHCl_3$).

11ξ-Hydroxy: ***Hydroxydilophol***
[69204-66-6]
$C_{20}H_{34}O_2$ 306.487
Isol. from *Dictyota mansonii*. Oil. $[\alpha]_D^{20}$ -35 (c, 1.4 in $CHCl_3$).

Amico, V. *et al., Chem. Comm.*, 1976, 1024 (*isol*)
Sun, H.H. *et al., J.O.C.*, 1979, **44**, 1354 (*Hydroxydilophol*)
Enoki, N. *et al., Chem. Lett.*, 1984, 459 (*cryst struct*)
Ishitsuka, M. *et al., Tet. Lett.*, 1986, **27**, 2639 (*isol*)
König, G.M. *et al., Phytochemistry*, 1991, **30**, 3679 (*isol, pmr, cmr*)

Dilopholide D-890

[153415-49-7]

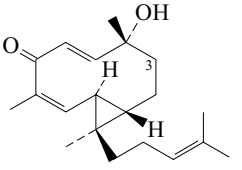


$C_{22}H_{32}O_4$ 360.492
Constit. of *Dilophus ligulatus*. Oil. $[\alpha]_D$ -113.7 (c, 0.86 in $CHCl_3$). λ_{max} 217 (ϵ 5624) (MeOH) (Berdy).

Bouaicha, N. *et al., J. Nat. Prod.*, 1993, **56**, 1747 (*isol, pmr, cmr*)

Dilopholone D-891

[70142-88-0]



$C_{20}H_{30}O_2$ 302.456
Constit. of *Dilophus prolificans*. Oil. $[\alpha]_D^{20}$ +172 (c, 0.3 in $CHCl_3$).

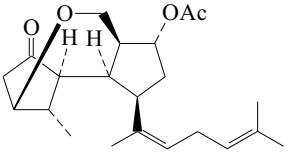
3α-Acetoxy: ***Acetoxydilopholone***
[70142-87-9]
$C_{22}H_{32}O_4$ 360.492
Cryst. Mp 179°. $[\alpha]_D^{20}$ -58 (c, 0.5 in $CHCl_3$).

3β-Acetoxy: ***Epiacetoxydilopholone***. epi-*Acetoxydilopholone*
[70191-50-3]
$C_{22}H_{32}O_4$ 360.492
Isol. from *Dilophus prolificans*. Cryst.
Mp 104-105°. $[\alpha]_D^{20}$ +162 (c, 0.32 in $CHCl_3$).

Enoki, N. *et al., Chem. Lett.*, 1964, 459
Kazlauskas, R. *et al., Tet. Lett.*, 1978, 4155

Dilophus ether D-892

[121940-50-9]

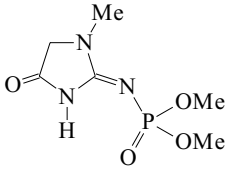


$C_{22}H_{32}O_4$ 360.492
Constit. of alga *Dilophus okamurai*. Antifeedant. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -69 (c, 0.860 in $CHcl_3$).

Kurata, K. *et al., Tet. Lett.*, 1989, **30**, 1567

Dimethyl N^2-creatininylphosphate D-893

[145644-08-2]



$C_6H_{12}N_3O_4P$ 221.152
Isol. from the sponge *Ulosa ruetzleri*.
Mp 154-155°.

Van Wagenen, B.C. *et al., J.O.C.*, 1993, **58**, 335 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)

Dimethyl sulfide D-894

Thiobismethane, 9CI. Methyl sulfide
[75-18-3]
MeSMe
C_2H_6S 62.135
Manuf. by reaction of methanol and hydrogen sulfide. Isol. from green and red algae and higher plants. Selective reducing agent; reagent for *ortho*-alkylation of aromatic amines. Used with diborane as effective reducing agent for esters, amides, etc. Liq. d_4^{25} 1.44.
Fp -98.27. Bp 37.5-38°.

▶ Highly flammable, fl. p. -34°, autoignition temp. 206°. Skin and eye irritant. LD_{50} (rat, orl) 3300 mg/kg. Stench. PV5075000

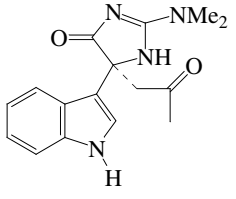
S-*Oxide:* See Dimethyl sulfoxide in *The Combined Chemical Dictionary.*

S,S-*Dioxide:* See Dimethyl sulfone in *The Combined Chemical Dictionary.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 264B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 425A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 347B (*ir*)
Finckh, J. *et al., Ber.*, 1894, **27**, 1239 (*synth*)
McAllan, D.T. *et al., J.A.C.S.*, 1951, **73**, 3627 (*synth*)
Pettit, G.R. *et al., Can. J. Chem.*, 1964, **42**, 2357 (*pmr*)
Scott, J.D. *et al., J. Chem. Phys.*, 1973, **59**, 6577 (*uv*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 260 (*use*)
Zack, N.R. *et al., J. Fluorine Chem.*, 1975, **5**, 153 (*ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 365 (*rev, tox*)
Cataliotti, R.S. *et al., Can. J. Phys.*, 1986, **64**, 100 (*ir, Raman*)
Piras, P.P. *et al., Synthesis*, 1990, 329 (*synth*)
Casida, J.E. *et al., J. Agric. Food Chem.*, 1992, **40**, 1425 (*pmr, cmr*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **3**, 2135-2138 (*use*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0878
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TFP000

2-(Dimethylamino)-1,5-dihydro-5-(1*H*-indol-3-yl)-5-(2-oxopropyl)-4*H*-imidazol-4-one, 9CI D-895

[205117-53-9]

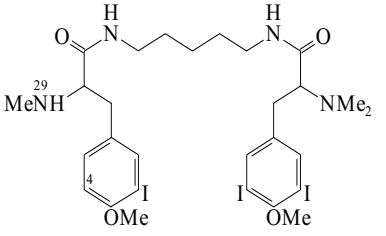


$C_{16}H_{18}N_4O_2$ 298.344
Isol. from the marine tunicate *Dendrodoa grossularia*. Powder. Mp 265-266°. $[\alpha]_D$ -15 (c, 0.14 in MeOH).

Loukaci, A. *et al., J. Nat. Prod.*, 1998, **61**, 519-522 (*isol, pmr, cmr*)

α-(Dimethylamino)-3,5-diiodo-*N*-[5-[[3-(3-iodo-4-methoxyphenyl)-2-(methylamino)-1-oxopropyl]amino]pentyl]-4-methoxybenzenepropanamide, 9CI D-896

3-(3,5-Diiodo-4-methoxyphenyl)-2-dimethylamino-3′-(3-iodo-4-methoxyphenyl)-2′-methylamino-N,N′-*(1,5-pentanediyl)bispropanamide*
[149196-93-0]



$C_{28}H_{39}I_3N_4O_4$ 876.354
Alkaloid from the colonial ascidian *Aplidium* sp. Glutathione reductase inhibitor. Gum. $[\alpha]_D$ -0.74 (c, 0.24 in $CHCl_3$). λ_{max} 210 (ε 40000); 222 (ε 39000); 278 (ε 9200) (EtOH) (Berdy).

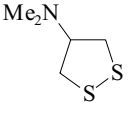
N^{29}-*Me:* ***3-(3,5-Diiodo-4-methoxyphenyl)-3′-(3-iodo-4-methoxyphenyl)-N,N′-(1,5-pentanediyl)bis[2-dimethylaminopropanamide]***
[149196-91-8]
$C_{29}H_{41}I_3N_4O_4$ 890.381
From *Aplidium* sp. Cytotoxic. Shows inhibition of glutathione reductase activity. Needles ($CHCl_3$/EtOAc).
Mp 135-137°. $[\alpha]_D$ -0.23 (c, 0.51 in $CHCl_3$).

4-Iodo, N^{29}-*Me:* ***N,N′-(1,5-Pentanediyl)bis[3-(3,5-diiodo-4-methoxyphenyl)-2-dimethylaminopropanamide]***
[149196-92-9]
$C_{29}H_{40}I_4N_4O_4$ 1016.277
From *Aplidium* sp. Cytotoxic. Shows inhibition of glutathione reductase activity. Needles ($CHCl_3$/EtOAc).
Mp 114-116°. $[\alpha]_D$ -0.2 (c, 0.35 in $CHCl_3$). λ_{max} 207 (ε 32000); 275 (ε 8400) (EtOH) (Berdy).

Carroll, A.R. *et al., Aust. J. Chem.*, 1993, **46**, 825-832 (*isol, uv, ir, pmr, cmr, ms, struct*)

4-Dimethylamino-1,2-dithiolane D-897

N,N-*Dimethyl-1,2-dithiolan-4-amine, 9CI, 8CI.* ***Nereistoxin***
[1631-58-9]



$C_5H_{11}NS_2$ 149.281
Isol. from the marine annelid worms *Lumbriconereis heteropoda* and *Lumbriconereis brevicirra*. Neurotoxin; shows unusual toxicity against insects, has been prod. synthetically. Marketed in Japan. Liq. Bp 212-213°. λ_{max} 330 (MeOH) (Berdy).

▶ JP0470000

Oxalate (1:1): [1631-52-3]
Mp 173-174° dec.

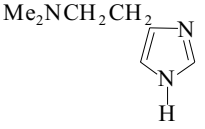
Picrate:
Needles (EtOH). Mp 169°.

Hashimoto, Y. *et al., Ann. N.Y. Acad. Sci.*, 1960, **90**, 669 (*isol*)
Okaichi, T. *et al., Agric. Biol. Chem.*, 1962, **26**, 224-227 (*struct, pmr, pharmacol*)
Konishi, K. *et al., Agric. Biol. Chem.*, 1970, **34**, 926; 935; 1549 (*synth, pmr, uv*)
Hashimoto, Y. *et al., Food-Drugs Sea, Proc. Conf., 3rd*, 1972, 129 (*rev, bibl*)
Satelle, D.B. *et al., Crop Prot. Agents Their Biol. Eval., Proc. Int. Conf.*, 1975, 421 (*pharmacol*)

4-[2-(Dimethylamino)ethyl]imidazole, 8CI D-898

N,N-*Dimethyl-1*H-*imidazole-4-ethanamine, 9CI*. **N$^{\alpha}$,N$^{\alpha}$-*Dimethylhistamine*.** *Hippospongine*†

[673-46-1]



$C_7H_{13}N_3$ 139.2

The application of the name Hippospongine to this compound is tentative. Alkaloid from *Echinocereus blanckii*, *Echinocereus triglochidiatus*, *Echinocereus triglochidiatus neomexicanus*, *Casimiroa edulis* seeds (Cactaceae, Rutaceae), the sponges *Geodia gigas* and *Ianthella* sp., and from skin extracts of amphibians, e.g. *Leptodactylus pentadactylus labyrinthicus* and *Nyctimystes disrupta* and from basidiomycete *Coprinus comatus*.

▶ NI4840000

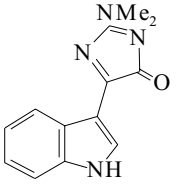
Hydrochloride (1:2): Mp 182-184°.

Dipicrate: Mp 229-230°.

Ackermann, D. *et al., Z. Biol. (Munich)*, 1924, **82**, 278 (*isol*)
Garforth, B. *et al., J.C.S.*, 1935, 489 (*synth*)
Huebner, C.F. *et al., J.A.C.S.*, 1949, **71**, 3942 (*synth*)
List, P.H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1958, **291**, 502 (*isol*)
Major, R.T. *et al., J.O.C.*, 1958, **23**, 1564 (*isol*)
Ling, J.S.L. *et al., J. Pharmacol. Exp. Ther.*, 1958, **122**, 44A (*pharmacol*)
Erspamer, V. *et al., Experientia*, 1963, **19**, 346 (*occur*)
Ingle, P.H.B. *et al., J. Pharm. Pharmacol.*, 1963, **15**, 620 (*synth*)
Erspamer, V. *et al., Arch. Biochem. Biophys.*, 1964, **105**, 620 (*occur*)
German, V.F. *et al., J. Pharm. Sci.*, 1971, **60**, 495 (*isol, pmr, ms*)
Roseghini, M. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1976, **54**, 31 (*occur*)
Roseghini, M. *et al., Z. Naturforsch., C*, 1976, **31**, 118 (*occur*)
Ferrigni, N.R. *et al., J. Ethnopharmacol.*, 1982, **5**, 359 (*isol*)
Wagner, H. *et al., Planta Med.*, 1982, **45**, 95 (*isol*)
Romero, M.L. *et al., J. Chromatogr.*, 1983, **281**, 245 (*hplc*)
Ferrigni, N.R. *et al., Rev. Latinoam. Quim.*, 1984, **14**, 131; *CA*, **101**, 23790a (*pmr, cmr*)

2-(Dimethylamino)-5-(1*H*-indol-3-yl)-4*H*-imidazol-4-one, 9CI D-899

[103590-22-3]



$C_{13}H_{12}N_4O$ 240.264

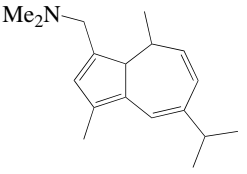
First report of a 4*H*-imidazol-4-one as a nat. prod. Isol. from the tunicate *Dendrodoa grossularia*. Orange needles (MeOH). Mp 356-358°. Sensitive to light in soln. λ_{max} 213 (ϵ 15300); 261 (ϵ 7140); 284 (ϵ 6010); 343 (ϵ 5120); 430 (ϵ 5360) (EtOH) (Derep).

Guyot, M. *et al., Tet. Lett.*, 1986, **27**, 2621-2622 (*isol, uv, ir, pmr, cmr, ms, struct, synth*)
Dalkafouki, A. *et al., Tet. Lett.*, 1991, **32**, 5325 (*synth*)

1-(Dimethylaminomethyl)-5-isopropyl-3,8-dimethylazulene D-900

N,N,*3,8-Tetramethyl-5-(1-methylethyl)-1-azulenemethanamine, 9CI*. N,N-*Dimethylamino-3-guaiazulenylmethane*

[88141-88-2]



$C_{18}H_{25}N$ 255.402

Constit. of blue gorgonian (family Paramuriceidae). Viscous blue oil. λ_{max} 242 (ϵ 28000); 293 (ϵ 31400); 305 (sh) (ϵ); 351 (ϵ 4400); 368 (ϵ 4400); 620 (ϵ 420) ($CHCl_3$/HI salt) (Derep). λ_{max} 247 (ϵ 23600); 293 (ϵ 36600); 307 (sh) (ϵ 18500); 355 (ϵ 5560); 372 (ϵ 4870); 612 (ϵ 460) ($CHCl_3$) (Derep).

[93801-01-5]

Li, M.K.W. *et al., Tet. Lett.*, 1984, **25**, 4707-4708 (*isol, struct*)

Dimethylarsinic acid, 9CI D-901

Cacodylic acid. Hydroxydimethylarsine oxide. Ansar. Phytar. Many other names

[75-60-5]

$Me_2As(O)OH$

$C_2H_7AsO_2$ 137.998

Possesses H-bonded centrosymmetric dimer struct. Common metab. of arsenite and arsenate. Synth. from Me_2AsX (X = Cl, I). Occurs in *Mytilus edulis* (mussels), *Crassostrea gigas* (oysters), *Cerastoderma edulis* (cockles), *Hizikia fusiforme*, *Porphyra tenera*, *Fucus serratus* and many other marine organisms. Putative biosynthetic intermed. of arseno-substd. ribose compds. Herbicide; has been used in chronic eczema and as a tonic. Colourless odourless cryst. (MeOH, 2-propanol, EtOH). V. sol. H_2O; sol. EtOH; insol. Et_2O.
Mp 195-197° Mp 200°. pK_a 6.15 (25°).

▶ Skin and eye irritant. LD_{50} (rat, orl) 644 mg/kg. Exp. reprod. and teratogenic effects. Tumour promoting props. CH7525000

Na salt: [124-65-2] Defoliant.

▶ CH7700000

Propyl ester: Propyl dimethylarsinate. Dimethylpropoxyarsine oxide
[70096-42-3]
$C_5H_{13}AsO_2$ 180.078
Solid. Mp 37-38°. $Bp_{0.015}$ 109-110°.

Butyl ester: Butyl dimethylarsinate. Butoxydimethylarsine oxide
[16270-48-7]
$C_6H_{15}AsO_2$ 194.105
Liq. Bp_1 132°.

[53106-49-3, 69486-80-2]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 1016B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1137A (*ir*)
Challenger, F. *et al., J.C.S.*, 1935, 396-400 (*synth*)
Trotter, J. *et al., J.C.S.*, 1965, 4466-4471 (*cryst struct*)
Levskaya, G.S. *et al., Zh. Obshch. Khim.*, 1967, **37**, 905; *J. Gen. Chem. USSR (Engl. Transl.)*, 1967, **37**, 855 (*deriv*)
Stec, W.J. *et al., Inorg. Chem.*, 1972, **11**, 219 (*pe*)
Simon, A. *et al., Z. Anorg. Allg. Chem.*, 1973, **400**, 294 (*ir, Raman*)
Gruendler, H.-V. *et al., J. Mol. Struct.*, 1974, **21**, 149 (*Raman, ir*)
Vansant, F.K. *et al., J. Mol. Struct.*, 1974, **22**, 273 (*deriv, ir, Raman*)
Moore, L.O. *et al., Encycl. Chem. Process. Des.*, 1977, **3**, 396 (*rev*)
Zakirov, D.U. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1977, 910; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1977, 834 (*nqr*)
Dietz, E.A. *et al., Anal. Methods Pestic. Plant Growth Regul.*, 1978, **10**, 385
Cullen, W.R. *et al., Can. J. Microbiol.*, 1979, **25**, 1201-1205 (*occur*)
Gamayurova, V.S. *et al., Zh. Obshch. Khim.*, 1979, 49; 174; *J. Gen. Chem. USSR (Engl. Transl.)*, 1979, **49**, 153 (*deriv*)
Edmonds, J.S. *et al., J.C.S. Perkin 1*, 1983, 2375 (*pmr, cmr*)
Joannidou, M. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1984, **81**, 397 (*ir, Raman*)
Spall, W.D. *et al., Anal. Chem.*, 1986, **58**, 1340 (*hplc*)

Dangerous Prop. Ind. Mater. Rep., 1986, **6**, 33; *CA*, **104**, 191996 (*rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 66
Sastry, D.L. *et al., Chem. Phys. Lett.*, 1988, **146**, 422 (*cmr, nqr*)
Cullen, W.R. *et al., Chem. Rev.*, 1989, **89**, 713-764 (*rev*)
Shibata, Y. *et al., Appl. Organomet. Chem.*, 1990, **4**, 255-260 (*occur, anal*)
Pesticide Manual, 9th edn., 1991, 4910
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A954
Edmonds, J.S. *et al., Nat. Prod. Rep.*, 1993, **10**, 421-42 (*occur, biosynth, metab, rev*)
Yamamoto, S. *et al., Appl. Organomet. Chem.*, 1994, **8**, 197 (*tox*)
Le, S.X.C. *et al., Environ. Sci. Technol.*, 1994, **28**, 1598-1604 (*occur*)
Gomez-Ariza, J.L. *et al., Analyst (London)*, 2000, **125**, 401-407 (*occur*)
McSheehy, S. *et al., J. Anal. At. Spectrom.*, 2000, **15**, 79-87 (*occur, anal, ms*)
Madsen, A.D. *et al., J. Anal. At. Spectrom.*, 2000, **15**, 652-662 (*occur, anal, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, HKC000; HKC500

2-(Dimethylarsinothioyl)acetic acid D-902

$Me_2As(S)CH_2COOH$

$C_4H_9AsO_2S$ 196.102

Isol. from the urine of an Orcadian sheep feeding on seaweed.

Hansen, H.R. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 337-340 (*isol, synth, ms*)

N-[4-(Dimethylarsinoyl)butanoyl]aminoethylsulfonic acid D-903

N-*[4-(Dimethylarsinoyl)butanoyl]taurine*

[142732-42-1]

$Me_2As(O)CH_2CH_2CH_2CONHCH_2CH_2SO_3H$

$C_8H_{18}AsNO_5S$ 315.221

Constit. of the kidney of *Tridacna maxima*. Needles. Mp 215-216°.

Francesconi, K.A. *et al., J.C.S. Perkin 1*, 1992, 1349 (*isol, synth*)

2-(Dimethylarsinoyl)ethanol D-904

β-Hydroxyethyldimethylarsine oxide. Dimethyloxarsylethanol

[82563-93-7]

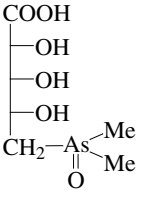
$Me_2As(O)CH_2CH_2OH$

$C_4H_{11}AsO_2$ 166.051

Synth. from the corresp. arsine and HgO, and from $[Me_2As(O)]_2O$ and 2-chloroethanol. Isol. from the brown kelp *Ecklonia radiata* anaerobically incubated. Prob. intermed. in the biosynth. of arsenobetaine from arsenic-contg. sugars in marine organisms. Needles (MeOH/Me_2CO). Mp 96° Mp 148-149.5° Mp 153-156°.

Edmonds, J.S. *et al., Experientia*, 1982, **38**, 643
Edmonds, J.S. *et al., J.C.S. Perkin 1*, 1983, 2375 (*pmr, cmr*)
Pham Ba Chi, *et al., Z. Anorg. Allg. Chem.*, 1983, **498**, 64 (*synth, pmr, ir*)
Kaise, T. *et al., Appl. Organomet. Chem.*, 1988, **2**, 339 (*synth, pmr, cmr, ms*)

5-(Dimethylarsinoyl)-D-2,3,4-trihydroxypentanoic acid D-905



$C_7H_{15}AsO_6$ 270.114

(2*R*,3*S*,4*S*)-*form*

5-Deoxy-5-(dimethylarsinoyl)-D-ribonic acid

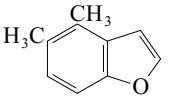
[370868-36-3]

Isol. from kidney of the giant clam *Tridacna derasa*.

Francesconi, K.A. *et al., Rapid Commun. Mass Spectrom.*, 2001, **15**, 1641-1646 (*isol, ms, struct*)

4,5-Dimethylbenzofuran D-906

[97457-29-9]



$C_{10}H_{10}O$ 146.188

Constit. of the red alga *Desmia hornemanni*.

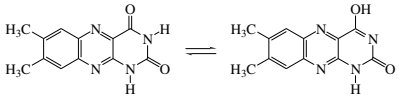
Higa, T. *et al., Tet. Lett.*, 1985, **26**, 2335

7,8-Dimethylbenzo[*g*]pteridine-2,4(1*H*,3*H*)-dione, 9CI D-907

7,8-Dimethylalloxazine. ***Lumichrome***

[1086-80-2]

[809279-55-8 (Isolumichrome)]



$C_{12}H_{10}N_4O_2$ 242.237

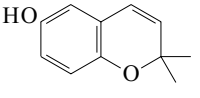
The 4-OH tautomer, called Isolumichrome in the lit., appears to be separately isolable. The reported Mp was the same. Irradiation product of Riboflavine, R-48. Prod. by *Micromonospora* sp. Tü 6368 and *Paecilomyces* sp. J300. Also isol. (as Isolumichrome) from the marine sponge *Cinachyrella australiensis*. Pale yellow cryst. ($CHCl_3$ or AcOH aq.). Spar. sol. H_2O, EtOH, $CHCl_3$. Mp 300° dec. Blue fluor. in soln. λ_{max} 211 (log ϵ 4.53); 242 (log ϵ 4.54); 252 (sh) (log ϵ 4.47); 258 (log ϵ 4.66); 331 (log ϵ 3.93); 377 (log ϵ 3.87) (MeOH).

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 768B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 894D (*ir*)
Karrer, P. *et al., Helv. Chim. Acta*, 1934, **17**, 1010 (*isol*)
Seng, F. *et al., Angew. Chem., Int. Ed.*, 1972, **11**, 1010 (*synth*)
Yoneda, F. *et al., J.A.C.S.*, 1976, **98**, 830 (*synth*)
Villemin, D. *et al., Synth. Commun.*, 1995, **25**, 2319 (*synth, ms*)
Sikorska, E. *et al., Pol. J. Chem. (Rocz. Chem.)*, 2003, **77**, 65-73 (*spectra*)
Kwon, H.C. *et al., Arch. Pharmacal Res.*, 2004, **27**, 604-609 (*isol, uv, pmr, cmr*)
Li, L. *et al., CA*, 2004, **142**, 52432n (*isol, Isolumichrome*)
Antal, N. *et al., J. Antibiot.*, 2005, **58**, 95-102; 103-110 (*isol, pmr, cmr*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 430

2,2-Dimethyl-2*H*-1-benzopyran-6-ol D-908

*6-Hydroxy-2,2-dimethyl-2*H*-1-benzopyran. 6-Hydroxy-2,2-dimethylchromene. 2,2-Dimethyl-6-chromenol*

[19012-99-8]



$C_{11}H_{12}O_2$ 176.215

Isol. from the marine urochordate *Aplidium californicum*. Antimutagenic agent. Cryst. (Et_2O/pentane). Mp 86-87°.

O-*Ribofuranoside:* ***Sterin A***

$C_{16}H_{20}O_6$ 308.33

Prod. by *Stereum hirsutum*. Antioxidant.

*Me ether: 6-Methoxy-2,2-dimethyl-2*H*-1-benzopyran. 6-Methoxy-2,2-dimethylchromene*

[22927-97-5]

$C_{12}H_{14}O_2$ 190.241

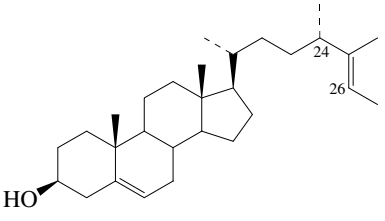
Isol. from *Ageratina aromatica, Ageratum conyzoides, Lactarius fuliginosus* and *Lactarius picinus*. Bp_6 125° $Bp_{0.5}$ 77°.

Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 2101 (*isol, deriv*)
Howard, B.M. *et al., Tet. Lett.*, 1979, **20**, 4449-4452 (*isol*)

Conca, E. *et al., Tet. Lett.*, 1981, **22**, 4327 (*isol, deriv*)
Talley, J.J. *et al., Synthesis*, 1983, 845 (*synth, deriv*)
Cortes, M.J. *et al., Heterocycles*, 1984, **22**, 1951 (*synth, deriv*)
Banerji, A. *et al., Indian J. Chem., Sect. B*, 1984, **23**, 885 (*synth*)
Timar, T. *et al., Magn. Reson. Chem.*, 1989, **27**, 303 (*cmr*)
Chauder, B.A. *et al., Synthesis*, 1998, 279-282 (*Me ether*)
Yun, B.-S. *et al., J. Antibiot.*, 2002, **55**, 208-210 (*Sterin A*)

24,26-Dimethylcholesta-5,25-dien-3-ol D-909

25-Ethylidene-27-norergost-5-en-3-ol



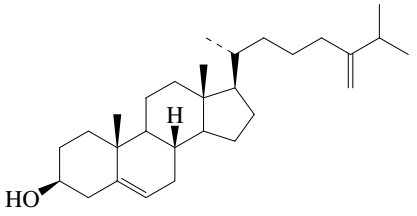
(3β,24*S*,25*E*)-*form*

$C_{29}H_{48}O$ 412.698

(3β,24*S*,25*E*)-*form*
Jaspisterol
[110012-19-6]
Constit. of the sponge *Jaspis stellifera*. Cryst. (MeOH). Mp 113-114°. $[\alpha]_D^{20}$ -44.1 (c, 10.3 in $CHCl_3$).

(3β,24*S*,25*Z*)-*form*
Isojaspisterol
[110012-18-5]
Constit. of the sponge *Jaspis stellifera*. Cryst. (MeOH). Mp 130-131°. $[\alpha]_D^{20}$ -52.8 (c, 8 in $CHCl_3$).
Cho, J.-H. *et al., J.O.C.*, 1987, **52**, 4517

27,27-Dimethylcholesta-5,25-dien-3-ol D-910

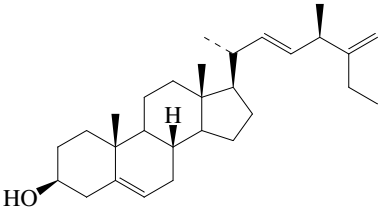


$C_{29}H_{48}O$ 412.698

3β-*form*
Azoricasterol
[810685-56-4]
Constit. of the deep-water sponge *Macandrewia azorica*. $[\alpha]_D^{20}$ -23 (c, 0.21 in CH_2Cl_2). $[\alpha]_D^{20}$ -40 (c, 0.02 in $CHCl_3$).
Gross, H. *et al., Naturwissenschaften*, 2004, **91**, 441-446

24,26-Dimethylcholesta-5,22,25(27)-trien-3-ol D-911

26-Methylergosta-5,22,25(27)-trien-3-ol

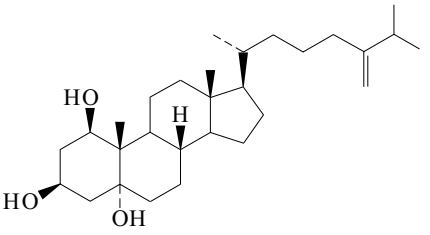


$C_{29}H_{46}O$ 410.682

(3β,22*E*,24*R*)-*form* [80525-47-9]
Isol. from the sponge *Pseudaxinella lunaecharta* from Senegal.
Sjöstrand, U. *et al., Steroids*, 1981, **38**, 355-364 (*isol, pmr, ms*)

27,27-Dimethylcholest-25-ene-1,3,5-triol D-912

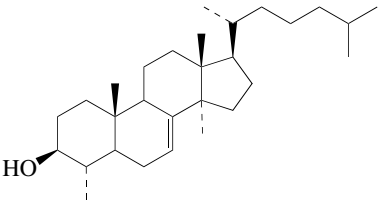
25-Methylene-22-homocholestane-1,3,5-triol



$C_{29}H_{50}O_3$ 446.712
Constit. of *Sinularia numerosa*.

(1β,3β,5α)-*form*
Numersterol B
[124596-65-2]
Constit. of *Sinularia numerosa*. Cryst. (Me_2CO/petrol). Mp 121-122°.
Su, J. *et al., J. Nat. Prod.*, 1989, **52**, 934 (*isol, pmr, cmr*)

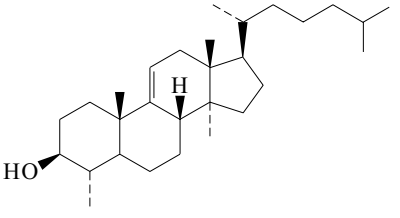
4,14-Dimethylcholest-7-en-3-ol D-913



$C_{29}H_{50}O$ 414.713

(3β,4α,5α)-*form* [28032-54-4]
Constit. of *Holothuria scabra*.
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*isol, ms*)

4,14-Dimethylcholest-9(11)-en-3-ol, 9CI D-914



$C_{29}H_{50}O$ 414.713

(3β,4α,5α)-*form* [68520-26-3]
Constit. of *Cucumaria fraudatrix*, *Cladolabes bifurcatus*, *Eupentacta fraudatrix*, *Holothuria nobilis*, *Holothuria scabra* and *Synapta maculata*. Cryst. Mp 154-155°. $[\alpha]_D^{22}$ +91.7 (c, 0.296 in MeOH).

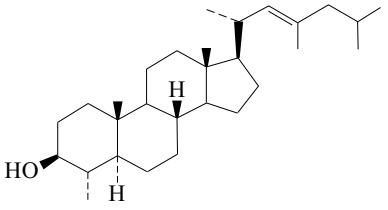
3-O-*Sulfate:* [151890-90-3]
$C_{29}H_{50}O_4S$ 494.778
Constit. of *Eupentacta fraudatrix*.

3-O-*β*-D-*Xylopyranoside:* [151890-77-6]
$C_{34}H_{58}O_5$ 546.829
Constit. of *Eupentacta fraudatrix*. Name incorr. in CAS.

Naora, M. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 1767-1776 (*synth*)
Kalinovskaya, N.I. *et al., Khim. Prir. Soedin.*, 1986, **22**, 185-187; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 172-174 (*isol, pmr, cmr*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*biosynth*)

Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*occur*)
Ponomarenko, L.P. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2001, **128**, 53-62 (*occur*)

4,23-Dimethylcholest-22-en-3-ol, 9CI D-915



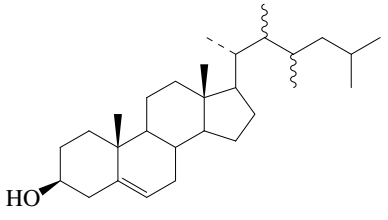
$C_{29}H_{50}O$ 414.713

(3β,4α,5α,22*E*)-*form*
24-Demethyldinosterol
[71962-35-1]
Constit. of *Gonyaulax diagenesis*, *Glenodinium foliaceum* and major sterol of dinoflagellate *Prorocentrum micans* of unknown origin. Cryst. ($CHCl_3$/MeOH). Mp 183-185°. $[\alpha]_D$ +3 (c, 0.45 in $CHCl_3$).

[70139-56-9]

Alam, M. *et al., J.O.C.*, 1979, **44**, 4466 (*isol*)
Withers, N.W. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1982, **79**, 3764 (*isol*)
Yamaguchi, T. *et al., Tohoku J. Agric. Res.*, 1986, **37**, 5 (*occur, dinoflagellate*)

22,23-Dimethylcholest-5-en-3-ol D-916

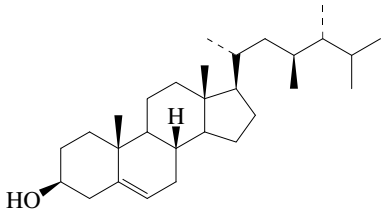


$C_{29}H_{50}O$ 414.713

(3β,22ξ,23ξ)-*form* [479411-45-5]
Constit. of a *Sinularia* sp. Cryst. (MeOH). Mp 186-188°. All four isomers earlier synthesised, but configs. not determined.
Gebreyesus, T. *et al., J.O.C.*, 1985, **50**, 154 (*synth, ms*)
Parvataneni, R. *et al., J. Indian Chem. Soc.*, 2002, **79**, 732-738 (*isol, pmr, cmr, ms*)

23,24-Dimethylcholest-5-en-3-ol D-917

23-Methylergost-5-en-3-ol
[77983-26-7]



(3β,23*S*,24*R*)-*form*

$C_{29}H_{50}O$ 414.713

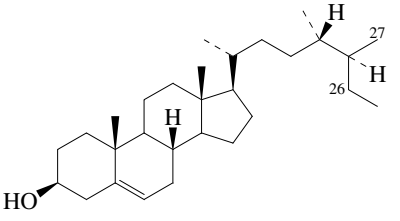
(3β,23*S*,24*R*)-*form* [86708-39-6]
Constit. of *Stelletta conulosa*.

(3β,23ξ,24ξ)-*form* [70755-55-4]
Minor sterol from dinoflagellate *Prorocentrum micans*. Isol. from *Patinopecten yessoensis* and *Gonyaulax polygramma*.

Zielinski, J. *et al., J.O.C.*, 1983, **48**, 3471-3477 (*isol, struct*)
Volkman, J.K. *et al., Lipids*, 1984, **19**, 456-465 (*Gonyaulax polygramma constit*)
Volkman, J.K. *et al., Phytochemistry*, 1999, **52**, 659-668 (*occur, dinoflagellates*)

24,26-Dimethylcholest-5-en-3-ol D-918

25-Ethyl-27-norergost-5-en-3-ol. 26-Methylergost-5-en-3-ol



$C_{29}H_{50}O$ 414.713

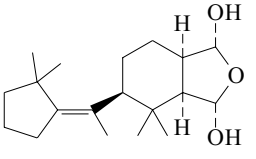
(3β,24*S*,25*S*)-*form*
Aplysterol
[38636-49-6]
Constit. of *Aplysina aerophoba*.
Cryst. (MeOH).
Mp 135-136°. $[\alpha]_D$ -25 ($CHCl_3$).

3-O-β-D-Xylopyranoside: [164728-33-0]
$C_{34}H_{58}O_5$ 546.829
Constit. of *Holothuria scabra*. Amorph. powder (MeOH).
Mp 230-232°. C-24 config. not confirmed.

25,27-Didehydro: 24,27-Dimethylcholesta-5,25-dien-3-ol. 27-Methylergosta-5,25-dien-3-ol. ***25-Dehydroaplysterol****. 25,26-Didehydroaplysterol*
[70354-61-9]
$C_{29}H_{48}O$ 412.698
Constit. of *Verongula cauliformis*. Cryst.
Mp 130-131.5°.

De Luca, P. *et al., J.C.S. Perkin 1*, 1972, 2132 (*isol*)
De Luca, P. *et al., Chem. Comm.*, 1973, 825 (*cryst struct*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195 (*pmr*)
Kokke, W.C.M.C. *et al., Tet. Lett.*, 1978, 4373-4376 (*25-Dehydroaplysterol*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 666-668 (*xyloside*)

5-[1-(2,2-Dimethylcyclopentylidene)ethyl]octahydro-4,4-dimethyl-1,3-isobenzofurandiol D-919

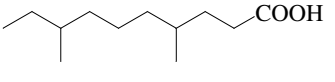


$C_{19}H_{32}O_3$ 308.46

Di-Ac: [117823-33-3]
$C_{23}H_{36}O_5$ 392.534
Constit. of *Spongionella gracilis*. Oil.
Mayol, L. *et al., Gazz. Chim. Ital.*, 1988, **118**, 559 (*isol, pmr, cmr*)

4,8-Dimethyldecanoic acid D-920

[28339-04-0]



$C_{12}H_{24}O_2$ 200.32
Constit. of the sponge *Suberites massa*. Also isol. from the ant *Atta colombica*. $Bp_{0.1}$ 99-100°.

Martin, M.M. *et al., Tetrahedron*, 1970, **26**, 307-319 (*isol, synth*)
Barnathan, G. *et al., J. Nat. Prod.*, 1993, **56**, 2104-2113 (*isol*)

4,9-Dimethyldecanoic acid D-921

$(H_3C)_2CH(CH_2)_4CH(CH_3)CH_2CH_2COOH$

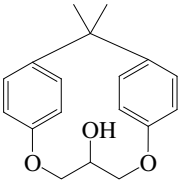
$C_{12}H_{24}O_2$ 200.32

Isol. from a halophilic *Bacillus* sp.

Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 256-259 (*isol, ms*)

11,11-Dimethyl-2,6-dioxatetracyclo[10.2.2.2^{7,10}]octadeca-1(14),7,9,12,15,17-hexaen-4-ol D-922

1,3-Di-O-*[2,2-di(*p-*phenylene)isopropylidene]glycerol*



$C_{18}H_{20}O_3$ 284.354

Constit. of *Sargassum parvivesiculosum*. Powder. λ_{max} 209; 229; 256; 277; 284 (MeOH).

Qi, S.-H. *et al., Chem. Pharm. Bull.*, 2004, **52**, 986-988 (*isol, pmr, cmr, ms*)

2,5-Dimethyldodecanoic acid D-923

2,5-Dimethyllauric acid

[100675-91-0]

$H_3C(CH_2)_6CH(CH_3)CH_2CH_2CH(CH_3)COOH$

$C_{14}H_{28}O_2$ 228.374

Isol. from the cyanobacterium *Lyngbya aestuarii*. Shows herbicidal activity. $[\alpha]_D^{22}$ -9.4 (c, 4.4 in MeOH). Config. not determined.

Me ester: [100675-92-1]

$C_{15}H_{30}O_2$ 242.401

Oil. $[\alpha]_D^{22}$ -15 (c, 0.77 in CCl_4).

(Z)-3-Acetoxy-3-bromo-1-propenyl ester: [139116-17-9]

$C_{19}H_{33}BrO_4$ 405.371

From a *Lyngbya* sp. Pale yellow oil. $[\alpha]_D$ -4.7 (c, 0.51 in $CHCl_3$).

Entzeroth, M. *et al., Phytochemistry*, 1985, **24**, 2875 (*isol*)
Hodder, A.R. *et al., J. Nat. Prod.*, 1991, **54**, 1668 (*deriv*)

4,10-Dimethyldodecanoic acid D-924

$H_3CCH_2CH(CH_3)(CH_2)_5CH(CH_3)CH_2CH_2COOH$

$C_{14}H_{28}O_2$ 228.374

Isol. from a halophilic *Bacillus* sp.

Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 256-259 (*isol, ms*)

4,11-Dimethyldodecanoic acid D-925

$(H_3C)_2CH(CH_2)_6CH(CH_3)CH_2CH_2COOH$

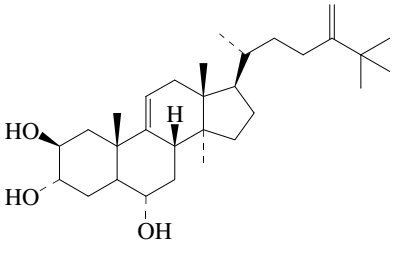
$C_{14}H_{28}O_2$ 228.374

Isol. from a halophilic *Bacillus* sp.

Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 256-259 (*isol, ms*)

14,25-Dimethylergosta-9(11),24(28)-diene-2,3,6-triol D-926

14,25-Dimethyl-24-methylenecholest-9(11)-ene-2,3,6-triol



$C_{30}H_{50}O_3$ 458.723

(2β,3α,5α,6α)-*form*

Trisulfate: ***Ibisterol sulfate C***

[350228-50-1]

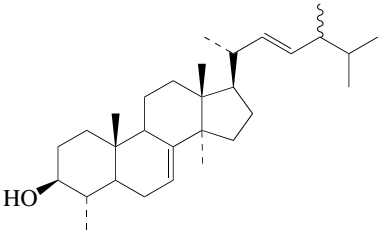
$C_{30}H_{50}O_{12}S_3$ 698.916

Constit. of a *Xestospongia* sp. Powder. $[\alpha]_D$ +27 (c, 0.29 in MeOH). λ_{max} 272 (ϵ 4838) (MeOH).

Lerch, M.L. *et al., Tetrahedron*, 2001, **57**, 4091-4094 (*isol, pmr, cmr*)

4,14-Dimethylergosta-7,22-dien-3-ol D-927

4,14,24-Trimethylcholesta-7,22-dien-3-ol



$C_{30}H_{50}O$ 426.724

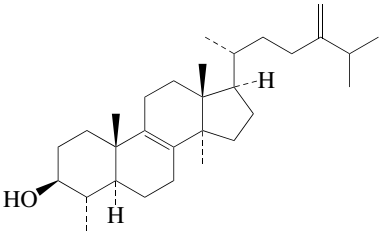
(3β,4α,5α,22*E*,24ξ)-*form* [214483-26-8]

Constit. of *Holothuria scabra*.

Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*isol, ms*)

4,14-Dimethylergosta-8,24(28)-dien-3-ol D-928

4,14-Dimethyl-24-methylenecholest-8-en-3-ol



$C_{30}H_{50}O$ 426.724

(3β,4α,5α)-*form*

Obtusifoliol

[16910-32-0]

Constit. of numerous plant spp. Minor constit. of the lipids of a marine unicellular green alga. Mp 144°.

3-Ketone: 4,14-Dimethylergosta-8,24(28)-dien-3-one. 4,14-Dimethyl-24-methylenecholest-8-en-3-one. ***Obtusifolione***

$C_{30}H_{48}O$ 424.709

Constit. of *Euphorbia piscatoria*. Cryst. (Me_2CO).

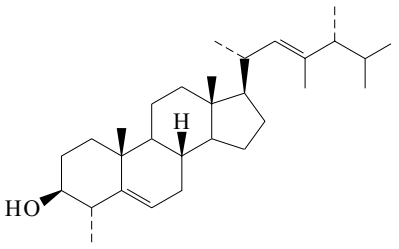
Mp 107-108°. $[\alpha]_D^{25}$ +82 (c, 1 in $CHCl_3$).

[89955-50-0, 121250-35-9]

Barrera, J.B. *et al., CA*, 1967, **67**, 108792g (*struct*)
Itoh, T. *et al., Phytochemistry*, 1978, **17**, 971 (*isol*)
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*occur, alga*)
De Pascual Teresa, J. *et al., Phytochemistry*, 1987, **26**, 1767 (*pmr, cmr*)
Xu, S. *et al., J. Chromatogr.*, 1988, **452**, 377 (*chromatog*)
Ferreira, M.J.U. *et al., Planta Med.*, 1994, **60**, 581 (*Obtosifolione*)

4,23-Dimethylergosta-5,22-dien-3-ol D-929

4,23,24-Trimethylcholesta-5,22-dien-3-ol

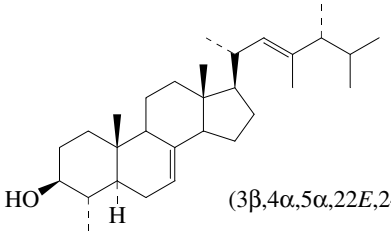


$C_{30}H_{50}O$ 426.724

(3β,4α,24*R*)-*form*
5-Dehydrodinosterol
[70329-25-8]
Constit. of *Crypthecodinium cohnii*, *Pyrocystis lunula* and *Zooxanthella microadriatica*.
Withers, N.W. *et al., Phytochemistry*, 1978, **17**, 1987-1989 (*isol*)
Bohlin, L. *et al., Phytochemistry*, 1981, **20**, 2397-2401 (*isol*)
Kokke, W.C.M.C. *et al., Steroids*, 1982, **40**, 307-318 (*isol*)

4,23-Dimethylergosta-7,22-dien-3-ol D-930

4,23,24-Trimethylcholesta-7,22-dien-3-ol



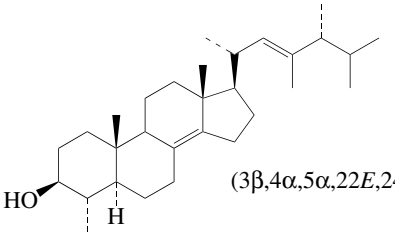
$C_{30}H_{50}O$ 426.724

(3β,4α,5α,22*E*,24*R*)-*form*
7-Dehydrodinosterol
[82637-05-6]
Isol. from various gorgonians and *Pseudostichopus trachus*.
22,23ξ-Dihydro: ***4,23-Dimethylergost-7-en-3-ol****. 4,23,24-Trimethylcholest-7-en-3-ol*
[214483-23-5]
$C_{30}H_{52}O$ 428.74
Constit. of *Pseudostichopus trachus* and *Bathyplotes natans*.

(3β,4α,5α,22*E*,24ξ)-*form* [199734-48-0]
Constit. of *Haliclona cinerea* and *Haliclona flavescens*.
Kokke, W.C.M.C. *et al., Phytochemistry*, 1982, **21**, 881-887 (*isol, pmr, ms*)
Elenkov, I. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1997, **118**, 155-157 (*Haliclona constit*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*isol, pmr, cmr*)

4,23-Dimethylergosta-8(14),22-dien-3-ol, 9CI D-931

4,23,24-Trimethylcholesta-8(14),22-dien-3-ol



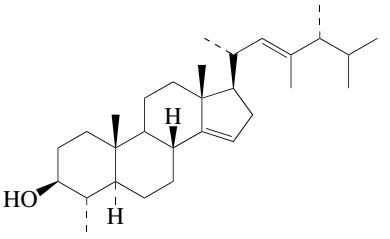
$C_{30}H_{50}O$ 426.724

(3β,4α,5α,22*E*,24*R*)-*form*
8(14)-Dehydrodinosterol
[82660-62-6]
Constit. of *Muriceopsis flavida*.

(3β,4α,5α,22*E*,24ξ)-*form* [78285-85-5]
Constit. of *Amphidinium carterae*.
Kokke, W.C.M.C. *et al., Phytochemistry*, 1981, **20**, 127-134; 1982, **21**, 881-887 (*isol*)

4,23-Dimethylergosta-14,22-dien-3-ol D-932

4,23,24-Trimethylcholesta-14,22-dien-3-ol

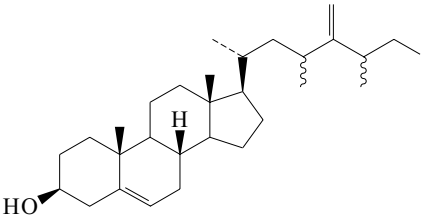


$C_{30}H_{50}O$ 426.724

(3β,5α,24*R*)-*form*
14-Dehydrodinosterol
Constit. of *Glenodinium* sp.
Cryst. (CH_2Cl_2).
Mp 174-178.5°.
Kokke, W.C.M.C. *et al., Phytochemistry*, 1981, **20**, 127-134 (*isol, pmr, ms*)

23,26-Dimethylergosta-5,24(28)-dien-3-ol D-933

25-Ethyl-23-methyl-27-norergosta-5,24(28)-dien-3-ol, 9CI. 23,26-Dimethyl-24-methylenecholest-5-en-3-ol

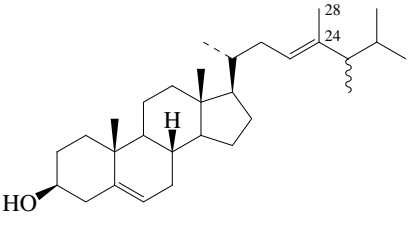


$C_{30}H_{50}O$ 426.724

(3β,23ξ,25ξ)-*form*
Remeisterol
[82866-33-9]
Constit. of the coral *Sinularia remei*.
Long, K. *et al., CA*, 1982, **97**, 107456h (*isol, uv, ir, pmr, cmr, ms*)

26,26-Dimethylergosta-5,23-dien-3-ol D-934

24,26,26-Trimethylcholesta-5,23-dien-3-ol



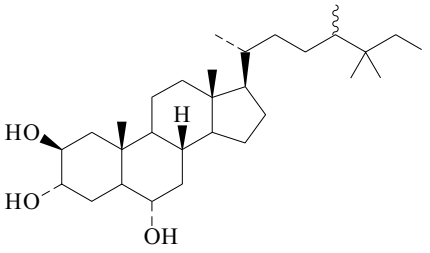
$C_{30}H_{50}O$ 426.724

(3β,23*E*,25ξ)-*form* [90195-41-8]
Minor constit. of lipids of a marine unicellular alga. Struct. not certain.

$\Delta^{24(28)}$-Isomer: ***26,26-Dimethylergosta-5,24(28)-dien-3-ol***.
24,26,26-Trimethylcholesta-5,24(28)-dien-3-ol
[90195-42-9]
$C_{30}H_{50}O$ 426.724
Minor constit. of lipids of a marine unicellular alga.
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*isol, pmr*)

25,26-Dimethylergostane-2,3,6-triol D-935

24,25,26-Trimethylcholestane-2,3,6-triol

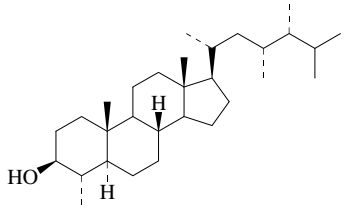


$C_{30}H_{54}O_3$ 462.755

(2β,3α,5α,6α,24ξ)-*form*
Tri-O-*sulfate:* ***Halistanol sulfate F***
[154205-18-2]
$C_{30}H_{54}O_{12}S_3$ 702.947
Constit. of sponge *Pseudaxinyssa digitata*.
Bifulco, G. *et al., J. Nat. Prod.*, 1994, **57**, 164-167 (*isol, pmr, cmr*)

4,23-Dimethylergostan-3-ol, 9CI D-936

4,23,24-Trimethylcholestan-3-ol. ***Dinostanol***
[79951-66-9, 84924-74-3, 86708-33-0, 86708-34-1, 86708-35-2, 86708-36-3, 86708-40-9]



(3β,4α,5α,23*R*,24*R*)-*form*

$C_{30}H_{54}O$ 430.756
Stereochem. of some isolates not fully determined. 23*S*- and 23*R*-isomers were distinguished among the dinoflagellate components.

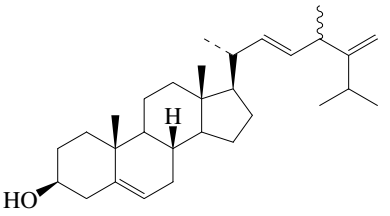
(3β,4α,5α,23*R*,24*R*)-*form* [86708-32-9]
[79951-66-9]
Isol. from a dinoflagellate symbiont of *Orbulina universa*. Also isol. from *Ascidia nigra* and *Scrobicularia plana*.
Cryst. (MeOH).
Mp 196-197°. $[\alpha]_D^{20}$ +35.6 (c, 1 in $CHCl_3$).

(3β,4α,5α,23*S*,24*R*)-*form* [86708-33-0]
Constit. of a *Siphonogorgia* sp. and *Scrobicularia plana*.
Cryst. (MeOH).
Mp 183-187°. $[\alpha]_D^{20}$ +8.3 (c, 0.78 in $CHCl_3$).

(3β,4α,5α,23ξ,24ξ)-*form* [91605-26-4]
Isol. from *Pseudostichopus trachus* and present in *Prorocentrum* spp. dinoflagellates.
Kokke, W.C.M.C. *et al., Phytochemistry*, 1982, **21**, 881-887 (*isol, pmr, ms*)
Zielinski, J. *et al., J.O.C.*, 1983, **48**, 3471-3477 (*isol, pmr, ms*)
Pettit, G.R. *et al., Steroids*, 1986, **47**, 321-326 (*cryst struct*)
Kokke, W.C.M.C. *et al., Biochem. Syst. Ecol.*, 1987, **15**, 475-478 (*Dinostanol*)
Shu, A.Y.L. *et al., J.C.S. Perkin 1*, 1987, 1291-1305 (*synth, pmr, ms*)
Volkman, J.K. *et al., Phytochemistry*, 1999, **52**, 659-668 (*occur, dinoflagellates*)

27,27-Dimethylergosta-5,22,25-trien-3-ol D-937

24,27,27-Trimethylcholesta-5,22,26-trien-3-ol

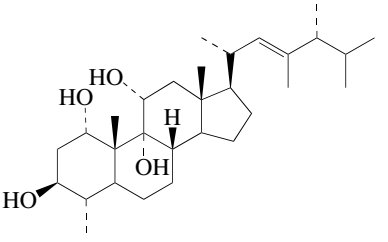


$C_{30}H_{48}O$ 424.709

(3β,22*E*,24ξ)-*form* [336808-40-3]
Constit. of *Axinyssa aplysinoides*.
Liang, L. *et al., Guangzhou Huaxue*, 2000, **25**, 26-28; *CA*, **134**, 323649y (*isol, pmr, cms*)
Liang, L. *et al., Zhongguo Haiyang Yaowu*, 2001, **20**, 1-4; *CA*, **135**, 301204t (*isol, pmr, cmr*)

4,23-Dimethylergost-22-ene-1,3,9,11-tetrol D-938

4,23,24-Trimethylcholest-22-ene-1,3,9,11-tetrol

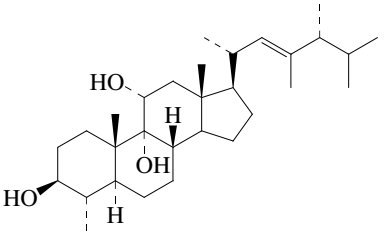


$C_{30}H_{52}O_4$ 476.738

(1α,3β,4α,9α,11α,22*E*,24*R*)-*form* [215929-18-3]
Constit. of *Pseudopterogorgia americana*.
Powder. $[\alpha]_D^{25}$ +0.88 (c, 1.1 in $CHCl_3$).
Rodriguez, A.D. *et al., Tet. Lett.*, 1998, **39**, 7645-7648 (*isol, pmr, cmr*)

4,23-Dimethylergost-22-ene-3,9,11-triol D-939

4,23,24-Trimethylcholest-22-ene-3,9,11-triol

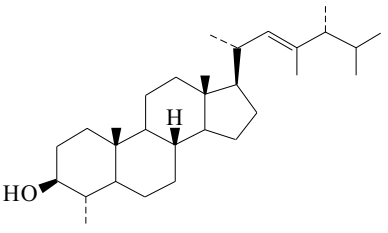


$C_{30}H_{52}O_3$ 460.739

(3β,4α,5α,11α,22*E*,24*R*)-*form* [88640-21-5]
Constit. of *Pseudopterogorgia americana*.
Musmar, M.F.N. *et al., Diss. Abstr. Int., B*, 1983, **44**, 1122 (*isol*)

4,23-Dimethylergost-22-en-3-ol D-940

4,23,24-Trimethylcholest-22-en-3-ol



$C_{30}H_{52}O$ 428.74

(3β,4α,5α,22*E*,24*R*)-*form*

Dinosterol. *Black Sea Sterol*

[58670-63-6]

Constit. of *Gonyaulax tamarensis*, *Styela plicata*, *Sarcophyton glaucum*, *Holothuria scabra*, *Pseudostichopus trachus*, *Synapta maculata* and dinoflagellate sediments. Occurs in dinoflagellates and rarely in other algae, and has been used as a marker of dinoflagellate contribution to organic sediments. Cryst. ($CHCl_3$/MeOH).

Mp 220-222°. $[\alpha]_D$ -6 (c, 0.52 in $CHCl_3$) (0).

3-Ac: [70329-28-1]

$C_{32}H_{54}O_2$ 470.777

Constit. of *Pseudoplexaura flagellosa*.

3-Ketone: 4,23-Dimethylergost-22-en-3-one. 4,23,24-Trimethylcholest-22-en-3-one. ***Dinosterone***

[70329-26-9]

Constit. of *Crypthecodinium cohnii*.

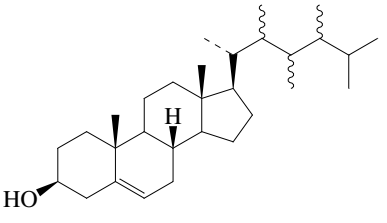
Cryst.

Mp 193-195°. Genus name erroneously given as Cryptocodinium.

Shimizu, Y. *et al., J.A.C.S.*, 1976, **98**, 1059-1060 (*isol*)
Finer, J. *et al., J.O.C.*, 1978, **43**, 1990-1992 (*cryst struct*)
Withers, N.W. *et al., Phytochemistry*, 1978, **17**, 1987-1989; 1979, **18**, 71-73 (*isol, 3-ketone, biosynth*)
Boon, J.J. *et al., Nature (London)*, 1979, **277**, 125-127 (*isol*)
Shu, A.Y.L. *et al., Tet. Lett.*, 1981, **22**, 4627-4630 (*synth*)
Kobayashi, M. *et al., Steroids*, 1982, **40**, 209-221 (*Dinosterol, Sarcophyton constit, pmr, ms*)
Zollo, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **85**, 559-560 (*occur*)
Giner, J.-L. *et al., J.O.C.*, 1991, **56**, 2357-2363 (*biosynth*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*occur*)
Volkman, J.K. *et al., Phytochemistry*, 1999, **52**, 659-668 (*occur, dinoflagellates*)
Reynolds, W.F. *et al., Magn. Reson. Chem.*, 2001, **39**, 94-97 (*Ac*)

22,23-Dimethylergost-5-en-3-ol D-941

22,23,24-Trimethylcholest-5-en-3-ol



$C_{30}H_{52}O$ 428.74

(3β,22ξ,23ξ,24ξ)-*form*

22,23,24-Trimethylcholesterol

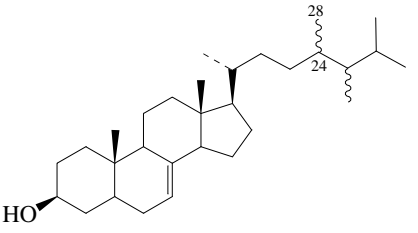
[223271-77-0]

Constit. of *Bugula neritina*.

Kerr, R.G. *et al., J. Nat. Prod.*, 1999, **62**, 468-470

26,26-Dimethylergost-7-en-3-ol D-942

24,26,26-Trimethylcholest-7-en-3-ol



$C_{30}H_{52}O$ 428.74

(3β,24ξ,25ξ)-*form*

Thymosiosterol

[226894-40-2]

Constit. of a *Thymosiopsis* sp.

Cryst.

Mp 136-137°. $[\alpha]_D$ +6 (c, 0.2 in $CHCl_3$).

24,28-Didehydro: 26,26-Dimethylergosta-7,24(28)-dien-3-ol. 26,26-Dimethyl-24-methylenecholest-7-en-3-ol. ***Δ^{24}-Thymosiosterol***

[226894-41-3]

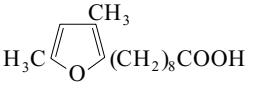
$C_{30}H_{50}O$ 426.724

Constit. of a *Thymosiopsis* sp. Cryst.

Mp 125-127°. $[\alpha]_D$ +10 (c, 0.2 in $CHCl_3$).

Bultel-Poncé, V. *et al., Tet. Lett.*, 1999, **40**, 2955-2956 (*isol, pmr, cmr*)

3,5-Dimethyl-2-furannonanoic acid D-943



$C_{15}H_{24}O_3$ 252.353

Et ester:

$C_{17}H_{28}O_3$ 280.406

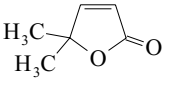
Isol. from the brown alga *Acrocarpia paniculata*. Liq.

Kaylauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 165

5,5-Dimethyl-2(5*H*)-furanone, 9CI D-944

4,4-Dimethyl-2-butenolide

[20019-64-1]



$C_6H_8O_2$ 112.128

Aroma component of hop extract, and of lavender, sagebrush, narcissus and salmon oils. Liq. with burnt camphor-menthol odour. Bp 210° Bp_{14} 94° Bp_{10} 80°. n_D^{18} 1.4470.

Haynes, L.J. *et al., J.C.S.*, 1946, 954 (*synth*)
Nobuhara, A. *et al., Agric. Biol. Chem.*, 1970, **11**, 1745 (*synth, props*)
King, G.S. *et al., J.C.S. Perkin 1*, 1974, 1499 (*synth, pmr, ms, gc*)
Torii, S. *et al., J.O.C.*, 1974, **39**, 2486 (*synth*)
Barluenga, J. *et al., Chem. Comm.*, 1986, 183 (*synth, cmr*)
Tanikaga, R. *et al., Synthesis*, 1986, 416 (*synth*)
Alper, H. *et al., J.O.C.*, 1991, **56**, 5357 (*synth*)

N,*N*-Dimethylglycine, 9CI D-945

Dimethylaminoacetic acid. Dimethylamine-N-*acetic acid*

[1118-68-9]

Me_2NCH_2COOH

$C_4H_9NO_2$ 103.121

Isol. from the ascidian *Atriolum robustum*. Hygroscopic cryst.

Mp 183° Mp 179-181°. pK_a 9.88 (25°).

▶ MB9865000

Hydrochloride: [2491-06-7]
Cryst. (Me_2CO/butanol). Mp 189-190°.

▶ MB9995000

Me ester: [7148-06-3]
$C_5H_{11}NO_2$ 117.147
Liq. Bp 135° Bp_{30} 51°.

▶ MC0011000

Et ester: [33229-89-9]
$C_6H_{13}NO_2$ 131.174
Liq. Bp 150° Bp_{12} 48-49°.

▶ MB9990000

Et ester, hydrochloride: Mp 88-90°. Extremely deliquescent.

Benzyl ester:
$C_{11}H_{15}NO_2$ 193.245
Mp 116° (as hydrochloride).

Chloride: (Dimethylamino)acetyl chloride
[51552-16-0]
C_4H_8ClNO 121.566
Needles (as hydrochloride). Mp 110-113° dec. (hydrochloride).

Amide: 2-(Dimethylamino)acetamide, 9CI
[6318-44-1]
$C_4H_{10}N_2O$ 102.136
Mp 61-62° Mp 95-95.8°.

Dimethylamide: [13574-14-6]
$C_6H_{14}N_2O$ 130.189
Bp_{34} 99-100°.

▶ AB7975000

Nitrile: (Dimethylamino)acetonitrile, 9CI. Cyano(dimethylamino)methane
[926-64-7]
$C_4H_8N_2$ 84.121
Liq. Bp 137-138° Bp_{41} 63°. n_D^{20} 1.4100.

▶ LD_{50} (rat, orl) 50 mg/kg; LD_{50} (rbt, skn) 170 mg/kg. Toxic if swallowed and in contact with skin. AL9450000

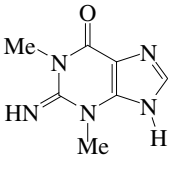
Hydrazide: [5787-71-3]
$C_4H_{11}N_3O$ 117.15
Mp 214° (as dihydrochloride).

[60853-81-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 570C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 868B; 1068B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 732C; 814C (*ir*)
Sadtler Standard NMR Spectra, 27051 (*pmr*)
Turner, R.A. *et al., J.A.C.S.*, 1946, **68**, 1607 (*nitrile, amide*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 2761
Olomucki, M. *et al., Bull. Soc. Chim. Fr.*, 1963, 2067 (*synth*)
Ikutani, T. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 1679 (*synth*)
Cameron, T.S. *et al., J.C.S. Dalton*, 1973, 2626 (*cryst struct*)
Marsh, R.E. *et al., J. Crystallogr. Spectrosc. Res.*, 1983, **13**, 245 (*cryst struct*)
Hercules, D.M. *et al., Anal. Chem.*, 1985, **57**, 698 (*ms*)
van Koten, G. *et al., Organometallics*, 1991, **10**, 2467 (*esters*)
Kehraus, S. *et al., J. Med. Chem.*, 2004, **47**, 2243-2255 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DOS200

1,3-Dimethylguanine D-946

1,2,3,7-Tetrahydro-2-imino-1,3-dimethyl-6H-purin-6-one
[224801-13-2]



$C_7H_9N_5O$ 179.181
Isol. from the ascidian *Botrylloides leachi*. Solid. λ_{max} 201 (log ϵ 3.7); 263 (log ϵ 3.3) (MeOH).

Lindsay, B.S. *et al., J. Nat. Prod.*, 1999, **62**, 638-639 (*isol, uv, pmr, cmr, ms*)

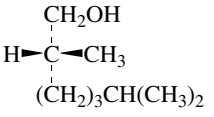
19,21-Dimethylheptacosanoic acid D-947

[93673-93-9]
$H_3C(CH_2)_5CH(CH_3)CH_2CH(CH_3)(CH_2)_{17}COOH$
$C_{29}H_{58}O_2$ 438.776
Isol. from the sponge *Strongylophora durissima*.

Dasgupta, A. *et al., Lipids*, 1984, **19**, 768-776 (*isol*)

2,6-Dimethyl-1-heptanol, 9CI D-948

[2768-12-9]



(*R*)-*form*

$C_9H_{20}O$ 144.256

(*R*)-*form* [59983-44-7]
Oil. Bp_{16} 92-95° Bp_{12} 90°. $[\alpha]_D^{25}$ +10.8 (c, 2 in C_6H_6).

O-*Sulfate:* [160098-17-9]
$C_9H_{20}O_4S$ 224.321
Isol. from the ascidian *Polycitor adriaticus* and *Halocynthia papillosa*. Constit. of the kairomone secreted by *Daphnia pulex*. Cytotoxic. Amorph. (as Na or K salt). $[\alpha]_D$ +4.7 (c, 0.01 in MeOH).

(S)*-*form [79397-71-0]
Bp 100-105°. $[\alpha]_D^{25}$ -11 (c, 2 in C_6H_6).

(±)-*form* [87247-02-7]
Oil. Bp_8 82.5-84°.

O-*Sulfate:* [160116-60-9]
$C_9H_{20}O_4S$ 224.321
Isol. from the ascidian *Halocynthia roretzi*. Antibacterial and antifungal agent.

[84606-47-3]

Hoever, H. *et al., Annalen*, 1965, **685**, 89 (*synth*)
Cohen, N. *et al., J.O.C.*, 1976, **41**, 3505 (*synth*)
Chan, K.-K. *et al., J.O.C.*, 1977, **42**, 3829 (*synth*)
Cohen, N. *et al., Helv. Chim. Acta*, 1981, **64**, 1158 (*synth*)
Helmchen, G. *et al., Tet. Lett.*, 1983, **24**, 1235 (*synth*)
Crispino, A. *et al., J. Nat. Prod.*, 1994, **57**, 1575-1577 (*sulfate, isol, pmr, cmr*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 1994, **57**, 1606-1609 (*Halocynthia, sulfate*)
De Rosa, S. *et al., J. Nat. Prod.*, 1997, **60**, 462-463 (*abs config*)
Aiello, A. *et al., J. Nat. Prod.*, 2000, **63**, 1590-1592 (*sulfate, activity*)
Yasumoto, K. *et al., Chem. Pharm. Bull.*, 2006, **54**, 271-274 (*Daphnia sulfates*)

2,6-Dimethyl-5-heptenal, 9CI D-949

Melonal. FEMA 2389
[106-72-9]
$(H_3C)_2C{=}CHCH_2CH_2CH(CH_3)CHO$
$C_9H_{16}O$ 140.225
Constit. of the mollusc *Melibe leonina* and a pheromone of the ant *Lasius carniolicus*. Oil.

▶ Skin and eye irritant. MJ8797000

(±)-*form*
Perfumery and flavouring ingredient.
Liq. with melon-like odour and taste. Bp_{100} 116-124°.

Oxime: [22457-24-5]
$C_9H_{17}NO$ 155.239
$Bp_{0.9}$ 80-81°.

Semicarbazone: Mp 135°.

2,4-Dinitrophenylhydrazone: Mp 87°.

1-Carboxylic acid: 2,6-Dimethyl-5-heptenoic acid
$C_9H_{16}O_2$ 156.224
Constit. of *Melibe leonina*. Oil.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 737C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 561A (*ir*)

Dominguez, X.A. *et al., CA*, 1956, **50**, 8445 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 793 (*rev, tox*)
Ayer, S.W. *et al., Experientia*, 1983, **39**, 255-256 (*isol*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DSD775
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

18,24-Dimethylhexacosanoic acid D-950

$H_3CCH_2CH(CH_3)(CH_2)_5CH(CH_3)(CH_2)_{16}COOH$
$C_{28}H_{56}O_2$ 424.749
Isol. from sponge *Cinachyrella alloclada*.

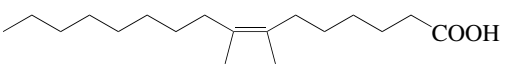
Barnathan, G. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2003, **135**, 297-308 (*isol, ms*)

7,8-Dimethylhexadecanoic acid D-951

[122706-66-5]
$H_3C(CH_2)_7CH(CH_3)CH(CH_3)(CH_2)_5COOH$
$C_{18}H_{36}O_2$ 284.481
Found in fish oils.

Ratnayake, W.M.N. *et al., Lipids*, 1989, **24**, 630-637 (*occur*)

7,8-Dimethyl-7-hexadecenoic acid D-952

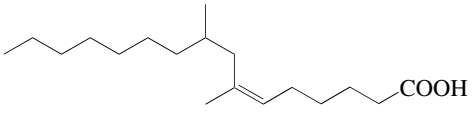


$C_{18}H_{34}O_2$ 282.465
Not in CAS.

(Z)-form
Isol. from the fish oils of *Brevoortia tyrannus* and *Oncorhynchus nerka*.

Ratnayake, W.M.N. *et al., Lipids*, 1989, **24**, 630-637 (*isol*)

7,9-Dimethyl-6-hexadecenoic acid D-953



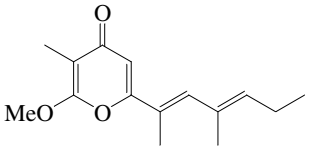
$C_{18}H_{34}O_2$ 282.465

(Z)-form [163632-69-7]
Isol. from the gorgonian *Leptogorgia piccola*.

Miralles, J. *et al., Lipids*, 1995, **30**, 459 (*isol, struct*)

6-(1,3-Dimethyl-1,3-hexadienyl)-2-methoxy-3-methyl-4*H*-pyran-4-one, 9CI D-954

7-Methylcyercene B



(1'*E*,3'*E*)-*form*

$C_{15}H_{20}O_3$ 248.321

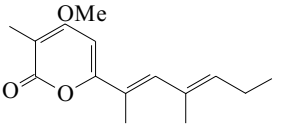
(1′E,3′E)-form [144938-28-3]
Isol. from *Ercolania funerea*. Ichthyotoxic. λ_{max} 227 (ϵ 13000); 288 (ϵ 10700) (MeOH) (Berdy).

(1′E,3′Z)-form [127848-75-3]
Isol. from *Cyerce nigricans*. λ_{max} 248 (ϵ 6700) (MeOH).

Roussis, V. *et al., Experientia*, 1990, **46**, 327-329 (*isol, pmr, cmr*)
Vardaro, R.R. *et al., Tetrahedron*, 1992, **48**, 9561-9566 (*isol, struct, pmr, cmr*)

6-(1,3-Dimethyl-1,3-hexadienyl)-4-methoxy-3-methyl-2*H*-pyran-2-one, 9CI D-955

7-Methylcyercene 2



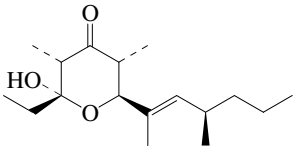
$C_{15}H_{20}O_3$ 248.321

(E,E)-form [144938-30-7]
Isol. from *Ercolania funerea*.

Vardaro, R.R. *et al., Tetrahedron*, 1992, **48**, 9561 (*isol, struct*)

6-(1,3-Dimethyl-1-hexenyl)-2-ethyltetrahydro-2-hydroxy-3,5-dimethyl-4*H*-pyran-4-one, 9CI D-956

[91466-58-9]

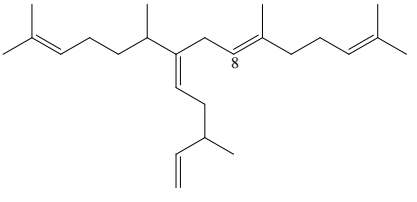


Absolute Configuration

$C_{17}H_{30}O_3$ 282.422
Isol. from the mollusc *Siphonaria australis*.
$[\alpha]_D$ +22.3 (c, 0.84 in $CHCl_3$).

Hochlowski, J.E. *et al., J.O.C.*, 1984, **49**, 3838 (*isol, pmr*)
Sundram, U.N. *et al., Tet. Lett.*, 1992, **33**, 437 (*synth, abs config*)
Lister, T. *et al., Aust. J. Chem.*, 2004, **57**, 787-797 (*synth, abs config*)

6-(1,5-Dimethyl-4-hexenyl)-3,9,13-trimethyl-1,5,8,12-tetradecatetraene D-957



(5*E*,8*E*)-*form*

$C_{25}H_{42}$ 342.607

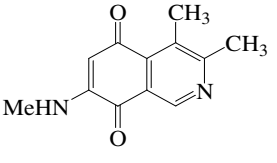
(5E,8E)-form [269060-02-8]
Constit. of *Pleurosigma intermedium*.

(5E,8Z)-form [269060-03-9]
Constit. of *Pleurosigma intermedium*.

Belt, S.T. *et al., Chem. Comm.*, 2000, 501-502 (*isol, pmr, cmr*)

3,4-Dimethyl-7-(methylamino)-5,8-isoquinolinedione D-958

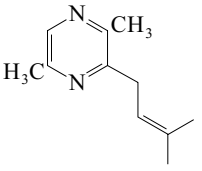
3,4-Dimethyl-7-(methylamino)-5,8-isoquinolinequinone



$C_{12}H_{12}N_2O_2$ 216.239
Prod. by the marine-derived *Streptomyces* sp. B1848. Red solid.
λ_{max} 232; 273; 339; 447 (MeOH).

Shaaban, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*isol, pmr, cmr, ms*)

2,5-Dimethyl-3-(3-methyl-2-butenyl)pyrazine, 9CI **D-959**
3-Isopentyl-2,5-dimethylpyrazine. 2,5-Dimethyl-3-prenylpyrazine

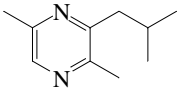


$C_{11}H_{16}N_2$ 176.261
Isol. from the ant *Iridomyrmex humilis*. Prod. by a marine bacterium.

2′,3′-Dihydro: 2,5-Dimethyl-3-(3-methylbutyl)pyrazine, 9CI
[18433-98-2]
$C_{11}H_{18}N_2$ 178.277
Isol. from the ants *Anochetus kempfi*, *Anochetus mayri*, *Mesoponera castanea* and *Mesoponera castaneicolor*. Prod. by various marine bacteria.

Cairll, G.W.K. *et al., Aust. J. Chem.*, 1974, **27**, 879
Fales, H.M. *et al., Tetrahedron*, 1988, **44**, 5045 (*deriv*)
Jones, T.H. *et al., J. Nat. Prod.*, 1999, **62**, 1343-1345 (*isol, deriv*)
Dickschat, J.S. *et al., Eur. J. Org. Chem.*, 2005, 4141-4153 (*marine isol*)
Dickschat, J.S. *et al., J. Chem. Ecol.*, 2005, **31**, 925-947 (*marine isol*)

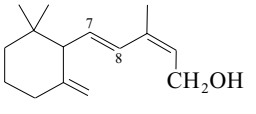
2,5-Dimethyl-3-(2-methylbutyl)pyrazine **D-960**
[72668-36-1]



$C_{11}H_{18}N_2$ 178.277
Prod. by the marine bacterium *Sulfitobacter pontiacus*.

Dickschat, J.S. *et al., Eur. J. Org. Chem.*, 2005, 4141-4153 (*isol, synth, pmr, cmr, ms*)

5-(2,2-Dimethyl-6-methylenecyclohexyl)-3-methyl-2,4-pentadien-1-ol, 9CI **D-961**
γ-Ionylideneethanol
[99297-86-6]



(2*Z*,4*E*)–*form*

$C_{15}H_{24}O$ 220.354
Terpenoid antibiotic. Isol. from *Cercospora cruenta*. Plant growth inhibitor. Oil.

3,5-Dinitrobenzoyl:
Cryst. (Et_2O/hexane). Mp 98.5°. $[\alpha]_D^{21}$ +18 (c, 0.1 in $CHCl_3$).

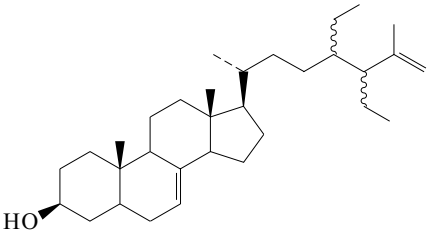
7,8-Dihydro: γ-Monocyclofarnesol
[33526-22-6]
$C_{15}H_{26}O$ 222.37
Formed from mevalonic acid by a *Helminthosporium siccans* enzyme extract. Oil. $[\alpha]_D$ +17.6 (EtOH).

9,10-Dihydro: ***2,3-Dihydro-γ-ionylideneethanol***
$C_{15}H_{26}O$ 222.37
Prod. by *Cercospora cruenta*.
$[\alpha]_D^{20}$ -13 (c, 0.02 in EtOH).

Carboxylic acid, 7,8-dihydro, 2,3-dihydroxypropyl ester: [97530-71-7]
$C_{18}H_{30}O_4$ 310.433
Isol. from the nudibranch *Archidoris montereyensis*. Oil. $[\alpha]_D$ +9.7 (c, 0.3 in $CHCl_3$).

Suzuki, K.T. *et al., Chem. Comm.*, 1971, 527 (*γ-Monocyclofarnesol*)
Oritani, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 2819 (*isol, props*)
Gustafson, K. *et al., Tetrahedron*, 1985, **41**, 1101-1108 (*Archidoris glyceride*)
Ungur, N. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 1263-1273 (*propyl ester, stereochem*)
Yamamoto, H. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 810-816 (*2,3-Dihydroionylideneethanol*)

26,27-Dimethyl-26-methylenestigmast-7-en-3-ol **D-962**
24-Ethyl-26,27-dimethyl-26-methylenecholest-7-en-3-ol. 24-Ethyl-26,26,27-trimethylcholesta-7,26(30)-dien-3-ol

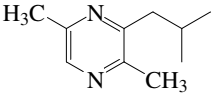


$C_{32}H_{54}O$ 454.778

(3β,24ξ,25ξ)-*form* [129620-25-3]
Constit. of a *Xestospongia* sp.

Kerr, R.G. *et al., J.O.C.*, 1991, **56**, 58 (*isol, pmr*)

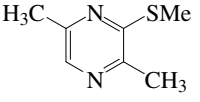
2,5-Dimethyl-3-(2-methylpropyl)pyrazine **D-963**
3-Isobutyl-2,5-dimethylpyrazine
[32736-94-0]



$C_{10}H_{16}N_2$ 164.25
Prod. by various marine bacteria.

Dickschat, J.S. *et al., Eur. J. Org. Chem.*, 2005, 4141-4153 (*isol, synth, pmr, cmr, ms*)

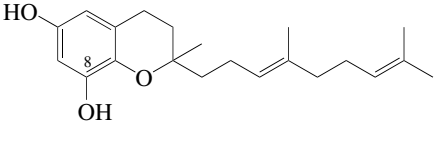
2,5-Dimethyl-3-(methylthio)pyrazine **D-964**
[59021-08-8]



$C_7H_{10}N_2S$ 154.235
Prod. by the marine bacterium *Sulfitobacter pontiacus*. Pale yellow liq.

Dickschat, J.S. *et al., Eur. J. Org. Chem.*, 2005, 4141-4153 (*isol, synth, pmr, cmr, ms*)

2-(4,8-Dimethyl-3,7-nonadienyl)-3,4-dihydro-6,8-dihydroxy-2-methyl-2*H*-1-benzopyran **D-965**
2-(4,8-Dimethyl-3,7-nonadienyl)-6,8-dihydroxy-2-methylchroman

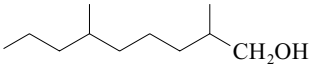


$C_{21}H_{30}O_3$ 330.466

(+)-*form*
*8-Me ether: 2-(4,8-Dimethyl-3,7-nonadienyl)-3,4-dihydro-8-methoxy-2-methyl-2*H*-1-benzopyran-6-ol, 9CI*
[184100-45-6]
$C_{22}H_{32}O_3$ 344.493

Isol. from the mollusc *Cratena peregrina*.
$[\alpha]_D^{25}$ +5.6 (c, 0.25 in $CHCl_3$). λ_{max} 218 (ϵ 3525); 291 (ϵ 3190) (MeOH).
Ciavatta, M.L. *et al., Gazz. Chim. Ital.*, 1996, **126**, 707-710 (*isol, pmr, cmr, uv, ms, cd*)

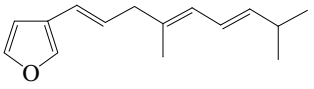
2,6-Dimethyl-1-nonanol D-966



$C_{11}H_{24}O$ 172.31

O-*Sulfate:* [133084-58-9]
$C_{11}H_{24}O_4S$ 252.374
Isol. from the sea cucumber *Cucumaria frondosa*. Amorph. solid (as Na salt).
Mp 180-190° dec. (Na salt). $[\alpha]_D$ +2.3 (c, 0.001 in $CHCl_3$).
Findlay, J.A. *et al., J. Nat. Prod.*, 1991, **54**, 302-304 (*isol, ir, pmr, cmr, ms*)

3-(4,8-Dimethyl-1,4,6-nonatrienyl)furan D-967

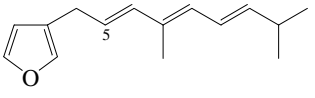


$C_{15}H_{20}O$ 216.322

(4E,7E,9E)-form
Isodehydrodendrolasin†
[230302-24-6]
Constit. of *Euryspongia deliculata*.
Pale yellow oil. Farnesane numbering. λ_{max} 221 (sh); 242 (log ϵ 4.47) (hexane).
Clark, R.J. *et al., J. Nat. Prod.*, 1999, **62**, 915-916 (*isol, pmr, cmr*)

3-(4,8-Dimethyl-2,4,6-nonatrienyl)furan D-968

Dehydrodendrolasin



(5E,7E,9E)-form

$C_{15}H_{20}O$ 216.322
Sesquiterpenoid numbering shown.

(5E,7E,9E)-form [41060-02-0]
Constit. of *Pleraplysilla spinifera*, *Ceratosoma brevicaudatum* and *Dysidea herbacea*.
Oil.

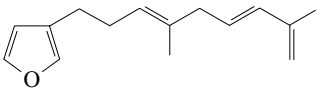
(5E,7Z,9E)-form
Constit. of *Ceratosoma brevicaudatum*. Incorr. indexed by CAS as (*Z,Z,E*)-isomer.

(5Z,7E,9E)-form [187335-07-5]
[81619-65-0]
Constit. of *Dysidea herbacea*.
Oil. λ_{max} 252 (ϵ 19950); 270 (ϵ 30900) (hexane) (Derep).

[117569-45-6]

Cimino, G. *et al., Tetrahedron*, 1972, **28**, 4761-4767 (*isol, struct*)
Dunlop, R.W. *et al., Aust. J. Chem.*, 1982, **35**, 95-103 (*Dysidea herbacea constits*)
Ksebati, M.B. *et al., J. Nat. Prod.*, 1988, **51**, 857-861 (*Ceratostoma brevicaudatum constits, isol, struct, pmr, cmr*)
Uenishi, J. *et al., Tetrahedron*, 1997, **53**, 2439-2448 (*synth*)

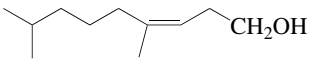
3-(4,8-Dimethyl-3,6,8-nonatrienyl)furan D-969



$C_{15}H_{20}O$ 216.322

(3′E,6′E)-form
Isodehydrodendrolasin†
[147663-94-3]
Constit. of *Hypselodoris cantabrica, Hypselodoris tricolor* and *Hypselodoris villafrance*. Ichthyotoxin. Antifeedant. λ_{max} 230 (ϵ 9430); 274 (ϵ 3510) (Et_2O) (Berdy).
Fontana, A. *et al., J. Chem. Ecol.*, 1993, **19**, 339 (*isol*)

4,8-Dimethyl-3-nonen-1-ol D-970

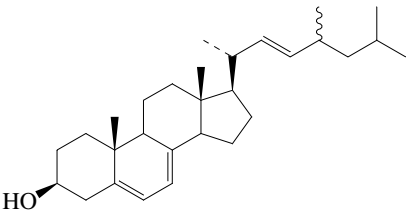


$C_{11}H_{22}O$ 170.294

(Z)-form
O-*Sulfate:* [195619-95-5]
$C_{11}H_{22}O_4S$ 250.358
Constit. of brittle star *Ophiocoma echinata* and of *Microcosmus vulgaris*. Antiproliferative agent. Powder. CAS number refers to Na salt.
Roccatagliata, A.J. *et al., J. Nat. Prod.*, 1997, **60**, 285-286 (*isol, pmr, cmr, ir*)
Aiello, A. *et al., Tetrahedron*, 1997, **53**, 11489-11492 (*isol, pmr, cmr*)

26,26-Dimethyl-27-norergosta-5,7,22-trien-3-ol D-971

24,26,26-Trimethyl-27-norcholest-5,7,22-trien-3-ol



$C_{29}H_{46}O$ 410.682

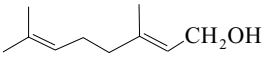
(3β,22E,24ξ)-form [473909-17-0]
Constit. of *Agelas sceptrum*. Cryst. ($CHCl_3$). Mp 123-124°. $[\alpha]_D^{25}$ +134 (c, 1.1 in $CHCl_3$).
Hu, J.-F. *et al., Steroids*, 2002, **67**, 743-747 (*isol, pmr, cmr*)

20,22-Dimethyloctacosanoic acid D-972

[93673-94-0]
$H_3C(CH_2)_5CH(CH_3)CH_2CH(CH_3)(CH_2)_{18}COOH$
$C_{30}H_{60}O_2$ 452.803
Isol. from the sponge *Strongylophora durissima*.
Dasgupta, A. *et al., Lipids*, 1984, **19**, 768-776 (*isol*)

3,7-Dimethyl-2,6-octadien-1-ol D-973

[624-15-7]



(E)–form

$C_{10}H_{18}O$ 154.252

(E)-form
Geraniol. *Geranyl alcohol. Lemonol. β-Geraniol. FEMA 2507*
[106-24-1]

Most coml. geraniol is prod. synthetically from 3,7-Dimethyl-1, 6-octadien-3-ol or β-Pinene. Found in free state and as esters in many essential oils including geranium oil. Honeybee *Apis mellifera* Nasonov pheromone lure. Most prolific natural source is palmarosa oil (70-85%). Detected by gc-ms in the bryozoan *Conopeum seuratum*. Extensively used in perfumery. Flavouring agent. Glutathion S transferase inhibitor showing anticarcinogenic props. Antiaflatoxigenic. Oil with sweet rose odour. Bp 230°. n_D^{30} 1.4777. λ_{max} 195 (ϵ 19000) (MeOH) (Berdy).

▶ Skin irritant. LD_{50} (rat, orl) 3600 mg/kg. RG5830000

(Z)-form

Nerol. *Neryl alcohol. β-Nerol. FEMA 2770*

[106-25-2]

Constit. of many essential oils including neroli and bergamot oils. Nasonov pheromone of the honeybee *Apis mellifera*. In essential oils it is a minor component always accompanied by geraniol. Detected by gc-ms in the bryozoan *Conopeum seuratum*. Used in perfumery and food flavouring.

Oil with flowery odour. Bp 225-226°. n_D^{20} 1.4744.

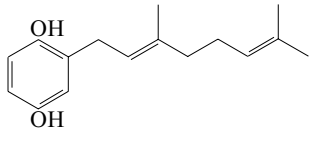
▶ Skin irritant. LD_{50} (rat, orl) 4500 mg/kg. RG5840000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 148D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 224C; 225A; 968A; 968B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 219A; 219B; 668D (*ir*)
Burrell, J.W.K. *et al., J.C.S.(C)*, 1966, 2144-2154 (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037-1064 (*ir*)
Howell, A.R. *et al., J.C.S. Perkin 1*, 1990, 2715-2720 (*synth*)
Eisenreich, W. *et al., Tet. Lett.*, 1997, **38**, 3889-3892 (*biosynth*)
Luan, F. *et al., Phytochemistry*, 2002, **60**, 451-459 (*biosynth*)
Dubey, V.S. *et al., Phytochemistry*, 2003, **63**, 257-264 (*biosynth*)

2-(3,7-Dimethyl-2,6-octadienyl)-1,4-benzenediol D-974

(3,7-Dimethyl-2,6-octadienyl)hydroquinone, 8CI. 2-Geranylhydroquinone. ***Geroquinol, INN***. *Beradia. B158*

[10457-66-6]



$C_{16}H_{22}O_2$ 246.349

For higher homologues see Farnesylhydroquinone, F-13 and 2-Polyprenyl-1,4-benzenediol, P-547. Isol. from trichomes of *Phacelia ixodes*. Also prod. by cultured cells of *Lithospermum erythrorhizon* and by a tunicate *Aplidium savignyi*. Radioprotectant agent. Intermed. in biosynth. of 5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione. Shows significant cytotoxic activity and antioxidative props. Oil. Log P 4.84 (calc).

▶ Contact allergen.

3′-Hydroxy, 2′,3′-dihydro: ***2-(3-Hydroxy-3,7-dimethyl-6-octenyl)-1,4-benzenediol***
[124596-53-8]
$C_{16}H_{24}O_3$ 264.364
Metab. of *Amaroucium multiplicatum*. Prod. by a tunicate *Aplidium savignyi*. Shows significant cytotoxic activity and antioxidative props. Oil.

7′-Hydroxy, 6′,7′-dihydro: ***2-(7-Hydroxy-3,7-dimethyl-2-octenyl)-1,4-benzenediol***
[203524-75-8]
$C_{16}H_{24}O_3$ 264.364
Constit. of an *Aplydium* sp. Oil. λ_{max} 294 (ϵ 4250) (MeOH).

*Δ$^{1'}$-Isomer(*E-*), 3′-hydroxy:* ***2-(3-Hydroxy-3,7-dimethyl-1,6-octadienyl)-1,4-benzenediol***
[124596-54-9]
$C_{16}H_{22}O_3$ 262.348
Metab. of *Amaroucium multiplicatum*. Oil.

*Δ$^{1'}$-Isomer(*Z-*), 3′-hydroxy:* [264202-56-4]
$C_{16}H_{22}O_3$ 262.348
Constit. of *Cordia alliodora*. Yellow gum. $[\alpha]_D^{25}$ -8.8 (c, 0.5 in $CHCl_3$). λ_{max} 220 (log ϵ 4.18); 264 (sh) (log ϵ 3.5); 332 (log ϵ 3.36) (MeOH).

*Δ$^{1'}$-Isomer(*E-*), 3′ξ-methoxy: 2-(3-Methoxy-3,7-dimethyl-1,6-octadienyl)-1,4-benzenediol*
[459174-32-4]
$C_{17}H_{24}O_3$ 276.375
Constit. of *Aplidium conicum*. Orange oil. $[\alpha]_D^{27}$ +13.2 (c, 0.2 in $CHCl_3$).

Quinone: See 2-(3,7-Dimethyl-2,6-octadienyl)-1,4-benzoquinone, D-975

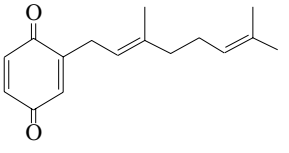
[80496-91-9]

Fr. Pat., 1964, M2694; *CA*, 1964, **61**, 15940e (*synth, pharmacol, tox*)
Rudali, G. *et al., C. R. Hebd. Seances Soc. Biol. Ses Fil.*, 1966, **160**, 1365-1369 (*pharmacol*)
Sato, A. *et al., J. Nat. Prod.*, 1989, **52**, 975-981 (*Amaroucium multiplicatum constits*)
Ippen, H. *et al., Dermatol. Clin.*, 1990, **8**, 67 (*tox*)
Rueda, A. *et al., Nat. Prod. Lett.*, 1998, **11**, 127-130 (*7′-hydroxy 6′,7′-dihydro, activity*)
Aknin, M. *et al., J. Agric. Food Chem.*, 1999, **47**, 4175-4177 (*Aplidium savignyi constits, activity*)
Ioset, J.-R. *et al., J. Nat. Prod.*, 2000, **63**, 424-426 (*Cordia alliodora constit*)
Garrido, L. *et al., J. Nat. Prod.*, 2002, **65**, 1328-1331 (*Δ$^{1'}$-isomer 3′-methoxy*)

2-(3,7-Dimethyl-2,6-octadienyl)-1,4-benzoquinone D-975

Geranylbenzoquinone

[61977-06-8]



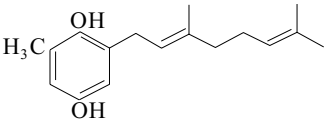
$C_{16}H_{20}O_2$ 244.333
Isol. from trichomes of *Phacelia ixodes* and from *Aplidium* sp. Yellow oil.

▶ Causes allergic contact dermatitis.

Hydroquinone: See 2-(3,7-Dimethyl-2,6-octadienyl)-1,4-benzenediol, D-974

Inouye, H. *et al., Phytochemistry*, 1979, **18**, 1301
Reynolds, G.W. *et al., Phytochemistry*, 1979, **18**, 1567 (*isol, synth*)
Naruta, Y. *et al., J.O.C.*, 1980, **45**, 4097 (*synth*)
Reynolds, G.W. *et al., Planta Med.*, 1981, **43**, 187 (*isol*)
Yazaki, K. *et al., Chem. Pharm. Bull.*, 1986, **34**, 2290

2-(3,7-Dimethyl-2,6-octadienyl)-6-methyl-1,4-benzenediol D-976



$C_{17}H_{24}O_2$ 260.375

(E)-form

2-Geranyl-6-methyl-1,4-benzenediol
[81532-05-0]
Sol. MeOH, C_6H_6. λ_{max} 241 (ϵ 17400) (MeOH) (Berdy).

1-Me ether: 3-(3,7-Dimethyl-2,6-octadienyl)-4-methoxy-5-methylphenol. 3-Geranyl-4-methoxy-5-methylphenol
$C_{18}H_{26}O_2$ 274.402
Constit. of a *Cystophora* sp. Oil. $Bp_{1.5}$ 200°.

4-Me ether: 2-(3,7-Dimethyl-2,6-octadienyl)-4-methoxy-6-methylphenol. 2-Geranyl-4-methoxy-6-methylphenol
$C_{18}H_{26}O_2$ 274.402
Constit. of the rhizomes of *Atractylodes lancea*. Yellow oil.

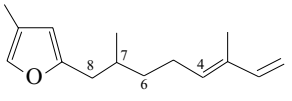
Di-Me ether: 2-(3,7-Dimethyl-2,6-octadienyl)-1,4-dimethoxy-6-methylbenzene. 2-Geranyl-1,4-dimethoxy-6-methylbenzene
[81532-03-8]
$C_{19}H_{28}O_2$ 288.429
Constit. of a *Cystophora* sp. Oil. $Bp_{1.5}$ 182°.

1,4-Quinone: 2-(3,7-Dimethyl-2,6-octadienyl)-6-methylbenzoquinone
[81532-02-7]
$C_{17}H_{22}O_2$ 258.36
Constit. of a *Cystophora* sp. and from *Atractylodes lancea*. Yellow oil. $Bp_{1.5}$ 210°.

Capon, R.J. *et al., Phytochemistry*, 1981, **20**, 2598-2600 (*1-Me, di-Me, quinone, isol*)
Resch, M. *et al., J. Nat. Prod.*, 1998, **61**, 347-350 (*isol, quinone, pmr, cmr*)
Resch, M. *et al., Planta Med.*, 2001, **67**, 437-442 (*4-Me ether*)

2-(2,6-Dimethyl-5,7-octadienyl)-4-methylfuran, 9CI D-977

[85679-59-0]



$C_{15}H_{22}O$ 218.338
Constit. of *Sinularia capillosa*. Oil.

6,7-Didehydro: ***2-(2,6-Dimethyl-2,5,7-octatrienyl)-4-methylfuran***
[85679-61-4]
$C_{15}H_{20}O$ 216.322
Constit. of *Sinularia capillosa*.

7,8-Didehydro: ***2-(2,6-Dimethyl-1,5,7-octatrienyl)-4-methylfuran***
$C_{15}H_{20}O$ 216.322
Constit. of *Sinularia capillosa*. Oil.

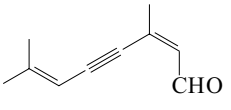
4Z-Isomer, 6,7-didehydro: [85679-62-5]
$C_{15}H_{20}O$ 216.322
Constit. of *Sinularia capillosa*. Oil.

4Z-Isomer, 7,8-didehydro: [85679-63-6]
Constit. of *Sinularia capillosa*.
Oil.

$\Delta^{3,15}$-Isomer, 6E,7-didehydro: ***4-Methyl-2-(2-methyl-6-methylene-2,7-octadienyl)furan***
[93590-09-1]
$C_{15}H_{20}O$ 216.322
Constit. of *Alcyonium palmatum*. Oil.

Bowden, B.F. *et al., Aust. J. Chem.*, 1983, **36**, 371
Cimino, G. *et al., J. Nat. Prod.*, 1984, **47**, 877-878 (*Aleyonium constit*)

3,7-Dimethyl-2,6-octadien-4-ynal D-978

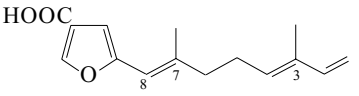


$C_{10}H_{12}O$ 148.204

(Z)-form
Taxifolial D
[142474-79-1]
Constit. of *Caulerpa taxifolia*.
Oil. λ_{max} 259 (ϵ 22000); 322 (ϵ 15800); 355 (ϵ 6300) (MeOH) (Berdy).
▶ Toxic.

Guerriero, A. *et al., Helv. Chim. Acta*, 1992, **75**, 689 (*isol, pmr, cmr*)

5-(2,6-Dimethyl-1,5,7-octatrienyl)-3-furancarboxylic acid D-979



(3E,7E)–form

$C_{15}H_{18}O_3$ 246.305

(3E,7E)-form
Constit. of *Sinularia capillosa* and *Sinularia lochmodes*. Shows antiinflammatory props. Cryst.
Mp 94.5-95.5°.

Me ester: [85679-64-7]
$C_{16}H_{20}O_3$ 260.332
Constit. of *Sinularia capillosa*. Oil. λ_{max} 208 (ϵ 16980); 236 (ϵ 21877); 258 (ϵ 24547) (EtOH) (Derep).

7,8-Dihydro: 5-(2,6-Dimethyl-5,7-octadienyl)-3-furancarboxylic acid
[85679-68-1]
$C_{15}H_{20}O_3$ 248.321
Constit. of *Sinularia capillosa* and *Sinularia lochmodes*. Oil.

7,8-Dihydro, Me ester: [85679-65-8]
$C_{16}H_{22}O_3$ 262.348
Constit. of *Sinularia capillosa*. Oil.

(3Z,7E)-form [64597-82-6]
Constit. of *Sinularia gonatodes*.
Cryst. (petrol).
Mp 99-100°.

Me ester: [64597-84-8]
Constit. of *Sinularia capillosa*.
Oil.

7,8-Dihydro: [85679-69-2]
Constit. of *Sinularia capillosa*.
Oil.

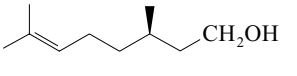
7,8-Dihydro, Me ester: [85679-66-9]
Constit. of *Sinularia capillosa*.
Oil.

[105072-13-7]

Coll, J.C. *et al., Tet. Lett.*, 1977, **18**, 1539-1542 (*Sinularia gonatodes constit*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1983, **36**, 371 (*isol*)
Park, S.K. *et al., J. Korean Chem. Soc.*, 1994, **38**, 749-752 (*isol*)
Williams, D.H. *et al., Tetrahedron*, 1996, **52**, 4245 (*synth*)

3,7-Dimethyl-6-octen-1-ol D-980

Citronellol. *β-Rhodinol. β-Citronellol. Yacarol. Rhodinol*†
[106-22-9]



(R)–form

$C_{10}H_{20}O$ 156.267
Occurs in many essential oils, usually as a partial racemate. Obt. mainly from geranium oil or synthetically. Widely used fragrance material for floral perfumes. Flavour for use in citrus compositions. Both enantiomers and the racemate are among the most widely used fragrance materials, used in floral compositions. Esters used in foods etc. are mostly of unreported enantiomeric composition. They are given here under the racemate and the props. reported presumably refer to the racemic forms.
▶ Fl. p. >100°. Skin irritant. LD_{50} (rat, orl) 3450 mg/kg. LD_{50} (rbt, skn) 2650 mg/kg. RH3400000

(R)-form [1117-61-9]
Constit. of black cumin (*Nigella sativa*) seeds and *Cymbopogon distans*. A common constit. of plant oils, esp. in the Rutaceae. Also isol. from alligator secretions. Richest source is *Boronia citriodora* oil (80%). Mostly prod. by partial or total synth.
Oil with sweet rose odour and bitter taste. d^{20} 0.86. Bp 108° $Bp_{0.5}$ 68°. $[\alpha]_D$ +5.45 (neat). n_D^{20} 1.4558.

(*S*)-*form* [7540-51-4]
Constit. of geranium and citronella oils. Used in perfumery and flavourings.
Oil with sweet odour, more delicate than *R*-enantiomer, and sweet peach-like taste. $Bp_{0.5}$ 68-70°. $[\alpha]_D$ -4.76.

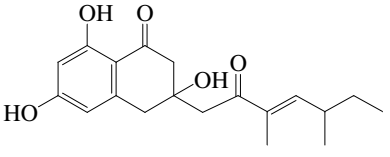
(±)-*form*
FEMA 2309
[26489-01-0] Bp 213-215° Bp_{12} 107-108°.

(ξ)-*form*
Identified in esterified form in the bryozoan *Conopeum seuratum*.
[22850-15-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 145C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 216B; 216C; 217A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 213A; 213C; 213D (*ir*)
Burrell, J.W.K. *et al., J.C.S.(C)*, 1966, 2144 (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037-1064 (*ir*)
Shono, T. *et al., Tet. Lett.*, 1974, 1295-1298 (*synth*)
Hidai, M. *et al., Chem. Comm.*, 1975, 170-171 (*synth*)
Corey, E.J. *et al., J.O.C.*, 1976, **41**, 380-381 (*synth*)
Chan, K.-K. *et al., J.O.C.*, 1976, **41**, 3497-3505 (*synth*)
Lanza, E. *et al., Phytochemistry*, 1977, **16**, 1555-1560 (*biosynth*)
Hiroma, M. *et al., J.O.C.*, 1985, **50**, 127-129 (*synth*)
Hadjieva, P. *et al., Z. Naturforsch., C*, 1987, **42**, 1019-1022 (*occur, bryozoan*)
Sharma, A. *et al., Annalen*, 1996, 529-531 (*resoln, pmr, ir*)

3-(3,5-Dimethyl-2-oxo-3-heptenyl)-3,4-dihydro-3,6,8-trihydroxy-1(2*H*)-naphthalenone D-981

3-(3,5-Dimethyl-2-oxo-3-heptenyl)-3,6,8-trihydroxy-1-tetralone

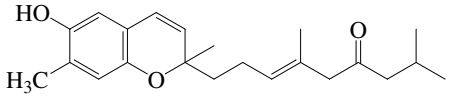


$C_{19}H_{24}O_5$ 332.396

(3ξ,3′*E*,5′ξ)-*form*
Prod. by the marine fungus *Keissleriella* sp. YS4108. Antifungal agent. Yellowish gum. $[\alpha]_D^{20}$ -23.6 (c, 0.06 in $CHCl_3$).
Liu, C.H. *et al., Planta Med.*, 2002, **68**, 363-365 (*isol, pmr, cmr*)

2-(4,8-Dimethyl-6-oxo-3-nonenyl)-6-hydroxy-2,7-dimethyl-2*H*-1-benzopyran D-982

*9-(6-Hydroxy-2,7-dimethyl-2*H*-1-benzopyran-2-yl)-2,6-dimethyl-6-nonen-4-one, 9CI*

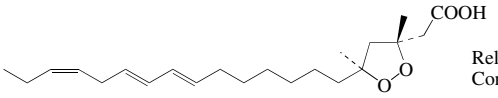


$C_{22}H_{30}O_3$ 342.477

(2ξ,3′*E*)-*form* [369380-52-9]
Isol. from *Leminda millecra*.
Orange oil. λ_{max} 222 (log ϵ 4.43); 267 (log ϵ 3.68); 331 (log ϵ 3.11) (MeOH).
McPhail, K.L. *et al., J. Nat. Prod.*, 2001, **64**, 1183-1190 (*isol, pmr, cmr, ms*)

3,5-Dimethyl-5-(7,9,12-pentadecatrienyl)-1,2-dioxolane-3-acetic acid D-983

3,5-Epidioxy-3,5-dimethyl-12,14,17-eicosatrienoic acid

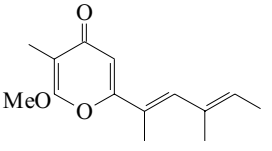


$C_{22}H_{36}O_4$ 364.524

(3*R,5*S**,7′*E*,9′*E*,12′*Z*)-*form***
Isol. from the sponge *Plakinastrella* sp.
Pale yellow oil.
Me ester:
$C_{23}H_{38}O_4$ 378.551
Isol. from *Plakinastrella* sp. Oil. $[\alpha]_D$ -28.5 (c, 0.2 in $CHCl_3$).
λ_{max} 228 (ϵ 37000); 264 (ϵ 5000); 275 (ϵ 4700) (hexane).
Qureshi, A. *et al., J. Nat. Prod.*, 1998, **61**, 1539-1542 (*isol, uv, ir, pmr, cmr*)

6-(1,3-Dimethyl-1,3-pentadienyl)-2-methoxy-3-methyl-4*H*-pyran-4-one, 9CI D-984

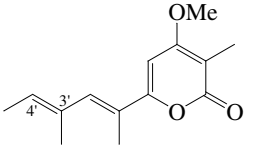
7-Methyl-12-norcyercene B



$C_{14}H_{18}O_3$ 234.294

(*E,E*)-*form* [144938-29-4]
Isol. from *Ercolania funerea*. Ichthyotoxic. λ_{max} 229 (ϵ 10320); 276 (ϵ 6785) (MeOH) (Berdy).
Vardaro, R.R. *et al., Tetrahedron*, 1992, **48**, 9561 (*isol, struct*)

6-(1,3-Dimethyl-1,3-pentadienyl)-4-methoxy-3-methyl-2*H*-pyran-2-one, 9CI D-985



(*E,E*)-*form*

$C_{14}H_{18}O_3$ 234.294

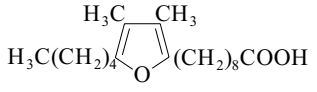
(1′*E*,3′*E*)-*form*
Phomenin A. *Phomapyrone A. 7-Methylcyercene 1*
[144938-31-8]
Prod. by *Phoma tracheiphila* and *Leptosphaeria maculans*/*Phoma lingam*. Also isol. from the mollusc *Ercolania funerea*. Phytotoxin. Solid. λ_{max} 255 (log ϵ 4.01); 342 (log ϵ 4.05) ($CHCl_3$).
*3′,4′-Dihydro, 4′-oxo: 6-(1,3-Dimethyl-4-oxo-1-pentenyl)-4-methoxy-3-methyl-2*H*-pyran-2-one.* ***Phomapyrone E***
$C_{14}H_{18}O_4$ 250.294
Prod. by *Leptosphaeria maculans*/*Phoma lingam*. λ_{max} 230; 335 (no solvent reported).

(1′*E*,3′*Z*)-*form*
Phomenin B
[155233-35-5]
Prod. by *Phoma tracheiphila*.

(1′*Z*)-*form*
3′ξ,4′ξ-Epoxide: ***Phomapyrone G***
$C_{14}H_{18}O_4$ 250.294
Prod. by *Leptosphaeria maculans*/*Phoma lingam*. λ_{max} 230; 330 (no solvent reported).

Vardaro, R.R. *et al., Tetrahedron*, 1992, **48**, 9561-9566 (*isol, struct*)
Tringali, C. *et al., Nat. Prod. Lett.*, 1993, **3**, 101 (*isol*)
Pedras, M.S.C. *et al., Phytochemistry*, 1994, **36**, 1315; 2005, **66**, 81-87 (*Phomapyrones, isol, pmr, cmr, ms, biosynth*)

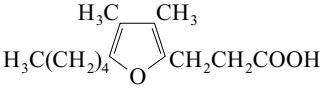
3,4-Dimethyl-5-pentyl-2-furannonanoic acid D-986
10,13-Epoxy-11,12-dimethyl-10,12-octadecadienoic acid. ***F_3 acid***
[57818-40-3]



$C_{20}H_{34}O_3$ 322.487
Present in fish oils. Also found in human and bovine blood plasma as phospholipid.

Glass, R.L. *et al., Lipids*, 1974, **9**, 1004; 1975, **10**, 695; 1977, **12**, 828
Gunstone, F.D. *et al., J. Sci. Food Agric.*, 1978, **29**, 539
Puchta, V. *et al., Annalen*, 1987, 25 (*occur*)
Scheinkönig, J. *et al., Annalen*, 1991, 451 (*biosynth*)
Batna, A. *et al., Annalen*, 1991, 861 (*biosynth*)
Spiteller, G. *et al., Lipids*, 2005, **40**, 755-771 (*rev, synth, occur*)

3,4-Dimethyl-5-pentyl-2-furanpropanoic acid D-987
4,7-Epoxy-5,6-dimethyl-4,6-dodecadienoic acid
[66612-08-6]

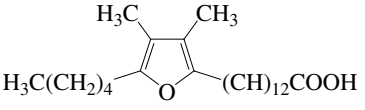


$C_{14}H_{22}O_3$ 238.326
Constit. of the soft corals *Sarcophyton glaucum* and *Sarcophyton gemmatum*. λ_{max} 225 (ϵ 7400) (MeOH).

[66612-07-5]

Groweiss, A. *et al., Experientia*, 1978, **34**, 299 (*isol*)

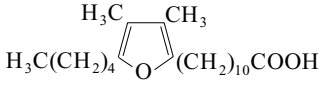
3,4-Dimethyl-5-pentyl-2-furantridecanoic acid D-988
14,17-Epoxy-15,16-dimethyl-14,16-heneicosadienoic acid. ***F_8 acid***
[57818-43-6]



$C_{24}H_{42}O_3$ 378.594
Constit. of fish oils.

Glass, R.L. *et al., Lipids*, 1975, **10**, 695-702 (*isol*)
Scheinkönig, J. *et al., Annalen*, 1991, 451-453 (*biosynth*)
Spiteller, G. *et al., Lipids*, 2005, **40**, 755-771 (*rev, occur, synth*)

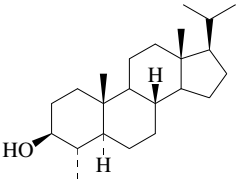
3,4-Dimethyl-5-pentyl-2-furanundecanoic acid, 9CI D-989
12,15-Epoxy-13,14-dimethyl-12,14-eicosadienoic acid. ***F_6 acid***
[57818-36-7]



$C_{22}H_{38}O_3$ 350.54
The most common member of a series of furanoid acids varying in chain length and in the number of methyl groups; see also 3-Methyl-5-pentyl-2-furannonanoic acid, M-449. Present in fish lipids and reaching high proportions in starved fish. Component of F acid fraction present in human and beef blood serum.

Glass, R.L. *et al., Lipids*, 1977, **12**, 828
Gunstone, F.D. *et al., J. Sci. Food Agric.*, 1978, **29**, 539
Puchta, V. *et al., Annalen*, 1988, 25 (*occur*)
Batna, A. *et al., Annalen*, 1991, 861 (*biosynth*)
Spitller, G. *et al., Lipids*, 2005, **40**, 755-771 (*rev, occur, synth*)

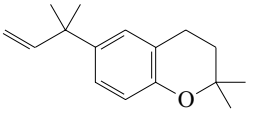
4,20-Dimethylpregnan-3-ol D-990
4-Methyl-23,24,25,26,27-pentanorcholestan-3-ol



$C_{23}H_{40}O$ 332.568

(3β,4α,5α)-*form* [242467-53-4]
Sterol from the Black Sea hydrozoan *Obelia longissima*.
De Rosa, S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1999, **123**, 229-233

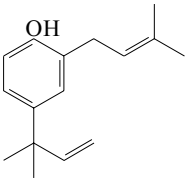
6-(1,1-Dimethyl-2-propenyl)-3,4-dihydro-2,2-dimethyl-2*H*-1-benzopyran D-991
6-(1,1-Dimethyl-2-propenyl)-2,2-dimethylchroman. 6-(1,1-Dimethylallyl)-2,2-dimethylchroman
[73215-08-4]



$C_{16}H_{22}O$ 230.349
Isol. from the brown alga *Perithalia caudata* (Sporochnaceae). Oil. Possible artifact.

Blackman, A.J. *et al., Aust. J. Chem.*, 1979, **32**, 2783 (*synth, pmr*)
Rochfort, S.J. *et al., J. Nat. Prod.*, 1994, **57**, 849 (*isol*)

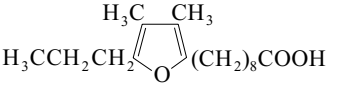
4-(1,1-Dimethyl-2-propenyl)-2-(3-methyl--2-butenyl)phenol D-992
[73215-04-0]



$C_{16}H_{22}O$ 230.349
Constit. of *Perithalia caudata*. Also from the brown alga *Sporochnus pedunculatus*. Antibacterial and antifungal agent. Oil.

Blackman, A.J. *et al., Aust. J. Chem.*, 1979, **32**, 2783
Gunasekera, L.S. *et al., Int. J. Pharmacogn.*, 1995, **33**, 253 (*isol*)

3,4-Dimethyl-5-propyl-2-furannonanoic acid, 9CI D-993
10,13-Epoxy-11,12-dimethyl-10,12-hexadecadienoic acid. ***F_1 acid***
[57818-38-9]

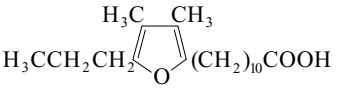


$C_{18}H_{30}O_3$ 294.433
Present in fish oils. Also found in human and bovine blood plasma as phospholipid.

Glass, R.L. *et al., Lipids*, 1974, **9**, 1004; 1975, **10**, 695; 1977, **12**, 828
Gunstone, F.D. *et al., J. Sci. Food Agric.*, 1978, **29**, 539

Puchta, V. *et al., Annalen*, 1988, 25 (*occur*)
Scheinkönig, J. *et al., Annalen*, 1991, 451 (*biosynth*)
Batna, A. *et al., Annalen*, 1991, 861 (*biosynth*)
Spiteller, G. *et al., Lipids*, 2005, **40**, 755-771 (*rev, synth, occur*)

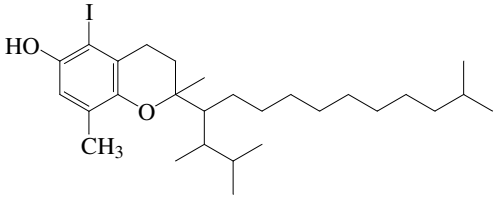
3,4-Dimethyl-5-propyl-2-furanundecanoic acid, 9CI D-994
12,15-Epoxy-13,14-dimethyl-12,14-octadecadienoic acid. ***F_4 acid***
[57818-41-4]



$C_{20}H_{34}O_3$ 322.487
Present in fish oils. Also found in human and bovine blood plasma as phospholipids.

Glass, R.L. *et al., Lipids*, 1974, **9**, 1004; 1975, **10**, 695; 1977, **12**, 828
Gunstone, F.D. *et al., J. Sci. Food Agric.*, 1978, **29**, 539
Puchta, V. *et al., Annalen*, 1988, 25 (*occur*)
Scheinkönig, J. *et al., Annalen*, 1991, 451 (*biosynth*)
Batna, A. *et al., Annalen*, 1991, 858 (*biosynth*)
Spiteller, G. *et al., Lipids*, 2005, **40**, 755-771 (*rev, synth, occur*)

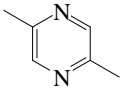
2-[1-(1,2-Dimethylpropyl)-10-methylundecyl]-3,4-dihydro-5-iodo-2,8-dimethyl-2*H*-1-benzopyran-6-ol, 9CI D-995
[161187-78-6]



$C_{28}H_{47}IO_2$ 542.583
Isol. from *Ascophyllum nodosum*. Antioxidant. Lipid peroxidation inhibitor. CA name and struct. in abstract do not match.

Japan. Pat., 1994, 94 298 753; *CA*, **122**, 160372p (*isol*)

2,5-Dimethylpyrazine, 9CI D-996
FEMA 3272
[123-32-0]



$C_6H_8N_2$ 108.143
Component of urinary signalling pheromone in the tree shrew *Tupaia belangeri* and the pine vole *Microtus pinetorum*. Prod. by *Chondromyces crocatus*. Isol. from an arctic marine bacterium. Used as flavour additive and odorant in foods. Liq. or solid with potato chip flavour. Sol. H_2O, EtOH, Et_2O.
Mp 15°. Bp 155°. pK_{a1} 1.85; pK_{a2} -4.6 (27°, H_2SO_4 aq.). pK_{a1} 1.99; pK_{a2} -4.42 (25°, H_2O). Steam-volatile. Odour threshold 1800 ppb in H_2O.

▶ Fl. p. 64° (oc). LD_{50} (rat, orl) 1020 mg/kg. UQ2800000

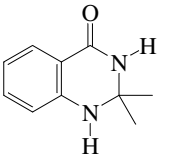
Picrate: Mp 157°.

Mono-oxide: [6890-37-5]
$C_6H_8N_2O$ 124.142
Needles (C_6H_6). Mp 105-108°. Subl.0.001 100.

1,4-Dioxide: [6890-38-6]
$C_6H_8N_2O_2$ 140.141
Needles ($CHCl_3$). Mp 280° dec.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 840D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 398C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1556C (*ir*)
Newbold, G.T. *et al., J.C.S.*, 1947, 1183-1185 (*1-oxide, 1,4-dioxide*)
Langdon, W.K. *et al., Ind. Eng. Chem. Prod. Res. Dev.*, 1964, **3**, 8 (*synth*)
Wilen, S.H. *et al., Chem. Ind. (London)*, 1969, **8**, 237 (*synth*)
Paudler, W.W. *et al., Org. Mass Spectrom.*, 1970, **4**, 513 (*ms*)
Paudler, W.W. *et al., Org. Magn. Reson.*, 1971, **3**, 217 (*nmr*)
Oertel, R.P. *et al., Anal. Chem.*, 1972, **44**, 1589 (*Raman*)
Bus, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1973, **92**, 123 (*ir*)
Gumbley, S.J. *et al., J. Het. Chem.*, 1985, **22**, 1143 (*props*)
von Stralendorff, F. *et al., J. Chem. Ecol.*, 1987, **13**, 655
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DTU600
Boyer, M.L. *et al., J. Chem. Ecol.*, 1989, **15**, 649
Eiermann, U. *et al., Chem. Ber.*, 1990, **123**, 523 (*uv*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 874 (*use, occur*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*marine isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DTU600

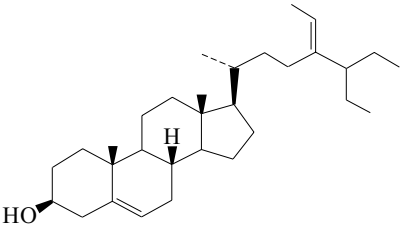
2,2-Dimethyl-4(1*H*,3*H*)-quinazolinone D-997



$C_{10}H_{12}N_2O$ 176.218
Prod. by *Cytophaga marinoflava* sp. AM13.1. Amorph. solid.

Shaaban, M. *et al., J. Nat. Prod.*, 2002, **65**, 1660-1663 (*isol*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*isol, pmr, ms*)

26,27-Dimethylstigmasta-5,24(28)-dien-3-ol D-998
24-Ethylidene-26,27-dimethylcholest-5-en-3-ol



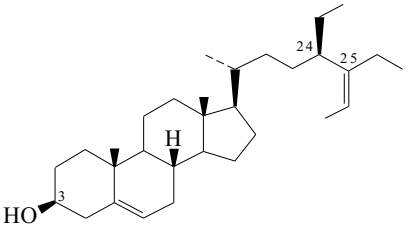
(3β,24*E*)–*form*

$C_{31}H_{52}O$ 440.751

(3β,24*E*)-*form*
28-Methylxestosterol
Isol. from the sponge *Strongylophora durissima*. Cryst. Mp 116-117°. $[\alpha]_D^{20}$ -37 (c, 0.009 in $CHCl_3$).

(3β,24*Z*)-*form*
Cryst. Mp 130-131°. $[\alpha]_D^{20}$ -15 (c, 0.02 in $CHCl_3$).
Li, L.N. *et al., Tet. Lett.*, 1981, **22**, 4639-4642 (*isol*)

26,27-Dimethylstigmasta-5,25-dien-3-ol D-999
24-Ethyl-26,27-dimethylcholesta-5,25-dien-3-ol

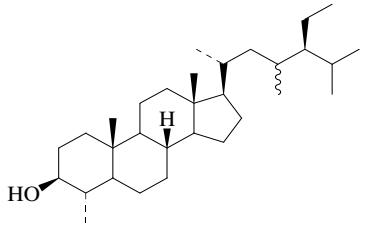


$C_{31}H_{52}O$ 440.751

(3β,24*R*,25*Z*)-*form*
26-Methylstrongylosterol
Constit. of the sponge *Strongylophora durissima*. Cryst. Mp 107-108°. $[\alpha]_D^{20}$ -15 (c, 0.017 in $CHCl_3$).

(3β,24*R*,25*E*)-*form*
Constit. of *Strongylophora durissima*. Cryst. Mp 90-91°. $[\alpha]_D^{20}$ -21 (c, 0.002 in $CHCl_3$).
Li, L.N. *et al., Tet. Lett.*, 1981, **22**, 4639-4642 (*isol*)

4,23-Dimethylstigmastan-3-ol D-1000
24-Ethyl-4,23-dimethylcholestan-3-ol



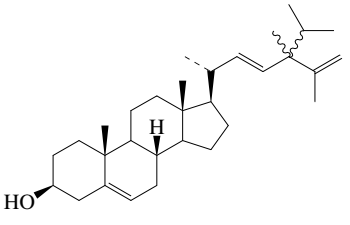
(3β,4α,23ξ,24*S*)-*form*

$C_{31}H_{56}O$ 444.783

(3β,4α,23ξ,24*S*)-*form* [351443-75-9]
Constit. of a *Cladiella* sp. Cryst. (MeOH). Mp 185-186°. $[\alpha]_D^{25}$ +11.5 (c, 0.1 in $CHCl_3$).

(3β,4α,23ξ,24ξ)-*form*
Component of dinoflagellate *Prorocentrum micans* sterols from an Adriatic red tide bloom.
Piretti, M.V. *et al., J. Phycol.*, 1997, **33**, 61 (*occur, dinoflagellate*)
Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 2001, **40**, 405-409 (*isol, pmr, cmr*)

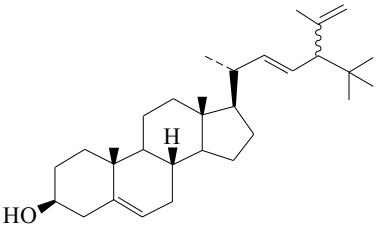
24,28-Dimethylstigmasta-5,22,25-trien-3-ol D-1001
24-Isopropyl-24-methylcholesta-5,22,25-trien-3-ol



$C_{31}H_{50}O$ 438.735

(3β,22*E*,24ξ)-*form* [102054-52-4]
Constit. of a *Pseudaxinyssa* sp.
22,23-Dihydro: 24,28-Dimethylstigmasta-5,25-dien-3-ol. 24-Isopropyl-24-methylcholesta-5,25-dien-3-ol
[102054-51-3]
$C_{31}H_{52}O$ 440.751
Constit. of a *Pseudaxinyssa* sp.
22,23,25,26-Tetrahydro: ***24,28-Dimethylstigmast-5-en-3-ol****. 24-Isopropyl-24-methylcholest-5-en-3-ol*
[102054-50-2]
$C_{31}H_{54}O$ 442.767
Constit. of a *Pseudaxinyssa* sp.
Tam Ha, T.B. *et al., Steroids*, 1985, **45**, 263-276 (*isol, pmr, ms*)

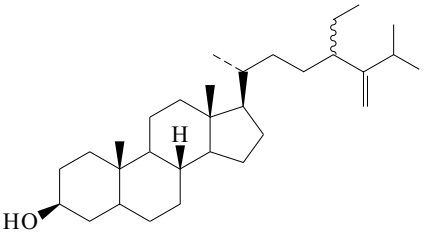
25,28-Dimethylstigmasta-5,22,28-trien-3-ol, 9CI D-1002
*28,28-Dimethylstigmasta-5,22,25-trien-3-ol, 9CI. 24-Isopropenyl-25-methylcholesta-5,22-dien-3-ol. 24-*tert*-Butylcholesta-5,22,25-trien-3-ol*



$C_{31}H_{50}O$ 438.735
Has been named both as 25,28- and 28,28-dimethyl in CAS. Both names are valid, but 25,28-dimethyl should take priority.

(3β,22*E*,24ξ)-*form*
Epipolasterol
[195972-43-1]
Metab. of sponges *Halichondria* sp. and *Epipolasis* sp.
Ac: [97484-58-7]
Cryst. (MeOH). Mp 124-127°. $[\alpha]_D^{20}$ -49 (c, 0.2 in $CHCl_3$).
*22,23-Dihydro: 25,28-Dimethylstigmasta-5,28-dien-3-ol. 28,28-Dimethylstigmasta-5,25-dien-3-ol. 24-Isopropenyl-25-methylcholest-5-en-3-ol. 24-*tert*-Butylcholesta-5,25-dien-3-ol.*
Axinyssasterol*. 22,23-Dihydroepipolasterol*
[86105-68-2]
[195972-45-3]
$C_{31}H_{52}O$ 440.751
Constit. of the sponges *Pseudaxinyssa* sp. and *Epipolasis* sp.
Li, X. *et al., Tet. Lett.*, 1983, **24**, 665-668 (*Axinyssasterol*)
Shubina, L.K. *et al., Khim. Prir. Soedin.*, 1985, **21**, 232; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 217 (*isol. Halichondria*)
Kerr, R.G. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1997, **117**, 561-563 (*Epipolasterols*)

26,26-Dimethylstigmast-25(27)-en-3-ol D-1003
24-Ethyl-26,26-dimethylcholest-25(27)-en-3-ol



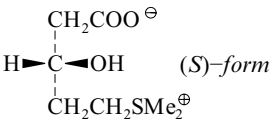
$C_{31}H_{54}O$ 442.767

3β-*form* [129620-26-4]
Constit. of a *Xestospongia* sp.
Kerr, R.G. *et al., J.O.C.*, 1991, **56**, 58 (*isol, pmr*)

5-Dimethylsulfonio 2-amino-4-hydroxypentanoate D-1004
(4-Amino-4-carboxy-2-hydroxybutyl)dimethylsulfonium hydroxide inner salt, 9CI
[117845-16-6]
$Me_2S^{\oplus}CH_2CH(OH)CH_2CH(NH_2)COO^{\ominus}$
$C_7H_{15}NO_3S$ 193.266
Isol. from the alga *Lophocladia lallemandi*.
Sciuto, S. *et al., J. Nat. Prod.*, 1988, **51**, 1017

5-Dimethylsulfonio 3-hydroxypentanoate **D-1005**

(4-Carboxy-3-hydroxybutyl)dimethylsulfonium hydroxide inner salt, 9CI. ***Gonyol***



(*S*)–*form*

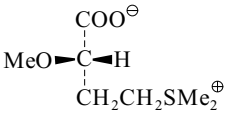
$C_7H_{14}O_3S$ 178.252

(S)-form [154277-23-3]
Isol. from the dinoflagellate *Gonyaulax polyedra*.
Oil. $[\alpha]_D^{25}$ +3.7 (c, 0.3 in H_2O).

Nakamura, H. *et al., Tet. Lett.*, 1993, **34**, 8481-8484 (*isol, pmr, cmr, synth*)

4-Dimethylsulfonio 2-methoxybutanoate **D-1006**

(3-Carboxy-3-methylpropyl)dimethylsulfonium hydroxide inner salt, 9CI
[122279-95-2]



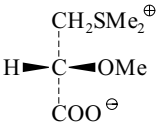
$C_7H_{14}O_3S$ 178.252

(S)-form [81920-17-4]
Isol. from the red alga *Rytiphloea tinctoria* and from *Vidalia volubilis*.
Syrup. $[\alpha]_D^{25}$ -26.6 (c, 1 in H_2O).

Sciuto, S. *et al., Phytochemistry*, 1982, **21**, 227-228 (*isol, struct*)
Patti, A. *et al., J. Nat. Prod.*, 1992, **55**, 53-57 (*isol*)

3-Dimethylsulfonio 2-methoxypropanoate **D-1007**

(2-Carboxy-2-methoxyethyl)dimethylsulfonium hydroxide inner salt, 9CI



(*R*)–*form*

$C_6H_{12}O_3S$ 164.225

(R)-form [147427-22-3]
Isol. from the red alga *Digenea simplex*.
$[\alpha]_D^{25}$ +33 (c, 0.5 in H_2O).

Patti, A. *et al., J. Nat. Prod.*, 1993, **56**, 432 (*isol*)

2-(Dimethylsulfonio)acetic acid **D-1008**

(Carboxymethyl)dimethylsulfonium hydroxide inner salt, 9CI. Dimethylacetothetin. Dimethylthetin. Thetin
[4727-41-7]
$Me_2S^{\oplus}CH_2COO^{\ominus}$
$C_4H_8O_2S$ 120.172
Zwitterion. Isol. from the red alga *Digenea simplex*. Fish feeding stimulant. Cryst. + $1H_2O$ (EtOH/Et_2O).
Mp 67-69° (as monohydrate) Mp 143.5-144.5° (anhydr.). pK_a 1.5.

Hydrochloride: [10132-50-0]
$C_4H_9ClO_2S$ 156.633
Cryst. (EtOH/Et_2O). Mp 134.5-135.5°.

Me ester, chloride: [19643-32-4]
$C_5H_{11}ClO_2S$ 170.659
Mp 107-108°.

Me ester, bromide: (Carbomethoxymethyl)dimethylsulfonium bromide
[19643-31-3]
$C_5H_{11}BrO_2S$ 215.111
Cryst. (EtOH/Et_2O). Mp 175-177° (81-82°).

Et ester, bromide: (Carbethoxymethyl)dimethylsulfonium bromide
[5187-82-6]
$C_6H_{13}BrO_2S$ 229.137
Mp 85-87°.

► WR7600000

[19643-24-4, 24220-08-4, 114827-81-5]

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 393E (*ir*)
du Vigneaud, V. *et al., J. Biol. Chem.*, 1948, **174**, 477 (*synth*)
Klee, W.A. *et al., Biochemistry*, 1967, **6**, 988 (*conformn, ir*)
Payne, G.B. *et al., J.O.C.*, 1967, **32**, 3351 (*synth, ester*)
Ratts, K.W. *et al., J.O.C.*, 1968, **33**, 70 (*synth, ir, pmr*)
Johnson, A.W. *et al., J.O.C.*, 1969, **34**, 1240 (*synth*)
Rutolo, D.A. *et al., Org. Prep. Proced. Int.*, 1969, **1**, 111 (*synth, ester*)
Patti, S. *et al., J. Nat. Prod.*, 1993, **56**, 432 (*isol*)

2,12-Dimethyltetradecanoic acid **D-1009**

$H_3CCH_2CH(CH_3)(CH_2)_9CH(CH_3)COOH$
$C_{16}H_{32}O_2$ 256.428
Isol. from a halophilic *Bacillus* sp.

Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 256-259 (*isol, ms*)

2,13-Dimethyltetradecanoic acid **D-1010**

$(H_3C)_2CH(CH_2)_{10}CH(CH_3)COOH$
$C_{16}H_{32}O_2$ 256.428
Isol. from a halophilic *Bacillus* sp.

Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 256-259 (*isol, ms*)

4,13-Dimethyltetradecanoic acid **D-1011**

$(H_3C)_2CH(CH_2)_8CH(CH_3)CH_2CH_2COOH$
$C_{16}H_{32}O_2$ 256.428
Isol. from a halophilic *Bacillus* sp.

Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 256-259 (*isol, ms*)

9,13-Dimethyltetradecanoic acid **D-1012**

$(H_3C)_2CH(CH_2)_3CH(CH_3)(CH_2)_7COOH$
$C_{16}H_{32}O_2$ 256.428
Isol. from the sponge *Calyx podatypa*.

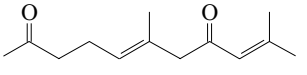
Carballeira, N.M. *et al., J. Nat. Prod.*, 2000, **63**, 666-669 (*isol, synth, pmr, cmr*)

10,13-Dimethyltetradecanoic acid **D-1013**

[121981-41-7]
$(H_3C)_2CHCH_2CH_2CH(CH_3)(CH_2)_8COOH$
$C_{16}H_{32}O_2$ 256.428
Isol. from the sponge *Ectyoplasia ferox*.

Carballeira, N.M. *et al., Lipids*, 1989, **24**, 371 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2000, **63**, 666-669 (*synth*)

6,10-Dimethyl-5,9-undecadiene-2,8-dione **D-1014**

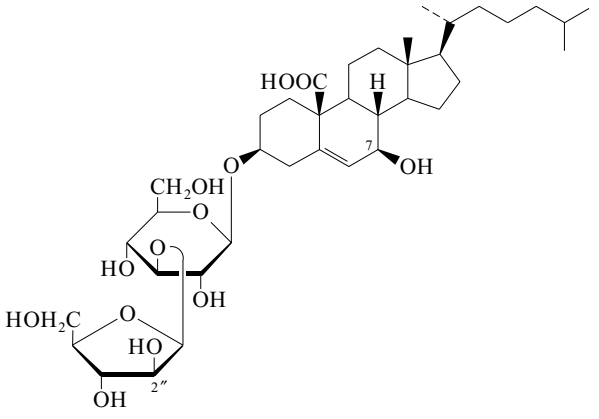


$C_{13}H_{20}O_2$ 208.3
Constit. of *Cystoseira crinita*. Oil.

Amico, V. *et al., Phytochemistry*, 1980, **19**, 2759

Dimorphoside A D-1015

3-[(3-O-β-D-Arabinofuranosyl-β-D-glucopyranosyl)oxy]-7-hydroxycholest-5-en-19-oic acid
[108179-46-0]

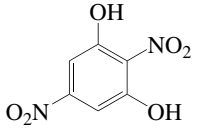


$C_{38}H_{62}O_{13}$ 726.9
Constit. of gorgonian *Anthoplexaura dimorpha*. Cell division inhibitor. Amorph. solid. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{23}$ -59 (c, 0.38 in MeOH).

7-Deoxy, 2″Ac: ***Dimorphoside B***
[108179-45-9]
$C_{40}H_{64}O_{13}$ 752.938
Constit. of *Anthoplexaura dimorpha*. Amorph. solid. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{23}$ -12 (c, 0.3 in MeOH).
Fusetani, N. *et al., Tet. Lett.*, 1987, **28**, 1187

2,5-Dinitro-1,3-benzenediol D-1016

2,5-Dinitroresorcinol



$C_6H_4N_2O_6$ 200.107

3-Me ether: 3-Methoxy-2,5-dinitrophenol
$C_7H_6N_2O_6$ 214.134
Isol. from the marine-derived *Flavobacterium* sp. T436.
Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005,

3,5-Dinitro-1,2-benzenediol, 9CI D-1017

3,5-Dinitropyrocatechol, 8CI. 3,5-Dinitrocatechol
[7659-29-2]
$C_6H_4N_2O_6$ 200.107
Used for photometric detn. of Nb, Ti, V, W, rare earth metals. Yellow needles (EtOH). Sol. alkalis, EtOH, Me_2CO; spar. sol. H_2O; insol. C_6H_6, $CHCl_3$. Mp 164°. pK_{a1} 3.39; pK_{a2} 10.03 (25°, 0.1*M* $NaClO_4$ 4% EtOH).

▶ CZ8947010

Di-Ac:
$C_{10}H_8N_2O_8$ 284.182
Mp 112°.

1-Me ether: 2-Methoxy-4,6-dinitrophenol. 3,5-Dinitroguaiacol
[63975-57-5]
$C_7H_6N_2O_6$ 214.134
Isol. from the seaweed *Marginisporum aberrans*. Prod. by the marine-derived *Flavobacterium* sp. T436. Yellow cryst. (C_6H_6). Mp 80° Mp 123-124°. λ_{max} 213 (ε 21400); 266 (ε 9550); 332 (ε 6460); 410 (ε 1100) (MeOH) (Derep).

2-Me ether: 2-Methoxy-3,5-dinitrophenol. 4,6-Dinitroguaiacol
$C_7H_6N_2O_6$ 214.134
Prod. by the marine-derived *Flavobacterium* sp. T436. Yellow cryst.
Mp 123°.

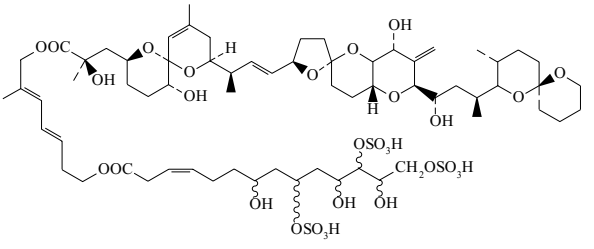
2-Me ether, Ac: [36383-37-6]
$C_9H_8N_2O_7$ 256.171
Mp 114°.

Di-Me ether: 1,2-Dimethoxy-3,5-dinitrobenzene. 3,5-Dinitroveratrole
[13661-34-2]
$C_8H_8N_2O_6$ 228.161
Cryst. (EtOH). Mp 102°.

Polecoff, F. *et al., J.C.S.*, 1918, **113**, 650 (*deriv*)
Heertjes, P.M. *et al., J.C.S.*, 1954, 1868 (*synth*)
Iorio, M.A. *et al., Ann. Chim. (Rome)*, 1959, **49**, 379 (*synth*)
Ohta, K. *et al., Phytochemistry*, 1977, **16**, 1085-1086 (*Marginisporum, isol*)
Lobiński, R. *et al., Anal. Sci.*, 1988, **4**, 629 (*detn, V*)
Marczenko, Z. *et al., Talanta*, 1988, **34**, 1001 (*detn, V*)
Lobiński, R. *et al., Anal. Chim. Acta*, 1989, **226**, 281 (*detn, Nb*)
Kawakami, T. *et al., J.C.S. Perkin 1*, 2000, 1259-1264 (*di-Me ether, synth, pmr, ir*)
Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*Flavobacterium, isol*)

Dinophysistoxin 4 D-1018

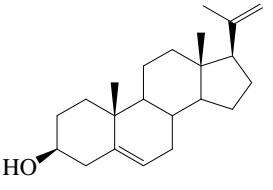
DTX4
[162795-98-4]



$C_{66}H_{104}O_{30}S_3$ 1473.728
Ester of Okadaic acid, O-90. Isol. from the dinoflagellate *Prorocentrum lima*. Phosphatase inhibitor. Solid. Sol. H_2O. Mp 300° dec. $[\alpha]_D^{26}$ -12 (c, 0.1 in MeOH). λ_{max} 230 (MeCN). λ_{max} 230 (MeCN) (Berdy).
Hu, T. *et al., Chem. Comm.*, 1995, 597; 1623 (*isol, pmr, cmr, biosynth*)

23,24-Dinorchola-5,20-dien-3-ol D-1019

23,24-Bisnorchola-5,20-dien-3-ol

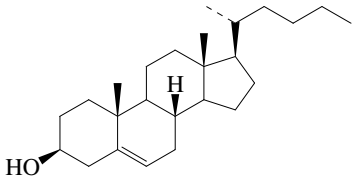


$C_{22}H_{34}O$ 314.51

3β-*form* [17879-91-3]
Sterol present in sponge *Damiriana hawaiiana* and *Cladophora vagabunda*.

20,21-Dihydro: 23,24-Dinorchol-5-en-3-ol. 23,24-Bisnorchol-5-en-3-ol. 20-Methylpregn-5-en-3-ol. 23,24,25,26,27-Pentanorcholest-5-en-3-ol. Gunneribol
[1042-59-7]
$C_{22}H_{36}O$ 316.526
Sterol present in sponge *Damiriana hawaiiana*.
Mp 135-136°.
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476 (*Damiriana hawaiiana constits*)
Elenkov, I. *et al., Phytochemistry*, 1995, **38**, 457-459 (*Cladophora vagabunda constit*)

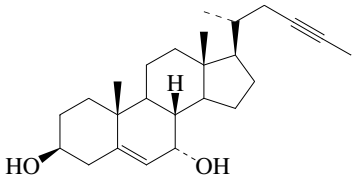
26,27-Dinorcholest-5-en-3-ol D-1020



$C_{25}H_{42}O$ 358.606

3β-*form* [2790-32-1]
Isol. from sponge *Damiriana hawaiiana*.
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476

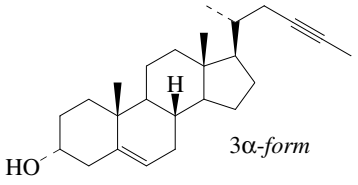
26,27-Dinorcholest-5-en-23-yne-3,7-diol D-1021



$C_{25}H_{38}O_2$ 370.574

(3β,7α)-*form*
Gelliusterol A
[351198-06-6]
Constit. of a *Gellius* sponge.
$[\alpha]_D$ -25.7 (c, 0.07 in MeOH). λ_{max} 230 (ϵ 176) (MeOH).
7-Ketone: 3-Hydroxy-26,27-dinorcholest-5-en-23-yn-7-one. ***Gelliusterol B***
[351198-07-7]
$C_{25}H_{36}O_2$ 368.558
Constit. of a *Gellius* sponge.
$[\alpha]_D$ -16.6 (c, 0.02 in MeOH). λ_{max} 237 (ϵ 283) (MeOH).
Gallimore, W.A. *et al., J. Nat. Prod.*, 2001, **64**, 741-744 (*isol, pmr, cmr*)

26,27-Dinorcholest-5-en-23-yn-3-ol D-1022



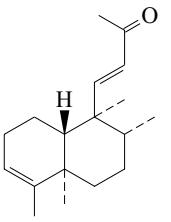
$C_{25}H_{38}O$ 354.575

3α-*form*
5β,6-Dihydro: ***26,27-Dinorcholest-23-yn-3-ol***
[123158-88-3]
$C_{25}H_{40}O$ 356.59
Minor sterol from *Calyx nicaeensis*, prob. as an endobacterial metab.

3β-*form* [63015-89-4]
Constit. of *Calyx nicaeensis.*
Cryst. (MeOH).
Mp 104-105°. $[\alpha]_D$ -42.2.
Ac: Mp 137-140°. $[\alpha]_D$ -33.7 (c, 3 in $CHCl_3$).
5β,6-Dihydro: [123158-89-4]
Isol. from sponge *Calyx nicaeensis*, prob. as a prod. of endobacterial metab.
Steiner, E. *et al., Helv. Chim. Acta*, 1977, **60**, 475-481 (*isol, synth*)
Itoh, T. *et al., J.A.C.S.*, 1983, **105**, 4407-4416 (*synth*)
Ha, T.B.T. *et al., Steroids*, 1989, **53**, 487-489 (*dihydro*)

14,15-Dinor-3,11-clerodadien-13-one D-1023

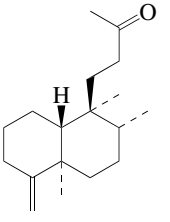
14,15-Bisnor-3,11-clerodadien-13-one



$C_{18}H_{28}O$ 260.419

ent-form
14,15-Bisnor-3,11-kolavadien-13-one. 14,15-Dinor-3,11-kolavadien-13-one
[126582-61-4]
Constit. of *Polyalthia viridis.*
Gum.
11,12-Dihydro: **ent-*14,15-Dinor-3-cleroden-3-one***. ent-*14,15-Bisnor-3-cleroden-3-one*
[130466-21-6]
$C_{18}H_{30}O$ 262.434
Isol. from *Parentucellia latifolia* and a *Mycale* sp. Oil. $[\alpha]_D$ -41.6 (c, 0.4 in $CHCl_3$).
Kijjoa, A. *et al., Phytochemistry*, 1990, **29**, 653 (*isol, pmr, cmr*)
Urones, J.G. *et al., Phytochemistry*, 1990, **29**, 2223 (*11,12-dihydro*)
Capon, R.J. *et al., J. Nat. Prod.*, 1997, **60**, 1261-1264 (*11,12-dihydro*)

14,15-Dinor-4(18)-cleroden-13-one D-1024

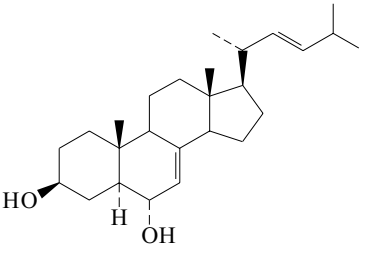


$C_{18}H_{30}O$ 262.434

ent-form [82205-28-5]
Constit. of a *Mycale* sp.
Oil. $[\alpha]_D$ +43 (c, 1.2 in $CHCl_3$).
13ξ-Alcohol: **ent-*14,15-Dinor-4(18)-cleroden-13-ol***
[199116-49-9]
$C_{18}H_{32}O$ 264.45
Constit. of a *Mycale* sp. Oil. $[\alpha]_D$ -27 (c, 0.2 in $CHCl_3$).
Albericci, M. *et al., Tetrahedron*, 1982, **38**, 1881-1890 (*synth*)
Capon, R.J. *et al., J. Nat. Prod.*, 1997, **60**, 1261-1264 (*isol, pmr, cmr*)

26,27-Dinorergosta-7,22-diene-3,6-diol, 9CI D-1025

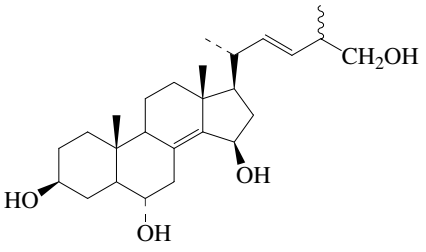
24-Norcholesta-7,22-diene-3,6-diol



$C_{26}H_{42}O_2$ 386.617

(3β,5α,6α,22*E*)-*form*
Constit. of *Spongionella gracilis*.
Cryst. (MeOH/petrol).
Mp 188-190°.
Madaio, A. *et al., J. Nat. Prod.*, 1989, **52**, 952 (*isol, pmr*)

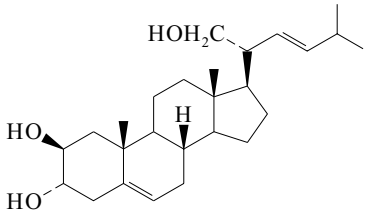
26,27-Dinorergosta-8(14),22-diene-3,6,15,25-tetrol D-1026
24-Norcholesta-8(14),22-diene-3,6,15,26-tetrol



$C_{26}H_{42}O_4$ 418.615

(3β,6α,15β,22*E*,24ξ)-*form* [195064-46-1]
Constit. of *Acodontaster conspicuus*.
$[\alpha]_D$ -15.7 (c, 1 in MeOH).
De Marino, S. *et al., J. Nat. Prod.*, 1997, **60**, 959-966 (*isol, pmr, cmr*)

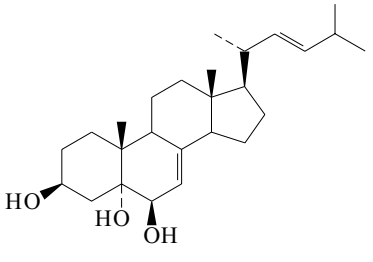
26,27-Dinorergosta-5,22-diene-2,3,21-triol, 9CI D-1027
24-Norcholesta-5,22-diene-2,3,21-triol



$C_{26}H_{42}O_3$ 402.616

(2β,3α,22*E*)-*form*
3,21-Di-O-*sulfate:* [161470-24-2]
$C_{26}H_{42}O_9S_2$ 562.744
Constit. of *Ophiopholis aculeata* and *Ophiura texturata*.
$[\alpha]_D$ -10.4.
Fedorov, S.N. *et al., J. Nat. Prod.*, 1994, **57**, 1631-1637 (*3,21-disulfate, isol, pmr, cmr*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1995, **58**, 189-196 (*3,21-disulfate, isol, pmr, cmr*)

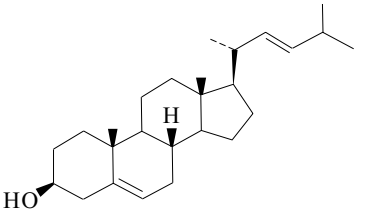
26,27-Dinorergosta-7,22-diene-3,5,6-triol D-1028
24-Norcholesta-7,22-diene-3,5,6-triol



$C_{26}H_{42}O_3$ 402.616

(3β,5α,6β,22*E*)-*form* [112058-02-3]
Constit. of *Heliometra glacialis maxima* and the sponge *Spongionella gracilis*.
Cryst. (MeOH).
Mp 215-217°.
Piccialli, V. *et al., J. Nat. Prod.*, 1987, **50**, 915-920 (*isol*)
Shubina, L.K. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **119**, 505-511 (*isol*)

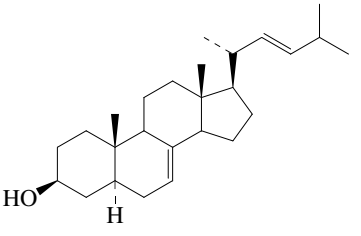
26,27-Dinorergosta-5,22-dien-3-ol, 9CI D-1029
24-Norcholesta-5,22-dien-3-ol



$C_{26}H_{42}O$ 370.617

(3β,22*E*)-*form* [38788-81-7]
Constit. of *Pseudostichopus trachus*, *Placopecten magellanicus*, *Bugula neritina*, *Mytilus edulis* (blue mussel), *Mya arenaria* and other crustaceans, molluscs and sponges such as *Damiriana hawaiiana*, *Echinus esculentus*, *Echinocardium cordatum*, *Antedon bifida*, *Ophiocomina nigra*, *Crassostrea virginica*, *Cucumaria lactea*, *Arctica islandica*, *Henricia sanguinolenta*, *Marthasterias glacialis* and *Polizoa opuntia*.
Cryst.
Mp 138-140° (122-124°). $[\alpha]_D$ -31 ($CHCl_3$).
3-O-*Sulfate:* [82563-91-5]
[151890-94-7]
$C_{26}H_{42}O_4S$ 450.681
Constit. of *Eupentacta fraudatrix*, *Cucumaria lactea*, *Echinus esculentus*, *Echinocardium cordatum*, *Antedon bifida* and *Ophiocomina nigra*.
[34428-92-7, 52745-87-6 (3β,22*Z*-form), 76250-41-4, 77880-46-7]
Idler, D.R. *et al., Steroids*, 1970, **16**, 451-461 (*isol, struct*)
Fryberg, M. *et al., Chem. Comm.*, 1971, 1194-1195 (*synth*)
Viala, J. *et al., Bull. Soc. Chim. Fr.*, 1972, 3626-3627 (*pmr, ms*)
Metayer, A. *et al., Tet. Lett.*, 1974, 595-598 (*synth*)
Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*isol, ms*)
Sheikh, Y.M. *et al., Steroids*, 1975, **26**, 129-136 (*synth*)
Delseth, C *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476 (*isol, sponge*)
Goodfellow, R.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **76**, 575-578 (*occur, sulfate*)
Palermo, J.A. *et al., Steroids*, 1996, **61**, 2-6 (*occur*)
Kerr, R.G. *et al., J. Nat. Prod.*, 1999, **62**, 468-470 (*isol, Bugula*)

26,27-Dinorergosta-7,22-dien-3-ol D-1030
24-Norcholesta-7,22-dien-3-ol



$C_{26}H_{42}O$ 370.617

(3β,5α,22*E*)-*form*
Asterosterol. *Asterosterin*
[30674-32-9]
Constit. of *Asterias amurensis*, *Cucumaria* sp., *Eupentacta fraudatrix*, *Holothuria nobilis*, *Placopecten magellanicus* and clams and oysters.
Cryst. (MeOH).
Mp 130-131°. $[\alpha]_D$ -6.4 (c, 1 in $CHCl_3$).
3-O-*Sulfate:* [446840-57-9]

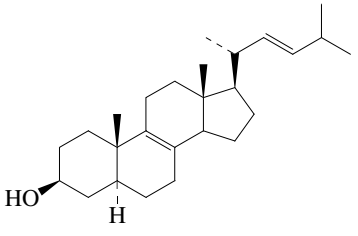
[151891-04-2]
$C_{26}H_{42}O_4S$ 450.681
Constit. of the starfish *Leptasterias alaskensis* and the sea cucumber *Eupentacta fraudatrix*.

3-O-β-D-Xylopyranoside: [74219-31-1]
$C_{31}H_{50}O_5$ 502.733
Constit. of *Eupentacta fraudatrix*.

Idler, D.R. *et al., Steroids*, 1970, **16**, 451-461 (*Placopecten magellanicus constit*)
Kobayashi, M. *et al., Tetrahedron*, 1973, **29**, 1193-1196 (*Asterias amurensis constit*)
Boll, P.M. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 270-271 (*synth*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1974, **22**, 236-238 (*synth*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*occur*)
Kapustina, I.I. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2002, **37**, 515-519 (*sulfate*)

26,27-Dinorergosta-8,22-dien-3-ol, 9CI D-1031

24-Norcholesta-8,22-dien-3-ol

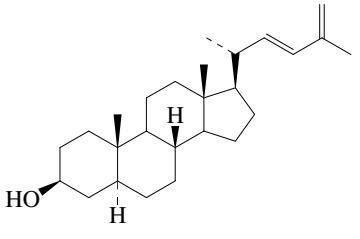


$C_{26}H_{42}O$ 370.617

(3β,5α,22*E*)-*form* [85733-78-4]
Constit. of the sponge *Axinella cannabina*.

Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol*)

26,27-Dinorergosta-22,24-dien-3-ol D-1032



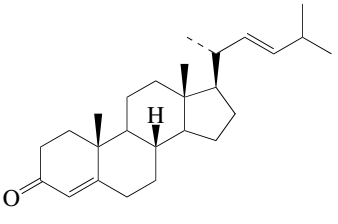
$C_{26}H_{42}O$ 370.617

(3β,5α,22*E*)-*form* [242467-55-6]
Isol. from the Black Sea hydrozoan *Obelia longissima*.

De Rosa, S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1999, **123**, 229-233

26,27-Dinorergosta-4,22-dien-3-one D-1033

24-Norcholesta-4,22-dien-3-one
[182257-20-1]



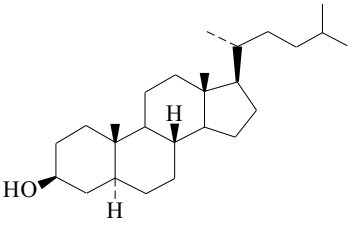
$C_{26}H_{40}O$ 368.601

(*E*)-*form* [55688-45-4]
Constit. of the sponge *Stelletta clarella* and dried prawns (*Nematopalaemon tenuipes*).

Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*isol, pmr, ms*)
Indap, M.M. *et al., Indian J. Exp. Biol.*, 1996, **34**, 588-589; *CA*, **125**, 270867y (*isol, pmr*)

26,27-Dinorergostan-3-ol, 9CI D-1034

24-Norcholestan-3-ol



$C_{26}H_{46}O$ 374.649

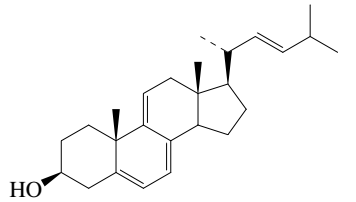
(3β,5α)-*form*
Halostanol
[69977-26-0]
Constit. of *Terpios zeteki* and sponges *Suberites japonicus*, *Synops* sp. and *Artemisia apollinis*.
Oil.

5,6-Didehydro: 26,27-Dinorergost-5-en-3-ol. 24-Norcholest-5-en-3-ol. ***24-Norcholesterol***
[38819-44-2]
$C_{26}H_{44}O$ 372.633
Present in giant clam *Placopecten magellanicus*.

Idler, D.R. *et al., Steroids*, 1976, **27**, 155 (*24-Norcholesterol*)
Ballentine, J.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1979, **63**, 119-123 (*Synops constit*)
Delseth, C. *et al., Helv. Chim. Acta*, 1979, **62**, 101
Dmitrenok, P.S. *et al., Khim. Prir. Soedin.*, 1988, **24**, 461; *Chem. Nat. Compd. (Engl. Transl.)*, 397 (*isol*)
Seldes, A.M. *et al., Z. Naturforsch., C*, 1990, **45**, 83 (*isol*)

26,27-Dinorergosta-5,7,9(11),22-tetraen-3-ol D-1035

24-Norcholesta-5,7,9(11),22-tetraen-3-ol



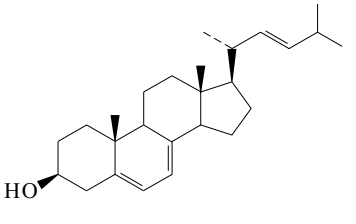
$C_{26}H_{38}O$ 366.586

(3β,22*E*)-*form* [85733-68-2]
Constit. of the sponge *Axinella cannabina*.

Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol, pmr, ms*)

26,27-Dinorergosta-5,7,22-trien-3-ol, 9CI D-1036

24-Norcholesta-5,7,22-trien-3-ol

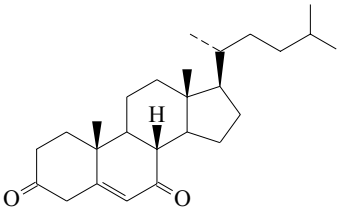


$C_{26}H_{40}O$ 368.601

(3β,22*E*)-*form*
Crassosterol
[78094-00-5]
Constit. of *Crassostrea virginica*. Also (stereochem. not explicit) in sponge *Tethya amamensis.*
Teshima, S.-I. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1981, **68**, 177 (*isol, pmr*)
Teshima, S. *et al., Lipids*, 1983, **18**, 193-197 (*occur, Tethya*)

26,27-Dinorergost-5-ene-3,7-dione D-1037

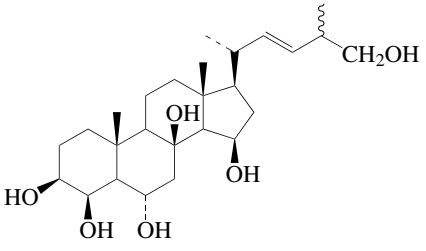
24-Norcholest-5-ene-3,7-dione. ***Somalenone***
[178494-82-1]



$C_{26}H_{40}O_2$ 384.601
Isol. from the red alga *Melanothamnus somalensis.* Amorph. powder. λ_{max} 240 (MeOH).
Ahmad, V.U. *et al., Phytochemistry*, 1996, **42**, 1141-1143 (*isol, pmr, cmr*)

26,27-Dinorergost-22-ene-3,4,6,8,15,25-hexol D-1038

24-Norcholest-22-ene-3,4,6,8,15,26-hexol

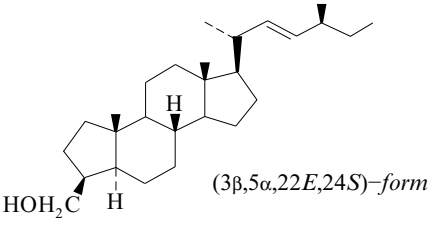


$C_{26}H_{44}O_6$ 452.63

(3β,4β,5α,6α,8β,15β,22*E*,24ξ)-*form* [781646-83-1]
Constit. of *Acodontaster conspicuus* and *Certonardoa semiregularis.*
$[\alpha]_D$ +8.6 (c, 1 in MeOH).
3-O-*(2,4-Di*-O-*methyl-β-D-xylopyranoside):* ***Tumidoside A***
[877175-40-1]
$C_{33}H_{56}O_{10}$ 612.799
Constit. of *Henricia tumida.*
$[\alpha]_D^{20}$ -5.3 (c, 0.13 in MeOH).
De Marino, S. *et al., J. Nat. Prod.*, 1997, **60**, 959-966 (*isol, pmr, cmr*)
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 1654-1660 (*isol*)
Levina, E.V. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2005, **31**, 467-474 (*Tumidoside A*)

A,27-Dinorergost-22-ene-3-methanol, 9CI D-1039

3-Hydroxymethyl-A-norpatinosterol



(3β,5α,22*E*,24*S*)–*form*

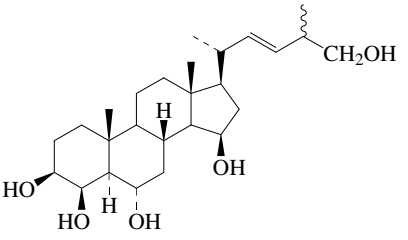
$C_{27}H_{46}O$ 386.66

(3β,5α,22*E*,24*S*)-*form* [83704-12-5]
Isol. from *Acanthella aurantiaca*.

(3ξ,5α,22*E*,24*S*)-*form*
Isol. from *Teichaxinella morchella* as acetate.
[78285-95-7]
Bohlin, L. *et al., J.C.S. Perkin 1*, 1981, 1023
Bohlin, L. *et al., J.O.C.*, 1982, **47**, 5309 (*isol, pmr*)

26,27-Dinorergost-22-ene-3,4,6,15,25-pentol D-1040

24-Norcholest-22-ene-3,4,6,15,25-pentol

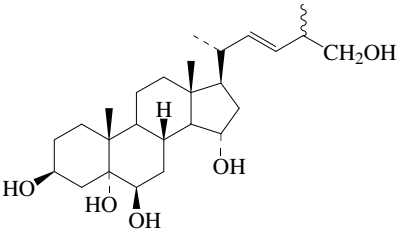


$C_{26}H_{44}O_5$ 436.631

(3β,4β,5α,6α,15β,22*E*,24ξ)-*form*
Certonardosterol B3
[781646-84-2]
Constit. of *Certonardoa semiregularis.*
Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 1654-1660 (*isol, pmr, cmr*)

26,27-Dinorergost-22-ene-3,5,6,15,25-pentol D-1041

24-Norcholest-22-ene-3,5,6,15,26-pentol

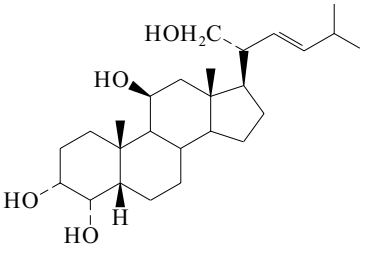


$C_{26}H_{44}O_5$ 436.631

(3β,5α,6β,15α,22*E*,24ξ)-*form*
25-O-*Sulfate:* [874351-58-3]
$C_{26}H_{44}O_8S$ 516.695
Constit. of *Ctenodiscus crispatus* and *Henricia leviuscula*.
Amorph. $[\alpha]_D$ +7 (c, 0.1 in MeOH). $[\alpha]_D$ +2 (c, 0.1 in MeOH).
Kicha, A.A. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2005, **54**, 1266-1271 (*Ctenodiscus crispatus constit*)
Ivanchina, N.V. *et al., J. Nat. Prod.*, 2006, **69**, 224-228 (*Henricia leviuscula constit*)

26,27-Dinorergost-22-ene-3,4,11,21-tetrol D-1042

24-Norcholest-22-ene-3,4,11,21-tetrol

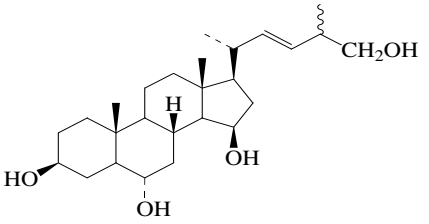


$C_{26}H_{44}O_4$ 420.631

(3α,4α,5β,11β,22*E*)-*form*

3,21-Di-O-*sulfate:* [180305-82-2]
$C_{26}H_{44}O_{10}S_2$ 580.76
Constit. of *Ophioplocus januarii*. Powder. $[\alpha]_D^{25}$ +10.9 (c, 0.62 in MeOH).
Roccatagliata, A.J. *et al., J. Nat. Prod.*, 1996, **59**, 887-889 (*isol, pmr, cmr*)

26,27-Dinorergost-22-ene-3,6,15,25-tetrol D-1043

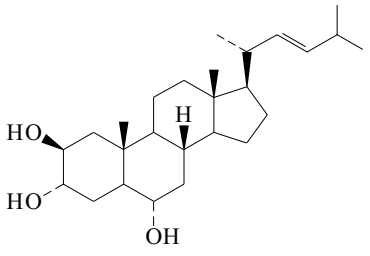


$C_{26}H_{44}O_4$ 420.631

(3β,5α,6α,15β,22*E*,24ξ)-*form*
Certonardosterol H
[517900-56-0]
Constit. of *Certonardoa semiregularis*.
Cryst. $[\alpha]_D^{21}$ -7.5 (c, 0.11 in MeOH).
Wang, W. *et al., J. Nat. Prod.*, 2003, **66**, 384-391 (*Certonardosterol H*)

26,27-Dinorergost-22-ene-2,3,6-triol D-1044

24-Methyl-26,27-dinorcholest-22-ene-2,3,6-triol



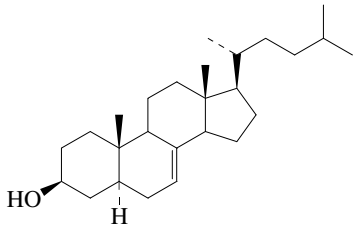
$C_{26}H_{44}O_3$ 404.632

(2β,3α,5α,6α,22*E*)-*form*

Tri-O-*sulfate:* ***Halistanol sulfate D***
[143049-15-4]
$C_{26}H_{44}O_{12}S_3$ 644.824
Constit. of an *Epipolasis* sp. Thrombin Inhibitor. $[\alpha]_D^{21}$ +13.7 (c, 0.56 in MeOH).
Kanazawa, S. *et al., Tetrahedron*, 1992, **48**, 5467 (*isol, pmr, cmr*)

26,27-Dinorergost-7-en-3-ol D-1045

24-Norcholest-7-en-3-ol

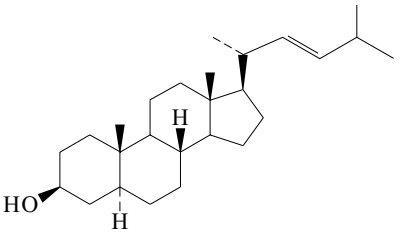


$C_{26}H_{44}O$ 372.633

(3β,5α)-*form* [128111-50-2]
Constit. of *Bathyplotes natans*.
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347

26,27-Dinorergost-22-en-3-ol, 9CI D-1046

24-Norcholest-22-en-3-ol

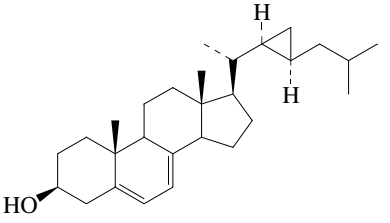


$C_{26}H_{44}O$ 372.633

(3β,5α,22*E*)-*form* [58560-37-5]
Well distributed in marine organisms, such as *Haliclona chilensis*, *Esperiopsis edwardii*, *Salpa thompsoni*, *Axinella damicornis*, *Polizoa opuntia*, *Hymeniacidon perleve*, *Mesidothea entomon*, *Echinaster sepositus*, *Bathyplotes natans*, *Holothuria nobilis*, *Trochostoma orientale* and *Patinopecten yessoensis*.
Cryst. (MeOH).
Mp 85° Mp 119-121° (double Mp).
3-O-*Sulfate:* [152005-14-6]
$C_{26}H_{44}O_4S$ 452.697
Constit. of *Eupentacta fraudatrix*.
3-O-*β-D-Xylopyranoside:* [74219-30-0]
$C_{31}H_{52}O_5$ 504.749
Constit. of *Eupentacta fraudatrix*.
Erdman, T.R. *et al., Tetrahedron*, 1972, **28**, 5163-5173 (*isol*)
Kobayashi, M. *et al., Steroids*, 1975, **26**, 605 (*isol*)
De Simone, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **66**, 351-357 (*occur, sponges*)
Dini, A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **71**, 285-288 (*occur*)
Seldes, A.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **81**, 119-122 (*occur, sponges*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Palermo, J.A. *et al., Steroids*, 1996, **61**, 2-6 (*occur*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*occur*)

28,33-Dinorgorgosta-5,7-dien-3-ol, 9CI D-1047

22,23-Methylenecholesta-5,7-dien-3-ol. *23,24-Didemethylgorgosta-5,7-dien-3-ol*

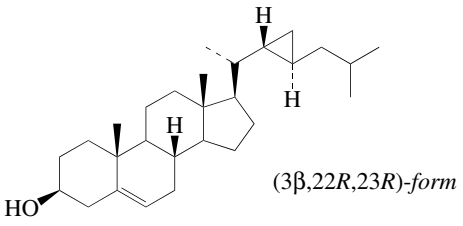


$C_{28}H_{44}O$ 396.655

(3β,22*R*,23*R*)-*form* [85733-77-3]
Constit. of the sponge *Axinella cannabina*.
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol, pmr, cmr*)

28,33-Dinorgorgost-5-en-3-ol, 9CI D-1048

22,23-Methylenecholest-5-en-3-ol



(3β,22*R*,23*R*)-*form*

$C_{28}H_{46}O$ 398.671

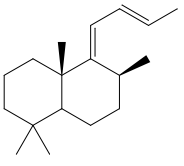
(3β,22*R*,23*R*)-*form*

22,23-Methylenecholesterol. 23,24-Didemethylgorgosterol
[75871-95-3]
Constit. of the sponges *Dysidea* sp. and *Xestospongia* sp. and corals *Lobophytum crassum* and *Siphonogorgia* sp.
Cryst. (MeOH aq.).
Mp 179-180°. $[\alpha]_D^{20}$ -61.3 (c, 7.1 in $CHCl_3$).

(3β,22*S*,23*S*)-*form* [75917-89-4]
Constit. of a *Hyrtios* sponge.

Blanc, P.A. *et al., J.A.C.S.*, 1980, **102**, 7113-7114; 1981, **103**, 7036 (*isol, pmr*)
Lang, R.W. *et al., J.O.C.*, 1982, **47**, 625-633 (*synth, pmr, cmr, abs config*)
Koch, P. *et al., Helv. Chim. Acta*, 1983, **66**, 2431-2436 (*Hyrtios constit*)
Zimmerman, M.P. *et al., J.A.C.S.*, 1984, **106**, 5602-5612 (*synth, cryst struct*)
Kim, D. *et al., Arch. Pharmacal Res.*, 1992, **15**, 374-375 (*synth*)
Venkateswarlu, Y. *et al., J. Nat. Prod.*, 1997, **60**, 1301-1302 (*Lobophytum crassum constit*)

15,16-Dinor-9(11),12-labdadiene D-1049



$C_{18}H_{30}$ 246.435

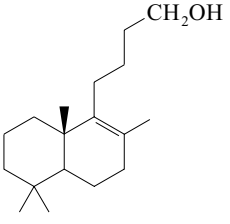
(9*E*,12*E*)-*form*

Sigmosceptrin A
[204980-39-2]
Isol. from the marine sponge *Sigmosceptrella* sp.
Yellow oil. $[\alpha]_D$ +38.1 (c, 9.9 in $CHCl_3$). λ_{max} 250 (ϵ 22000) ($CHCl_3$).

Bassett, S. *et al., Aust. J. Chem.*, 1997, **50**, 1137-1143 (*isol, pmr, cmr, ms*)

15,16-Dinor-8-labden-14-ol D-1050

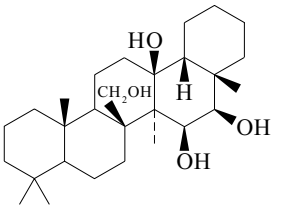
Luffarin Y
[145398-75-0]



$C_{18}H_{32}O$ 264.45
Constit. of *Luffariella geometrica*. Oil. $[\alpha]_D^{20}$ +72.3 (c, 1.6 in $CHCl_3$).

Butler, M.-S. *et al., Aust. J. Chem.*, 1992, **45**, 1705 (*isol, pmr, cmr*)

29,30-Dinor-13,15,16,26-oleananetetrol D-1051



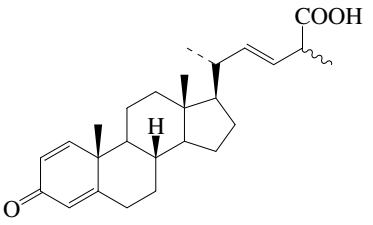
$C_{28}H_{48}O_4$ 448.685

(13β,15β,16β)-*form* [166534-28-7]
Constit. of *Nephthea albida*.
Cryst.
Mp 234-236°.

Fu, J. *et al., Huanan Ligong Daxue Xuebao, Ziran Kexueban*, 1995, **25**, 120-124; *CA*, **123**, 139301a (*isol, pmr, cmr*)

26,27-Dinor-3-oxoergosta-1,4,22-trien-28-oic acid D-1052

24-Nor-3-oxocholesta-1,4,22-trien-26-oic acid



$C_{26}H_{36}O_3$ 396.569

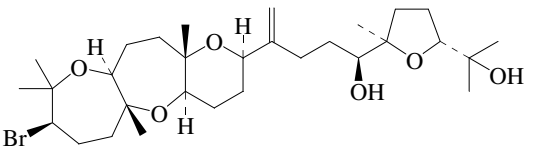
(22*E*,25ξ)-*form*

Me ester: [862288-90-2]
$C_{27}H_{38}O_3$ 410.595
Constit. of *Anthomastus bathyproctus*. Amorph. powder. $[\alpha]_D^{25}$ +8.5 (c, 0.1 in $CHCl_3$). λ_{max} 245 (log ϵ 4.01) (MeOH).

Mellado, G.G. *et al., J. Nat. Prod.*, 2005, **68**, 1111-1115

Dioxepandehydrothyrsiferol D-1053

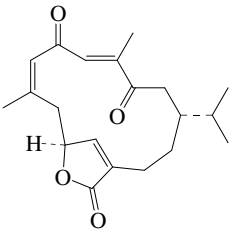
[346583-59-3]



$C_{30}H_{51}BrO_6$ 587.633
Constit. of *Laurencia viridis*. Amorph. solid. $[\alpha]_D^{25}$ +39 (c, 0.07 in $CHCl_3$).

Manríquez, C.P. *et al., Tetrahedron*, 2001, **57**, 3117-3123 (*isol, pmr, cmr*)

3,6-Dioxo-4,7,11,15-cembratetraen-20,10-olide D-1054



(1*R*,4*E*,7*Z*,10*S*)-*form*

$C_{20}H_{24}O_4$ 328.407

(1*R*,4*E*,7*Z*,10*S*)-*form*
Isoepilophodione A
[118101-24-9]
Metab. of *Gersemia rubiformis*.
Pale yellow oil. $[\alpha]_D^{25}$ +138 (c, 0.55 in CH_2Cl_2). λ_{max} 208 (ϵ 16200); 246 (ϵ 12800) (MeOH) (Derep).

(1*R*,4*Z*,7*Z*,10*S*)-*form*
Isoepilophodione B
From *Gersemia rubiformis*.
Pale yellow oil. $[\alpha]_D^{25}$ +298 (c, 0.4 in CH_2Cl_2). λ_{max} 212 (ϵ 13100); 267 (ϵ 14400) (MeOH) (Derep).

(1*S*,4*E*,7*Z*,10*S*)-*form*
Isolophodione
[82407-61-2]
Metab. of *Lophogorgia alba*.
Cryst.
Mp 172-175°. $[\alpha]_D^{18}$ -231.8 (c, 1.0 in $CHCl_3$).

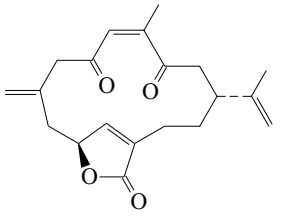
(1*S*,4*Z*,7*E*,10*R*)-*form*
Epilophodione
Constit. of *Gersemia rubiformis*.
Needles (CH_2Cl_2/MeOH).
Mp 153-155°. $[\alpha]_D^{25}$ +136.2 (c, 0.42 in $CHCl_3$). λ_{max} 211 (ϵ 14100); 264 (ϵ 10900) (MeOH) (Derep).

(1*S*,4*Z*,7*E*,10*S*)-*form*
Lophodione
[82443-67-2]
Metab. of the gorgonian coral *Lophogorgia alba*.
Cryst. (EtOAc/2,3,3-trimethylpentane).
Mp 172-174°. $[\alpha]_D^{23}$ -274.6 (c, 0.8 in $CHCl_3$). λ_{max} 211 (ϵ 14100); 264 (ϵ 10900) (MeOH) (Derep).

*4*R*,5*S*-Epoxide: 4,5-Epoxy-3,6-dioxo-7,11,15-cembratrien-20,10-olide.* ***Epoxylophodione***
[82407-62-3]
$C_{20}H_{24}O_5$ 344.407
Metab. of *Lophogorgia alba*. Solid. $[\alpha]_D^{23}$ -114.4 (c, 1.1 in $CHCl_3$).

Bandurraga, M.M. *et al., Tetrahedron*, 1982, **38**, 305 (*cryst struct*)
Williams, D. *et al., J.O.C.*, 1987, **52**, 332 (*isol*)
Williams, D.E. *et al., Can. J. Chem.*, 1988, **66**, 2928 (*isol, pmr, cmr*)

3,6-Dioxo-4,8(19),11,15-cembratetraen-20,10-olide D-1055

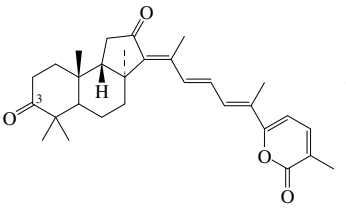


$C_{20}H_{24}O_4$ 328.407

(1*R*,4*Z*,10*S*)-*form*
Isoepilophodione C
[118025-70-0]
Metab. of *Gersemia rubiformis*.
Oil. $[\alpha]_D^{25}$ -170 (c, 0.26 in CH_2Cl_2). λ_{max} 230 (ϵ 2500) (MeOH) (Derep).

Williams, D.E. *et al., Can. J. Chem.*, 1988, **66**, 2928 (*isol, pmr, cmr*)

3,12-Dioxo-13,15,17(20),22,24-isomalabaricapentaen-26,22-olide D-1056



(8α,9β,13*E*,15*E*,17(20)*E*)-*form*

$C_{30}H_{38}O_4$ 462.628

(8α,9β,13*E*,15*E*,17(20)*E*)-*form*
Stellettin A
[160796-24-7]
Constit. of *Stelletta tenuis*.
Yellow needles (EtOAc/petrol). Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 234-235°. $[\alpha]_D^{20}$ +28.8 (c, 0.16 in MeOH). λ_{max} 312 (log ϵ 4.03); 396 (log ϵ 4.35); 417 (log ϵ 4.24) (EtOH). λ_{max} 248 (ϵ 4188); 302 (ϵ 11720); 312 (ϵ 12780); 396 (ϵ 30100) (MeOH) (Berdy).

3-Alcohol: 3-Hydroxy-12-oxo-13,15,17(20),22,24-isomalabricapentaen-26,22-olide

3β-Alcohol, 3-Ac: ***Stellettin C***
[184885-07-2]
$C_{32}H_{42}O_5$ 506.681
Constit. of a *Stelletta* sp. Yellow solid. $[\alpha]_D$ -250 (c, 0.51 in $CHCl_3$). λ_{max} 313 (log ϵ 4.24); 395 (log ϵ 4.48); 418 (log ϵ 4.39) (EtOH).

(8α,9β,13*Z*,15*E*,17(20)*E*)-*form*
Stellettin B
[84048-10-2]
[184885-91-4]
Constit. of the sponges *Stelletta* sp. and *Jaspis stellifera*.
Unstable yellow prisms (CH_2Cl_2/Et_2O).
Mp 258-260° (266-268°). $[\alpha]_D^{25}$ +87 (c, 0.8 in $CHCl_3$). λ_{max} 302 (sh) (ϵ 6200); 314 (ϵ 8780); 396 (ϵ 29600); 417 (ϵ 23800) (MeOH) (Derep).

3β-Alcohol, 3-Ac: ***Stellettin D***
[184885-08-3]
$C_{32}H_{42}O_5$ 506.681
Constit. of a *Stelletta* sp. Yellow solid. $[\alpha]_D$ -19.4 (c, 1 in $CHCl_3$). λ_{max} 313 (log ϵ 4.23); 400 (log ϵ 4.54); 418 (log ϵ 4.45) (EtOH). λ_{max} 313 (ϵ 16600); 395 (ϵ 33100); 418 (ϵ 29800) (MeOH) (Berdy).

*22*S*,23-Dihydro: 3,12-Dioxo-13,15,17(20),24-isomalabaricatetraen-26,22-olide.* ***22,23-Dihydrostellettin B***
[823808-55-5]
$C_{30}H_{40}O_4$ 464.644
Constit. of *Rhabdastrella* aff. *distincta*.

22,23-Dihydro, 3β-alcohol: 3-Hydroxy-12-oxo-13,15,17(20),24-isomalabaricatetraen-26,22-olide
$C_{30}H_{42}O_4$ 466.659

22,23-Dihydro, 3β-alcohol, 3-Ac: ***22,23-Dihydrostellettin D***
[854203-78-4]
$C_{32}H_{44}O_5$ 508.697
Constit. of a *Jaspis* sp. Yellow amorph. powder.

[76915-24-7]

Ravi, B.N. *et al., J.O.C.*, 1981, **46**, 1998 (*isol*)
McCabe, T. *et al., Tet. Lett.*, 1982, **23**, 3307 (*isol, cryst struct*)
Su, J.Y. *et al., J. Nat. Prod.*, 1994, **57**, 1450 (*Stellettin A*)
McCormick, J.L. *et al., J. Nat. Prod.*, 1996, **59**, 1047-1050 (*isol, pmr, cmr, derivs*)
Lv, F. *et al., J. Nat. Prod.*, 2004, **67**, 2033-2036 (*22,23-Dihydrostellettin B*)
Tang, S.A. *et al., Chin. Chem. Lett.*, 2005, **16**, 353-355 (*22,23-Dihydrostellettin D*)

4,5-Dioxopentanoic acid D-1057

4-Oxoglutaraldehydic acid, 8CI. β-Glyoxylpropanoic acid. γ-Ketoglutaric semialdehyde. DOVA

[5976-90-9]

$OHCCOCH_2CH_2COOH$

$C_5H_6O_4$ 130.1

Metabolite of the green alga *Scenedesmus obliquus*. Intermed. in the biosynth. of 5-aminolevulinate, a biosynthetic precursor of chlorophyll and other porphyrins. Grey, glassy solid. Unstable.

Dioxime:

$C_5H_8N_2O_4$ 160.129

Prisms. Mp 136°.

Bis(phenylhydrazone): Mp 153.5-154°.

Et ester: [91479-18-4]

$C_7H_{10}O_4$ 158.154

Green oil. Unstable.

2,3-Diaminonaphthalene deriv.: Benzo[g]quinoxaline-2-propanoic acid, 9CI

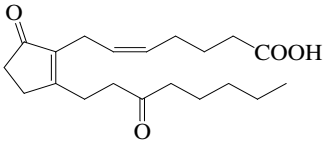
[25470-39-7]

$C_{15}H_{12}N_2O_2$ 252.272

Solid (EtOH).

Olivard, J. *et al., J.O.C.*, 1968, **33**, 2552 (*synth*)
Beale, S.I. *et al., Phytochemistry*, 1979, **18**, 441 (*synth*)
Doernemann, D. *et al., Biochim. Biophys. Acta*, 1980, **628**, 35; 1988, **964**, 61 (*synth, pmr, ms, ir, uv, isol*)
Mitschka, R. *et al., Tetrahedron*, 1981, **37**, 4521 (*synth*)
Morton, K.A. *et al., J. Clin. Invest.*, 1983, **71**, 1744 (*biosynth*)
Cooper, K. *et al., J.C.S. Perkin 1*, 1984, 779 (*Et ester*)
Meisch, H.U. *et al., Biochim. Biophys. Acta*, 1985, **841**, 319 (*biosynth*)
Breu, V. *et al., Biochim. Biophys. Acta*, 1988, **964**, 61 (*isol*)
Kotzabasis, K. *et al., Biochim. Biophys. Acta*, 1989, **977**, 309 (*biosynth*)

9,15-Dioxo-5,8(12)-prostadienoic acid D-1058



$C_{20}H_{30}O_4$ 334.455

(Z)-form

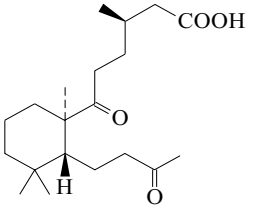
Me ester:

$C_{21}H_{32}O_4$ 348.481

Isol. from the coral *Sarcophyton crassocaule*. Pale yellow oil. λ_{max} 237 ($CHCl_3$).

Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 2000, **63**, 1425-1426

8,9-Dioxo-8,9-seco-15-labdanoic acid D-1059



$C_{20}H_{34}O_4$ 338.486

(ent-13S)-form

2-Acetoxy-3-hydroxypropyl ester: [138909-54-3]

$C_{25}H_{42}O_7$ 454.603

Constit. of *Austrodoris kerguelensis*. Oil. $[\alpha]_D$ -9 (c, 0.24 in $CHCl_3$).

3-Acetoxy-2-hydroxypropyl ester: [138909-55-4]

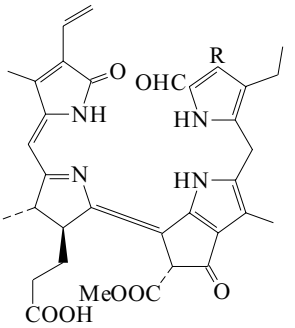
$C_{25}H_{42}O_7$ 454.603

Constit. of *Austrodoris kerguelensis*. Oil. $[\alpha]_D$ -7 (c, 0.17 in $CHCl_3$).

Davies-Coleman, M.T. *et al., Tetrahedron*, 1991, **47**, 9743 (*isol, pmr, cmr*)

4,5-Dioxo-4,5-secophaeophorbide a D-1060

[155656-02-3]



R = CH_3

$C_{35}H_{38}N_4O_7$ 626.708

Isol. from the microalga *Chlorella protothecoides*. Product of chlorophyll catabolism. λ_{max} 278; 312 (CH_2Cl_2/MeOH).

Iturraspe, J. *et al., Phytochemistry*, 1994, **35**, 1387 (*isol, uv, pmr, ms*)

4,5-Dioxo-4,5-secophaeophorbide b D-1061

[155656-00-1]

As 4,5-Dioxo-4,5-secophaeophorbide a, D-1060 with

R = CHO

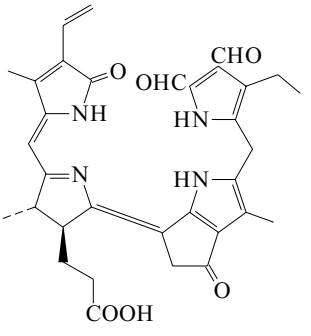
$C_{35}H_{36}N_4O_8$ 640.691

Isol. from the microalga *Chlorella protothecoides*. Product of chlorophyll catabolism. λ_{max} 278; 326 (CH_2Cl_2).

Iturraspe, J. *et al., Phytochemistry*, 1994, **35**, 1387 (*isol, uv, pmr, ms*)

4,5-Dioxo-4,5-secopyrophaeophorbide b D-1062

[155656-01-2]



$C_{33}H_{34}N_4O_6$ 582.655

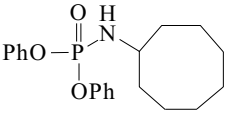
Isol. from *Chlorella protothecoides*. Product of chlorophyll catabolism.

Iturraspe, J. *et al., Phytochemistry*, 1994, **35**, 1387 (*isol, pmr, cmr, uv*)

Diphenyl cyclooctylphosphoramidate, 9CI D-1063

PB-1. GB1 Toxin†

[86126-37-6]



$C_{20}H_{26}NO_3P$ 359.404

Toxin from the red tide dinoflagellate *Ptychodiscus brevis*. Appears to be a metab. of *P. brevis*, although the possibility that it may be derived from an unsuspected contaminant in the artificial culture

medium cannot be totally excluded. λ_{max} 259 (sh) (ϵ); 262 (ϵ 475); 268 (sh) (ϵ) (MeOH) (Derep). λ_{max} 259; 262 (ϵ 475); 268 (MeOH) (Berdy).

DiNovi, M. *et al., Tet. Lett.*, 1983, **24**, 855 (*isol, uv, pmr, cmr, struct, synth*)

2,4-Diphenyl-1-butene, 8CI D-1064

1,1′-(1-Methylene-1,3-propanediyl)bisbenzene, 9CI. SD-2
[16606-47-6]
$H_2C{=}CHPhCH_2CH_2Ph$
$C_{16}H_{16}$ 208.302
Isol. from the starfish *Pteraster militaris.* Oil. $Bp_{2.5}$ 140° (lit. gives a pressure range).

Marion, L. *et al., Can. J. Res., Sect. B*, 1938, **16**, 213
Parkhurst, R.M. *et al., J.O.C.*, 1963, **28**, 120 (*synth, ir, pmr*)
Mayo, F.R. *et al., J.A.C.S.*, 1968, **90**, 1289 (*synth, ir*)
Kurze, J. *et al., Angew. Makromol. Chem.*, 1970, **12**, 25
Yayli, N. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 556 (*isol, pmr, cmr*)
Kawamura, Y. *et al., Shokuhin Eisegaku Zasshi*, 1998, **39**, 110-119; *CA*, **129**, 42008w; **130**, 251409n (*detn*)
Ohyama, K. *et al., Environ. Health Perspect.*, 2001, **109**, 699-703 (*tox*)

1,5-Diphenyl-1,4-pentadiene D-1065

1,1′-(1,4-Pentadiene-1,5-diyl)bisbenzene, 9CI
[52267-15-9]
$PhCH{=}CHCH_2CH{=}CHPh$
$C_{17}H_{16}$ 220.313

(*E,E*)-*form* [26057-48-7]
Oil. $Bp_{0.5}$ 170°.

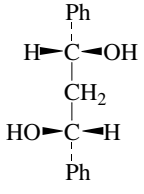
(*E,Z*)-*form* [26057-49-8]
Isol. from *Caulerpa racemosa*.
Oil.

(*Z,Z*)-*form* [26057-47-6]
No phys. props. reported. Obt. chromatographically.

Brenner, S. *et al., Isr. J. Chem.*, 1969, **7**, 735 (*synth, pmr*)
Boyle, P.H. *et al., J.O.C.*, 1973, **38**, 826 (*synth*)
Shoppee, C.W. *et al., J.C.S. Perkin 1*, 1975, 765 (*synth*)
Komatsu, K. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2470 (*synth*)
Tolbert, L.M. *et al., J.A.C.S.*, 1990, **112**, 9519 (*synth, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 1992, **55**, 496-499 (*isol, pmr, cmr*)

1,3-Diphenyl-1,3-propanediol D-1066

[5471-97-6]



(1*R*,3*R*)-*form*

$C_{15}H_{16}O_2$ 228.29

(1*R*,3*R*)-*form* [77291-92-0]
Needles ($CHCl_3$). Mp 151.5-153°. $[\alpha]_D^{20}$ +67.5 (c, 0.3 in EtOH) (100% ee).

(1*S*,3*S*)-*form* [108391-15-7]
Mp 160-161°. $[\alpha]_D^{26}$ -72 (MeOH).

(1*RS*,3*RS*)-*form*
(±)-form
[5355-61-3]
Cryst. (CH_2Cl_2/pentane). Mp 135-139° (125-126°).

(1*RS*,3*SR*)-*form*
meso-*form*
[5381-86-2]
Isol. from a *Nephthea* sp.
Cryst. (CH_2Cl_2/pentane).
Mp 104-105°.
[59825-14-8]

Ito, K. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 3367 (*synth*)
Barluenga, J. *et al., J.C.S. Perkin 1*, 1983, 3019 (*synth*)
Todesco, R. *et al., J.O.C.*, 1983, **48**, 4963 (*synth, pmr*)
Bakos, J. *et al., Tet. Lett.*, 1984, **25**, 4965 (*synth*)
Yamamoto, K. *et al., Chem. Comm.*, 1987, 334 (*synth*)
Chen, K. *et al., Tet. Lett.*, 1987, **28**, 155 (*synth*)
Silins, E. *et al., Zh. Strukt. Khim.*, 1987, **28**, 92 (*cryst struct*)
Tiecco, M. *et al., Tetrahedron*, 1988, **44**, 2261 (*synth*)
Ray, A.K. *et al., J. Nat. Prod.*, 1991, **54**, 854 (*isol, bibl, pmr*)
Barbero, A. *et al., J.C.S. Perkin 1*, 1997, 1329-1352 (*synth, ir, pmr*)
Roos, G.H.P. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 991-1000 (*1R,3R-form, synth, nmr*)

1,3-Diphenyl-1-propanone, 9CI D-1067

ω-Benzylacetophenone. Phenethyl phenyl ketone. Dihydrochalcone. Hydrocinnamophenone. Hydrochalcone
[1083-30-3]
$PhCOCH_2CH_2Ph$
$C_{15}H_{14}O$ 210.275
Isol. from *Phallus impudicus* (common stinkhorn). Also from *Pteraster militaris.* Leaflets (EtOH).
Mp 72-73°. Bp 360°.

Oxime: [5371-55-1]
$C_{15}H_{15}NO$ 225.29
Needles (EtOH aq.). Mp 87°.

2,4-Dinitrophenylhydrazone: [5371-54-0]
Mp 143-145°.

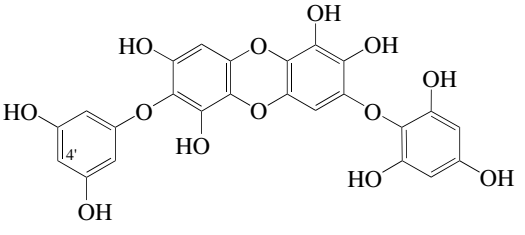
Semicarbazone: [33745-39-0]
Cryst. (EtOH). Mp 148-148.5°.

Di-Et acetal: 1,1-Diethoxy-1,3-diphenylpropane
$C_{19}H_{24}O_2$ 284.397
Liq. d_4^{22} 1.04. Bp_{18} 189°.

Org. Synth., Coll. Vol., 4, 1963, 101 (*synth*)
Freunel, B. *et al., Planta Med.*, 1968, 123; *CA*, **70**, 54869 (*isol*)
Shemyakin, M.M. *et al., Tetrahedron*, 1971, **27**, 2811 (*synth*)
Weber, F.G. *et al., Tetrahedron*, 1973, **29**, 2479 (*synth, pmr*)
Yayli, N. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 556 (*isol*)
Judaš, N. *et al., Acta Cryst. C*, 1995, **51**, 2656 (*cryst struct*)
Pande, P.P. *et al., Synth. Commun.*, 1998, **28**, 4193-4200 (*synth, ir, pmr*)
Wang, H. *et al., Synth. Commun.*, 1999, **29**, 129-134 (*synth, ir, pmr*)

Diphlorethohydroxycarmalol D-1068

7-(3,5-Dihydroxyphenoxy)-3-(2,4,6-trihydroxyphenoxy)dibenzo[b,e][1,4]dioxin-1,2,6,8-tetrol, 9CI
[138529-04-1]

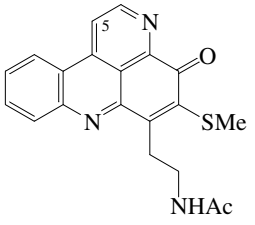


$C_{24}H_{16}O_{13}$ 512.383
Constit. of *Carpophyllum maschalocarpum.* Isol. as nona-Ac.

4′-(3,5-Dihydroxyphenoxy): ***Triphloroethohydroxycarmalol***
[138529-05-2]
$C_{30}H_{20}O_{16}$ 636.478
Constit. of *Carpophyllum maschalocarpum.* Isol. as undeca-Ac.
Li, S.-M. *et al., Phytochemistry*, 1991, **30**, 3417-3421 (*isol, pmr, cmr*)

Diplamine D-1069

[123794-30-9]



$C_{20}H_{17}N_3O_2S$ 363.439

Related to *N*-Deacylcystodytin, D-34. Alkaloid from the tunicate *Diplosoma* sp. Exhibits antitussive and antitumour activity. Burnt-orange solid.
Mp 202-204° dec. λ_{max} 263 (ϵ 24900); 300 (ϵ 14700); 377 (ϵ 6000) (MeOH) (Derep).

N-*De-Ac,* N-*(3-methylbutanoyl):* ***Lissoclin A***
[158761-12-7]
$C_{23}H_{23}N_3O_2S$ 405.52
Alkaloid from the tropical ascidian *Lissoclinum* sp. and *Didemnum* sp. Orange needles (MeOH).
Mp 202-204°. λ_{max} 263 (ϵ 28000); 300 (ϵ 17000); 383 (ϵ 6800); 450 (ϵ 4900) (MeOH) (Berdy).

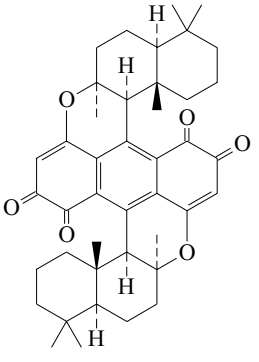
N-*De-Ac,* N-*tigloyl:* ***Lissoclin B****. (Demethylthio)cystodytin B*
[158761-13-8]
$C_{23}H_{21}N_3O_2S$ 403.504
Alkaloid from *Lissoclinum* sp. and *Didemnum* sp. Orange solid.
λ_{max} 263 (ϵ 28000); 300 (ϵ 17000); 383 (ϵ 6800); 450 (ϵ 4900) (MeOH) (Berdy).

De(methylthio), 5-methylthio: ***Isodiplamine***
[496909-75-2]
$C_{20}H_{17}N_3O_2S$ 363.439
Alkaloid from *Lissoclinum notti*. Green solid.
Mp 208-210°. λ_{max} 215 (log ϵ 4.68); 274 (log ϵ 4.16); 320 (log ϵ 4.01); 406 (log ϵ 4) (MeOH/TFA).

Charyulu, G.A. *et al., Tet. Lett.*, 1989, **30**, 4201-4202 (*isol, uv, ir, pmr, cmr, struct*)
Szczepankiewicz, B.G. *et al., J.O.C.*, 1994, **59**, 3512-3513 (*synth*)
Searle, P.A. *et al., J.O.C.*, 1994, **59**, 6600-6605 (*Lissoclins*)
Ciufolini, M.A. *et al., J.A.C.S.*, 1995, **117**, 12460 (*synth*)
Appleton, D.R. *et al., Tetrahedron*, 2002, **58**, 9779-9783 (*Isodiplamine*)

Dipuupehedione D-1070

[178115-90-7]

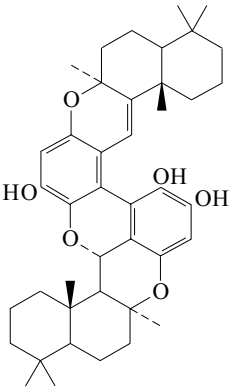


$C_{42}H_{50}O_6$ 650.853
Constit. of *Hyrtios* sp. Red glassy solid. Incorrect MF given in paper.

Bourguet-Kondracki, M.-L. *et al., Tet. Lett.*, 1996, **37**, 3861-3864 (*isol, pmr, cmr*)

Dipuupehetriol D-1071

[151345-11-8]

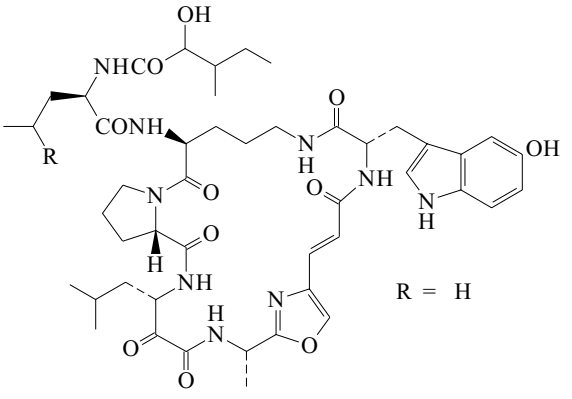


$C_{42}H_{54}O_6$ 654.885
Constit. of a marine Verongid sponge.
$[\alpha]_D$ -18 (c, 0.136 in MeOH). λ_{max} (solvent not reported) (Derep). λ_{max} 206 (ϵ 24400); 230 (ϵ 18600); 292 (ϵ 13100); 342 (ϵ 7760); 518 (ϵ 1010) (MeOH) (Derep).

Hamann, N.T. *et al., J.O.C.*, 1993, **58**, 6565-6569 (*isol, pmr, cmr*)
Urban, S. *et al., J. Nat. Prod.*, 1996, **59**, 900 (*abs config*)

Discobahamin A D-1072

[155547-93-6]



$C_{47}H_{65}N_9O_{11}$ 932.084
Cyclic peptide antibiotic. Constit. of the marine sponge *Discodermia* sp. Antifungal agent. Pale yellow gum. Sol. MeOH. $[\alpha]_D^{24}$ -29 (c, 0.5 in MeOH). λ_{max} 203 (ϵ 1400); 220 (ϵ 10200); 267 (ϵ 6800); 305 (ϵ 1500) (MeOH) (Berdy).

Gunasekera, S.P. *et al., J. Nat. Prod.*, 1994, **57**, 79 (*isol, pmr, cmr*)

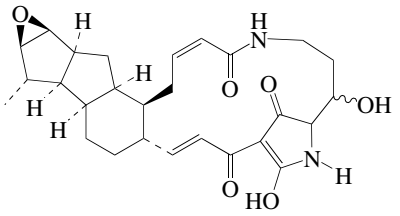
Discobahamin B D-1073

[155547-94-7]
As Discobahamin A, D-1072 with
R = $-CH_3$
$C_{48}H_{67}N_9O_{11}$ 946.111
Cyclic peptide antibiotic. Constit. of the marine sponge *Discodermia* sp. Antifungal agent. Pale yellow gum. Sol. MeOH. $[\alpha]_D^{24}$ -31 (c, 0.1 in MeOH). λ_{max} 203 (ϵ 1400); 220 (ϵ 10200); 267 (ϵ 6800); 305 (ϵ 1500) (MeOH) (Berdy).

Gunasekera, S.P. *et al., J. Nat. Prod.*, 1994, **57**, 79 (*isol, pmr, cmr*)

Discodermide D-1074

[134458-00-7]

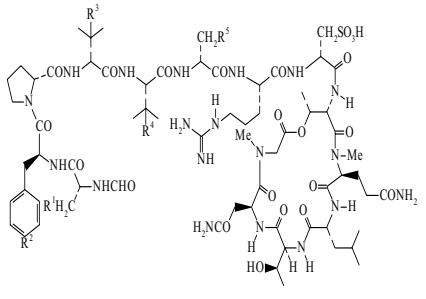


$C_{27}H_{34}N_2O_6$ 482.575

Tetramic acid deriv. Isol. from the sponge *Discodermia dissoluta*. Antifungal and antitumour agent.
Mp *ca.*200° (dec.). $[\alpha]_D$ +97.5 (c, 0.2 in $CHCl_3$/MeOH). λ_{max} 238 (ϵ 16500); 313 (ϵ 9650) (MeOH).

Gunasekera, S.P. *et al., J.O.C.*, 1991, **56**, 4830-4833 (*isol, uv, pmr, cmr*)

Discodermin D-1075



Cyclic peptide antibiotic complex. Struct. revised in 1994. Found in *Discodermia kiiensis*. Possibly a metab. of a symbiotic organism. Shows antimicrobial and cytotoxic activity. Inhibits the development of starfish embryos.

Discodermin A [94552-47-3]

$C_{77}H_{116}N_{20}O_{22}S$ 1705.95
Tumour promotion activity inhibitor. PLA2 inhibitor. Sol. H_2O, DMSO, MeOH; fairly sol. EtOH; poorly sol. EtOH, $CHCl_3$. Mp 226-227°. $[\alpha]_D^{22}$ -6.3 (c, 0.7 in MeOH). Has $R^1 = R^2 = H$, $R^3 = R^4 = CH_3$, R^5 = 1*H*-indol-3-yl. λ_{max} 276 (ϵ 6200); 282 (ϵ 6500); 292 (ϵ 5600) (MeOH) (Derep). λ_{max} 276 (ϵ 6200); 282 (ϵ 6500); 292 (ϵ 5600) (MeOH) (Berdy).

Discodermin B [96156-14-8]

$C_{76}H_{114}N_{20}O_{22}S$ 1691.923
PLA2 inhibitor. Sol. MeOH. Mp 217-219°. $[\alpha]_D^{23}$ -3.2 (c, 1.0 in MeOH). Has $R^1 = R^2 = R^3 = H$, $R^4 = CH_3$, R^5 = 1*H*-indol-3-yl. λ_{max} 276 (ϵ 6200); 282 (ϵ 6500); 292 (ϵ 5600) (MeOH) (Derep). λ_{max} 275 (ϵ 5030); 282 (ϵ 5340); 290 (ϵ 4600) (MeOH) (Berdy).

Discodermin C [96182-34-2]

$C_{76}H_{114}N_{20}O_{22}S$ 1691.923
PLA2 inhibitor. Sol. MeOH. Mp 222-224°. $[\alpha]_D^{23}$ -6.6 (c, 1.0 in MeOH). Has $R^1 = R^2 = R^4 = H$, $R^3 = CH_3$, R^5 = 1*H*-indol-3-yl. λ_{max} 276 (ϵ 6200); 282 (ϵ 6500); 292 (ϵ 5600) (MeOH) (Derep). λ_{max} 275 (ϵ 5450); 282 (ϵ 5810); 290 (ϵ 4950) (MeOH) (Berdy).

Discodermin D [96156-13-7]

$C_{75}H_{112}N_{20}O_{22}S$ 1677.897
PLA2 inhibitor. Sol. MeOH. Mp 215-219°. $[\alpha]_D^{23}$ -4.7 (c, 1 in MeOH). Has $R^1 = R^2 = R^3 = R^4 = H$, R^5 = 1*H*-indol-3-yl. λ_{max} 276 (ϵ 6200); 282 (ϵ 6500); 292 (ϵ 5600) (MeOH) (Derep). λ_{max} 275 (ϵ 4800); 282 (ϵ 5150); 290 (ϵ 4980) (MeOH) (Berdy).

Discodermin E [159436-26-7]

$C_{76}H_{116}N_{20}O_{23}S$ 1709.939
$[\alpha]_D^{23}$ -7.1 (c, 0.01 in MeOH). Has $R^1 = R^2 = H$, $R^3 = R^4 = CH_3$, R^5 = 2-aminobenzoyl. λ_{max} 232 (ϵ 26720); 258 (ϵ 7160); 368 (ϵ 3040) (MeOH) (Berdy).

Discodermin F [160016-17-1]

$C_{78}H_{118}N_{20}O_{22}S$ 1719.977
Toxic to *Asterina pectinifera*. Amorph. solid. $[\alpha]_D^{23}$ -6.7 (c, 0.8 in MeOH). Has $R^1 = R^2 = H$, $R^3 = CH_3$, $R^4 = CH_2CH_3$, R^5 = 1*H*-indol-3-yl. λ_{max} 217 (ϵ 42100); 275 (ϵ 3880); 282 (ϵ 4070); 290 (ϵ 3390) (MeOH) (Berdy).

Discodermin G [160016-18-2]

$C_{78}H_{118}N_{20}O_{22}S$ 1719.977
Toxic to *Asterina pectinifera*. Amorph. solid. $[\alpha]_D^{23}$ -6.8 (c, 0.6 in MeOH). Has $R^1 = R^3 = R^4 = CH_3$, $R^2 = H$, R^5 = 1*H*-indol-3-yl. λ_{max} 217 (ϵ 49200); 275 (ϵ 3970); 282 (ϵ 4230); 290 (ϵ 3640) (MeOH) (Berdy).

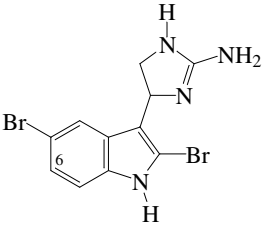
Discodermin H [160016-19-3]

$C_{77}H_{116}N_{20}O_{23}S$ 1721.95
Toxic to *Asterina pectinifera*. Amorph. solid. $[\alpha]_D^{23}$ -5.8 (c, 0.6 in MeOH). Has $R^1 = H$, $R^2 = OH$, $R^3 = R^4 = CH_3$, R^5 = 1*H*-indol-3-yl. λ_{max} 274 (ϵ 4510); 280 (ϵ 4730); 289 (ϵ 3680) (MeOH) (Berdy).

Matsunaga, S. *et al., Tet. Lett.*, 1984, **25**, 5165; 1985, **26**, 855 (*spectra*)
Matsunaga, S. *et al., J. Nat. Prod.*, 1985, **48**, 236 (*isol*)
Ryu, G. *et al., Tet. Lett.*, 1994, **35**, 8251 (*Discodermin E*)
Ryu, G. *et al., Tetrahedron*, 1994, **50**, 13409-13416 (*Discodermins A-H, pmr, cmr, struct*)

Discodermindole D-1076

[133523-28-1]



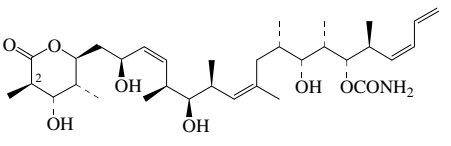
$C_{11}H_{10}Br_2N_4$ 358.035
Alkaloid from the sponge *Discodermia polydiscus*. Cytotoxic. Viscous oil. $[\alpha]_D^{20}$ -27 (c, 1 in MeOH). λ_{max} 224 (ϵ 34000); 282 (ϵ 5700); 292 (ϵ 6100); 300 (ϵ 5000) (MeOH) (Derep).

6-Hydroxy: ***6-Hydroxydiscodermindole***
$C_{11}H_{10}Br_2N_4O$ 374.034
Isol. from *Discodermia polydiscus*.
$[\alpha]_D^{21}$ -41.6 (c, 0.1 in MeOH). λ_{max} 215 (log ϵ 4.34); 260 (log ϵ 3.94); 310 (log ϵ 4.79) (MeOH).

Sun, H.H. *et al., J.O.C.*, 1991, **56**, 4307-4308 (*isol, uv, ir, pmr, cmr, ms*)
Cohen, J. *et al., Pharm. Biol.*, 2004, **42**, 59-61 (*6-Hydroxydiscodermindole*)

Discodermolide D-1077

Disermolide, INN
[127943-53-7]



Absolute Configuration

$C_{33}H_{55}NO_8$ 593.799
Constit. of *Discodermia dissoluta*. Immunosuppressant. Antineoplastic agent. Cryst.
Mp 115-116°. $[\alpha]_D^{25}$ +7.2 (c, 0.72 in MeOH). λ_{max} 210 (ϵ 35400); 226 (sh) (ϵ 19500); 235 (ϵ 12500) (MeOH) (Derep).

O-*Decarbamoyl:* ***19-Deaminocarbonyldiscodermolide****. 19-Decarbamoyldiscodermolide*
[358968-11-3]
$C_{32}H_{54}O_7$ 550.774
Isol. from a *Discodermia* sp. Solid. $[\alpha]_D^{21}$ +18 (c, 0.1 in MeOH).

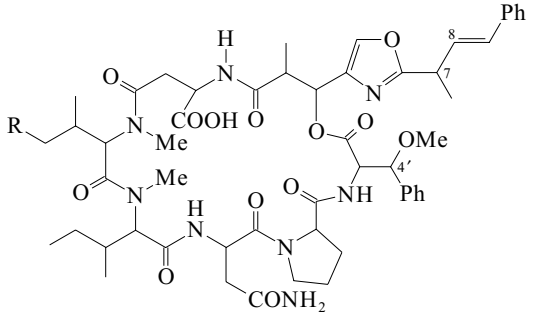
2-Epimer: ***2-Epidiscodermolide***
[358968-12-4]
$C_{33}H_{55}NO_8$ 593.799
Isol. from a *Discodermia* sp. Solid. $[\alpha]_D^{21}$ +10.7 (c, 0.1 in MeOH).

2-Demethyl: ***2-Demethyldiscodermolide***
[358968-10-2]
$C_{32}H_{53}NO_8$ 579.773
Isol. from a *Discodermia* sp. Solid. $[\alpha]_D^{21}$ +10.2 (c, 0.1 in MeOH).

Gunasekera, S.P. *et al., J.O.C.*, 1990, **55**, 4912-4915; 1991, **56**, 1346 (*isol, pmr, cmr, cryst struct*)
Longley, R.E. *et al., Ann. N.Y. Acad. Sci.*, 1993, **696**, 94-107 (*rev, pharmacol*)
Nerenberg, J.B. *et al., J.A.C.S.*, 1993, **115**, 12621-12622 (*synth*)
Marshall, J.A. *et al., J.O.C.*, 1998, **63**, 7885-7892 (*synth*)
Smith, A.B. *et al., J.A.C.S.*, 2000, **122**, 8654-8664 (*synth*)
Smith, A.B. *et al., Org. Lett.*, 2001, **3**, 695-698 (*synth*)
Broker, L.E. *et al., Cancer Res.*, 2002, **62**, 4081-4088 (*pharmacol*)
Gunasekera, S.P. *et al., J. Nat. Prod.*, 2002, **65**, 1643-1648 (*O-decarbamoyl, 2-epimer, 2-demethyl*)
Paterson, I. *et al., Eur. J. Org. Chem.*, 2003, 2193-2208 (*rev, synth*)
Harried, S.S. *et al., J.O.C.*, 2003, **68**, 6646-6660 (*synth*)
Francavilla, C. *et al., Org. Lett.*, 2003, **5**, 1233-1236 (*synth*)
Mickel, S.J. *et al., Org. Process Res. Dev.*, 2004, **8**, 101-130 (*synth*)
Arefolov, A. *et al., J.A.C.S.*, 2005, **127**, 5596-5603 (*synth*)
Paterson, I. *et al., J.O.C.*, 2005, **70**, 150-160 (*synth, bibl*)
Smith, A.B. *et al., Org. Lett.*, 2005, **7**, 1825-1828 (*synth*)

Discokiolide A D-1078

[141266-02-6]



R = H

$C_{53}H_{70}N_8O_{13}$ 1027.182

Depsipeptide antibiotic. Isol. from marine sponge *Discodermia kiiensis*. Cytotoxic agent. $[\alpha]_D^{25}$ -52.3 (c, 1 in MeOH) (as Me ester). λ_{max} 251 (ϵ 19500) (MeOH).

Tada, H. *et al., Chem. Lett.*, 1992, 431-434 (*isol, struct*)

Discokiolide B D-1079

[141266-03-7]
As Discokiolide A, D-1078 with
R = CH_3
$C_{54}H_{72}N_8O_{13}$ 1041.209

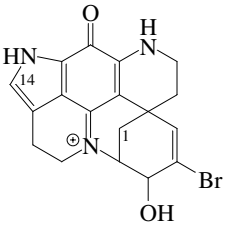
Depsipeptide antibiotic. Isol. from the marine sponge *Discodermia kiiensis*. Cytotoxic. $[\alpha]_D^{25}$ -43.5 (c, 1 in MeOH) (as Me ester). λ_{max} 251 (ϵ 19500) (MeOH) (Derep).

Δ^7-Isomer: ***Discokiolide D***
[141266-05-9]
$C_{54}H_{72}N_8O_{13}$ 1041.209
Isol. from *Discodermia kiiensis*. Cytotoxic. $[\alpha]_D^{25}$ -49.5 (c, 0.6 in MeOH) (as Me ester). λ_{max} 258 (ϵ 15900) (MeOH) (Derep).

4′-Demethoxy: ***Discokiolide C***
[141266-04-8]
$C_{53}H_{70}N_8O_{12}$ 1011.182
Isol. from *Discodermia kiiensis*. Cytotoxic. $[\alpha]_D^{25}$ -28.7 (c, 0.6 in MeOH) (as Me ester). λ_{max} 252 (ϵ 18200) (MeOH) (Derep).

Tada, H. *et al., Chem. Lett.*, 1992, 431 (*isol, struct*)

Discorhabdin V D-1080



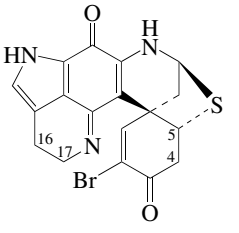
$C_{18}H_{17}BrN_3O_2^{\oplus}$ 387.255
Alkaloid from the sponge *Tsitsikamma pedunculata*. Dark green solid (as trifluoroacetate salt).

14-Bromo, 1-hydroxy: ***14-Bromo-1-hydroxydiscorhabdin V***
$C_{18}H_{16}Br_2N_3O_3^{\oplus}$ 482.151
Alkaloid from *Tsitsikamma flavus* and *Tsitsikamma pedunculata*. Brown solid (as trifluoroacetate salt).

Antunes, E.M. *et al., J. Nat. Prod.*, 2004, **67**, 1268-1276 (*isol, cd, pmr, cmr*)

Discorhabdin A D-1081

Prianosin A
[112515-41-0]



$C_{18}H_{14}BrN_3O_2S$ 416.297

Closely related to Discorhabdin C, D-1082. Alkaloid from the marine sponge *Prianos melanos* and *Latrunculia brevis*. Exhibits potent antineoplastic activity. Green solid (as hydrochloride). Mp 300°. $[\alpha]_D^{24}$ +248 (c, 0.19 in $CHCl_3$). $[\alpha]_D$ +400 (c, 0.05 in MeOH) (hydrochloride). λ_{max} 335 (ϵ 14000); 473 (ϵ 1000) (MeOH/KOH) (Derep). λ_{max} 248 (ϵ 29500); 353 (ϵ 11000); 430 (sh); 567 (ϵ 900) (MeOH) (Derep).

4,5-Didehydro: ***Discorhabdin B***
[115439-61-7]
$C_{18}H_{12}BrN_3O_2S$ 414.282
Isol. from a *Latrunculia* sp. Cytotoxic agent. Green solid (hydrochloride). Sol. DMSO; fairly sol. MeOH, H_2O.
Mp >360° (hydrochloride). $[\alpha]_D$ +400 (c, 0.2 in MeOH) (hydrochloride). λ_{max} 248 (ϵ 30600); 309 (ϵ 10800); 357 (ϵ 10600); 567 (ϵ 1100) (MeOH). λ_{max} 231 (ϵ 22500); 306 (ϵ 14700) (MeOH/NaOH) (Berdy).

16,17-Didehydro: ***Prianosin B***
[116302-35-3]
$C_{18}H_{12}BrN_3O_2S$ 414.282
Alkaloid from *Prianos melanos*. Cytotoxic agent. Red cryst. Sol. EtOAc, MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 250-251° dec. $[\alpha]_D^{30}$ +360 (c, 0.1 in $CHCl_3$). λ_{max} 228 (ϵ 17800); 263 (ϵ 15000); 410 (sh) (ϵ); 430 (ϵ 11200) (MeOH) (Derep).

4,5,16,17-Tetradehydro: ***Discorhabdin Q***
[224447-29-4]
$C_{18}H_{10}BrN_3O_2S$ 412.266

Alkaloid from the sponges *Latrunculia purpurea* and *Zyzzya* spp. Orange solid. $[\alpha]_D$ -452.4 (c, 0.004 in $CHCl_3$). $[\alpha]_D$ -904 (c, 0.01 in MeOH). λ_{max} 222 (ϵ 28200); 428 (ϵ 9900) (MeOH).

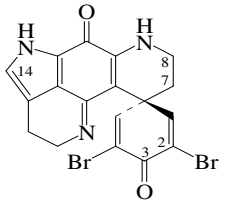
Debromo, 4,5-didehydro: ***Discorhabdin I***
[663597-85-1]
$C_{18}H_{13}N_3O_2S$ 335.386
Isol. from *Latrunculia brevis*. Cytotoxic. Green solid (as trifluoroacetate salt).
Mp >250° (blackens at 193°) (trifluoroacetate salt). $[\alpha]_D^{25}$ -562.8 (c, 0.13 in MeOH). λ_{max} 309 (log ϵ 3.72); 374 (sh); 556 (log ϵ 2.81) (MeOH) (trifluoroacetate salt).

Debromo, 4,5-didehydro, 1,2-epoxide: ***Discorhabdin R***
$C_{18}H_{13}N_3O_3S$ 351.385
Alkaloid from the sponges *Latrunculia* sp. and *Negombata* sp. Green solid. $[\alpha]_D^{20}$ +161 (c, 0.1 in MeOH). Config. of epoxide not determined. λ_{max} 202 (ϵ 7600); 255 (ϵ 9000); 262 (ϵ 9200); 287 (ϵ 5400); 326 (ϵ 3500); 368 (ϵ 3800); 567 (ϵ 600) (MeOH).

Kobayashi, J. *et al., Tet. Lett.*, 1987, **28**, 4939-4942 (*uv, ir, pmr, cmr, cryst struct, abs config*)
Cheng, J. *et al., J.O.C.*, 1988, **53**, 4621-4624 (*Prianosins*)
Perry, N.B. *et al., Tetrahedron*, 1988, **44**, 1727-1734 (*Discorhabdin B*)
Dijoux, M.-G. *et al., J. Nat. Prod.*, 1999, **62**, 636-637 (*Discorhabdin Q*)
Ford, J. *et al., J. Nat. Prod.*, 2000, **63**, 1527-1528 (*Discorhabdin R*)
Tohma, H. *et al., Angew. Chem., Int. Ed.*, 2002, **41**, 348-350 (*Discorhabdin A, synth*)
Tohma, H. *et al., J.A.C.S.*, 2003, **125**, 11235-11240 (*Discorhabdin A, synth*)
Reyes, F. *et al., J. Nat. Prod.*, 2004, **67**, 463-465 (*Discorhabdin I*)
Harayama, Y. *et al., Curr. Org. Chem.*, 2005, **9**, 1567-1588 (*rev, synth*)
Antunes, E.M. *et al., Nat. Prod. Rep.*, 2005, **22**, 62-72 (*rev*)

Discorhabdin C D-1082

[105372-81-4]



$C_{18}H_{13}Br_2N_3O_2$ 463.128
Pigment from a sponge of the genus *Latrunculia*. Sol. DMSO; fairly sol. MeOH.
Mp 360° (as hydrochloride). λ_{max} 245 (ϵ 28500); 351 (ϵ 10000); 545 (ϵ 500) (MeOH/HCl) (Derep). λ_{max} 337 (ϵ 13000); 481 (ϵ 1500) (MeOH/KOH) (Derep). λ_{max} 245 (ϵ 28500); 250 (ϵ 14600); 351 (ϵ 10000); 355 (ϵ 7700); 545 (ϵ 500) (MeOH) (Berdy).
▶ Highly cytotoxic; LD_{50} (mus, ipr) 2 mg/kg.

*13-*N*-Me:* ***Discorhabdin P***
[219566-63-9]
$C_{19}H_{15}Br_2N_3O_2$ 477.154
Isol. from a sponge of the *Batzella* sp. Cytotoxic agent.
Mp >360° (blackens at 162°). λ_{max} 200 (log ϵ 4.26); 245 (log ϵ 4.28); 337 (log ϵ 4); 488 (log ϵ 3.49) (MeOH).

3-Alcohol: ***3-Dihydrodiscorhabdin C***
$C_{18}H_{15}Br_2N_3O_2$ 465.143
Isol. from *Tsitsikamma pedunculata*. Red solid (as trifluoroacetate). λ_{max} 239 (ϵ 23700); 351 (ϵ 6030); 551 (ϵ 740) (MeOH) (trifluoroacetate).

7,8-Didehydro, 3-alcohol: ***7,8-Didehydro-3-dihydrodiscorhabdin C****. 3-Dihydro-7,8-dehydrodiscorhabdin C*
$C_{18}H_{13}Br_2N_3O_2$ 463.128
Isol. from the sponges *Tsitsikamma flavus* and *Tsitsikamma pedunculata*. Olive-green solid.

14-Bromo: ***14-Bromodiscorhabdin C***
[182928-53-6]
$C_{18}H_{12}Br_3N_3O_2$ 542.024
Isol. from the South African latrunculid sponge *Tsitsikamma pedunculata* and another sponge. Exhibits antimicrobial activity. λ_{max} 242; 317; 374 (MeOH) (Berdy).

14-Bromo, 3-alcohol: ***14-Bromo-3-dihydrodiscorhabdin C***
[182928-55-8]
$C_{18}H_{14}Br_3N_3O_2$ 544.04
Isol. from *Tsitsikamma flavus*, *Tsitsikamma pedunculata* and another sponge. Exhibits antimicrobial activity. λ_{max} 242; 317; 374 (MeOH) (Berdy).

14-Bromo, 7,8-didehydro, 3-alcohol: ***14-Bromo-7,8-didehydro-3-dihydrodiscorhabdin C****. 14-Bromo-3-dihydro-7,8-didehydrodiscorhabdin C*
$C_{18}H_{12}Br_3N_3O_2$ 542.024
Isol. from *Tsitsikamma pedunculata*. Green solid.

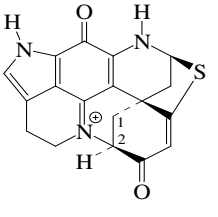
2-Debromo: ***Discorhabdin E***
[159308-95-9]
$C_{18}H_{14}BrN_3O_2$ 384.232
Alkaloid from the New Zealand sponge *Latrunculia* cf. *bocagei*. Red solid (as trifluoroacetate). λ_{max} 201 (ϵ 14500); 244 (ϵ 18000); 360 (ϵ 7300); 551 (ϵ 1000) (MeOH) (Berdy).

2-Debromo, 7,8-didehydro, 1,2-dihydro: ***Discorhabdin G***†
[172961-01-2]
$C_{18}H_{14}BrN_3O_2$ 384.232
Not to be confused with Discorhabdin G, D-1084. Alkaloid from the Antarctic sponge *Latrunculia apicalis*. Antimicrobial agent. Green pigment (as trifluoroacetate). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +27 (c, 0.063 in MeOH). λ_{max} 210 (ϵ 7500); 250 (ϵ 8100); 322 (ϵ 3200); 402 (ϵ 2300); 610 (ϵ 600) (MeOH).

Perry, N.B. *et al., J.O.C.*, 1986, **51**, 5476-5478 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Nishiyama, S. *et al., Tet. Lett.*, 1991, **32**, 4151 (*synth*)
Kita, Y. *et al., J.A.C.S.*, 1992, **114**, 2175 (*synth*)
Copp, B.R. *et al., J.O.C.*, 1994, **59**, 8233-8238 (*Discorhabdin E*)
Tao, X.L. *et al., Tetrahedron*, 1994, **50**, 2017 (*synth*)
Yang, A. *et al., J. Nat. Prod.*, 1995, **58**, 1596-1599 (*Discorhabdin G*)
Sadanandan, E.V. *et al., J.O.C.*, 1995, **60**, 1800 (*synth*)
Hooper, G.J. *et al., Tet. Lett.*, 1996, **37**, 7135 (*14-Bromodiscorhabdin C, 14-Bromodihydrodiscorhabdin C*)
Roberts, D. *et al., J.O.C.*, 1997, **62**, 568 (*synth*)
Gunasekera, S.P. *et al., J. Nat. Prod.*, 1999, **62**, 173-175 (*Discorhabdin P*)
Aubart, K.M. *et al., J.O.C.*, 1999, **64**, 16-22 (*synth*)
Antunes, E.M. *et al., J. Nat. Prod.*, 2004, **67**, 1268-1276 (*14-Bromo-3-dihydro-7,8-didehydrodiscorhabdin C, 3-Dihydro-7,8-didehydrodiscorhabdin C*)
Harayama, Y. *et al., Curr. Org. Chem.*, 2005, **9**, 1567-1588 (*rev, synth*)

Discorhabdin D D-1083

Prianosin D
[115384-95-7]



$C_{18}H_{14}N_3O_2S^{\oplus}$ 336.393
Alkaloid from the New Zealand sponge *Latrunculia brevis* and from the Okinawan marine sponge *Prianos melanos*. Exhibits significant *in vivo* antitumour and antineoplastic activity and antimicrobial action. Also induces $Ca^{2\oplus}$ release from sarcoplasmic reticulum. Green solid.
Mp 300°. $[\alpha]_D^{26}$ +344 (c, 0.01 in MeOH). Unstable in soln. λ_{max} 250 (ϵ 18100); 284 (ϵ 11100); 325 (ϵ 6600); 392 (ϵ 6950) (MeOH) (Derep). λ_{max} 262 (ϵ 30900); 290 (ϵ 15500); 368 (ϵ 9550) (MeOH/KOH) (Derep). λ_{max} 248 (ϵ 22400); 281 (ϵ 14100); 320 (ϵ 8510); 395 (ϵ 8910); 584 (ϵ 692) (MeOH) (Derep).

*1*R*-Hydroxy:* ***Discorhabdin L***
$C_{18}H_{14}N_3O_3S^{\oplus}$ 352.393
Alkaloid from *Latrunculia brevis*. Cytotoxic. Green solid (as TFA salt). Mp >250°. Blackens at 160° (TFA salt). λ_{max} 268 (log ϵ 3.75); 310 (sh); 352 (log ϵ 3.59); 550 (log ϵ 2.65) (MeOH) (TFA salt).

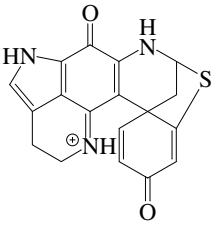
1ξ-Amino: ***1-Aminodiscorhabdin D***
$C_{18}H_{15}N_4O_2S^{\oplus}$ 351.408
Isol. from *Latrunculia bellae*. Dark green solid.

1ξ-(Carboxymethylamino): ***Discorhabdin N***
$C_{20}H_{17}N_4O_4S^{\oplus}$ 409.445
Isol. from *Latrunculia bellae*. Red-brown solid.

1ξ-Methoxy: ***1-Methoxydiscorhabdin D***
$C_{19}H_{16}N_3O_3S^{\oplus}$ 366.42
Isol. from *Latrunculia bellae*. Brown solid.

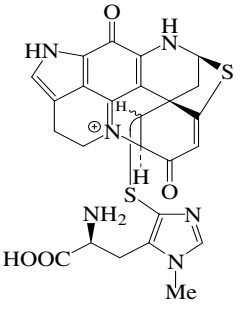
Perry, N.B. *et al., J.O.C.*, 1988, **53**, 4127-4128 (*isol, uv, ir, pmr, cmr*)
Cheng, J.F. *et al., J.O.C.*, 1988, **53**, 4621-4624 (*isol, uv, ir, pmr, cmr, ms, cd*)
Kobayashi, J. *et al., Tet. Lett.*, 1991, **32**, 1227-1228 (*struct*)
Reyes, F. *et al., J. Nat. Prod.*, 2004, **67**, 463-465 (*Discorhabdin L*)
Antunes, E.M. *et al., J. Nat. Prod.*, 2004, **67**, 1268-1276 (*Discorhabdin N, 1-Aminodiscorhabdin D, 1-Methoxydiscorhabdin D*)
Antunes, E.M. *et al., Nat. Prod. Rep.*, 2005, **22**, 62-72 (*rev*)

Discorhabdin G† D-1084



$C_{18}H_{14}N_3O_2S^{\oplus}$ 336.394
Not to be confused with Discorhabdin G in D-1082. Alkaloid from the sponge *Latrunculia bellae*. Dark yellow-brown solid.
Antunes, E.M. *et al., J. Nat. Prod.*, 2004, **67**, 1268-1276 (*isol, pmr, cmr*)

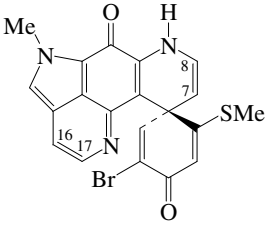
Discorhabdin H D-1085



$C_{25}H_{23}N_6O_4S_2^{\oplus}$ 535.627
Alkaloid from the sponge *Strongylodesma algoensis*. Dark green solid.

Antunes, E.M. *et al., J. Nat. Prod.*, 2004, **67**, 1268-1276 (*isol, pmr, cmr*)

Discorhabdin T D-1086



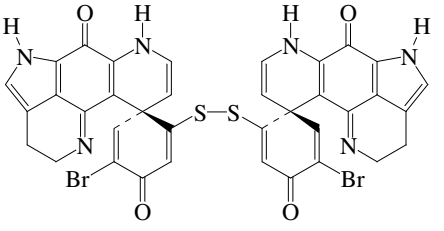
$C_{20}H_{14}BrN_3O_2S$ 440.32
Isol. from the sponge *Batzella* sp. Cytotoxic. Dark orange solid. λ_{max} 225 (log ϵ 4.11); 245 (log ϵ 3.97); 305 (log ϵ 3.65); 412 (log ϵ 3.55); 432 (log ϵ 3.65) (MeOH).

7,8-Dihydro: ***Discorhabdin S***
$C_{20}H_{16}BrN_3O_2S$ 442.335
Isol. from a *Batzella* sp. Cytotoxic. Dark orange solid. λ_{max} 225 (log ϵ 4.54); 260 (log ϵ 4.27); 305 (log ϵ 4.04); 400 (log ϵ 3.94); 422 (log ϵ 4.14) (MeOH).

16,17-Dihydro: ***Discorhabdin U***
$C_{20}H_{16}BrN_3O_2S$ 442.335
Isol. from a *Batzella* sp. Cytotoxic. Dark orange solid. λ_{max} 205 (log ϵ 4.42); 242 (log ϵ 4.22); 287 (log ϵ 4.01); 340 (log ϵ 3.95); 425 (log ϵ 3.12) (MeOH).

Gunasekera, S.P. *et al., J. Nat. Prod.*, 2003, **66**, 1615-1617 (*isol, pmr, cmr*)

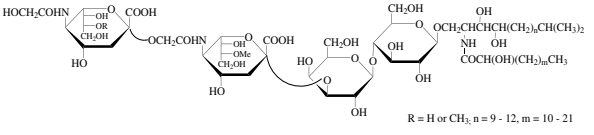
Discorhabdin W D-1087



$C_{36}H_{22}Br_2N_6O_4S_2$ 826.548
Isol. from a New Zealand *Latrunculia* sp.
$[\alpha]_D^{20}$ +220 (c, 0.05 in MeOH). λ_{max} 203; 241; 301; 444 (TFA/MeCN aq.).

Lang, G. *et al., J. Nat. Prod.*, 2005, **68**, 1796-1798 (*isol, pmr, cmr*)

Aphelasterias japonica Disialoganglioside D-1088

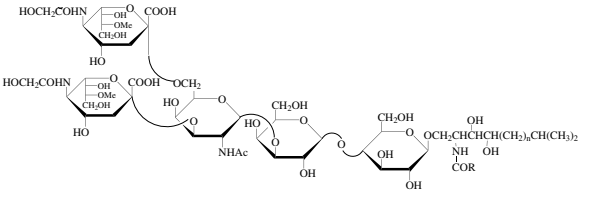


Isol. from the starfish *Aphelasterias japonica*.

[110183-19-2]

Smirnova, G.P. *et al., Biochim. Biophys. Acta*, 1987, **920**, 47-55 (*isol, struct*)

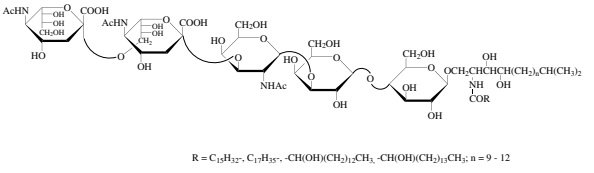
Asterias amurensis Disialoganglioside D-1089



Isol. from the starfish *Asterias amurensis*. CAS no. not found 8-14CI.

Kochetkov, N.K. *et al., Biochim. Biophys. Acta*, 1982, **712**, 650-658 (*isol, struct*)

Evasterias retifera Disialoganglioside D-1090

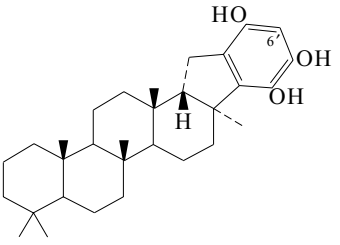


Isol. from the starfish *Evasterias retifera*. CAS no. not found 8-14CI.

Kochetkov, N.K. *et al., Biochim. Biophys. Acta*, 1982, **712**, 650-658 (*isol, struct*)

Disidein D-1091

*17,17*a*-Dihydro-4,4,8,17-tetramethyl-3′*H*-indeno[1′,2′:17,17*a*]-D-homoandrost-17-ene-4′,6′,7′-triol, 9CI. Dysidein*
[56012-79-4]



$C_{31}H_{46}O_3$ 466.703
Constit. of *Dysidea pallescens*. Cryst. (Et_2O).
Mp 260° dec. $[\alpha]_D$ +24 (c, 2.3 in dioxan). Genus name given as Disidea. λ_{max} 287 (ϵ 4990) (MeOH) (Derep).

Tri-Ac:
Cryst. (MeOH). Mp 143-145°.

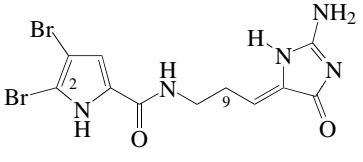
6′-Chloro: ***6′-Chlorodisidein***
$C_{31}H_{45}ClO_3$ 501.147
Constit. of *Dysidea pallescens*. Cryst.
Mp 158-159°. $[\alpha]_D$ +22.1 (c, 2 in $CHCl_3$).

6′-Bromo: ***6′-Bromodisidein***
$C_{31}H_{45}BrO_3$ 545.599
Constit. of *Dysidea pallescens*. Cryst.
Mp 159-160°. $[\alpha]_D$ +24.2 (c, 2.5 in $CHCl_3$).

Cimino, G. *et al., Tetrahedron*, 1975, **31**, 271 (*isol, struct*)
Cimino, G. *et al., Tetrahedron*, 1987, **43**, 4777 (*cryst struct, abs config, derivs*)

Dispacamide A D-1092

[177744-33-1]



$C_{11}H_{11}Br_2N_5O_2$ 405.048
Major alkaloid from the Caribbean sponges *Agelas dispar* and *Agelas clathrodes*. Exhibits remarkable antihistamine activity. Amorph. solid.

2-Debromo: ***Dispacamide B***. *2-Debromodispacamide A*
[177744-34-2]
$C_{11}H_{12}BrN_5O_2$ 326.152
Major alkaloid from the sponges *Agelas conifera* and *Agelas longissima*. Shows remarkable antihistamine activity.

9-Hydroxy: ***Dispacamide C***
[197448-22-9]
$C_{11}H_{11}Br_2N_5O_3$ 421.048
Alkaloid from *Agelas* spp. λ_{max} 227 (ϵ 11200); 272 (ϵ 12500) (MeOH).

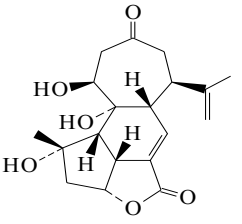
2-Debromo, 9-hydroxy: ***Dispacamide D***. *Mukanadin A*
[197448-24-1]
$C_{11}H_{12}BrN_5O_3$ 342.152
Alkaloid from *Agelas* spp. and *Axinella verrucosa*.

2-Debromo, 9-methoxy: ***9-Methoxydispacamide B***. *9-O-Methylmukanadin A*
$C_{12}H_{14}BrN_5O_3$ 356.178
Isol. from *Axinella verrucosa*.

Cafieri, F. *et al., Tet. Lett.*, 1996, **37**, 3587-3590 (*isol, uv, ir, pmr, cmr*)
Cafieri, F. *et al., Bioorg. Med. Chem. Lett.*, 1997, **7**, 2283-2288 (*isol, pmr, cmr*)
Lindel, T. *et al., Tet. Lett.*, 1997, **38**, 8935-8938 (*synth*)
Uemoto, H. *et al., J. Nat. Prod.*, 1999, **62**, 1581-1583 (*Mukanadine A*)
Fresneda, P.M. *et al., Tet. Lett.*, 2001, **42**, 851-854 (*synth*)
Aiello, A. *et al., Bioorg. Med. Chem.*, 2006, **14**, 17-24 (*9-Methoxydispacamide B*)

Dissectolide A D-1093

[163597-21-5]

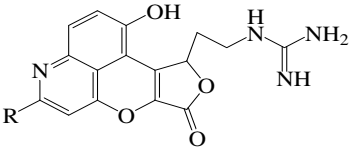


$C_{19}H_{24}O_6$ 348.395
Constit. of *Sinularia dissecta*. Cryst.
Mp 254-256°. $[\alpha]_D$ +91 (c, 0.5 in Py).

Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1995, 188 (*isol, pmr, cmr*)

Distomadine A D-1094

[549521-28-0]



R = H

$C_{16}H_{14}N_4O_4$ 326.311
Isol. from the ascidian *Pseudodistoma aureum*. Yellow powder.
Mp 232° dec. $[\alpha]_D^{20}$ +47 (c, 0.3 in MeOH). Fluorescent.

Pearce, A.N. *et al., Tet. Lett.*, 2003, **44**, 3897-3899 (*isol, pmr, cmr*)

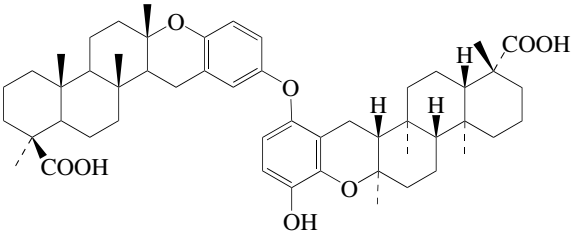
Distomadine B D-1095

[549521-30-4]
As Distomadine A, D-1094 with
R = COOH
$C_{17}H_{14}N_4O_6$ 370.321
Isol. from the ascidian *Pseudodistoma aureum*.

Pearce, A.N. *et al., Tet. Lett.*, 2003, **44**, 3897-3899 (*isol, pmr, cmr*)

Distrongylophorine D-1096

[211686-51-0]

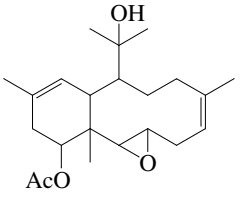


$C_{52}H_{70}O_8$ 823.12
Constit. of a *Strongylophora* sp. Cream powder. λ_{max} 206 (ϵ 5000); 230 (ϵ 1500); 295 (ϵ 1200) (MeOH) (Berdy).

Balbin-Oliveros, M. *et al., J. Nat. Prod.*, 1998, **61**, 948-952 (*isol, pmr, cmr*)

Aplysia Diterpenoid D-1097

[149064-80-2]



$C_{22}H_{34}O_4$ 362.508
Constit. of an *Aplysia* sp.
$[\alpha]_D$ -45.3 (c, 0.07 in $CHCl_3$).

Yamaguchi, Y. *et al., Kinki Daigaku Rikogakubu Kenkyu Hokoku*, 1992, **2**, 73-81; *CA*, **119**, 91581e (*isol, pmr*)

1,16-Dithiocyanato-8-hexadecanol D-1098

Thiocyanatin A
$NCS(CH_2)_8CH(OH)(CH_2)_7SCN$
$C_{18}H_{32}N_2OS_2$ 356.596

(±)-*form* [382595-10-0]
Isol. from a marine sponge *Oceanapia* sp. Nematocidal agent. Oil.

Capon, R.J. *et al., J.O.C.*, 2001, **66**, 7765-7769 (*isol, synth, pmr, cmr, ms*)

1,16-Dithiocyanato-7-hexadecene D-1099

Thiocyanatin C
$NCS(CH_2)_8CH{=}CH(CH_2)_6SCN$
$C_{18}H_{30}N_2S_2$ 338.58

(*E*)-*form* [382595-40-6]
Isol. from the marine sponge *Oceanapia* sp. Nematocidal agent. Isol. as a mixt. with.

Capon, R.J. *et al., J.O.C.*, 2001, **66**, 7765-7769 (*isol, synth, pmr, cmr, ms*)

1,16-Dithiocyanato-8-hexadecene D-1100

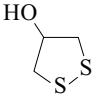
Thiocyanatin B
$NCS(CH_2)_7CH{=}CH(CH_2)_7SCN$
$C_{18}H_{30}N_2S_2$ 338.58

(*E*)-*form* [382595-18-8]
Isol. from a marine sponge *Oceanapia* sp. Nematocidal agent. Isol. as a mixt. with.

Capon, R.J. *et al., J.O.C.*, 2001, **66**, 7765-7769 (*isol, synth, pmr, cmr, ms*)

1,2-Dithiolan-4-ol, 9CI D-1101

4-Hydroxy-1,2-dithiolane
[27550-66-9]



$C_3H_6OS_2$ 122.212
Constit. of stem and bark of the mangrove plant *Bruguiera cylindrica*. Yellow oil.

S^1-*Oxide* (cis-): ***Brugierol***
[36437-85-1]
$C_3H_6O_2S_2$ 138.211
Constit. of *Bruguiera cylindrica* and *Bruguiera conjugata*. Cryst. (EtOAc).
Mp 84-85°. Config. revised in 2005. Possible artifact.

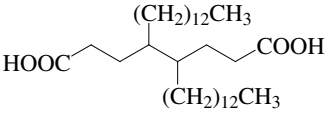
S^1-*Oxide* (trans-): ***Isobrugierol***
[36437-86-2]
$C_3H_6O_2S_2$ 138.211
Constit. of *Bruguiera cylindrica* and *Bruguiera conjugata*. Liq.
Config. revised in 2005. Possible artifact.

S^1,S^1-*Dioxide:* ***Bruguiesulfurol***
$C_3H_6O_3S_2$ 154.211
Constit. of the flowers of the mangrove *Bruguiera gymnorrhiza*. Cryst. ($CHCl_3$). λ_{max} 283 (log ϵ 1.58); 285 (log ϵ 1.57) (MeOH).

Kato, A. *et al., Tet. Lett.*, 1972, **13**, 203-206; 2959-2960 (*isol, synth*)
Kato, A. *et al., Phytochemistry*, 1976, **15**, 220-221 (*isol, ir, uv, pmr*)
Kato, A. *et al., Chem. Lett.*, 1978, 1219 (*synth*)
Bao, S. *et al., Helv. Chim. Acta*, 2005, **88**, 2757-2763 (*oxides, config*)
Homhual, S. *et al., Planta Med.*, 2006, **72**, 248-254 (*Bruguiesulfurol*)

4,5-Ditridecyloctanedioic acid D-1102

4,4′-Biheptadecanoic acid

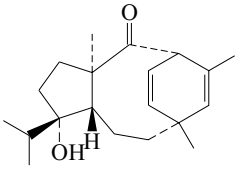


$C_{34}H_{66}O_4$ 538.893
Prod. by the marine-derived *Myrothecium* sp. Z16.
Mp 132-135°.

Liu, J.Y. *et al., J. Appl. Microbiol.*, 2006, **100**, 195-202 (*isol, pmr, cmr*)

Divarinone D-1103

[140679-92-1]



$C_{20}H_{30}O_2$ 302.456
Constit. of *Dictyota divaricata*. Oil. $[\alpha]_D$ -38.9 (c, 0.97 in $CHCl_3$).

Trimurtulu, G. *et al., Tet. Lett.*, 1992, **33**, 729 (*isol, pmr, cmr*)

Divercin V41 D-1104

[218289-96-4]
Peptide containing 43 amino acid residues and 2 disulfide bonds; shows high homology with and. Prod. by *Carnobacterium divergens* V41 isol. from fish viscera. Bacteriocin.

Métivier, A. *et al., Microbiology (Reading, U.K.)*, 1998, **144**, 2837-2844 (*isol, struct*)

Divergicin M35 D-1105

Peptide containing 43 amino acid residues incl. 4 cysteine residues. Prod. by *Carnobacterium divergens* M35 isol. from a commercial sample of frozen smoked mussels. Bacteriocin.

Tahiri, I. *et al., Int. J. Food Microbiol.*, 2004, **97**, 123-136 (*isol*)

4,19-Docosadiene-2,9,11,13,21-pentayn-1-ol, 9CI D-1106

Dehydrosiphonochalynol
[73247-90-2]
$HC{\equiv}CCH{=}CH(CH_2)_4C{\equiv}CC{\equiv}CC{\equiv}C(CH_2)_3CH{=}CH$
$C{\equiv}CCH_2OH$
$C_{22}H_{22}O$ 302.415

(4*Z*,9*Z*)-*form*
Isol. from sponges *Callyspongia* sp. and *Siphonochalina* sp. Pale yellow oil. λ_{max} 252; 267; 283; 308 (MeOH).

Rotem, M. *et al., Tet. Lett.*, 1979, 3193-3196 (*isol, uv, ir, pmr*)
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2003, **66**, 679-681 (*isol, pmr, cmr*)

5,9-Docosadienoic acid D-1107

[29564-66-7]
$H_3C(CH_2)_{11}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{22}H_{40}O_2$ 336.557

(5*E*,9*E*)-*form* [132171-23-4]
Isol. from the sponge *Plakortis halichondroides*.
Nitrile: [485322-60-9]
$C_{22}H_{39}N$ 317.557
Oil.

(5*Z*,9*Z*)-*form* [118885-06-6]
Constit. of sea anemones and sponges.
Characterised spectroscopically.

[118885-08-8]

Ayanoglu, E. *et al., Chem. Phys. Lipids*, 1988, **47**, 165-175 (*synth, pmr*)
Carballeira, N.M. *et al., Lipids*, 1990, **25**, 835-840 (*isol, ir, cmr*)
Carballeria, N. *et al., J. Nat. Prod.*, 1995, **58**, 1689-1694; 1998, **61**, 1049-1052 (*Z,Z-form, isol*)
Takahashi, S. *et al., Tetrahedron*, 2003, **59**, 1627-1638 (*E,E-form, nitrile, pmr, cmr*)

7,13-Docosadienoic acid D-1108

[64003-19-6]
$H_3C(CH_2)_7CH{=}CH(CH_2)_4CH{=}CH(CH_2)_5COOH$
$C_{22}H_{40}O_2$ 336.557

(7*Z*,13*Z*)-*form* [73536-71-7]
Constit. of *Scapharca broughtoni* and *Hymeniacidon sanguinea*.
Ayanoglu, E. *et al., Lipids*, 1982, **17**, 617-625 (*isol*)
Zhukova, N.V. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **83**, 643-646 (*isol*)
Christie, W.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1994, **109**, 245-252 (*isol*)

7,15-Docosadienoic acid D-1109

[3516-53-8]
$H_3C(CH_2)_5CH{=}CH(CH_2)_6CH{=}CH(CH_2)_5COOH$
$C_{22}H_{40}O_2$ 336.557

(7*Z*,15*Z*)-*form* [73536-72-8]
Constit. of *Dysidea fragilis* and *Scapharca broughtoni*.
Zhukova, N.V. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **83**, 643-646 (*isol*)
Christie, W.W. *et al., Lipids*, 1992, **27**, 640-644 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1994, **57**, 1152-1159 (*isol*)

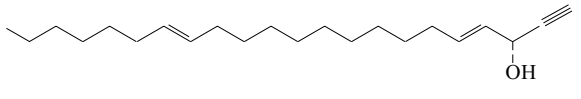
3,15-Docosadien-1-yne D-1110

$H_3C(CH_2)_5CH{=}CH(CH_2)_{10}CH{=}CHC{\equiv}CH$
$C_{22}H_{38}$ 302.542

(3*E*,15*Z*)-*form* [144259-04-1]
Isol. from the marine sponge *Cribrochalina vasculum*. Toxic to brine shrimp. Immunosuppressant. λ_{max} 225 (ε 14000) (hexane) (Berdy).
Aiello, A. *et al., J. Nat. Prod.*, 1992, **55**, 1275

4,15-Docosadien-1-yn-3-ol D-1111

[139722-81-9]
[151329-65-6, 178034-50-9]



(3*R*,4*E*,15*E*)–*form*

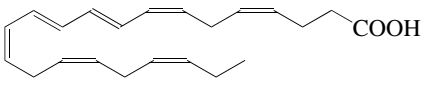
$C_{22}H_{38}O$ 318.542

(3*R*,4*E*,15*E*)-*form* [129364-94-9]
Isol. from the sponge *Cribrochalina vasculum*. Shows cytotoxic and immunosuppressive props. $[\alpha]_D$ -44 (c, 0.2 in MeOH). λ_{max} 202; 204 (ε 1400) (MeOH) (Berdy).

(3*R*,4*E*,15*Z*)-*form*
Isol. from the sponge *Cribrochalina vasculum*.
Gum. $[\alpha]_D$ -16.5 (c, 2.8 in MeOH). λ_{max} 202 (ε 1400) (MeOH) (Derep).

(3*S*,4*E*,15*Z*)-*form* [173938-16-4]
Isol. from *Cribrochalina vasculum*.
Oil. $[\alpha]_D$ +21.5 (c, 1.1 in MeOH).
Gunasekera, S.P. *et al., J.O.C.*, 1990, **55**, 6223 (*isol, pmr, cmr*)
Aiello, A. *et al., J. Nat. Prod.*, 1992, **55**, 1275 (*isol, pmr*)
Kulkarni, B.A. *et al., J.O.C.*, 1993, **58**, 5964 (*synth*)
Guo, Y.-W. *et al., Tetrahedron*, 1994, **50**, 13261 (*isol, pmr*)
Hallock, Y.F. *et al., J. Nat. Prod.*, 1995, **58**, 1801 (*isol, pmr, cmr, abs config*)
Ohtani, T. *et al., J.C.S. Perkin 1*, 1996, 961 (*synth*)
Morishita, K. *et al., J.C.S. Perkin 1*, 1999, 513-518 (*synth, abs config*)

4,7,9,11,13,16,19-Docosaheptaenoic acid D-1112

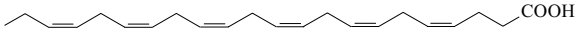


$C_{22}H_{30}O_2$ 326.478

(4*Z*,7*Z*,9*E*,11*E*,13*Z*,16*Z*,19*Z*)-*form*
Stellaheptaenoic acid
[167228-00-4]
Isol. from the green alga *Anadyomene stellata*.
Mikhailova, M.V. *et al., Lipids*, 1995, **30**, 583-589 (*isol, struct, pmr, ms*)

4,7,10,13,16,19-Docosahexaenoic acid D-1113

[2091-24-9]
[25167-62-8]



$C_{22}H_{32}O_2$ 328.494
▶ JR1230200

(*all-Z*)-*form*
Clupanodonic acid. ***Doconexent, INN***. *Cervonic acid*
[6217-54-5]
[32839-18-2]
Metabolic prod. of present in fish oils and in many phospholipids. Tuna eyeballs are a major source. Isol. from the sponge *Microciona prolifera*. Nutriceutical with antioxidation props. Extensively marketed as a dietary supplement in Japan. Essential for the functional development of nervous system including retina. Modulates arachidonic metab. and has antiinflammatory effects. May also depress platelet aggregation, augment efficiency of anticancer drugs, prevent arrhythmia and reduce serum cholesterol. Platelet aggregation inhibitor. Antihypertensive and antihypercholesterolaemic activities. Putative nootropic agent. Log P 7.44 (uncertain value) (calc). Component of Omega-3 Marine Triglycerides.
Me ester: [2566-90-7]
[301-01-9]
$C_{23}H_{34}O_2$ 342.52
Oil.
Et ester: [81926-94-5]
[84494-72-4]
$C_{24}H_{36}O_2$ 356.547
Oil.
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 786B (*nmr*)
Hands, A.R. *et al., Biochem. J.*, 1963, **87**, 263
Beach, D.H. *et al., Biochim. Biophys. Acta*, 1974, **369**, 16 (*biosynth*)
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206 (*isol*)
Sanders, T.A.B. *et al., Am. J. Clin. Nutr.*, 1978, **31**, 805
Moreno, V.J. *et al., Lipids*, 1979, **14**, 15 (*biosynth*)
Selivonchick, D.P. *et al., Lipids*, 1979, **14**, 66 (*isol*)
Dyerberg, J. *et al., Nutr. Rev.*, 1986, **44**, 125 (*rev*)
Hahn, S. *et al., J.A.C.S.*, 1988, **110**, 8177-8124 (*isol*)
Bazan, N.G. *et al., Prog. Clin. Biol. Res.*, 1989, **312**, 95 (*rev*)
Kim, H.Y. *et al., Prostaglandins*, 1990, **40**, 539 (*metab*)

Anderson, R.E. *et al., Adv. Exp. Med. Biol.*, 1992, **318**, 285 (*rev*)
Aursand, M. *et al., Chem. Phys. Lipids*, 1992, **62**, 239 (*cmr*)
Taber, D.F. *et al., J.O.C.*, 1995, **60**, 139-142 (*Et ester, synth, pmr, cmr, ir, ms*)
Sandri, J. *et al., J.O.C.*, 1995, **60**, 6627 (*synth, ir, pmr, cmr*)
Stillwell, W. *et al., Chem. Phys. Lipids*, 2003, **126**, 1-27 (*props*)

Docosane D-1114

[629-97-0]

$H_3C(CH_2)_{20}CH_3$

$C_{22}H_{46}$ 310.605

Constit. of green alga *Scenedesmus acutus* and moth scales of the corn earworm *Heliothis zea*. Also isol. from higher plant sources. Has kairomone activity. Cryst. (Et_2O).

Mp 47°. Bp_{15} 224°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 6B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 5B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 6C (*ir*)
Levene, P.A. *et al., J. Biol. Chem.*, 1915, **20**, 528
Minami, Y. *et al., CA*, 1953, 1422e (*synth*)
Hunter, G.L.K. *et al., Phytochemistry*, 1966, **5**, 807 (*isol*)
Jones, R.L. *et al., Environ. Entomol.*, 1973, **2**, 593 (*isol*)
Snyder, R.G. *et al., J. Chem. Phys.*, 1978, **68**, 4156 (*ir*)
Kakemoto, M. *et al., Nippon Kagaku Kaishi*, 1979, 80 (*glc, ms*)

4,8,12,15,19-Docosapentaenoic acid D-1115

[2548-85-8]

[25448-00-4, 32839-34-2]

$H_3CCH_2CH{=}CHCH_2CH_2CH{=}CHCH_2CH{=}CHCH_2CH_2CH{=}CHCH_2CH_2CH{=}CHCH_2CH_2COOH$

$C_{22}H_{34}O_2$ 330.509

The name Clupanodonic acid was prev. applied to a mixt. of this with 4,7,10,13,16,19-Docosahexaenoic acid, D-1113. It is now applied to the hexaenoic acid alone. Constit. of many fish oils e.g. sardine, mackerel and herring.

Me ester: d_{15} 0.94. $Bp_{0.07}$ 169-170°. n_D^{15} 1.4933.

Tsujimoto, M. *et al., Chem. Zentralbl.*, 1923, **1**, 38
Toyama, Y. *et al., Bull. Chem. Soc. Jpn.*, 1935, **10**, 433; 441 (*isol, struct*)
Baudent, P. *et al., C. R. Trav. Fac. Sci. Univ. Aix-Marseille*, 1941, **1**, 79; 1942, 86; 1943, 127 (*isol, struct*)
Varanasi, U. *et al., Biochim. Biophys. Acta*, 1975, **409**, 304 (*isol*)

7,10,13,16,19-Docosapentaenoic acid, 9CI D-1116

[2234-74-4]

[25448-00-4, 32839-34-2]

$H_3C(CH_2CH{=}CH)_5(CH_2)_5COOH$

$C_{22}H_{34}O_2$ 330.509

Metab. of Linolenic acid.

(all-*Z*)-*form* [24880-45-3]

Widespread occurrence in marine organisms e.g. *Dysidea fragilis*. d_4^{20} 0.92. n_D^{20} 1.4928.

[124020-08-2]

Myagkova, G.I. *et al., CA*, 1967, **66**, 94666 (*synth*)
Frangulyan, G.A. *et al., Khim. Prir. Soedin.*, 1987, **23**, 205-212; *Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 168-173 (*isol, pmr, cmr*)
Grandgirard, A. *et al., Lipids*, 1989, **24**, 799-804 (*synth*)
Christie, W.W. *et al., Lipids*, 1992, **27**, 640-644 (*isol*)
Kuklev, D.V. *et al., Bioorg. Khim.*, 1996, **22**, 219-222; *Sov. J. Bioorg. Chem. (Engl. Transl.)*, 1996, **22**, 192-195; *CA*, **125**, 221425 (*all-Z-form*)

4,7,10,13-Docosatetraenoic acid D-1117

$H_3C(CH_2)_7CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH_2COOH$

$C_{22}H_{36}O_2$ 332.525

(4*Z*,7*Z*,10*Z*,13*E*)-*form* [230295-20-2]

Isol. from scallop *Pecten maximus*.

(*all-Z*)-*form* [34711-40-5]

Constit. of *Pargrus major*.

Kunai, W.H. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1971, **352**, 542-548 (*synth*)
Marty, Y. *et al., J. Chromatogr., A*, 1999, **839**, 119-127
Kraffe, E. *et al., Lipids*, 2006, **41**, 491-497 (*isol*)

7,10,13,16-Docosatetraenoic acid D-1118

[2091-25-0]

$H_3C(CH_2)_4(CH{=}CHCH_2)_4(CH_2)_4COOH$

$C_{22}H_{36}O_2$ 332.525

(*all-Z*)-*form*

Adrenic acid

[81276-10-0]

[28874-58-0]

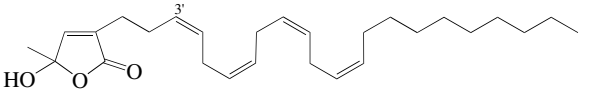
Constit. of canine adrenal gland and marine sponge *Microciona prolifera*. Metabolic prod. of linoleic acid.

Oil.

Chang, T.C.L. *et al., J. Lipid Res.*, 1962, **3**, 170; *Biochemistry*, 1963, **2**, 592
Comai, K. *et al., Lipids*, 1975, **10**, 555 (*isol*)
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206 (*isol, biosynth*)
William, G. *et al., J. Am. Oil Chem. Soc.*, 1977, **54**, 328 (*isol*)
Golovnya, R.V. *et al., Prikl. Biokhim. Mikrobiol.*, 1978, **14**, 609 (*glc, ms*)
Beckman, J.K. *et al., Lipids*, 1979, **14**, 262 (*isol*)

3-(3,6,9,12-Docosatetraenyl)-5-hydroxy-5-methyl-2(5*H*)-furanone D-1119

2-(3,6,9,12-Docosatetraenyl)-4-hydroxy-4-methyl-2-buten-4-olide



$C_{27}H_{42}O_3$ 414.627

Sol. MeOH, EtOAc; poorly sol. H_2O. λ_{max} 224 (ε 5000) (MeOH) (Derep).

(*all-Z*)-*form*

Flavalactone 4

[81346-98-7]

Obt. from the Japanese gorgonian *Euplexaura flava*.

Oil.

*3′,4′-Dihydro: 3-(6,9,12-Docosatrienyl)-5-hydroxy-5-methyl-2(5*H*)-furanone.* ***Flavalactone 3***

[81346-97-6]

$C_{27}H_{44}O_3$ 416.643

From *Euplexaura flava*. Granulation inhibitor. Antiinflammatory agent. Oil. Sol. MeOH, EtOAc; poorly sol. H_2O. λ_{max} 224 (ε 5000) (MeOH) (Derep).

Kituchi, H. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1172-1176 (*isol, ir, pmr, cmr*)

4,13,19-Docosatriene-2,9,11,21-tetrayn-1-ol D-1120

$HC{\equiv}CCH{=}CH(CH_2)_4CH{=}CHC{\equiv}CC{\equiv}C(CH_2)_3CH{=}CHC{\equiv}CCH_2OH$

$C_{22}H_{24}O$ 304.431

(4*Z*,13*Z*,19*Z*)-*form*

Callyspongenol C

Isol. from a *Callyspongia* sp.

Pale yellow oil. λ_{max} 218 (log ε 4.04) (MeOH).

13,14-Dihydro: 4,19-Docosadiene-2,9,11,21-tetrayn-1-ol. ***Callyspongenol B***

$C_{22}H_{26}O$ 306.447

Isol. from a *Callyspongia* sp. Pale yellow oil. λ_{max} 218 (log ε 4.04) (MeOH).

Youssef, D.T.A. *et al., J. Nat. Prod.*, 2003, **66**, 679-681 (*isol, pmr, cmr*)

3,10,19-Docosatriene-1,8,21-triyne D-1121

Aikupikanyne C

$HC{\equiv}CCH{=}CH(CH_2)_7CH{=}CHC{\equiv}C(CH_2)_3CH{=}CHC{\equiv}CH$

$C_{22}H_{28}$ 292.463

(3*Z*,10*E*,19*Z*)-*form*
Isol. from a *Callyspongia* sp.
Oil.
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2000, **63**, 1406-1410

7,13,16-Docosatrienoic acid D-1122

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CH(CH_2)_4CH{=}CH(CH_2)_5COOH$
$C_{22}H_{38}O_2$ 334.541

(*all-Z*)-*form* [83474-14-0]
Constit. of *Petrosia ficiformis*.
Ayanoglu, E. *et al., Lipids*, 1982, **17**, 617-625 (*isol*)

13,16,19-Docosatrienoic acid D-1123

[59708-86-0]
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_{11}COOH$
$C_{22}H_{38}O_2$ 334.541

(*all-Z*)-*form* [28845-86-5]
Isol. from rape seed oil. Widespread among marine organisms. Found in lipids of egg yolk, embryo of dogfish and in lipids and phospholipids of pancreatic islets.
[108698-01-7]
Haeffner, E. *et al., Lipids*, 1970, **5**, 430 (*isol, struct*)
Moreno, V.J. *et al., Lipids*, 1979, **14**, 15; 313 (*biosynth*)
Diaz, G.B. *et al., Lipids*, 1988, **23**, 1125; 1990, **25**, 724 (*occur*)
Berger, A. *et al., Lipids*, 1990, **25**, 473 (*biosynth*)

15-Docosene-1,3-diyn-5-one, 9CI D-1124

$H_3C(CH_2)_5CH{=}CH(CH_2)_9COC{\equiv}CC{\equiv}CH$
$C_{22}H_{34}O$ 314.51

(*Z*)-*form*
Debromorenierin 1
[63987-88-2]
Constit. of *Reniera fulva*.
Oil. λ_{max} 236 (ϵ 5 800), 246 (9 320), 262 (12 900) and 276 nm (8 700) (MeOH). λ_{max} 236 (ϵ 5800); 246 (ϵ 9320); 262 (ϵ 12900); 276 (ϵ 8700) (MeOH) (Derep).
Cimino, G. *et al., Tet. Lett.*, 1977, 1325 (*ir, uv, pmr*)

3-Docosene-1,11,13,15,21-pentayne, 9CI D-1125

$HC{\equiv}CCH{=}CH(CH_2)_6C{\equiv}CC{\equiv}CC{\equiv}C(CH_2)_4C{\equiv}CH$
$C_{22}H_{24}$ 288.432

(*Z*)-*form*
Siphonochalyne
[73247-89-9]
Isol. from the sponge *Siphonochalina* sp.
Dihydro: ***Dihydrosiphonochalyne***
[73203-57-3]
$C_{22}H_{26}$ 290.447
From *Siphonochalina* sp. Exact struct. not determined.
Rotem, M. *et al., Tet. Lett.*, 1979, 3193-3196 (*isol, struct, ir, uv, pmr*)

19-Docosene-2,9,11,13,21-pentayn-1-ol D-1126

$HC{\equiv}CCH{=}CH(CH_2)_4C{\equiv}CC{\equiv}CC{\equiv}C(CH_2)_5C{\equiv}CCH_2OH$
$C_{22}H_{24}O$ 304.431

(*Z*)-*form*
Siphonochalynol
[73233-09-7]
Isol. from the sponge *Siphonochalina* sp.
Rotem, M. *et al., Tet. Lett.*, 1979, 3193 (*isol, struct, ir, uv, pmr*)

19-Docosene-2,10,12,14,21-pentayn-1-ol D-1127

Aikupikanyne E
$HC{\equiv}CCH{=}CH(CH_2)_3C{\equiv}CC{\equiv}CC{\equiv}C(CH_2)_6C{\equiv}CCH_2OH$
$C_{22}H_{24}O$ 304.431

(*Z*)-*form*
Isol. from a *Callyspongia* sp.
Oil.
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2000, **63**, 1406-1410

19-Docosene-2,7,13,21-tetrayn-1-ol D-1128

Callyspongenol A
$HC{\equiv}CCH{=}CH(CH_2)_4C{\equiv}C(CH_2)_4C{\equiv}C(CH_2)_3C{\equiv}CCH_2OH$
$C_{22}H_{28}O$ 308.463

(*Z*)-*form*
Isol. from a *Callyspongia* sp.
Pale yellow oil. λ_{max} 216 (log ϵ 4.05) (MeOH).
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2003, **66**, 679-681 (*isol, pmr, cmr*)

3-Docosene-1,8,21-triyne D-1129

Octahydrosiphonochalyne
$HC{\equiv}C(CH_2)_{11}C{\equiv}C(CH_2)_3CH{=}CHC{\equiv}CH$
$C_{22}H_{32}$ 296.495

(*Z*)-*form* [73203-56-2]
Isol. from *Callyspongia* sp. and *Siphonochalina* sp.
Oil.
Rotem, M. *et al., Tet. Lett.*, 1979, 3193-3196 (*isol*)
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2000, **63**, 1406-1410 (*isol, pmr, cmr, struct*)

11-Docosenoic acid D-1130

[506-36-5]
[25378-26-1]
$H_3C(CH_2)_9CH{=}CH(CH_2)_9COOH$
$C_{22}H_{42}O_2$ 338.573

(*E*)-*form*
Catelaidic acid
[62600-37-7]
Constit. of partially hydrogenated fish oil.

(*Z*)-*form*
Cetoleic acid
[1002-96-6]
[28929-01-3]
Esters occur commonly in oil from marine mammals and fish and rapeseed.
Mp 33-33.7°.
Toyama, Y. *et al., CA*, 1928, **22**, 575 (*isol*)
Ackman, R.G. *et al., Fette, Seifen, Anstrichm.*, 1977, **79**, 15
Gudbjarnason, S. *et al., Biochim. Biophys. Acta*, 1977, **487**, 10
Kirk, R.S. *et al., J. Sci. Food Agric.*, 1978, **29**, 880 (*glc*)
Loew, F.M. *et al., Nutr. Metab.*, 1978, **22**, 207
Thomas, D.C. *et al., Arch. Microbiol.*, 1978, **117**, 239

13-Docosenoic acid D-1131

[25378-26-1]
$H_3C(CH_2)_7CH{=}CH(CH_2)_{11}COOH$
$C_{22}H_{42}O_2$ 338.573
Present in lipids of *Physalia physalis* (Portuguese-man-of-war). Antineoplastic agent. Log P 9.86 (uncertain value) (calc).

(*E*)-*form*
Brassidic acid
[506-33-2]
Cryst. (EtOH). Mp 61.5°. Bp_{30} 282° Bp_{10} 256°.
Me ester: [7439-44-3]
$C_{23}H_{44}O_2$ 352.599
Mp 34-35°.
Et ester: [116723-91-2]

$C_{24}H_{46}O_2$ 366.626
Mp 30.5°.

Nitrile:
$C_{22}H_{41}N$ 319.573
Mp 22°. Bp_{17} 257°.

Anhydride:
$C_{44}H_{82}O_3$ 659.13
Mp 64°.

(*Z*)-*form*
Erucic acid
[112-86-7]
[28929-01-3]
An important vegetable fatty acid, mainly confined to seed fats of the families Cruciferae and Tropaelaceae (e.g. rape, mustard and wallflower seeds). Occurs widely in marine organisms.
Cryst. (MeCN).
Mp 33.5°. Pharmacol. active isomer. Undergoes solid-state phase transitions.

Me ester: [1120-34-9]
Oil. Bp_5 221-222°. Ir ν 1744 cm^{-1}.

Et ester: [37910-77-3] Bp_5 229-230°.

Chloride: [7459-29-2]
$C_{22}H_{41}ClO$ 357.018
Mp 14°.

Amide: 13-Docosenamide. Newtron S
[112-84-5]
$C_{22}H_{43}NO$ 337.588
Isol from the cerebrospinal fluid of humans, cats and rats. Antiblocking agent/lubricant for polymers. Sleep inducer.
Mp 94° (65-66°).

Nitrile: [73170-89-5] Bp 238-240°.

Anhydride: [103213-60-1]
Mp 47.5-48°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 501D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 784A; 1221C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 588C (*ir*)
Holde, D. *et al., Ber.*, 1923, **56**, 2052-2058 (*anhydrides*)
Org. Synth., Coll. Vol., 2, 1943, 258 (*synth*)
Bowman, R.E. *et al., J.C.S.*, 1950, 177 (*synth*)
Lakizo, V.I. *et al., CA*, 1968, **69**, 2475g (*synth*)
Niewiadomski, H. *et al., Przem. Chem.*, 1969, **48**, 659; *CA*, **72**, 78; 293 (*rev*)
Chang, S.P. *et al., J. Am. Oil Chem. Soc.*, 1972, **49**, 422 (*synth*)
Mitcham, D. *et al., J. Am. Oil Chem. Soc.*, 1973, **50**, 446 (*ir*)
Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*Physalia physalis constit*)
Barrette, J.P. *et al., J. Assoc. Off. Anal. Chem.*, 1976, **59**, 855 (*glc*)
Yamada, K. *et al., J.O.C.*, 1978, **43**, 2076 (*synth*)
Kaneko, F. *et al., Acta Cryst. C*, 1992, **48**, 1060; 1993, **49**, 1232 (*cryst struct, erucic acid*)
Painuly, P. *et al., J. Chromatogr.*, 1992, **590**, 139 (*purifn*)
Kling, M.R. *et al., J.C.S. Perkin 1*, 1993, 1183 (*synth, ir, ms*)
Lerner, R. *et al., Science (Washington, D.C.)*, 1995, **268**, 1506 (*isol, amide*)

15-Docosenoic acid D-1132

[14134-54-4]
[25378-26-1]

$H_3C(CH_2)_5CH{=}CH(CH_2)_{13}COOH$
$C_{22}H_{42}O_2$ 338.573

(*Z*)-*form* [17735-97-6]
[28929-01-3]
Constit. of the sponge *Pseudaxinella* cf. *lunaecharta*. Occurs in *Brassica campestris* and other rape oils. Found in pig brain sphingolipids.

[62732-79-0, 82683-31-6]

Kishimoto, Y. *et al., J. Lipid Res.*, 1963, **4**, 437; 1964, **5**, 98 (*isol, struct*)
Sebedio, S.L. *et al., Lipids*, 1982, **17**, 469 (*isol*)
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol*)

17-Docosenoic acid D-1133

$H_3C(CH_2)_3CH{=}CH(CH_2)_{15}COOH$
$C_{22}H_{42}O_2$ 338.573

(*Z*)-*form* [132998-37-9]
Constit. of the sponges *Amphimedon compressa* and *Hymeniacidon sanguinea*.

Carballeira, N.M. *et al., J. Nat. Prod.*, 1992, **55**, 333-339 (*isol*)
Christie, W.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1994, **109**, 245-252 (*isol*)

15-Docosen-1-yne D-1134

$HC{\equiv}C(CH_2)_{12}CH{=}CH(CH_2)_5CH_3$
$C_{22}H_{40}$ 304.558

(*Z*)-*form* [73233-10-0]
Isol. from the marine sponge *Siphonochalina* sp.
Rotem, M. *et al., Tet. Lett.*, 1979, 3193 (*isol*)

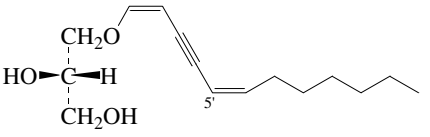
3,5-Dodecadien-2-amine D-1135

2-Amino-3,5-dodecadiene
$H_3C(CH_2)_5CH{=}CHCH{=}CHCH(NH_2)CH_3$
$C_{12}H_{23}N$ 181.32

(±)-(3*E*,5*Z*)-*form* [134387-52-3]
Constit. of the ascidian *Pseudodistoma novaezelandiae*. λ_{max} 233 (MeOH) (Berdy).
Perry, N.B. *et al., Aust. J. Chem.*, 1991, **44**, 627-633 (*isol, uv, pmr, cmr*)

3-(1,5-Dodecadien-3-ynyloxy)-1,2-propanediol D-1136

Glycerol 1-(1,5-dodecadien-3-ynyl) ether



$C_{15}H_{24}O_3$ 252.353

(*S,Z,Z*)-*form*
Petroraspailyne A1
[219917-14-3]
Isol. from a *Petrosia* sp.
$[\alpha]_D^{25}$ -3.2 (c, 0.08 in MeOH). λ_{max} 276 (log ϵ 3.74); 291 (log ϵ 3.58) (MeOH).

5′,6′-Dihydro: 3-(1-Dodecen-3-ynyloxy)-1,2-propanediol. Glycerol 1-(1-dodecen-3-ynyl) ether. ***Petroraspailyne B1***
[219917-17-6]
$C_{15}H_{26}O_3$ 254.369
Isol. from a *Petrosia* sp.
$[\alpha]_D^{25}$ +0.5 (c, 0.21 in MeOH). λ_{max} 237 (log ϵ 3.57) (MeOH).
Seo, Y. *et al., J. Nat. Prod.*, 1999, **62**, 122-126

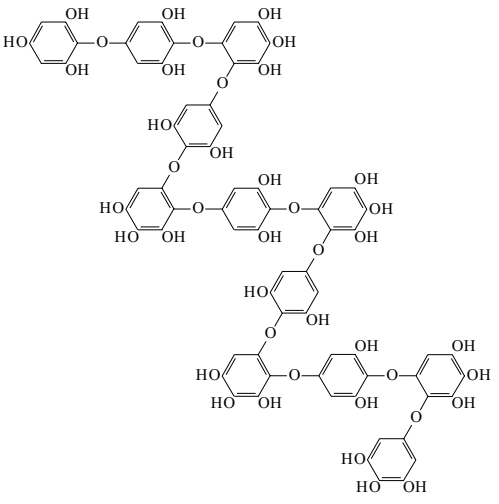
2,4-Dodecadiyn-1-ol D-1137

[95667-32-6]
$H_3C(CH_2)_6C{\equiv}CC{\equiv}CCH_2OH$
$C_{12}H_{18}O$ 178.274
Isol. from the stony coral *Montipora* sp. Cytotoxic.
Mp 34-36°.

Doolittle, R.E. *et al., Synthesis*, 1984, 730-732 (*synth*)
Wityak, J. *et al., Synth. Commun.*, 1991, **21**, 977-979 (*synth*)
Coll, J.C. *et al., Mar. Biol. (Berlin)*, 1994, **118**, 177-182 (*isol*)
Fiandanese, V. *et al., J. Organomet. Chem.*, 2005, **690**, 3004-3008 (*synth, ir, pmr, cmr, ms*)

Dodecafuhalol A D-1138

[164176-32-3]



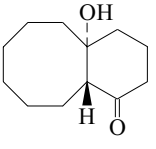
$C_{72}H_{50}O_{42}$ 1587.162

Constit. of the brown alga *Sargassum spinuligerum*.

Glombitza, K.-W. *et al., Phytochemistry*, 1995, **38**, 987-995 (*isol, pmr, cmr, ms*)

Dodecahydro-4*a*-hydroxy-1(2*H*)-benzocyclooctenone, 9CI D-1139

1-Hydroxybicyclo[6.4.0]dodecan-9-one



$C_{12}H_{20}O_2$ 196.289

(R*,R*)-form

trans-*form*

[167900-48-3]

Constit. of the leaves of *Rhizophora mucronata*.

Viscous solid.

Lakshmi, V. *et al., Planta Med.*, 1995, **61**, 382-383 (*isol, pmr, cmr*)

Dodecanal D-1140

Lauric aldehyde. Laurylaldehyde. FEMA 2615

[112-54-9]

$H_3C(CH_2)_{10}CHO$

$C_{12}H_{24}O$ 184.321

Occurs in peel oil from *Chamaecyparis lawsonia*, *Citrus* spp. and kumquat. Also present in ginger, coriander, chervil, and scallop. A common component of lepidopteran pheromones. Occurs in secretions from heads of the bees *Andrena* sp. Perfumery ingredient. Flavouring agent. Cryst. with fatty, woody taste. Poorly sol. H_2O. d_{25}^{25} 0.83.

Mp 44.5°. Bp_{100} 184-185° Bp_{22} 142-143°.

▶ Skin and eye irritant. LD_{50} (rat, orl) 23000 mg/kg. JR1910000

Oxime: [13372-76-4]

[106915-67-7, 106915-68-8]

$C_{12}H_{25}NO$ 199.336

Mp 73°.

2,4-Dinitrophenylhydrazone: [1726-78-9]

Mp 106°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 361B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 469D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 556B (*ir*)
Kraft, F. *et al., Ber.*, 1880, **13**, 1413-1418 (*synth*)
Davies, R.R. *et al., J.C.S.*, 1943, 84-86 (*synth*)
Ikeda, R.M. *et al., J. Agric. Food Chem.*, 1962, **10**, 98-102 (*isol*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 483 (*rev, tox*)
Boss, B.D. *et al., Anal. Chem.*, 1976, **48**, 417-420 (*glc, ms*)
Tengoe, J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **55**, 179-188 (*occur*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DXT000
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1542-1543 (*occur, props*)
Aurell, M.J. *et al., Tetrahedron*, 1997, **53**, 10883-10898 (*synth, pmr*)
Sharma, A. *et al., J.O.C.*, 1999, **22**, 8059-8062 (*synth, ir, pmr*)
Singh, R.S. *et al., Chem. Eur. J.*, 2002, **8**, 900-909 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

1-Dodecanol D-1141

Dodecyl alcohol. Lauryl alcohol. FEMA 2617

[112-53-8]

$H_3C(CH_2)_{10}CH_2OH$

$C_{12}H_{26}O$ 186.337

Isol. from plant sources, e.g. oil of *Furcraea gigantea*, apple and banana. Used in perfumery. Sulfuric esters are used as wetting agents and detergents. Flavouring agent. Cryst. (EtOH aq.) with fatty, waxy flavour.

Mp 24° Mp 26°. Bp 260-262° Bp_{18} 145-148°.

▶ Severe skin irritant. LD_{50} (rat, orl) *ca.* 13000 mg/kg. JR5775000

2-Propenoyl: Dodecyl propenoate. Lauryl acrylate

[2156-97-0]

$C_{15}H_{28}O_2$ 240.385

Constit. of the alga *Dictyota volubilis*. Bp_5 110°.

[27342-88-7]

Wright, A.D. *et al., J. Nat. Prod.*, 1990, **53**, 845-861 (*propenoate, isol*)

2-Dodecanone D-1142

[6175-49-1]

$H_3C(CH_2)_9COCH_3$

$C_{12}H_{24}O$ 184.321

Detected in rue oils, tomato leaf oil and *Cannabis sativa* oil. Also in hop oil (*Humulus lupulus*) and oil of *Schisandra nigra*. Isol. from an arctic marine bacterium. Antifungal agent.

Mp 21°. Bp_{100} 177-178° $Bp_{3.5}$ 101°. n_D^{20} 1.4340.

2,4-Dinitrophenylhydrazone: [81874-90-0]

Mp 81°.

Semicarbazone:

Needles (EtOH). Mp 122-123°.

Pickard, R.H. *et al., J.C.S.*, 1911, **99**, 57 (*synth*)
Asinger, F. *et al., Ber.*, 1944, **77**, 73 (*synth*)
U.S. Pat., 1968, 3 365 499; *CA*, **69**, 35440 (*manuf*)
Yeo, A.N.H. *et al., Chem. Comm.*, 1970, 987 (*ms*)
Cooke, M.P. *et al., J.O.C.*, 1973, **38**, 4082 (*synth*)
Bente, P.F. *et al., J. Phys. Chem.*, 1975, **79**, 713 (*ms*)
Kabalka, G.W. *et al., J. Chem. Educ.*, 1976, **53**, 549 (*synth*)
Hokanson, E.C. *et al., J.O.C.*, 1985, **50**, 462 (*synth, pmr*)
McDowell, P.G. *et al., Phytochemistry*, 1988, **27**, 2519 (*isol*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*marine isol*)

3,6,9-Dodecatrienoic acid D-1143

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2COOH$

$C_{12}H_{18}O_2$ 194.273

(all-Z)-form [92340-48-2]

Constit. of the female gametes of *Analipus japonicus*. Possible precursor of algal sex attractants.

[82461-32-3]

Kodama, K. *et al., Phytochemistry*, 1993, **33**, 1039 (*isol, synth, pmr, cmr*)

3,6,9-Dodecatrien-1-ol, 9CI D-1144

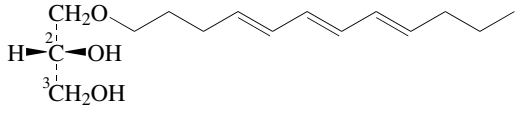
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH_2OH$

$C_{12}H_{20}O$ 180.289

(3*Z*,6*Z*,9*Z*)-*form* [81345-02-0]
Isol. from the ascidian *Botrylloides giganteum*.
Amorph. solid. λ_{max} 274 (MeOH).
O-*Sulfate:*
$C_{12}H_{20}O_4S$ 260.354
Isol. from *Daphnia pulex*. Kairomone. Counterion not identified.
Sandri, J. *et al., J.O.C.*, 1995, **60**, 6627 (*synth, pmr, cmr, ir*)
Granato, A.C. *et al., Quim. Nova*, 2005, **28**, 192-198 (*isol, pmr, cmr*)
Yasumoto, K. *et al., Tet. Lett.*, 2005, **46**, 4765-4767 (*sulfate*)

3-(4,6,8-Dodecatrienyloxy)-1,2-propanediol D-1145

1-O-*(4,6,8-Dodecatrienyl)glycerol. Glycerol 1-(4,6,8-dodecatrienyl) ether*



(*R*,all-*E*)-*form*

$C_{15}H_{26}O_3$ 254.369
Closely related to the Fecapentaenes.

(*R*,*all-E*)-*form*
2-O-*(4-Hydroxybenzoyl):* ***Bretonin A***
[123231-45-8]
$C_{22}H_{30}O_5$ 374.476
Isol. from an unidentified marine demosponge. Oil. $[\alpha]_D^{25}$ -7 (c, 0.13 in $CHCl_3$) (as di-Ac). Opt. rotn. of parent compd. too small to measure.
3-O-*(4-Hydroxybenzoyl):* ***Isobretonin A***
[123231-46-9]
$C_{22}H_{30}O_5$ 374.476
Isol. from an unidentified marine demosponge. Oil. $[\alpha]_D^{25}$ +7.3 (c, 0.11 in $CHCl_3$). Abs. config. is *S*-.

(2*S*,4′*E*,6′*Z*,8′*E*)-*form*
2-O-*(4-Hydroxybenzoyl):* ***Bretonin B***
[137623-93-9]
$C_{22}H_{30}O_5$ 374.476
Isol. from an unidentified marine demosponge.
Guella, G. *et al., Helv. Chim. Acta*, 1989, **72**, 1121-1124 (*isol, uv, pmr, cmr, struct*)
Mancini, I. *et al., Helv. Chim. Acta*, 1991, **74**, 941-950 (*synth, abs config*)
Solladie, G. *et al., J.O.C.*, 1996, **61**, 4369-4370 (*synth, Isobretonin A*)

11-Dodecene-2,4-diyn-1-ol D-1146

Montiporyne G
$H_2C{=}CH(CH_2)_5C{\equiv}CC{\equiv}CCH_2OH$
$C_{12}H_{16}O$ 176.258
Isol. from the coral *Montipora* sp. Cytotoxic. Light yellow oil.
Methoxyacetyl: [125906-55-0]
$C_{15}H_{20}O_3$ 248.321
Isol. from the hermatypic coral *Montipora* sp. Shows ichthyotoxicity. Sol. MeOH, Me_2CO.
2-Hydroxyethyl ether: 2-(11-Dodecene-2,4-diynyloxy)ethanol. ***Montiporyne H***
$C_{14}H_{20}O_2$ 220.311
Isol. from a *Montipora* sp. Yellow oil.
Higa, T. *et al., Chem. Lett.*, 1990, 145 (*isol, struct*)
Alam, N. *et al., J. Nat. Prod.*, 2001, **64**, 1059-1063 (*Montiporyne H*)

2-Dodecenoic acid D-1147

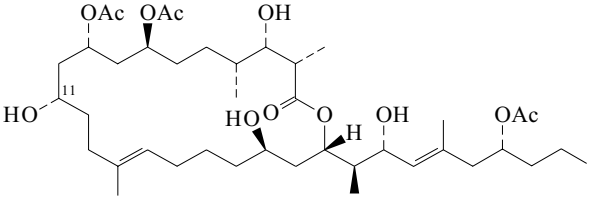
[4412-16-2]
$H_3C(CH_2)_8CH{=}CHCOOH$
$C_{12}H_{22}O_2$ 198.305

(*E*)-*form* [32466-54-9]
Mp 13-18°. Bp_3 155-158° $Bp_{0.15}$ 127-130°.
Me ester: [6208-91-9]
$C_{13}H_{24}O_2$ 212.331
Occurs in volatile component of pears. Oil. Bp_3 105°.
Et ester: [28290-90-6]
$C_{14}H_{26}O_2$ 226.358
Occurs in pears.
*2*R,*3*S-*Epoxide: 3-Nonyloxiranecarboxylic acid, 9CI. 2,3-Epoxydodecanoic acid*
$C_{12}H_{22}O_3$ 214.304
Isol. from the red alga *Gracilaria verrucosa*. Oil (as Me ester). $[\alpha]_D^{23}$ +36.4 (c, 0.11 in CH_2Cl_2) (Me ester).

(*Z*)-*form* [55928-65-9]
Org. Synth., Coll. Vol., 4, 1963, 398 (*synth*)
Creveling, R.K. *et al., J. Agric. Food Chem.*, 1970, **18**, 19 (*ir, pmr, ms, uv*)
Bus, J. *et al., Chem. Phys. Lipids*, 1976, **17**, 501; 1977, **18**, 130 (*cmr*)
Muto, S. *et al., Eur. J. Org. Chem.*, 2001, 4635-4638 (*Me ester*)
Popaj, K. *et al., Helv. Chim. Acta*, 2001, **84**, 180-186 (*Et ester, synth, ir, pmr, cmr*)
Shoeb, M. *et al., J. Nat. Prod.*, 2003, **66**, 1509-1511 (*2,3-Epoxydodecanoic acid*)

Dolabelide B D-1148

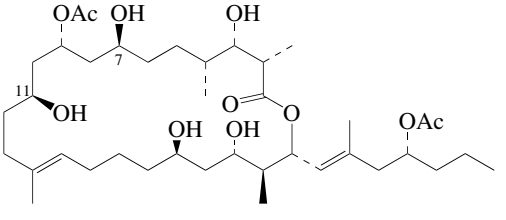
[169970-79-0]



$C_{41}H_{70}O_{12}$ 754.997
Macrolide antibiotic. Isol. from the sea hare *Dolabella auricularia*. Cytotoxic agent.
11-Ac: ***Dolabelide A***
[169970-80-3]
$C_{43}H_{72}O_{13}$ 797.034
Isol. from *Dolabella auricularia*. Cytotoxic agent. $[\alpha]_D^{25}$ -13.5 (c, 1.4 in $CHCl_3$).
Ojika, M. *et al., Tet. Lett.*, 1995, **36**, 7491-7494 (*isol, ir, pmr, cmr*)

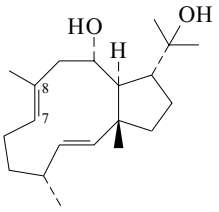
Dolabelide D D-1149

[185843-01-0]



$C_{39}H_{68}O_{11}$ 712.96
Macrolide antibiotic. Isol. from the sea hare *Dolabella auricularia*. Cytotoxic agent. Oil. $[\alpha]_D^{29}$ +2.6 (c, 0.3 in $CHCl_3$).
7,11-Di-Ac: ***Dolabelide C***
[185843-00-9]
$C_{43}H_{72}O_{13}$ 797.034
From *Dolabella auricularia*. Cytotoxic agent. Oil. $[\alpha]_D^{26}$ +10 (c, 0.2 in $CHCl_3$).
Suenaga, K. *et al., J. Nat. Prod.*, 1997, **60**, 155-157 (*isol, pmr, cmr*)
Park, P.K. *et al., J.A.C.S.*, 2006, **128**, 2796-2797 (*synth*)

2,7-Dolabelladiene-10,18-diol D-1150



$C_{20}H_{34}O_2$ 306.487

(2*E*,4*E*,10α)-*form* [60259-76-9]
Constit. of *Dolabella californica*.
Cryst.
Mp 152-153°. $[\alpha]_D^{20}$ -71.8 (c, 0.92 in $CHCl_3$).

10-Ac: ***10-Acetoxy-2,7-dolabelladien-18-ol***
[60259-77-0]
$C_{22}H_{36}O_3$ 348.525
Constit. of *Dolabella californica*. Cryst. Sol. MeOH, hexane; poorly sol. H_2O.
Mp 78°. $[\alpha]_D^{20}$ -101 (c, 1.32 in $CHCl_3$).

Di-Ac: ***10,18-Diacetoxy-2,7-dolabelladiene***
[62861-12-5]
$C_{24}H_{38}O_4$ 390.562
Constit. of *Dolabella californica*. Oil. $[\alpha]_D^{20}$ -80.5 (c, 2.6 in $CHCl_3$).

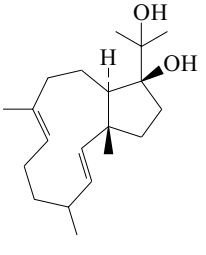
7β,8β-Epoxide: ***7,8-Epoxy-2-dolabellene-10,18-diol***
[86304-14-5]
$C_{20}H_{34}O_3$ 322.487
Isol. from digestive gland of sea hare *Aplysia dactylomela*. Cryst. (hexane).
Mp 171-172°. $[\alpha]_D$ +11 (c, 0.33 in $CHCl_3$).

7β,8β-Epoxide, di-Ac: [112727-25-0]
$C_{24}H_{38}O_5$ 406.561
Isol. from *Aplysia dactylomela* and *Aplysia depilans*. Oil. $[\alpha]_D^{25}$ +13 (c, 0.06 in $CHCl_3$).

18-Ac: 18-Acetoxy-2,7-dolabelladien-10-ol
$C_{22}H_{36}O_3$ 348.525
Constit. of *Dictyota dichotoma*. Oil. $[\alpha]_D^{25}$ -36.2 (c, 0.47 in $CHCl_3$).

Ireland, C. *et al., J.A.C.S.*, 1976, **98**, 4664-4665 (*cryst struct*)
Danise, B. *et al., Experientia*, 1977, **33**, 413-415 (*isol, epoxide di-Ac*)
Ireland, C. *et al., J.O.C.*, 1977, **42**, 3157-3162 (*isol, cmr, Ac derivs*)
Amico, V. *et al., Tetrahedron*, 1980, **36**, 1409 (*isol*)
González, A.G. *et al., Tet. Lett.*, 1983, **24**, 1075 (*isol, cryst struct, epoxide*)
González, A.G. *et al., J. Nat. Prod.*, 1987, **50**, 1158 (*isol*)
Piattelli, M. *et al., J. Nat. Prod.*, 1995, **58**, 697 (*pmr, cmr*)
Durán, R. *et al., Tetrahedron*, 1997, **53**, 8675-8688 (*18-Ac*)

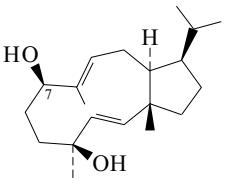
2,7-Dolabelladiene-12,18-diol D-1151



$C_{20}H_{34}O_2$ 306.487

(2*E*,4*E*,12β)-*form* [156351-70-1]
Constit. of *Dilophus mediterraneus*.
Oil. $[\alpha]_D$ -23.4 (c, 0.68 in $CHCl_3$).
Goez, C.E. *et al., Phytochem. Anal.*, 1994, **5**, 68 (*isol, pmr, cmr*)

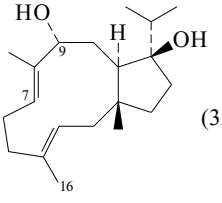
2,8-Dolabelladiene-4,7-diol D-1152



$C_{20}H_{34}O_2$ 306.487

(2*E*,4β,7β,8*E*)-*form*
7-Ac: 7-Acetoxy-2,8-dolabelladien-4-ol
$C_{22}H_{36}O_3$ 348.525
Constit. of a *Dictyota* sp. Cryst.
Mp 117-119°. $[\alpha]_D$ +99.8 (c, 0.54 in $CHCl_3$).
Gallardo, A. *et al., Rev. Latinoam. Quim.*, 1988, **19**, 86 (*isol, pmr, cmr*)

3,7-Dolabelladiene-9,12-diol D-1153



(3*E*,7*E*,9α)–*form*

$C_{20}H_{34}O_2$ 306.487

(3*E*,7*E*,9α)-*form*
Constit. of *Dictyota pardalis* f. *pseudohamata*.
Oil. $[\alpha]_D^{25}$ +36 (c, 0.43 in $CHCl_3$).

9-Ac:
$C_{22}H_{36}O_3$ 348.525
Constit. of *Dictyota pardalis* f. *pseudohamata*. Oil. $[\alpha]_D^{25}$ +20 (c, 0.5 in $CHCl_3$).

16-Acetoxy, 9-Ac: ***9,16-Diacetoxy-3,7-dolabelladien-12-ol***
$C_{24}H_{38}O_5$ 406.561
Constit. of *Dictyota pardalis* f. *pseudohamata*. Oil. $[\alpha]_D^{25}$ +13.9 (c, 0.82 in $CHCl_3$).

(3*E*,7*E*,9β)-*form*
Constit. of *Dictyota pardalis* f. *pseudohamata*.
Oil. $[\alpha]_D^{25}$ +6.4 (c, 0.4 in $CHCl_3$).

9-Ac: ***9-Acetoxy-3,7-dolabelladien-12-ol***
$C_{22}H_{36}O_3$ 348.525
Constit. of *Dictyota dichotoma* and *Dictyota pardalis* f. *pseudohamata*. Oil. $[\alpha]_D$ +2.3.

7ξ,8ξ-Epoxide, 9-Ac: ***9-Acetoxy-7,8-epoxy-3-dolabellen-12-ol***
$C_{22}H_{36}O_4$ 364.524
From *Dictyota dichotoma*. Oil. $[\alpha]_D$ -3.3 (c, 2.37 in $CHCl_3$).

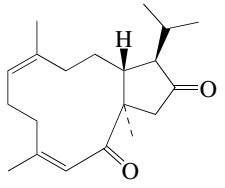
9-Ketone: From *Dictyota dichotoma* and *Dictyota pardalis* f. *pseudohamata*.
Oil. $[\alpha]_D$ +7.2 (c, 6.16 in $CHCl_3$).

7S,8S-Epoxide, 9-ketone: ***7,8-Epoxy-12-hydroxy-3-dolabellen-9-one***
$C_{20}H_{32}O_3$ 320.471
From *Dictyota dichotoma*. Oil. $[\alpha]_D$ -1.3 (c, 1.97 in $CHCl_3$). λ_{max} 231 (ϵ 5000) (MeOH) (Derep).

(3*E*,7*Z*,9β)-*form*
9-Ketone: ***12-Hydroxy-3,7-dolabelladien-9-one***
$C_{20}H_{32}O_2$ 304.472
Constit. of *Dictyota dichotoma* and *Dictyota pardalis* f. *pseudohamata*. Cryst. (petrol).
Mp 93-95°. $[\alpha]_D$ -53.3 (c, 1.96 in $CHCl_3$). λ_{max} 205 (ϵ 6700); 235 (ϵ 7200) (MeOH) (Derep).

3S,4S-Epoxide, 9-ketone: ***3,4-Epoxy-12-hydroxy-7-dolabellen-9-one***
$C_{20}H_{32}O_3$ 320.471
From *Dictyota dichotoma*. Cryst.
Mp 113-115°. $[\alpha]_D$ -32.7 (c, 0.3 in $CHCl_3$).
Rao, C.B. *et al., J.O.C.*, 1986, **51**, 2736
König, G.M. *et al., J. Nat. Prod.*, 1994, **57**, 1529 (*cryst struct*)
König, G.M. *et al., Tetrahedron*, 1994, **50**, 8011 (*isol, pmr, cmr, struct*)

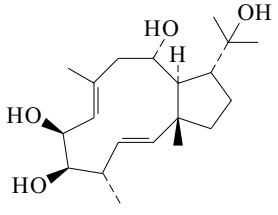
3,7-Dolabelladiene-2,13-dione D-1154



$C_{20}H_{30}O_2$ 302.456

(3*Z*,7*Z*)-*form*
Edudione
[163135-98-6]
Constit. of *Eunicea laciniata*.
Semisolid. $[\alpha]_D^{25}$ -92.4 (c, 9.0 in $CHCl_3$). λ_{max} 246 (ε 6421) (MeOH) (Berdy).
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1995, **58**, 226 (*isol, pmr, cmr*)

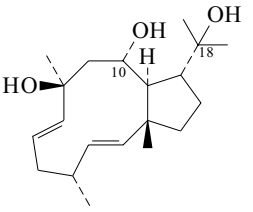
2,7-Dolabelladiene-5,6,10,18-tetrol D-1155



$C_{20}H_{34}O_4$ 338.486

(2*E*,4β*H*,5β,6β,7*E*,10α)-*form* [95186-44-0]
5,6-Di-Ac: [95660-68-7]
$C_{24}H_{38}O_6$ 422.561
Constit. of brown alga *Dilophus fasciola*. Phytotoxin. Ichthyotoxin. Cryst. ($CHCl_3$).
Mp 201-203°. $[\alpha]_D$ +11.1 (c, 2.1 in $CHCl_3$).
5,6,10-Tri-Ac: ***5,6,10-Triacetoxy-2,7-dolabelladien-18-ol***
[95186-42-8]
$C_{26}H_{40}O_7$ 464.598
Constit. of *Dilophus fasciola*. Phytotoxin. Ichthyotoxin. Oil.
$[\alpha]_D$ -25.4 (c, 1.6 in $CHCl_3$).
Tetra-Ac: ***5,6,10,18-Tetraacetoxy-2,7-dolabelladiene***
[95186-43-9]
$C_{28}H_{42}O_8$ 506.635
Constit. of *Dilophus fasciola*. Phytotoxin. Ichthyotoxin. Oil.
$[\alpha]_D$ +1.6 (c, 2.5 in $CHCl_3$).
5,6,18-Tri-Ac: 5,6,18-Triacetoxy-2,7-dolabelladien-10-ol
$C_{26}H_{40}O_7$ 464.598
Constit. of *Dictyota dichotoma*. Oil. $[\alpha]_D^{25}$ +10 (c, 0.11 in $CHCl_3$).
De Rosa, S. *et al., Tetrahedron*, 1984, **40**, 4991
Durán, R, *et al., Tetrahedron*, 1997, **53**, 8675-8688 (*5,6,18-Tri-Ac*)

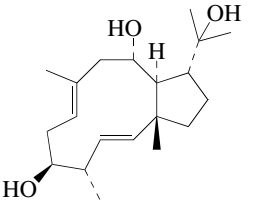
2,6-Dolabelladiene-8,10,18-triol D-1156



$C_{20}H_{34}O_3$ 322.487

(2*E*,4β*H*,6*E*,8β,10α)-*form* [62861-18-1]
Constit. of *Dolabella californica* and *Dictyota pfaffii*.
Cryst. (hexane).
Mp 168-169°. $[\alpha]_D^{26}$ -86 (c, 0.5 in $CHCl_3$).
10-Ac: [847556-55-2]
$C_{22}H_{36}O_4$ 364.524
Constit. of *Dictyota pfaffii*. Oil. $[\alpha]_D^{20}$ -60 (c, 0.5 in $CHCl_3$).
18-Ac: [62861-17-0]
$C_{22}H_{36}O_4$ 364.524
Constit. of *Dolabella californica*. Oil. $[\alpha]_D^{20}$ -45 (c, 1.9 in $CHCl_3$).
8,10-Di-Ac: [62861-16-9]
$C_{24}H_{38}O_5$ 406.561
Constit. of *Dolabella californica*. Oil. $[\alpha]_D^{20}$ -26.4 (c, 0.36 in $CHCl_3$).
8,18-Di-Ac: [62861-15-8]
Oil. $[\alpha]_D^{20}$ -33.3 (c, 0.4 in $CHCl_3$).
10,18-Di-Ac: [62861-14-7]
$C_{24}H_{38}O_5$ 406.561
Constit. of *Dolabella californica* and *Dictyota pfaffii*. Cryst.
Mp 136-137°. $[\alpha]_D^{20}$ -56.7 (c, 0.94 in $CHCl_3$).
Tri-Ac: [62861-13-6]
$C_{26}H_{40}O_6$ 448.598
Constit. of *Dolabella californica*. Oil. $[\alpha]_D^{20}$ -33.6 (c, 1.1 in $CHCl_3$).
Ireland, C. *et al., J.O.C.*, 1977, **42**, 3157-3162 (*isol*)
Barbosa, J.P. *et al., Biochem. Syst. Ecol.*, 2003, **31**, 1451-1453 (*di-Ac*)
Barbosa, J.P. *et al., Planta Med.*, 2004, **70**, 856-860 (*Dictyota pfaffii constits*)

2,7-Dolabelladiene-5,10,18-triol D-1157

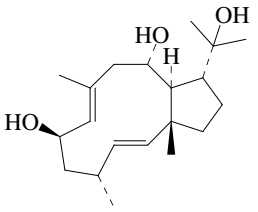


$C_{20}H_{34}O_3$ 322.487

(2*E*,4β*H*,5β,7*E*,10α)-*form*
5-Ac: ***5-Acetoxy-2,7-dolabelladiene-10,18-diol***
[193824-77-0]
$C_{22}H_{36}O_4$ 364.524
Constit. *Dictyota dichotoma*. Oil. $[\alpha]_D^{25}$ -6.7 (c, 0.15 in $CHCl_3$).
Durán, R. *et al., Tetrahedron*, 1997, **53**, 8675-8688 (*isol, pmr, cmr*)

2,7-Dolabelladiene-6,10,18-triol D-1158

[62861-22-7]



$C_{20}H_{34}O_3$ 322.487

(2*E*,7*Z*,10α)-*form*
Constit. of *Dolabella californica*.
Cryst. (Et_2O).
Mp 157-158°. $[\alpha]_D^{20}$ -29 (c, 0.9 in $CHCl_3$).

10-Ac: [62861-20-5]
$C_{22}H_{36}O_4$ 364.524
Constit. of *Dolabella californica*. Oil. $[\alpha]_D^{20}$ -0.4 (c, 0.7 in $CHCl_3$).

18-Ac: [62861-21-6]
$C_{22}H_{36}O_4$ 364.524
Constit. of *Dolabella californica*. Cryst.
Mp 153-154°. $[\alpha]_D^{20}$ +21.2 (c, 1.06 in $CHCl_3$).

6,10-Di-Ac: [62861-19-2]
$C_{24}H_{38}O_5$ 406.561
Constit. of *Dolabella californica*. Oil. $[\alpha]_D^{20}$ -4.7 (c, 0.17 in $CHCl_3$).

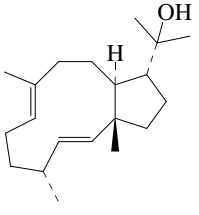
6-Ketone: 10,18-Dihydroxy-2,7-dolabelladien-6-one
$C_{20}H_{32}O_3$ 320.471

6-Ketone, di-Ac: [216770-29-5]
$C_{24}H_{36}O_5$ 404.545
Constit. of *Sigmosceptrella quadrilobata* and a *Dysidea* sp. Oil or amorph. solid. $[\alpha]_D^{25}$ -36 (c, 0.22 in $CHCl_3$) (-23.6). λ_{max} 243 (ϵ 7600) (hexane).

(2*E*,7*Z*,10α)-*form*

6-Ketone, di-Ac: [216770-33-1]
Isol. from a *Dysidea* sp.
Oil. $[\alpha]_D$ -19.4 (c, 0.36 in $CHCl_3$). λ_{max} 245 (ϵ 1700) ($CHCl_3$).
Ireland, C. *et al., J.O.C.*, 1977, **42**, 3157-3162 (*isol, pmr*)
Lu, Q. *et al., J. Nat. Prod.*, 1998, **61**, 1096-1100 (*ketone derivs*)
Costantino, V. *et al., Eur. J. Org. Chem.*, 1999, 227-230 (*ketone deriv*)

2,7-Dolabelladien-18-ol D-1159

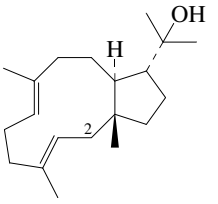


$C_{20}H_{34}O$ 290.488

(2*E*,4*R*,7*E*)-*form* [62861-23-8]
Isol. from *Dictyota dichotoma*, *Dictyota divaricata* and *Dolabella californica*.
Oil. $[\alpha]_D$ -76 (c, 1 in $CHCl_3$).

Ac: [193975-35-8]
$C_{22}H_{36}O_2$ 332.525
Constit. of *Dictyota dichotoma*. Oil. $[\alpha]_D^{25}$ -53.2 (c, 0.41 in $CHCl_3$).
Ireland, C. *et al., J.O.C.*, 1977, **42**, 3157-3162 (*isol, Dolabella*)
Amico, V. *et al., Tetrahedron*, 1980, **36**, 1409-1414 (*Dictyota dichotoma constit*)
König, G.M. *et al., Phytochemistry*, 1991, **30**, 3679-3682 (*Dictyota divaricata, isol, pmr, cmr*)
Durán, R. *et al., Tetrahedron*, 1997, **53**, 8675-8688 (*Ac*)

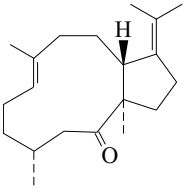
3,7-Dolabelladien-18-ol D-1160



$C_{20}H_{34}O$ 290.488

(3*E*,7*E*)-*form* [79405-81-5]
Constit. of *Dictyota dichotoma*.
Oil. $[\alpha]_D$ +27.5 (c, 1 in $CHCl_3$).
Amico, V. *et al., Phytochemistry*, 1981, **20**, 848-849

7,12(18)-Dolabelladien-2-one D-1161



$C_{20}H_{32}O$ 288.472

7E-form
Edunone
[163135-96-4]
Constit. of *Eunicea laciniata*.
Oil. $[\alpha]_D^{25}$ +17 (c, 8.45 in $CHCl_3$). λ_{max} 254 (ϵ 3300) (MeOH) (Berdy).
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1995, **58**, 226 (*isol, pmr, cmr*)

Dolabellanin D-1162

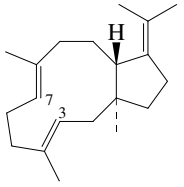
Dolabellanin A [125199-94-2]
Isol. from the albumen gland of the sea hare *Dolabella auricularia*. Shows antimicrobial and antifungal activity. Glycoprotein consisting of 4 subunits.

Dolabellanin B_2
Isol. from the body wall of *Dolabella auricularia*. Shows antimicrobial activity. Peptide containing 33 amino acid units.

Dolabellanin C [122462-72-0]
Isol. from body fluid of *Dolabella auricularia*. Shows antimicrobial and antifungal activity. Glycoprotein consisting of 3 subunits.

Dolabellanin P [123758-92-9]
Isol. from the purple fluid of the sea hare *Dolabella auricularia*. Cytolytic. Protein, a single polypeptide chain.
Yamazaki, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2179-2182 (*Dolabellanin P*)
Kisugi, J. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2773-2776; 1992, **40**, 1537-1539 (*Dolabellanin A*)
Kisugi, J. *et al., Dev. Comp. Immunol.*, 1989, **13**, 3-8 (*Dolabellanin C*)
Yamazaki, M. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1993, **105**, 141-146 (*rev*)
Iijima, R. *et al., Dev. Comp. Immunol.*, 2003, **27**, 305-311 (*Dolabellanin B_2*)

3,7,12(18)-Dolabellatriene D-1163



(1α,3*E*,7*E*,11β*H*)-*form*

$C_{20}H_{32}$ 272.473

(1α,3*E*,7*E*,11β*H*)-*form*

(-)-β-Araneosene. *Dolabellane 4*

Isol. from *Eunicea laciniata* and *Sordaria araneosa*.

Oil. $[\alpha]_D$ -149 (c, 0.8 in $CHCl_3$).

*3S,4*R-*Epoxide:* ***3,4-Epoxy-7,12(18)-dolabelladiene***

[404913-76-4]

$C_{20}H_{32}O$ 288.472

Constit. of a *Clavularia* sp. Cryst. $[\alpha]_D^{22}$ -214 (c, 1.28 in $CHCl_3$).

3α,4α:7ξ,8ξ-Diepoxide: ***3,4:7,8-Diepoxy-12(18)-dolabellene***

[129932-82-7]

$C_{20}H_{32}O_2$ 304.472

Metab. of *Dictyopteris delicatula*. Oil. $[\alpha]_D$ +86 (c, 0.4 in $CHCl_3$).

(1β,3*E*,7*E*,11α*H*)-*form*

(+)-β-Araneosene

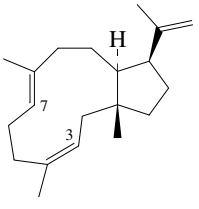
Prod. by *Phomopsis amygdali*.

$[\alpha]_D$ +106 (c, 0.3 in $CHCl_3$).

[133523-24-7, 166240-51-3]

Wright, A.D. *et al., J. Nat. Prod.*, 1990, **53**, 845-861 (*diepoxide*)
Shin, J. *et al., J.O.C.*, 1991, **56**, 3392-3398 (*isol, pmr, cmr*)
Jenny, L. *et al., Helv. Chim. Acta*, 1995, **78**, 715-729 (*(-)-β-Araneosene*)
Iguchi, K. *et al., Bull. Chem. Soc. Jpn.*, 2002, **75**, 131-136 (*3,4-epoxide, cryst struct*)
Sassa, T. *et al., Biosci., Biotechnol., Biochem.*, 2004, **68**, 1608-1610 (*(+)-β-Araneosene*)
Kingsbury, J.S. *et al., J.A.C.S.*, 2005, **127**, 13813-13815 (*synth*)

3,7,18-Dolabellatriene D-1164



(3*Z*,7*E*)-*form*

$C_{20}H_{32}$ 272.473

(3*Z*,7*E*)-*form* [341505-78-0]

Constit. of *Cyperus alopecuroides* essential oil.

3β,4β-Epoxide: ***3,4-Epoxy-7,18-dolabelladiene***

$C_{20}H_{32}O$ 288.472

Constit. of *Dictyota dichotoma*. Cryst. (EtOH).

Mp 63-64°. $[\alpha]_D$ +76.9 (c, 1.0 in $CHCl_3$). Stereochem. revised in 1995.

(3*E*)-*form*

7β,8α-Epoxide: ***7,8-Epoxy-3,18-dolabelladiene***

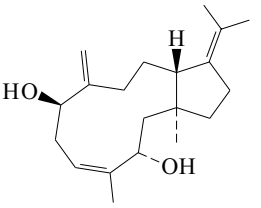
[193975-34-7]

$C_{20}H_{32}O$ 288.472

Constit. of *Dictyota dichotoma*. Oil. $[\alpha]_D^{25}$ +27.4 (c, 0.46 in $CHCl_3$).

Amico, V. *et al., Tetrahedron*, 1980, **36**, 1409 (*3,4-epoxide, isol*)
Piattelli, M. *et al., J. Nat. Prod.*, 1995, **58**, 697 (*3,4-epoxide, pmr, cmr, struct*)
Durán, R. *et al., Tetrahedron*, 1997, **53**, 8675 (*7,8-epoxide*)
Sonwa, M.M. *et al., Phytochemistry*, 2001, **56**, 321-326 (*isol, pmr, cmr*)

4,8(17),12(18)-Dolabellatriene-3,7-diol D-1165



$C_{20}H_{32}O_2$ 304.472

(1α,3α,4*Z*,7β,11β)-*form* [129932-81-6]

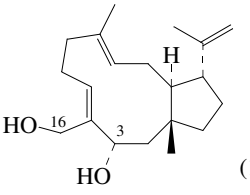
Constit. of brown alga *Dictyota pardarlis* f. *pseudohamata* A7749.

Cryst. (MeOH).

Mp 206-207°. $[\alpha]_D^{25}$ +66 (c, 0.005 in $CHCl_3$).

Wright, A.D. *et al., Tetrahedron*, 1990, **46**, 3851 (*isol*)
Wright, A.D. *et al., Helv. Chim. Acta*, 1991, **74**, 1801 (*cryst struct*)

4,8,18-Dolabellatriene-3,16-diol D-1166



(1*R*,3*S*,4*E*,8*E*,11*S*,12*R*)-*form*

$C_{20}H_{32}O_2$ 304.472

(1*R*,3*S*,4*E*,8*E*,11*S*,12*R*)-*form* [90985-73-2]

Metab. of brown alga *Dictyota* sp. Molluscicide. Cryst. (hexane). Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O.

Mp 104-105°. $[\alpha]_D$ +46.4 (c, 1.8 in EtOH).

3-Ac: ***3-Acetoxy-4,8,18-dolabellatrien-16-ol***

[90985-74-3]

$C_{22}H_{34}O_3$ 346.509

Metab. of *Dictyota* sp. Molluscicide. Shows cytotoxic activity. Cryst. (hexane). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O.

Mp 142-143°. $[\alpha]_D$ +19.8 (c, 1.0 in EtOH).

16-Ac: ***16-Acetoxy-4,8,18-dolabellatrien-3-ol***

$C_{22}H_{34}O_3$ 346.509

Isol. from *Dictyota* sp. Oil. $[\alpha]_D^{25}$ +43.9 (c, 1 in EtOH).

16-Aldehyde, 3-Ac: ***3-Acetoxy-4,8,18-dolabellatrien-16-al***

[93379-57-8]

$C_{22}H_{32}O_3$ 344.493

Metab. of *Dictyota* sp. Molluscicide. Viscous oil. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D$ +9.7 (c, 1.2 in EtOH). Aldehyde has 4*Z*-config. owing to change of (*R,S*)-priorities. λ_{max} 230 (ϵ 8100) (EtOH) (Berdy).

(1*R*,3*S*,4*Z*,8*E*,11*S*,12*R*)-*form*

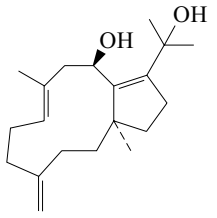
16-Aldehyde, 3-Ac: Isol. from a *Dictyota* sp.

Needles (EtOH).

Mp 72-73°. $[\alpha]_D^{25}$ -13.9 (c, 1 in EtOH). Aldehyde has (4*E*)-config.

Tringali, C. *et al., J. Nat. Prod.*, 1984, **47**, 615
Tringali, C. *et al., Tetrahedron*, 1984, **40**, 799

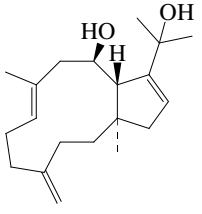
4(16),7,11-Dolabellatriene-10,18-diol D-1167



$C_{20}H_{32}O_2$ 304.472

(7*E*,10β)-*form*
Clavudiol A
Constit. of *Clavularia viridis*.
Cryst.
Mp 147-149°. $[\alpha]_D$ -45.9 (c, 0.3 in $CHCl_3$). λ_{max} 203 (ϵ 23000); 208 (ϵ 20000) (MeOH) (Derep).
Su, J. *et al., J.O.C.*, 1991, **56**, 2337 (*isol, pmr, cmr, abs config, cryst struct*)

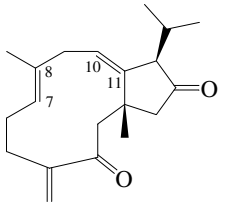
4(16),7,12-Dolabellatriene-10,18-diol D-1168



$C_{20}H_{32}O_2$ 304.472

(7*E*,10β)-*form*
Clavudiol B
Constit. of *Clavularia viridis*.
Oil. $[\alpha]_D^{20}$ -84.4 (c, 0.09 in MeOH).
Su, J. *et al., Chin. J. Chem.*, 1992, **10**, 155-160 (*isol, pmr, cmr*)

4(16),7,10-Dolabellatriene-3,13-dione D-1169

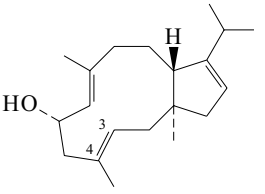


$C_{20}H_{28}O_2$ 300.44

(7*E*,10*Z*)-*form* [359415-65-9]
Constit. of *Clavularia inflata*.
Oil. $[\alpha]_D^{25}$ -92.3 (c, 0.1 in $CHCl_3$). λ_{max} 226 (log ϵ 4.24) (MeOH).
7α,8α-Epoxide: ***7,8-Epoxy-4(16),10-dolabelladiene-3,13-dione***
[359415-66-0]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Clavularia inflata*. Oil. $[\alpha]_D^{25}$ -82.3 (c, 0.09 in $CHCl_3$). λ_{max} 233 (log ϵ 4.22) (MeOH).
10β,11β-Epoxide: ***10,11-Epoxy-4(16),7-dolabelladiene-3,13-dione***
[359415-67-1]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Clavularia inflata*. Oil. $[\alpha]_D^{25}$ +56.2 (c, 0.06 in $CHCl_3$). λ_{max} 230 (log ϵ 4.28) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 2001, **64**, 1028-1031 (*isol, pmr, cmr*)

3,7,12-Dolabellatrien-6-ol D-1170

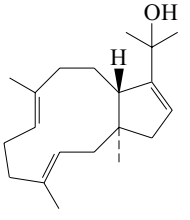
[135650-22-5]



$C_{20}H_{32}O$ 288.472
Metab. of *Dictyota divaricata*. Cryst. ($CHCl_3$/petrol).
Mp 125-127°. $[\alpha]_D$ -61.5 (c, 4 in $CHCl_3$).

3α,4α-Epoxide: ***3,4-Epoxy-7,12-dolabelladien-6-ol***
[135650-23-6]
$C_{20}H_{32}O_2$ 304.472
Metab. of *Dictyota divaricata*. Cryst. ($CHCl_3$/MeOH).
Mp 115-117°.
Rao, C.B. *et al., Phytochemistry*, 1991, **30**, 1971 (*isol, pmr, cmr*)

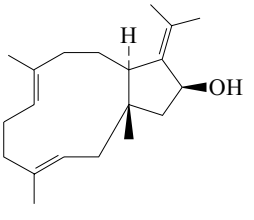
3,7,12-Dolabellatrien-18-ol D-1171



$C_{20}H_{32}O$ 288.472
Struct. revised in 1991.

(1α,3*E*,7*E*,11α)-*form*
Palominol
[126222-05-7]
Metab. of *Eunicea calyculata* and *Eunicea laciniata*.
Cryst.
Mp 52-53°. $[\alpha]_D^{27}$ -33.3 (c, 1 in $CHCl_3$).
Cáceres, J. *et al., Tetrahedron*, 1990, **46**, 341 (*isol*)
Shin, J. *et al., J.O.C.*, 1991, **56**, 3392 (*pmr, cmr, struct*)
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 1843 (*isol, pmr, cmr*)
Corey, E.J. *et al., Tet. Lett.*, 1998, **39**, 741-744 (*synth*)
Miyaoka, H. *et al., Tetrahedron*, 2003, **59**, 61-75 (*synth*)

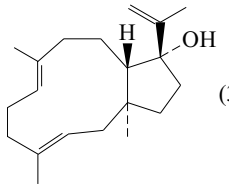
3,7,12(18)-Dolabellatrien-13-ol D-1172



$C_{20}H_{32}O$ 288.472

(3*E*,7*E*,13β)-*form*
Isopalominol
[153081-59-5]
Constit. of *Eunicea laciniata*.
Cryst.
Mp 117.3-119°.
[153153-28-7]
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 1843 (*isol, pmr, cmr*)

3,7,18-Dolabellatrien-12-ol D-1173



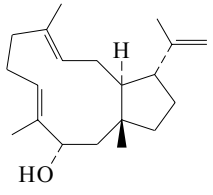
(3*E*,7*E*,12α)–*form*

$C_{20}H_{32}O$ 288.472

(3*E*,7*E*,12α)-*form*
Edunol†
[163135-89-5]
Constit. of *Eunicea laciniata*.
Oil. $[\alpha]_D^{25}$ -18.5 (c, 7.9 in $CHCl_3$).

(3*E*,7*E*,12β)-*form*
Isoedunol
[163252-97-9]
Constit. of *Eunicea laciniata*.
Oil. $[\alpha]_D^{25}$ -60.2 (c, 6.0 in $CHCl_3$).
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1995, **58**, 226 (*isol, pmr, cmr*)
Kingsbury, J.S. *et al., J.A.C.S.*, 2005, **127**, 13813-13815 (*synth*)

4,8,18-Dolabellatrien-3-ol D-1174

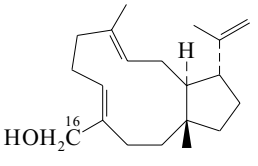


$C_{20}H_{32}O$ 288.472

(3α,4*E*,8*E*)-*form*
Constit. of a *Dictyota* sp.
Yellow oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +1.5 (c, 1 in EtOH).

Ac:
$C_{22}H_{34}O_2$ 330.509
Constit. of *Dictyota* sp. Cryst.
Mp 115-117°. $[\alpha]_D^{25}$ +52.2 (c, 1 in EtOH).
Tringali, C. *et al., Phytochemistry*, 1984, **23**, 1681 (*isol*)
Tringali, C. *et al., J. Nat. Prod.*, 1985, **48**, 484 (*deriv*)

4,8,18-Dolabellatrien-16-ol D-1175



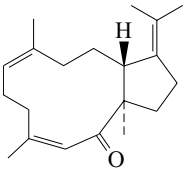
$C_{20}H_{32}O$ 288.472

(4*Z*,8*E*)-*form*
Constit. of a *Dictyota* sp.
Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +85 (c, 1 in EtOH).

Ac:
$C_{22}H_{34}O_2$ 330.509
From *Dictyota* sp. Oil. $[\alpha]_D^{25}$ +52.2 (c, 1 in EtOH).

16-Aldehyde: ***4,8,18-Dolabellatrien-16-al***
$C_{20}H_{30}O$ 286.456
From *Dictyota* sp. Yellow oil. $[\alpha]_D$ -72 (c, 1 in EtOH).
Tringali, C. *et al., Phytochemistry*, 1984, **23**, 1681 (*isol*)
Tringali, C. *et al., J. Nat. Prod.*, 1985, **48**, 484 (*deriv*)

3,7,12(18)-Dolabellatrien-2-one D-1176

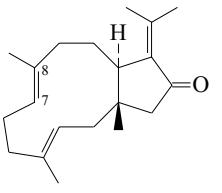


$C_{20}H_{30}O$ 286.456

(3*Z*,7*Z*)-*form*
Eduenone
[163135-97-5]
Constit. of *Eunicea laciniata*.
Oil. $[\alpha]_D^{25}$ -54 (c, 4.0 in $CHCl_3$). λ_{max} 244 (ϵ 4391) (MeOH) (Berdy).
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1995, **58**, 226 (*isol, pmr, cmr*)

3,7,12(18)-Dolabellatrien-13-one D-1177

[82798-98-9]

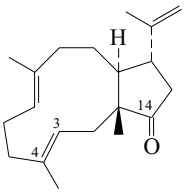


$C_{20}H_{30}O$ 286.456

(3*E*,7*E*)-*form*
Constit. of *Eunicea calyculata*.
Oil. $[\alpha]_D^{20}$ +31 (c, 0.88 in $CHCl_3$). Abs. config. revised in 1996.
λ_{max} 256 (ϵ 6900) (MeOH) (Berdy).

*7α,8α-Epoxide: 7,8-Epoxy-3*E*,12(18)-dolabelladien-13-one*
[82798-97-8]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Eunicea calyculata* and *Eunicea tourneforti*. Cryst. (Et_2O).
Mp 147-149° Mp 88-89°. $[\alpha]_D^{20}$ +61 (c, 1.29 in $CHCl_3$). $[\alpha]_D^{24}$ +100 (c, 0.2 in $CHCl_3$). λ_{max} 250 (ϵ 10100) (MeOH) (Berdy).
Look, S.A. *et al., J.O.C.*, 1982, **47**, 4129 (*struct, abs config*)
Govindan, M. *et al., J. Nat. Prod.*, 1995, **58**, 1174 (*isol, pmr, cmr*)
Corey, E.J. *et al., J.A.C.S.*, 1996, **118**, 1229 (*synth, abs config*)
Corey, E.J. *et al., Tet. Lett.*, 1998, **39**, 741-744 (*synth*)
Miyaoka, H. *et al., Tetrahedron*, 2003, **59**, 61-75 (*synth*)

3,7,18-Dolabellatrien-14-one D-1178



$C_{20}H_{30}O$ 286.456

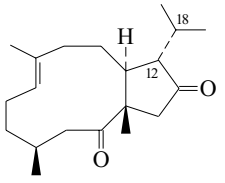
(3*E*,7*E*)-*form*
Constit. of *Dictyota dichotoma*.
Cryst. (EtOH).
Mp 53-54°. $[\alpha]_D$ -54.5 (c, 1.0 in $CHCl_3$).

3β,4β-Epoxide: ***3,4-Epoxy-7,18-dolabelladien-14-one***
$C_{20}H_{30}O_2$ 302.456
Isol. from *Dictyota dichotoma*. Cryst. (EtOH). Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 132-133°. $[\alpha]_D$ +109 (c, 1.0 in $CHCl_3$). Struct. revised in 1995.

14α-Alcohol, 3β,4β-epoxide: ***3,4-Epoxy-7,18-dolabelladien-14β-ol***
$C_{20}H_{32}O_2$ 304.472
Isol. from *Dictyota dichotoma*. Oil. $[\alpha]_D$ +48 (c, 0.5 in EtOH). Struct. revised in 1995.
Amico, V. *et al., Tetrahedron*, 1980, **36**, 1409
Piattelli, M. *et al., J. Nat. Prod.*, 1995, **58**, 697 (*pmr, cmr, struct*)

7-Dolabellene-2,13-dione D-1179

Dolabellane 6
[133523-26-9]

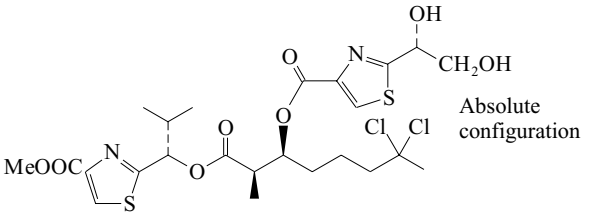


$C_{20}H_{32}O_2$ 304.472
Constit. of *Eunicea laciniata*. Oil. $[\alpha]_D$ -44 (c, 0.6 in $CHCl_3$).

12,18-Didehydro: 7,12(18)-Dolabelladiene-2,13-dione. ***Dolabellane 5***
[133523-25-8]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Eunicea laciniata*. Oil. $[\alpha]_D$ -27 (c, 0.7 in $CHCl_3$).
Shin, J. *et al., J.O.C.*, 1991, **56**, 3392-3398 (*isol, pmr, cmr*)

Dolabellin D-1180

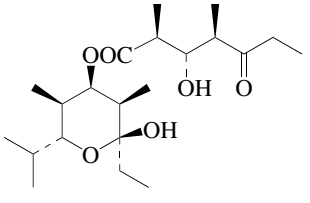
[165467-49-2]



$C_{24}H_{32}Cl_2N_2O_8S_2$ 611.563
Isol. from *Dolabella auricularia* and *Lyngbya majuscula*. Cytotoxic. Oil. Sol. MeOH, EtOAc; poorly sol. hexane. $[\alpha]_D^{28}$ -7.3 (c, 0.34 in $CHCl_3$). λ_{max} 204 (ϵ 29400); 236 (ϵ 14600) (MeOH).
Sone, H. *et al., J.O.C.*, 1995, **60**, 4774-4781 (*isol, synth uv, ir, pmr, cmr*)

Dolabriferol D-1181

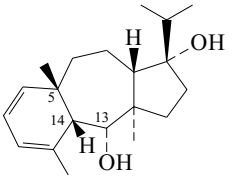
[181770-41-2]



$C_{21}H_{38}O_6$ 386.528
Isol. from the mollusc *Dolabrifera dolabrifera*.
Mp 112-114°. $[\alpha]_D^{25}$ -29.4 (c, 0.7 in $CHCl_3$).
Ciavatta, M.L. *et al., Tetrahedron*, 1996, **52**, 12831-12838 (*isol, ir, pmr, cmr, ms, cryst struct*)

1,3-Dolastadiene-9,13-diol D-1182

[135650-25-8]



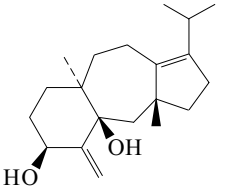
$C_{20}H_{32}O_2$ 304.472
Metab. of *Dictyota divaricata*. Oil. $[\alpha]_D$ +110.7 (c, 0.42 in $CHCl_3$).

13-Ac: 13-Acetoxy-1,3-dolastadien-9-ol
[135650-26-9]
$C_{22}H_{34}O_3$ 346.509
Metab. of *Dictyota divaricata*. Oil. $[\alpha]_D$ +41.4 (c, 2.13 in $CHCl_3$).

5,14-Diepimer: [135684-49-0]
$C_{20}H_{32}O_2$ 304.472
Metab. of *Dictyota divaricata*. Cryst.
Mp 107-108°.

5,14-Diepimer, 13-ketone: ***9-Hydroxy-1,3-dolastadien-13-one***
[135650-27-0]
$C_{20}H_{30}O_2$ 302.456
Metab. of *Dictyota divaricata*. Oil. $[\alpha]_D$ -344.9 (c, 0.88 in $CHCl_3$).
Rao, C.B. *et al., Phytochemistry*, 1991, **30**, 1971 (*isol, pmr, cmr*)

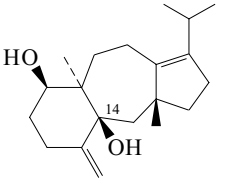
1(15),8-Dolastadiene-2,14-diol D-1183



$C_{20}H_{32}O_2$ 304.472

(2β,14β)-*form*
Isoamijiol
[75744-71-7]
Constit. of *Dictyota linearis.*
Cryst.
Mp 128-128.5°. $[\alpha]_D$ -45 ($CHCl_3$).
Ochi, M. *et al., Chem. Lett.*, 1980, 1229
Haruda, N. *et al., Chem. Comm.*, 1984, 1220 (*abs config*)
Begley, M.J. *et al., J.C.S. Perkin 1*, 1988, 1085 (*synth*)
Mehta, G. *et al., J.A.C.S.*, 1991, **113**, 5765 (*synth*)

1(15),8-Dolastadiene-4,14-diol D-1184

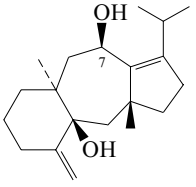


$C_{20}H_{32}O_2$ 304.472

(4β,14β)-*form*
Amijiol
[75744-70-6]
Constit. of *Dictyota linearis* and *Dictyota cervicornis.*
Cryst.
Mp 180-181°. $[\alpha]_D$ -126 ($CHCl_3$).
Ochi, M. *et al., Chem. Lett.*, 1980, 1229 (*isol*)
Teixeira, V.L. *et al., J. Nat. Prod.*, 1986, **49**, 570 (*isol*)

Piers, E. *et al., Chem. Comm.*, 1988, 125 (*synth*)
Majetich, G. *et al., Tet. Lett.*, 1990, **31**, 2239 (*synth*)

1(15),8-Dolastadiene-7,14-diol D-1185

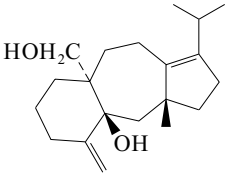


$C_{20}H_{32}O_2$ 304.472

(7β,14β)-*form*
7-Ac: ***7-Acetoxy-1(15),8-dolastadien-14-ol***
$C_{22}H_{34}O_3$ 346.509
Constit. of *Dictyota divaricata*. Oil. $[\alpha]_D^{25}$ -9.4 (c, 0.9 in $CHCl_3$).
Sun, H.H. *et al., Tetrahedron*, 1981, **37**, 1237

1(15),8-Dolastadiene-14,16-diol D-1186

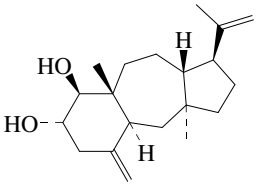
Dictindiol
[133882-84-5]



$C_{20}H_{32}O_2$ 304.472
Metab. of *Dictyota indica*. Gum. $[\alpha]_D$ -28.67 (c, 0.0035 in $CHCl_3$).
Ahmad, V.U. *et al., Phytochemistry*, 1991, **30**, 1015 (*isol, pmr, cmr*)

1(15),17-Dolastadiene-3,4-diol D-1187

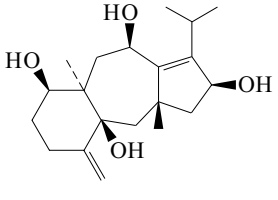
1(15),17-Clavularadiene-3,4-diol



$C_{20}H_{32}O_2$ 304.472

(3α,4β)-*form* [69301-38-8]
Constit.of *Clavularia inflata*.
Cryst.
Mp 78-80°. $[\alpha]_D$ +51 (c, 0.6 in $CHCl_3$).
Braekman, J.C. *et al., Tetrahedron*, 1978, **34**, 1551-1556 (*Clavularia inflata*)
Williams, D.R. *et al., J.A.C.S.*, 1993, **115**, 11654-11655 (*synth, abs config*)

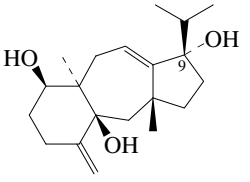
1(15),8-Dolastadiene-4,7,10,14-tetrol D-1188



$C_{20}H_{32}O_4$ 336.47

(4β,7β,10β,14β)-*form*
7-Ac: ***Deacetylamijidictyol***
[140475-71-4]
$C_{22}H_{34}O_5$ 378.508
Constit. of *Dictyota divaricata*. Amorph. powder. $[\alpha]_D^{27}$ -90 (c, 0.05 in MeOH).
7,10-Di-Ac: ***Amijidictyol***
[75744-69-3]
$C_{24}H_{36}O_6$ 420.545
Constit. of *Dictyota linearis.* Cryst.
Mp 187-189°. $[\alpha]_D$ -40 ($CHCl_3$).
10-Ketone: 4,7,14-Trihydroxy-1(15),8-dolastadien-10-one. ***Dichotenone A***
[639476-53-2]
$C_{20}H_{30}O_4$ 334.455
Constit. of *Dictyota dichotoma*. Cryst.
Mp 267-270°. $[\alpha]_D^{24}$ -66.6 (c, 0.0127 in Py). λ_{max} 242 (log ε 6.7) (MeOH).
Ochi, M. *et al., Chem. Lett.*, 1980, 1233
Li, L.N. *et al., Chin. Chem. Lett.*, 1991, **2**, 621 (*isol, pmr, cmr, deriv*)
Ali, M.S. *et al., Nat. Prod. Res.*, 2003, **17**, 301-306 (*Dichotenone A*)

1(15),7-Dolastadiene-4,9,14-triol D-1189



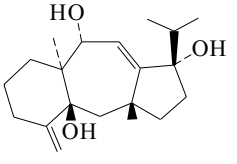
(4β,9α,14β)-*form*

$C_{20}H_{32}O_3$ 320.471

(4β,9α,14β)-*form* [80243-68-1]
Constit. of *Dictyota* spp.
Cryst.
Mp 179-180° Mp 220°. $[\alpha]_D$ -161 ($CHCl_3$). $[\alpha]_D$ -189 (c, 0.1 in MeOH).
4-Ac:
$C_{22}H_{34}O_4$ 362.508
Constit. of *Dictyota* spp. Cryst.
Mp 151°. $[\alpha]_D$ -40 (c, 1 in MeOH). λ_{max} 208 (ε 6700) (MeOH) (Berdy).

(4β,9β,14β)-*form*
Constit. of *Dictyota* sp.
Cryst.
Mp 160-161°. $[\alpha]_D$ -59 (c, 0.1 in $CHCl_3$).
Crews, P. *et al., J.O.C.*, 1982, **47**, 811 (*isol*)
Gonzalez, A.G. *et al., Tetrahedron*, 1983, **39**, 3355 (*isol, absol config, cryst struct*)
Teixeira, V.L. *et al., J. Nat. Prod.*, 1986, **49**, 570 (*isol*)

1(15),7-Dolastadiene-6,9,14-triol D-1190



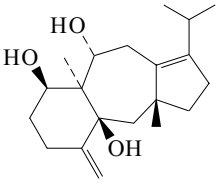
$C_{20}H_{32}O_3$ 320.471

(6α,9α,14β)-*form*
Dolatriol
[60259-78-1]
Constit. of *Dolabella auricularia*, *Dolabella ecaudata* and *Stylocheilus longicauda*. Cytotoxic against P388 cells. Cryst. (Me_2CO/heptane).

Mp 235-236°.

6-Ac: [60259-79-2]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Dolabella auricularia*. Cytotoxic agent. Cryst. (Me_2CO/heptane).
Mp 210-212°.
Pettit, G.R. *et al., J.A.C.S.*, 1976, **98**, 4677-4678 (*isol, struct*)
Pettit, G.R. *et al., J. Nat. Prod.*, 1980, **43**, 752

1(15),8-Dolastadiene-4,6,14-triol D-1191

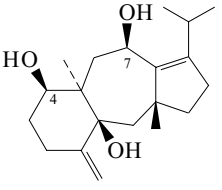


$C_{20}H_{32}O_3$ 320.471

(4β,6α,14β)-*form*
4,6-Di-Ac: [80243-70-5]
$C_{24}H_{36}O_5$ 404.545
Constit. of *Dictyota* spp. Yellow oil. $[\alpha]_D^{25}$ -144.6 (c, 1 in MeOH).
Crews, P. *et al., J.O.C.*, 1982, **47**, 811

1(15),8-Dolastadiene-4,7,14-triol D-1192

[80243-69-2]



$C_{20}H_{32}O_3$ 320.471

(4β,7β,14β)-*form*
Constit. of *Dictyota* spp. Histamine antagonist. Cryst. (C_6H_6/hexane). Poorly sol. hexane.
Mp 172° (163-166°). $[\alpha]_D$ -112 ($CHCl_3$). $[\alpha]_D$ -140 (c 0.005 in $CHCl_3$).

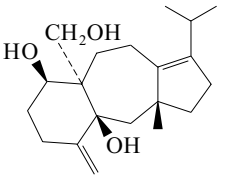
4-Ac: ***4-Acetoxy-1(15),8-dolastadiene-7,14-diol***
$C_{22}H_{34}O_4$ 362.508
Constit. of *Dictyota* spp. Cryst.
Mp 150°. $[\alpha]_D$ -122 (c, 0.1 in $CHCl_3$).

7-Ac: ***7-Acetoxy-1(15),8-dolastadiene-4,14-diol***
$C_{22}H_{34}O_4$ 362.508
Isol. from *Dictyota divaricata*. Oil. $[\alpha]_D^{25}$ -35.3 (c, 1.1 in $CHCl_3$).

4,7-Di-Ac: ***4,7-Diacetoxy-1(15),8-dolastadien-14-ol***
$C_{24}H_{36}O_5$ 404.545
Isol, from *Dictyota divaricata* and *Dictyota cervicornis*. Oil. $[\alpha]_D^{25}$ -44 (c, 1.1 in $CHCl_3$).
Crews, P. *et al., J.O.C.*, 1982, **47**, 811 (*isol*)
Gonzalez, A.G. *et al., Tetrahedron*, 1983, **39**, 3355 (*isol, abs config*)
Teixeira, V.L. *et al., J. Nat. Prod.*, 1986, **49**, 570 (*isol*)

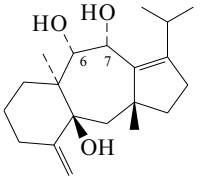
1(15),8-Dolastadiene-4,14,16-triol D-1193

Dictintriol
[133882-86-7]



$C_{20}H_{32}O_3$ 320.471
Metab. of *Dictyota indica*. Gum. $[\alpha]_D$ -63.4 (c, 1.8 in $CHCl_3$).
Ahmad, V.U. *et al., Phytochemistry*, 1991, **30**, 1015 (*isol, pmr, cmr*)

1(15),8-Dolastadiene-6,7,14-triol D-1194

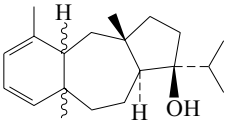


$C_{20}H_{32}O_3$ 320.471

(6*S*,7*R*,14*S*)-*form*
6,7-Di-Ac: 6,7-Diacetoxy-1(15),8-dolastadien-14-ol
[121531-32-6]
$C_{24}H_{36}O_5$ 404.545
Constit. of *Dictyota furcellata*. Cryst. (MeCN).
Mp 125.5-127°.
Dunlop, R.W. *et al., Aust. J. Chem.*, 1989, **42**, 315 (*isol, pmr, cmr, cryst struct*)

1,3-Dolastadien-9-ol D-1195

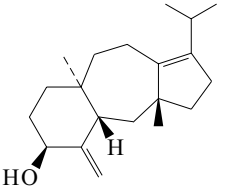
[135684-50-3]



$C_{20}H_{32}O$ 288.472
Metab. of *Dictyota divaricata*. Oil. $[\alpha]_D$ -34.4 (c, 1.25 in $CHCl_3$).

Stereoisomer:
$C_{20}H_{32}O$ 288.472
Metab. of *Dictyota divaricata*. Oil. $[\alpha]_D$ -80.1 (c, 2.47 in $CHCl_3$).
[135650-29-2]
Rao, C.B. *et al., Phytochemistry*, 1991, **30**, 1921 (*isol, pmr, cmr*)

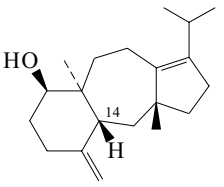
1(15),8-Dolastadien-2-ol D-1196



$C_{20}H_{32}O$ 288.472

(2β,14β)-*form*
14-Deoxyisoamijiol
[87745-21-9]
Constit. of *Dictyota linearis*.
Cryst. (hexane).
Mp 89-90°. $[\alpha]_D^{18}$ -2.6 (c, 0.09 in EtOH).
Ochi, M. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 661
Majetich, G. *et al., J.O.C.*, 1991, **56**, 3973 (*synth*)

1(15),8-Dolastadien-4-ol D-1197

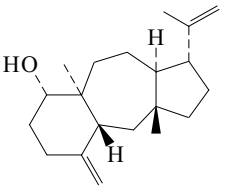


$C_{20}H_{32}O$ 288.472

(1β,14β)-*form*
14-Deoxyamijiol
Constit. of *Dictyota linearis*.
Cryst.
Mp 103-104°. $[\alpha]_D$ -79 ($CHCl_3$).
Ochi, M. *et al., Chem. Lett.*, 1980, 1229 (*isol*)
Majetich, G. *et al., Tet. Lett.*, 1990, **31**, 2239 (*synth*)

1(15),17-Dolastadien-4-ol D-1198

1(15),17-Clavularadien-4-ol

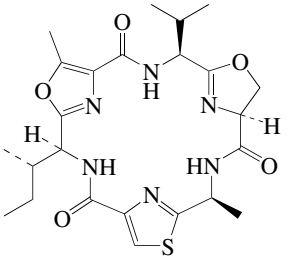


$C_{20}H_{32}O$ 288.472

(4α,9β*H*,14β)-*form* [69301-50-4]
Constit. of *Clavularia inflata*.
$[\alpha]_D$ +51 (c, 0.55 in $CHCl_3$).
Braekman, J.C. *et al., Tetrahedron*, 1978, **34**, 1551

Dolastatin I D-1199

[192800-84-3]



$C_{24}H_{32}N_6O_5S$ 516.62
Isol. from *Dolabella auricularia*. Cytotoxic agent. Amorph. powder. $[\alpha]_D^{30}$ -50 (c, 0.06 in $CHCl_3$). λ_{max} 198 (ϵ 27000); 220 (ϵ 20000) (MeCN).

Sone, H. *et al., Tetrahedron*, 1997, **53**, 8149-8154 (*isol, uv, ir, pmr, cmr*)
Kigoshi, H. *et al., Tetrahedron*, 1999, **55**, 12301-12308 (*synth*)

Dolastatin 1 D-1200

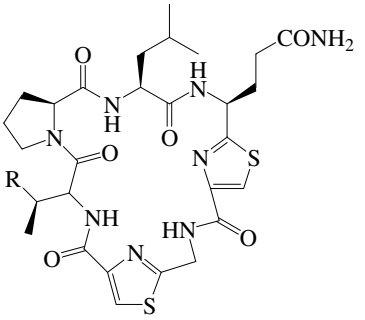
[79394-15-3]
Thiazole-peptide antibiotic. Struct. unknown. Isol. from *Dolabella auricularia* and *Aplysia pulmonica*. Cytotoxic agent. Powder. λ_{max} 218 (MeOH).
Pettit, G.R. *et al., J. Nat. Prod.*, 1981, **44**, 482-485

Dolastatin 2 D-1201

[79394-16-4]
Thiazole-peptide antibiotic. Struct. unknown. Isol. from *Dolabella auricularia* and *Aplysia pulmonica*. Cytotoxic agent. Powder. λ_{max} 217 (MeOH).
Pettit, G.R. *et al., J. Nat. Prod.*, 1981, **44**, 482-485

Dolastatin 3 D-1202

[80387-90-2]



R = CH_3

$C_{29}H_{40}N_8O_6S_2$ 660.817
Cyclic peptide antibiotic. Isol. from the Indian Ocean sea hare *Dolabella auricularia*, sponge *Aplysia pulmonica* and *Lyngbya majuscula*. Shows potent antineoplastic props. Inhibitor of HIV 1 integrase. Amorph. solid.
Mp 133-137°. $[\alpha]_D^{26}$ -35.5 (c, 0.09 in MeOH). λ_{max} 206 (ϵ 13940); 208; 238 (ϵ 8960) (MeOH) (Berdy).

Homologue (R = -CH_2CH_3): ***Homodolastatin 3***
[261373-24-4]
$C_{30}H_{42}N_8O_6S_2$ 674.844
Isol. from *Lyngbya majuscula*. Amorph. solid. λ_{max} 240 (ϵ 7000) (MeOH).

Pettit, G.R. *et al., J. Nat. Prod.*, 1981, **44**, 482-485 (*isol*)
Pettit, G.R. *et al., J.A.C.S.*, 1982, **104**, 905-907; 1987, **109**, 7581-7582 (*uv, ir, pmr, cmr, ms, struct, bibl, synth*)
Schmidt, U. *et al., Angew. Chem., Int. Ed.*, 1984, **23**, 725-726 (*struct*)
Hamada, Y. *et al., Tet. Lett.*, 1984, **25**, 5303-5306 (*synth*)
Bredenkamp, M.W. *et al., Annalen*, 1990, 871-875 (*synth, conformn*)
Holzapfel, C.W. *et al., Tetrahedron*, 1990, **46**, 649-660 (*synth*)
Pettit, G.R. *et al., Tetrahedron*, 1993, **49**, 9151
Mitchell, S.S. *et al., J. Nat. Prod.*, 2000, **63**, 279-282 (*Homodolastatin 3*)

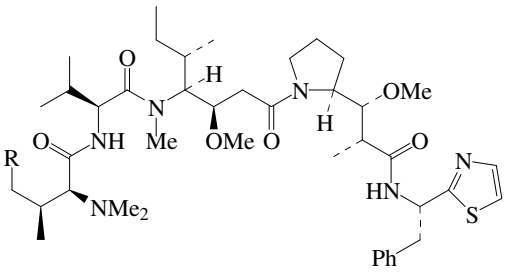
Dolastatin 4 D-1203

[79394-18-6]
Thiazole-peptide antibiotic. Struct. unknown. Isol. from *Dolabella auricularia* and *Aplysia pulmonica*. Cytotoxic agent. Powder.
Pettit, G.R. *et al., J. Nat. Prod.*, 1981, **44**, 482-485

Dolastatin 10 D-1204

NSC 376128

[110417-88-4]



R = H

$C_{42}H_{68}N_6O_6S$ 785.102

Peptide antibiotic. Isol. from *Dolabella auricularia* and *Symploca* sp. VP642. Antitumour and antimitotic agent. Shows fungicidal activity. Tubulin polymerisation inhibitor. Phase II clin. trial (2000). Lacked clinically significant activity. Amorph. powder ($MeOH/CH_2Cl_2$). Sol. MeOH, $CHCl_3$.

Mp 107-112°. $[\alpha]_D^{29}$ -68 (c, 0.01 in MeOH). λ_{max} 203 (log ϵ 4.39); 216 (ϵ 20200); 242 (ϵ 3610); 245 (log ϵ 3.63) (MeOH) (Derep).

Homologue (R = CH_3): ***Symplostatin 1***

[212007-18-6]

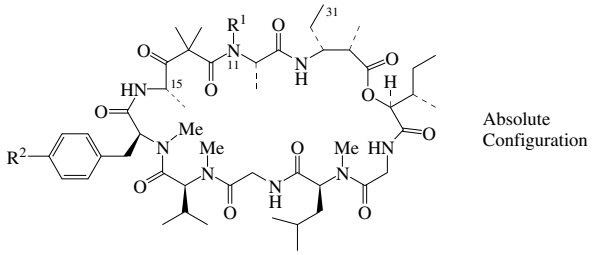
$C_{43}H_{70}N_6O_6S$ 799.129

Isol. from the cyanobacterium S*ymploca hydnoides*. Antitumour agent. Microtubule assembly inhibitor. $[\alpha]_D$ -45 (c, 1.6 in MeOH). λ_{max} 209 (ϵ 20420); 245 (ϵ 5430) (MeOH).

Pettit, G.R. *et al., J.A.C.S.*, 1987, **109**, 6883-6885 (*isol, struct*)
Pettit, G.R. *et al., J.A.C.S.*, 1989, **111**, 5463-5465 (*synth, abs config*)
Shioiri, T. *et al., Tetrahedron*, 1993, **49**, 1913-1924 (*synth*)
Pettit, G.R. *et al., Tetrahedron*, 1993, **49**, 9151-9170 (*isol, bibl*)
Pettit, G.R. *et al., J.O.C.*, 1994, **59**, 6127-6130 (*synth, cryst struct*)
Roux, F. *et al., Tetrahedron*, 1994, **50**, 5345-5360 (*synth*)
Alattia, T. *et al., Tetrahedron*, 1995, **51**, 2593-2604 (*pmr, cmr, conformn*)
Pettit, G.R. *et al., J.C.S. Perkin 1*, 1996, 853-858; 859-863 (*synth*)
Pettit, R.K. *et al., Antimicrob. Agents Chemother.*, 1998, **42**, 2961-2965 (*Dolastatin 10, activity*)
Harrigan, G.G. *et al., J. Nat. Prod.*, 1998, **61**, 1075-1077 (*Symplostatin 1*)
Munro, M.H.G. *et al., J. Biotechnol.*, 1999, **70**, 15-25 (*rev*)
Vaishampayan, U. *et al., Clin. Cancer Res.*, 2000, **6**, 1293-1301; 4205-4208 (*pharmacol*)
Luesch, H. *et al., J. Nat. Prod.*, 2001, **64**, 907-910 (*isol, activity, Symplostatin 1*)
Hoffman, M.A. *et al., Gynecol. Oncol.*, 2003, **89**, 95-98 (*clin trial*)
Mooberry, S.L. *et al., Int. J. Cancer*, 2003, **104**, 512-521 (*Symplostatin 1, pharmacol*)

Dolastatin 11 D-1205

[111517-68-1]



Absolute Configuration

R^1 = H, R^2 = -OMe

$C_{50}H_{80}N_8O_{12}$ 985.228

Depsipeptide antibiotic. Similar to Majusculamide C, M-39. Isol. from the sea hare *Dolabella auricularia* and from an assemblage of *Lyngbya majuscula* with *Schizothrix calcicola*. Cytotoxic. Powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 134-137°. $[\alpha]_D^{26}$ -143.9 (c, 0.33 in CH_2Cl_2). λ_{max} 225 (ϵ 6610); 277 (ϵ 2190); 283 (ϵ 1900) (MeOH) (Derep). λ_{max} 230; 278 (MeOH) (Berdy).

*11-*N*-Me:* ***Lyngbyastatin 1***

$C_{51}H_{82}N_8O_{12}$ 999.255

Isol. from the cyanobacterial assemblage of *Lyngbya majuscula* and *Schizothrix calcicola*. Cytokinesis inhibitor, cellular microfilament disrupter. Glassy oil. $[\alpha]_D^{27}$ -17 (c, 0.3 in MeOH). Shown to be a mixt. of C-15 epimers in 2003. λ_{max} 236 (log ϵ 3.15); 277 (log ϵ 2.8); 284 (log ϵ 2.75) (MeOH).

*31-Methyl, 11-*N*-Me:* ***Lyngbyastatin 3***

$C_{52}H_{84}N_8O_{12}$ 1013.282

Isol. from *Lyngbya majuscula*. Oil. $[\alpha]_D^{27}$ -62 (c, 0.12 in $CHCl_3$). λ_{max} 201 (log ϵ 4.23); 209 (log ϵ 3.98); 221 (log ϵ 3.87); 277 (log ϵ 3.45) (MeOH).

Pettit, G.R. *et al., Heterocycles*, 1989, **28**, 553-558 (*isol, struct*)
Pettit, G.R. *et al., Tetrahedron*, 1993, **49**, 9151-9170 (*isol, struct*)
Bates, R.B. *et al., J.A.C.S.*, 1997, **119**, 2111-2113 (*synth, abs config*)
Harrigan, G.G. *et al., J. Nat. Prod.*, 1998, **61**, 1221-1225 (*Lyngbyastatin 1*)
Bai, R. *et al., J. Nat. Prod.*, 2002, **65**, 1824-1829 (*Lyngbyastatin 1, synth, pmr, stereochem*)
Williams, P.G. *et al., J. Nat. Prod.*, 2003, **66**, 1356-1363 (*Lyngbyastatins*)
Ali, M.A. *et al., Bioorg. Med. Chem.*, 2005, **13**, 4138-4152 (*synth, conformn*)

Dolastatin 12 D-1206

[122054-77-7]

As Dolastatin 11, D-1205 with

$R^1 = CH_3$, R^2 = H

$C_{50}H_{80}N_8O_{11}$ 969.229

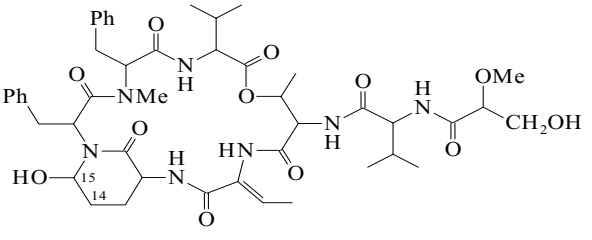
Depsipeptide antibiotic. Isol. from the sea hare *Dolabella auricularia*. Also obt. from the cyanobacterial assemblage *Lyngbya majuscula*/*Schizothrix calcicola* as an inseparable mixture with its C-15 epimer. Cytotoxic agent. Powder.

Mp 130-135°. $[\alpha]_D^{24}$ -98 (c, 0.01 in MeOH). Similar to Majusculamide C, M-39. λ_{max} 225 (ϵ 6610); 277 (ϵ 2190); 283 (ϵ 1900) (MeOH) (Derep). λ_{max} 224 (ϵ 6600) (MeOH) (Berdy).

Pettit, G.R. *et al., Heterocycles*, 1989, **28**, 553-558 (*isol, struct*)
Pettit, G.R. *et al., Tetrahedron*, 1993, **49**, 9151-9170 (*isol, struct*)
Bates, R.B. *et al., J.A.C.S.*, 1997, **119**, 2111 (*abs config*)
Harrigan, G.G. *et al., J. Nat. Prod.*, 1998, **61**, 1221-1225 (*isol*)
Williams, P.G. *et al., J. Nat. Prod.*, 2003, **66**, 1356-1363 (*isol, config*)

Dolastatin 13 D-1207

[120231-23-4]



$C_{46}H_{63}N_7O_{12}$ 906.043

Depsipeptide antibiotic. Isol. from the sea hare *Dolabella auricularia*. Cytotoxin. Cryst. (CH_2Cl_2/hexane).

Mp 286-289°. $[\alpha]_D$ +94 (c, 0.01 in MeOH). λ_{max} 220 (ϵ 1100) (MeOH) (Derep).

14,15-Didehydro: ***Dehydrodolastatin 13***

[120231-24-5]

$C_{46}H_{61}N_7O_{12}$ 904.028

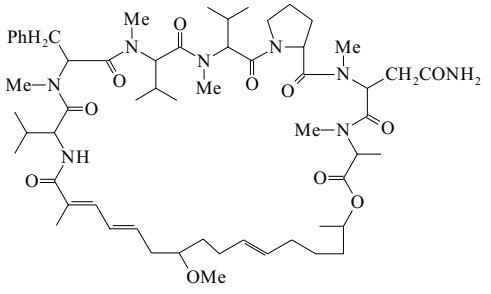
Isol. from *Dolabella auricularia*. Cytotoxin. Cryst. (CH_2Cl_2/hexane).

Mp 127-132°. $[\alpha]_D$ +38 (c, 0.005 in MeOH). λ_{max} 220 (ϵ 1100) (MeOH) (Derep). λ_{max} 220 (ϵ 12900) (MeOH) (Berdy).

Pettit, G.R. *et al., J.A.C.S.*, 1989, **111**, 5015-5017 (*isol*)
Kamano, Y. *et al., Tennen Yuki Kagobutsu Toronkai Koen Yoshishu*, 1989, **31**, 641-647; *CA*, **112**, 95756 (*isol, struct*)
Pettit, G.R. *et al., Tetrahedron*, 1993, **49**, 9151-9170 (*isol, struct*)

Dolastatin 14 D-1208

[126723-15-7]



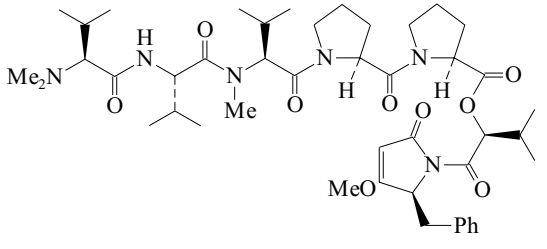
$C_{59}H_{92}N_8O_{11}$ 1089.423

Depsipeptide antibiotic. Isol. from *Dolabella auricularia*. Cytotoxic agent. Amorph.
Mp 123-125°. $[\alpha]_D^{24}$ -146 (c, 0.14 in MeOH). λ_{max} 211 (ϵ 23400); 262 (ϵ 14200) (MeOH).

Pettit, G.R. *et al., J.O.C.*, 1990, **55**, 2989-2990 (*isol, struct*)
Pettit, G.R. *et al., Tetrahedron*, 1993, **49**, 9151-9170 (*isol, struct*)

Dolastatin 15 D-1209

[123884-00-4]



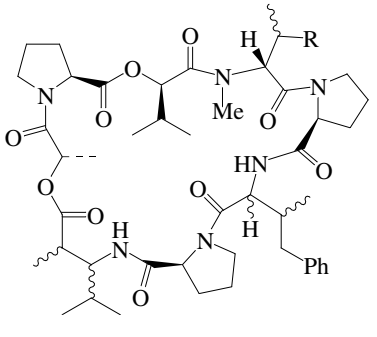
$C_{45}H_{68}N_6O_9$ 837.067

Peptide antibiotic. Isol. from the sea hare *Dolabella auricularia*. Cytotoxic agent. Microtubule inhibitor. Powder.
Mp 143-148°. $[\alpha]_D^{26}$ -26 (c, 0.01 in MeOH). λ_{max} 220 (ϵ 1290); 242 (ϵ 794) (MeOH) (Derep). λ_{max} 220 (ϵ 30200); 239 (ϵ 28840) (MeOH) (Berdy).

Pettit, G.R. *et al., J.O.C.*, 1989, **54**, 6005-6006 (*isol, struct*)
Patino, N. *et al., Tetrahedron*, 1992, **48**, 4115-4122 (*synth*)
Pettit, G.R. *et al., Tetrahedron*, 1993, **49**, 9151-9170 (*isol, struct*)
Pettit, G.R. *et al., Tetrahedron*, 1994, **50**, 12097 (*synth*)
Akaji, K. *et al., J.O.C.*, 1999, **64**, 405-411 (*synth*)

Dolastatin 16 D-1210

[192214-57-6]



R = CH_3

$C_{47}H_{70}N_6O_{10}$ 879.104

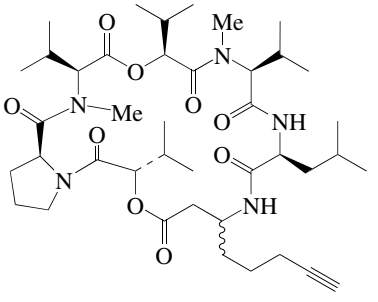
Depsipeptide antibiotic. Isol. from *Dolabella auricularia*. Cytotoxic agent. Amorph. powder. $[\alpha]_D^{20}$ +15.5 (c, 0.2 in MeOH).

*Homologue (R = -CH_2CH_3): **Homodolastatin 16***
$C_{48}H_{72}N_6O_{10}$ 893.131
Isol. from a Kenyan *Lyngbya majuscula*. Moderate cytotoxic agent. Pale yellow oil. $[\alpha]_D^{22}$ -25 (c, 0.19 in MeOH). Partial stereochem. has been determined.

Pettit, G.R. *et al., J. Nat. Prod.*, 1997, **60**, 752-754 (*isol, pmr, cmr*)
Davies-Coleman, M.T. *et al., J. Nat. Prod.*, 2003, **66**, 712-715 (*Homodolastatin 16*)

Dolastatin 17 D-1211

[205750-27-2]



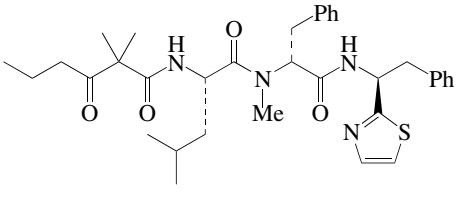
$C_{41}H_{67}N_5O_9$ 774.008

Depsipeptide antibiotic. Isol. from the sea hare *Dolabella auricularia*. Cytotoxic agent. Amorph. powder. $[\alpha]_D$ -145 (c, 0.1 in MeOH).

Pettit, G.R. *et al., Heterocycles*, 1998, **47**, 491-496 (*isol*)

Dolastatin 18 D-1212

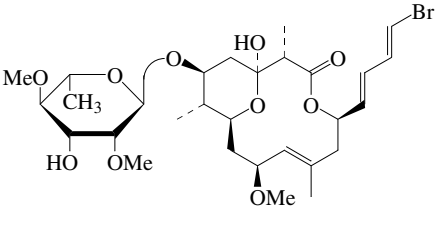
[190181-65-8]



$C_{35}H_{46}N_4O_4S$ 618.839
Isol. from *Dolabella auricularia*. Cytotoxic agent. Powder. $[\alpha]_D$ -2.3 (c, 0.1 in MeOH).

Pettit, G.R. *et al., Bioorg. Med. Chem. Lett.*, 1997, **7**, 827-832 (*isol, pmr, cmr*)
Pettit, G.R. *et al., J.O.C.*, 2004, **69**, 4019-4022 (*synth*)

Dolastatin 19 D-1213



Absolute Configuration

$C_{29}H_{45}BrO_{10}$ 633.573

Similar to Lyngbouilloside, L-299. Stereochem. revised in 2006. Isol. from *Dolabella auricularia*. Cytotoxic. Amorph. powder. $[\alpha]_D$ +7.5 (c, 0.04 in MeOH). λ_{max} 220; 250 (MeOH).

Pettit, G.R. *et al., J. Nat. Prod.*, 2004, **67**, 1252-1255 (*isol, pmr, cmr, ms*)
Paterson, I. *et al., Org. Lett.*, 2006, **8**, 2131-2134 (*synth, struct*)

Dolastatin A D-1214

[94700-27-3]

Peptide antibiotic. Struct. unknown. Isol. from a sea hare, *Dolabella* sp. Cytotoxic agent.

Eur. Pat., 1984, 124 984; *CA*, **102**, 72870f (*isol*)

Dolastatin B D-1215

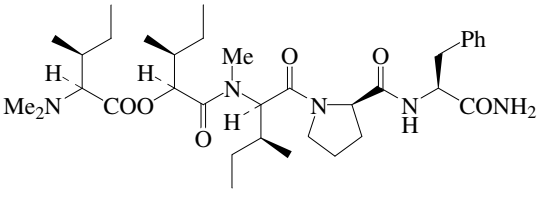
[94700-28-4]

Peptide antibiotic. Struct. unknown. Isol. from a sea hare, *Dolabella* sp. Cytotoxic agent.

Eur. Pat., 1984, 124 984; *CA*, **102**, 72870f (*isol*)

Dolastatin C D-1216

[155281-41-7]



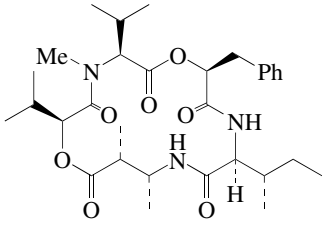
$C_{35}H_{57}N_5O_6$ 643.865

Isol. from *Dolabella auricularia*. Weak cytotoxic agent. Amorph. powder. $[\alpha]_D^{25}$ -136 (c, 0.066 in MeOH). λ_{max} 207 (ϵ 17500) (MeOH).

Sone, H. *et al., Tet. Lett.*, 1993, **34**, 8445-8448 (*isol, uv, pmr, cmr*)

Dolastatin D D-1217

[155180-52-2]



$C_{31}H_{47}N_3O_7$ 573.728

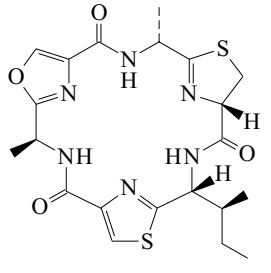
Isol. from *Dolabella auricularia*. Cytotoxic. Needles (hexane/CH_2Cl_2).

Mp 200-201°. $[\alpha]_D^{25}$ -73 (c, 0.13 in MeOH). λ_{max} 206 (ϵ 16300) (MeOH).

Sone, H. *et al., Tet. Lett.*, 1993, **34**, 8449-8452 (*isol, uv, pmr, cmr*)

Dolastatin E D-1218

[165967-00-0]



Absolute configuration

$C_{21}H_{26}N_6O_4S_2$ 490.606

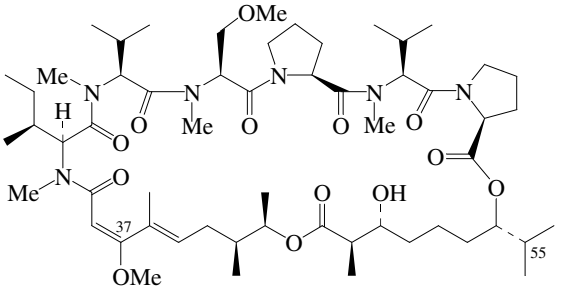
Cyclic peptide antibiotic. Isol. from the sea hare *Dolabella auricularia*. Cytotoxic agent. Powder. $[\alpha]_D^{27}$ -22 (c, 0.2 in MeOH). λ_{max} 205 (ϵ 26600); 213 (sh) (ϵ 23800); 240 (sh) (ϵ 13800) (MeOH) (Derep).

[170720-11-3, 170720-12-4]

Ojika, M. *et al., Tet. Lett.*, 1995, **36**, 5057-5058; 5059-5062 (*isol, synth, pmr, cmr, abs config*)

Dolastatin G D-1219

[174916-13-3]



Absolute Configuration

$C_{57}H_{96}N_6O_{13}$ 1073.418

Depsipeptide antibiotic. Isol. from the sea hare *Dolabella auricularia*. Cytotoxic agent. Prisms (hexane/C_6H_6).

Mp 138-139°. $[\alpha]_D^{25}$ -211 (c, 0.4 in MeOH). λ_{max} 205 (ϵ 38200); 250 (ϵ 9600) (MeOH).

37-O-*De-Me:* ***Nordolastatin G***

[180610-93-9]

$C_{56}H_{94}N_6O_{13}$ 1059.391

Isol. from *Dolabella auricularia*. Cytotoxic agent. Amorph. powder. $[\alpha]_D^{25}$ -183 (c, 0.1 in MeOH). Enolised diketone. λ_{max} 205 (ϵ 35900); 225 (sh) (ϵ 22700); 291 (ϵ 5000) (MeOH).

55-Demethyl: ***Lyngbyastatin 2***

$C_{56}H_{94}N_6O_{13}$ 1059.391

Prod. by *Lyngbya majuscula*. Oil. $[\alpha]_D^{27}$ -218 (c, 0.04 in MeOH). λ_{max} 202 (log ϵ 4.61); 225 (sh) (log ϵ 4.28); 250 (log ϵ 3.94) (MeOH).

55-Demethyl, 37-O-*de-Me:* ***Norlyngbyastatin 2***

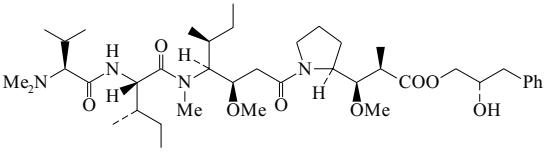
$C_{55}H_{92}N_6O_{13}$ 1045.364

Prod. by *Lyngbya majuscula*. Oil. $[\alpha]_D^{27}$ -179 (c, 0.05 in MeOH). Enolised β-diketone. λ_{max} 202 (log ϵ 4.58); 227 (sh) (log ϵ 4.28); 290 (log ϵ 2.95) (MeOH).

Mutou, T. *et al., J.O.C.*, 1996, **61**, 6340-6345 (*isol, uv, ir, pmr, cmr*)
Mutou, T. *et al., Tet. Lett.*, 1996, **37**, 7299-7302 (*synth, struct*)
Luesch, H. *et al., J. Nat. Prod.*, 1999, **62**, 1702-1706 (*Lyngbyastatin 2, Norlyngbyastatin 2*)

Dolastatin H D-1220

[173327-16-7]

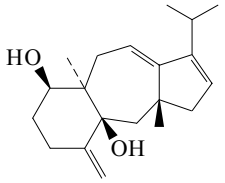


$C_{41}H_{70}N_4O_8$ 747.026

Peptide antibiotic. Isomer of Isodolastatin H, I-170. Isol. from the sea hare *Dolabella auricularia*. Cytotoxic agent. Powder. $[\alpha]_D^{25}$ -56 (c, 0.04 in MeOH). λ_{max} 208 (ϵ 23000) (MeOH).

Sone, H. *et al., J.A.C.S.*, 1996, **118**, 1874-1880 (*isol, uv, ir, pmr, cmr*)

1(15),7,9-Dolastatriene-4,14-diol D-1221



$C_{20}H_{30}O_2$ 302.456

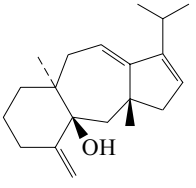
(4β,14β)-*form*
Constit. of *Dictyota cervicornis.*
Cryst. (EtOH aq.).
Mp 145°. $[\alpha]_D^{25}$ -190 (c, 3.35 in $CHCl_3$).

4-Ac: ***4-Acetoxy-1(15),7,9-dolastatrien-14-ol***
$C_{22}H_{32}O_3$ 344.493
Constit. of *Dictyota divaricata* and *Dictyota cervicornis.*
Histamine antagonist. Oil. $[\alpha]_D^{25}$ -128.5 (c, 9.5 in $CHCl_3$). λ_{max} 243 (ϵ 7000) (MeOH) (Berdy).

Sun, H.H. *et al., Tetrahedron*, 1981, **37**, 1237 (*cryst struct*)
Gonzalez, A.G. *et al., Tetrahedron*, 1983, **39**, 3355 (*abs config*)
Teixeira, V.L. *et al., J. Nat. Prod.*, 1986, **49**, 570 (*isol*)

1(15),7,9-Dolastatrien-14-ol D-1222

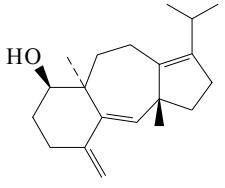
[80243-67-0]



$C_{20}H_{30}O$ 286.456
Constit. of *Dictyota* spp. Oil.

Crews, P. *et al., J.O.C.*, 1982, **47**, 811
Piers, E. *et al., J.O.C.*, 1986, **51**, 3405 (*synth*)
Mehta, G. *et al., J.A.C.S.*, 1991, **113**, 5765 (*synth*)
Piers, E. *et al., Can. J. Chem.*, 1992, **70**, 1204 (*synth*)

1(15),8,13-Dolastatrien-4-ol D-1223



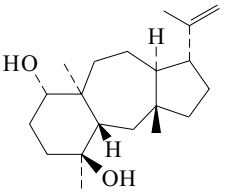
$C_{20}H_{30}O$ 286.456

4β-*form*
Amijitrienol
[87745-20-8]
Constit. of *Dictyota linearis.*
Cryst. (hexane).
Mp 129-129.5°. $[\alpha]_D^{18}$ +15.1 (c, 0.09 in EtOH).

Ochi, M. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 661
Piers, E. *et al., Can. J. Chem.*, 1992, **70**, 1204 (*synth*)

17-Dolastene-1,4-diol D-1224

17-Clavularene-1,4-diol

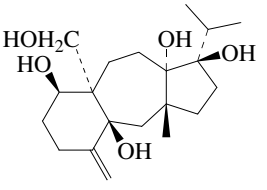


$C_{20}H_{34}O_2$ 306.487

(1β,4α,9β*H*,14β)-*form*
Constit. of *Clavularia inflata.*
Cryst.
Mp 165-167°. $[\alpha]_D$ +9 (c, 0.8 in $CHCl_3$).

Braekman, J.C. *et al., Tetrahedron*, 1978, **34**, 1551

1(15)-Dolastene-4,8,9,14,16-pentol D-1225

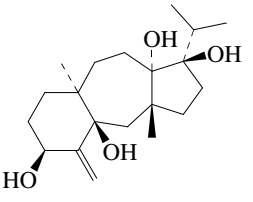


$C_{20}H_{34}O_5$ 354.486

(4β,8α,9β,14β)-*form*
Dichotopentaol
[626201-72-7]
Constit. of *Dictyota dichotoma.*
Cryst.
Mp 112-115°. $[\alpha]_D^{24}$ -20 (c, 0.09 in Py).

Ali, M.S. *et al., Nat. Prod. Res.*, 2003, **17**, 281-286 (*isol, pmr, cmr*)

1(15)-Dolastene-2,8,9,14-tetrol D-1226

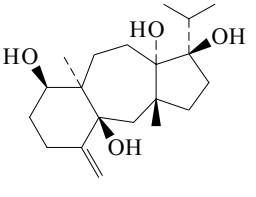


$C_{20}H_{34}O_4$ 338.486

(2β,8α,9β,14β)-*form*
Dichototetraol
[626201-71-6]
Constit. of *Dictyota dichotoma.*
Gum. $[\alpha]_D^{24}$ -28.9 (c, 0.076 in $CHCl_3$).

Ali, M.S. *et al., Nat. Prod. Res.*, 2003, **17**, 281-286 (*isol, pmr, cmr*)

1(15)-Dolastene-4,8,9,14-tetrol D-1227

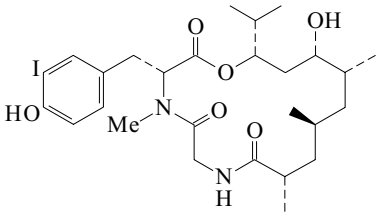


$C_{20}H_{34}O_4$ 338.486

(4β,9β,14β)-*form* [117383-30-9]
Constit. of *Dictyota cervicornis* and *Dictyota dichotoma*.
Cryst.
Mp 196-199°. $[\alpha]_D$ -80.7 (c, 1 in $CHCl_3$).
Kelecom, A. *et al., Phytochemistry*, 1988, **27**, 2907
Ali, M.S. *et al., Nat. Prod. Res.*, 2003, **17**, 281-286 (*isol, pmr, cmr*)

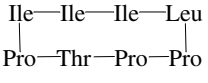
Doliculide D-1228

[156953-84-3]



$C_{27}H_{41}IN_2O_6$ 616.535
Depsipeptide antibiotic. Isol. from *Dolabella auricularia*. Cytotoxic agent. Needles (CH_2Cl_2/hexane). Sol. MeOH, DMSO, Me_2CO, C_6H_6, $CHCl_3$, EtOAc, EtOH.
Mp 173-174°. $[\alpha]_D^{24}$ -25.5 (c, 0.6 in MeOH). λ_{max} 207 (ϵ 27300); 227 (sh) (ϵ 11000); 284 (ϵ 3100) (MeOH).
Ishiwata, H. *et al., J.O.C.*, 1994, **59**, 4710 (*isol, pmr, cmr*)
Ishiwata, H. *et al., Tetrahedron*, 1994, **50**, 12853 (*synth*)
Ghosh, A.K. *et al., Org. Lett.*, 2001, **3**, 635-638 (*synth*)
Hanessian, S. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2004, **101**, 11996-12001 (*synth*)

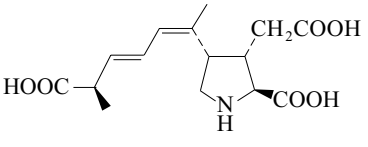
Dominicin D-1229



$C_{43}H_{72}N_8O_9$ 845.09
Isol. from the sponge *Eurypon laughlini*. Prisms.
Mp 168-171°. $[\alpha]_D^{25}$ -118.7 (c, 7.8 in MeOH).
Williams, D.E. *et al., J. Nat. Prod.*, 2005, **68**, 327-330 (*isol, pmr, cmr, cryst struct*)

Domoic acid D-1230

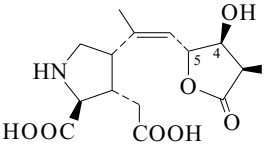
2-Carboxy-4-(5-carboxy-1-methyl-1,3-hexadienyl)-3-pyrrolidineacetic acid, 9CI
[14277-97-5]



$C_{15}H_{21}NO_6$ 311.334
Constit. of the red algae *Chondria armata* and *Alsidium corallinum*. Also isol. from toxin contaminated edible mussels (*Mytilus edulis*) containing diatom *Nitzschia multiseries* (formerly *Nitzschia pungens*). Ionotropic glutamate (kainate) receptor agonist. Neurotoxin. Amnesic shellfish poison. Vermifuge, insecticide. Needles + $2H_2O$. Sol. H_2O, AcOH; fairly sol. MeOH, EtOH; poorly sol. Me_2CO, C_6H_6.
Mp 213° dec. $[\alpha]_D^{12}$ -109.6 (H_2O). λ_{max} 242 (ϵ 24300) (H_2O at pH 2) (Derep). λ_{max} 242 (ϵ 26100) (H_2O pH 7) (Derep). λ_{max} 242 (ϵ 17500) (H_2O) (Berdy).
▶ Toxic, LD_{50} 10mg/kg (mus). UX9665100
(1′E)-Isomer: ***Isodomoic acid E***
[126872-96-6]
$C_{15}H_{21}NO_6$ 311.334
Isol. from mussel (*Mytilus edulis*).
$[\alpha]_D^{25}$ -19.5 (H_2O).
(3′Z)-Isomer: ***Isodomoic acid D***
[101977-26-8]
$C_{15}H_{21}NO_6$ 311.334
Isol. from mussel (*Mytilus edulis*).
$[\alpha]_D^{25}$ -72 (H_2O). λ_{max} 213 (ϵ 5030) (MeOH) (Berdy).
(1′E,3′Z)-Isomer: ***Isodomoic acid F***
[127761-30-2]
$C_{15}H_{21}NO_6$ 311.334
Isol. from mussel (*Mytilus edulis*).
$[\alpha]_D^{25}$ -85 (H_2O).
5′-Epimer: ***5′-Epidomoic acid***
$C_{15}H_{21}NO_6$ 311.334
Isol. from mussel and contaminating microalga *Nitzschia pungens*.
$[\alpha]_D^{24}$ -48.8 (c, 0.18 in H_2O). λ_{max} 242 (no solvent reported).
Daigo, K. *et al., Yakugaku Zasshi*, 1959, **79**, 350; 353; 356; 365; *CA*, **53**, 14218d (*isol, algae*)
Takemoto, T. *et al., Yakugaku Zasshi*, 1966, **86**, 874 (*pmr, struct*)
Impellizzeri, G. *et al., Phytochemistry*, 1975, **14**, 1549 (*isol, algae*)
Ohfune, Y. *et al., J.A.C.S.*, 1982, **104**, 3511-3513 (*synth, struct*)
Thibault, P. *et al., Biomed. Mass Spectrom.*, 1989, **18**, 373 (*ms*)
Wright, J.L.C. *et al., Can. J. Chem.*, 1989, **67**, 481; 1990, **68**, 22 (*Domoic acid, Isodomoic acids, isol, mussels*)
Falk, M. *et al., Can. J. Chem.*, 1989, **67**, 1421 (*uv*)
Tryphonas, L. *et al., Toxicol. Pathol.*, Pt. 2, 1990, **18**, 165 (*rev, tox*)
Walter, J.A. *et al., Can. J. Chem.*, 1992, **70**, 1156 (*pmr, cmr*)
Walter, J.A. *et al., Can. J. Chem.*, 1994, **72**, 430-436 (*5′-Epidomoic acid*)
Parsons, A.F. *et al., Tetrahedron*, 1996, **52**, 4149-4174 (*rev*)
Food Sci. Technol., Seafood and Freshwater Toxins, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*revs*)
Clayden, J. *et al., Tetrahedron*, 2005, **61**, 5713-5724 (*rev*)

Domoilactone A D-1231

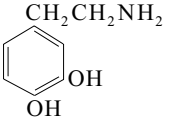
[101899-46-1]



$C_{15}H_{21}NO_7$ 327.333
Isol. from the red alga *Chondria armata*. λ_{max} 200 (ϵ 5700) (MeOH) (Derep).
4,5-Diepimer: ***Domoilactone B***
[101977-27-9]
$C_{15}H_{21}NO_7$ 327.333
From *Chondria armata*. λ_{max} 200 (ϵ 5700) (MeOH) (Derep).
Maeda, M. *et al., Tet. Lett.*, 1987, **28**, 633 (*isol, struct*)

Dopamine, BAN, INN D-1232

4-(2-Aminoethyl)-1,2-benzenediol, 9CI. 2-(3,4-Dihydroxyphenyl)ethylamine. 3,4-Dihydroxyphenethylamine. Hydroxytyramine. Oxytyramine. Cardiosteril. Dopastat. Intropin. NSC 169105. ASL 279. Many other names
[51-61-6]



$C_8H_{11}NO_2$ 153.18
Occurs in animals, esp. in the brain and nervous system, and in several higher plants, such as broom (*Cytisus scoparius*), banana (*Musa sapientum*) and *Hermidium alipes* (preferred genus name *Mirabilis*), and in the marine alga *Monostroma fuscum*. Also isol. from marine animals (e.g. *Metridium* sp.). Adrenergic, sympathomimetic agent. Antihypotensive, cardiotonic, antiparkinsonian agent. Central neurotransmitter and precursor of

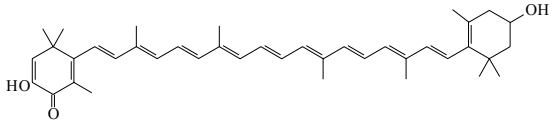
noradrenaline. Log P 0.02 (calc). Autoxidises very readily as free base.

▶ LD_{50} (rat, ipr) 163 mg/kg. Exp. reprod. and teratogenic effects. UX1088000

Tocher, R.D. *et al., Can. J. Bot.*, 1966, **44**, 605-608 (*Monostroma fuscum constit*)
Lenicque, P.M. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1977, **56**, 31-34 (*Metridium senile constit*)

β-Doradecin D-1233

3′-Hydroxy-β,β-carotene-3,4-dione. 3′-Hydroxy-3,4-diketo-β-carotene. Dehydroadonixanthin. 3-Hydroxyeuglenanone
[31460-54-5]

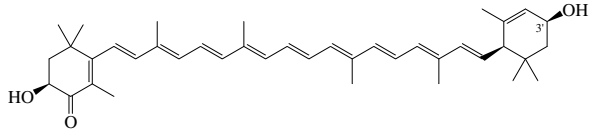


$C_{40}H_{52}O_3$ 580.849
Isol. as an ester from goldfish (*Carassius auratus*) and as an ester from Pacific salmon. Also obt. on saponification of Adonixanthin. λ_{max} 465 (EtOH). λ_{max} 455 (hexane).

Egger, K. *et al., Phytochemistry*, 1965, **4**, 609
Katayama, T. *et al., Int. J. Biochem.*, 1970, **1**, 438 (*isol*)
Kitahara, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1984, **78**, 859 (*isol*)

α-Doradexanthin D-1234

3,3′-Dihydroxy-β,ϵ-caroten-4-one. Papilioerythrin
[29125-77-7]



$C_{40}H_{54}O_3$ 582.865
Carotenoid from the goldfish *Carassius auratus* and from the integument of butterfly *Papilio xuthus*. Also isol. from the hermit crab *Clibanarius erythropus*. λ_{max} 466; 486 (C_6H_6). λ_{max} 453 (petrol).

3′-Ketone: ***Papilioerythrinone****. 3-Hydroxy-β,ϵ-carotene-3′,4-dione*
[60147-71-9]
$C_{40}H_{52}O_3$ 580.849
Isol. from pupae of *Papilio xuthus* and carapaces of *Paralithodes brevipes*.

3′-Epimer: ***Fritschiellaxanthin***
[68474-14-6]
$C_{40}H_{54}O_3$ 582.865
Isol. from the green alga *Fritschiella tuberosa*, the crab *Sesarma hematocheir* and from Cyprinidae eggs.

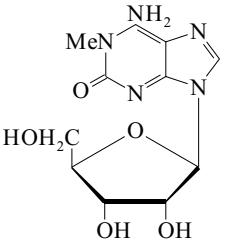
6′-Epimer: ***4-Ketolutein D***
[210761-24-3]
$C_{40}H_{54}O_3$ 582.865
Constit. of *Branchiostegus japonicus*.

3′,6′-Diepimer: ***4-Ketolutein F***
[210761-25-4]
$C_{40}H_{54}O_3$ 582.865
Constit. of *Branchiostegus japonicus*.

Harashima, K. *et al., Agric. Biol. Chem.*, 1976, **40**, 711 (*Papilioerythrinone*)
Castillo, R. *et al., Comp. Biochem. Physiol.*, 1978, **59**, 67 (*isol*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1978, **61**, 1962
Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **83**, 335 (*occur*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 334
Tsushima, M. *et al., Fish. Sci.*, 1998, **64**, 464-468 (*Ketoluteins*)

Doridosine D-1235

N,6-Didehydro-1,2,3,6-tetrahydro-1-methyl-2-oxoadenosine, 9CI. 1-Methylisoguanosine
[73027-05-1]



$C_{11}H_{15}N_5O_5$ 297.27
Nucleoside antibiotic. Obt. from the marine sponges *Tedania digitata* and *Anisodoris nobilis*. Shows antiinflammatory and muscle relaxant props. Long-acting hypertensive agent. Cryst. (H_2O). Sol. MeOH, H_2O; poorly sol. Me_2CO, hexane. Mp 266-267° (262-263°). $[\alpha]_D^{24}$ -65.4 (c, 1.0 in DMSO) $[\alpha]_D^{22}$ -54.6 (c, 1.0 in H_2O). Log P -4.17 (calc). λ_{max} 237 (ϵ 5600); 283 (ϵ 12900) (dil HCl) (Derep). λ_{max} 253 (ϵ 8400); 292 (ϵ 11200) (dil. NaOH) (Derep). λ_{max} 250 (ϵ 8600); 294 (ϵ 11400) (H_2O at pH 6.3) (Derep). λ_{max} 250 (ϵ 9400); 299 (ϵ 11500) (MeOH) (Berdy). λ_{max} 234 (ϵ 7000); 283 (ϵ 13700) (HCl) (Berdy). λ_{max} 286 (ϵ 7500) (pH 12 buffer) (Berdy).

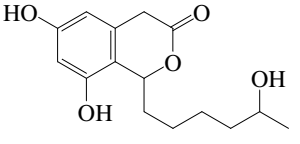
▶ LD_{50} (mus, orl) 1000 mg/kg.

[70639-65-5]

Cook, A.F. *et al., J.O.C.*, 1980, **45**, 4020 (*isol, synth, cmr, ms*)
Fuhrman, F.A. *et al., Science (Washington, D.C.)*, 1980, **207**, 193-195; 1981, **212**, 557 (*isol, pharmacol*)
Quinn, R.J. *et al., Tet. Lett.*, 1980, **21**, 567 (*isol, struct, synth*)
Kim, Y.H. *et al., J. Nat. Prod.*, 1981, **44**, 206-214 (*isol, struct, pharmacol*)
Wong, R.L. *et al., Acta Cryst. C*, 1984, **40**, 1409 (*cryst struct*)
Nachman, R.J. *et al., J.C.S. Perkin 1*, 1985, 1315 (*synth*)
Davies, L.P. *et al., Trends Pharmacol. Sci.*, 1985, **6**, 143 (*isol, rev*)
Chern, J.-W. *et al., J.O.C.*, 1991, **56**, 4213 (*synth*)

Dothiorelone D D-1236

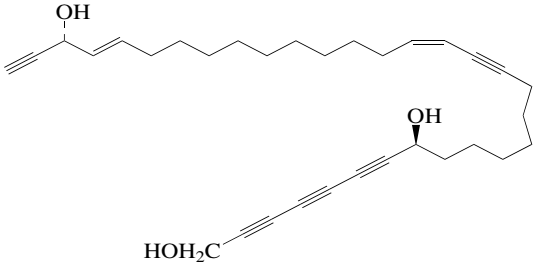
*1,4-Dihydro-6,8-dihydroxy-1-(5-hydroxyhexyl)-3*H*-2-benzopyran-3-one, 9CI*
[849758-69-6]



$C_{15}H_{20}O_5$ 280.32
Prod. by the mangrove fungus *Dothiorella* sp. Cytotoxic.

Yu, Q. *et al., CA*, 2004, **142**, 388784y (*isol*)

17,28-Dotriacontadiene-2,4,6,15,31-pentayne-1,8,30-triol D-1237

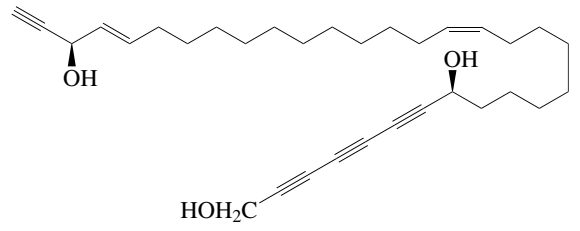


$C_{32}H_{42}O_3$ 474.682

Probable stereochem. shown.

(8*S*,17*Z*,28*E*,30*R*)-*form*
Triangulyne E
[182314-11-0]
Isol. from the sponge *Pellina triangulata*. Cytotoxic agent. Powder. $[\alpha]_D$ -11.4 (c, 0.4 in $CHCl_3$). λ_{max} 203 (log ϵ 3.7); 227 (log ϵ 4) (MeOH). λ_{max} 203 (ϵ 5010); 227 (ϵ 10000) (MeOH) (Berdy).
Dai, J.-R. *et al., J. Nat. Prod.*, 1996, **59**, 860-865 (*isol, uv, ir, pmr, cmr, ms*)

16,28-Dotriacontadiene-2,4,6,31-tetrayne-1,8,30-triol D-1238

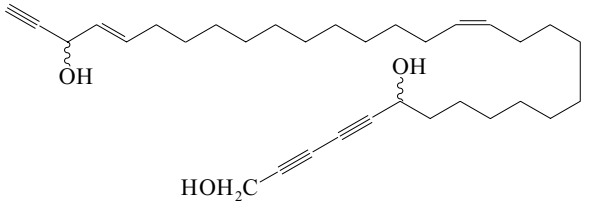


$C_{32}H_{46}O_3$ 478.714

(8*S*,16*Z*,28*E*,30*R*)-*form*
Triangulyne A
[182313-95-7]
Isol. from the sponge *Pellina triangulata*. Cytotoxic agent. Powder. $[\alpha]_D$ -15 (c, 1.6 in $CHCl_3$). λ_{max} 204 (log ϵ 3.5); 230 (log ϵ 3); 242 (log ϵ 2.8); 257 (log ϵ 2.6) (MeOH). λ_{max} 204 (ϵ 3160); 230 (ϵ 1000); 242 (ϵ 631); 257 (ϵ 400) (MeOH) (Berdy).
Dai, J.-R. *et al., J. Nat. Prod.*, 1996, **59**, 860-865 (*isol, uv, ir, pmr, cmr, ms*)

16,28-Dotriacontadiene-2,4,31-triyne-1,6,30-triol, 9CI D-1239

Melyne B
[115276-18-1]



$C_{32}H_{50}O_3$ 482.745
Isol. from *Xestospongia* sp.
$[\alpha]_D$ -7.2 (c, 4.0 in $CHCl_3$). λ_{max} 230 (ϵ 360); 240 (ϵ 330); 255 (ϵ 200) (MeOH) (Derep).

16,17-Dihydro: 28-Dotriacontene-2,4,31-triyne-1,6,30-triol. ***Pellynol E***
$C_{32}H_{52}O_3$ 484.761
Isol. from a *Theonella* sp. Gum. $[\alpha]_D$ -8.3 (c, 0.6 in $CHCl_3$).
Quinoa, E. *et al., Tet. Lett.*, 1988, **29**, 2037 (*isol, struct*)
Fu, X. *et al., J. Nat. Prod.*, 1999, **62**, 1336-1338 (*Pellynol E*)

17,28-Dotriacontadiene-2,4,31-triyne-1,6,30-triol D-1240

$HC{\equiv}CCH(OH)CH{=}CH(CH_2)_9CH{=}CH(CH_2)_{10}CH(OH)C{\equiv}CC{\equiv}CCH_2OH$

$C_{32}H_{50}O_3$ 482.745

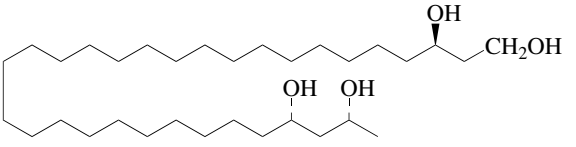
(-)-(17*Z*,28*E*)-*form*
Pellynol B
[186248-10-2]
Isol. from the sponge *Pellina triangulata*. Exhibits cytotoxic activity to human cell lines. $[\alpha]_D$ -7.6 (c, 0.3 in $CHCl_3$).
Fu, X. *et al., Tetrahedron*, 1997, **53**, 799 (*isol, ir, pmr, cmr*)
Rashid, M.A. *et al., Nat. Prod. Lett.*, 2000, **14**, 387-392 (*isol, activity*)

21,25-Dotriacontadienoic acid D-1241

$H_3C(CH_2)_5CH{=}CHCH_2CH_2CH{=}CH(CH_2)_{19}COOH$
$C_{32}H_{60}O_2$ 476.825

(*Z*,*Z*)-*form* [187657-42-7]
Isol. from the sponge *Haliclona cinerea*.
Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*isol, ms*)

1,3,29,31-Dotriacontanetetrol D-1242



$C_{32}H_{66}O_4$ 514.871

(3*R*,29*S*,31*R*)-*form*
1-O-α-D-*Glucopyranoside:*
$C_{38}H_{76}O_9$ 677.013
Isol. from *Chlorogloeopsis fritschii* and *Fischerella muscicola*.
1-O-α-D-*Mannopyranoside:*
$C_{38}H_{76}O_9$ 677.013
Isol. from *Chlorogloeopsis fritschii*.
29-Ketone, 1-O-α-D-*glucopyranoside:*
$C_{38}H_{74}O_9$ 674.997
Isol. from *Chlorogloeopsis fritschii* and *Fischerella muscicola*.
$[\alpha]_D$ +24 (c, 1.3 in $CHCl_3$/MeOH).
29-Ketone, 1-O-α-D-*mannopyranoside:*
$C_{38}H_{74}O_9$ 674.997
Isol. from *Chlorogloeopsis fritschii*.
Gambacorta, A. *et al., Phytochemistry*, 1998, **48**, 801-805

5,9,21,25-Dotriacontatetraenoic acid D-1243

$H_3C(CH_2)_5CH{=}CHCH_2CH_2CH{=}CH(CH_2)_{10}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{32}H_{56}O_2$ 472.793

(*all-Z*)-*form* [187657-46-1]
Isol. from the sponge *Haliclona cinerea*.
Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*isol, ms*)

5,9,25-Dotriacontatrienoic acid D-1244

$H_3C(CH_2)_5CH{=}CH(CH_2)_{14}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{32}H_{58}O_2$ 474.809

(*all-Z*)-*form* [187657-44-9]
Isol. from the sponge *Haliclona cinerea*.
Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*isol, ms*)

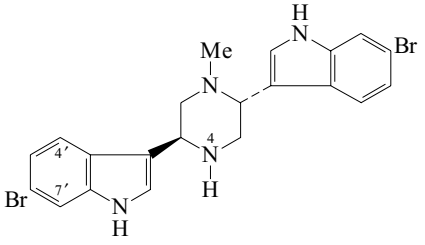
Dracotoxin D-1245

[140609-96-7]
Major toxic component of the venom of the Greater Weever fish *Trachinus draco*. Exhibits membrane depolarizing and hemolytic activities.
Chhatwal, I. *et al., Toxicon*, 1992, **30**, 87-93 (*isol, props, bibl*)

Dragmacidin A D-1246

*3,3′-(1-Methyl-2,5-piperazinediyl)bis[6-bromo-1*H*-indole], 9CI. 2,5-Bis(6-bromo-3-indolyl)-1-methylpiperazine*

[128364-31-8]



$C_{21}H_{20}Br_2N_4$ 488.224

Alkaloid from the marine sponges *Hexadella* sp., *Dragmacidon* spp., *Spongosorites* spp. and from tunicate *Didemnum candidum*. Cytotoxic. Shows antifungal, antiviral and antiinflammatory activity. Pale yellow powder.

N^4-*Me:* ***Dragmacidin B***

[128629-37-8]

$C_{22}H_{22}Br_2N_4$ 502.251

Alkaloid from the sponge *Hexadella* sp. Pale yellow powder.

7′-Bromo, 4′-hydroxy: ***Dragmacidin***. *Biemnidin*

[114582-72-8]

$C_{21}H_{19}Br_3N_4O$ 583.119

Alkaloid from the deep-water sponge *Dragmacidon* sp. Cytotoxic agent. Powder. $[\alpha]_D^{20}$ -3 (c, 13.2 in Me_2CO). λ_{max} 220 (ϵ 52600); 275 (ϵ 11700); 286 (sh) (ϵ 10900); 293 (sh) (ϵ 10100) (MeOH) (Derep).

N-*De-Me: 3,3′-(2,5-Piperazinediyl)bis[6-bromo-1*H*-indole]. 2,5-Bis(6-bromo-3-indolyl)piperazine.* ***Dragmacidin C***

[135048-54-3]

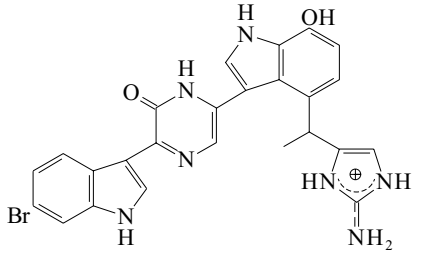
$C_{20}H_{18}Br_2N_4$ 474.197

Alkaloid from the marine tunicate *Didemnum candidum*. Opaque glass. $[\alpha]_D$ 0.

Eur. Pat., 1988, 284 337; *CA*, **111**, 50423 (*Biemnidin*)
Kohmoto, S. *et al., J.O.C.*, 1988, **53**, 3116-3118 (*isol, uv, ir, pmr, cmr, ms, struct*)
Morris, D.A. *et al., Tetrahedron*, 1990, **46**, 715-720 (*isol, pmr, struct*)
Fahy, E. *et al., J. Nat. Prod.*, 1991, **54**, 564-569 (*Dragmacidin C*)
Jiang, B. *et al., J.O.C.*, 1994, **59**, 6823-6827 (*Dragmacidin, synth*)
Whitlock, C.R. *et al., Tet. Lett.*, 1994, **35**, 371-374 (*Dragmacidin B, synth*)
Kawasaki, T. *et al., Org. Lett.*, 2000, **2**, 3027-3029 (*synth*)
Miyake, F.Y. *et al., Org. Lett.*, 2000, **2**, 3185-3187 (*Dragmacidin B, synth*)
Kawasaki, T. *et al., Tet. Lett.*, 2002, **43**, 4245-4248 (*Dragmacidin B, Dragmacidin C, synth*)
Garg, N.K. *et al., Tet. Lett.*, 2005, **46**, 2423-2426 (*Dragmacidin B, synth*)

Dragmacidin D D-1247

[142979-34-8]



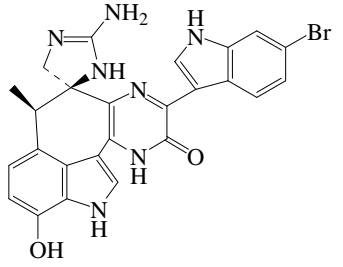
$C_{25}H_{21}BrN_7O_2^{\oplus}$ 531.391

Alkaloid from a deep-water marine sponge *Spongosorites* sp. Exhibits antimicrobial activity. Also inhibits the *in vitro* growth of P388 murine and A589 human lung tumour cell lines, and *in vitro* replication of feline leukaemia virus. Yellow solid. $[\alpha]_D$ +12 (c, 0.95 in EtOH). λ_{max} 213 (ϵ 43000); 270 (ϵ 14400); 383 (ϵ 20700) (EtOH) (Berdy). λ_{max} 214 (ϵ 54000); 280 (ϵ 16400); 452 (ϵ 19946) (EtOH-HCl) (Berdy).

Wright, A.E. *et al., J.O.C.*, 1992, **57**, 4772 (*isol, uv, pmr, cmr, struct*)
Capon, R.J. *et al., J. Nat. Prod.*, 2002, **61**, 660-662 (*isol, cmr*)
Garg, N.K. *et al., J.A.C.S.*, 2002, **124**, 13179-13184 (*synth*)

Dragmacidin E D-1248

[206061-75-8]



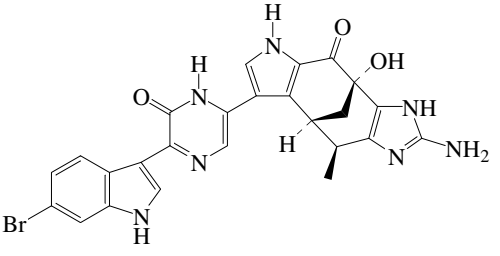
Relative Configuration

$C_{25}H_{20}BrN_7O_2$ 530.383

Tautomeric with the hydroxypyrazine form. Isol. from the sponge *Spongosorites* sp. Inhibitor of serine-threonine protein phosphatases. Yellow solid. $[\alpha]_D$ -34 (c, 0.9 in EtOH). Fluorescent. λ_{max} 211 (ϵ 46200); 281 (ϵ 7530); 427 (ϵ 27700) (EtOH). λ_{max} 427 (ϵ 26400) (EtOH/HCl). λ_{max} 410 (ϵ 26100) (EtOH/NaOH).

Capon, R.J. *et al., J. Nat. Prod.*, 1998, **61**, 660-662 (*isol, uv, pmr, cmr*)

Dragmacidin F D-1249



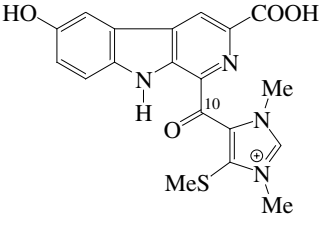
$C_{25}H_{20}BrN_7O_3$ 546.382

Alkaloid from the sponge *Halicortex* sp. Antiviral agent. Pale yellow solid. $[\alpha]_D^{25}$ -159 (c, 0.4 in MeOH). Mp >260°. λ_{max} 207 (ϵ 14000); 274 (ϵ 6460); 280 (ϵ 6430); 388 (ϵ 9600) (MeOH).

Cutignano, A. *et al., Tetrahedron*, 2000, **56**, 3743-3748 (*isol*)
Garg, N.K. *et al., J.A.C.S.*, 2004, **126**, 9552-9553 (*synth*)

Dragmacidonamine A D-1250

3-Carboxyhyrtiomanzamine



$C_{19}H_{17}N_4O_4S^{\oplus}$ 397.434

Counterion not specified. Charge is delocalised. Related to Hyrtiomanzamine, H-1031. Alkaloid from the sponge *Dragmacidon* sp. Amorph. yellow solid. λ_{max} 221; 254; 317 (MeOH).

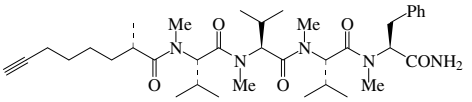
10-Deoxo: ***Dragmacidonamine B***

$C_{19}H_{19}N_4O_3S^{\oplus}$ 383.45

Alkaloid from *Dragmacidon* sp. Brownish oil. λ_{max} 222; 242; 282 (MeOH).

Pedpradab, S. *et al., J. Nat. Prod.*, 2004, **67**, 2113-2116 (*isol*)

Dragonamide D-1251

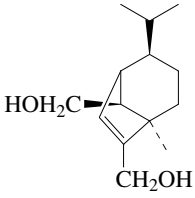


$C_{37}H_{59}N_5O_5$ 653.904
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{20}$ -260.8 (c, 2.6 in CH_2Cl_2).

Jimenez, J.I. *et al., J. Nat. Prod.*, 2001, **64**, 200-203 (*isol, pmr, cmr*)
Chen, H. *et al., Tetrahedron*, 2005, **61**, 11132-11140 (*synth, config*)

Drechslerine A D-1252

[405157-84-8]

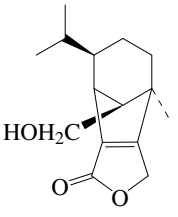


$C_{14}H_{24}O_2$ 224.342
Metab. of *Drechslera dematioidea*. Cryst.
Mp 125°. $[\alpha]_D^{22}$ -25 (c, 0.1 in EtOH).

Osterhage, C. *et al., J. Nat. Prod.*, 2002, **65**, 306-313 (*isol, pmr, cmr*)

Drechslerine B D-1253

[405157-85-9]

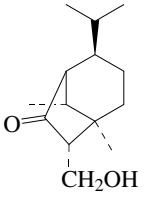


$C_{15}H_{22}O_3$ 250.337
Metab. of *Drechslera dematioidea*. Oil. $[\alpha]_D^{22}$ -42 (c, 0.1 in EtOH). λ_{max} 235 (log ϵ 3.63) (EtOH).

Osterhage, C. *et al., J. Nat. Prod.*, 2002, **65**, 306-313 (*isol, pmr, cmr*)

Drechslerine C D-1254

[405157-87-1]

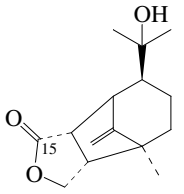


$C_{14}H_{24}O_2$ 224.342
Metab. of *Drechslera dematioidea*. Amorph. powder. $[\alpha]_D^{22}$ -13 (c, 0.15 in EtOH). λ_{max} 220 (log ϵ 3.08) (EtOH).

Osterhage, C. *et al., J. Nat. Prod.*, 2002, **65**, 306-313 (*isol, pmr, cmr*)

Drechslerine D D-1255

[405157-88-2]



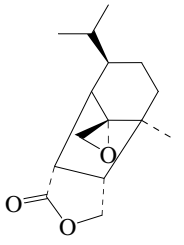
$C_{15}H_{22}O_3$ 250.337
Metab. of *Drechslera dematioidea*. Oil. $[\alpha]_D^{22}$ -90 (c, 0.4 in EtOH). λ_{max} 217 (log ϵ 3.1) (EtOH).

15β-Alcohol, 15-Me ether: ***Drechslerine E***
[405157-89-3]
$C_{16}H_{26}O_3$ 266.38
Metab. of *Drechslera dematioidea*. Amorph. powder. $[\alpha]_D^{22}$ +12 (c, 0.4 in EtOH). λ_{max} 264 (log ϵ 2.43) (EtOH).

Osterhage, C. *et al., J. Nat. Prod.*, 2002, **65**, 306-313 (*isol, pmr, cmr*)

Drechslerine F D-1256

[405157-90-6]

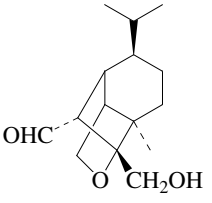


$C_{15}H_{22}O_3$ 250.337
Metab. of *Drechslera dematioidea*. Amorph. powder. $[\alpha]_D^{22}$ -35.5 (c, 0.2 in EtOH). λ_{max} 226 (log ϵ 3.14) (EtOH).

Osterhage, C. *et al., J. Nat. Prod.*, 2002, **65**, 306-313 (*isol, pmr, cmr*)

Drechslerine G D-1257

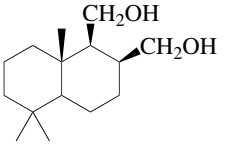
[405157-91-7]



$C_{15}H_{24}O_3$ 252.353
Metab. of *Drechslera dematioidea*. Oil. $[\alpha]_D^{22}$ -7.2 (c, 0.47 in EtOH). λ_{max} 264 (log ϵ 2.98) (EtOH).

Osterhage, C. *et al., J. Nat. Prod.*, 2002, **65**, 306-313 (*isol, pmr, cmr*)

11,12-Drimanediol D-1258



$C_{15}H_{28}O_2$ 240.385

Di-Ac: [178961-85-8]
$C_{19}H_{32}O_4$ 324.459

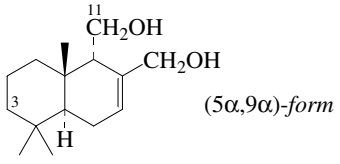
Constit. of *Dysidea fusca* and another *Dysidea* sp. Oil. $[\alpha]_D^{25}$ +37.2 (c, 0.1 in MeOH). $[\alpha]_D$ +47 (c, 0.4 in $CHCl_3$).

Dialdehyde: ***11,12-Drimanedial***
[151751-75-6]
$C_{15}H_{24}O_2$ 236.353
Constit. of a *Dysidea* sp. Oil. $[\alpha]_D$ +8.5 (c, 0.55 in $CHCl_3$).

12-Carboxylic acid, 11-aldehyde: ***11-Oxo-12-drimanoic acid***
$C_{15}H_{24}O_3$ 252.353
Constit. of *Dysidea fusca*. Oil. $[\alpha]_D$ +47 (c, 0.4 in $CHCl_3$).

Butler, M.S. *et al., Aust. J. Chem.*, 1993, **46**, 1255-1267 (*11,12-Drimanediol, 11,12-Drimanedial*)
Montagnac, A. *et al., J. Nat. Prod.*, 1996, **59**, 866 (*di-Ac, 11-Oxo-12-drimanoic acid*)
Paul, V.J. *et al., J. Nat. Prod.*, 1997, **60**, 1115-1120 (*11,12-Drimanediol*)
Barrero, A.F. *et al., J. Nat. Prod.*, 1999, **62**, 1488-1491 (*synth*)

7-Drimene-11,12-diol D-1259



(5α,9α)-*form*

$C_{15}H_{26}O_2$ 238.369

(5α,9α)-*form*

11,12-Dialdehyde: ***Isopolygodial***. *Isotadeonal*
[5956-39-8]
$C_{15}H_{22}O_2$ 234.338
Constit. of *Polygonum hydropiper* and other plant spp. Oil. Bp_1 145-153°. $[\alpha]_D$ -237.4 (EtOH). λ_{max} 227 (ε 10000) (MeOH).

(5α,9β)-*form* [34437-62-2]
Constit. of *Drimys winterii* and *Mniopetalum* sp.
Oil. $[\alpha]_D^{23}$ -6.5 (c, 0.2 in $CHCl_3$).

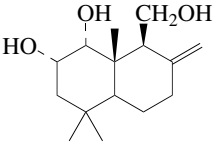
11,12-Dialdehyde: 7-Drimene-11,12-dial. ***Polygodial***. *Tadeonal*
[6754-20-7]
$C_{15}H_{22}O_2$ 234.338
Isol. from *Polygonum hydropiper*, *Drimys lanceolata* and other plants, also molluscs *Dendrodoris krebsii*, *Dendrodoris limbata*, *Dendrodoris nigra* and *Dendrodoris tuberculosa* and sponges *Dysidea* spp. Used as reagent for separation of enantiomeric primary amines. Shows antinociceptive activity. Shows antibacterial and antifungal activity. Plant growth regulator (inhibits rice husk germination, promotes root elongation in rice). Helicocide. Insect growth regulator. Insect antifeedant properties. Needles (petrol). Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane.
Mp 57° (50°). $Bp_{0.8}$ 138-140°. $[\alpha]_D$ -210 (90% EtOH). 'Hot' taste. λ_{max} 223 (ε 6000) (MeOH) (Derep). λ_{max} 231 (ε 11800); 295 (ε 76) (MeOH) (Berdy).
▶ Skin irritant.

11-Carboxylic acid, 12-aldehyde: 12-Oxo-7-drimen-11-oic acid. ***Polygonic acid***
[98204-84-3]
$C_{15}H_{22}O_3$ 250.337
Constit. of *Polygonum hydropiper*. Cryst.
Mp 96-97°. $[\alpha]_D^{23}$ -31 (c, 1.06 in $CHCl_3$).

[79732-75-5]

Loder, J.W. *et al., Aust. J. Chem.*, 1962, **15**, 322; 389 (*isol, uv, ir, pmr*)
Ohsuka, A. *et al., Nippon Kagaku Zasshi*, 1963, **84**, 748 (*Isotadeonal*)
Kubo, I. *et al., Chem. Comm.*, 1976, 1013 (*isol, struct*)
Ohsuka, A. *et al., Chem. Lett.*, 1979, 63 (*synth, Isotadeonal*)
Okuda, R.K. *et al., J.O.C.*, 1983, **48**, 1866 (*Polgodial*)
Jalali-Naini, M. *et al., Tetrahedron*, 1983, **39**, 749 (*synth*)
Cortés, M.J. *et al., Chem. Ind. (London)*, 1985, 735 (*synth*)
Cimino, G. *et al., Experientia*, 1985, **41**, 1335 (*Polygodial, isol*)
Fukuyama, Y. *et al., Phytochemistry*, 1985, **24**, 1521 (*Polygonic acid*)
Mori, K. *et al., Tetrahedron*, 1986, **42**, 273 (*synth*)
Caprioli, V. *et al., J. Nat. Prod.*, 1987, **50**, 146 (*synth*)
Brooks, C.J. *et al., J. Chromatogr.*, 1988, **438**, 108 (*use*)
Jansen, B.J.M. *et al., J.O.C.*, 1988, **53**, 855 (*synth*)
Banthorpe, D.V. *et al., Phytochemistry*, 1989, **28**, 1631 (*biosynth*)
Kuschel, A. *et al., J. Antibiot.*, 1994, **47**, 733; 1017 (*isol, pmr, cmr*)
Van Beek, T.A. *et al., Phytochem. Anal.*, 1994, **5**, 19 (*isol, hplc*)
Brown, G.D. *et al., Phytochemistry*, 1994, **35**, 975 (*isol, pmr, cmr*)
Urones, J.G. *et al., Tet. Lett.*, 1994, **35**, 3781 (*synth*)
Gómez, P.M. *et al., Tetrahedron*, 1994, **50**, 10995 (*synth*)
Gómez, M. *et al., Tetrahedron*, 1995, **51**, 1845 (*synth*)
Barrero, A.F. *et al., Tetrahedron*, 1995, **51**, 7435 (*synth*)
Toyooka, N. *et al., Tetrahedron*, 1997, **53**, 6313 (*synth*)
Filho, V.C. *et al., J. Ethnopharmacol.*, 1998, **62**, 223-227 (*activity, Polygodial*)

8(12)-Drimene-1,2,11-triol D-1260



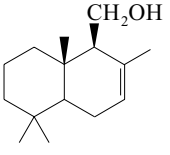
$C_{15}H_{26}O_3$ 254.369

(1α,2α)-*form*

Tri-Ac: [194020-45-6]
$C_{21}H_{32}O_6$ 380.48
Constit. of *Cadlina marginata*. Oil.

Dumdei, E.J. *et al., Can. J. Chem.*, 1997, **75**, 773-789 (*isol, pmr, cmr*)

7-Drimen-11-ol D-1261



$C_{15}H_{26}O$ 222.37

(5α,9β,10β)-*form*
Drimenol
[468-68-8]
Constit. of *Drimys winteri* and *Warburgia ugandensis*. Plant growth regulator (inhibits cress root growth, promotes wheat seed germination). Cryst. (C_6H_6).
Mp 97.8°. $Bp_{3.5}$ 150.5-151°. $[\alpha]_D^{17}$ -19.1 (C_6H_6).

O-*Hexadecanoyl:*
$C_{31}H_{56}O_2$ 460.782
Constit. of *Lactarius uvidus*.

O-*Octadecanoyl:*
$C_{33}H_{60}O_2$ 488.836
Constit. of *Lactarius uvidus*.

O-*(9-Octadecenoyl):*
$C_{33}H_{58}O_2$ 486.82
Constit. of *Lactarius uvidus*.

O-*(9,12-Octadecadienoyl):*
$C_{33}H_{56}O_2$ 484.804
Constit. of *Lactarius uvidus*.

O-*(6-Oxooctadecanoyl): 6-Ketostearoyldrimenol. Drimenol lactarinate*
$C_{33}H_{58}O_3$ 502.819
Constit. of *Lactarius uvidus*. Waxy solid.
Mp 22-23°. $[\alpha]_D^{20}$ +7.24 (c, 1.3 in $CHCl_3$).

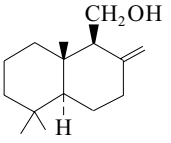
Carboxylic acid, 2,3-dihydroxypropyl ester: [89188-16-9]
$C_{18}H_{30}O_4$ 310.433
Isol. from the nudibranch *Archidoris montereyensis*.
$[\alpha]_D$ +23.1 (c, 0.9 in $CHCl_3$).

Carboxylic acid, 3-acetoxy-2-hydroxypropyl ester: [97530-70-6]
$C_{20}H_{32}O_5$ 352.47
Isol. from *Archidoris montereyensis*.

Appel, H.H. *et al., J.C.S.*, 1959, 3322-3332 (*isol, struct*)
Wenkert, E. *et al., J.A.C.S.*, 1964, **86**, 2044-2050 (*synth*)

Huneck, S. *et al., Phytochemistry*, 1972, **11**, 2429-2434 (*activity*)
Pelletier, S.W. *et al., J.O.C.*, 1975, **40**, 1607-1609 (*synth*)
Nishizawa, M. *et al., Tet. Lett.*, 1983, **24**, 2581-2584 (*(±)-form, synth*)
Gustafson, K. *et al., Tetrahedron*, 1985, **41**, 1101-1108 (*Archidoris glycerides*)
Garlaschelli, L. *et al., J. Nat. Prod.*, 1994, **57**, 905-910 (*esters*)
Polovinka, M.P. *et al., J.O.C.*, 1994, **59**, 1509-1517 (*(±)-form, synth*)
Barrero, A.F. *et al., Tetrahedron*, 1995, **51**, 7435-7450 (*synth*)
Ungur, N. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 1263-1273 (*carboxylic acid deriv*)
Lagnel, B.M.F. *et al., Synthesis*, 2000, 1907-1916 (*synth, ir, pmr, cmr*)

8(12)-Drimen-11-ol D-1262



$C_{15}H_{26}O$ 222.37

(5α,9β,10β)-*form*

Albicanol

[54632-04-1]

Constit. of *Diplophyllum albicans* and *Diplophyllum taxifolium*. Also from mollusc *Cadlina luteomarginata*. Shows ichthyotoxic and antitumour promoting activity. Needles.

Mp 68-70°. $[\alpha]_D^{25}$ +13 (c, 0.5 in $CHCl_3$).

Ac: ***Albicanyl acetate***

[83679-71-4]

[81767-36-4]

$C_{17}H_{28}O_2$ 264.407

Constit. of *Cadlina luteomarginata*. Shows ichthyotoxic and antitumour promoting activity. Oil. $[\alpha]_D^{23}$ +26.2 (c, 1.3 in $CHCl_3$).

2,4-Dihydroxycinnamoyl: [80358-00-5]

$C_{24}H_{32}O_4$ 384.514

Constit. of *Bazzania* spp. Oil.

3,4-Dihydroxycinnamoyl: [80357-99-9]

$C_{24}H_{32}O_4$ 384.514

Constit. of *Bazzania* spp. Cryst.

Mp 179-180°. $[\alpha]_D$ -18.3 (c, 3.2 in MeOH).

11-Aldehyde: 8(12)-Drimen-11-al. ***Albicanal***

[155551-30-7]

$C_{15}H_{24}O$ 220.354

Constit. of *Diplophyllum serrulatum*. Oil. $[\alpha]_D^{22}$ -69.8 (c, 3.1 in $CHCl_3$).

11-Carboxylic acid: 8(12)-Drimen-11-oic acid. ***Albicanic acid***

[112608-74-9]

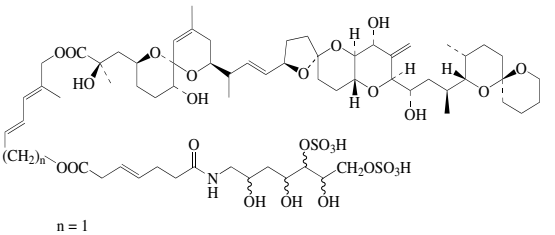
$C_{15}H_{24}O_2$ 236.353

Constit. of *Diplophyllum serrulatum*. Oil. $[\alpha]_D^{21}$ -23.2 (c, 0.07 in $CHCl_3$).

Ohta, Y. *et al., Tetrahedron*, 1977, **33**, 617 (*isol*)
Toyota, M. *et al., Phytochemistry*, 1981, **20**, 2359-2366 (*isol*)
Hellou, J. *et al., Tetrahedron*, 1982, **38**, 1875-1879 (*isol*)
Armstrong, R.J. *et al., Can. J. Chem.*, 1986, **64**, 1002 (*synth*)
Ragoussis, V. *et al., J.C.S. Perkin 1*, 1987, 987 (*synth*)
Shishido, K. *et al., Chem. Comm.*, 1989, 1093 (*synth*)
Toyota, M. *et al., Phytochemistry*, 1994, **35**, 1263 (*Albicanal, Albicanic acid*)
Barrero, A.F. *et al., Tet. Lett.*, 1994, **35**, 2945 (*synth*)
Weyerstahl, P. *et al., Annalen*, 1995, 1389 (*synth*)
Nakano, T. *et al., J. Chem. Res., Synop.*, 1995, 330 (*synth*)
Barrero, A.F. *et al., Tetrahedron*, 1995, **51**, 7435 (*synth*)
Dumdei, E.J. *et al., Can. J. Chem.*, 1997, **75**, 773-789 (*isol, pmr, cmr*)
Kubanek, J. *et al., J.O.C.*, 1997, **62**, 7239-7246 (*Albicanyl acetate, pmr, cmr, biosynth*)
Ito, H. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1190-1195 (*Albicanol, Albicanol acetate, activity*)
Anilkumar, A.T. *et al., Tetrahedron*, 2000, **56**, 1899-1904 (*synth*)
Toshima, H. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 1244-1247 (*synth, pmr, cmr*)

DTX 5a D-1263

[172923-84-1]



n = 1

$C_{65}H_{101}NO_{27}S_2$ 1392.635

Isol. from the dinoflagellate *Prorocentrum maculosum*. Serine phosphatase inhibitor, allelopathic agent, phycotoxin. Sol. H_2O.

Hu, T. *et al., Tet. Lett.*, 1995, **36**, 9273-9276 (*isol, struct*)
Macpherson, G.R. *et al., J.O.C.*, 2003, **68**, 1659-1664 (*biosynth*)

DTX 5b D-1264

[172960-97-3]

As DTX 5a, D-1263 with

n = 2

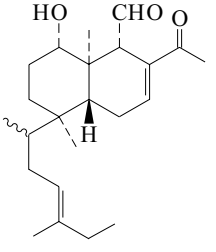
$C_{66}H_{103}NO_{27}S_2$ 1406.662

Isol. from dinoflagellate *Prorocentrum maculosum*. Serine phosphatase inhibitor, allelopathic agent, phycotoxin. Sol. H_2O.

Hu, T. *et al., Tet. Lett.*, 1995, **36**, 9273-9276 (*isol, struct*)
Macpherson, G.R. *et al., J.O.C.*, 2003, **68**, 1659-1664 (*biosynth*)

Durbinal B D-1265

[165337-79-1]



$C_{23}H_{36}O_3$ 360.536

Constit. of a *Psammoclemma* sp. Oil. $[\alpha]_D$ -12.5 (c, 1.4 in $CHCl_3$). Genus name given as alternative sp. Psammoclema.

Ac: ***Durbinal A***

[165406-95-1]

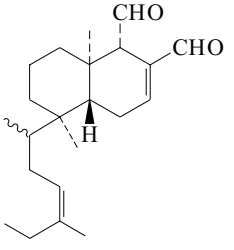
$C_{25}H_{38}O_4$ 402.573

Constit. of a *Psammoclemma* sp. Oil. $[\alpha]_D$ +5.6 (c, 2.5 in $CHCl_3$).

Rudi, A. *et al., Tet. Lett.*, 1995, **36**, 4853 (*isol, pmr, cmr*)

Durbinal C D-1266

[165337-80-4]



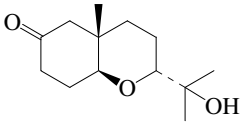
$C_{22}H_{34}O_2$ 330.509

Constit. of a *Psammoclemma* sp. Oil. $[\alpha]_D$ -14.5 (c, 0.9 in $CHCl_3$). Genus name given as alternative spelling Psammoclema.

Rudi, A. *et al., Tet. Lett.*, 1995, **36**, 4853 (*isol, pmr, cmr*)

Durgamone D-1267

[233607-67-5]

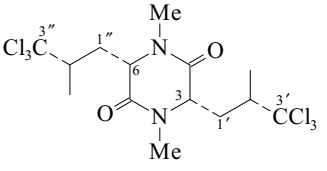


$C_{13}H_{22}O_3$ 226.315
Constit. of *Ptilocaulis spiculifer*. Oil. $[\alpha]_D$ -28.5 (c, 0.1 in MeOH). Probably derived from Abudinol, A-28.

Rudi, A. *et al., Tetrahedron*, 1999, **55**, 5555-5566 (*isol, pmr, cmr*)

Dysamide A D-1268

[149377-31-1]



$C_{14}H_{20}Cl_6N_2O_2$ 461.04
Alkaloid from the sponge *Dysidea fragilis* and a coelenterate *Zoanthus* sp. Osteoporotic agent. Prisms (Me_2CO/petrol).
Mp 118-119°. $[\alpha]_D$ -36.6 (c, 0.265 in MeOH).

*1′,3-Didehydro(*E*-):* ***1,4-Dimethyl-3-(3,3,3-trichloro-2-methylpropyl)-6-(3,3,3-trichloro-2-methylpropylidene)-2,5-piperazinedione, 9CI. Dihydrodysamide C***
[70359-79-4]
$C_{14}H_{18}Cl_6N_2O_2$ 459.025
Isol. from the sponge *Dysidea herbacea*.
Mp 106-107°. $[\alpha]_D^{20}$ -144 (c, 0.5 in $CHCl_3$).

*1′,3-Didehydro(*E*-), N^1-de-Me:* ***N^1-Demethyldihydrodysamide C***
[320425-24-9]
[149732-67-2]
$C_{13}H_{16}Cl_6N_2O_2$ 444.998
Alkaloid from *Dysidea herbacea*.
$[\alpha]_D$ -93.3 (c, 1.84 in $CHCl_3$).

*1′,3-Didehydro(*Z*-):* ***Dysamide I***
[213817-92-6]
$C_{14}H_{18}Cl_6N_2O_2$ 459.025
Alkaloid from *Dysidea chlorea*.
$[\alpha]_D$ -135.9 (c, 0.85 in EtOH).

*1′,1″,3,6-Tetradehydro(3*E*,6*Z*-):* ***Dysamide C***
[149355-71-5]
$C_{14}H_{16}Cl_6N_2O_2$ 457.009
Alkaloid from *Dysidea fragilis*. Needles (Me_2CO/petrol, 1:2).
Mp 196-197°. $[\alpha]_D$ -7.3 (c, 0.041 in MeOH).

*1′,1″,3,6-Tetradehydro(*Z,Z*-):* ***Dysamide E***
[161754-34-3]
$C_{14}H_{16}Cl_6N_2O_2$ 457.009
Isol. from *Dysidea fragilis*. Needles. $[\alpha]_D$ -308 (c, 0.54 in EtOH).

3ξ-Hydroxy: ***Dysamide P***
[213817-99-3]
$C_{14}H_{20}Cl_6N_2O_3$ 477.04
Alkaloid from *Dysidea chlorea*.
$[\alpha]_D$ -19.3 (c, 1.15 in EtOH/CH_2Cl_2).

*4″-Hydroxy, 1′,3-didehydro(*E*-):* ***Dysamide O***
[213817-98-2]
$C_{14}H_{18}Cl_6N_2O_3$ 475.024
Alkaloid from *Dysidea chlorea*.
$[\alpha]_D$ -80.8 (c, 0.13 in EtOH).

*6ξ-Hydroxy, 1′,3-didehydro(*E*-):* ***Dysamide Q***
[213818-00-9]
$C_{14}H_{18}Cl_6N_2O_3$ 475.024
Alkaloid from *Dysidea chlorea*. Isol. as a mixture with its C-6 epimer, Dysamide R.

*6ξ-Hydroxy, 1′,3-didehydro(*Z*-)(1):* ***Dysamide S***
[213818-02-1]
[213818-03-2]
$C_{14}H_{18}Cl_6N_2O_3$ 475.024
Alkaloid from *Dysidea chlorea*. Isol. as a mixture with its C-6 epimer, Dysamide T.

*6ξ-Hydroxy, 1′,3-didehydro(*Z*-)(2): Dysamide T*
$C_{14}H_{18}Cl_6N_2O_3$ 475.024
Alkaloid from *Dysidea chlorea*.

3′-Dechloro: ***Dysamide D***
[190510-98-6]
$C_{14}H_{21}Cl_5N_2O_2$ 426.596
Isol. from *Dysidea fragilis*. Needles (Et_2O).
Mp 141-142°. $[\alpha]_D$ +4 (c, 1.5 in $CHCl_3$).

*3′-Dechloro, 1′,3-didehydro(*Z*-):* ***Dysamide N***
[213817-97-1]
$C_{14}H_{19}Cl_5N_2O_2$ 424.58
Alkaloid from *Dysidea chlorea*.
$[\alpha]_D$ -50 (c, 0.04 in EtOH).

*3′-Dechloro, 1′,2′,3,3′-tetradehydro(*Z*-):* ***Dysamide J***
[213685-90-6]
$C_{14}H_{17}Cl_5N_2O_2$ 422.564
Alkaloid from *Dysidea chlorea*.
$[\alpha]_D$ -186.8 (c, 0.19 in EtOH). λ_{max} 270 (ε 6960) (EtOH).

*3″-Dechloro, 1′,3-didehydro(*E*-):* ***Dysamide K***
[213817-94-8]
$C_{14}H_{19}Cl_5N_2O_2$ 424.58
Alkaloid from *Dysidea chlorea*.
$[\alpha]_D$ -72.7 (c, 0.33 in EtOH).

*3″-Dechloro, 1′,3-didehydro(*Z*-):* ***Dysamide L***
[213817-95-9]
$C_{14}H_{19}Cl_5N_2O_2$ 424.58
Alkaloid from *Dysidea chlorea*.
$[\alpha]_D$ -63.3 (c, 0.12 in EtOH).

3′,3″-Didechloro: ***Dysamide B***
[149355-70-4]
$C_{14}H_{22}Cl_4N_2O_2$ 392.151
Alkaloid from *Dysidea fragilis*. Needles (Me_2CO/petrol, 1:1).
Mp 147-149°. $[\alpha]_D$ +13.7 (c, 0.117 in MeOH).

*3′,3″-Didechloro, 1′,3-didehydro(*E*-):* ***Didechlorodihydrodysamide C***
[210356-27-7]
$C_{14}H_{20}Cl_4N_2O_2$ 390.135
Alkaloid from *Dysidea herbacea*.
$[\alpha]_D$ +2.4 (c, 0.13 in $CHCl_3$).

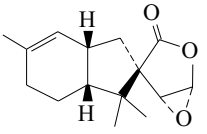
*3′,3″-Didechloro, 1′,3-didehydro(*Z*-):* ***Dysamide M***
[213817-96-0]
$C_{14}H_{20}Cl_4N_2O_2$ 390.135
Alkaloid from *Dysidea chlorea*.
$[\alpha]_D$ -35 (c, 0.2 in EtOH).

*3′,3″,3″-Tridechloro, 1′,3-didehydro(*E*-):* ***Dysamide U***
[320592-93-6]
$C_{14}H_{21}Cl_3N_2O_2$ 355.69
Alkaloid from *Dysidea* sp.
$[\alpha]_D$ -23 (c, 0.05 in EtOH).

Kazlauskas, R. *et al., Tet. Lett.*, 1978, 4945-4948 (*pmr, cmr, struct*)
Su, J.Y. *et al., J. Nat. Prod.*, 1993, **56**, 637-642 (*isol, ir, pmr, cmr, ms, cryst struct, Dysamides A-C*)
Su, J.Y. *et al., Huaxue Xuebao*, 1995, **53**, 90; *CA*, **122**, 183509c (*Dysamide E*)
Dumdei, E.J. *et al., Aust. J. Chem.*, 1997, **50**, 139-144 (*Dihydrodysamides C, Demethyldihydrodysamide C*)
Fu, X. *et al., J. Nat. Prod.*, 1997, **60**, 695-696; 1998, **61**, 1226-1231 (*Dysamides D,E,I-T*)
Fu, X. *et al., Chin. J. Chem.*, 2000, **18**, 882-885 (*Dysamide U*)
Durow, A.C. *et al., Org. Lett.*, 2006, **8**, 5401-5404 (*synth*)

Dysetherin D-1269

[97920-19-9]

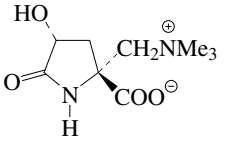


$C_{15}H_{20}O_3$ 248.321
Constit. of *Dysidea etheria*. Oil. $[\alpha]_D$ -28.5 (c, 0.85 in $CHCl_3$).

Schram, T.J. *et al., J.O.C.*, 1985, **50**, 4155
Cameron, G.M. *et al., Tetrahedron*, 2000, **56**, 5247-5252 (*pmr, cmr*)

Dysibetaine D-1270

[247166-12-7]

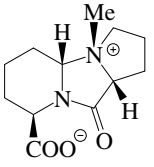


Relative Configuration

$C_9H_{16}N_2O_4$ 216.236
Isol. from the marine sponge *Dysidea herbacea*.
$[\alpha]_D^{20}$ -7.3 (c, 0.26 in H_2O).

Sakai, R. *et al., Tet. Lett.*, 1999, **40**, 6941-6944 (*isol, pmr, cmr, cryst struct*)
Snider, B.B *et al., Org. Lett.*, 2001, **3**, 1761-1763 (*synth*)
Wardrop, D.J. *et al., Chem. Comm.*, 2004, 1230-1231 (*synth*)
Langlois, N. *et al., J.O.C.*, 2004, **69**, 7558-7564 (*synth*)

Dysibetaine PP D-1271



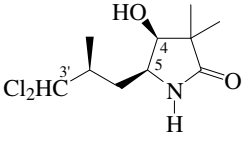
Relative Configuration

$C_{12}H_{18}N_2O_3$ 238.286
Isol. from the marine sponge *Dysidea herbacea*. Amorph. solid.
$[\alpha]_D^{18}$ -70.3 (c, 0.24 in H_2O).

Sakai, R. *et al., J.O.C.*, 2004, **69**, 1180-1185 (*isol, pmr, cmr*)
Ijzendoorn, D.R. *et al., Org. Lett.*, 2006, **8**, 239-242 (*synth*)

Dysidamide C D-1272

5-(3,3-Dichloro-2-methylpropyl)-4-hydroxy-3,3-dimethyl-2-pyrrolidinone, 9CI
[133738-40-6]



Absolute Configuration

$C_{10}H_{17}Cl_2NO_2$ 254.155
Constit. of the Red Sea sponge *Lamellodysidea herbacea*. Needles.
$[\alpha]_D$ -41 (c, 1 in MeOH).

N-*(4,4-Dichloro-3-methylbutanoyl):* ***Dysidamide B***
[133738-39-3]
$C_{15}H_{23}Cl_4NO_3$ 407.162
Constit. of *Lamellodysidea herbacea*.
$[\alpha]_D$ +6 (c, 0.16 in $CHCl_3$).

N-*(4,4,4-Trichloro-3ξ-methylbutanoyl):* ***Dysidamide E***
$C_{15}H_{22}Cl_5NO_3$ 441.607
Constit. of *Lamellodysidea herbacea*. Glass. $[\alpha]_D$ -3.5 (c, 0.3 in CH_2Cl_2).

3′-Chloro: ***Dysidamide F***
$C_{10}H_{16}Cl_3NO_2$ 288.6
Constit. of *Lamellodysidea herbacea*. Needles.
Mp 171-172°. $[\alpha]_D$ -36 (c, 0.84 in CH_2Cl_2).

3′-Chloro, N-*(4,4-dichloro-3ξ-methylbutanoyl):* ***Dysidamide D***
$C_{15}H_{22}Cl_5NO_3$ 441.607
Constit. of *Lamellodysidea herbacea*. Glass. $[\alpha]_D$ -4 (c, 0.15 in CH_2Cl_2).

3′-Chloro, N-*(4,4,4-trichloro-3*S*-methylbutanoyl): 4-Hydroxy-3,3-dimethyl-1-(4,4,4-trichloro-3-methyl-1-oxobutyl)-5-(3,3,3-trichloro-2-methylpropyl)-2-pyrrolidinone, 9CI.* ***Dysidamide***
[117694-99-2]
$C_{15}H_{21}Cl_6NO_3$ 476.052
Alkaloid from the Red Sea sponge *Lamellodysidea herbacea*.
Neurotoxin. Needles (petrol).
Mp 133° (123-124°). $[\alpha]_D$ -16.1 (c, 2.76 in CH_2Cl_2).

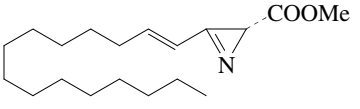
3′-Chloro, 4-ketone: ***Dysidamide G***
$C_{10}H_{14}Cl_3NO_2$ 286.584
Constit. of *Lamellodysidea herbacea*. Needles.
Mp 109°. $[\alpha]_D$ -38.5 (c, 0.75 in CH_2Cl_2). Data refers to mixt. with 5-epimer.

3′-Chloro, 4-ketone, N-*(4,4,4-trichloro-3ξ-methylbutanoyl):* ***Dysidamide H***
$C_{15}H_{19}Cl_6NO_3$ 474.036
Constit. of *Lamellodysidea herbacea*. Glass. $[\alpha]_D$ -62.8 (c, 0.6 in CH_2Cl_2).

5-Epimer, 3′-chloro, 4-ketone: ***5-Epidysidamide G***
$C_{10}H_{14}Cl_3NO_2$ 286.584
Constit. of *Lamellodysidea herbacea*. Isol. as a mixt. with 5-epimer.

Carmely, S. *et al., Aust. J. Chem.*, 1990, **43**, 1881-1883 (*Dysidamide*)
Isaacs, S. *et al., J. Nat. Prod.*, 1991, **54**, 83-91 (*isol, pmr, cmr, ms*)
Sauleau, P. *et al., Tetrahedron*, 2005, **61**, 955-963 (*isol, pmr, cmr*)

Dysidazirine D-1273



(*R,E*)-*form*

$C_{19}H_{33}NO_2$ 307.475

(*R,E*)-*form* [113507-74-7]
Isol. from Fijian marine sponge, *Dysidea fragilis*.
Low melting solid. Sol. MeOH, $CHCl_3$. $[\alpha]_D$ -165 (c, 0.5 in MeOH). λ_{max} 222 (ϵ 16600) (MeOH) (Berdy).
► Cytotoxic.

(*S,E*)-*form* [163013-15-8]
From *Dysidea fragilis*.
Oil. $[\alpha]_D$ +47.2 (c, 1.08 in $CHCl_3$). Erroneous MF in paper.

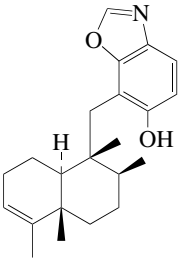
(*Z*)-*form* [172140-90-8]
Minor constit. of *Dysidea fragilis*.
Oil. C-2 config. not detd.

Molinski, T.F. *et al., J.O.C.*, 1988, **53**, 2103 (*isol, uv, pmr, ms, abs config*)
Salomon, C.E. *et al., J. Nat. Prod.*, 1995, **58**, 1463 (*isol, uv, ir, pmr, cmr, ms, cd*)
Davis, F.A. *et al., J.A.C.S.*, 1995, **117**, 3651 (*synth*)

Dysidea benzoxazole D-1274

7-[(1,2,3,4,4a,7,8,8a-Octahydro-1,2,4a,5-tetramethyl-1-naphthalenyl)methyl]-6-benzoxazolol, 9CI

[193157-85-6]



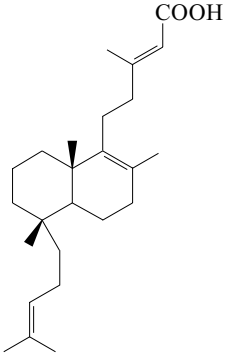
$C_{22}H_{29}NO_2$ 339.477

Not named in paper. Related to Avarol, A-766. Constit. of a *Dysidea* sp. Oil.

Stewart, M. *et al., Aust. J. Chem.*, 1997, **50**, 341-347 (*isol, pmr, cmr*)

Dysideapalaunic acid D-1275

[116002-89-2]



$C_{25}H_{40}O_2$ 372.59

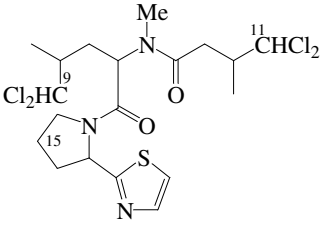
Metab. of a *Dysidea* sp. Inhibits aldose reductase. Oil. $[\alpha]_D$ +61 ($CHCl_3$).

Nakagawa, M. *et al., Abstr. Pap. Symp. Chem. Nat. Prod. Jpn., 28th*, 1986, 200; *CA*, **106**, 96126b (*isol, activity*)

Hagiwara, H. *et al., J.C.S. Perkin 1*, 1991, 343-350 (*synth, struct, abs config*)

Singh, M. *et al., Planta Med.*, 1999, **65**, 2-8 (*rev*)

Dysideaproline A D-1276



$C_{19}H_{27}Cl_4N_3O_2S$ 503.318

Similar to Dysidenin, D-1280. Isol. from a *Dysidea* sp. Pale yellow oil. $[\alpha]_D^{23}$ +16.5 (c, 0.02 in MeOH). λ_{max} 213 (ϵ 8295); 239 (ϵ 4400) (MeOH).

N-*De-Me:* ***Dysideaproline C***

$C_{18}H_{25}Cl_4N_3O_2S$ 489.291

Isol. from a *Dysidea* sp. Pale yellow oil. $[\alpha]_D^{23}$ +23.5 (c, 0.02 in MeOH). λ_{max} 212 (ϵ 6210); 239 (ϵ 3920) (MeOH).

9-Dechloro: ***Dysideaproline F***

$C_{19}H_{28}Cl_3N_3O_2S$ 468.873

Isol. from a *Dysidea* sp. Pale yellow oil. $[\alpha]_D^{23}$ +18.8 (c, 0.02 in MeOH). λ_{max} 215 (ϵ 6040); 236 (ϵ 4135) (MeOH).

11-Dechloro: ***Dysideaproline D***

$C_{19}H_{28}Cl_3N_3O_2S$ 468.873

Isol. from a *Dysidea* sp. Pale yellow oil. $[\alpha]_D^{23}$ +28.8 (c, 0.02 in MeOH). λ_{max} 215 (ϵ 5800); 237 (ϵ 4095) (MeOH).

9,9-Bis(dechloro): ***Dysideaproline E***

$C_{19}H_{29}Cl_2N_3O_2S$ 434.428

Isol. from a *Dysidea* sp. Pale yellow oil. $[\alpha]_D^{23}$ +45.5 (c, 0.02 in MeOH). λ_{max} 214 (ϵ 5500); 235 (ϵ 4335) (MeOH).

15-Methyl: ***Dysideaproline B***

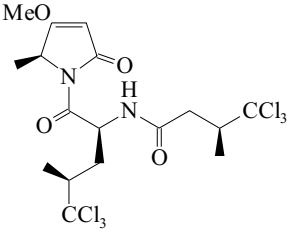
$C_{20}H_{29}Cl_4N_3O_2S$ 517.345

Isol. from a *Dysidea* sp. Pale yellow oil. $[\alpha]_D^{23}$ +37.5 (c, 0.02 in MeOH). λ_{max} 214 (ϵ 5885); 240 (ϵ 3270) (MeOH).

Harrigan, G.G. *et al., J. Nat. Prod.*, 2001, **64**, 1133-1138

Dysideapyrrolidone D-1277

[151805-42-4]



$C_{17}H_{22}Cl_6N_2O_4$ 531.088

Isol. from the marine sponge *Dysidea herbacea* (Dictyoceratida). Feeding deterrent. Prisms.

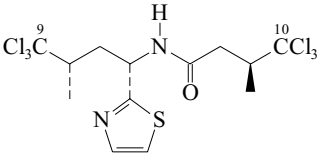
Mp 165-166°. $[\alpha]_D$ +16.6 (c, 0.4 in $CHCl_3$). λ_{max} 215 (ϵ 5100); 238 (ϵ 14000) ($CHCl_3$). λ_{max} 215 (ϵ 5100); 238 (ϵ 14000) (MeOH) (Berdy).

Unson, M.D. *et al., J.O.C.*, 1993, **58**, 6336 (*isol, uv, ir, pmr, cmr*)

Dysideathiazole D-1278

*4,4,4-Trichloro-3-methyl-*N*-[4,4,4-trichloro-3-methyl-1-(2-thiazolyl)butyl]butanamide, 9CI*

[151805-43-5]



$C_{13}H_{16}Cl_6N_2OS$ 461.064

Isol. from the marine sponge *Dysidea herbacea* (Dictyoceratida). Feeding deterrent. Needles.

Mp 176-177°. $[\alpha]_D$ -71.8 (c, 2 in $CHCl_3$). λ_{max} 202 (ϵ 6865); 241 (ϵ 5900) ($CHCl_3$). λ_{max} 202 (ϵ 6865); 241 (ϵ 5900) (MeOH) (Berdy).

N-*Me:* **N-*Methyldysideathiazole***

[151805-44-6]

$C_{14}H_{18}Cl_6N_2OS$ 475.091

Isol. from *Dysidea herbacea*. Feeding deterrent. Needles.

Mp 96°. $[\alpha]_D$ -108.3 (c, 2 in $CHCl_3$). λ_{max} 205 (ϵ 6530); 243 (ϵ 4325) ($CHCl_3$). λ_{max} 205 (ϵ 6530); 243 (ϵ 4325) (MeOH) (Berdy).

10-Dechloro: ***10-Dechlorodysideathiazole***

[151805-45-7]

$C_{13}H_{17}Cl_5N_2OS$ 426.62

Isol. from *Dysidea herbacea*. Feeding deterrent. Oil. $[\alpha]_D$ -57.5 (c, 0.6 in $CHCl_3$). λ_{max} 245 (ϵ 4040) ($CHCl_3$). λ_{max} 244 (ϵ 4040) (MeOH) (Berdy).

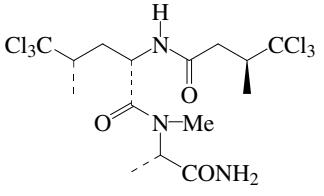
10-Dechloro, N-*Me:* ***10-Dechloro-N-methyldysideathiazole***
[151805-46-8]
$C_{14}H_{19}Cl_5N_2OS$ 440.646
Isol. from *Dysidea herbacea*. Feeding deterrent. Prisms. Mp 118-119°. $[\alpha]_D$ -98.9 (c, 0.5 in $CHCl_3$). λ_{max} 245 (ϵ 4040) ($CHCl_3$). λ_{max} 244 (ϵ 4040) (MeOH) (Berdy).

9,10-Bisdechloro, N-*Me:* ***9,10-Didechloro-N-methyldysideathiazole***
[151805-47-9]
$C_{14}H_{20}Cl_4N_2OS$ 406.202
Isol. from *Dysidea herbacea*. Feeding deterrent. Oil. $[\alpha]_D$ -79.9 (c, 3.2 in $CHCl_3$). λ_{max} 214 (ϵ 4270); 241 (ϵ 4880) ($CHCl_3$). λ_{max} 214 (ϵ 4270); 241 (ϵ 4880) (MeOH) (Berdy).

[151908-88-2]

Unson, M.D. *et al., J.O.C.*, 1993, **58**, 6336-6343 (*isol, uv, ir, pmr, cmr, cryst struct*)

Dysidenamide D-1279

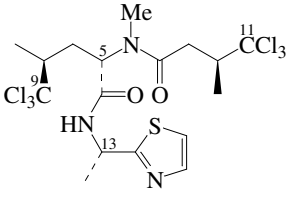


$C_{15}H_{23}Cl_6N_3O_3$ 506.081
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D$ -40.3 (c, 0.96 in CH_2Cl_2). Related to Dysidenin, D-1280.

Jimenez, J.I. *et al., J. Nat. Prod.*, 2001, **64**, 200-203

Dysidenin D-1280

5,5,5-Trichloro-4-methyl-2-[methyl(4,4,4-trichloro-3-methyl-1-oxobutyl)amino]-N-*[1-(2-thiazolyl)ethyl]pentanamide, 9CI*
[65647-65-6]



$C_{17}H_{23}Cl_6N_3O_2S$ 546.17
Peptide antibiotic. Metab. of the sponge *Dysidea herbacea* from the Great Barrier Reef; also isol. in small amt. from a specimen from the New Guinea coast. Shows antibiotic props. Ichthyotoxin. Iodine transport inhibitor. Needles (hexane). Sol. MeOH, $CHCl_3$.
Mp 98-99°. $[\alpha]_D^{21}$ -98 (c, 0.5 in $CHCl_3$). λ_{max} 240 (ϵ 3980) (MeOH) (Derep).

N^6-*De-Me:* ***Nordysidenin***
[331970-05-9]
$C_{16}H_{21}Cl_6N_3O_2S$ 532.143
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D$ -56.7 (c, 0.76 in CH_2Cl_2).

N^6-*De-Me,* N^{12}-*Me:* ***Pseudodysidenin***
[331970-03-7]
[383898-07-5]
$C_{17}H_{23}Cl_6N_3O_2S$ 546.17
Isol. from *Lyngbya majuscula*. Cryst. $[\alpha]_D$ -96.9 (c, 0.03 in $CHCl_3$).

5-Epimer: ***Isodysidenin***
[67528-34-1]
$C_{17}H_{23}Cl_6N_3O_2S$ 546.17
Toxic constit. of *Dysidea herbacea* from New Guinea. Ichthyotoxin. Iodine transport inhibitor. Amorph. solid. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{22}$ +47 (c, 0.88 in $CHCl_3$). λ_{max} 240 (ϵ 3980) (MeOH) (Derep). λ_{max} 238 (ϵ 3311) (MeOH) (Berdy).

13-Epimer: ***Neodysidenin***
[294638-50-9]
$C_{17}H_{23}Cl_6N_3O_2S$ 546.17
Isol. from *Dysidea herbacea*.
$[\alpha]_D$ -52.1 (c, 0.16 in $CHCl_3$). λ_{max} 241 (ϵ 4300) (MeOH).

13-Demethyl: ***13-Demethyldysidenin***
[81801-19-6]
$C_{16}H_{21}Cl_6N_3O_2S$ 532.143
From *Dysidea herbacea* (Great Barrier Reef). Gum. $[\alpha]_D^{20}$ -97 (c, 1.23 in $CHCl_3$). λ_{max} 240 (ϵ 3980) (MeOH) (Derep).

13-Demethyl, 5-epimer: ***13-Demethylisodysidenin***
[81754-76-9]
$C_{16}H_{21}Cl_6N_3O_2S$ 532.143
From *Dysidea herbacea* (Great Barrier Reef) and *Oscillatoria spongeliae*. Antihypertensive agent. Gum. $[\alpha]_D^{20}$ +52 (c, 2.6 in $CHCl_3$). λ_{max} 242 (ϵ 14000) (MeOH) (Berdy).

13-Demethyl, 5-epimer, 9-dechloro: ***9-Monodechloro-13-demethylisodysidenin***
[81754-77-0]
$C_{16}H_{22}Cl_5N_3O_2S$ 497.698
From *Dysidea herbacea* (Great Barrier Reef). Gum. $[\alpha]_D^{20}$ +69 (c, 0.27 in $CDCl_3$).

13-Demethyl, 5-epimer, 11-dechloro: ***11-Monodechloro-13-demethylisodysidenin***
[81747-68-4]
$C_{16}H_{22}Cl_5N_3O_2S$ 497.698
From *Dysidea herbacea* (Great Barrier Reef). Gum. $[\alpha]_D^{20}$ +85 (c, 1.04 in $CHCl_3$).

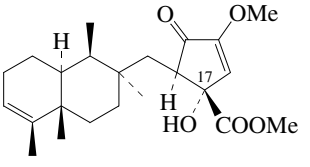
13-Demethyl, 5-epimer, 9,11-bisdechloro: ***9,11-Didechloro-13-demethylisodysidenin***
[189297-59-4]
$C_{16}H_{23}Cl_4N_3O_2S$ 463.253
From *Dysidea herbacea*.
$[\alpha]_D$ +174 (c, 0.04 in $CHCl_3$).

13-Demethyl, 13-isopropyl: [383898-06-4]
$C_{19}H_{27}Cl_6N_3O_2S$ 574.223
From *Dysidea herbacea*.

Kazlauskas, R. *et al., Tet. Lett.*, 1977, 3183 (*isol, ms, ir, uv, pmr, cmr, struct*)
Charles, C. *et al., Tet. Lett.*, 1978, 1519 (*isol, ir, pmr, struct, Isodysidenin*)
Erickson, K.L. *et al., Aust. J. Chem.*, 1982, **35**, 31 (*derivs*)
Biskupiak, J.E. *et al., Tet. Lett.*, 1984, **25**, 2935 (*abs config*)
Dumdei, E.J. *et al., Aust. J. Chem.*, 1997, **50**, 139-144 (*isol, derivs, pmr, cmr, ms*)
MacMillan, J.B. *et al., Org. Lett.*, 2000, **2**, 2721-2723 (*Neodysidenin*)
Dumrongchai, N. *et al., ACGC Chem. Res. Commun.*, 2001, **13**, 17-22; *CA*, 2002, **136**, 67123n (*13-de-Me-13-isopropyl*)
Jimenez, J.I. *et al., J. Nat. Prod.*, 2001, **64**, 200-203 (*Nordysidenin, Pseudodysidenin*)

Dysidenone A D-1281

[346706-48-7]



$C_{23}H_{34}O_5$ 390.519
Constit. of a *Dysidea* sp. Amorph. λ_{max} 250 (log ϵ 3.6) (MeOH).

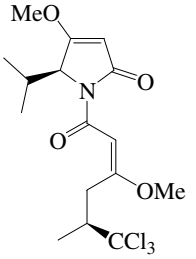
17-Epimer: ***Dysidenone B***
[346706-49-8]
$C_{23}H_{34}O_5$ 390.519
Constit. of a *Dysidea* sp. Amorph.

Giannini, C. *et al., J. Nat. Prod.*, 2001, **64**, 612-615 (*isol, pmr, cmr*)

Dysidine† D-1282

1,5-Dihydro-4-methoxy-5-(1-methylethyl)-1-(6,6,6-trichloro-3-methoxy-5-methyl-1-oxo-2-hexenyl)-2H-pyrrol-2-one, 9CI

[63079-71-0]



Absolute Configuration

$C_{16}H_{22}Cl_3NO_4$ 398.712

Constit. of the marine sponge *Dysidea herbacea* and prod. by *Streptomyces galilaeus* ATCC 31534. Shows antibiotic props. Needles (hexane). Sol. MeOH, acids, C_6H_6, DMSO, $CHCl_3$; poorly sol. H_2O, hexane.

Mp 127-129°. $[\alpha]_D^{25}$ +141 (c, 1 in $CHCl_3$). λ_{max} 226 (ϵ 15850); 264 (ϵ 26920) (EtOH) (Derep). λ_{max} 228 (E1%/1cm 570); 258 (E1%/1cm 375); 288 (E1%/1cm 145); 433 (E1%/1cm 160) (MeOH) (Berdy). λ_{max} 239 (E1%/1cm 588); 288 (E1%/1cm 160); 315 (E1%/1cm 80); 525 (E1%/1cm 175) (MeOH/NaOH) (Berdy).

▶ LD_{50} (mus, ipr) 40 - 80 mg/kg.

(-)-*form*

Synthetic.

Needles (hexane). Mp 130°. $[\alpha]_D$ -139 (c, 0.3 in $CHCl_3$).

(ξ)-*form*

[91279-96-8]

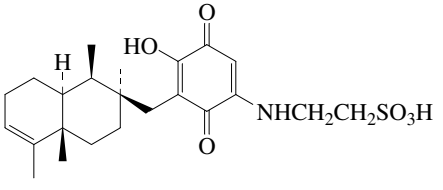
Trace constit. of *Carteriospongia flabellifera*.

[91279-96-8]

Hofheinz, W. *et al., Helv. Chim. Acta*, 1977, **60**, 660 (*isol, uv, cd, ir, pmr, cmr, ms, abs config, cryst struct*)
Köhler, H. *et al., Helv. Chim. Acta*, 1984, **67**, 1783 (*synth*)
Williard, P.G. *et al., J.O.C.*, 1984, **49**, 3489 (*synth, ir, pmr, cmr*)
Schmitz, F.J. *et al., J. Nat. Prod.*, 1988, **51**, 745-748; 1112 (*isol*)

Dysidine† D-1283

[346706-47-6]



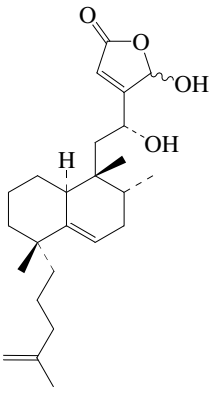
$C_{23}H_{33}NO_6S$ 451.583

Not to be confused with Dysidine, D-1282. Isol. from a sponge, *Dysidea* sp. Inhibitor of human phospholipase A_2. Deep purple cryst. $[\alpha]_D^{25}$ +19 (c, 1 in MeOH). λ_{max} 228 (log ϵ 4.43); 334 (log ϵ 4.15) (EtOH).

Giannini, C. *et al., J. Nat. Prod.*, 2001, **64**, 612-615

Dysidiolide D-1284

[182136-94-3]



$C_{25}H_{38}O_4$ 402.573

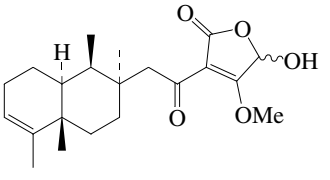
Constit. of *Dysidea etheria*. Inhibitor of protein phosphatase CDC25A. Cytotoxic agent. Shows antitumour activity. Cryst. ($MeOH/CH_2Cl_2$).

Mp 186-187°. $[\alpha]_D^{24}$ -11.1 (c, 0.6 in CH_2Cl_2/MeOH). Related to Cladocoran B, C-668.

Gunasekera, S.P. *et al., J.A.C.S.*, 1996, **118**, 8759-8760 (*isol, pmr, cmr, cryst struct*)
Corey, E.J. *et al., J.A.C.S.*, 1997, **119**, 12425-12431 (*synth*)
Boukoulvalas, J. *et al., J.O.C.*, 1998, **63**, 228-229 (*synth*)
Takahashi, M. *et al., Bioorg. Med. Chem. Lett.*, 2000, **10**, 2571-2574 (*activity*)
Piers, E. *et al., Org. Lett.*, 2000, **2**, 2483-2486 (*synth*)
Paczkowski, R. *et al., Org. Lett.*, 2000, **2**, 3967-3969 (*synth*)
Takahashi, M. *et al., Tet. Lett.*, 2000, **41**, 2111-2114 (*synth*)
Miyaoka, H. *et al., J.O.C.*, 2001, **66**, 1429-1435 (*synth*)
Jung, M.E. *et al., Org. Lett.*, 2001, **3**, 2113-2115 (*synth*)
Demeke, D. *et al., Tetrahedron*, 2002, **58**, 6531-6544 (*synth*)
Kaliappan, K.P. *et al., Tet. Lett.*, 2004, **45**, 8207-8209 (*synth*)

Dysidotronic acid D-1285

[281664-79-7]



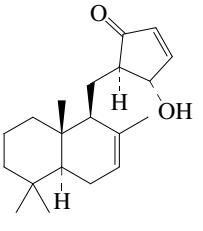
$C_{21}H_{30}O_5$ 362.465

Constit. of a *Dysidea* sp. Human phospholipase A_2 inhibitor. Solid. $[\alpha]_D$ +44.7.

Giannini, C. *et al., Tet. Lett.*, 2000, **41**, 3257-3260 (*isol, pmr, cmr*)

Dysienone D-1286

[852931-99-8]



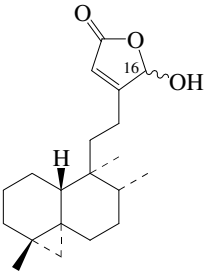
$C_{20}H_{30}O_2$ 302.456

Constit. of a *Dysidea* sp. Yellow oil. $[\alpha]_D^{25}$ -12.5 (c, 0.07 in $CHCl_3$).

Pérez-García, E. *et al., J. Nat. Prod.*, 2005, **68**, 653-658 (*Dysienone*)

Dysifragin D-1287

[252721-96-3]

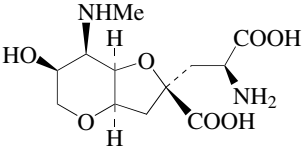


$C_{15}H_{26}O_2$ 238.369
Constit. of *Dysidea fragilis.*
$[\alpha]_D^{21}$ +13 (c, 1.3 in $CHCl_3$) (synthetic).

Shen, Y.-C. *et al., Chin. Pharm. J. (Taipei)*, 1999, **51**, 213-218; *CA*, **132**, 47791t (*isol, pmr, cmr*)
Uyanik, M. *et al., Bioorg. Med. Chem.*, 2005, **13**, 5055-5065 (*synth, cryst struct, abs config, pmr, cmr*)

Dysiherbaine D-1288

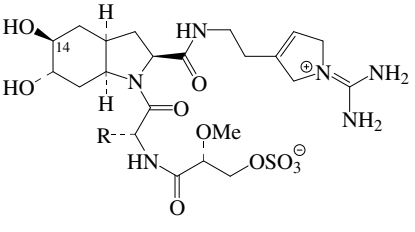
[185245-55-0]



$C_{12}H_{20}N_2O_7$ 304.299
Zwitterionic amino acid. Isol. from the sponge *Dysidea herbacea.* Neurotoxin. $[\alpha]_D^{26}$ -3.5 (c, 0.4 in H_2O).

Sakai, R. *et al., J.A.C.S.*, 1997, **119**, 4112 (*isol, ir, pmr, cmr*)
Masaki, H. *et al., J.A.C.S.*, 2000, **122**, 5216-5217 (*synth*)
Snider, B.B. *et al., Org. Lett.*, 2000, **2**, 635-638 (*synth*)
Sasaki, M. *et al., Tet. Lett.*, 2000, **41**, 3923-3926 (*synth*)
Phillips, D. *et al., J.O.C.*, 2002, **67**, 3194-3201 (*synth*)

Dysinosin A D-1289



Absolute Configuration

R = -$CH_2CH(CH_3)_2$

$C_{26}H_{44}N_6O_{10}S$ 632.734
Isol. from an Australian sponge of the family Dysideidae. Inhibitor of Factor VIIa and thrombin. Amorph. solid.

Carroll, A.R. *et al., J.A.C.S.*, 2002, **124**, 13340-13341 (*isol, struct*)
Hanessian, S. *et al., J.A.C.S.*, 2002, **124**, 13342-13343 (*synth*)

Dysinosin C D-1290

As Dysinosin A, D-1289 with
R = -$CH(CH_3)_2$

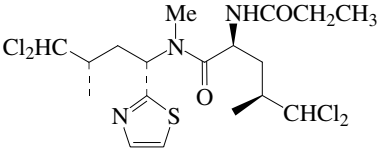
$C_{25}H_{42}N_6O_{10}S$ 618.707
Isol. from the sponge *Lamellodysidea chlorea*. Inhibitor of factor VIa and thrombin. Amorph. solid. Stereochem. not confirmed. λ_{max} 202 (log ϵ 3.92) (MeOH).

De-O-*sulfo:* ***Dysinosin D***
$C_{25}H_{42}N_6O_7$ 538.643
Isol. from *Lamellodysidea chlorea*. Amorph. solid.

14-O-α-D-*Glucopyranoside:* ***Dysinosin B***
$C_{31}H_{52}N_6O_{15}S$ 780.849
Isol. from *Lamellodysidea chlorea*. Amorph. solid. $[\alpha]_D^{25}$ +72 (c, 0.02 in MeOH). λ_{max} 203 (log ϵ 4.2) (MeOH).

Carroll, A.R. *et al., J. Nat. Prod.*, 2004, **67**, 1291-1294 (*isol, pmr, cmr*)

Dysithiazolamide D-1291



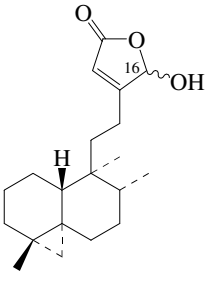
Absolute Configuration

$C_{18}H_{27}Cl_4N_3O_2S$ 491.307
Isol. from an unidentified *Dysidea* sp.
$[\alpha]_D$ -35 (c, 0.08 in CH_2Cl_2).

Ardá, A. *et al., Tetrahedron*, 2005, **61**, 10093-10098 (*isol, pmr, cmr*)

Dytesinin A D-1292

[309964-71-4]



$C_{20}H_{30}O_3$ 318.455
Constit. of a *Cystodytes* sp. Amorph. solid. $[\alpha]_D^{25}$ 0 (c, 1 in $CHCl_3$).

16-Deoxy: ***Dytesinin B***
[309964-72-5]
$C_{20}H_{30}O_2$ 302.456
Constit. of a *Cystodytes* sp. Amorph. solid. $[\alpha]_D^{25}$ -37 (c, 0.25 in $CHCl_3$). .

Shimbo, K. *et al., Tetrahedron*, 2000, **56**, 7923-7926 (*isol, pmr, cmr*)

Eburnetoxin E-1

[83382-09-6]

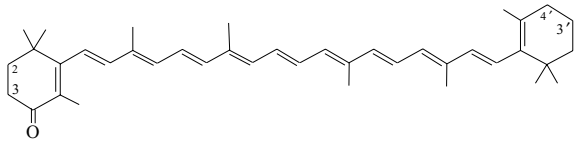
Protein. Isol. from venom of *Conus eburneus*. Vasoactive agent. Vasoconstrictor.

Kobayashi, J. *et al., Life Sci.*, 1982, **31**, 1085-1091 (*isol*)

Echinenone E-2

β,β-Caroten-4-one. Myxoxanthin. Aphanine. Echininone

[432-68-8]



$C_{40}H_{54}O$ 550.866

Orange pigment originally isol. from the gonads of sea urchins. Xanthophyll of cyanobacteria. Found in echinoids, crustacea, green algae and sponges. Violet cryst. (petrol).

Mp 178-179°.

4-Alcohol: ***Isocryptoxanthin****. β,β-Caroten-4-ol. 4-Hydroxy-β-carotene. Myxoxanthol. Aphanol*

[472-62-8]

$C_{40}H_{56}O$ 552.882

Isol. from blue-green algae.

2-Hydroxy: ***2-Hydroxyechinenone****. 2-Hydroxy-β,β-caroten-4-one*

[100459-63-0]

$C_{40}H_{54}O_2$ 566.865

Isol. from *Daphnia magna*.

3S-Hydroxy: ***3-Hydroxyechinenone***

[72843-12-0]

$C_{40}H_{54}O_2$ 566.865

Isol. from *Adonis annua*, *Rhizobium lupini*, fish eggs, algae. Prisms (Me_2CO/petrol).

Mp 155-157°. λ_{max} 457 (petrol). λ_{max} 466 (EtOH).

3′-Hydroxy: ***3′-Hydroxyechinenone***

[4481-36-1]

$C_{40}H_{54}O_2$ 566.865

Main carotenoid component of several genera of cyanobacteria, present as carotenoid-protein complex. Isol. from *Arthrospira* sp. λ_{max} 458 (Me_2CO). λ_{max} 450 (hexane).

4′-Hydroxy: ***4′-Hydroxyechinenone***

[2213-17-4]

$C_{40}H_{54}O_2$ 566.865

Isol. from the spindle shell *Fusinus perplexus*, goldfish eggs, green algae and other spp. Rosettes (Et_2O/petrol).

Mp 189-190° (175°). λ_{max} 458 (EtOH). λ_{max} 454 (petrol).

4′-Ethoxy: ***4′-Ethoxy-β,β-caroten-4-one****. 4′-Ethoxy-4-keto-β-carotene*

[54897-06-2]

$C_{42}H_{58}O_2$ 594.919

Occurs in the Echinodermata. Plates ($CHCl_3$/EtOH or C_6H_6/MeOH).

Mp 163-164° (154-156°). λ_{max} 459 (hexane).

3′,4′-Didehydro: ***3′,4′-Didehydro-β,β-caroten-4-one****. 4-Keto-3′,4′-dehydro-β-carotene*

[991-90-2]

$C_{40}H_{52}O$ 548.85

Occurs in the decapod crustacean *Xantho poressa*. Red-purple plates (C_6H_6/MeOH).

Mp 192-194°. Poss. artifact.

3′,4′-Didehydro, 4-alcohol: ***3′,4′-Didehydro-β,β-caroten-4-ol****. 3′,4′-Dehydro-4-hydroxy-β-carotene*

[4441-44-5]

$C_{40}H_{54}O$ 550.866

Isol. from *Pallasea cancelloides* from Lake Baikal. λ_{max} 460 (petrol).

[4339-77-9]

Goodwin, T.W. *et al., Biochem. J.*, 1956, **63**, 481
Petracek, F.J. *et al., J.A.C.S.*, 1956, **78**, 1427 (*synth*)
Entschel, R. *et al., Helv. Chim. Acta*, 1958, **41**, 402 (*synth*)
Akhtar, M. *et al., J.C.S.*, 1959, 4058 (*synth*)
Krinsky, N.I. *et al., Arch. Biochem. Biophys.*, 1960, **91**, 271 (*3-Hydroxyechinenone*)
Jansen, S.L. *et al., Acta Chem. Scand.*, 1965, **19**, 1166 (*synth, 4′-hydroxy*)
Egger, K. *et al., Phytochemistry*, 1965, **4**, 609 (*3-Hydroxyechinenone*)
Surmatis, J.D. *et al., Helv. Chim. Acta*, 1970, **53**, 974 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 1854 (*occur*)
Francis, G.W. *et al., Phytochemistry*, 1972, **11**, 2347 (*Isocryptoxanthin*)
Hsieh, L.K. *et al., J. Bacteriol.*, 1974, **118**, 385 (*biosynth*)
Czeczuga, B. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1975, **50**, 259 (*3′,4′-Didehydro-β,β-caroten-4-ol*)
Cooper, R.D.G. *et al., J.C.S. Perkin 1*, 1975, 2195 (*synth, 3-hydroxy*)
Czeczuga, B. *et al., Hydrobiologia*, 1977, **53**, 271 (*occur, deriv*)
Watts, C.D. *et al., Org. Mass Spectrom.*, 1978, **10**, 1102 (*ms*)
Beyer, P. *et al., Helv. Chim. Acta*, 1979, **62**, 2551 (*isol, 3-hydroxy*)
Holt, T.K. *et al., Biochim. Biophys. Acta*, 1981, **637**, 408 (*3′-hydroxy*)
Liaaen-Jensen, S. *et al., Biochem. Syst. Ecol.*, 1982, **10**, 167-174 (*occur, sponges*)
Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **81**, 905; 1986, **83**, 335 (*isol, 4′-hydroxy, 3-hydroxy*)
Foss, P. *et al., Acta Chem. Scand., Ser. B*, 1986, **40**, 157 (*2-Hydroxyechinenone*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 57; 282; 283; 294; 295 (*bibl*)

Echinobetaine A E-3

$MeOCH_2CH(COO^{\ominus})CH_2N^{\oplus}Me_3$

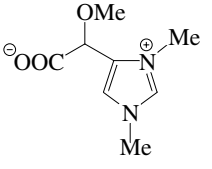
$C_8H_{17}NO_3$ 175.227

Isol. from the sponge *Echinodictyum* sp. Nematocide. $[\alpha]_D^{22}$ -49 (c, 0.6 in MeOH).

Capon, R.J. *et al., J. Nat. Prod.*, 2005, **68**, 179-182 (*isol, synth*)

Echinobetaine B E-4

*4-(Carboxymethoxymethyl)-1,3-dimethyl-1*H*-imidazolium hydroxide inner salt*



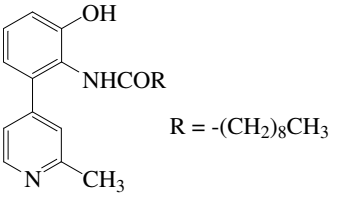
$C_8H_{12}N_2O_3$ 184.194

Positive charge delocalised over the two Ns. Isol. from the sponge *Echinodictyum* sp. Nematocidal agent. $[\alpha]_D$ +30 (c, 0.6 in MeOH) (as TFA salt). λ_{max} 214 (ϵ 2340) (MeOH) (TFA salt).

Capon, R.J. *et al., Org. Biomol. Chem.*, 2005, **3**, 118-122 (*isol, synth, pmr, cmr*)

Echinoclathrine A E-5

[223774-66-1]



$C_{22}H_{30}N_2O_2$ 354.491

Alkaloid from the Okinawan sponge *Echinoclathria* sp. Immunosuppressant. Amorph. solid (hexane/EtOAc).

Mp 143-144°. λ_{max} 256 (ϵ 7500) (MeOH).

Kitamura, A. *et al., Tetrahedron*, 1999, **55**, 2487-2492 (*isol, uv, ir, pmr, cmr, ms*)

Echinoclathrine C E-6

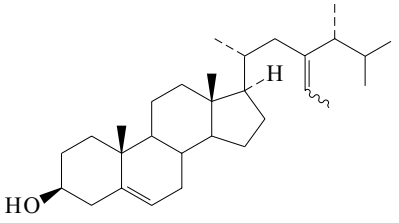
[223775-02-8]
As Echinoclathrine A, E-5 with
R = -$(CH_2)_{11}CH_2SH$
$C_{25}H_{36}N_2O_2S$ 428.638
Alkaloid from the Okinawan sponge *Echinoclathria* sp. Amorph. solid (hexane/EtOAc).
Mp 121-122°. λ_{max} 259 (ϵ 11700) (MeOH).

S-*Ac:* ***Echinoclathrine B***
[223774-86-5]
$C_{27}H_{38}N_2O_3S$ 470.675
Alkaloid from an *Echinoclathria* sp. Immunosuppressant.
Amorph. solid (hexane/EtOAc).
Mp 135-136°. λ_{max} 257 (ϵ 4200) (MeOH).

Kitamura, A. *et al., Tetrahedron*, 1999, **55**, 2487-2492 (*isol, uv, ir, pmr, cmr, ms*)

Echinoflorasterol E-7

23-Ethylidene-5-ergosten-3-ol, 9CI
[85617-75-0]



$C_{30}H_{50}O$ 426.724
Isol. from the gorgonian *Echinogorgia flora*.

Li, R. *et al., CA*, 1983, **98**, 176537t (*isol, pmr, cmr, ir*)

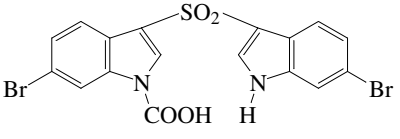
Echinoidin E-8

Anthocidaris crassispina *Lectin*
Multimeric glycoprotein with a subunit consisting of 147 amino acid residues with one carbohydrate chain. Each polypeptide chain contains 7 half-cystines, 6 of which form intrachain disulfide bonds and the other forms an interchain bond. Isol. from the coelomic fluid of the sea urchin *Anthocidaris crassispina*. Lectin.

Giga, Y. *et al., J. Biol. Chem.*, 1987, **262**, 6197-6203 (*struct*)

Echinosulfone A E-9

[246037-89-8]

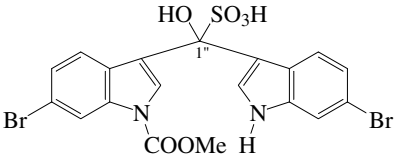


$C_{17}H_{10}Br_2N_2O_4S$ 498.151
Isol. from the sponge *Echinodictyum* sp. Orange oil. λ_{max} 221 (ϵ 42000); 250 (sh) (ϵ 14000); 280 (ϵ 17000); 320 (sh) (ϵ 9000) (MeOH).

Ovenden, S.P.B. *et al., J. Nat. Prod.*, 1999, **62**, 1246-1249 (*isol, ir, pmr, cmr, uv*)

Echinosulfonic acid C E-10

[246037-85-4]



$C_{19}H_{14}Br_2N_2O_6S$ 558.203
Isol. from the sponge *Echinodictyum* sp. Antibacterial agent.
Orange oil. λ_{max} 222 (ϵ 47000); 276 (ϵ 8800) (MeOH).

1″-Me ether: ***Echinosulfonic acid B***
[246037-60-5]
$C_{20}H_{16}Br_2N_2O_6S$ 572.23
Isol. from *Echinodictyum* sp. and *Psammoclemma* sp. Orange oil. λ_{max} 223 (ϵ 39000); 276 (ϵ 8000) (MeOH).

1″-Et ether: ***Echinosulfonic acid A***
[246036-86-2]
$C_{21}H_{18}Br_2N_2O_6S$ 586.257
Isol. from *Echinodictyum* sp. Orange oil. λ_{max} 223 (ϵ 42000); 276 (ϵ 8000) (MeOH).

1″-Deoxy: ***Echinosulfonic acid D***
$C_{19}H_{14}Br_2N_2O_5S$ 542.204
Isol. from the sponge *Psammoclemma* sp. Cytotoxic. Brown amorph. solid. λ_{max} 285 (MeCN/trifluoracetic acid).

Ovenden, S.P.B. *et al., J. Nat. Prod.*, 1999, **62**, 1246-1249 (*isol, ir, pmr, cmr, uv*)
Rubnov, S. *et al., Nat. Prod. Res.*, 2005, **19**, 75-79; 2006, **20**, 517 (*Echinosulfonic acid D*)

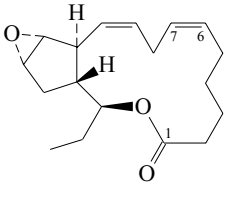
Echotoxins E-11

Three proteins, Echotoxins 1-3; Echotoxin 2 contains 226 aminoacid residues. Isol. from the salivary gland of the marine gastropod *Monoplex echo*. Haemolytic agents.

Shiomi, K. *et al., Toxicon*, 2002, **40**, 563-571 (*isol*)
Kawashima, Y. *et al., Toxicon*, 2003, **42**, 491-497 (*struct*)

Ecklonialactone A E-12

[121923-95-3]



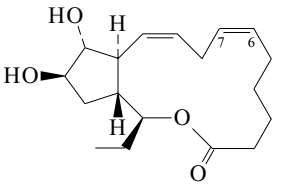
$C_{18}H_{26}O_3$ 290.402
Oxylipin. Metab. of brown alga *Ecklonia stolonifera*. Feeding deterrent. Cryst. (EtOH).
Mp 96-98°. $[\alpha]_D$ -87.7 (c, 1.02 in $CHCl_3$).

6,7-Dihydro: ***Ecklonialactone B***
[121923-96-4]
$C_{18}H_{28}O_3$ 292.417
Metab. of *Ecklonia stolonifera*. Feeding deterrent. Cryst. (EtOH).
Mp 64-66°. $[\alpha]_D$ -49.3 (c, 1.08 in $CHCl_3$).

Kurata, K. *et al., Chem. Lett.*, 1989, 267-270 (*cryst struct*)
Todd, J.S. *et al., J. Nat. Prod.*, 1994, **57**, 171-174 (*abs config*)

Ecklonialactone C E-13

[149633-54-5]



$C_{18}H_{28}O_4$ 308.417

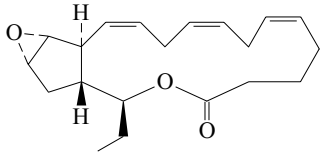
Oxylipin. Metab. of the brown alga *Ecklonia stolonifera*. Oil. $[\alpha]_D^{15}$ -197 (c, 0.66 in $CHCl_3$).

6,7-Dihydro: ***Ecklonialactone D***
[149633-55-6]
$C_{18}H_{30}O_4$ 310.433
Metab. of *Ecklonia stolonifera*. Oil. $[\alpha]_D^{15}$ -135 (c, 0.74 in $CHCl_3$).

Kurata, K. *et al., Phytochemistry*, 1993, **33**, 155-159 (*isol, pmr, cmr, ms*)

Ecklonialactone E E-14

[149633-56-7]

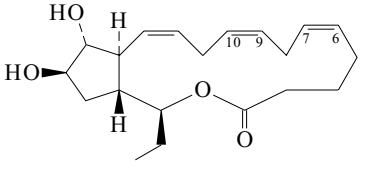


$C_{20}H_{28}O_3$ 316.439
Metab. of the brown alga *Ecklonia stolonifera*. Oil. $[\alpha]_D^{18}$ -62.1 (c, 1.04 in $CHCl_3$).

Kurata, K. *et al., Phytochemistry*, 1993, **33**, 155 (*isol, pmr, cmr*)
Todd, J.S. *et al., J. Nat. Prod.*, 1994, **57**, 171 (*abs config*)

Ecklonialactone F E-15

[149633-57-8]

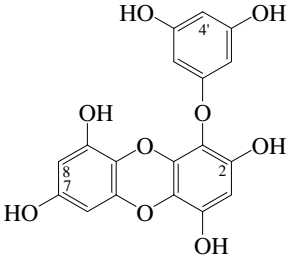


$C_{20}H_{30}O_4$ 334.455
Metab. of the brown alga *Ecklonia stolonifera*. Oil. $[\alpha]_D^{15}$ -83.5 (c, 1.01 in $CHCl_3$).

Kurata, K. *et al., Phytochemistry*, 1993, **33**, 155 (*isol, pmr, cmr*)

Eckol E-16

4-(3,5-Dihydroxyphenoxy)dibenzo[b,e][1,4]dioxin-1,3,6,8-tetrol, 9CI
[88798-74-7]



$C_{18}H_{12}O_9$ 372.287

Numbering systems vary. Constit. of the brown algae *Ecklonia kurome*, *Ecklonia maxima*, *Eisenia arborea*and *Eisenia bicyclis*. Inhibitor of α_2-Macroglobulin, glycation and α-amylase. Cryst. Mp 243-244°. λ_{max} 232 (ϵ 26700); 292 (ϵ 6200) (MeOH).

O^2*-(2,4,6-Trihydroxyphenyl):* ***2-Phloroeckol***
[89444-89-3]
$C_{24}H_{16}O_{12}$ 496.383
Constit. of *Ecklonia kurome*, *Ecklonia maxima* and *Eisenia arborea*. α_2-Macroglobulin inhibitor. Cryst.
Mp 206-207°. λ_{max} 232 (ϵ 40000); 292 (ϵ 3400) (MeOH) (Berdy).

O^7*-(2,4,6-Trihydroxyphenyl):* ***7-Phloroeckol***
$C_{24}H_{16}O_{12}$ 496.383
Constit. of the brown alga *Eisenia bicyclis*. Light brown powder. λ_{max} 233 (ϵ 30700); 292 (ϵ 4900) (MeOH).

4′-Bromo: ***4′-Bromoeckol***
[96820-13-2]
$C_{18}H_{11}BrO_9$ 451.184
Constit. of the brown alga *Eisenia arborea*. Isol. as hexa-Ac.

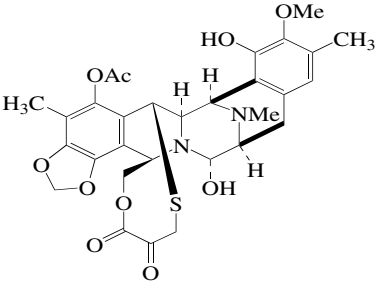
4′-Iodo: ***4′-Iodoeckol***
[96820-14-3]
$C_{18}H_{11}IO_9$ 498.184
Constit. of the brown alga *Eisenia arborea*. Isol. as hexa-Ac.

8-Hydroxy: ***8-Hydroxyeckol***
[96820-18-7]
$C_{18}H_{12}O_{10}$ 388.287
Constit. of the brown alga *Eisenia arborea*. Isol. as hepta-Ac.

Glombitza, K.-W. *et al., Phytochemistry*, 1985, **24**, 543-551 (*isol, pmr, cmr*)
Fukuyama, Y. *et al., Chem. Pharm. Bull.*, 1989, **37**, 349-353 (*cryst struct*)
Okada, Y. *et al., J. Nat. Prod.*, 2004, **67**, 103-105 (*isol, cmr, 7-Phloroeckol*)

Ecteinascidin 594 E-17

[184300-09-2]

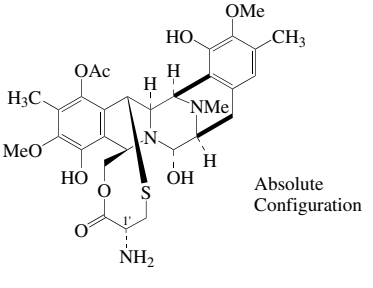


$C_{30}H_{32}N_2O_{10}S$ 612.656
Isol. from the Caribbean tunicate *Ecteinascidia turbinata*. Shows potent inhibition of DNA and RNA synth. and of RNA polymerase activity. Weakly cytotoxic against several cell lines. Light yellow solid. $[\alpha]_D^{22}$ -58 (c, 1.1 in MeOH). λ_{max} 207 (ϵ 60500); 230 (sh) (ϵ 11000); 287 (ϵ 2900) (MeOH).

Sakai, R. *et al., J.A.C.S.*, 1996, **118**, 9017-9023 (*isol, uv, pmr, cmr, ms, struct*)

Ecteinascidin 597 E-18

[184300-07-0]



$C_{30}H_{37}N_3O_9S$ 615.703

Isol. from the Caribbean tunicate *Ecteinascidia turbinata*. Shows potent inhibition of DNA and RNA synthesis and of RNA polymerase activity. Weakly cytotoxic against several cell lines. Light brown solid. $[\alpha]_D^{25}$ -49 (c, 0.17 in MeOH). λ_{max} 207 (ϵ 46000); 230 (sh) (ϵ 15000); 278 (ϵ 3500); 285 (ϵ 3800) (no solvent reported). λ_{max} 207 (ϵ 46000); 278 (ϵ 3500); 285 (ϵ 3800) (MeOH) (Berdy).

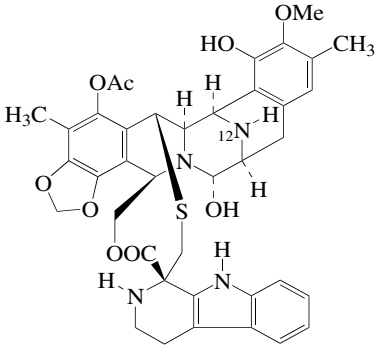
N-*De-Me:* ***Ecteinascidin 583***
[184300-08-1]
$C_{29}H_{35}N_3O_9S$ 601.676
From *Ecteinascidia turbinata*. Shows potent inhibition of DNA and RNA synthesis and of RNA polymerase activity. Weakly cytotoxic against several cell lines. Light yellow solid. $[\alpha]_D^{22}$ -47 (c, 0.14 in $CHCl_3$/MeOH, 6:1). λ_{max} 207 (ϵ 48000); 230 (sh) (ϵ 9200); 280 (ϵ 2100); 290 (ϵ 2300) (no solvent reported). λ_{max} 207 (ϵ 48000); 280 (ϵ 2100); 290 (ϵ 2300) (MeOH) (Berdy).

1′-Deamino, 1′-oxo: ***Ecteinascidin 596***
[184300-10-5]
$C_{30}H_{34}N_2O_{10}S$ 614.672
Trace constit. of *Ecteinascidia turbinata*. Observed only in a MeOH adduct. Tentative struct.

Sakai, R. *et al., J.A.C.S.*, 1996, **118**, 9017 (*isol, uv, ir, cd, pmr, cmr, ms, struct*)

Ecteinascidin 722 E-19

[144285-84-7]



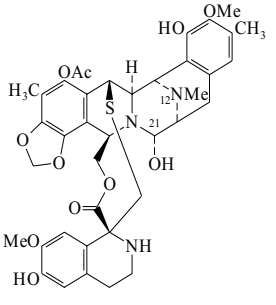
$C_{39}H_{40}N_4O_9S$ 740.832
Isol. from the tunicate *Ecteinascidia turbinata*. Cytotoxic agent. Yellow powder.
Mp 160-164°. $[\alpha]_D$ -40 (c, 1.64 in $CHCl_3$).

N^{12}-*Me:* ***Ecteinascidin 736***
[144285-85-8]
$C_{40}H_{42}N_4O_9S$ 754.859
Isol. from *Ecteinascidia turbinata*. Cytotoxic agent. Fine needles (MeCN aq.).
Mp 140-150° dec. $[\alpha]_D$ -76 (c, 0.5 in $CHCl_3$).

Pat. Coop. Treaty (WIPO), 1992, 92 09 607; *CA*, **117**, 205189z (*isol*)
Sakai, R. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1992, **89**, 11456-11460 (*isol*)

Ecteinascidin 743 E-20

Trabectedin, INN, USAN*. Yondelis. ET 743. NSC 648766*
[114899-77-3]



$C_{39}H_{43}N_3O_{11}S$ 761.848

Alkaloid from the ascidian *Ecteinascidia turbinata*. Antineoplastic agent. Investigated for treatment of a variety of human tumours incl. soft tissue sarcomas, osteosarcoma, melanoma and breast cancer. Mechanisms of action include inhibition of minor-groove-interacting transcription factors. In phase II clinical trials (2003). Granted orphan drug status by FDA (2004) for the treatment of soft tissue sarcoma. Sol. MeOH, CH_2Cl_2, C_6H_6; poorly sol. hexane, H_2O. λ_{max} 203 (ϵ 62000); 240 (sh) (ϵ 9000); 288 (ϵ 6500) (0.1*N* HCl) (Derep). λ_{max} 235 (ϵ 38000); 252 (sh) (ϵ 9000); 295 (ϵ 6500) (0.1*N* KOH) (Derep). λ_{max} 202 (ϵ 81000); 240 (sh) (ϵ 15000); 287 (ϵ 6200) (MeOH) (Derep). λ_{max} 202 (ϵ 81000); 284 (ϵ 6600); 289 (ϵ 6400) (MeOH) (Berdy).

S-*Oxide:* ***Ecteinascidin 759B***
[114899-29-5]
$C_{39}H_{43}N_3O_{12}S$ 777.848
From *Ecteinascidia turbinata*. Antineoplastic agent. Struct. revised in 2002. Formerly thought to be an *N*-oxide.

N^{12}-*Oxide:* ***Ecteinascidin 759C****. ET 759C*
[146663-68-5]
$C_{39}H_{43}N_3O_{12}S$ 777.848
From *Ecteinascidia turbinata*. Prisms (MeCN).
Mp 150° dec. $[\alpha]_D^{25}$ -55 (c, 0.22 in $CHCl_3$).

N^{12}-*De-Me:* ***Ecteinascidin 729***
[114899-27-3]
$C_{38}H_{41}N_3O_{11}S$ 747.821
From tunicate *Ecteinascidia turbinata*. Antineoplastic agent, immunoregulator. Sol. MeOH, C_6H_6, CH_2Cl_2; poorly sol. hexane, H_2O. λ_{max} 203 (ϵ 62000); 240 (sh) (ϵ 9000); 288 (ϵ 6500) (0.1*N* HCl) (Derep). λ_{max} 235 (ϵ 38000); 252 (sh) (ϵ 9000); 295 (ϵ 6500) (0.1*N* KOH) (Derep). λ_{max} 202 (ϵ 81000); 240 (sh) (ϵ 15000); 287 (ϵ 6200) (MeOH) (Derep). λ_{max} 202 (ϵ 61000); 283 (ϵ 5000); 284 (ϵ 4700) (MeOH) (Berdy). λ_{max} 204 (ϵ 61000); 283 (ϵ 4800); 289 (ϵ 4300) (MeOH-HCl) (Berdy). λ_{max} 215 (ϵ 33800); 258 (ϵ 8200); 290 (ϵ 6400) (MeOH/NaOH) (Berdy).

21-Ketone: ***Ecteinascidin 759A***
[114899-30-8]
$C_{39}H_{41}N_3O_{11}S$ 759.832
From *Ecteinascidia turbinata*. Formerly thought to be an *N*-oxide.

21-Deoxy: ***Ecteinascidin 745***
[114899-28-4]
$C_{39}H_{43}N_3O_{10}S$ 745.849
From *Ecteinascidia turbinata*. Antineoplastic agent, immunoregulator. Sol. MeOH, CH_2Cl_2, C_6H_6; poorly sol. hexane, H_2O. λ_{max} 202 (ϵ 52000); 281 (ϵ 5600); 287 (ϵ 5400) (MeOH) (Berdy). λ_{max} 204 (ϵ 51000); 281 (ϵ 5200); 287 (ϵ 5200) (MeOH/HCl) (Berdy). λ_{max} 215 (ϵ 36000); 254 (ϵ 8300); 290 (ϵ 5900); 298 (ϵ 5800) (MeOH/NaOH) (Berdy).

21-Deoxy, 21-cyano: ***Ecteinascidin 770***
[114899-80-8]
$C_{40}H_{42}N_4O_{10}S$ 770.859
From *Ecteinascidia turbinata* and *Ecteinascidia thurstoni*. Antineoplastic agent, immunoregulator. Prisms (MeOH). Sol. MeOH, CH_2Cl_2, C_6H_6; poorly sol. hexane, H_2O.
Mp 216-218° dec. $[\alpha]_D^{24}$ -58.5 (c, 1 in $CHCl_3$). λ_{max} 216 (ϵ 66000); 234 (ϵ 55000); 240 (ϵ 58000); 263 (ϵ 25000); 299 (ϵ 22000); 329 (ϵ 3900); 342 (ϵ 3200) (MeOH) (Berdy). λ_{max} 216 (ϵ 71000); 234 (ϵ 57000); 240 (ϵ 58000); 263 (ϵ 29000); 299 (ϵ 24000); 329 (ϵ 5700); 342 (ϵ 4900) (MeOH/HCl) (Berdy). λ_{max} 216 (ϵ 57000); 234 (ϵ 57000); 240 (ϵ 58000); 263 (ϵ 28000); 299 (ϵ 22000); 329 (ϵ 4900); 342 (ϵ 3700) (MeOH/NaOH) (Berdy).

21-Deoxy, 21-cyano, S-*oxide:* ***Ecteinascidin 786***
[442851-31-2]
$C_{40}H_{42}N_4O_{11}S$ 786.858
From *Ecteinascidia thurstoni*. Prisms (MeOH).
Mp 197-199° dec. $[\alpha]_D^{24}$ -156.9 (c, 0.6 in $CHCl_3$).

Wright, A.E. *et al., J.O.C.*, 1990, **55**, 4508 (*isol, struct*)
Rinehart, K.L. *et al., J.O.C.*, 1990, **55**, 4512-4515 (*isol, struct*)
Sakai, R. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1992, **89**, 11456-11460 (*Ecteinascidin 759C*)
Kerr, R.G. *et al., J. Nat. Prod.*, 1995, **58**, 1618 (*biosynth*)
Jimeno, J.M. *et al., Drugs of the Future*, 1996, **21**, 1155-1165 (*rev*)
Sakai, R. *et al., J.A.C.S.*, 1996, **118**, 9017 (*cd, abs config*)
Corey, E.J. *et al., J.A.C.S.*, 1996, **118**, 9202 (*synth*)

Moore, B.M. *et al., J.A.C.S.*, 1997, **119**, 5475 (*drug-DNA adduct*)
Zewail-Foote, M. *et al., J. Med. Chem.*, 1999, **42**, 2493-2497 (*pharmacol*)
Saito, N. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1549-4557 (*synth*)
Martinez, E.J. *et al., Org. Lett.*, 2000, **2**, 993-996 (*synth*)
Jin, S. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2000, **97**, 6775-6779 (*pharmacol*)
Minuzzo, M. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2000, **97**, 6780-6784 (*pharmacol*)
Ryan, D.P. *et al., Clin. Cancer Res.*, 2001, **7**, 231-242 (*clin trial*)
Erba, E. *et al., Eur. J. Cancer*, 2001, **37**, 97-105 (*pharmacol*)
Zewail-Foote, M. *et al., J.A.C.S.*, 2001, **123**, 6485-6495 (*pharmacol*)
Cvetkovic, R.S. *et al., Drugs*, 2002, **62**, 1185-1192 (*rev*)
Suwanborirux, K. *et al., J. Nat. Prod.*, 2002, **65**, 935-937 (*Ecteinascidins 770, 786*)
Endo, A. *et al., J.A.C.S.*, 2002, **124**, 6552-6554 (*synth*)
Sainz-Diaz, C.I. *et al., Acta Cryst. C*, 2003, **59**, o197-o198 (*cryst struct*)
Nicolaou, K.C. *et al., Classics in Total Synthesis II: More Targets, Strategies, Methods*, Wiley-VCH, 2003, 109 (*rev, synth*)
Menchaca, R. *et al., J.O.C.*, 2003, **68**, 8859-8866 (*synth*)
Zheng, S. *et al., Angew. Chem., Int. Ed.*, 2006, **45**, 1754-1759 (*synth*)
Chen, J. *et al., J.A.C.S.*, 2006, **128**, 87-89 (*synth*)

Ectyonin E-21

[52350-24-0]

Struct. unknown. Isol. from *Microciona prolifera*. Antimicrobial agent. Cryst. Sol. MeOH, Et_2O, hexane; poorly sol. H_2O, Me_2CO, $CHCl_3$.

Nigrelli, R.F. *et al., Zoologica*, 1959, **44**, 173-176 (*isol*)
Bose, A.K. *et al., CA*, 1974, **80**, 130700r (*isol*)

Eel intestinal pentapeptide E-22

[138149-60-7]

Gly-Phe-Trp-Asn-Lys

$C_{32}H_{42}N_8O_7$ 650.733

Isol. from eel (*Anguilla japonica*) gut.

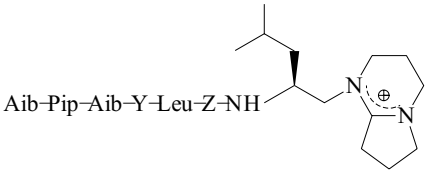
Uesaka, T. *et al., Biochem. Biophys. Res. Commun.*, 1991, **180**, 828-832 (*isol*)

Efrapeptin E-23

Efrastatin. Antibiotic A 23871. A 23871

[56645-91-1]

Ac–Pip–Aib–Pip–Aib–X–Leu–β–Ala–Gly–Aib–



Efrapeptin	C	X= Z= Aib, Y= Gly
Efrapeptin	D	X= Aib, Y= Gly, Z= Iva
Efrapeptin	E	X= Z= Iva, Y= Gly
Efrapeptin	F	X= Aib, Y= Ala, Z= Iva
Efrapeptin	G	X= Z= Iva, Y= Ala

Oligopeptide antibiotic complex. Prod. by the fungus *Tolypocladium niveum* and *Tolypocladium geodes*. Possesses insect toxicity. Potent inhibitor of mitochondrial ATPase and photophosphorylation in chloroplasts.

Efrapeptin C [138145-54-7]

$C_{80}H_{137}N_{18}O_{16}$ 1607.073

Sol. MeOH, $CHCl_3$. $[\alpha]_D^{22}$ -2.5 (c, 0.08 in $CHCl_3$). λ_{max} 208 (ϵ); 230 (sh) (ϵ) (MeOH) (Derep). λ_{max} 209 (MeOH) (Berdy).

Efrapeptin D [71503-60-1]

$C_{81}H_{140}N_{18}O_{16}$ 1622.108

$[\alpha]_D^{22}$ -3.1 (c, 0.32 in $CHCl_3$). λ_{max} 208 (ϵ); 230 (sh) (ϵ) (MeOH) (Derep). λ_{max} 208; 230 (MeOH) (Berdy).

Efrapeptin E [138168-07-7]

$C_{82}H_{142}N_{18}O_{16}$ 1636.135

$[\alpha]_D^{22}$ -2.2 (c, 0.37 in $CHCl_3$). λ_{max} 208 (ϵ); 230 (sh) (ϵ) (MeOH) (Derep). λ_{max} 208 (MeOH) (Berdy).

Efrapeptin F [131353-66-7]

$C_{82}H_{142}N_{18}O_{16}$ 1636.135

Sol. MeOH, $CHCl_3$. $[\alpha]_D^{22}$ -5 (c, 0.4 in $CHCl_3$). λ_{max} 208 (ϵ); 230 (sh) (ϵ) (MeOH) (Derep). λ_{max} 208; 230 (MeOH) (Berdy).

Efrapeptin G [138145-55-8]

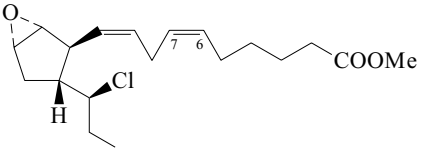
$C_{83}H_{143}N_{18}O_{16}$ 1649.154

Also prod. by an *Acremonium* sp. isol. from the marine sponge *Teichaxinella* sp. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{22}$ -5.3 (c, 0.42 in $CHCl_3$). λ_{max} 208 (ϵ); 230 (sh) (ϵ) (MeOH) (Derep). λ_{max} 208 (MeOH) (Berdy).

Susa, J.B. *et al., Mol. Pharmacol.*, 1975, **11**, 166 (*props*)
Lucero, H. *et al., Arch. Biochem. Biophys.*, 1978, **186**, 9
Kohlbrenner, W.E. *et al., Arch. Biochem. Biophys.*, 1979, **198**, 598
Jackson, C.G. *et al., Biochem. Soc. Trans.*, 1979, **7**, 224 (*hplc*)
Bullough, D.A. *et al., Biochem. Int.*, 1982, **4**, 543
Shaw, I.M. *et al., Can. J. Chem.*, 1986, **64**, 164
Krasnoff, S.B. *et al., J. Chem. Ecol.*, 1991, **17**, 1953 (*isol*)
Gupta, S. *et al., J.O.C.*, 1992, **57**, 2306 (*isol, pmr, cmr, struct*)
Jost, M. *et al., Angew. Chem., Int. Ed.*, 2002, **41**, 4267-4269 (*Efrapeptin C, synth*)
Boot, C.M. *et al., J. Nat. Prod.*, 2006, **69**, 83-92 (*Efrapeptin G, marine isol*)

Egregiachloride A E-24

[152218-33-2]



$C_{19}H_{29}ClO_3$ 340.889

Constit. of the marine brown alga *Egregia menziesii*.

$[\alpha]_D^{27}$ -12 (c, 0.44 in $CHCl_3$).

6,7-Dihydro: ***Egregiachloride B***

[152218-34-3]

$C_{19}H_{31}ClO_3$ 342.905

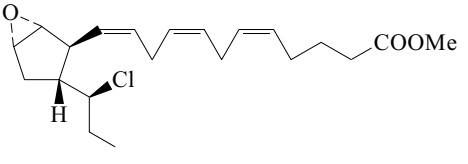
Constit. of *Egregia menziesii*.

$[\alpha]_D^{27}$ -12 (c, 0.87 in $CHCl_3$).

Todd, J.S. *et al., Tet. Lett.*, 1993, **34**, 7689 (*isol, pmr, cmr*)

Egregiachloride C E-25

[152218-35-4]



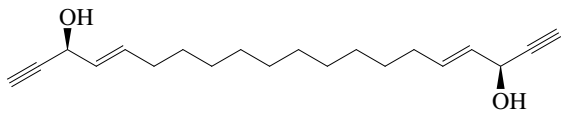
$C_{21}H_{31}ClO_3$ 366.927

Constit. of the brown alga *Egregia menziesii*.

$[\alpha]_D^{27}$ -13 (c, 0.14 in $CHCl_3$).

Todd, J.S. *et al., Tet. Lett.*, 1993, **34**, 7689 (*isol, pmr, cmr*)

4,16-Eicosadiene-1,19-diyne-3,18-diol E-26



$C_{20}H_{30}O_2$

(3S,4E,16E,18S)-form
Isol. from the sponge *Callyspongia pseudoreticulata*.
Amorph. solid. $[\alpha]_D^{20}$ +26 (c, 1 in MeOH).
Braekman, J.C. *et al., J. Nat. Prod.*, 2003, **66**, 871-872 (*isol, pmr, cmr, ms*)

5,9-Eicosadienoic acid E-27

5,9-Icosadienoic acid
$H_3C(CH_2)_9CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{20}H_{36}O_2$ 308.503

(Z,Z)-form [133530-14-0]
Constit. of *Erylus formosus* and *Stoichactis helianthus.*
Carballeira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 305-309; 1994, **57**, 1688-1695

6,11-Eicosadienoic acid E-28

6,11-Icosadienoic acid
[25448-01-5]
$H_3C(CH_2)_7CH{=}CH(CH_2)_3CH{=}CH(CH_2)_4COOH$
$C_{20}H_{36}O_2$ 308.503

(Z,Z)-form [122458-81-5]
Isol. from the sponges *Amphimedon complanata* and *Euryspongia rosea*.
Carballeira, N.M. *et al., Lipids*, 1989, **24**, 665-668 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 315-317 (*isol*)
Kulkarni, B.A. *et al., Molecules*, 1997, **2**, 3-6; 99 (*synth*)

6,14-Eicosadienoic acid E-29

6,14-Icosadienoic acid
[25448-01-5]
$H_3C(CH_2)_4CH{=}CH(CH_2)_6CH{=}CH(CH_2)_4COOH$
$C_{20}H_{36}O_2$ 308.503

(E,E)-form [132171-19-8]
Isol. from the sponge *Plakortis halichondroides.*
Carballeira, N.M. *et al., Lipids*, 1990, **25**, 835-840 (*isol, ir, cmr*)

9,13-Eicosadienoic acid E-30

9,13-Icosadienoic acid
$H_3C(CH_2)_5CH{=}CHCH_2CH_2CH{=}CH(CH_2)_7COOH$
$C_{20}H_{36}O_2$ 308.503

(Z,Z)-form [187657-28-9]
Isol. from the sponge *Haliclona cinerea.*
Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*isol, ms*)

10,15-Eicosadienoic acid E-31

10,15-Icosadienoic acid
[25448-01-5, 32839-28-4]
$H_3C(CH_2)_3CH{=}CH(CH_2)_3CH{=}CH(CH_2)_8COOH$
$C_{20}H_{36}O_2$ 308.503

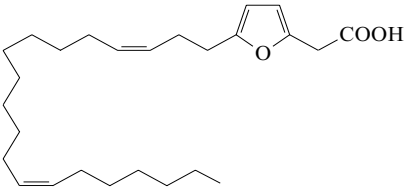
(Z,Z)-form [145930-75-2]
Isol. from the marine opisthobranch *Haminoea templadoi*. Genus name given as the alternate spelling Haminea.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1992, **55**, 1783 (*isol*)
Kulkarni, B.A. *et al., J. Nat. Prod.*, 1994, **57**, 537 (*synth*)

11,15-Eicosadienoic acid E-32

11,15-Icosadienoic acid
[133530-13-9]
[25448-01-5, 32839-28-4]
$H_3C(CH_2)_3CH{=}CHCH_2CH_2CH{=}CH(CH_2)_9COOH$
$C_{20}H_{36}O_2$ 308.503
Constit. of the sponge *Amphimedon complanata*. Isol. as Me ester.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 315 (*isol*)
Kulkarni, B.A. *et al., Org. Prep. Proced. Int.*, 1993, **25**, 333 (*synth*)

5-(3,13-Eicosadienyl)-2-furanacetic acid, 9CI E-33

3,6-Epoxy-3,5,9,19-hexacosatetraenoic acid

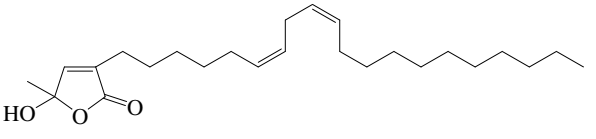


$C_{26}H_{42}O_3$ 402.616

(Z,Z)-form [136337-71-8]
Constit. of the steryl esters of the sponge *Dictyonella incisa*.
Ciminiello, P. *et al., Experientia*, 1991, **47**, 739 (*isol*)

3-(6,9-Eicosadienyl)-5-hydroxy-5-methyl-2(5*H*)-furanone E-34

2-(6,9-Eicosadienyl)-4-hydroxy-4-methyl-2-buten-4-olide

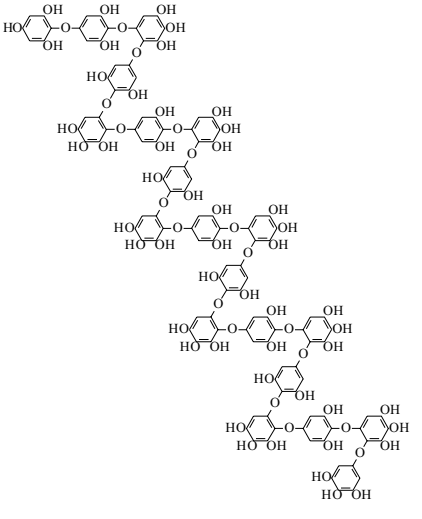


$C_{25}H_{42}O_3$ 390.605

(Z,Z)-form
Flavalactone 2
[81346-96-5]
Isol. from the Japanese gorgonian *Euplexaura flava*.
Oil. λ_{max} 224 (ϵ 5000) (MeOH) (Derep).
Kituchi, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1172-1176 (*isol, ir, pmr, cmr*)

Eicosafuhalol A E-35

[164176-36-7]



$C_{120}H_{82}O_{70}$ 2643.926

Constit. of the brown alga *Sargassum spinuligerum*. Largest phlorotannin isol. pure to date (1995).

Glombitza, K.-W. *et al., Phytochemistry*, 1995, **38**, 987-995 (*isol, pmr, cmr, ms*)

1,16-Eicosanediol E-36

1,16-Icosanediol
[20301-19-3]
$H_3C(CH_2)_3CH(OH)(CH_2)_{14}CH_2OH$
$C_{20}H_{42}O_2$ 314.551

(ξ)-*form*

Di-O-*sulfate:* [131985-12-1]
$C_{20}H_{42}O_8S_2$ 474.679
Isol. from the starfish *Asterias forbesi*.
Mp 154° dec. (as di-Na salt). Isol. as di-Na salt to which CAS no. refers.

1-O-*Sulfate, 16*-O-*[6*-O-*deoxy-β-*D*-glucopyranosyl-(1→2)-6-deoxy-β-*D*-glucopyranoside]:* ***Forbesin***
[131985-11-0]
$C_{32}H_{62}O_{13}S$ 686.9
Isol. from *Asterias forbesi*.
Mp 168° dec. (as Na salt). CAS no. refers to Na salt.

(±)-*form*
Mp 60-64°.

Findlay, J.A. *et al., J. Nat. Prod.*, 1990, **53**, 1015-1018 (*isol, pmr, cmr, ms*)

Eicosanoic acid E-37

Arachidic acid. Icosanoic acid. Arachic acid
[506-30-9]
$H_3C(CH_2)_{18}COOH$
$C_{20}H_{40}O_2$ 312.535
Constit. of arachis (*Arachis hypogaea*) (ground-nut) oil glycerides. Widely distributed in other seed oils. Present in lipids of *Physalia physalis* (Portuguese-man-of-war). Cryst. (EtOH). Sol. $CHCl_3$, hexane; poorly sol. H_2O.
Mp 77°. Bp_1 203-205°.

► JX3780000

Me ester: [1120-28-1]
$C_{21}H_{42}O_2$ 326.562
Mp 45.8-46.3°. Bp_{10} 215-216° Bp_2 188°.

Et ester: [18281-05-5]
$C_{22}H_{44}O_2$ 340.588
Constit. of *Cassia javanica* leaves.
Mp 41.4-42°. Bp_{100} 295-297° Bp_2 186-187°.

Amide:
$C_{20}H_{41}NO$ 311.55
Mp 109°.

Nitrile:
$C_{20}H_{39}N$ 293.535
Mp 49.5°.

Hexacosyl ester: Hexacosyl eicosanoate
[17318-45-5]
$C_{46}H_{92}O_2$ 677.232
Constit. of the waxes of *Desmodium* sp., *Nardostachys* sp., *Scutellaria* sp. and green tobacco leaves.

Heptadecyl ester: Heptadecyl eicosanoate
[36610-58-9]
$C_{37}H_{74}O_2$ 550.99
Constit. of *Valeriana wallichi*.
Mp 62.8-63.2°.

[14923-81-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 486A; 610A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 758A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 632B (*ir*)
Adam, N.K. *et al., J.C.S.*, 1925, **127**, 72 (*synth*)
Sy, M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1954, **239**, 1813 (*synth*)
Radler, F. *et al., Aust. J. Chem.*, 1965, **18**, 1059 (*isol*)
Marosi, L. *et al., Annalen*, 1973, 584 (*props, cryst struct*)
Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*Physalia physalis constit*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EAF000

2-Eicosanone E-38

Methyl octadecyl ketone. 2-Icosanone
[29703-52-4]
$H_3C(CH_2)_{17}COCH_3$
$C_{20}H_{40}O$ 296.535
Constit. of *Euonymus latifolius* leaves. Cryst. (EtOH).
Mp 58-59°.

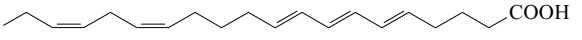
Oxime:
$C_{20}H_{41}NO$ 311.55
Cryst. (EtOH). Mp 73-74°.

Semicarbazone:
Cryst. (EtOH). Mp 128°.

Pangborn, M.C. *et al., J.A.C.S.*, 1936, **58**, 10-14 (*synth*)
Breusch, F.L. *et al., Chem. Ber.*, 1953, **86**, 684-688 (*synth*)
Ulubelen, A. *et al., Phytochemistry*, 1973, **12**, 1824 (*Euonymus latifolius constit*)
Xiao, D. *et al., Fenxi Huaxue*, 2004, **32**, 1621-1623; *CA*, **143**, 23210 (*Spheciospongia vagabunda constit*)

5,7,9,14,17-Eicosapentaenoic acid E-39

5,7,9,14,17-Icosapentaenoic acid
[25378-27-2, 32839-30-8]



(5*E*,7*E*,9*E*,14*Z*,17*Z*)–*form*

$C_{20}H_{30}O_2$ 302.456

(5*E*,7*E*,9*E*,14*Z*,17*Z*)-*form* [108543-67-5]
Isol. from the red algae *Murraya periclados* and *Ptilota filicina*.

(5*E*,7*Z*,9*E*,14*Z*,17*Z*)-*form* [121979-44-0]
Isol. from the red alga *Farlowia mollis*.

(5*Z*,7*E*,9*E*,14*Z*,17*Z*)-*form* [108526-93-8]
Isol. from *Murraya periclados* and *Ptilota filicina*.

Lopez, A. *et al., Lipids*, 1987, **22**, 190-194 (*isol*)
Solem, M.L. *et al., Lipids*, 1989, **24**, 256-260 (*isol*)
Bernart, M.W. *et al., Phytochemistry*, 1994, **36**, 1233-1240 (*isol*)

5,8,10,12,14-Eicosapentaenoic acid E-40

5,8,10,12,14-Icosapentaenoic acid
[25378-27-2, 32839-30-8]
$H_3C(CH_2)_4CH{=}CHCH{=}CHCH{=}CHCH{=}CHCH_2CH{=}CH(CH_2)_3COOH$
$C_{20}H_{30}O_2$ 302.456

(5*Z*,8*Z*,10*E*,12*E*,14*Z*)-*form*
Bosseopentaenoic acid
[133205-91-1]
Formed from arachidonic acid (see 5,8,11,14-Eicosatetraenoic acid) in the red alga *Bossiella orbigniana*.

Burgess, J.R. *et al., Lipids*, 1991, **26**, 162 (*isol*)
Gerwick, W.H. *et al., Phytochemistry*, 1993, **34**, 1029 (*synth*)

5,8,11,14,17-Eicosapentaenoic acid E-41

5,8,11,14,17-Icosapentaenoic acid. EPA
[1553-41-9]
[25378-27-2, 32839-30-8]
$H_3CCH_2(CH{=}CHCH_2)_5CH_2CH_2COOH$
$C_{20}H_{30}O_2$ 302.456
Component of Omega-3 Marine Triglycerides.

► JX3830000

(*all-Z*)-*form*
Timnodonic acid. *Icosapent, INN*
[10417-94-4]

Present in fish oils as an acylglycerol and in animal phospholipids. Constit of various red algae. Nutriceutical with antioxidation props. Precursor of PG_3 series of prostaglandins. Platelet aggregation inhibitor. Allelopathic agent. Oil. Launched 1990. Granted fast track designation by FDA (2005) for the treatment of Huntington's disease

Et ester. Ethyl icosapentate, JAN. Ethyl EPA. MND 21. Miraxion. LAX 101
[86227-47-6]
$C_{22}H_{34}O_2$ 330.509
Isol. from fish oils. Antithrombotic agent.

[2734-47-6, 84494-70-2]

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 786A (*nmr*)
Teshima, S. *et al., CA*, 1978, **89**, 193306 (*isol, nmr*)
Von Schacky, C. *et al., J. Clin. Invest.*, 1985, **76**, 2446 (*metab, pharmacol*)
Eur. Pat., 1988, 292 846; *CA*, **111**, 63962 (*isol, Et ester*)
Corey, E.J. *et al., J.O.C.*, 1988, **53**, 5980 (*synth, ir, pmr, ms*)
Viala, J. *et al., Tet. Lett.*, 1992, **33**, 4897 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 991
Vatele, J.-M. *et al., Chem. Phys. Lipids*, 1995, **78**, 65 (*synth*)
Sandri, J. *et al., J.O.C.*, 1995, **60**, 6627 (*synth, ir*)
Suzuki, M. *et al., Phytochemistry*, 1996, **43**, 63 (*isol*)
Sayanova, O.V. *et al., Phytochemistry*, 2004, **65**, 147-158 (*biosynth*)
Boston, P.F. *et al., Prostaglandins, Leukotrienes, Essent. Fatty Acids*, 2004, **71**, 341-346 (*Et ester, pharmacol*)
Puri, B.K. *et al., Neurology*, 2005, **65**, 286-292 (*Et ester, pharmacol, clin trial*)

4,7,10,13-Eicosatetraenoic acid E-42

4,7,10,13-Icosatetraenoic acid
[27400-91-5]

$H_3C(CH_2)_5(CH{=}CHCH_2)_4CH_2COOH$
$C_{20}H_{32}O_2$ 304.472

(*all-Z*)-*form* [32907-97-4]
[31152-45-1]
Constit. of the sponge *Microciona prolifera*. Present in some animal phospholipids. Metab. of 9-Hexadecenoic acid.

Kunau, W.H. *et al., Eur. J. Biochem.*, 1974, **48**, 311
Hahn, S. *et al., J.A.C.S.*, 1988, **110**, 8117-8124 (*isol*)

5,7,9,14-Eicosatetraenoic acid E-43

5,7,9,14-Icosatetraenoic acid
$H_3C(CH_2)_4CH{=}CH(CH_2)_3CH{=}CHCH{=}CHCH{=}CH(CH_2)_3COOH$
$C_{20}H_{32}O_2$ 304.472

(5*Z*,7*E*,9*E*,14*Z*)-*form*
Isol. from red alga *Ptilota filicina*. λ_{max} 262; 272; 282 (EtOH).
Wise, M.L. *et al., Biochemistry*, 1994, **33**, 15223-15232

6,9,12,15-Eicosatetraenoic acid E-44

6,9,12,15-Icosatetraenoic acid
$H_3C(CH_2)_3CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_4COOH$
$C_{20}H_{32}O_2$ 304.472

(*all-Z*)-*form* [24257-11-2]
Constit. of freshwater and marine sponges, e.g. *Ectyoplasia ferox*.
Carballeira, N.M. *et al., Lipids*, 1989, **24**, 371-374 (*isol*)
Dembitsky, V.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1993, **106**, 825-831; 1994, **109**, 415-426 (*isol*)

8,11,14,17-Eicosatetraenoic acid E-45

8,11,14,17-Icosatetraenoic acid
[2091-26-1]
[27400-91-5]

$H_3CCH_2(CH{=}CHCH_2)_4(CH_2)_5COOH$
$C_{20}H_{32}O_2$ 304.472

(*all-Z*)-*form* [24880-40-8]
[31152-45-1]
Present in fish oils and in animal phospholipids. Metab. of α-Linolenic acid.
Nicolasev, V. *et al., CA*, 1974, **81**, 117622
Dhopeshwarkor, G. *et al., Lipids*, 1976, **11**, 689

10,13,16,19-Eicosatetraenoic acid E-46

10,13,16,19-Icosatetraenoic acid
$H_2C{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_8COOH$
$C_{20}H_{32}O_2$ 304.472
Isol. from the marine bivalve *Megangulus zyonoensis.*

Kawashima, H. *et al., Lipids*, 2004, **39**, 265-271 (*isol*)

5,9,13-Eicosatrienoic acid E-47

5,9,13-Icosatrienoic acid
$H_3C(CH_2)_5CH{=}CHCH_2CH_2CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{20}H_{34}O_2$ 306.487

(*all-Z*)-*form* [161925-90-2]
Isol. from *Haliclona cinerea* and *Stoichactis helianthus.*
Carballeira, N.M. *et al., J. Nat. Prod.*, 1994, **57**, 1688-1695 (*isol*)
Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*isol, ms*)

8,11,14-Eicosatrienoic acid E-48

8,11,14-Icosatrienoic acid
[7324-41-6]
[27070-56-0]

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_6COOH$
$C_{20}H_{34}O_2$ 306.487

(*all-Z*)-*form*
Dihomogammalinolenic acid. γ-Homolinolenic acid. Dihomo-γ-linolenic acid
[1783-84-2]
Minor component of animal phospholipids. Constit. of *Sargassum pallidum*. Metab. of Linoleic acid. Precursor of PG_1 series of prostaglandins. Intermediate for 8,9-Leukotriene C_3.

N-*(2-Hydroxyethyl)amide: Homo-γ-linolenylethanolamide*
[150314-34-4]
$C_{22}H_{39}NO_2$ 349.556
Isol. from porcine brain. Endogenous cannabinoid receptor agonist.

Struijk, C.B. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1966, **85**, 1241 (*synth*)
Hanus, L. *et al., J. Med. Chem.*, 1993, **36**, 3032-3034 (*amide deriv, synth, pharmacol*)
Pertwee, R. *et al., Eur. J. Pharmacol.*, 1994, **259**, 115-120; 1995, **287**, 145-152 (*amide deriv, pharmacol*)
Groza, N.V. *et al., Bioorg. Khim.*, 1998, **24**, 458-461 (*synth*)
Zhukova, N.V. *et al., Phytochemistry*, 1999, **50**, 1209-1211 (*isol*)

4-Eicosene-1,14,19-triyn-3-ol E-49

Aikupikanyne D
$HC{\equiv}C(CH_2)_3C{\equiv}C(CH_2)_8CH{=}CHCH(OH)C{\equiv}CH$
$C_{20}H_{28}O$ 284.441

(3ξ,4*E*)-*form*
Isol. from a *Callyspongia* sp.
Oil. Incorrect MF given in ref.

Youssef, D.T.A. *et al., J. Nat. Prod.*, 2000, **63**, 1406-1410

9-Eicosenoic acid, 9CI E-50

9-Icosenoic acid
[506-31-0]
[26764-41-0]

$H_3C(CH_2)_9CH{=}CH(CH_2)_7COOH$
$C_{20}H_{38}O_2$ 310.519

(*E*)-*form*
Gadelaidic acid
Cryst. (MeOH). Mp 54°.

Amide:
$C_{20}H_{39}NO$ 309.534
Mp 90-91°.

(*Z*)-*form*
Gadoleic acid
[29204-02-2]
[28933-89-3]
Constit. of fish oil glycerides.
Mp 23-23.5°. $Bp_{0.1}$ 170°.
Et ester:
$C_{22}H_{42}O_2$ 338.573
$Bp_{0.1}$ 154-155°.
Amide: Mp 78-79°.
Boughton, B.W. *et al., J.C.S.*, 1952, 671 (*synth*)

11-Eicosenoic acid E-51

11-Icosenoic acid
[2462-94-4]
[26764-41-0]
$H_3C(CH_2)_7CH{=}CH(CH_2)_9COOH$
$C_{20}H_{38}O_2$ 310.519
Present in lipids of *Physalia physalis* (Portuguese-man-of-war).

(*E*)-*form* [62322-84-3]
Mp 49-51°.

(Z)-*form*
Gondoic acid
[5561-99-9]
[28933-89-3]
Constit. of rape oil and fish oils as glyceride. Also in other plant oils, e.g. false flax (*Camelina sativa*), and swede (*Brassica napobrassica*). Isol. from the sponge *Amphimedon complanata*.
Cryst. (Me_2CO/hexane).
Mp 24-25°.
Me ester: [2390-09-2]
$C_{21}H_{40}O_2$ 324.546
Mp -45°.
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 783C; 988B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 686A (*ir*)
Fieser, L.F. *et al., J.A.C.S.*, 1948, **70**, 71 (*synth*)
Argoudelis, C.J. *et al., Lipids*, 1968, **3**, 379 (*struct, ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 742 (*occur*)
Spencer, F. *et al., Chem. Phys. Lipids*, 1973, **11**, 215 (*synth*)
Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*Physalia physalis constit*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 315-317 (*Amphimedon, isol*)

12-Eicosenoic acid E-52

12-Icosenoic acid
[66570-12-5]
[26764-41-0]
$H_3C(CH_2)_6CH{=}CH(CH_2)_{10}COOH$
$C_{20}H_{38}O_2$ 310.519
Isol. from the sponge *Eurypongia rosea*.
[28933-89-3, 69119-91-1, 69120-01-0, 82683-04-3, 82683-16-7]
Carballeira, N.M. *et al., Lipids*, 1989, **24**, 665-668 (*isol*)

13-Eicosenoic acid, 9CI E-53

13-Icosenoic acid
[14134-51-1]
[26764-41-0]
$H_3C(CH_2)_5CH{=}CH(CH_2)_{11}COOH$
$C_{20}H_{38}O_2$ 310.519
Present in lipids of *Physalia physalis* (Portuguese-man-of-war).

(*Z*)-*form*
Paullinic acid
[17735-94-3]
[28933-89-3]
Isol. from herring oil and rapeseed oil and from various Sapindaceae. Constit. of the sponge *Trikentrion loeve.*
[69119-92-2, 69120-02-1, 82683-17-8]
Kishimoto, Y. *et al., J. Lipid Res.*, 1964, **5**, 98 (*isol, struct*)
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206 (*isol*)
Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*Physalia physalis constit*)
Richter, I. *et al., Z. Naturforsch., C*, 1978, **33**, 629 (*synth*)
Yu, Q.T. *et al., Lipids*, 1989, **24**, 79 (*ms*)
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol, Trikentrion*)
Spitzer, V. *et al., Phytochemistry*, 1996, **42**, 1357 (*isol*)

14-Eicosenoic acid E-54

14-Icosenoic acid
[45269-91-8]
[26764-41-0, 82683-18-9 (E-)]
$H_3C(CH_2)_4CH{=}CH(CH_2)_{12}COOH$
$C_{20}H_{38}O_2$ 310.519

(*Z*)-*form* [17735-95-4]
[28933-89-3]
Constit.of the sponge *Pseudaxinella* cf. *lunaecharta*.
Cryst. (EtOH).
Mp 42.5°.
Baker, C.D. *et al., J.C.S.*, 1963, 489 (*synth*)
Ackman, R.G. *et al., J. Gas Chromatogr.*, 1967, **5**, 489 (*chromatog*)
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol*)

15-Eicosenoic acid E-55

15-Icosenoic acid
[2654-73-1]
[26764-41-0]
$H_3C(CH_2)_3CH{=}CH(CH_2)_{13}COOH$
$C_{20}H_{38}O_2$ 310.519

(*Z*)-*form* [34739-80-5]
[28933-89-3]
A minor component of lipids from marine sources.
Ackman, R.G. *et al., Lipids*, 1966, **1**, 341
Vickery, J.R. *et al., Phytochemistry*, 1971, **10**, 123

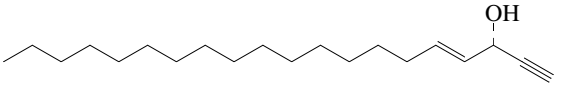
16-Eicosenoic acid E-56

16-Icosenoic acid
$H_3CCH_2CH_2CH{=}CH(CH_2)_{14}COOH$
$C_{20}H_{38}O_2$ 310.519

(*Z*)-*form* [82683-05-4]
Constit. of the sponge *Trikentrion loeve* and fish oils.
Sacchi, R. *et al., J. Am. Oil Chem. Soc.*, 1993, **70**, 225-228 (*isol*)
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol*)

4-Eicosen-1-yn-3-ol E-57

4-Icosen-1-yn-3-ol
[139722-80-8]



$C_{20}H_{36}O$ 292.504
λ_{max} 202 (ϵ 1400) (MeOH) (Derep).

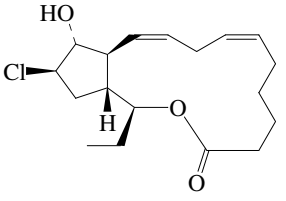
(3*S*,4*E*)-*form* [129364-93-8]
Isol. from the marine sponge *Cribrochalina vasculum*.
Solid (prev. descr. as gum). $[\alpha]_D$ +18.3 (c, 0.4 in MeOH) (+3.8).
Nat. prod. may be a partial racemate.

(±)-(*E*)-*form* [146333-80-4]
Gum.

[146333-83-7]

Gunasekera, S.P. *et al., J.O.C.*, 1990, **55**, 6223 (*isol, pmr, cmr*)
U.S. Pat., 1992, 5 166 379; *CA*, **118**, 124061 (*synth*)
Kulkarni, B.A. *et al., Coll. Czech. Chem. Comm.*, 1993, **58**, 1711 (*synth*)
Hallock, Y.F. *et al., J. Nat. Prod.*, 1995, **58**, 1801 (*isol, abs config*)
Sharma, A. *et al., Tetrahedron: Asymmetry*, 1998, **9**, 2635-2639 (*synth*)
Lu, W. *et al., Tetrahedron*, 1999, **55**, 4649-4654 (*synth*)
Gung, B.W. *et al., Synth. Commun.*, 2002, **32**, 2733-2740 (*synth, pmr, cmr*)

Eiseniachloride A E-58



$C_{18}H_{27}ClO_3$ 326.862

Oxylipin. Related to Ecklonialactone C, E-13. Isol. from the brown alga *Eisenia bicyclis*. Oil. $[\alpha]_D^{20}$ -149 (c, 0.07 in $CHCl_3$).

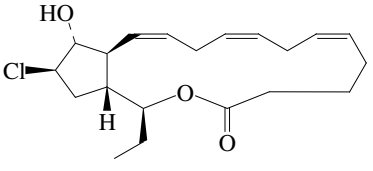
6,7-Dihydro: ***Eiseniachloride B***
$C_{18}H_{29}ClO_3$ 328.878
Isol. from *Eisenia bicyclis*. Oil. $[\alpha]_D^{20}$ -126 (c, 0.06 in $CHCl_3$).

Iodo analogue: ***Eiseniaiodide A***
$C_{18}H_{27}IO_3$ 418.314
Isol. from *Eisenia bicyclis*. Oil.

Iodo analogue, 6,7-dihydro: ***Eiseniaiodide B***
$C_{18}H_{29}IO_3$ 420.33
Isol. from *Eisenia bicyclis*. Oil. $[\alpha]_D^{20}$ -193 (c, 0.08 in $CHCl_3$).

Kousaka, K. *et al., J. Nat. Prod.*, 2003, **66**, 1318-1323 (*isol, pmr, cmr*)

Eiseniachloride C E-59



$C_{20}H_{29}ClO_3$ 352.9

Oxylipin. Related to Ecklonialactone F, E-15. Isol. from the brown alga *Eisenia bicyclis*. Oil. $[\alpha]_D^{20}$ -128 (c, 0.07 in $CHCl_3$).

Kousaka, K. *et al., J. Nat. Prod.*, 2003, **66**, 1318-1323 (*isol, pmr, cmr*)

Eisenin E-60

N-*[N²-(5-Oxoprolyl)glutaminyl]alanine, 9CI. Pyroglutamylglutaminylalanine*
5-OxoPro-Gln-Ala-OH
$C_{13}H_{20}N_4O_6$ 328.324

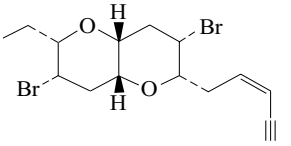
L-L-L-*form* [21477-57-6]
Peptide occurring in *Eisenia bicyclis*. Carcinostatic agent with an immunopotentiating effect. Cryst. (EtOH or MeOH aq.). Sol. acids.
Mp 224-226°. $[\alpha]_D$ -52.8 (c, 6.5 in H_2O).
▶ LD_{50} =5g/kg.

Amide: Eiseninamide
$C_{13}H_{21}N_5O_5$ 327.339
Cryst. (H_2O). Mp 251-254° dec. $[\alpha]_D$ -46 (c, 2.0 in H_2O).

Katakai, R. *et al., J.O.C.*, 1974, **39**, 180 (*synth*)
U.K. Pat., 1985, 2 114 128; *CA*, **103**, 206536h (*pharmacol*)

Elatenyne E-61

[105013-69-2]



$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of *Laurencia elata*. Pale-yellow oil. $[\alpha]_D^{25}$ +16.83 (c, 1.4 in CH_2Cl_2). λ_{max} 224 (ϵ 12600); 233 (sh) (ϵ 9770) (EtOH) (Derep).

Hall, J.G. *et al., Aust. J. Chem.*, 1986, **39**, 1401

Eledoisin, 9CI, INN E-62

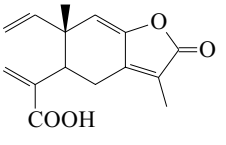
ELD 950. Eloisin. FI 6225
[69-25-0]
5-OxoPro-Pro-Ser-Lys-Asp-Ala-Phe-Ile-Gly-Leu-Met-NH_2
$C_{54}H_{85}N_{13}O_{15}S$ 1188.41
A tachykinin from the posterior salivary glands of *Eledone* spp. Neurokinin receptor agonist. Stimulates extravascular smooth muscle, has powerful vasodilatory and hypotensive action and in certain spp. causes salivation and increased capillary permeability (ophthalmic use). Powder + 1½ H_2O.
Mp 230° dec. $[\alpha]_D^{22}$ -44 (c, 1 in 95% AcOH).
▶ JX8688000

N^{ϵ}-*(Lys)*-tert-*Butoxycarbonyl:* Mp 200° dec. $[\alpha]_D$ -57 (95% AcOH).

[39877-24-2]

Erdös, E.G. *et al., Adv. Pharmacol.*, 1966, **4**, 1 (*rev*)
Bernardi, L. *et al., Gazz. Chim. Ital.*, 1967, **97**, 34 (*analogues*)
Pietta, P.G. *et al., J.O.C.*, 1974, **39**, 44 (*synth*)
De Marco, A. *et al., Int. J. Pept. Protein Res.*, 1975, **7**, 437 (*pmr, cmr*)
Nan, H. *et al., Adv. Mass Spectrom.*, 1978, **7B**, 1518 (*ms*)
Gillespie, J.S. *et al., Br. J. Pharmacol.*, 1978, **62**, 267 (*activity, deriv*)
De Castiglione, R. *et al., Biopolymers*, 1983, **22**, 507 (*rev, pharmacol, manuf, props*)
Kuhl, P. *et al., Monatsh. Chem.*, 1984, **115**, 423 (*partial synth*)
Carpino, L.A. *et al., J.O.C.*, 1991, **56**, 2635 (*synth*)
Geraghty, D.P. *et al., Mol. Pharmacol.*, 1992, **41**, 147
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1364
Wilson, J.C. *et al., Biochemistry*, 1994, **33**, 6802 (*conformn, cd, nmr*)
Bjorup, P. *et al., Bioorg. Med. Chem.*, 1998, **6**, 891-901 (*synth*)

1,3,7(11),8-Elematetraen-12,8-olid-15-oic acid E-63



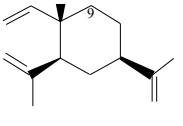
$C_{15}H_{16}O_4$ 260.289

Me ester: [128008-17-3]
$C_{16}H_{18}O_4$ 274.316
Constit. of *Pseudopterogorgia* sp. Gum. $[\alpha]_D$ +19 (c, 0.05 in $CHCl_3$).

Chan, W.R. *et al., Tetrahedron*, 1990, **46**, 1499 (*isol, struct*)

1,3,11-Elematriene E-64

β-Elemene
[33880-83-0]



(−)–*form*

$C_{15}H_{24}$ 204.355

(+)-*form* [13833-25-5]
Isol. from *Libanotis transcaucasica*, *Curcuma aromatica* and coelenterate *Eunicea succinea*. Poorly sol. hexane. $[\alpha]_D$ +14.2 (c, 2.8 in $CHCl_3$). n_D^{20} 1.4945.
▶ LD_{50} (mus, ipr) 278.7 mg/kg.

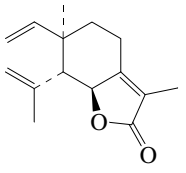
7-Epimer: ***Iso-β-elemene***
[783322-21-4]
$C_{15}H_{24}$ 204.355
Constit. of *Saccogyna viticulosa*. Oil.

(-)-*form* [515-13-9]
Constit. of sweet-flag and juniper oils, *Chrysanthemum* spp., *Mentha* spp. *Doona* spp. and others. Antineoplastic agent. Cytotoxic to P388 and KB cell lines. Oil. $Bp_{15.5}$ 117-124°. $[\alpha]_D^{20}$ -11.1 ($CHCl_3$).
▶ GU9660000

10-Epimer: (-)-cis-*β*-*Elemene*
[674819-49-9]
$C_{15}H_{24}$ 204.355
Constit. of *Scapania undulata*. Oil.

Pigulevskii, G.V. *et al., J. Org. Chem. USSR (Engl. Transl.)*, 1962, **32**, 3054 (*isol*)
Irie, T. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 1053 (*isol, ir, pmr*)
Hunter, G.L.K. *et al., J. Food Sci.*, 1964, **29**, 25 (*isol*)
Patil, L.J. *et al., Tet. Lett.*, 1967, 2273 (*synth*)
Gopichand, Y. *et al., J. Nat. Prod.*, 1984, **47**, 607-614 (*Eunicea succinea constit*)
McMurry, J.E. *et al., Tet. Lett.*, 1985, **26**, 2171 (*synth*)
Wang, X.-W. *et al., Drugs of the Future*, 1998, **23**, 266-270 (*rev*)
Duh, C.Y. *et al., J. Nat. Prod.*, 1999, **62**, 1518 (*isol, activity*)
Kozmin, S.A. *et al., J.A.C.S.*, 1999, **121**, 9562-9573 (*synth*)
Kim, D. *et al., Tetrahedron*, 2001, **57**, 1247-1252 (*synth*)
Adio, A.M. *et al., Phytochemistry*, 2004, **65**, 199-206 (*Scapania undulata constit*)
Hackl, T. *et al., Phytochemistry*, 2004, **65**, 2261-2275 (*Iso-β-elemene*)

1,3,7(11)-Elematrien-12,6-olide E-65

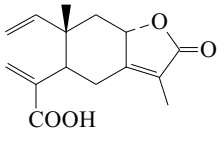


$C_{15}H_{20}O_2$ 232.322

(*ent*-6α)-*form* [865668-52-6]
Constit. of a *Eunicea* sp.
Amorph. powder. $[\alpha]_D^{25}$ +18.8 (c, 1.2 in $CHCl_3$). λ_{max} 220 (ϵ 9400) (MeOH).

Garzón, S.P. *et al., J. Nat. Prod.*, 2005, **68**, 1354-1359

1,3,7(11)-Elematrien-12,8-olid-15-oic acid E-66



$C_{15}H_{18}O_4$ 262.305

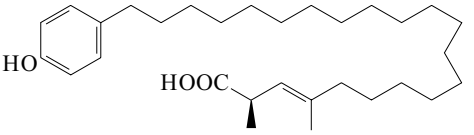
8α-*form*

Me ester: ***Edwardsolide C***
[158515-38-9]
$C_{16}H_{20}O_4$ 276.332
Constit. of *Maasella edwardsi*.
$[\alpha]_D$ +2.7 (c, 0.5 in MeOH).

Bifulco, G. *et al., Nat. Prod. Lett.*, 1993, **3**, 167 (*isol, pmr, cmr*)

Elenic acid E-67

22-(4-Hydroxyphenyl)-2,4-dimethyl-3-docosenoic acid



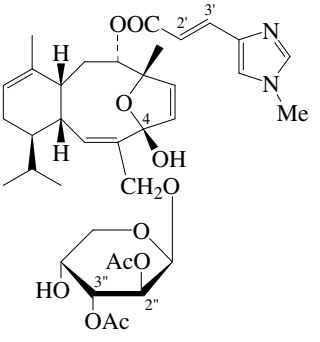
$C_{30}H_{50}O_3$ 458.723
λ_{max} 250 (ϵ 2840) (MeOH) (Derep).

(2*R*,3*E*)-*form* [163564-63-4]
Isol. from a sponge *Plakinastrella* sp. Inhibitor of topoisomerase II. Cytotoxic agent. Amorph. powder. $[\alpha]_D$ -27.2 (c, 2.2 in $CHCl_3$) (natural). $[\alpha]_D^{25}$ -31 (c, 0.31 in $CHCl_3$) (synthetic). λ_{max} 250 (ϵ 2839) (MeOH) (Berdy).

Juagdan, E.G. *et al., Tet. Lett.*, 1995, **36**, 2905 (*isol, uv, ir, pmr, cmr, ms*)
Takanashi, S. *et al., J.C.S. Perkin 1*, 1998, 1603-1606 (*synth, ir, pmr, cmr*)
Hoye, R.C. *et al., J.O.C.*, 1999, **64**, 2450-2453 (*synth*)

Eleuthoside A† E-68

[180692-76-6]



$C_{36}H_{48}N_2O_{11}$ 684.782
Constit. of *Eleutherobia aurea*. Inhibits tubulin polym. induction. Shows strong cytotoxic and antitumour effects. Oil. $[\alpha]_D$ -9 (c, 0.2 in $CHCl_3$).

3″-De-Ac: ***Desmethyleleutherobin***. *Demethyleleutherobin*
[259670-83-2]
$C_{34}H_{46}N_2O_{10}$ 642.745
Constit. of *Erythropodium caribaeorum*.

4-Me ether, 2″-de-Ac: ***Isoeleutherobin A***
[259728-67-1]
$C_{35}H_{48}N_2O_{10}$ 656.772
Constit. of *Erythropodium caribaeorum*. Underwent preclinical evaluation as anticancer drug (2001), but is no longer being pursued due to lack of material availability

4-Me ether, 3″-de-Ac: ***Eleutherobin***
[174545-76-7]
$C_{35}H_{48}N_2O_{10}$ 656.772
Isol. from the soft coral *Eleutherobia* cf. *albiflora* and *Erythropodium caribaeorum*. Cytotoxin with microtubule stabilising props. Shows potent antitumour activity. Amorph. solid. $[\alpha]_D^{25}$ -49.3 (c, 3 in MeOH). λ_{max} 290 (log ϵ 3.82) (MeOH).

4-Me ether, 2″,3″-dide-Ac: ***Deacetyleleutherobin***
[213824-30-7]
$C_{33}H_{46}N_2O_9$ 614.734
Constit. of *Erythropodium caribaeorum*.

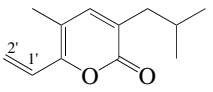
2′Z-Isomer, 4-Me ether, 3″-de-Ac: ***Z-Eleutherobin***
[259670-84-3]
$C_{35}H_{48}N_2O_{10}$ 656.772
Constit. of *Erythropodium caribaeorum*.

Schiff, P.B. *et al., Nature (London)*, 1979, **277**, 665-667 (*activity*)
U.S. Pat., 1995, 5 473 057; *CA*, **124**, 194297 (*Eleutherobin*)
Ketzinel, S. *et al., J. Nat. Prod.*, 1996, **59**, 873-875 (*Eleuthoside A*)

Lindel, T. *et al., J.A.C.S.*, 1997, **119**, 8744-8745 (*Eleutherobin*)
Long, B.H. *et al., Cancer Res.*, 1998, **58**, 1111-1117 (*Eleutherobin, activity*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)
Nicolaou, K.C. *et al., J.A.C.S.*, 1998, **120**, 8661-8673; 8674-8680 (*synth, activity*)
Gutteridge, C. E. *et al., J.A.C.S.*, 1999, **121**, 6563-6579 (*synth*)
Rayl, A.J.S. *et al., The Scientist*, 1999, **13**, 1-3 (*clinical*)
Roberge, M. *et al., Cancer Res.*, 2000, **60**, 5052-5058 (*activity*)
Cinel, B. *et al., Org. Lett.*, 2000, **2**, 257-260 (*Deacetyleleutherobin, Isoeleutherobin A, Desmethyleleutherobin, Z-Eleutherobin*)
Britton, R. *et al., Tet. Lett.*, 2001, **42**, 2953-2956 (*isol, biosynth*)
Castoldi, D. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 588-591 (*Eleutherobin, synth*)

Elijopyrone D E-69

*6-Ethenyl-5-methyl-3-(2-methylpropyl)-2*H*-pyran-2-one, 9CI*
[180839-65-0]



$C_{12}H_{16}O_2$ 192.257
Constit. of a marine actinomycete CNB 880. Oil.

1′,2′-Dihydro: ***Elijopyrone C***
[180839-64-9]
$C_{12}H_{18}O_2$ 194.273
Isol. from marine actinomycete CNB 880. Oil. λ_{max} 212; 308 (MeOH) (Berdy).

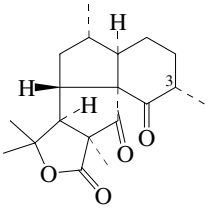
1′,2′-Dihydro, 1′-hydroxy: ***Elijopyrone A***
[180839-62-7]
$C_{12}H_{18}O_3$ 210.272
Isol. from marine actinomycete CNB 880. Oil. λ_{max} 202 (ϵ 9332); 216 (ϵ 3311); 302 (ϵ 6761) (MeOH) (Berdy).

1′,2′-Dihydro, 1′-oxo: ***Elijopyrone B***
[180839-63-8]
$C_{12}H_{16}O_3$ 208.257
Constit. of marine actinomycete CNB 880. Oil. λ_{max} 202 (ϵ 7943); 238 (ϵ 2187); 315 (ϵ 4168) (MeOH) (Berdy).

Toske, S.G. *et al., Nat. Prod. Lett.*, 1995, **6**, 303-308 (*Elijopyrones A-D*)

Elisabanolide E-70

[214355-47-2]



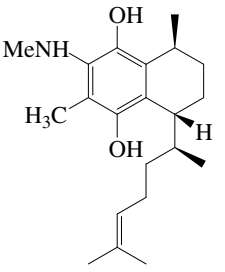
$C_{19}H_{26}O_4$ 318.412
Constit. of *Pseudopterogorgia elisabethae.* Cryst. $[\alpha]_D^{25}$ -39 (c, 0.4 in $CHCl_3$).

3-Epimer: ***3-Epielisabanolide***
[261712-75-8]
$C_{19}H_{26}O_4$ 318.412
Constit. of *Pseudopterogorgia elisabethae.* Cryst. $[\alpha]_D^{25}$ -4 (c, 1.5 in $CHCl_3$).

Rodríguez, A.D. *et al., J.O.C.*, 1998, **63**, 7083-7091 (*isol, pmr, cmr, cryst struct*)
Rodríguez, A.D. *et al., J.O.C.*, 2000, **65**, 1390-1398 (*3-epimer, pmr, cmr, cryst struct*)

Elisabethamine E-71

[294202-41-8]

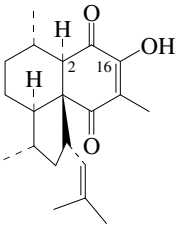


$C_{21}H_{33}NO_2$ 331.497
Alkaloid from *Pseudopterogorgia elisabethae.* Cytotoxic agent. Yellow gum. $[\alpha]_D^{20}$ +89. λ_{max} 292 (no solvent reported).

Ata, A. *et al., Tet. Lett.*, 2000, **41**, 5821-5825 (*isol, pmr, cmr*)

Elisabethin A E-72

[214355-39-2]



$C_{20}H_{28}O_3$ 316.439
Constit. of *Pseudopterogorgia elisabethae.* Cryst. $[\alpha]_D^{25}$ +133 (c, 0.45 in $CHCl_3$). λ_{max} 211 (ϵ 6500); 278 (ϵ 6000) (MeOH).

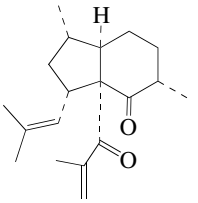
2α-Hydroxy: ***Elisabethin D***
[261712-73-6]
$C_{20}H_{28}O_4$ 332.439
Constit. of *Pseudopterogorgia elisabethae.* Cryst. $[\alpha]_D^{25}$ +6.4 (c, 1.2 in $CHCl_3$). λ_{max} 208 (ϵ 6100); 280 (ϵ 1300) (MeOH).

2α-Hydroxy, 16-Ac: Elisabethin D acetate
[261712-74-7]
$C_{22}H_{30}O_5$ 374.476
Constit. of *Pseudopterogorgia elisabethae.* Oil. $[\alpha]_D^{25}$ +26.3 (c, 2.8 in $CHCl_3$). λ_{max} 208 (ϵ 7000); 252 (ϵ 4000) (MeOH).

Rodríguez, A.D. *et al., J.O.C.*, 1998, **63**, 7083-7091; 2000, **65**, 1390-1398 (*isol, pmr, cmr, cryst struct*)
Heckrodt, T.J. *et al., J.A.C.S.*, 2003, **125**, 4680-4681 (*synth*)

Elisabethin B E-73

[214355-42-7]

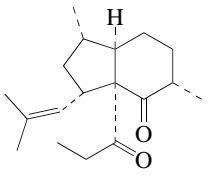


$C_{19}H_{28}O_2$ 288.429
Constit. of *Pseudopterogorgia elisabethae.* Oil. $[\alpha]_D^{25}$ -99 (c, 1.1 in $CHCl_3$). λ_{max} 225 (ϵ 2300) (MeOH).

Rodríguez, A.D. *et al., J.O.C.*, 1998, **63**, 7083-7091 (*isol, pmr, cmr*)
Waizumi, N. *et al., J.A.C.S.*, 2003, **125**, 13022-13023 (*synth*)

Elisabethin C E-74

[214355-44-9]

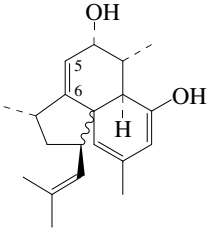


$C_{18}H_{28}O_2$ 276.418
Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{25}$ -31.2 (c, 0.5 in $CHCl_3$).

Rodríguez, A.D. *et al., J.O.C.*, 1998, **63**, 7083-7091 (*isol, pmr, cmr*)
Miyaoka, H. *et al., Tet. Lett.*, 2002, **43**, 7773-7775 (*synth, abs config*)

Elisabethin E E-75

[737006-84-7]



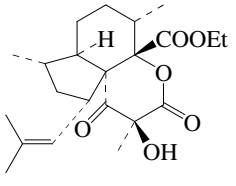
$C_{20}H_{28}O_2$ 300.44
Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{20}$ +39 (c, 0.58 in $CHCl_3$). λ_{max} 232; 269 (MeOH).

5,6α-Dihydro: ***Elisabethin F***
[737006-88-1]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{20}$ +46 (c, 0.24 in $CHCl_3$). λ_{max} 231; 271 (MeOH).

Ata, A. *et al., Helv. Chim. Acta*, 2004, **87**, 1090-1098 (*isol, pmr, cmr*)

Elisabetholide E-76

[290353-49-0]

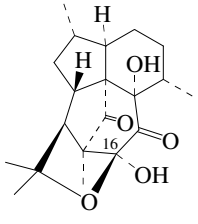


$C_{22}H_{32}O_6$ 392.491
Constit. of *Pseudopterogorgia elisabethae*. Yellow oil. $[\alpha]_D^{25}$ +21.9 (c, 2 in $CHCl_3$).

Rodríguez, A.D. *et al., Tet. Lett.*, 2000, **41**, 5177-5180 (*isol, pmr, cmr*)

Elisapterosin A E-77

[261712-76-9]



Relative Configuration

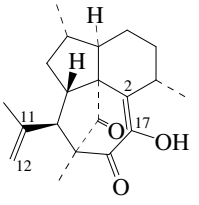
$C_{20}H_{28}O_5$ 348.438
Constit. of *Pseudopterogorgia elisabethae*. Cryst. $[\alpha]_D^{25}$ +140.7 (c, 1.4 in $CHCl_3$).

16-Deoxy: ***Elisapterosin E***
[549503-63-1]
$C_{20}H_{28}O_4$ 332.439
Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{25}$ +51.5 (c, 0.34 in $CHCl_3$).

Rodríguez, A.D. *et al., J.O.C.*, 2000, **65**, 1390-1398 (*Elisapterosin A*)
Shi, Y.-P. *et al., Tet. Lett.*, 2003, **44**, 3249-3253 (*Elisapterosin E*)

Elisapterosin B E-78

[261712-77-0]



Relative Configuration

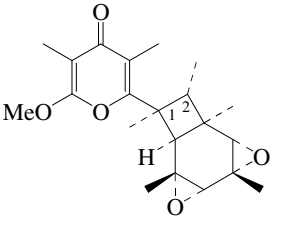
$C_{20}H_{26}O_3$ 314.424
Constit. of *Pseudopterogorgia elisabethae*. Cryst. $[\alpha]_D^{25}$ -3 (c, 4.4 in $CHCl_3$). λ_{max} 212 (ϵ 8500); 288 (ϵ 3400) (MeOH).

11-Hydroxy, 11,12-dihydro: ***Elisapterosin C***
[325691-47-2]
$C_{20}H_{28}O_4$ 332.439
Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{25}$ -71.4 (c, 0.7 in $CHCl_3$). λ_{max} 210 (ϵ 5000); 240 (ϵ 3800); 286 (ϵ 6300) (MeOH).

2α-Hydroxy, 2,17-dihydro, 17-ketone: ***Elisapterosin D***
[549503-62-0]
$C_{20}H_{26}O_4$ 330.423
Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{25}$ +248 (c, 0.5 in $CHCl_3$). λ_{max} 204 (ϵ 5300); 252 (ϵ 2000) (MeOH).

Rodríguez, A.D. *et al., J.O.C.*, 2000, **65**, 1390-1398 (*Elisapterosin B, isol, pmr, cmr, cryst struct*)
Rodríguez, A.D. *et al., Tetrahedron*, 2000, **56**, 9015-9023 (*Elisapterosin C*)
Kim, A.I. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 1267-1270 (*synth*)
Waizumi, N. *et al., J.A.C.S.*, 2003, **125**, 13022-13023 (*synth*)
Shi, Y.-P. *et al., Tet. Lett.*, 2003, **44**, 3249-3253 (*Elisapterosin D*)
Boezio, A.A. *et al., Angew. Chem., Int. Ed.*, 2004, **44**, 6046-6050 (*synth*)
Harrowven, D.C. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 1221-1222 (*synth*)

Elysiapyrone A E-79



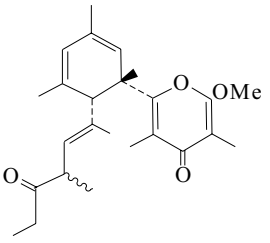
$C_{21}H_{28}O_5$ 360.449
Related to 15-Nortridachione, N-239. Isol. from the sea slug *Elysia diomedea*. Oil. $[\alpha]_D^{25}$ +37 (c, 0.08 in $CHCl_3$).

1,2-Diepimer: ***Elysiapyrone B***
$C_{21}H_{28}O_5$ 360.449
Isol. from *Elysia diomedea*. Oil. $[\alpha]_D^{25}$ +225 (c, 0.08 in $CHCl_3$).

Cueto, M. *et al., Org. Lett.*, 2005, **7**, 415-418 (*isol, pmr, cmr, ms*)

Elysione E-80

[103590-21-2]



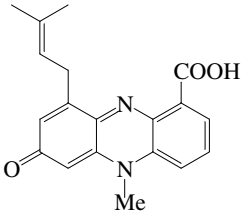
$C_{25}H_{34}O_4$ 398.541

Metab. of mollusc *Elysia chlorotica*. Oil. $[\alpha]_D$ +213 (c, 0.31 in $CHCl_3$). λ_{max} 255 (ϵ 15000) (MeOH) (Derep).

Dawe, R.D. *et al., Tet. Lett.*, 1986, **27**, 2559-2562 (*isol*)

Endophenazine B E-81

*5-Methyl-9-(3-methyl-2-butenyl)-7-oxo-1(5*H*)-phenazinecarboxylic acid*



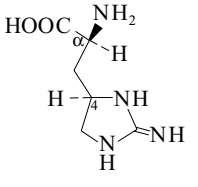
$C_{19}H_{18}N_2O_3$ 322.363

Prod. by various strains of the endosymbiotic *Streptomyces anulatus*. Active against gram-positive bacteria and some fungi. Violet solid. λ_{max} 236 (log ϵ 4.33); 283 (log ϵ 4.44); 374 (log ϵ 3.86); 516 (log ϵ 3.89); 545 (sh) (MeOH).

Gebhardt, K. *et al., J. Antibiot.*, 2002, **55**, 794-800; 801-806 (*isol, pmr, cmr, ms, activity*)

Enduracididine E-82

*α,2-Diamino-4,5-dihydro-1*H*-imidazole-4-propanoic acid, 9CI*



(α*S*,4*R*)*-form*

$C_6H_{12}N_4O_2$ 172.186

(α*S*,4*R*)-*form* [21209-39-2]

Isol. from seeds of *Lonchocarpus sericeus*. Component of Enduracidin A. Mp 235-236° (as hydrobromide).

N$^{\alpha}$*-(6-Bromo-1*H*-indol-3-ylcarbonyl):* **N$^{\alpha}$*-(6-Bromo-1*H*-indol-3-ylcarbonyl)enduracididine***

$C_{15}H_{16}BrN_5O_3$ 394.227

Isol. from the ascidian *Leptoclinides dubius*. Sol. MeOH, butanol. $[\alpha]_D^{20}$ +16.5 (c, 0.8 in MeOH). λ_{max} 222 (log ϵ 2.98); 250 (log ϵ 2.63); 282 (log ϵ 2.39) (MeOH). λ_{max} 222 (ϵ 1122); 250 (ϵ 1350); 282 (ϵ 1288) (MeOH) (Berdy).

(α*R*,4*R*)-*form*

Alloenduracididine

[21380-32-5]

Component of Enduracidin A. Mp 249-252° (as hydrobromide).

Horii, S. *et al., J. Antibiot.*, 1968, **21**, 665-667 (*isol*)
Tsuji, S. *et al., Chem. Lett.*, 1975, 1281-1284 (*synth*)
Fellows, L.E. *et al., Phytochemistry*, 1977, **16**, 1957-1959 (*isol, ms, ir, pmr, cmr*)
Garcia, A. *et al., J. Nat. Prod.*, 1996, **59**, 782-785 (*6-Bromoindolylcarbonylenduracididine*)

Enkephalins E-83

[59141-40-1]

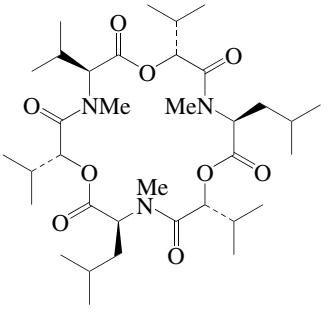
H-Tyr-Gly-Gly-Phe-X-OH, X = Met or Leu

Many syntheses descr. Pentapeptides isol. from several CNS and peripheral tissues. [Met^5]-enkephalin is derived from β-lipotropin (residues 61-65). Also obt. from the cyanobacterial assemblage *Lyngbya majuscula* / *Schizothrix calcicola* as an inseparable mixt. with its C-15 epimer. Both peptides have antinociceptive activity but this is v. transient due to the rapid inactivation by enkephalinases. Hundreds of analogues have been prepd. and evaluated as analgesics in the hope of finding a long-acting non-addictive material.

[58569-55-4, 58822-25-6]

Hughes, J. *et al., Nature (London)*, 1975, **258**, 277
Dhotre, B.J. *et al., J. Indian Chem. Soc.*, 1978, **55**, 1128 (*synth*)
Tregear, T.W. *et al., Circ. Res.*, (Suppl. 1), 1980, **46**, 1 (*rev*)
Coy, D.H. *et al., Pharmacol. Ther.*, 1980, **10**, 657
Beddell, C.R. *et al., Prog. Med. Chem.*, 1980, **17**, 1 (*rev*)
Olson, R.D. *et al., Psychoendocrinology*, 1980, **5**, 47 (*rev*)
Hill, R.C. *et al., Drug Ther. (Biomed. Inf. Corp.)*, 1982, 99 (*rev, pharmacol*)
Aloisi, F. *et al., Isr. J. Med. Sci.*, 1982, **18**, 183 (*activity*)
Vavrek, R.J. *et al., Life Sci.*, 1982, **31**, 2249 (*struct, biol activity*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 6201
Kambara, H. *et al., Org. Mass Spectrom.*, 1982, **17**, 67 (*ms*)
Renugopalakrishnan, V. *et al., NIDA Res. Monogr.*, 1986, **69**, 332 (*conformn, ir, pmr*)
Doi, M. *et al., Pept. Chem.*, 1986, **24**, 131 (*cryst struct, Met^5-Enkephalin*)
Griffin, J.F. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1986, **83**, 3272 (*cryst struct, Leu^5-Enkephalin*)
Kawasaki, K. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1044 (*synth*)
Aubry, A. *et al., Biopolymers*, 1989, **28**, 27 (*cryst struct, Leu^5-Enkephalin*)
Picone, D. *et al., Eur. J. Biochem.*, 1990, **192**, 433 (*conformn*)
Brinkman, H.R. *et al., Synth. Commun.*, 1991, **21**, 459 (*synth, Leu^5-Enkephalin, Met^5-Enkephalin*)
Masiukiewicz, E. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1672-1675 (*synth, Met^5-Enkephalin*)
Harrigan, G.G. *et al., J. Nat. Prod.*, 1998, **61**, 1221-1225 (*isol*)

Enniatin G E-84



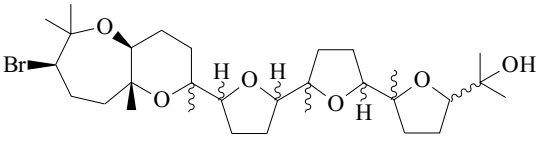
$C_{35}H_{61}N_3O_9$ 667.882

Depsipeptide antibiotic. Prod. by the mangrove fungus *Halosarpheia* sp. 732. Powder. Mp 125-127°. $[\alpha]_D^{25}$ -52.7 (c, 0.29 in $CHCl_3$). λ_{max} 239 (ϵ 5510) ($CHCl_3$).

Lin, Y.-C. *et al., Aust. J. Chem.*, 2002, **55**, 225-227 (*isol, pmr, cmr, ms*)

Enshuol E-85

[171370-52-8]



$C_{30}H_{51}BrO_6$ 587.633

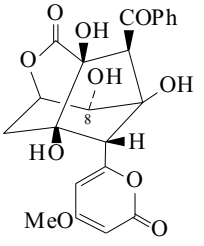
Constit. of *Laurencia omaezakiana*. Oil. $[\alpha]_D^{22}$ +22.7 (c, 1 in $CHCl_3$).

Matsuo, T. *et al., Chem. Lett.*, 1995, 1043 (*isol, pmr, cmr*)

Enterocin E-86

*7-Benzoylhexahydro-4*a*,6,7*a*,8-tetrahydroxy-5-(4-methoxy-2-oxo-2*H*-pyran-6-yl)-3,6-methanocyclopenta[*c*]pyran-1(3*H*)-one, 9CI. Vulgamycin. A 5294. WS 8096. Antibiotic A 5294. Antibiotic WS 8096*

[59678-46-5]



$C_{22}H_{20}O_{10}$ 444.394

Isol. from *Streptomyces candidus, Streptomyces viridochromogenes, Streptomyces hygroscopicus* and *Streptomyces maritimus* BD-26T. Also from a marine ascidian *Didemnum* sp. Active against gram-positive and -negative bacteria esp. *Enterobacteria*. Shows synergism with Streptomycin and Chloramphenicol. Needles (MeOH/EtOH).

Mp 171-173° (163-167°). $[\alpha]_D^{20}$ -10.5 (c, 1 in MeOH). λ_{max} 250 (ϵ 14700); 283 (ϵ 9950) (MeOH) (Derep).

▶ PB9245500

8-O-*Docosanoyl: 8-Docosanoylenterocin. Enterocin 8-behenate*
[172960-83-7]
$C_{44}H_{62}O_{11}$ 766.967

Isol. from a *Didemnum* sp. Non-cryst. solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D$ -75.5 (c, 0.2 in MeOH). λ_{max} 203 (ϵ 58000); 248 (ϵ 19100); 284 (ϵ 12700) (MeOH) (Berdy). λ_{max} 205 (ϵ 57000); 246 (ϵ 19600); 282 (ϵ 11600); 385 (ϵ 3010) (MeOH/NaOH) (Berdy).

8-O-*Eicosanoyl: 8*-O-*Eicosanoylenterocin. Enterocin 8-arachidate*
[172960-84-8]
$C_{42}H_{58}O_{11}$ 738.914

Isol. from a *Didemnum* sp. Non-cryst. solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D$ -81 (c, 0.15 in MeOH). λ_{max} 203 (ϵ 57200); 247 (ϵ 20400); 287 (ϵ 12900) (MeOH) (Berdy). λ_{max} 205 (ϵ 78000); 244 (ϵ 19800); 282 (ϵ 12000); 382 (ϵ 4000) (MeOH/NaOH) (Berdy).

8-Deoxy: ***8-Deoxyenterocin***
[108605-51-2]
$C_{22}H_{20}O_9$ 428.395

From *Streptomyces* sp. L11-1. Also from *Didemnum* sp.

Mp 218-220°. $[\alpha]_D$ -31.5 (c, 1 in MeOH).

6-Epimer, 8-deoxy: [178233-35-7]
$C_{22}H_{20}O_9$ 428.395

Prod. by a marine *Streptomyces* sp. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D$ -22.9 (c, 1 in MeOH). λ_{max} 207 (ϵ 21500); 239 (ϵ 9980); 281 (ϵ 10750) (MeOH).

Miyairi, N. *et al., J. Antibiot.*, 1976, **29**, 227-235 (*isol*)
Tokuma, N. *et al., J. Antibiot.*, 1976, **29**, 1114-1116 (*cryst struct*)
Haruo, S. *et al., Tet. Lett.*, 1976, 4367-4370 (*cmr, struct*)
Japan. Pat., 1979, 79 135 300; *CA*, **86**, 167581 (*isol*)
Japan. Pat., 1985, 85 123 487; *CA*, **104**, 33028 (*derivs*)
Japan. Pat., 1987, 87 56 487; *CA*, **107**, 5763 (*8-deoxy*)
Kang, H. *et al., J.O.C.*, 1996, **61**, 1543-1546 (*isol, uv, ir, pmr, cmr, ms, 8-deoxy, 8-esters*)
Sitachitta, N. *et al., Tetrahedron*, 1996, **52**, 8073-8080 (*isol, 8-deoxy, 6-epimer-8-deoxy*)
Xiang, L. *et al., J. Bacteriol.*, 2003, **185**, 399-404 (*biosynth, isol*)

Enticin E-87

Peptide containing 69 (*Aplysia californica*) or 72 (*Aplysia brasiliana*) amino acid residues. Present in albumen glands of *Aplysia californica* and *Aplysia brasiliana*. Water-borne pheromone that acts in concert with attractin to stimulate mate attraction.

Cummins, S.F. *et al., J. Biol. Chem.*, 2004, **279**, 25614-25622 (*isol*)

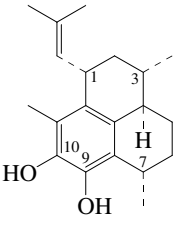
Epiactins E-88

Three polypeptides with MW *ca.* 19500 Da. Isol. from the sea anemone *Epiactis prolifera*. Cytotoxins. Epiactin B is the major toxin.

[82852-42-4 (Epiactin A), 82852-43-5 (Epiactin B), 82852-44-6 (Epiactin C)]

Bernheimer, A.W. *et al., Arch. Biochem. Biophys.*, 1982, **217**, 174-180 (*isol*)

8,10,12,14-Epiamphilectatetraene-9,10-diol E-89



(1α,3α,7α)-*form*

$C_{20}H_{28}O_2$ 300.44

Stereochem. varies between different recent refs. and may not be certain. Pseudopterosins reported simultaneously by 3 different groups with much duplication of names. They are confused in CAS.

(1α,3α,7α)-*form*

Stereochem. revised in 2000.

10-O-*α-D-Arabinopyranoside: Pseudopterosin T*†. *Pseudopterosin Y*
[791846-70-3]
$C_{25}H_{36}O_6$ 432.556

Constit. of *Pseudopterogorgia elisabethae*. Powder. $[\alpha]_D^{20}$ -54.2 (c, 1 in $CHCl_3$). $[\alpha]_D^{25}$ -38 (c, 0,89 in MeOH). λ_{max} 228 (ϵ 28400); 278 (ϵ 7500); 284 (ϵ 6800) (MeOH). λ_{max} 212 (ϵ 15100); 232 (sh); 276 (sh); 285 (ϵ 1770) (MeOH).

10-O-*(3-O-Acetyl-α-D-arabinopyranoside): Pseudopterosin U*†. *Pseudopterosin V*†
[791846-28-1]
$C_{27}H_{38}O_7$ 474.593

Constit. of *Pseudopterogorgia elisabethae*. Powder. $[\alpha]_D^{25}$ -63 (c, 0.31 in MeOH). $[\alpha]_D^{20}$ -78.3 (c, 1.2 in $CHCl_3$). λ_{max} 207 (ϵ 21100); 232 (sh); 274 (sh); 285 (ϵ 2130) (MeOH). λ_{max} 228 (ϵ 37000); 277 (ϵ 6800); 284 (ϵ 7500) (MeOH).

10-O-*(4-O-Acetyl-α-D-arabinopyranoside): Pseudopterosin U*†. *Pseudopterosin V*†
[791846-63-4]
$C_{27}H_{38}O_7$ 474.593

Constit. of *Pseudopterogorgia elisabethae*. Powder. $[\alpha]_D^{20}$ -32.9 (c, 1.1 in $CHCl_3$). $[\alpha]_D^{25}$ -90 (c, 0.88 in MeOH). λ_{max} 228 (ϵ 22300); 277 (ϵ 6500); 284 (ϵ 6300) (MeOH). λ_{max} 211 (ϵ 21900); 232 (sh); 276 (sh); 285 (ϵ 2020) (MeOH).

10-O-*(2,4-Di-O-acetyl-α-D-arabinopyranoside):* ***Pseudopterosin X***
[791846-67-8]
$C_{29}H_{40}O_8$ 516.63

Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{20}$ -39 (c, 1.3 in $CHCl_3$). λ_{max} 228 (ϵ 33800); 277 (ϵ 6800); 284 (ϵ 5100) (MeOH).

10-O-*(3,4-Di-O-acetyl-α-D-arabinopyranoside):* ***Pseudopterosin W***
[791846-65-6]
$C_{29}H_{40}O_8$ 516.63

Constit. of *Pseudopterogorgia elisabethae*. Amorph. solid. $[\alpha]_D^{20}$ -54.8 (c, 1.3 in $CHCl_3$). λ_{max} 228 (ϵ 35000); 277 (ϵ 13000); 284 (ϵ 9000) (MeOH).

10-O-*(2-Acetyl-β-D-xylopyranoside):* ***Pseudopterosin M***
[433717-30-7]
$C_{27}H_{38}O_7$ 474.593

Constit. of *Pseudopterogorgia elisabethae*.
$[\alpha]_D^{20}$ -85 (MeOH). λ_{max} 226; 282 (MeOH).

10-O-*(3-Acetyl-β-D-xylopyranoside):* ***Pseudopterosin N***

[433717-40-9]
$C_{27}H_{38}O_7$ 474.593
Constit. of *Pseudopterogorgia elisabethae.*
$[\alpha]_D^{20}$ -87 (MeOH). λ_{max} 226; 280 (MeOH).

10-O-*(4-Acetyl-β-D-xylopyranoside):* ***Pseudopterosin O***
[433717-38-5]
Constit. of *Pseudopterogorgia elisabethae.*
$[\alpha]_D^{20}$ -75 (MeOH). λ_{max} 226; 279 (MeOH).

10-O-*α-L-Fucopyranoside: Pseudopterosin P*†. *Pseudopterosin T*†
[741259-81-4]
$C_{26}H_{38}O_6$ 446.583
Constit. of *Pseudopterogorgia elisabethae.* Powder. $[\alpha]_D^{25}$ -29 (c, 0.52 in MeOH). $[\alpha]_D^{20}$ -31.8 (c, 1 in $CHCl_3$). λ_{max} 213 (ϵ 24300); 232 (sh); 276 (sh); 285 (ϵ 1400) (MeOH). λ_{max} 228 (ϵ 32800); 277 (ϵ 9400); 284 (ϵ 7400) (MeOH).

9-O-*α-L-Fucopyranoside:* ***Pseudopterosin G***
[128733-03-9]
$C_{26}H_{38}O_6$ 446.583
Constit. of *Pseudopterogorgia elisabethae.* Antiinflammatory agent. Oil. $[\alpha]_D$ -56.8 (c, 2.3 in $CHCl_3$). λ_{max} 226 (ϵ 20800); 275 (ϵ 2770); 285 (ϵ 3350) (MeOH) (Derep).

9-O-*(2-Acetyl-α-L-fucopyranoside):* ***Pseudopterosin H***
[128802-17-5]
$C_{28}H_{40}O_7$ 488.62
Constit. of *Pseudopterogorgia elisabethae.* Antiinflammatory agent. Oil. $[\alpha]_D$ -52.1 (c, 1.3 in $CHCl_3$). λ_{max} 228 (ϵ 10000); 275 (ϵ 1450); 286 (ϵ 1900) (MeOH) (Derep). λ_{max} 229; 276; 280 (MeOH) (Berdy).

9-O-*(3-Acetyl-α-L-fucopyranoside):* ***Pseudopterosin I***
[128733-04-0]
$C_{28}H_{40}O_7$ 488.62
Constit. of *Pseudopterogorgia elisabethae.* Antiinflammatory agent. Oil. $[\alpha]_D$ -44 (c, 1.2 in $CHCl_3$). λ_{max} 228 (ϵ 10000); 275 (ϵ 1450); 286 (ϵ 1900) (MeOH) (Derep).

9-O-*(4-Acetyl-α-L-fucopyranoside):* ***Pseudopterosin J***
[128733-05-1]
$C_{28}H_{40}O_7$ 488.62
Constit. of *Pseudopterogorgia elisabethae.* Antiinflammatory agent. Oil. $[\alpha]_D$ -52.9 (c, 2.2 in $CHCl_3$). λ_{max} 228 (ϵ 10000); 275 (ϵ 1450); 286 (ϵ 1900) (MeOH) (Derep). λ_{max} 227 (ϵ 13000); 276 (ϵ 1900); 284 (ϵ 2400) (MeOH) (Berdy).

10-O-*(2*-O-*Acetyl-α-L-fucopyranoside): Pseudopterosin S*†
$C_{28}H_{40}O_7$ 488.62
Constit. of *Pseudopterogorgia elisabethae.* Powder. $[\alpha]_D^{25}$ -48 (c, 0.18 in MeOH). λ_{max} 208 (ϵ 20500); 232 (sh); 276 (sh); 284 (ϵ 1200) (MeOH).

10-O-*(3*-O-*Acetyl-α-L-fucopyranoside): Pseudopterosin Q*†. *Pseudopterosin R*†
[741259-86-9]
$C_{28}H_{40}O_7$ 488.62
Constit. of *Pseudopterogorgia elisabethae.* Powder. $[\alpha]_D^{25}$ -34 (c, 0.28 in MeOH). $[\alpha]_D^{20}$ -43.6 (c, 1 in $CHCl_3$). λ_{max} 208 (ϵ 25900); 234 (sh); 276 (sh); 285 (ϵ 1150) (MeOH). λ_{max} 228 (ϵ 31500); 278 (ϵ 9800); 284 (ϵ 7500) (MeOH).

10-O-*(4*-O-*Acetyl-α-L-fucopyranoside): Pseudopterosin P*†. *Pseudopterosin Q*†
[741259-85-8]
$C_{28}H_{40}O_7$ 488.62
Constit. of *Pseudopterogorgia elisabethae.* Powder. $[\alpha]_D^{25}$ -53 (c, 0.56 in MeOH). $[\alpha]_D^{20}$ -107.2 (c, 1.3 in $CHCl_3$). λ_{max} 214 (ϵ 23700); 232 (sh); 276 (sh); 285 (ϵ 1670) (MeOH). λ_{max} 228 (ϵ 35000); 277 (ϵ 7000); 284 (ϵ 9000) (MeOH).

10-O-*(2,4-Di*-O-*acetyl-α-L-fucopyranoside): Pseudopterosin S*†
[741260-09-3]
$C_{30}H_{42}O_8$ 530.657
Constit. of *Pseudopterogorgia elisabethae.* Powder. $[\alpha]_D^{20}$ -11.2 (c, 1.3 in $CHCl_3$). λ_{max} 228 (ϵ 29300); 277 (ϵ 6500); 284 (ϵ 7600) (MeOH).

10-O-*(3,4-Di*-O-*acetyl-α-L-fucopyranoside): Pseudopterosin R*†
$C_{30}H_{42}O_8$ 530.657
Constit. of *Pseudopterogorgia elisabethae.* Powder. $[\alpha]_D^{20}$ -45 (c, 1.1 in $CHCl_3$). λ_{max} 228 (ϵ 36700); 277 (ϵ 8500); 284 (ϵ 11000) (MeOH).

(1α,3β,7β)-*form*

9-O-*α-L-Fucopyranoside:* ***Pseudopterosin K***
[128820-74-6]
$C_{26}H_{38}O_6$ 446.583
Constit. of *Pseudopterogorgia elisabethae.* Antiinflammatory agent. Oil. $[\alpha]_D$ -111 (c, 2.1 in $CHCl_3$). λ_{max} 226 (ϵ 20800); 275 (ϵ 2770); 285 (ϵ 3350) (MeOH) (Derep). λ_{max} 277 (ϵ 2000); 284 (ϵ 2300) (MeOH) (Berdy).

9-O-*(3-Acetyl-α-L-fucopyranoside):* ***Pseudopterosin L***
[128819-90-9]
$C_{28}H_{40}O_7$ 488.62
Constit. of *Pseudopterogorgia elisabethae.* Antiinflammatory agent. Oil. $[\alpha]_D$ -112 (c, 1.1 in $CHCl_3$). λ_{max} 228 (ϵ 10000); 275 (ϵ 1450); 286 (ϵ 1900) (MeOH) (Derep). λ_{max} 278 (ϵ 1300); 284 (ϵ 1500) (MeOH) (Berdy).

(1β,3α,7α)-*form*

Pseudopterosin aglycone

10-O-*α-D-Arabinopyranoside:* ***Pseudopterosin F***
[124645-98-3]
$C_{25}H_{36}O_6$ 432.556
Constit. of *Pseudopterogorgia elisabethae.* Antiinflammatory agent. Needles.
Mp 200° dec. $[\alpha]_D$ -243.2 (c, 0.5 in MeOH). λ_{max} 247; 285; 295 (MeOH/KOH) (Derep). λ_{max} 230 (ϵ 11200); 278 (ϵ 2060); 283 (ϵ 2200) (MeOH) (Derep).

10-O-*(2,3-Di*-O-*acetyl-α-D-arabinopyranoside):* ***Pseudopterosin Z***
[791846-80-5]
$C_{29}H_{40}O_8$ 516.63
Constit. of *Pseudopterogorgia elisabethae.* Powder. $[\alpha]_D^{20}$ -142.6 (c, 0.9 in $CHCl_3$). λ_{max} 228 (ϵ 21700); 277 (ϵ 18700); 284 (ϵ 4500) (MeOH).

9-O-*β-D-Xylopyranoside:* ***Pseudopterosin A***. *Resilience™*
[104855-20-1]
$C_{25}H_{36}O_6$ 432.556
Isol. from *Pseudopterogorgia elisabethae.* Shows high antiinflammatory and analgesic activities. Elastase stimulant used in cosmetic antiwrinkle creams. Amorph. solid. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{20}$ -85 (c, 0.69 in $CHCl_3$). λ_{max} 247; 285; 295 (MeOH/KOH) (Derep). λ_{max} 230 (ϵ 11200); 278 (ϵ 2060); 283 (ϵ 2200) (MeOH) (Derep).

9-O-*(2-Acetyl-β-D-xylopyranoside):* ***Pseudopterosin B***
[104855-21-2]
$C_{27}H_{38}O_7$ 474.593
From *Pseudopterogorgia elisabethae.* Antiinflammatory agent and analgesic. Oil. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{20}$ -55.2 (c, 2.1 in $CHCl_3$). λ_{max} 227 (ϵ 11000); 276 (ϵ 1500); 285 (ϵ 2200) (MeOH) (Derep). λ_{max} 230 (ϵ 6000); 274 (ϵ 1400); 285 (ϵ 1600) (MeOH) (Berdy). λ_{max} 288; 294 (MeOH/NaOH) (Berdy).

9-O-*(3-Acetyl-β-D-xylopyranoside):* ***Pseudopterosin C***
[104881-78-9]
$C_{27}H_{38}O_7$ 474.593
From *Pseudopterogorgia elisabethae.* Potent antiinflammatory agent and analgesic. Used in skin care prods., claimed to prevent skin ageing. Cryst. (EtOAc/EtOH). Sol. MeOH, $CHCl_3$.
Mp 113.5-115°. $[\alpha]_D^{20}$ -77 (c, 1.09 in $CHCl_3$). Log P 4.99 (uncertain value) (calc). λ_{max} 227 (ϵ 11000); 276 (ϵ 1500); 285 (ϵ 2200) (MeOH) (Derep). λ_{max} 229 (ϵ 9600); 275 (ϵ 1500); 282 (ϵ 1700) (MeOH) (Berdy). λ_{max} 285; 295 (MeOH/NaOH) (Berdy).

9-O-*(4-Acetyl-β-D-xylopyranoside):* ***Pseudopterosin D***
[104855-22-3]
$C_{27}H_{38}O_7$ 474.593
From *Pseudopterogorgia elisabethae.* Antiinflammatory agent and analgesic. Oil. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{20}$ -107.3 (c, 0.55 in $CHCl_3$). λ_{max} 227 (ϵ 11000); 276 (ϵ 1500); 285 (ϵ 2200) (MeOH) (Derep). λ_{max} 230 (ϵ 6500); 272 (ϵ 3300); 282 (ϵ 3100) (MeOH) (Berdy). λ_{max} 284; 295 (MeOH/NaOH).

10-O-*α-L-Fucopyranoside:* ***Pseudopterosin E***
[121011-80-1]
$C_{26}H_{38}O_6$ 446.583

Constit. of *Pseudopterogorgia elisabethae.* Antiinflammatory, lipoxygenase inhibitor, degranulation inhibitor, leucotriene formn. inhibitor. Amorph. $[\alpha]_D$ -255 (c, 0.4 in MeOH). λ_{max} 226 (ϵ 20800); 275 (ϵ 2770); 285 (ϵ 3350) (MeOH) (Derep).

9-Ac:
$C_{22}H_{30}O_3$ 342.477
Constit. of *Pseudopterogorgia elisabethae.* Prob. struct. Obt. only as an inseparable mixt. with 10-Ac.

*9-Ac, 10-*O*-β-D-xylopyranoside:* ***Pseudopterosin P***
[737006-62-1]
$C_{27}H_{38}O_7$ 474.593
Constit. of *Pseudopterogorgia elisabethae.* Gum. $[\alpha]_D^{20}$ +122 (c, 0.48 in $CHCl_3$). λ_{max} 227; 280 (MeOH).

*9-Ac, 10-*O*-(3-*O*-acetyl-β-D-xylopyranoside):* ***Pseudopterosin Q***†
[737006-76-7]
$C_{29}H_{40}O_8$ 516.63
Constit. of *Pseudopterogorgia elisabethae.* Gum. $[\alpha]_D^{20}$ +124 (c, 0.67 in $CHCl_3$). λ_{max} 229; 281 (MeOH).

*9-Ac, 10-*O*-β-L-xylopyranoside:* ***Pseudopterosin P***†
$C_{27}H_{38}O_7$ 474.593
Constit. of *Pseudopterogorgia elisabethae.* Gum. $[\alpha]_D^{20}$ +122 (c, 0.48 in $CHCl_3$). λ_{max} 227; 280 (MeOH).

10-Ac:
$C_{22}H_{30}O_3$ 342.477
Isol. from *Pseudopterogorgia elisabethae.* Prob. struct. Obt. only as an inseparable mixt. with 9-Ac.

9-Me ether:
$C_{21}H_{30}O_2$ 314.467
Constit. of *Pseudopterogorgia elisabethae.* Oil.

(1β,3β,4β,7β)-*form*
8,10,12,14-Amphilectatetraene-9,10-diol

9-Ac: [890028-31-6]
$C_{22}H_{30}O_3$ 342.477
Constit. of *Pseudopterogorgia elisabethae.* Interconverts with 10-Ac.

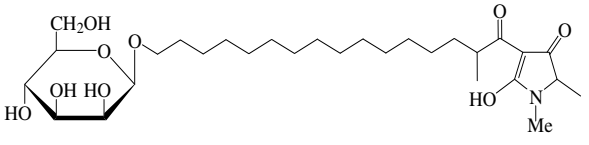
10-Ac: [890028-30-5]
$C_{22}H_{30}O_3$ 342.477
Constit. of *Pseudopterogorgia elisabethae.* Interconverts with 9-Ac.

9,10-Quinone: ***8(13),11,14-Amphilectatriene-9,10-dione***
[889890-61-3]
$C_{20}H_{26}O_2$ 298.424
Constit. of *Pseudopterogorgia elisabethae.* Orange oil. $[\alpha]_D^{25}$ +146 (c, 0.1 in MeOH). λ_{max} 208 (ϵ 27700); 280 (ϵ 2100) (MeOH).

Look, S.A. *et al., J.O.C.*, 1986, **51**, 5140 (*isol, cryst struct*)
Broka, C.A. *et al., J.O.C.*, 1988, **53**, 1584 (*synth*)
Harvis, C.A. *et al., Tet. Lett.*, 1988, **29**, 4361-4364 (*acetates*)
Roussis, V. *et al., J.O.C.*, 1990, **55**, 4916 (*Pseudopterosins E-L, isol, cryst struct*)
Ganguly, A.K. *et al., Pure Appl. Chem.*, 1990, **62**, 1289 (*synth, bibl*)
McCombie, S.W. *et al., Tet. Lett.*, 1991, **32**, 2087 (*synth*)
Lazerwith, S.E. *et al., Org. Lett.*, 2000, **2**, 2389-2392 (*stereochem*)
Chow, R. *et al., J.C.S. Perkin 1*, 2001, 2344-2355 (*synth*)
Kocienski, P.J. *et al., J.C.S. Perkin 1*, 2001, 2356-2366 (*synth*)
Mydlarz, L.D. *et al., Chem. Biol.*, 2003, **10**, 1051-1056 (*biosynth*)
Kohl, A.C. *et al., Mar. Drugs*, 2003, **1**, 54-65 (*biosynth*)
Ata, A. *et al., Tetrahedron*, 2003, **59**, 4215-4222 (*Pseudopterosins M,N,O*)
Ata, A. *et al., Helv. Chim. Acta*, 2004, **87**, 1090-1098 (*Pseudopterosins P and Q*)
Rodriguez, I.I. *et al., J. Nat. Prod.*, 2004, **67**, 1672-1680 (*Pseudopterosins P-Z*)
Harrowven, D.C. *et al., Tet. Lett.*, 2004, **45**, 2089-2091 (*synth*)
Duque, C. *et al., Tetrahedron*, 2004, **60**, 10627-10635 (*Pseudopterosins P-V*)
Duque, C. *et al., Tetrahedron*, 2006, **62**, 4205-4213 (*Amphilectatane derivs*)

Epicoccamide E-90

[606139-26-8]

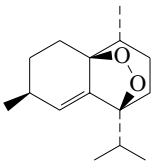


$C_{29}H_{51}NO_9$ 557.723

Tetramic acid deriv. Metab. of the fungus *Epicoccum purpurascens* derived from the jellyfish *Aurelia aurita*. Amorph. powder. $[\alpha]_D^{20}$ -10.3 (c, 0.1 in EtOH). λ_{max} 282 (ϵ 7940) (EtOH).

Wright, A.D. *et al., Org. Biomol. Chem.*, 2003, **1**, 507-510 (*isol, cd, pmr, cmr, ms*)

1,7-Epidioxy-5-cadinene E-91

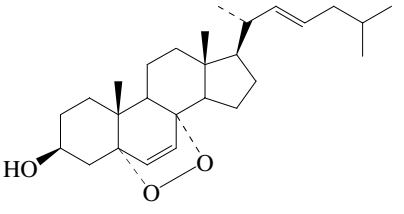


$C_{15}H_{24}O_2$ 236.353

(1β,4β,7β,10α)-*form* [178888-22-7]
Constit. of *Phyllidiopsis krempfi.*
$[\alpha]_D^{23}$ +36 (c, 0.08 in $CHCl_3$).

Okino, T. *et al., Tetrahedron*, 1996, **52**, 9447-9454 (*isol, pmr, cmr*)

5,8-Epidioxycholesta-6,22-dien-3-ol E-92

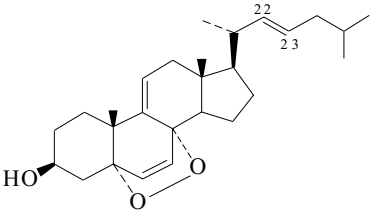


$C_{27}H_{42}O_3$ 414.627

(3β,5α,8α,22*E*)-*form* [75246-76-3]
Constit. of *Luffariella* cf. *variabilis* and *Dendrodoa grossularia.*

Jiménez, C. *et al., J. Nat. Prod.*, 1986, **49**, 905-909 (*isol*)
Gauvin, A. *et al., Can. J. Chem.*, 2000, **78**, 986-992 (*isol, pmr, cmr*)

5,8-Epidioxycholesta-6,9(11),22-trien-3-ol E-93



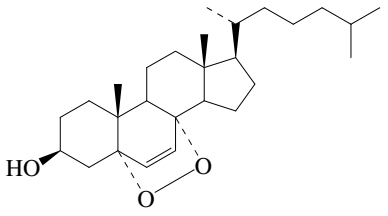
$C_{27}H_{40}O_3$ 412.611

(3β,5α,8α,22*E*)-*form* [78370-85-1]
Constit. of *Ascidia nigra, Dendrogyra cylindrus* and *Thalysias juniperina.*
Oil.

22,23-Dihydro: ***5,8-Epidioxycholesta-6,9(11)-dien-3-ol***
[78342-39-9]
$C_{27}H_{42}O_3$ 414.627
Constit. of *Ascidia nigra, Dendrogyra cylindrus, Thalysias juniperina, Ciona intestinalis, Metridium senile* and *Phallusia mamillata.* Oil.
Mp 164-166°. $[\alpha]_D^{20}$ +95.3 ($CHCl_3$).

Gunatilaka, A.A.L. *et al., J.O.C.*, 1981, **46**, 3860-3866 (*isol, pmr, ms, hplc*)
Guyot, M. *et al., Tet. Lett.*, 1981, **22**, 1391-1392 (*isol*)
Castedo, L. *et al., An. Quim., Ser. C*, 1983, **79**, 454-455 (*dihydro, isol*)
Findlay, J.A. *et al., Steroids*, 1984, **44**, 261-265 (*isol*)

5,8-Epidioxycholest-6-en-3-ol E-94



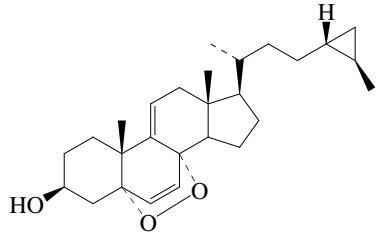
$C_{27}H_{44}O_3$ 416.643

(3β,5α,8α)-*form* [14231-33-5]
Constit. of *Perinereis aibuhitensis*, molluscs and sponges. Also isol. from tunicate *Cynthia savignyi*. Shows antibacterial, antifungal and cytotoxic activities. Cryst.
Mp 102-105°. $[\alpha]_D^{25}$ -30 (c, 0.5 in $CHCl_3$).

24,25-Didehydro: 5,8-Epidioxycholesta-6,24-dien-3-ol
[1715-89-5]
[106518-66-5]
$C_{27}H_{42}O_3$ 414.627
Constit. of *Ascidiella aspersa*, *Dendrodoa grossularia* and *Aplysia punctata*.

Calderon, J.S. *et al., Rev. Latinoam. Quim.*, 1982, **13**, 49-52 (*occur, sponges*)
Castedo, L. *et al., An. Quim., Ser. C*, 1983, **79**, 454-455 (*isol*)
Jiménez, C. *et al., J. Nat. Prod.*, 1986, **49**, 905-909 (*24,25-didehydro, isol, synth*)
Takahashi, K. *et al., Acta Cryst. C*, 1991, **47**, 2581-2583 (*cryst struct, Ac*)
Seo, Y. *et al., Haeyang Yongu*, 1996, **18**, 83-87; *CA*, **125**, 297377 (*isol, pmr, cmr*)
Aknin, M. *et al., J. Am. Oil Chem. Soc.*, 1998, **75**, 1679-1681 (*isol*)
Gauvin, A. *et al., Can. J. Chem.*, 2000, **78**, 986-992 (*isol, pmr*)
Abourriche, A. *et al., Farmaco*, 2000, **55**, 492-494 (*isol, activity*)
Minh, C.V. *et al., Arch. Pharmacal Res.*, 2004, **27**, 734-737 (*isol, pmr, cmr*)

5,8-Epidioxy-24,26-cyclocholesta-6,9(11)-dien-3-ol E-95



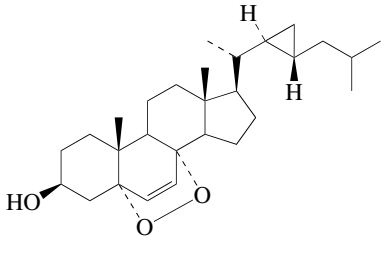
$C_{27}H_{40}O_3$ 412.611

(3β,5α,8α,24*R*,25*R*)-*form* [193270-80-3]
Isol. from sponge *Tethya* sp.

Seo, Y. *et al., Bull. Korean Chem. Soc.*, 1997, **18**, 631-635

5,8-Epidioxy-23,24-didemethylgorgost-6-en-3-ol E-96

5,8-Epidioxy-22,23-cyclopropacholest-6-en-3-ol. *5,8-Epidioxy-22,23-methylenecholest-6-en-3-ol*

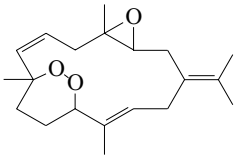


$C_{28}H_{44}O_3$ 428.654

(3β,5α,8α)-*form* [169564-96-9]
Constit. of *Sinularia maxima* and *Sinularia gibberosa*.
Needles (MeOH).
Mp 156-158°. $[\alpha]_D^{27}$ -16.5 (c, 2.09 in $CHCl_3$).

Anjaneyulu, A.S.R. *et al., J. Chem. Res., Synop.*, 1995, 142 (*isol, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 819-825 (*isol, pmr, cmr*)

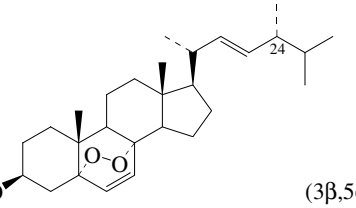
8,11-Epidioxy-3,4-epoxy-1(15),6,12-cembratriene E-97



$C_{20}H_{30}O_3$ 318.455
Constit. of a *Lobophytum* coral. Gum. $[\alpha]_D^{30}$ +1.72 (c, 0.58 in $CHCl_3$).

Subrahmanyam, C. *et al., Tetrahedron*, 1992, **48**, 3111 (*isol, pmr*)

5,8-Epidioxyergosta-6,22-dien-3-ol E-98



(3β,5α,8α,22*E*,24*R*)-*form*

$C_{28}H_{44}O_3$ 428.654

(3β,5α,8α,22*E*,24*R*)-*form*
Ergosterol peroxide. *5α,8α-Peroxyergosterol*
[2061-64-5]
Widely distributed in fungi and lichens. Also obt. from leaves of *Ananas comosus* (pineapple), *Ajuga remota*, the sponge *Axinella cannabina*, the crinoid *Gymnocrinus richeri*, from *Typha latifolia*, *Ascidia nigra*, *Dendrogyra cylindrus*, *Thalysias juniperina*, lichens *Peltigera aphthosa* and *Peltigera dolichorrhiza* and other biol. sources. Active against mycobacterium tuberculosis. Possesses antitumour activity. Cryst. (MeOH).
Mp 181.5-183° (176-198°). $[\alpha]_D$ -29 (c, 0.8 in $CHCl_3$).
▶ KE7289000

3-O-β-D-Glucopyranoside: [140447-22-9]
$C_{34}H_{54}O_8$ 590.796
Constit. of *Cordyceps sinensis* and *Lactarius volemus.*
$[\alpha]_D^{25}$ -15.6.

Ac: [23869-16-1]
Cryst. (Me_2CO). Mp 202.5-203.5°. $[\alpha]_D$ -23 (c, 0.65 in $CHCl_3$).

Octadecanoyl: [644994-62-7]
$C_{46}H_{78}O_4$ 695.12
Constit. of *Ruprechtia triflora*. Amorph. powder. $[\alpha]_D^{25}$ +13 (c, 0.2 in CH_2Cl_2).

3-(2-Hydroxy-4-methoxy-6-propylbenzoyl): ***5,8-Peroxyergosteryl divaricatinate***
[55485-60-4]
$C_{39}H_{56}O_6$ 620.868
Constit. of *Haematomma ventosum*. Cryst. (EtOAc).
Mp 171-172°.

(3β,5α,8α,22*E*,24*S*)-*form*
5,8-Epidioxycampesta-6,22-dien-3-ol
[55722-34-4]
Constit. of *Ascidia nigra*, *Dendrogyra cylindrus*, *Thalysias juniperina* and *Spirastrella abata*.
Oil.

(3β,5α,8α,22*E*,24ξ)-*form* [75197-39-6]
Constit. of *Biemna fortis*, *Luffariella* cf. *variabilis*, *Centaurea diffusa*, *Adalaria* sp. and sea pen *Virgularia* sp.

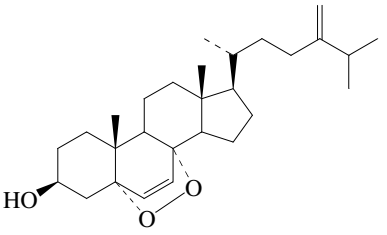
(3β,5β,8β,22*E*,24*R*)-*form* [40071-60-1]
Isol. from *Typha latifolia*.

3-O-*β*-D-*Glucopyranoside:* [348144-81-0]
Constit. of *Lactarius volemus* (tawny milkcap mushroom).

Windaus, A. *et al., Annalen*, 1928, **460**, 225-235 (*Ergosterol peroxide, synth*)
Windaus, A. *et al., Z. Phys. Chem.*, 1942, **276**, 280-281 (*isol, struct*)
Wieland, P. *et al., Helv. Chim. Acta*, 1947, **30**, 1028-1030 (*isol*)
Bauslaugh, G. *et al., Nature (London)*, 1964, **202**, 1218 (*isol*)
Takahashi, R. *et al., Phytochemistry*, 1972, **11**, 1850 (*isol*)
Fattorusso, G. *et al., Gazz. Chim. Ital.*, 1974, **104**, 409-413 (*Typha peroxides*)
Bruun, T. *et al., Acta Chem. Scand., Ser. B*, 1975, **29**, 274-275 (*divaricatinate, isol, synth*)
Pakrashi, S.C. *et al., Indian J. Chem.*, 1975, **13**, 755-756 (*Ergosterol peroxide, isol*)
Stonard, R.J. *et al., Steroids*, 1980, **36**, 81-86 (*3β,5α,8α,22E,24ξ-form, isol*)
Gunatilaka, A.A.C. *et al., J.O.C.*, 1981, **46**, 3860-3866 (*Ergosterol peroxide, 3β,5α,8α,22E,24S-form, isol, pmr, hplc*)
Stoiloo, I. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1984, **79**, 493-497 (*3β,5α,8α,22E,24ξ-form, isol*)
Matsueda, S. *et al., Chem. Ind. (London)*, 1985, 411 (*Ergosterol peroxide, synth, props*)
Della Greca, M. *et al., Gazz. Chim. Ital.*, 1990, **120**, 391-392 (*isol, pmr, cmr, bibl*)
Bok, J.W. *et al., Phytochemistry*, 1999, **51**, 891-898 (*glucoside*)
Cantrell, C.L. *et al., Planta Med.*, 1999, **65**, 732-734 (*isol, activity*)
Yue, J.-M. *et al., Phytochemistry*, 2001, **56**, 801-806 (*Lactarius volemus constit*)
Woldemichael, G.M. *et al., Planta Med.*, 2003, **69**, 628-631 (*octadecanoyl*)
Wang, J.-F. *et al., Acta Cryst. E*, 2004, **60**, o764-o765 (*cryst struct*)

5,8-Epidioxyergosta-6,24(28)-dien-3-ol E-99

5,8-Epidioxy-24-methylenecholest-6-en-3-ol

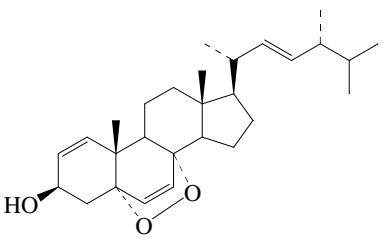


$C_{28}H_{44}O_3$ 428.654

(3β,5α,8α)-*form* [55688-50-1]
[55688-47-6 (Ac)]
Isol. from *Tethya aurantia*, *Metridium senile*, *Dendrodoa grossularia*, *Thalysias juniperina*, *Ascidia nigra*, *Adalaria* sp., seapen *Virgularia* sp. and *Actinia equina*.
No phys. props. reported.

Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*Tethya constit*)
Gunatilaka, A.A.L. *et al., J.O.C.*, 1981, **46**, 3860-3866 (*isol, pmr, ms*)
Findlay, J.A. *et al., Steroids*, 1984, **44**, 261-265 (*Metridium constit*)
Jiménez, C. *et al., J. Nat. Prod.*, 1986, **49**, 905-909 (*isol*)

5,8-Epidioxyergosta-1,6,22-trien-3-ol E-100

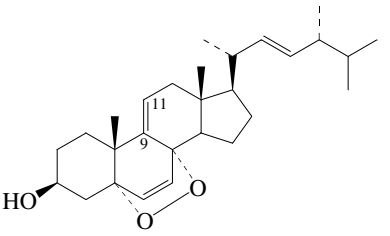


$C_{28}H_{42}O_3$ 426.638

(3β,5α,8α,22*E*,24*R*)-*form* [870486-71-8]
Constit. of *Laurencia cartilaginea*.

Yang, X.-Y. *et al., Guangpu Shiyanshi*, 2005, **22**, 12-16; *CA*, **144**, 19295p

5,8-Epidioxyergosta-6,9(11),22-trien-3-ol E-101



(3β,5α,8α,22*E*,24*R*)-*form*

$C_{28}H_{42}O_3$ 426.638

(3β,5α,8α,22*E*,24*R*)-*form* [86363-50-0]
Constit. of *Typha latifolia*.

O-*β*-D-*Glucopyranoside:* [366006-32-8]
$C_{34}H_{52}O_8$ 588.78
Constit. of *Chlorophyllum molybdites*. Amorph. powder. $[\alpha]_D^{25}$ +5.6 (c, 2 in MeOH).

22,23-Dihydro: ***5,8-Epidioxyergosta-6,9(11)-dien-3-ol***
[50627-03-7]
$C_{28}H_{44}O_3$ 428.654
Constit. of *Metridium senile*.

(3β,5α,8α,22*E*,24*S*)-*form* [78342-38-8]
Constit. of *Ascidia nigra*, *Dendrogyra cylindrus* and *Thalysias juniperina*.

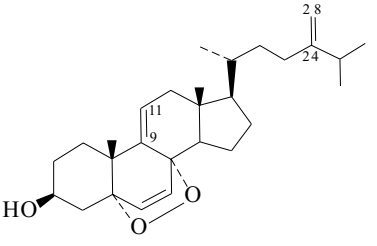
(3β,5α,8α,22*E*,24ξ)-*form* [299159-52-7]
Constit. of *Luffariella* cf. *variabilis*.

22,23-Dihydro: [78418-45-8]
Constit. of *Ascidia nigra*, *Dendrogyrus cylindrus* and *Thalysias juniperina*.
Oil.

Gunatilaka, A.A.L. *et al., J.O.C.*, 1981, **46**, 3860-3866 (*22,23-dihydro*)
Findlay, J.A. *et al., Steroids*, 1984, **44**, 261-265 (*22,23-dihydro, isol*)
Della Greca, M. *et al., Gazz. Chim. Ital.*, 1990, **120**, 391 (*isol, pmr, cmr, bibl*)
Gauvin, A. *et al., Can. J. Chem.*, 2000, **78**, 986-992 (*isol, pmr*)
Yoshikawa, K. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1030-1032 (*glucoside*)

5,8-Epidioxyergosta-6,9(11),24(28)-trien-3-ol E-102

5,8-Epidioxy-24-methylcholesta-6,9(11),24(28)-trien-3-ol.
5,8-Epidioxy-24-methylenecholesta-6,9(11)-dien-3-ol



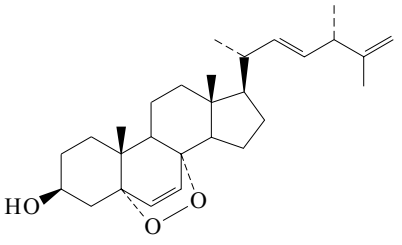
$C_{28}H_{42}O_3$ 426.638

(3β,5α,8α)-*form* [78342-37-7]
Constit. of *Ascidia nigra*.
Oil.

Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*isol*)
Gunatilaka, A.A.L. *et al., J.O.C.*, 1981, **46**, 3860-3866 (*isol, pmr, ms, hplc*)

5,8-Epidioxyergosta-6,22,25-trien-3-ol E-103

5,8-Epidioxy-24-methylcholesta-6,22,25-trien-3-ol



$C_{28}H_{42}O_3$ 426.638

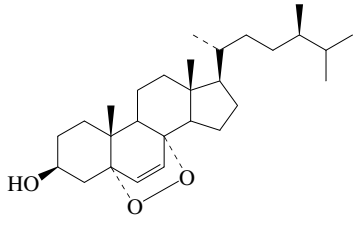
(3β,5α,8α,22*E*,24*S*)-*form*
Axinysterol
[151606-24-5]
Constit. of an *Axinyssa* spp.
Cryst.
Mp 114-115°. $[\alpha]_D^{26}$ -7.7 (c, 0.16 in $CHCl_3$). Not to be confused with Axinyssasterol, 22,23-Dihydro.

9,11-Didehydro: 5,8-Epidioxyergosta-6,9(11),22,25-tetraen-3-ol.
9,11-Didehydroaxinysterol. *9(11)-Dehydroaxinysterol*
[475282-79-2]
$C_{28}H_{40}O_3$ 424.622
Constit. of an *Axinyssa* sponge. Amorph. solid. $[\alpha]_D^{25}$ +78.9 (c, 0.89 in $CHCl_3$).

Iguchi, K. *et al., Steroids*, 1993, **58**, 410-413 (*isol, pmr, cmr*)
Zhi, Y. *et al., CA*, 1995, **122**, 210100w (*isol, pmr, cmr*)
Iwashima, M. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1286-1289 (*9,11-didehydro*)

5,8-Epidioxyergost-6-en-3-ol E-104

5,8-Epidioxy-24-methylcholest-6-en-3-ol



(3β,5α,8α,24*R*)-*form*

$C_{28}H_{46}O_3$ 430.67

(3β,5α,8α,24*R*)-*form* [299159-51-6]
Constit. of *Luffariella* cf. *variabilis.*

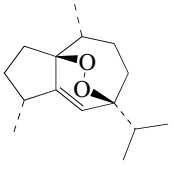
(3β,5α,8α,24*S*)-*form* [82227-99-4]
Constit. of *Luffariella* cf. *variabilis.*

(3β,5α,8α,24ξ)-*form* [75197-38-5]
Constit. of *Dendrogyra cylindrus* and *Thalysias juniperina*.
Oil.

Gunatilaka, A.A.L. *et al., J.O.C.*, 1981, **46**, 3860-3866 (*isol, pmr, cmr*)
Gauvin, A. *et al., Can. J. Chem.*, 2000, **78**, 986-992 (*isol, pmr*)

1,7-Epidioxy-5-guaiene E-105

1,7-Endoperoxy-5-guaiene

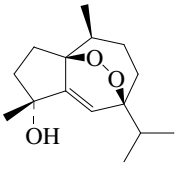


$C_{15}H_{24}O_2$ 236.353

(1β,4α,7β,10α)-*form* [105281-47-8]
Constit. of an *Axinyssa* sponge. Antifouling agent. $[\alpha]_D$ -49.4 (c, 0.27 in $CHCl_3$).

Hirota, H. *et al., Tetrahedron*, 1998, **54**, 13971-13980 (*isol, pmr, cmr*)

1,7-Epidioxy-5-guaien-4-ol E-106

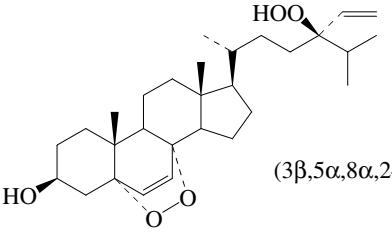


$C_{15}H_{24}O_3$ 252.353

(1β,4α,7β,10β)-*form*
Peroxygibberol
[862377-77-3]
Constit. of *Sinularia gibberosa*.
Oil. $[\alpha]_D^{25}$ +22.4 (c, 1.25 in $CHCl_3$).

Ahmed, A.F. *et al., J. Nat. Prod.*, 2005, **68**, 1208-1212 (*Peroxygibberol*)

5,8-Epidioxy-24-hydroperoxystigmasta-6,28-dien-3-ol E-107



(3β,5α,8α,24*R*)-*form*

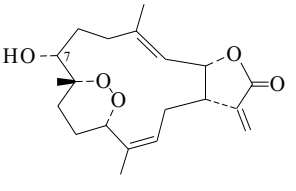
$C_{29}H_{46}O_5$ 474.679

(3β,5α,8α,24*R*)-*form* [217455-29-3]
Constit. of *Lendenfeldia chondrodes.*

(3β,5α,8α,24*S*)-*form* [217455-30-6]
Constit. of *Lendenfeldia chondrodes.*

Sera, Y. *et al., J. Nat. Prod.*, 1999, **62**, 152-154 (*isol, pmr, cmr*)

8,11-Epidioxy-7-hydroxy-3,12,15(17)-cembratrien-16,2-olide E-108



(1*S*,2*S*,3*E*,7*R*,8*R*,11*S*,12*Z*)–*form*

$C_{20}H_{28}O_5$ 348.438

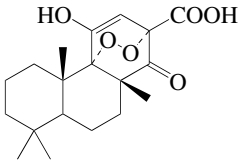
(1*S*,2*S*,3*E*,7*R*,8*R*,11*S*,12*Z*)-*form*
*Ac: **7-Epidenticulatolide***
$C_{22}H_{30}O_6$ 390.475
Constit. of *Lobophytum denticulatum*. Cryst. (Et_2O).
Mp 125-126°. $[\alpha]_D$ -58.4 (c, 2.3 in $CHCl_3$).

(1*S*,2*S*,3*E*,7*S*,8*R*,11*S*,12*Z*)-*form*
*Ac: **Denticulatolide**. Cembranolide C*
[99250-17-6]
$C_{22}H_{30}O_6$ 390.475
Constit. of soft coral *Lobophytum denticulatum* and from *Sinularia mayi* and *Sarcophyton crassocaule.* Icthyotoxin. Cryst. (hexane/CH_2Cl_2).

Mp 129-130.5°. $[\alpha]_D$ +1.4 (c, 0.5 in $CHCl_3$). λ_{max} 210 (MeOH) (Derep). λ_{max} 212 (EtOH) (Berdy).

Uchio, Y. *et al., Tet. Lett.*, 1985, **26**, 4487 (*cryst struct*)
Fukazawa, Y. *et al., Tet. Lett.*, 1986, **27**, 1825 (*conformn*)
Kusumi, T. *et al., Tet. Lett.*, 1988, **29**, 4731-4734 (*Denticulatolide, abs config*)
Uchio, Y. *et al., Bull. Chem. Soc. Jpn.*, 1992, **65**, 1182 (*7-Epidenticulatolide, cryst struct*)

9,13-Epidioxy-11-hydroxy-15-nor-14-oxo-11-isocopalen-16-oic acid E-109

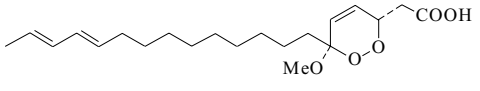


$C_{19}H_{26}O_6$ 350.411

Ac, Me ester: ***Aplypallidioxone***
[200497-15-0]
$C_{22}H_{30}O_7$ 406.475
Constit. of *Aplysilla pallida*. Needles (CH_2Cl_2/petrol).
Mp 170-171°.

Hambley, T.W. *et al., Aust. J. Chem.*, 1997, **50**, 903-909 (*isol, pmr, cmr*)

3,6-Epidioxy-6-methoxy-4,16,18-eicosatrienoic acid E-110

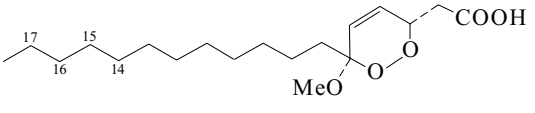


$C_{21}H_{34}O_5$ 366.497

Me ester: Methyl 3,6-epidioxy-6-methoxy-4,16,18-eicosatrienoate
$C_{22}H_{36}O_5$ 380.523
Constit. of sponge *Plakortis lita*. Antitumour agent. Solid.
Mp 47.5°. $[\alpha]_D^{20}$ +36.4 (c, 1.1 in MeOH).

Sakemi, S. *et al., Tetrahedron*, 1987, **43**, 263

3,6-Epidioxy-6-methoxy-4-octadecenoic acid E-111



$C_{19}H_{34}O_5$ 342.475

Me ester: Methyl 3,6-epidioxy-6-methoxy-4-octadecenoate
$C_{20}H_{36}O_5$ 356.501
Constit. of sponge *Plakortis lita*. Antitumour agent. Solid.
Mp 49°. $[\alpha]_D^{20}$ +38.1 (c, 5.3 in MeOH).

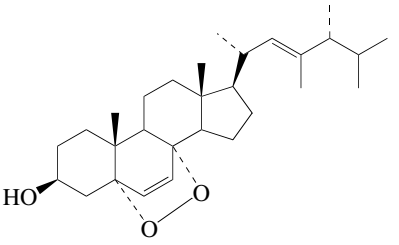
16,17-Didehydro, Me ester: Methyl 3,6-epidioxy-6-methoxy-4,16-octadecadienoate
$C_{20}H_{34}O_5$ 354.486
Constit. of sponge *Plakortis lita*. Antitumour agent. Solid.
Mp 37.5°. $[\alpha]_D^{20}$ +41.4 (c, 2.9 in MeOH).

14,15,16,17-Tetradehydro, Me ester: Methyl 3,6-epidioxy-6-methoxy-4,14,16-octadecatrienoate
$C_{20}H_{32}O_5$ 352.47
Constit. of sponge *Plakortis lita*. Antitumour agent. Solid.
Mp 38-39°. $[\alpha]_D^{20}$ +40.8 (c, 4.9 in MeOH).

Sakemi, S. *et al., Tetrahedron*, 1987, **43**, 263

5,8-Epidioxy-23-methylergosta-6,22-dien-3-ol E-112

5,8-Epidioxy-23,24-dimethylcholesta-6,22-dien-3-ol



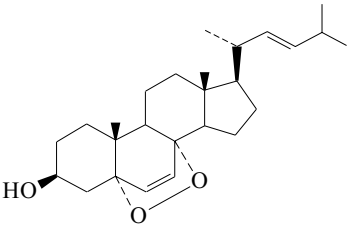
$C_{29}H_{46}O_3$ 442.681

(3β,22*E*,24*R*)-*form* [211486-11-2]
Constit. of *Lentinus edodes* (shiitake).
Amorph. powder. $[\alpha]_D^{16}$ -37 (c, 0.05 in $CHCl_3$).

3-O-Sulfate: [488730-63-8]
$C_{29}H_{46}O_6S$ 522.745
Constit. of *Odontella aurita*. Amorph. solid. $[\alpha]_D$ -1.2 (c, 0.23 in MeOH).

Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1998, **46**, 944-950 (*isol, pmr, cmr*)
Toume, K. *et al., Phytochemistry*, 2002, **61**, 359-360 (*sulfate*)

5,8-Epidioxy-24-norcholesta-6,22-dien-3-ol E-113



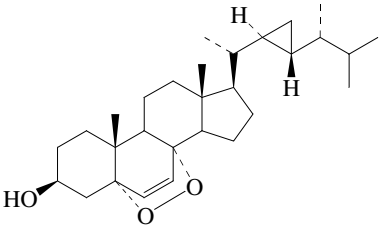
$C_{26}H_{40}O_3$ 400.6

(3β,5α,8α,22*E*)-*form* [75179-58-7]
Constit. of *Ascidia nigra, Dendrogyra cylindrus* and *Thalysias juniperina*. Also from the sea pen *Virgularia* sp.
Oil.

Stonard, R.J. *et al., Steroids*, 1980, **36**, 81-86
Gunatilaka, A.A.L. *et al., J.O.C.*, 1981, **46**, 3860

5,8-Epidioxy-23-norgorgost-6-en-3-ol E-114

5,8-Endoperoxy-23-demethylgorgost-6-en-3-ol



(3β,5α,8α)-*form*

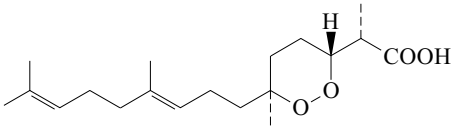
$C_{29}H_{46}O_3$ 442.681

(3β,5α,8α)-*form* [256377-68-1]
Constit. of a *Sinularia* sp.
Amorph. powder.
Mp 159-160°. $[\alpha]_D^{26}$ +35 (c, 0.1 in $CHCl_3$).

Ac: [162290-41-7]
$C_{31}H_{48}O_4$ 484.718
Constit. of *Sinularia maxima*. Cryst.
Mp 148-151°. $[\alpha]_D^{27}$ +25.7 (c, 1.8 in $CHCl_3$).

(3β,5α,8α,22ξ,23ξ,24ξ)-*form* [171262-15-0]
Constit. of a *Lobophytum* sp.
Subrahmanyan, C. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 1114-1115 (*isol, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., J. Chem. Res., Synop.*, 1995, 142 (*Ac*)
Anjaneyulu, A.S.R. *et al., Tetrahedron*, 1995, **51**, 10997-11010 (*isol*)
Sheu, J.H. *et al., J. Nat. Prod.*, 2000, **63**, 149-151 (*isol*)

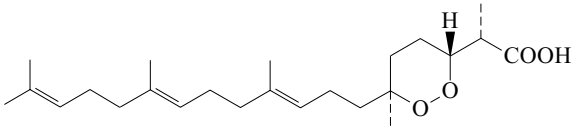
4,7-Epidioxy-1-nor-10,14-phytadien-2-oic acid E-115



$C_{19}H_{32}O_4$ 324.459
Possibly a norsesterterpene.

(3*S*,4*R*,7*S*,10*E*)-*form*
Constit. of an unidentified sponge.
$[\alpha]_D^{25}$ +52.2 (c, 5.65 in $CHCl_3$) (Me ester).
Capon, R.J. *et al., Tetrahedron*, 1985, **41**, 3391-3404 (*isol, pmr*)

4,7-Epidioxy-1-nor-16-prenyl-10,14-phytadien-2-oic acid E-116

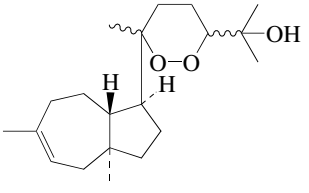


$C_{24}H_{40}O_4$ 392.578

(3*S*,4*S*,7*S*,10*E*,14*E*)-*form*
Constit. of an unidentified sponge.
$[\alpha]_D^{25}$ -60 (c, 9.5 in $CHCl_3$) (Me ester).
Capon, R.J. *et al., Tetrahedron*, 1985, **41**, 3391-3404 (*isol, pmr*)

13,17-Epidioxy-3-sphenoloben-18-ol E-117

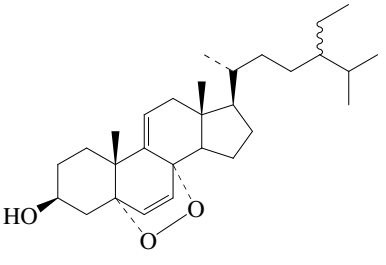
Peroxypolasol
[215440-72-5]



$C_{20}H_{34}O_3$ 322.487
Constit. of an *Epipolasis* sp. Oil. $[\alpha]_D^{25}$ +21.5 (c, 0.6 in $CHCl_3$).
Umeyama, A. *et al., J. Nat. Prod.*, 1998, **61**, 1435-1436 (*isol, pmr, cmr*)

5,8-Epidioxystigmasta-6,9(11)-dien-3-ol E-118

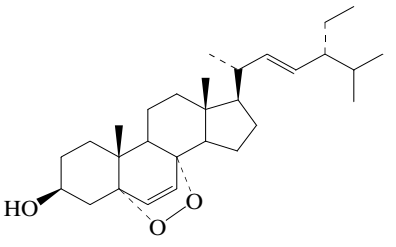
5,8-Epidioxy-24-ethylcholesta-6,9(11)-dien-3-ol



$C_{29}H_{46}O_3$ 442.681

(3β,5α,8α,24ξ)-*form* [78342-40-2]
Constit. of *Ascidia nigra*, *Dendrogyra cylindrus*, *Thalysias juniperina*, *Phallusia manillata*, *Dendrodoa grossularia* and *Spirastrella abata*.
Oil.
Gunatilaka, A.A.L. *et al., J.O.C.*, 1981, **46**, 3860-3866 (*isol*)
Guyot, M. *et al., Tet. Lett.*, 1981, **22**, 1391-1392 (*isol*)
Jimenez, C. *et al., J. Nat. Prod.*, 1986, **49**, 905-909 (*isol, pmr, ms*)
Im, K.S. *et al., Saengyak Hakhoechi*, 2000, **31**, 401-406 (*isol*)

5,8-Epidioxystigmasta-6,22-dien-3-ol E-119



(3β,5α,8α,22*E*,24*R*)-*form*

$C_{29}H_{46}O_3$ 442.681

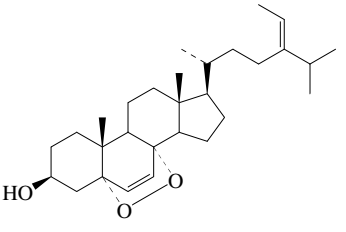
(3β,5α,8α,22*E*,24*R*)-*form* [103190-14-3]
Constit. of *Luffariella* cf. *variabilis*.

(3β,5α,8α,22*E*,24*S*)-*form* [82228-00-0]
Constit. of *Luffariella* cf. *variabilis*.
22,23-Dihydro: ***5,8-Epidioxystigmast-6-en-3-ol***
[193270-93-8]
Constit. of *Luffariella* cf. *variabilis*, *Dendrodoa grossularia* and a *Tethya* sp.

(3β,5α,8α,22*E*,24ξ)-*form* [75296-48-9]
Isol. from *Spirastrella abata*, *Pleraplysilla papyracea*, *Ascidia nigra*, *Dendrogyra cylindrus*, *Thalysias juniperina*, *Virgularia* spp., *Adalaria* sp., the freshwater mussel *Anodonta cygnea* and many other marine spp. Genus name misspelt in the lit. as Pleraphysilla.
22,23-Dihydro: [75246-77-4]
[55688-49-8]
Isol. from *Ascidia nigra*, *Dendrogyra cylindrus*, *Thalysias juniperina*, *Centaurea diffusa*, *Aplysilla gracialis*, *Aplysia dactylomela*, *Gymnocrinus richeri*, *Spirastrella abata* and many other marine spp.
Stonard, R.J. *et al., Steroids*, 1980, **36**, 81-86 (*24ξ-form, occur*)
Gunatilaka, A.A.L. *et al., J.O.C.*, 1981, **46**, 3860-3866 (*24ξ-form, occur*)
Jiménez, C. *et al., J. Nat. Prod.*, 1986, **49**, 905-909 (*24ξ-form 22,23-dihydro, isol*)
De Riccardis, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **100**, 647-651 (*24ξ-form 22,23-dihydro, occur*)
Bobzin, S. *et al., J. Chem. Ecol.*, 1992, **18**, 309-322 (*24ξ-form 22,23-dihydro, occur*)
Gauvin, A. *et al., Can. J. Chem.*, 2000, **78**, 986-992 (*isol, pmr*)
Im, K.S. *et al., Saengyak Hakhoechi*, 2000, **31**, 401-406 (*24ξ-form, isol*)

5,8-Epidioxystigmasta-6,24(28)-dien-3-ol E-120

5,8-Epidioxy-24-ethylcholesta-6,24(28)-dien-3-ol. *5,8-Epidioxy-24-ethylidenecholest-6-en-3-ol*



(3β,5α,8α,24(28*E*))-*form*

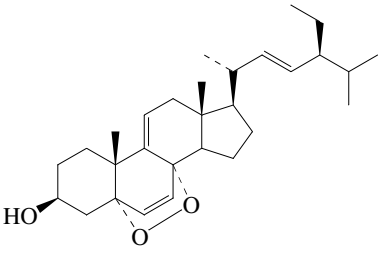
$C_{29}H_{46}O_3$ 442.681

(3β,5α,8α,24(28)*E*)-*form* [78370-84-0]
Constit. of *Ascidia nigra*, *Dendrogyra cylindrus* and *Dendrodoa grossularia*.
Oil. The 24-config. is shown as *E*- but descr. in the text as *Z*-. It is prob. *E*- as in fucosterol.

(3β,5α,8α,24(28)*Z*)-*form*
Isol. from *Dendrodoa grossularia*.
Gunatilaka, A.A.L. *et al., J.O.C.*, 1981, **46**, 3860-3866 (*isol, pmr, ms, hplc*)
Jimenez, C. *et al., J. Nat. Prod.*, 1986, **49**, 905-909 (*isol, pmr, ms*)

5,8-Epidioxystigmasta-6,9(11),22-trien-3-ol E-121

5,8-Epidioxy-24-ethylcholesta-6,9(11),22-trien-3-ol

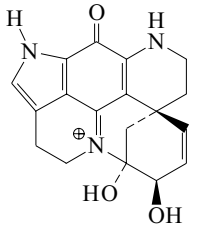


$C_{29}H_{44}O_3$ 440.665

(3β,5α,8α,22*E*,24*S*)-*form* [98495-36-4]
Constit. of *Metridium senile*.
Findlay, J.A. *et al., Steroids*, 1984, **44**, 261-265 (*isol*)

Epinardine A E-122

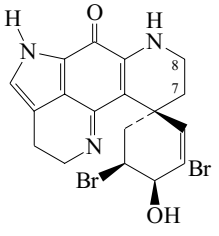
[178822-54-3]



$C_{18}H_{18}N_3O_3^{\oplus}$ 324.358
Alkaloid from an unidentified deep-water green demosponge collected in the South Indian Ocean. Green powder (counterion unspecified). λ_{max} 245 (ϵ 9800); 367 (ϵ 6800); 570 (ϵ 740) (MeOH).
D'Ambrosio, M. *et al., Tetrahedron*, 1996, **52**, 8899 (*isol, uv, cd, pmr, cmr, struct*)

Epinardine B E-123

[178822-55-4]



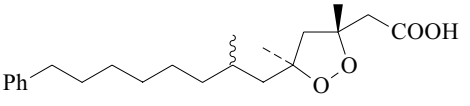
$C_{18}H_{17}Br_2N_3O_2$ 467.159
Alkaloid from an unidentified deep-water green demosponge collected in the South Indian Ocean. Grey-green powder. λ_{max} 200 (ϵ 11600); 248 (ϵ 9300); 340 (ϵ 4050); 390 (ϵ 3130) (MeOH).
λ_{max} 248 (ϵ 9300); 340 (ϵ 4050); 390 (ϵ 3130) (MeOH) (Berdy).

7,8-Didehydro: ***Epinardine C***
[178822-56-5]
$C_{18}H_{15}Br_2N_3O_2$ 465.143
Isol. from an unidentified deep-water demosponge. Strongly cytotoxic towards L1210 and doxorubicin-resistant L1210/DX murine lymphocytic leukaemia cells *in vitro*. Green powder. λ_{max} 210 (ϵ 11400); 250 (ϵ 5900); 290 (ϵ 4400); 370 (ϵ 3200); 535 (ϵ 374) (MeOH).

8α-Methoxy: ***Epinardine D***
[178822-57-6]
$C_{19}H_{19}Br_2N_3O_3$ 497.185
Isol. from an unidentified deep-water green demosponge. Green powder. Converted to Epinardin C on long standing in Me_2CO soln. λ_{max} 205 (ϵ 35000); 242 (ϵ 31000); 335 (ϵ 24000); 480 (ϵ 2000) (MeOH).
D'Ambrosio, M. *et al., Tetrahedron*, 1996, **52**, 8899 (*isol, uv, cd, pmr, cmr, struct*)

Epiplakinic acid E E-124

3,5-Dimethyl-5-(2-methyl-8-phenyloctyl)-1,2-dioxolane-3-acetic acid, 9CI
[159984-99-3]

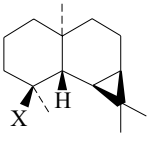


$C_{22}H_{34}O_4$ 362.508

Me ester: [159985-03-2]
$C_{23}H_{36}O_4$ 376.535
Isol. from the sponge *Plakinastrella onkodes*. Cytotoxic agent. Oil. $[\alpha]_D$ +7.5 (c, 0.6 in $CDCl_3$).
Horton, P.A. *et al., J. Nat. Prod.*, 1994, **57**, 1374 (*isol, pmr, cmr*)

Epipolasin A E-125

4-Isothiocyanatomaaliane



(+)–*form*

X = –NCS

$C_{16}H_{25}NS$ 263.446

(+)-*form* [97950-05-5]
Metab. of the sponge *Epipolasis kushimotoensis*.
Cryst. $[\alpha]_D$ +7.6 (c, 1.0 in $CHCl_3$).

(-)-*form*
Metab. of the sponges *Acanthella pulcherrima* and *Axinyssa* sp. and the mollusc *Cadlina luteomarginata*.
Oil. $[\alpha]_D$ -8 (c, 1.3 in $CHCl_3$).

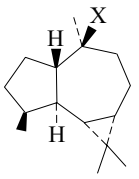
Formamide: ***4-Formylaminomaaliane***
[83631-20-3]
$C_{16}H_{27}NO$ 249.395
Metab. of an *Acanthella* sp. and *Cadlina luteomarginata*. Has -NHCHO replacing -NCS.

[83631-19-0]

Thompson, J.E. *et al., Tetrahedron*, 1982, **38**, 1865-1873 (*isol, pmr, ms*)
Tada, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1941
Capon, R.J. *et al., Aust. J. Chem.*, 1988, **41**, 979 (*isol*)
Simpson, J.S. *et al., Aust. J. Chem.*, 1997, **50**, 1123-1127 (*isol, pmr, cmr, ms*)

Epipolasin B E-126

[97950-06-6]



X = —NCS

$C_{16}H_{25}NS$ 263.446
Metab. of the sponge *Epipolasis kushimotoensis*. Cryst. Mp 92°. $[\alpha]_D$ +91.2 (c, 1.0 in $CHCl_3$).

Tada, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1941

Epipolasinthiourea A E-127

[97915-89-4]
As Epipolasin A, E-125 with
X = –$NHCSNHCH_2CH_2Ph$
$C_{24}H_{36}N_2S$ 384.628
Metab. of sponge *Epipolasis kushimotoensis*. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Tada, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1941

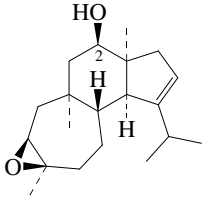
Epipolasinthiourea B E-128

[97915-90-7]
As Epipolasin B, E-126 with
X = –$NHCSNHCH_2CH_2Ph$
$C_{24}H_{36}N_2S$ 384.628
Metab. of sponge *Epipolasis kushimotoensis*. Oil. Sol. MeOH, $CHCl_3$.

Tada, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1941

Epipolol E-129

[367965-40-0]

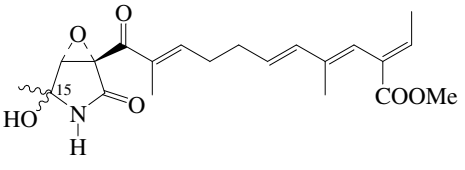


$C_{20}H_{32}O_2$ 304.472
Constit. of *Epipolasis reiswigi*. Oil. $[\alpha]_D^{24}$ +16.4 (c, 1.8 in $CHCl_3$).

2-Ketone: ***Epipolone***
[367965-38-6]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Epipolasis reiswigi*. Oil. $[\alpha]_D^{24}$ -6.7 (c, 0.4 in $CHCl_3$).
Rodríguez, A.D. *et al., J.O.C.*, 2001, **66**, 6364-6368 (*isol, pmr, cmr*)

Epolactaene E-130

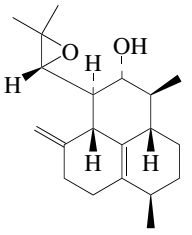
[167782-17-4]



$C_{21}H_{27}NO_6$ 389.447
Nat. product is a diastereoisomeric mixture at C-15. Prod. by the marine fungus *Penicillium* sp. BM1689-P. Neuritogenic agent. Amorph. solid. Sol. MeOH, EtOH, DMSO; fairly sol. $CHCl_3$, EtOAc; poorly sol. H_2O, hexane. $[\alpha]_D^{26}$ +32 (c, 0.1 in MeOH). Similar to Fusarin C. λ_{max} 232 (ϵ 21800); 280 (ϵ 15600) (MeOH) (Berdy).

Kakeya, H. *et al., J. Antibiot.*, 1995, **48**, 733-735 (*isol, ir, uv, pmr, cmr*)
Kuramochi, K. *et al., Tet. Lett.*, 1999, **40**, 7371-7374 (*synth*)
Marumoto, S. *et al., Tetrahedron*, 1999, **55**, 7129-7144; 7145-7156 (*synth, abs config*)
Hayashi, Y. *et al., J.O.C.*, 2002, **67**, 9443-9448 (*synth*)

14,15-Epoxy-8(13),11(20)-amphilectadien-2-ol E-131

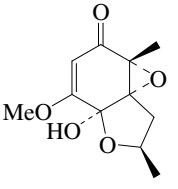


$C_{20}H_{30}O_2$ 302.456

2α-form

Ac: ***Sinulobatin C***
[189456-04-0]
$C_{22}H_{32}O_3$ 344.493
Constit. of *Sinularia nanolobata*. Amorph. solid. $[\alpha]_D^{25}$ +98.2 (c, 0.23 in $CHCl_3$).
Yamada, K. *et al., Tetrahedron*, 1997, **53**, 4569-4578 (*isol, pmr, cmr*)

Epoxyanserinone A E-132

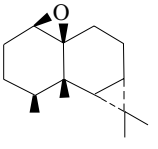


Absolute Configuration

$C_{11}H_{14}O_5$ 226.229
Prod. by a mixture of strains of the marine *Penicillium corylophilum*. Powder. $[\alpha]_D^{27}$ -115 (c, 0.1 in MeOH). λ_{max} 250 (log ϵ 3.9) (CH_2Cl_2).

Diastereoisomer: ***Epoxyanserinone B***
$C_{11}H_{14}O_5$ 226.229
Prod. by a mixt. of strains of *Penicillium corylophilum*. Powder. $[\alpha]_D^{27}$ +245 (c, 0.2 in MeOH).
Gautschi, J.T. *et al., J. Nat. Prod.*, 2004, **67**, 362-367 (*isol, pmr, cmr*)
Gautschi, J.T. *et al., J. Nat. Prod.*, 2004, **67**, 1638 (*abs config*)

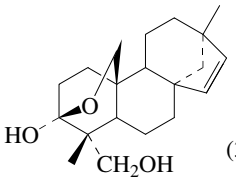
1,10-Epoxyaristolane E-133



$C_{15}H_{24}O$ 220.354

(1β,10β)-*form*
1,10-Epoxy-β-aristolane
[87332-34-1]
Constit. of the sea pen *Scytalium splendens*.
Oil. $[\alpha]_D^{25}$ -24.1 (c, 0.332 in $CHCl_3$).
Do, M.N. *et al., J.O.C.*, 1983, **48**, 4410,

3,20-Epoxy-15-beyerene-3,18-diol E-134



(3α*OH*)-*form*

$C_{20}H_{30}O_3$ 318.455

(3α*OH*)-*form*

Excoecarin D

[263545-01-3]

Constit. of *Excoecaria agallocha*.

Cryst.

Mp 177.5-179.5°. $[\alpha]_D^{25}$ -37.8 (c, 1 in $CHCl_3$).

(*ent*-3α*OH*)-*form*

Rhizophorin B

Constit. of *Rhizophora mucronata*.

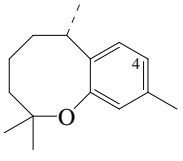
Cryst. ($CHCl_3$/MeOH).

Mp 220°. $[\alpha]_D^{25}$ -59.2 (c, 1.9 in $CHCl_3$). May be identical with Excoecarin D.

Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 2000, **39**, 803-807 (*Rhizophorin B*)

Konishi, T. *et al., J. Nat. Prod.*, 2000, **63**, 344-346 (*Excoecarin D, isol, pmr, cmr, cryst struct*)

1,11-Epoxy-1,3,5-bisabolatriene E-135



$C_{15}H_{22}O$ 218.338

(*S*)-*form*

Helianane

[187874-54-0]

Constit. of *Haliclona fascigera*.

Amorph. solid. $[\alpha]_D$ +8 (c, 1 in CH_2Cl_2). λ_{max} 230 (log ϵ 3.58); 276 (log ϵ 3.65); 282 (sh) (log ϵ 3.66) (no solvent reported).

4-Chloro: ***4-Chloro-1,11-epoxy-1,3,5-bisabolatriene***

[869700-58-3]

$C_{15}H_{21}ClO$ 252.783

Constit. of *Spirastrella hartmani*. Pale yellow oil. $[\alpha]_D^{25}$ +80 (c, 0.01 in $CHCl_3$).

4-Bromo: ***4-Bromo-1,11-epoxy-1,3,5-bisabolatriene***

[869700-59-4]

$C_{15}H_{21}BrO$ 297.234

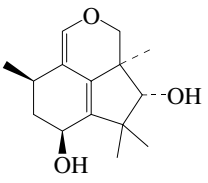
Constit. of *Spirastrella hartmani*. Pale yellow oil. $[\alpha]_D^{25}$ +2.8 (c, 0.02 in $CHCl_3$).

Harrison, B. *et al., J.O.C.*, 1997, **62**, 2646-2648 (*Helianane*)

Sabui, S.K. *et al., Tet. Lett.*, 2004, **45**, 9653-9655 (*Helianane*)

Martín, M.J. *et al., J. Nat. Prod.*, 2005, **68**, 1554-1555 (*4-bromo, 4-chloro*)

10,15-Epoxy-1(10),5(9)-botryadiene-4,7-diol E-136



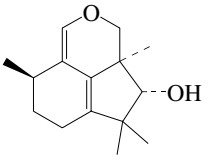
$C_{15}H_{22}O_3$ 250.337

(4β,7α)-*form* [850715-21-8]

Metab. of a *Geniculosporium* sp. isol. from a *Polysiphonia* sp. Gum. $[\alpha]_D^{25}$ +29 (c, 0.18 in CH_2Cl_2).

Krohn, K. *et al., J. Nat. Prod.*, 2005, **68**, 400-405 (*isol, pmr, cmr*)

10,15-Epoxy-1(10),5(9)-botryadien-7-ol E-137



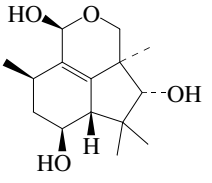
$C_{15}H_{22}O_2$ 234.338

7α-*form* [850715-20-7]

Metab. of a *Geniculosporium* sp. isol. from a *Polysiphonia* sp. Gum. $[\alpha]_D^{25}$ +7 (c, 0.01 in CH_2Cl_2).

Krohn, K. *et al., J. Nat. Prod.*, 2005, **68**, 400-405 (*isol, pmr, cmr*)

10,15-Epoxy-1(9)-botryene-4,7,10-triol E-138



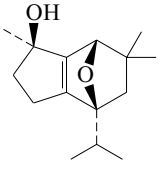
$C_{15}H_{24}O_4$ 268.352

(4β,7α,10β)-*form* [850715-19-4]

Metab. of a *Geniculosporium* sp. isol. from a *Polysiphonia* sp. Gum. $[\alpha]_D^{25}$ +67.9 (c, 0.02 in CH_2Cl_2). Incorrect name in ref.

Krohn, K. *et al., J. Nat. Prod.*, 2005, **68**, 400-405 (*isol, pmr, cmr*)

2,5-Epoxy-1(6)-brasilen-9-ol E-139



$C_{15}H_{24}O_2$ 236.353

(2β,5β,9β)-*form*

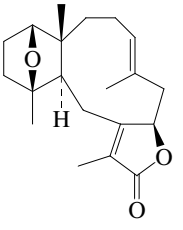
Metab. of *Laurencia obtusa*.

Cryst. (Et_2O/cyclohexane).

Mp 121-123°. $[\alpha]_D^{25}$ +5 (c, 2.5 in EtOH).

Caccmese, S. *et al., J. Nat. Prod.*, 1990, **53**, 1287 (*isol, pmr, cmr*)

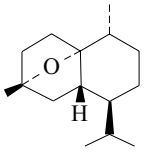
11,14-Epoxy-4,8(17)-briaradien-18,7-olide E-140



$C_{20}H_{28}O_3$ 316.439

(4*E*,7β,11β,14β)-*form*
Pachyclavulariolide A
[325691-32-5]
Constit. of *Pachyclavularia violacea*.
Amorph. solid. $[\alpha]_D$ +17.1 (c, 2 in MeOH).
Xu, L. *et al., Tetrahedron*, 2000, **56**, 9031-9037 (*isol, pmr, cmr*)

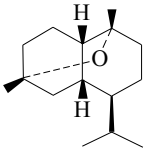
1,4-Epoxycadinane E-141



$C_{15}H_{26}O$ 222.37

(1α,4α,6β,7β,10α)-*form* [73772-79-9]
Constit. of *Dilophus fasciola*.
Cryst.
Mp 54-55°. $[\alpha]_D$ -46.6 (c, 1 in $CHCl_3$).
Fattorusso, E. *et al., Gazz. Chim. Ital.*, 1979, **109**, 589
Rogers, C. *et al., Can. J. Chem.*, 1993, **71**, 611 (*synth*)

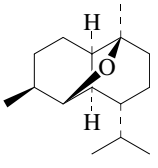
4,10-Epoxycadinane E-142



$C_{15}H_{26}O$ 222.37

(1β,4α,6β,7β,10α)-*form*
4,10-Epoxymuurolane
[70470-08-5]
Constit. of *Dilophus fasciola*.
Oil. $[\alpha]_D$ +15.4 (c, 1 in EtOH).
Amico, V. *et al., Experientia*, 1979, **35**, 450

5,10-Epoxycadinane E-143

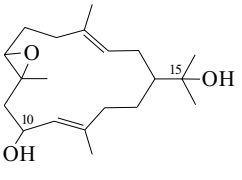


$C_{15}H_{26}O$ 222.37

(1α,4β,5β,6α,7α,10β)-*form*
5,10-Epoxymuurolane
[274675-51-3]
Constit. of *Gorgonia ventalina*.
$[\alpha]_D$ -18.9.
Tsitsimpikou, C. *et al., Nat. Prod. Lett.*, 1999, **14**, 17-23 (*isol, pmr, cmr*)

7,8-Epoxy-3,11-cembradiene-10,15-diol E-144

[83864-66-8]



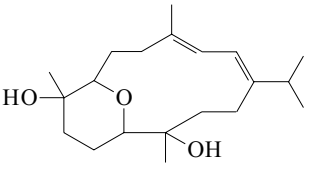
$C_{20}H_{34}O_3$ 322.487
Oil. $[\alpha]_D$ -44.8 (c, 0.14 in $CHCl_3$).

10-Ac: [83864-64-6]
$C_{22}H_{36}O_4$ 364.524
Constit. of *Nephthea brassica*. Oil. $[\alpha]_D$ -30.6.

10,15-Di-Ac: [83864-63-5]
$C_{24}H_{38}O_5$ 406.561
Constit. of *Nephthea brassica*. Oil. $[\alpha]_D$ -34.
Blackman, A.J. *et al., Aust. J. Chem.*, 1982, **35**, 1873

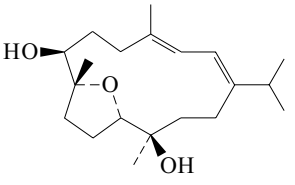
7,11-Epoxy-1,3-cembradiene-8,12-diol E-145

[147217-21-8]



$C_{20}H_{34}O_3$ 322.487
Constit. of a *Eunicea* sponge. Oil. $[\alpha]_D$ -85.8 (c, 0.9 in MeOH).
Shin, J. *et al., Tetrahedron*, 1993, **49**, 515 (*isol, pmr, cmr*)

8,11-Epoxy-1,3-cembradiene-7,12-diol E-146

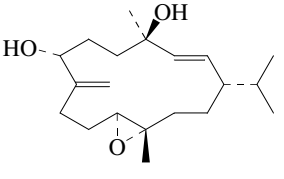


$C_{20}H_{34}O_3$ 322.487

(1*E*,3*E*,7β,8α,11α,12β)-*form* [147217-19-4]
Constit. of a *Eunicea* sponge.
Cryst. (Me_2CO).
Mp 131-132°. $[\alpha]_D$ -85.8 (c, 0.8 in MeOH).

7-Ac: [147217-20-7]
$C_{22}H_{36}O_4$ 364.524
Constit. of a *Eunicea* sponge. Cryst. (Me_2CO/hexane).
Mp 96-98°. $[\alpha]_D$ -35.3 (c, 0.5 in MeOH).
Shin, J. *et al., Tetrahedron*, 1993, **49**, 515 (*isol, pmr, cmr, cryst struct*)

11,12-Epoxy-2,8(19)-cembradiene-4,7-diol E-147



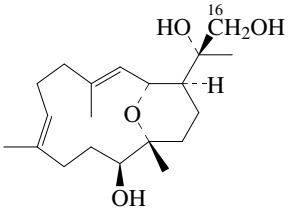
(1*S*,2*E*,4*R*,7*R*,11*S*,12*S*)-*form*

$C_{20}H_{34}O_3$ 322.487

(1*S*,2*E*,4*R*,7*R*,11*S*,12*S*)-*form* [461025-33-2]
Constit. of a *Sarcophyton* sp.
Powder. $[\alpha]_D^{25}$ +14.2 (c, 0.14 in $CHCl_3$). λ_{max} 203 (ε 2100) (MeOH).

(1*S*,2*E*,4*R*,7*S*,11*S*,12*S*)-*form* [461025-32-1]
Constit. of a *Sarcophyton* sp.
Powder. $[\alpha]_D^{25}$ +20.7 (c, 0.14 in $CHCl_3$). λ_{max} 203 (ε 1800) (MeOH).
Pham, N.B. *et al., J. Nat. Prod.*, 2002, **65**, 1147-1150 (*isol, pmr, cmr*)

2,12-Epoxy-3,7-cembradiene-11,15,16-triol E-148



$C_{20}H_{34}O_4$ 338.486

(1*S*,2*R*,3*E*,7*E*,11*S*,12*R*,15*S*)-*form* [824957-47-3]
Oil.

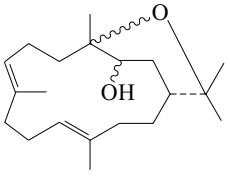
11-Ac: [824957-44-0]
$C_{22}H_{36}O_5$ 380.523
Constit. of a *Eunicea* sp. Oil. $[\alpha]_D^{20}$ +78 (c, 1 in $CHCl_3$).

16-Deoxy, 16-chloro: 16-Chloro-2,12-epoxy-3,7-cembradiene-11,15-diol

16-Deoxy, 16-chloro, 11-Ac: [824957-45-1]
$C_{22}H_{35}ClO_4$ 398.969
Constit. of a *Eunicea* sp. Oil. $[\alpha]_D^{20}$ +77.4 (c, 1 in $CHCl_3$).

Wei, X. *et al., Tetrahedron*, 2004, **60**, 11813-11819 (*isol, pmr, cmr*)

4,15-Epoxy-7,11-cembradien-3-ol E-149

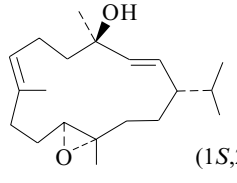


$C_{20}H_{34}O_2$ 306.487

(1*R*,3ξ,4ξ,7*E*,11*E*)-*form*
Decaryiol
[78039-78-8]
Constit. of *Sarcophyton decaryi*.
Cryst. (Me_2CO/petrol).
Mp 126-128.5°. $[\alpha]_D^{24}$ +69 (c, 1.3 in $CHCl_3$).

Carmely, S. *et al., J.O.C.*, 1981, **46**, 4279

11,12-Epoxy-2,7-cembradien-4-ol E-150



(1*S*,2*E*,3*R*,7*E*,11*S*,12*S*)–*form*

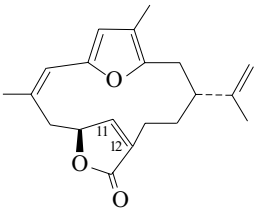
$C_{20}H_{34}O_2$ 306.487

(1*S*,2*E*,3*R*,7*E*,11*S*,12*S*)-*form*
Trocheliophorol
[68042-99-9]
Constit. of *Sarcophyton trocheliophorum*.
Oil.

(1ξ,2*E*,3ξ,7*E*,11ξ,12ξ)-*form*
Constit. of *Solenopodium stechei*.
Oil. $[\alpha]_D$ -28 (c, 0.16 in $CHCl_3$).

Groweiss, A. *et al., Bull. Soc. Chim. Belg.*, 1978, **87**, 277
Raldugin, V.A. *et al., Khim. Prir. Soedin.*, 1980, **16**, 844 (*synth*)
Carmely, S. *et al., J.O.C.*, 1981, **46**, 4279 (*stereochem*)
Bloor, S.J. *et al., J.O.C.*, 1992, **57**, 1205 (*isol, pmr, cmr*)

3,6-Epoxy-3,5,7,11,15-cembrapentaen-20,10-olide E-151



$C_{20}H_{24}O_3$ 312.408

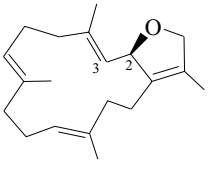
(1*R*,7*Z*,10*S*)-*form*
Rubifolide
[106231-29-2]
Constit. of *Gersemia rubiformis* and *Tochuina tetraquetra*.
Cryst. (CH_2Cl_2/MeOH).
Mp 159-160°. $[\alpha]_D^{25}$ +31.7 (c, 0.39 in $CHCl_3$). λ_{max} 279 (ϵ 16433) (MeOH) (Derep).

11α,12α-Epoxide: 3,6:11,12-Diepoxy-3,5,7,15-cembratetraen-20,10-olide. ***Coralloidolide A***
[107748-88-9]
$C_{20}H_{24}O_4$ 328.407
Isol. from *Alcyonium coralloides*. Cryst.
Mp 112-113°. $[\alpha]_D^{20}$ -66.1 (c, 0.36 in EtOH). Rel. config. only detd.

Williams, D.E. *et al., Can. J. Chem.*, 1987, **65**, 2244
D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1987, **70**, 63 (*Coralloidolide A*)
Williams, D. *et al., J.O.C.*, 1987, **52**, 332 (*Rubifolide*)
Marshall, J.A. *et al., J.O.C.*, 1997, **62**, 4313-4320 (*synth*)

2,16-Epoxy-1(15),3,7,11-cembratetraene E-152

*2,4,5,8,9,12,13,15*a-*Octahydro-3,6,10,14-tetramethylcyclotetradeca[*b*]furan, 9CI*



(2*R*,3*E*,7*E*,11*E*)–*form*

$C_{20}H_{30}O$ 286.456

(2*R*,3*E*,7*E*,11*E*)-*form*

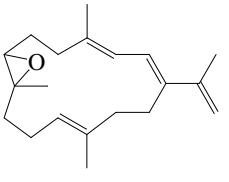
*(3*S*,4*R*)-Epoxide: 2,16:3,4-Diepoxy-1(15),7,11-cembratriene.* ***3,4-Epoxysarcophytonin***
$C_{20}H_{30}O_2$ 302.456
Constit. of a *Sarcophyton* sp. Oil. $[\alpha]_D$ -52.8 (c, 0.38 in $CHCl_3$).
Has (2*S*)-config.

(2ξ,3*E*,7*E*,11*E*)-*form*
Sarcophytonin A. *Deoxysarcophytoxide*
[70645-54-4]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D$ -92 (c, 2.3 in $CHCl_3$).

7,8-Epoxide: See 2,16:7,8-Diepoxy-1(15),3,11-cembratriene, D-424

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1979, **27**, 2382 (*isol, pmr, cmr*)
Nichitani, K. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2514 (*synth*)
Miyaoka, H. *et al., Chem. Lett.*, 1996, 239 (*epoxide*)

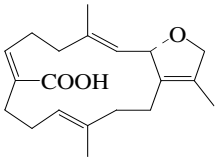
7,8-Epoxy-1,3,11,15-cembratetraene E-153



$C_{20}H_{30}O$ 286.456

(1*E*,3*E*,7ξ,8ξ,11*E*)-*form* [75222-57-0]
Constit. of *Sarcophyton crassocaule*.
Oil. $[\alpha]_D$ -14.4 (c, 0.1 in $CHCl_3$). λ_{max} 271 (sh) (ϵ 17300); 281 (ϵ 22500); 292 (sh) (ϵ 17300) (EtOH).
Bowden, B.F. *et al., Aust. J. Chem.*, 1980, **33**, 879-884 (*isol, pmr, cmr*)

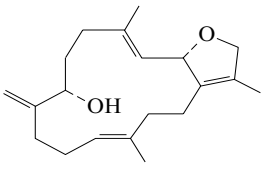
2,16-Epoxy-1(15),3,7,11-cembratetraen-19-oic acid E-154



$C_{20}H_{28}O_3$ 316.439

(2*S*,3*E*,7*Z*,11*E*)-*form*
Me ester: ***13-Dehydroxysarcoglaucol***
[541509-67-5]
$C_{21}H_{30}O_3$ 330.466
Constit. of *Sarcophyton cherbonnieri*. Solid. $[\alpha]_D^{23}$ +100.8 (c, 0.08 in MeOH). λ_{max} 205 (ϵ 10500) (MeOH).
Gross, H. *et al., Org. Biomol. Chem.*, 2003, **1**, 944-949 (*isol, pmr, cmr*)

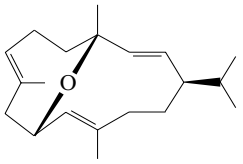
2,16-Epoxy-1(15),3,8(19),11-cembratetraen-7-ol E-155



$C_{20}H_{30}O_2$ 302.456

(2*S*,3*E*,7*S*,11*E*)-*form*
Sarcophytonin E
Constit. of a *Sarcophyton* sp.
Oil. $[\alpha]_D^{25}$ +120 (c, 2.06 in $CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 3055 (*isol, pmr, cmr*)

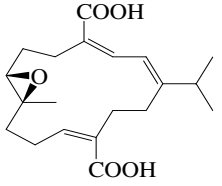
4,10-Epoxy-2,7,11-cembratriene E-156



$C_{20}H_{32}O$ 288.472

(2*E*,7*E*,11*E*)-*form*
Metab. of *Sarcophyton* sp.
Oil.
Anthoni, V. *et al., Tet. Lett.*, 1991, **32**, 2825 (*isol, pmr, cmr*)

7,8-Epoxy-1,3,11-cembratriene-18,20-dioic acid E-157

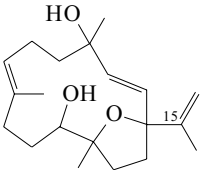


$C_{20}H_{28}O_5$ 348.438

(1*E*,3*Z*,7*S*,8*S*,11*Z*)-*form*
Di-Me ester: ***Sarcophytonolide B***
[862248-72-4]
$C_{22}H_{32}O_5$ 376.492
Constit. of a *Sarcophyton* sp. Oil. $[\alpha]_D^{20}$ +118 (c, 1.65 in $CHCl_3$). λ_{max} 217 (log ϵ 3.48); 287 (log ϵ 3.35) (MeOH).
Jia, R. *et al., Helv. Chim. Acta*, 2005, **88**, 1028-1033 (*Sarcophytonolide B*)

1,12-Epoxy-2,7,15-cembratriene-4,11-diol E-158

[152965-72-5]

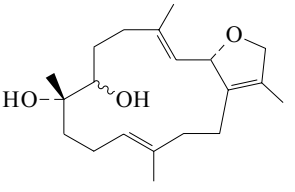


$C_{20}H_{32}O_3$ 320.471
Constit. of *Sinularia ovispiculata*. Cryst.
Mp 156-158°. $[\alpha]_D^{25}$ +81 (c, 0.59 in MeOH).

15,16-Dihydro: ***1,12-Epoxy-2,7-cembradiene-4,11-diol***
[152965-71-4]
$C_{20}H_{34}O_3$ 322.487
Isol. from *Sinularia ovispiculata*. Cryst.
Mp 143-145°. $[\alpha]_D^{25}$ +113.5 (c, 0.1 in $CHCl_3$).
Rao, C.B. *et al., J. Nat. Prod.*, 1993, **56**, 2003 (*isol, pmr, cmr*)

2,16-Epoxy-1(15),3,11-cembratriene-7,8-diol E-159

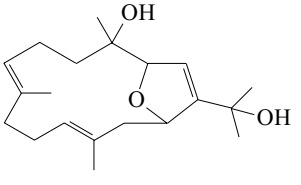
[131615-64-0]



$C_{20}H_{32}O_3$ 320.471

(2*S*,3*E*,7ξ,8*S*,11*E*)-*form*
Sarcophytonin C
[131549-79-6]
Constit. of a *Sarcophyton* coral.
Oil. $[\alpha]_D^{27}$ +90 (c, 1.09 in $CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2442 (*isol, pmr, cmr*)

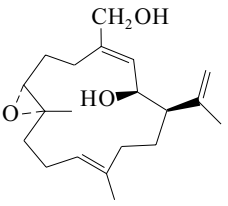
3,14-Epoxy-1,7,11-cembratriene-4,15-diol E-160



$C_{20}H_{32}O_3$ 320.471

(3ξ,4ξ,7*E*,11*E*,14ξ)-*form* [177714-93-1]
Constit. of *Sinularia gibberosa*.
Oil. $[\alpha]_D^{25}$ -10.6 (c, 0.24 in $CHCl_3$). λ_{max} 208 (log ϵ 3.9) (MeOH). λ_{max} 208 (ϵ 7940) (MeOH) (Berdy).
Duh, C.-Y. *et al., J. Nat. Prod.*, 1996, **59**, 595-598 (*isol, pmr, cmr*)

7,8-Epoxy-3,11,15-cembratriene-2,18-diol E-161



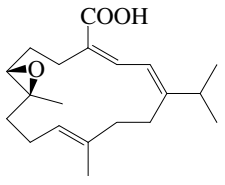
$C_{20}H_{32}O_3$ 320.471

(1*R*,3*E*,7*R*,8*R*,11*E*)-*form*
Asperdiol
[64180-67-2]
Constit. of *Eunicea asperula* and *Eunicea tourneforti*.
Cryst. (Me_2CO/hexane).
Mp 109-110°. $[\alpha]_D^{20}$ -87 ($CHCl_3$).

18-Ac: ***Asperdiol acetate***
$C_{22}H_{34}O_4$ 362.508
Constit. of *Eunicea succinea*. Oil. $[\alpha]_D^{25}$ -52.4 (c, 2.5 in $CHCl_3$). λ_{max} 206 (ϵ 9900) (MeOH) (Berdy).

Weinheimer, A.J. *et al., Tet. Lett.*, 1977, 1295 (*isol, struct*)
Martin, G.E. *et al., Tet. Lett.*, 1979, 2195 (*cmr*)
Still, W.C. *et al., J.O.C.*, 1983, **48**, 4785 (*synth*)
Aoki, M. *et al., Tet. Lett.*, 1983, **24**, 2267 (*synth*)
Marshall, J.A. *et al., J.O.C.*, 1986, **51**, 858 (*synth*)
Kato, T. *et al., J.O.C.*, 1987, **52**, 1803 (*synth*)
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 1134-1138 (*18-Ac*)

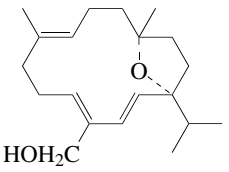
7,8-Epoxy-1,3,11-cembratrien-18-oic acid E-162



$C_{20}H_{30}O_3$ 318.455

(1*E*,3*Z*,7*S*,8*S*,11*E*)-*form*
Me ester: ***Sarcophytonolide A***
[862248-71-3]
$C_{21}H_{32}O_3$ 332.482
Constit. of a *Sarcophyton* sp. Oil. $[\alpha]_D^{20}$ +1.8 (c, 0.57 in $CHCl_3$). λ_{max} 283 (log ϵ 3.15) (MeOH).
Jia, R. *et al., Helv. Chim. Acta*, 2005, **88**, 1028-1033 (*Sarcophytonolide A*)

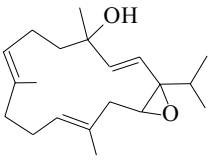
1,4-Epoxy-7,11,13-cembratrien-20-ol E-163



$C_{20}H_{32}O_2$ 304.472

(1*R,4*R**)-*form***
Ac: ***Lobophynin A***
[192222-17-6]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Lobophytum schoedei*. Oil. $[\alpha]_D^{22}$ -22.9 (c, 0.12 in $CHCl_3$).
Yamada, K. *et al., J. Nat. Prod.*, 1997, **60**, 798-801 (*isol, pmr, cmr*)

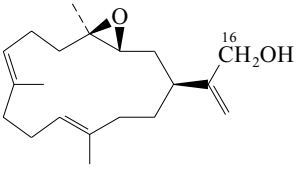
1,14-Epoxy-2,7,11-cembratrien-4-ol E-164



$C_{20}H_{32}O_2$ 304.472

(2*E*,7*E*,11*E*)-*form*
Sarcophytol C
[77394-01-5]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D$ +121 (c, 1.4 in $CHCl_3$).
Nakagawa, T. *et al., Chem. Pharm. Bull.*, 1981, **29**, 82

3,4-Epoxy-7,11,15(17)-cembratrien-16-ol E-165



$C_{20}H_{32}O_2$ 304.472

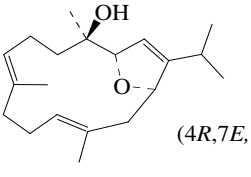
(3*R*,4*R*,7*E*,11*E*)-*form*
Pseudoplexaurol
[148149-83-1]
Constit. of *Pseudoplexaura porosa*.
Oil. $[\alpha]_D^{26}$ -21.5 (c, 3.4 in $CHCl_3$).

16-Aldehyde: 3,4-Epoxy-7,11,15(17)-cembratrien-16-al. ***Pseudoplexaural***
$C_{20}H_{30}O_2$ 302.456
Constit. of *Eunicea succinea*. Oil. $[\alpha]_D^{25}$ -2.8 (c, 1.4 in $CHCl_3$).

16-Carboxylic acid: 3,4-Epoxy-7,11,15(17)-cembratrien-16-oic acid. ***Pseudoplexauric acid***
$C_{20}H_{30}O_3$ 318.455
Constit. of *Eunicea mammosa*.
$[\alpha]_D^{25}$ -15.18 (c, 2.7 in $CHCl_3$) (as Me ester).

Rodríguez, A.D. *et al., Experientia*, 1993, **49**, 179 (*isol, pmr, cmr*)
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 1101 (*isol, pmr, cmr*)
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 1134-1138 (*Pseudoplexaural*)
Li, S.H. *et al., Chin. Chem. Lett.*, 2002, **13**, 820-823 (*synth*)

3,14-Epoxy-1,7,11-cembratrien-4-ol E-166



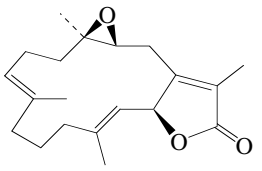
(4*R*,7*E*,11*E*)-*form*

$C_{20}H_{32}O_2$ 304.472

(4*R*,7*E*,11*E*)-*form*
Marasol
[137894-83-8]
Constit. of *Plexaura flexuosa*.
Oil. $[\alpha]_D^{29}$ +173.9 (c, 0.7 in $CHCl_3$).

(4*S*,7*E*,11*E*)-*form* [122053-16-1]
Constit. of *Sarcophyton glaucum*.
Kobayashi, M. *et al., Tennen Yuki Kagobutsu Toronkai Koen Yoshishu*, 1988, **30**, 212-219; *CA*, **112**, 56331g (*Sarcophyton glaucum constit*)
Peniston, M. *et al., J. Nat. Prod.*, 1991, **54**, 1009-1016 (*Marasol, isol, pmr, cmr*)

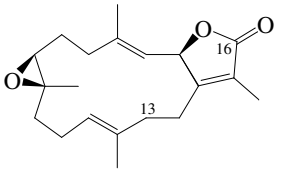
3,4-Epoxy-1(15),7,12-cembratrien-16,14-olide E-167



$C_{20}H_{28}O_3$ 316.439

(3*S*,4*R*,7*E*,12*E*,14*S*)-*form*
***Sarcophytolide*†**
[205445-12-1]
Constit. of *Sarcophyton glaucum*. Shows wide range of antimicrobial activity. Neuroprotectant. Cryst.
Mp 142°.
Badaria, F.A. *et al., Int. J. Pharmacogn.*, 1997, **35**, 284-287; *CA*, **128**, 255276y (*isol, pmr, cmr, activity*)
Badaria, F.A. *et al., Toxicol.*, 1998, **131**, 133-143 (*isol, cmr, activity*)

7,8-Epoxy-1(15),3,11-cembratrien-16,2-olide E-168

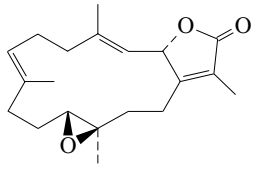


$C_{20}H_{28}O_3$ 316.439

(2*R*,3*E*,7*S*,8*S*,11*E*)-*form*
Sarcophine
[55038-27-2]
Constit. of *Sarcophyton glaucum*, *Lobophytum* sp. and *Sinularia gibberosa*. Ichthyotoxin; tumorigenesis inhibitor; inhibitor of acetylcholine esterase and ATPase. Cryst. (Me_2CO/petrol).
Mp 133-134°. $[\alpha]_D^{25}$ +92 (c, 1 in $CHCl_3$). λ_{max} 222 (ϵ 10000) (MeOH) (Derep).
▶ RR1108000
13-Acetoxy: ***13-Acetoxysarcophine***
$C_{22}H_{30}O_5$ 374.476
Constit. of a *Lobophytum* sp. Enzyme inhibitor. $[\alpha]_D$ +58 ($CHCl_3$).

(2*S*,3*E*,7*S*,8*S*,11*E*)-*form*
2-Episarcophine
Constit. of *Sarcophyton glaucum*.
Cryst.
Mp 70°. $[\alpha]_D$ -16. λ_{max} 222 (ϵ 10000) (MeOH) (Derep).
[84984-71-4]
Bernstein, J. *et al., Tetrahedron*, 1974, **30**, 2817 (*isol*)
Kashman, Y. *et al., Tetrahedron*, 1974, **30**, 3615 (*isol*)
Suleimova, A.M. *et al., Khim. Prir. Soedin.*, 1990, 762-765 (*13-Acetoxysarcophine*)
El Sayed, K.A. *et al., J.O.C.*, 1998, **63**, 7449-7455 (*analogues, activity*)
Gross, H. *et al., Org. Biomol. Chem.*, 2004, **2**, 1133-1138 (*abs config*)

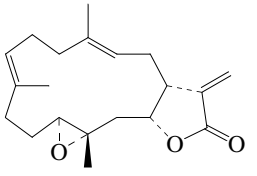
11,12-Epoxy-1(15),3,7-cembratrien-16,2-olide E-169



$C_{20}H_{28}O_3$ 316.439

(2α,3*E*,7*E*,11β,12β)-*form*
Isosarcophine. *Sartrochine*
[132160-45-3]
Constit. of *Sinularia mayi*.
Oil. $[\alpha]_D$ +235.3 (c, 0.14 in $CHCl_3$).
Kusumi, T. *et al., Chem. Lett.*, 1990, 1315 (*isol, pmr*)
Wu, Y.C. *et al., J. Chin. Chem. Soc. (Taipei)*, 1992, **39**, 355 (*isol, pmr, cmr*)
Su, J.Y. *et al., Huaxue Xuebao*, 1994, **52**, 813-816 (*Sartrochine*)

11,12-Epoxy-3,7,15(17)-cembratrien-16,14-olide E-170



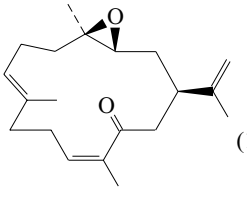
(1*R*,3*E*,7*E*,11*S*,12*S*,14*R*)-*form*

$C_{20}H_{28}O_3$ 316.439

(1*R*,3*E*,7*E*,11*S*,12*S*,14*R*)-*form*
***Crassolide*†**
[313674-26-9]
Constit. of *Sarcophyton crassocaule.*
Oil. $[\alpha]_D^{25}$ +127.1 (c, 0.21 in $CHCl_3$). λ_{max} 233 (log ϵ 4.3) (MeOH).

(1*R*,3*E*,7*E*,11*S*,12*S*,14*S*)-*form*
Lobophytolide
[55593-54-9]
Constit. of *Lobophytum cristigalli*.
Cryst.
Mp 137-138°. $[\alpha]_D$ +7 (c, 0.4 in $CHCl_3$). λ_{max} 210 (ϵ 6540) (EtOH) (Derep).
Karlsson, R. *et al., Acta Cryst. B*, 1977, **33**, 2032 (*Lobophytolide*)
Duh, C.-Y. *et al., J. Nat. Prod.*, 2000, **63**, 1634-1637 (*Crassolide*)

3,4-Epoxy-7,11,15-cembratrien-13-one E-171



(1*R*,3*R*,4*R*,7*E*,11*Z*)–*form*

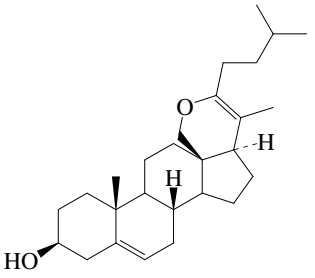
$C_{20}H_{30}O_2$ 302.456

(1*R*,3*R*,4*R*,7*E*,11*Z*)-*form* [152378-27-3]
Constit. of *Eunicea mammosa*.
Oil. $[\alpha]_D^{25}$ -5.38 (c, 2.6 in $CHCl_3$). λ_{max} 235 (ϵ 12000) (hexane) (Derep).

(1*S*,3*S*,4*S*,7*E*,11*E*)-*form* [65634-83-5]
Constit. of an unidentified soft coral.
Oil. $[\alpha]_D^{20}$ +12.78 (c, 1.65 in $CHCl_3$).

(1*S*,3*S*,4*S*,7*E*,11*Z*)-*form* [65622-45-9]
Constit. of an unidentified soft coral.
Oil. $[\alpha]_D^{20}$ +8.8 (c, 1.6 in $CHCl_3$).
Ravi, B.N. *et al., J.O.C.*, 1978, **43**, 2127-2131 (*soft coral constits*)
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 1101-1113 (*Eunicea mammosa constit*)

18,22-Epoxycholesta-5,20(22)-dien-3-ol E-172



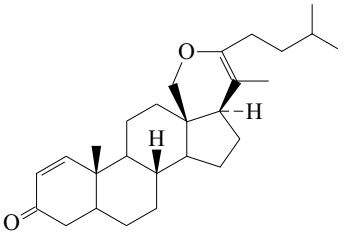
$C_{27}H_{42}O_2$ 398.628

3β-*form* [674819-46-6]
Constit. of *Axinella* cf. *bidderi*.
Powder. $[\alpha]_D^{25}$ +178.6 (c, 0.056 in CH_2Cl_2).

5α,6-Dihydro: ***18,22-Epoxycholest-20(22)-en-3-ol***
[675106-22-6]
$C_{27}H_{44}O_2$ 400.643
Constit. of *Axinella* cf. *bidderi*. Powder. $[\alpha]_D^{25}$ +101.7 (c, 0.118 in CH_2Cl_2).
Funel, C. *et al., J. Nat. Prod.*, 2004, **67**, 491-494 (*isol, pmr, cmr*)

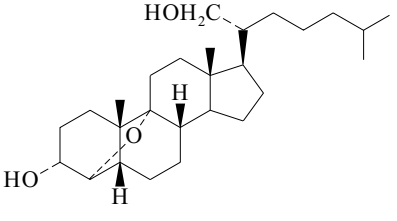
18,22-Epoxycholesta-1,20(22)-dien-3-one E-173

[161776-75-6]



$C_{27}H_{40}O_2$ 396.612
Constit. of *Alcyonium gracillimum*. Cryst.
Mp 52-53°. $[\alpha]_D$ +34 (c, 0.5 in $CDCl_3$).
Seo, Y. *et al., Tetrahedron*, 1995, **51**, 2497 (*isol, pmr, cmr*)

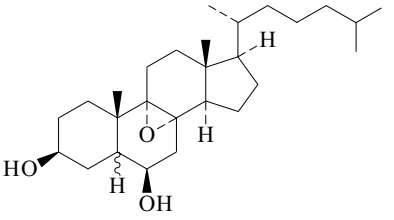
4,9-Epoxycholestane-3,21-diol E-174



$C_{27}H_{46}O_3$ 418.659

(3α,4α,5β,9α)-*form*
Amorph. solid.
Disulfate: [143503-20-2]
$C_{27}H_{46}O_9S_2$ 578.787
Constit. of *Ophiomastix annulosa*. Amorph. solid. $[\alpha]_D$ +53.4.
D'Auria, M.V. *et al., Tet. Lett.*, 1992, **33**, 4641-4644 (*isol, pmr, cmr*)

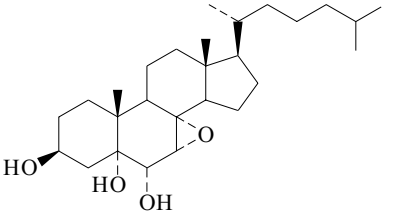
8,9-Epoxycholestane-3,6-diol, 9CI E-175



$C_{27}H_{46}O_3$ 418.659

(3β,5ξ,6β,8α,9α)-*form*
Elistanol
[54408-47-8]
Isol. from *Pseudopterogorgia elisabethae.*
Campbell, D.C. *et al., Diss. Abstr. Int., B*, 1974, **35**, 1566 (*isol*)

7,8-Epoxycholestane-3,5,6-triol E-176



$C_{27}H_{46}O_4$ 434.658

(3β,5α,6α,7α,8α)-*form* [71135-08-5]
Constit. of *Acabaria undulata.*
Cryst.
Mp 169-171°.

3-Ac: [73532-24-8]
$C_{29}H_{48}O_5$ 476.695
Mp 195-196°.

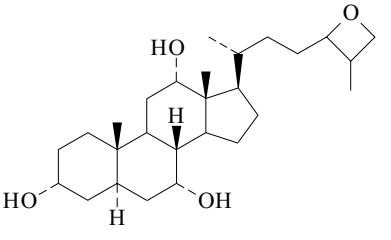
3,6-Di-Ac: [71831-88-4]
$C_{31}H_{50}O_6$ 518.732
Mp 190-191°.

24,25-Didehydro: 7,8-Epoxycholest-24-ene-3,5,6-triol
[177856-28-9]
$C_{27}H_{44}O_4$ 432.642
Constit. of *Acabaria undulata.*

24,25-Didehydro, 3,6-di-Ac:
Cryst. Mp 152-153°.

Rodewald, W. *et al., Tet. Lett.*, 1979, 169 (*synth, ir, pmr*)
Anastasia, M. *et al., Tet. Lett.*, 1979, 3323 (*synth*)
Fujimoto, Y. *et al., Chem. Comm.*, 1985, 10 (*synth*)
Shin, J. *et al., J. Nat. Prod.*, 1996, **59**, 679 (*isol, pmr, cmr*)

24,26-Epoxycholestane-3,7,12-triol, 8CI E-177

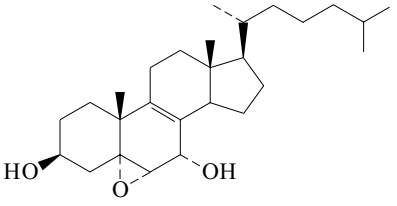


$C_{27}H_{46}O_4$ 434.658

(3α,5α,7α,12α)-*form* [27857-12-1]
Cryst. (EtOAc/Me_2CO). Mp 221-222°. $[\alpha]_D^{24}$ +31.8 (c, 0.68 in EtOH).

(3α,5β,7α,12α)-*form*
Anhydrochimerol
[28979-27-3]
Obt. from hydrolysis of bile salts of *Chimaera monstrosa*.
Mp 180°. $[\alpha]_D$ +41.5 (EtOH).
Okuda, K. *et al., J. Biochem. (Tokyo)*, 1962, **51**, 441 (*isol*)
Bridgwater, R.J. *et al., Biochem. J.*, 1963, **87**, 28 (*synth, 3α,5β,7α,12α-form*)
Anderson, I.G. *et al., Biochem. J.*, 1970, **116**, 581 (*synth, 3α,5α,7α, 12α-form*)

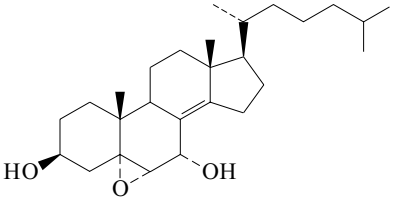
5,6-Epoxycholest-8-ene-3,7-diol E-178



$C_{27}H_{44}O_3$ 416.643

(3β,5α,6α,7α)-*form*
Melithasterol A
[133883-08-6]
Constit. of *Melithaea ocracea* and *Spongia officinalis*.
Cryst. (MeOH). Mp 175-177°. $[\alpha]_D^{26}$ -68 (c, 2,46 in $CHCl_3$).
*22,23-Didehydro (*E-*): 5,6-Epoxycholesta-8,22-diene-3,7-diol.*
Melithasterol C
[133883-09-7]
$C_{27}H_{42}O_3$ 414.627
Constit. of *Melithaea ocracea*. Cryst. (MeOH).
Mp 165-166°. $[\alpha]_D^{26}$ -66 (c, 0.66 in $CHCl_3$).
Di-Ac: [92804-68-7]
Cryst. (MeOH). Mp 188-190°. $[\alpha]_D^{20}$ -99.7 (c, 0.38 in $CHCl_3$).
Kobayashi, M. *et al., J.C.S. Perkin 1*, 1991, 1177 (*isol, pmr, cmr*)
Migliuolo, A. *et al., Steroids*, 1993, **58**, 134-140 (*isol, pmr, cmr*)
Ramesh, P. *et al., J. Nat. Prod.*, 2000, **63**, 1420-1421 (*synth*)

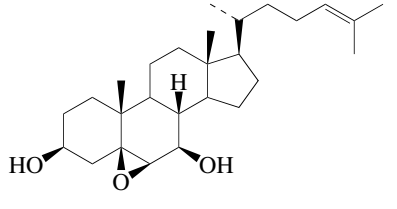
5,6-Epoxycholest-8(14)-ene-3,7-diol E-179



$C_{27}H_{44}O_3$ 416.643

(3β,5α,6α,7α)-*form* [49759-22-0]
Constit. of *Ircinia fasciculata* and *Spongia officinalis*.
Di-Ac: [92804-67-6]
Cryst. Mp 171-173° (138-140°). $[\alpha]_D$ -91.4 (c, 0.17 in $CHCl_3$).
Migliuolo, A. *et al., Steroids*, 1993, **58**, 134-140 (*isol, pmr, cmr, cryst struct*)
Venkateswarlu, Y. *et al., J. Nat. Prod.*, 1996, **59**, 876-877 (*isol, pmr, cmr*)

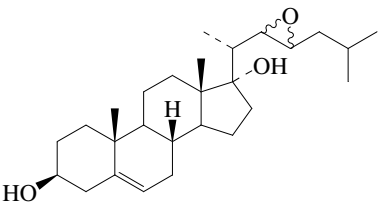
5,6-Epoxycholest-24-ene-3,7-diol E-180



$C_{27}H_{44}O_3$ 416.643

(3β,5β,6β,7β)-*form* [201800-60-4]
Constit. of *Gersemia fruticosa*. Apoptosis inducer. Plates.
Mp 122-123°. $[\alpha]_D$ +49.5 (c, 2.87 in MeOH).
Koljak, R. *et al., Tetrahedron*, 1998, **54**, 179-186 (*isol, pmr, cmr*)

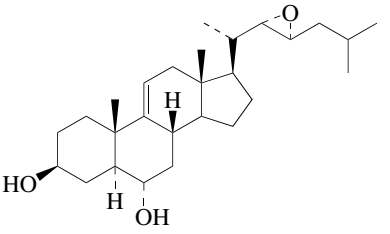
22,23-Epoxycholest-5-ene-3,17-diol E-181



$C_{27}H_{44}O_3$ 416.643

(3β,17α,22ξ,23ξ)-*form* [675106-21-5]
Constit. of *Axinella* cf. *bidderi*.
Funel, C. *et al., J. Nat. Prod.*, 2004, **67**, 491-494 (*isol, pmr, cmr*)

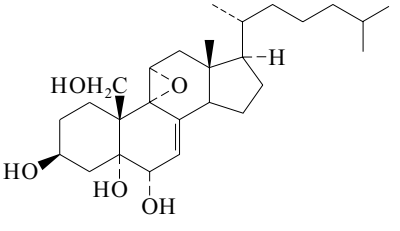
22,23-Epoxycholest-9(11)-ene-3,6-diol E-182



$C_{27}H_{44}O_3$ 416.643

(3β,5α,6α,22*S*,23*S*)-*form*
3-O-*β*-D-*Glucuronopyranoside, 6-sulfate:* ***Downeyoside C***
[174286-15-8]
$C_{33}H_{52}O_{12}S$ 672.833
Constit. of *Henricia downeyae*.
$[\alpha]_D$ -16.6.
3-O-*[α*-L-*Arabinopyranosyl-(1→2)-β*-D-*glucuronopyranoside], 6-sulfate:* ***Downeyoside H***
[174286-20-5]
$C_{38}H_{60}O_{16}S$ 804.948
Constit. of *Henricia downeyae*.
$[\alpha]_D$ -5.5.
Palagiano, E. *et al., J. Nat. Prod.*, 1996, **59**, 348-354 (*isol, pmr, cmr*)

9,11-Epoxycholest-7-ene-3,5,6,19-tetrol E-183



$C_{27}H_{44}O_5$ 448.642

(3β,5α,6α,9α,11α)-*form* [84473-34-7]
6-Ac: ***Dysideasterol A***. *ECTA*
[84473-32-5]
[101387-40-0]
$C_{29}H_{46}O_6$ 490.679

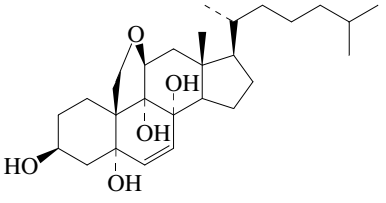
Constit. of sponge *Dysidea arenaria*. Reverses Fluconazole resistance in multidrug-efflux resistant fungi. Cryst. ($CHCl_3$/hexane).
Mp 204-205° Mp 229-230°. $[\alpha]_D^{26}$ +42.6 (c, 0.07 in $CHCl_3$)
$[\alpha]_D^{20}$ +60 (c, 0.13 in $CHCl_3$).

22,23-Didehydro: 9,11-Epoxycholesta-7,22-diene-3,5,6,19-tetrol
$C_{27}H_{42}O_5$ 446.626

*22,23-Didehydro(*E-*), 6-Ac:* ***Dysideasterol B***
[851318-94-0]
$C_{29}H_{44}O_6$ 488.663
Constit. of a *Dysidea* sp. Powder. $[\alpha]_D^{20}$ +42 (c, 0.11 in $CHCl_3$).

Gunasekera, S.P. *et al., J.O.C.*, 1983, **48**, 885 (*isol*)
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1985, **33**, 3129 (*struct*)
Jacob, M.R. *et al., J. Nat. Prod.*, 2003, **66**, 1618-1622 (*activity*)
Huang, X.-C. *et al., Helv. Chim. Acta*, 2005, **88**, 281-289 (*cryst struct*)

11,19-Epoxycholest-6-ene-3,5,8,9-tetrol E-184

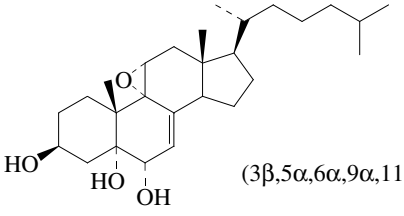


$C_{27}H_{44}O_5$ 448.642

(3β,5α,8α,9α,11β)-*form* [115150-55-5]
[115150-56-6 (3-Ac)]
Isol. from the sponge *Dysidea tupha*. Ichthyotoxin. Toxic to the fish *Lebistes reticulatus* and the sponge *Ephydatia fluviatilis*. Cryst. (Me_2CO) (as 3-Ac).
Mp 223-224° (3-Ac). $[\alpha]_D$ +10.5 (c, 0.4 in $CHCl_3$) (3-Ac).

Braeckman, J.C. *et al., Bull. Soc. Chim. Belg.*, 1988, **97**, 293-296; *CA*, **109**, 35460w (*isol, pmr, cmr*)

9,11-Epoxycholest-7-ene-3,5,6-triol E-185



(3β,5α,6α,9α,11α)-*form*

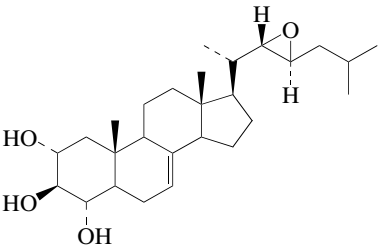
$C_{27}H_{44}O_4$ 432.642

(3β,5α,6α,9α,11α)-*form*
6-Ac: [268735-57-5]
$C_{29}H_{46}O_5$ 474.679
Constit. of a *Dysidea* sp. Powder. $[\alpha]_D^{24}$ +32 (c, 0.13 in $CHCl_3$).
λ_{max} 231 (log ϵ 0.66); 244 (log ϵ 0.47) (CH_2Cl_2).

(3β,5α,6β,9α,11α)-*form* [120152-00-3]
Isol. from marine gastropod *Planaxis sulcatus*.
Cryst. (Me_2CO).
Mp 237-239°. $[\alpha]_D^{20}$ -29.1 (c, 0.3 in $CHCl_3$).

Alam, M. *et al., Steroids*, 1988, **52**, 45 (*isol*)
Migliuolo, A. *et al., Steroids*, 1991, **56**, 154 (*synth, pmr, cmr*)
Leone, P. de A. *et al., J. Nat. Prod.*, 2000, **63**, 694-697 (*Dysidea constit*)

22,23-Epoxycholest-7-ene-2,3,4-triol E-186



$C_{27}H_{44}O_4$ 432.642

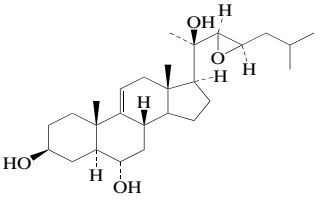
(2α,3β,4α,22*S*,23*S*)-*form*
4-Sulfate: ***Acanthosterol sulfate C***
[215113-05-6]
$C_{27}H_{44}O_7S$ 512.706
Constit. of an *Acanthodendrilla* sp.
$[\alpha]_D^{25}$ +23 (c, 0.054 in MeOH).

4-Sulfate, 2-Ac: ***Acanthosterol sulfate H***
[215113-10-3]
$C_{29}H_{46}O_8S$ 554.744
Constit. of an *Acanthodendrilla* sp.
$[\alpha]_D^{25}$ -6.9 (c, 0.054 in MeOH).

4-Sulfate, 3-Ac: ***Acanthosterol sulfate B***
[215113-04-5]
$C_{29}H_{46}O_8S$ 554.744
Constit. of an *Acanthodendrilla* sp.
$[\alpha]_D^{25}$ +23 (c, 0.054 in MeOH). Error in CAS entry for this compound.

Tsukamoto, S. *et al., J. Nat. Prod.*, 1998, **61**, 1374-1378 (*isol, pmr, cmr*)

22,23-Epoxycholest-9(11)-ene-3,6,20-triol E-187



(3β,5α,6α,20*R*,22*R*,23*R*)-*form*

$C_{27}H_{44}O_4$ 432.642

(3β,5α,6α,20*R*,22*R*,23*R*)-*form*
6-O-[β-D-Fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate: ***Tenuispinoside A***
[105404-82-8]
$C_{56}H_{92}O_{28}S$ 1245.392
Constit. of *Coscinasterias tenuispina*.
$[\alpha]_D$ -56.6 (MeOH) (as Na salt). Registry number refers to Na salt.

6-O-[β-D-Fucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate: ***Tenuispinoside B***
[105377-92-2]
$C_{56}H_{92}O_{27}S$ 1229.393
Constit. of *Coscinasterias tenuispina*.
$[\alpha]_D$ -11.9 (MeOH) (as Na salt). Registry number refers to Na salt.

(3β,5α,6α,20*R*,22*R*,23*S*)-*form*
6-O-[6-Deoxy-β-D-glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate: ***Asteroside A***
[115225-65-5]
$C_{56}H_{92}O_{28}S$ 1245.392

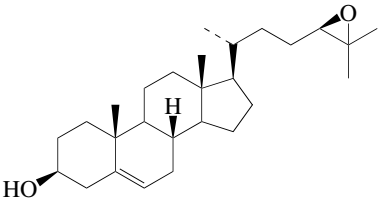
Constit. of *Asterias amurensis.*
$[\alpha]_D$ +5.8 (MeOH).

6-O-[β-D-Glucopyranosyl-(1→3)-β-D-fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate: ***Nipoglycoside A***
[154073-58-2]
$C_{62}H_{102}O_{33}S$ 1407.534
Constit. of *Distolasterias nipon.*
$[\alpha]_D$ +45 (MeOH).

6-O-[β-D-Glucopyranosyl-(1→4)-[β-D-fucopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate: ***Antarcticoside C***
[181186-47-0]
$C_{63}H_{104}O_{33}S$ 1421.561
Constit. of a starfish (Echinasteridae).
$[\alpha]_D$ +4.3 (MeOH).

Riccio, R. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 869-893 (*Tenuispinosides*)
Riccio, R. *et al., J.C.S. Perkin 1*, 1988, 1337-1347 (*Asterioside A*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1993, **56**, 1786-1798 (*Nipoglycoside A*)
De Marino, S. *et al., Gazz. Chim. Ital.*, 1996, **126**, 667-672 (*Antarcticoside C*)

24,25-Epoxycholest-5-en-3-ol, 9CI E-188



(3β,24*R*)-*form*

$C_{27}H_{44}O_2$ 400.643

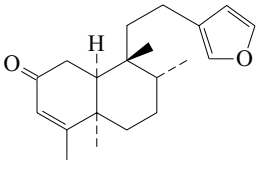
(3β,24*R*)-*form*
24R,25-Epoxycholesterol
[93528-37-1]
Cryst. Mp 166.5-168°.

(3β,24*S*)-*form*
24S,25-Epoxycholesterol
[77058-74-3]
Prod. of mammalian steroid biosynth. Isol. from human liver tissue.
Cryst.
Mp 160-162°.

(3b,24ξ)-*form* [72542-49-5]
Constit. of the red alga *Rissoella verruculosa.*
Nelson, J.A. *et al., J.A.C.S.*, 1981, **103**, 6974
Kabore, S.A. *et al., Phytochemistry*, 1983, **22**, 1239 (*isol*)
Spencer, T.A. *et al., J. Biol. Chem.*, 1985, **260**, 13391 (*isol*)
Emmons, G.T. *et al., J. Lipid Res.*, 1989, **30**, 133 (*synth*)
Tomkinson, N.C.O. *et al., J.O.C.*, 1998, **63**, 9919-9923 (*synth*)

15,16-Epoxy-3,13(16),14-clerodatrien-2-one E-189

[54274-56-5]



$C_{20}H_{28}O_2$ 300.44

(5α,8α)-*form*
Constit. of *Vellozia bicolor.*
Cryst. (hexane).
Mp 110°. $[\alpha]_D^{25}$ -84.1 (c, 0.94 in EtOH).

ent-form
Velamone
[210470-88-5]
Constit. of *Croton campestris.*
Yellow resin. λ_{max} 240 (ϵ 7869); 325 (ϵ 42) (EtOH).

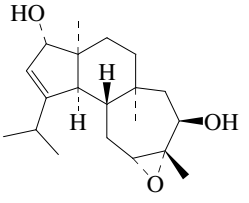
(*ent*-5α)-*form*
Raspailenone
[224778-75-0]
Constit. of a *Raspailia* sponge.
Oil. $[\alpha]_D$ +67.2 (c, 1.5 in MeOH). λ_{max} 214 (ϵ 5800); 246 (ϵ 5000) (MeOH).

(*ent*-5β,8α)-*form* [214897-38-8]
Constit. of *Croton ururucana.*
Oil. $[\alpha]_D^{20}$ -30 (c, 1.1 in $CHCl_3$).

[50490-44-3, 54165-70-7]

Pinto, A.C. *et al., Phytochemistry*, 1994, **37**, 1115 (*isol, pmr, cmr*)
West, L.M. *et al., Aust. J. Chem.*, 1998, **51**, 1097 (*Raspailenone*)
El Babili, F. *et al., Phytochemistry*, 1998, **48**, 165-169 (*Velamone*)
Lopes, M.T. *et al., Phytochemistry*, 1998, **49**, 171-174 (*isol, pmr, cmr*)

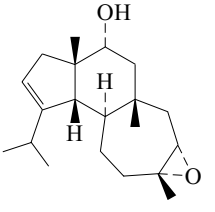
11,12-Epoxy-2-cyathene-1,13-diol E-190



$C_{20}H_{32}O_3$ 320.471

(1α,9α,11α,12α,13β)-*form*
Cyanthiwigin M
[481643-48-5]
Constit. of *Myrmekioderma styx.*
Gum. $[\alpha]_D$ +45 (c, 0.1 in MeOH). λ_{max} 206 (ϵ 5540) (MeOH).
Peng, J. *et al., Tetrahedron*, 2002, **58**, 7809-7819 (*isol, pmr, cmr*)

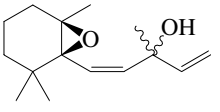
12,13-Epoxy-2-cyathen-8-ol E-191



$C_{20}H_{32}O_2$ 304.472

(8α,12α,13α)-*form*
Ac: 8α-Acetoxy-12α,13α-epoxy-2-cyathene
[144967-84-0]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Myrmekioderma styx.*
$[\alpha]_D^{22}$ -87.7 (c, 0.018 in CH_2Cl_2). λ_{max} 227 (ϵ 494) (EtOH) (Berdy).
Sennett, S.H. *et al., J. Nat. Prod.*, 1992, **55**, 1421 (*isol, pmr, cmr*)

5,6-Epoxy-7,10-cyclofarnesadien-9-ol E-192

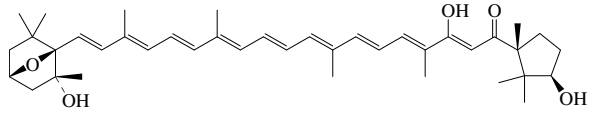


$C_{15}H_{24}O_2$ 236.353

(5β,6β,7*Z*,9ξ)-*form*

O-*Ac:* [636599-36-5]
$C_{17}H_{26}O_3$ 278.391
Constit. of *Laurencia obtusa*.
$[\alpha]_D^{25}$ -111 (c, 0.03 in $CHCl_3$).
Topcu, G. *et al., J. Nat. Prod.*, 2003, **66**, 1505-1508 (*isol, pmr, cmr*)

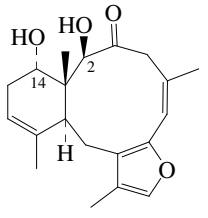
3,6-Epoxy-5,6-dihydro-3′,5,8′-trihydroxy-β,κ-caroten-6′-one E-193



$C_{40}H_{56}O_5$ 616.879

(3*S*,3′*S*,5*R*,5′*R*,6*R*)-*form* [256505-53-0]
Constit. of the oyster *Crassostrea gigas*.
Red amorph. solid. λ_{max} 464 (Et_2O).
Maoka, T. *et al., J. Nat. Prod.*, 2001, **64**, 578-581 (*isol, pmr, cmr*)

7,18-Epoxy-2,14-dihydroxy-5,7,11,17-briaratetraen-3-one E-194



$C_{20}H_{26}O_4$ 330.423

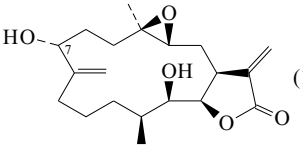
(2β,5*Z*,14α)-*form*

Di-Ac: [76364-86-8]
$C_{24}H_{30}O_6$ 414.497
Constit. of *Scytalium tentaculatum*. Foam. $[\alpha]_D^{20}$ -55 (c, 1.25 in CCl_4). λ_{max} 270 (ϵ 7600) (MeOH).

11α,12α-Epoxide: 7,18:11,12-Diepoxy-2,14-dihydroxy-5,7,17-briaratrien-3-one
[76353-46-3]
$C_{20}H_{26}O_5$ 346.422
Foam. $[\alpha]_D^{20}$ -160 (c, 1.1 in CCl_4). λ_{max} 271 (ϵ 5800) (MeOH).

11α,12α-Epoxide, 2-(3-methylbutanoyl), 14-Ac: [76364-85-7]
$C_{27}H_{36}O_7$ 472.577
Constit. of *Scytalium tentaculatum*. Foam. $[\alpha]_D^{20}$ -98.5 (c, 1.25 in CCl_4). λ_{max} 271 (ϵ 5500) (MeOH).
Ravi, B.N. *et al., Aust. J. Chem.*, 1980, **33**, 2307-2316 (*isol, pmr, cmr*)

3,4-Epoxy-7,13-dihydroxy-8(19),15(17)-cembradien-16,14-olide E-195



(1*S*,3*R*,4*R*,7*R*,12*S*,13*R*,14*R*)–*form*

$C_{20}H_{30}O_5$ 350.454

(1*S*,3*R*,4*R*,7*R*,12*S*,13*R*,14*R*)-*form*

7-Hydroperoxide, 13-Ac: ***Uprolide C acetate***
[165606-68-8]
$C_{22}H_{32}O_7$ 408.491
Constit. of *Eunicea mammosa*. Oil. $[\alpha]_D^{25}$ +7.2 (c, 7.0 in $CHCl_3$). Struct. revised in 2002.

Di-Ac: ***Uprolide C diacetate (incorr.)***
[165606-69-9]
$C_{24}H_{34}O_7$ 434.528
Constit. of *Eunicea mammosa*. Semisolid. $[\alpha]_D^{25}$ +7.2 (c, 7.1 in $CHCl_3$). The assigned name is no longer correct as the struct. of Uprolide C has been revised.

7-Hydroperoxide: 3,4-Epoxy-7-hydroperoxy-13-hydroxy-8(19),15(17)-cembradien-16,14-olide. ***Uprolide C***
[166197-34-8]
$C_{20}H_{30}O_6$ 366.453
Constit. of *Eunicea mammosa*. Oil. $[\alpha]_D^{25}$ -11.4 (c, 1.9 in MeOH). Struct. revised in 2002. Previously not recognised as a hydroperoxide.

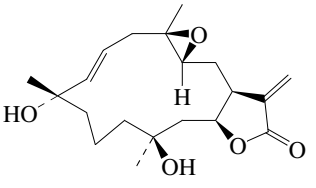
(1*S*,3*R*,4*R*,7*S*,12*S*,13*R*,14*R*)-*form*

7-Epiuprolide C

13-Ac: ***7-Epiuprolide C acetate***
[165880-77-3]
$C_{22}H_{32}O_6$ 392.491
Constit. of *Eunicea mammosa*. Oil. $[\alpha]_D^{25}$ +19 (c, 5.1 in $CHCl_3$).

Di-Ac: ***7-Epiuprolide C diacetate***
[165880-78-4]
$C_{24}H_{34}O_7$ 434.528
Constit. of *Eunicea mammosa*. Semisolid. $[\alpha]_D^{25}$ +17.5 (c, 8.3 in $CHCl_3$).
Rodríguez, A.D. *et al., Can. J. Chem.*, 1995, **73**, 643-654 (*isol, pmr, cmr*)
Shi, Y.-P. *et al., J. Nat. Prod.*, 2002, **65**, 1232-1241 (*struct*)

3,4-Epoxy-8,12-dihydroxy-6,15(17)-cembradien-16,14-olide E-196

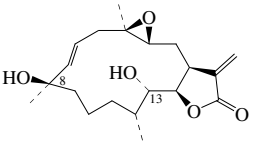


$C_{20}H_{30}O_5$ 350.454

(1*S*,3*S*,4*R*,6*E*,8*S*,12*S*,14*S*)-*form*

8-Hydroperoxide: ***Sarcophyocrassolide A***
$C_{20}H_{30}O_6$ 366.453
Constit. of *Sarcophyton crassocaule*. Cryst. (MeOH).
Mp 172-174°. λ_{max} 236 (no solvent reported).
Xu, X.-H. *et al., Chin. J. Chem.*, 2003, **21**, 1506-1509 (*isol, pmr, cmr, cryst struct*)

3,4-Epoxy-8,13-dihydroxy-6,15(17)-cembradien-16,14-olide E-197



(1*S*,3*R*,4*R*,6*E*,8*R*,12*R*,13*S*,14*R*)-*form*

$C_{20}H_{30}O_5$ 350.454

(1*S*,3*R*,4*R*,6*E*,8*R*,12*R*,13*S*,14*R*)-*form*

8-Hydroperoxide, 13-ketone: ***Uprolide I***
[461441-39-4]
$C_{20}H_{28}O_6$ 364.438
Constit. of *Eunicea pinta*. Gum. $[\alpha]_D^{25}$ -15.6 (c, 0.9 in $CHCl_3$). λ_{max} 214 (ϵ 3100) (MeOH).

(1*S*,3*R*,4*R*,6*E*,8*R*,12*R*,13*S*,14*S*)-*form*

8-Hydroperoxide, 13-ketone: ***Uprolide J***
[461441-40-7]
$C_{20}H_{28}O_6$ 364.438
Constit. of *Eunicea pinta*. Gum. $[\alpha]_D^{25}$ +12 (c, 0.25 in $CHCl_3$). λ_{max} 210 (ϵ 3550) (MeOH).

(1*S*,3*R*,4*R*,6*E*,8*R*,12*S*,13*R*,14*R*)-*form*

8-Epiuprolide A

13-Ac: ***8-Epiuprolide A acetate***
[165606-65-5]
$C_{22}H_{32}O_6$ 392.491
Constit. of *Eunicea mammosa*. Oil. $[\alpha]_D^{25}$ +12.03 (c, 9.12 in $CHCl_3$).

Di-Ac: ***8-Epiuprolide B diacetate (incorr.)***
[165606-66-6]
$C_{24}H_{34}O_7$ 434.528
Constit. of *Eunicea mammosa*. Oil. $[\alpha]_D^{25}$ -5.2 (c, 5.6 in $CHCl_3$). The assigned name is no longer correct as the struct. of 8-Epiuprolide B has been revised to a hydroperoxide.

8-Hydroperoxide: ***3,4-Epoxy-8-hydroperoxy-13-hydroxy-6,15(17)-cembradien-16,14-olide. 8-Epiuprolide B***
[165606-67-7]
$C_{20}H_{30}O_6$ 366.453
Constit. of *Eunicea mammosa*. Oil. $[\alpha]_D^{25}$ -17.7 (c, 2.3 in $CHCl_3$). Struct. revised in 2002. Not previously recognised as a hydroperoxide.

8-Hydroperoxide, 13-Ac: ***8-Epiuprolide B acetate***
[165880-74-0]
$C_{22}H_{32}O_7$ 408.491
Constit. of *Eunicea mammosa*. Oil. $[\alpha]_D^{25}$ -33 (c, 7.8 in $CHCl_3$). Struct. revised in 2002.

(1*S*,3*R*,4*R*,6*E*,8*S*,12*S*,13*R*,14*R*)-*form*

Uprolide A

13-Ac: ***Uprolide A acetate***
[166375-19-5]
$C_{22}H_{32}O_6$ 392.491
Constit. of *Eunicea mammosa*. Cryst.
Mp 210-211°. $[\alpha]_D^{25}$ +29.2 (c, 4.6 in $CHCl_3$).

Di-Ac: Uprolide B diacetate (incorr.)
[165880-76-2]
$C_{24}H_{34}O_7$ 434.528
Constit. of *Eunicea mammosa*. Semisolid. $[\alpha]_D^{25}$ +9.3 (c, 2.7 in $CHCl_3$). The assigned name is no longer correct as the struct. of Uprolide B has been revised.

8-Hydroperoxide: ***Uprolide B***
[166375-18-4]
$C_{20}H_{30}O_6$ 366.453
Constit. of *Eunicea mammosa*. Oil. $[\alpha]_D^{25}$ -22.3 (c, 5.4 in MeOH). Struct. revised in 2002. Not formerly recognised as a hydroperoxide.

8-Hydroperoxide, 13-Ac: ***Uprolide B acetate***
[165880-75-1]
$C_{22}H_{32}O_7$ 408.491
Constit. of *Eunicea mammosa*. Oil. $[\alpha]_D^{25}$ +30 (c, 4.9 in $CHCl_3$). Struct. revised in 2002.

(1*S*,3*R*,4*R*,6*E*,8*S*,12*R*,13*S*,14*R*)-*form*

13-Ketone: 3,4-Epoxy-8-hydroxy-13-oxo-6,15(17)-cembradien-16,14-olide. ***Uprolide K***
[461441-41-8]
$C_{20}H_{28}O_5$ 348.438
Constit. of *Eunicea pinta*. Gum. $[\alpha]_D^{25}$ -22 (c, 1 in $CHCl_3$). λ_{max} 212 (ε 3500) (MeOH).

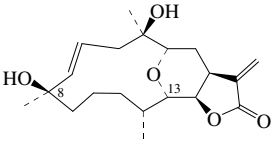
13-Ketone, 8-Ac: Uprolide K acetate
[460060-19-9]
$C_{22}H_{30}O_6$ 390.475
Constit. of *Eunicea pinta*. Gum. $[\alpha]_D^{25}$ -4 (c, 1 in $CHCl_3$). λ_{max} 206 (ε 2425) (MeOH).

8-Hydroperoxide: ***12,13-Bisepiuprolide B***
[200271-84-7]
$C_{20}H_{30}O_6$ 366.453
Constit. of *Eunicea succinea*. Oil. $[\alpha]_D^{25}$ -50.9 (c, 2.2 in $CHCl_3$). Struct. revised in 2002. Not formerly recognised as a hydroperoxide. λ_{max} 211 (ε 6200) (MeOH).

8-Hydroperoxide, 13-Ac: ***12,13-Bisepiuprolide B acetate***
[200271-85-8]
$C_{22}H_{32}O_7$ 408.491
Constit. of *Eunicea succinea*. Oil. $[\alpha]_D^{25}$ -52.6 (c, 4.3 in $CHCl_3$). Struct. revised in 2002. λ_{max} 218 (ε 4900) (MeOH).

8-Hydroperoxide, 13-ketone: 3,4-Epoxy-8-hydroperoxy-13-oxo-6,15(17)-cembradien-16,14-olide. ***Uprolide H***
[461441-38-3]
$C_{20}H_{28}O_6$ 364.438
Constit. of *Eunicea pinta*. Cryst.
Mp 161°. $[\alpha]_D^{25}$ -25.6 (c, 1 in $CHCl_3$). λ_{max} 216 (ε 4900) (MeOH).
Rodríguez, A.D. *et al., Can. J. Chem.*, 1995, **73**, 643-654 (*isol, pmr, cmr, cryst struct*)
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1998, **61**, 40-45 (*12,13-Bisepiuprolide B*)
Shi, Y.-P. *et al., J. Nat. Prod.*, 2002, **65**, 1232-1241 (*Uprolides, cryst struct*)

3,13-Epoxy-4,8-dihydroxy-6,15(17)-cembradien-16,14-olide E-198



(1*S*,3*S*,4*R*,6*E*,8*R*,12*R*,13*S*,14*R*)-*form*

$C_{20}H_{30}O_5$ 350.454

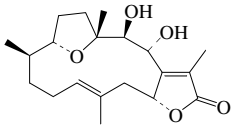
(1*S*,3*S*,4*R*,6*E*,8*R*,12*R*,13*S*,14*R*)-*form*

8-Hydroperoxide: 3,13-Epoxy-8-hydroperoxy-4-hydroxy-6,15(17)-cembradien-16,14-olide. ***Uproeunicin***
[200271-86-9]
$C_{20}H_{30}O_6$ 366.453
Constit. of *Eunicea succinea*. Oil. Struct. revised in 2002.

(1*S*,3*S*,4*R*,6*E*,8*S*,12*R*,13*R*,14*R*)-*form*

8-Hydroperoxide: ***Uprolide M***
[461441-43-0]
$C_{20}H_{30}O_6$ 366.453
Constit. of *Eunicea pinta*. Gum. λ_{max} 208 (ε 5000) (MeOH).
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1998, **61**, 40-45 (*isol, pmr, cmr*)
Shi, Y.-P. *et al., J. Nat. Prod.*, 2002, **65**, 1232-1241 (*isol, pmr, cmr, struct*)

4,7-Epoxy-2,3-dihydroxy-1(15),11-cembradien-16,14-olide E-199



(2*R**,3*S**,4*R**,7*S**,8*R**,11*E*,14*R**)-*form*

$C_{20}H_{30}O_5$ 350.454

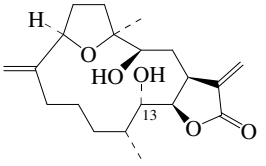
(2*R,3*S**,4*R**,7*S**,8*R**,11*E*,14*R**)-*form***
Pachyclavulariolide I
[369631-98-1]
Constit. of *Pachyclavularia violacea*.
Solid.
Mp 188-189°. $[\alpha]_D^{28}$ +88 (c, 1.03 in $CHCl_3$). λ_{max} 216 (ε 7927) (EtOH aq.).

Di-Ac: ***Pachyclavulariolide H***
[369631-97-0]
$C_{24}H_{34}O_7$ 434.528
Constit. of *Pachyclavularia violacea*. Solid.
Mp 215-216°. $[\alpha]_D^{28}$ -18 (c, 0.96 in $CHCl_3$). λ_{max} 216 (ε 15441) (EtOH aq.).

(2*R,3*S**,4*R**,7*S**,8*R**,11*E*,14*S**)-*form***
Pachyclavulariolide
[119770-11-5]
Constit. of *Pachyclavularia violacea*.
Cryst.
Mp 224-226°. $[\alpha]_D^{28}$ -10 (c, 3.59 in $CHCl_3$). λ_{max} 216 (ε 7927) (EtOH aq.).

Di-Ac: ***Pachyclavulariolide G***
[369631-96-9]
$C_{24}H_{34}O_7$ 434.528
Constit. of *Pachyclavularia violacea*. Cryst.
Mp 129-130°. $[\alpha]_D^{27}$ -122 (c, 0.86 in $CHCl_3$). λ_{max} 218 (ϵ 8345) (EtOH aq.).
Inman, W. *et al., J.O.C.*, 1989, **54**, 2526 (*isol, pmr, cmr*)
Sheu, J.-H. *et al., Tetrahedron*, 2001, **57**, 7639-7648 (*Pachyclavulariolides, cryst struct*)

4,7-Epoxy-3,13-dihydroxy-8(19),15(17)-cembradien-16,14-olide E-200



(1*S*,3*R*,4*S*,7*R*,12*R*,13*S*,14*R*)-*form*

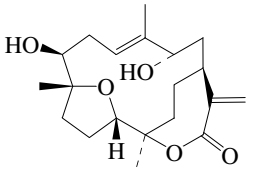
$C_{20}H_{30}O_5$ 350.454

(1*S*,3*R*,4*S*,7*R*,12*R*,13*S*,14*R*)-*form*
12,13-Bisepiuprolide D
3-Ac: ***12,13-Bisepiuprolide D acetate***
[200271-87-0]
$C_{22}H_{32}O_6$ 392.491
Constit. of *Eunicea succinea*. Oil. $[\alpha]_D^{25}$ -38.3 (c, 9.4 in $CHCl_3$). λ_{max} 207 (ϵ 8500) (MeOH).

(1*S*,3*R*,4*S*,7*R*,12*S*,13*R*,14*R*)-*form*
Uprolide D
[169217-43-0]
Constit. of *Eunicea mammosa*.
Oil. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{25}$ -19.9 (c, 0.7 in $CHCl_3$). λ_{max} 212 (ϵ 16500) (MeOH) (Berdy).
13-Ac: ***Uprolide D acetate***
[169275-29-0]
$C_{22}H_{32}O_6$ 392.491
Constit. of *Eunicea mammosa*. Oil. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{25}$ +45.6 (c, 0.7 in $CHCl_3$). λ_{max} 208 (ϵ 18700) (MeOH) (Berdy).

(1*S*,3*R*,4*S*,7*S*,12*S*,13*R*,14*R*)-*form*
Uprolide E
13-Ac: ***Uprolide E acetate***
[169217-44-1]
$C_{22}H_{32}O_6$ 392.491
Constit. of *Eunicea mammosa*. Oil. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{25}$ +68.3 (c, 0.75 in $CHCl_3$). λ_{max} 208 (ϵ 9900) (MeOH) (Berdy).
Rodriguéz, A.D. *et al., J. Nat. Prod.*, 1995, **58**, 1209; 1998, **61**, 40-45 (*isol, pmr, cmr*)

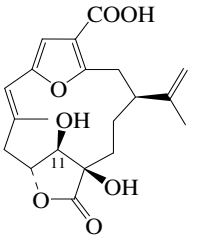
8,11-Epoxy-3,7-dihydroxy-4,15(17)-cembradien-16,12-olide E-201



$C_{20}H_{30}O_5$ 350.454

(1*S*,3*S*,4*E*,7*S*,8*R*,11*S*,12*R*)-*form*
Flexibolide
[184362-78-5]
Constit. of the coral *Sinularia flexibilis*.
Needles.
Mp 198-200°. $[\alpha]_D^{27}$ +31.3 (c, 1.3 in MeOH). λ_{max} 217 (MeOH).
Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 1997, **60**, 9-12 (*isol, pmr, cmr*)

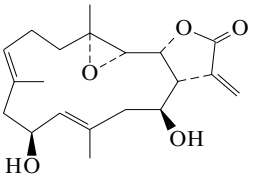
3,6-Epoxy-11,12-dihydroxy-3,5,7,15-cembratetraen-20,10-olid-18-oic acid E-202



$C_{20}H_{24}O_7$ 376.405

(7*E*,10*R*,11*R*)-*form*
11-Ac, Me ester: ***Sethukarailide***
[226561-97-3]
$C_{23}H_{28}O_8$ 432.469
Constit. of *Sinularia maxima*. Cryst.
Mp 177-180°. $[\alpha]_D^{25}$ +2.6 (c, 0.5 in $CHCl_3$). λ_{max} 235 (ϵ 5130); 250 (ϵ 4680) (MeOH).
Venkateswarlu, Y. *et al., J. Nat. Prod.*, 1999, **62**, 756-758 (*isol, pmr, cmr*)

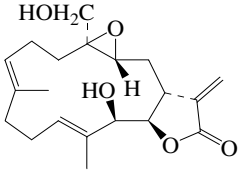
3,4-Epoxy-10,14-dihydroxy-7,11,15(17)-cembratrien-16,2-olide E-203



$C_{20}H_{28}O_5$ 348.438

(1*S*,2*S*,3*R*,4*S*,10*S*,14*S*)-*form*
Di-Ac: ***Lobomichaolide***
[145038-59-1]
$C_{24}H_{32}O_7$ 432.513
Constit. of *Lobophytum michaelae*. Prisms.
Mp 180-181°. $[\alpha]_D^{25}$ +54.9 (c, 0.16 in $CHCl_3$). λ_{max} 215 (ϵ 6310) (MeOH) (Berdy).
Wang, S.-K. *et al., J. Nat. Prod.*, 1992, **55**, 1430 (*isol, pmr, cmr, cryst struct*)

3,4-Epoxy-13,18-dihydroxy-7,11,15(17)-cembratrien-16,14-olide E-204



(1*R*,3*R*,4*S*,7*E*,11*E*,13*R*,14*R*)-*form*

$C_{20}H_{28}O_5$ 348.438

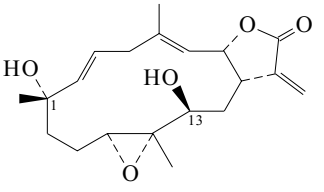
(1*R*,3*R*,4*S*,7*E*,11*E*,13*R*,14*R*)-*form*
Sinulariolide B
[852469-25-1]
Constit. of *Sinularia gibberosa*.
Cryst.
Mp 137-138°. $[\alpha]_D^{25}$ -134.3 (c, 0.05 in $CHCl_3$).

(1*R*,3*R*,4*S*,7*E*,11*E*,13*S*,14*R*)-*form*
Sinulariolide C
[852469-26-2]
Constit. of *Sinularia gibberosa*.
Oil. $[\alpha]_D^{25}$ -56.3 (c, 0.07 in $CHCl_3$).

(1ξ,3ξ,4ξ,7*E*,11*E*,13ξ,14ξ)(1)-*form*
Isol. from *Lobophytum crassum*.
OIl.
18-Ac: [77965-81-2]
$C_{22}H_{30}O_6$ 390.475
From *Lobophytum crassum*. Oil. $[\alpha]_D^{24}$ -81 (c, 1.3 in $CHCl_3$).

(1ξ,3ξ,4ξ,7*E*,11*E*,13ξ,14ξ)(2)-*form*
18-Ac: [78037-40-8]
From *Lobophytum crassum*.
Oil. $[\alpha]_D^{24}$ +16 (c, 0.9 in $CHCl_3$). 13-Epimer of the other isolated acetate.
Kashman, Y. *et al., J.O.C.*, 1981, **46**, 3592-3596 (*Lobophytum crassum constits*)
Li, G. *et al., J. Nat. Prod.*, 2005, **68**, 649-652 (*Sinulariolides B-C*)

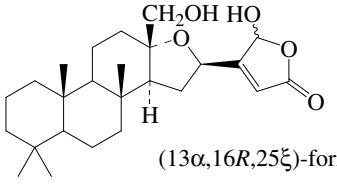
11,12-Epoxy-8,13-dihydroxy-3,6,15(17)-cembratrien-16,2-olide E-205



$C_{20}H_{28}O_5$ 348.438

(1*S*,2*S*,3*E*,6*E*,8*S*,11*S*,12*S*)-*form*
13-Ac: ***Mayolide C***
[114728-08-4]
$C_{22}H_{30}O_6$ 390.475
Constit. of *Sinularia mayi*. Oil. $[\alpha]_D$ +19 (c, 1.98 in $CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 488 (*isol, pmr, cmr*)
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1993, 458 (*struct*)

13,16-Epoxy-24,25-dihydroxy-17-cheilanthen-19,25-olide E-206



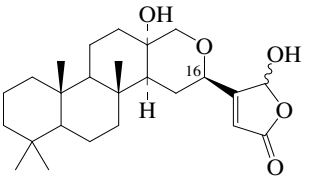
(13α,16*R*,25ξ)-form

$C_{25}H_{38}O_5$ 418.572

(13α,16*R*,25ξ)-*form*
Lintenolide F
[209167-25-9]
Constit. of *Cacospongia* cf. *linteiformis*.
Oil. $[\alpha]_D^{25}$ +54 (c, 0.03 in $CHCl_3$).
24-Ac: ***Spongianolide C***. *Lintenolide A*
[158931-47-6]
[209167-27-1]
$C_{27}H_{40}O_6$ 460.609
Constit. of a *Spongia* sp. and *Cacospongia* cf. *linteiformis*.
$[\alpha]_D$ +38 (c, 2 in MeOH).
24-(3-Hydroxybutanoyl): ***Spongianolide E***
$C_{29}H_{44}O_7$ 504.662
Constit. of a *Spongia* sp. Phospholipase A2 inhibitor. $[\alpha]_D$ +45 (c, 2.4 in MeOH). λ_{max} 212 (ϵ 9640) (MeOH) (Berdy).

(13α,16*S*,25ξ)-*form*
Lintenolide G
[209167-26-0]
Constit. of *Cacospongia* cf. *linteiformis*.
Oil. $[\alpha]_D^{25}$ -21 (c, 0.003 in $CHCl_3$).
24-Ac: ***Spongianolide D***. *Lintenolide B*
[158931-48-7]
[209167-28-2]
$C_{27}H_{40}O_6$ 460.609
Constit. of a *Spongia* sp. and *Cacospongia* cf. *linteiformis*.
$[\alpha]_D$ -16.9 (c, 1.1 in MeOH).
24-(3-Hydroxybutanoyl): ***Spongianolide F***
$C_{29}H_{44}O_7$ 504.662
Constit. of a *Spongia* sp. Phospholipase A inhibitor. $[\alpha]_D$ -9.4 (c, 0.7 in MeOH). λ_{max} 212 (ϵ 10300) (MeOH) (Berdy).
[154563-79-8, 154563-80-1]
He, H. *et al., Tet. Lett.*, 1994, **35**, 7189 (*Spongianolides*)
Conte, M.R. *et al., Tetrahedron*, 1994, **50**, 849 (*Lintenolides*)
Carotenuto, A. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1998, **119**, 119-123 (*Lintenolides F and G*)

16,24-Epoxy-13,25-dihydroxy-17-cheilanthen-19,25-olide E-207



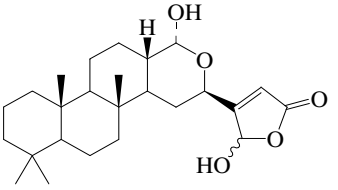
(13α,16*R*,25ξ)-*form*

$C_{25}H_{38}O_5$ 418.572

(13α,16*R*,25ξ)-*form*
Lintenolide D
[174024-97-6]
Constit. of *Cacospongia* cf. *linteiformis*. Antifeedant. Yellow solid.
$[\alpha]_D^{25}$ +93 (c, 0.004 in $CHCl_3$).

(13α,16*S*,25ξ)-*form*
Lintenolide E
[174024-99-8]
Constit. of *Cacospongia* cf. *linteiformis*. Antifeedant. Yellow solid.
$[\alpha]_D^{25}$ -29 (c, 0.004 in $CHCl_3$).
[174024-98-7, 174025-00-4]
Carotenuto, A. *et al., Annalen*, 1996, 77-81 (*isol, pmr, cmr*)

16,24-Epoxy-24,25-dihydroxy-17-cheilanthen-19,25-olide E-208



(24α,25ξ)-*form*

$C_{25}H_{38}O_5$ 418.572
Constit. of *Fasciospongia cavernosa*. Cryst. (MeOH).
Mp 119-121°. $[\alpha]_D$ +28.7 (c, 0.3 in $CHCl_3$).

(24α,25ξ)-*form*
24-Ac: ***Petrosaspongiolide M***
[209408-71-9]
$C_{27}H_{40}O_6$ 460.609
Constit. of *Petrosaspongia nigra*. Pla_2 inhibitor. Amorph. solid.
$[\alpha]_D$ -28.8 (c, 0.02 in $CHCl_3$). λ_{max} 224 (log ϵ 3.58) (MeOH).

(24β,25ξ)-*form*
24-Ac: ***Cavernosolide***
[193816-71-6]
$C_{27}H_{40}O_6$ 460.609
Constit. of *Fasciospongia cavernosa*. Cryst. (MeOH).
Mp 119-121°. $[\alpha]_D$ +28.7 (c, 0.3 in $CHCl_3$).

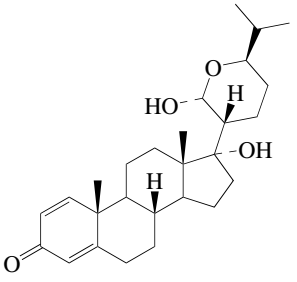
(24ξ,25ξ)-*form*

Petrosaspongiolide P

Constit. of *Petrosaspongia nigra*. Pla_2 inhibitor. Amorph. solid. $[\alpha]_D$ +13.8 (c, 0.001 in MeOH). λ_{max} 224 (MeOH) (Berdy).

De Rosa, S. *et al., J. Nat. Prod.*, 1997, **60**, 844-846 (*Cavernosolide*)
Randazzo, A. *et al., J. Nat. Prod.*, 1998, **61**, 571-575 (*Petrosaspongiolides*)
Soriente, A. *et al., Eur. J. Org. Chem.*, 2000, 947-953 (*abs config*)

21,24-Epoxy-17,21-dihydroxycholesta-1,4-dien-3-one E-209



$C_{27}H_{40}O_4$ 428.611

(17α,20*R*,21*R*,24*R*)-*form*

Anastomosacetal A

[185331-93-5]

Constit. of *Euplexaura anastomosans.*

Solid.

Mp 134-136°. $[\alpha]_D^{25}$ +22.3 (c, 0.4 in MeOH). λ_{max} 244 (ϵ 17500) (MeOH).

4,5-Dihydro: 21,24-Epoxy-17,21-dihydroxycholest-1-en-3-one.

Anastomosacetal B

[185331-94-6]

$C_{27}H_{42}O_4$ 430.626

Constit. of *Euplexaura anastomosans.* Solid.

Mp 107-108°. $[\alpha]_D^{25}$ +15.6 (c, 0.3 in MeOH). λ_{max} 230 (ϵ 14000) (MeOH).

1,2-Dihydro: 21,24-Epoxy-17,21-dihydroxycholest-4-en-3-one.

Anastomosacetal C

[185331-95-7]

$C_{27}H_{42}O_4$ 430.626

Constit. of *Euplexaura anastomosans.* Solid.

Mp 187-188°. $[\alpha]_D^{25}$ +23.3 (c, 0.3 in MeOH). λ_{max} 241 (ϵ 18000) (MeOH).

1,2,4,5-Tetrahydro: 21,24-Epoxy-17,21-dihydroxycholestan-3-one.

Anastomosacetal D

[185331-96-8]

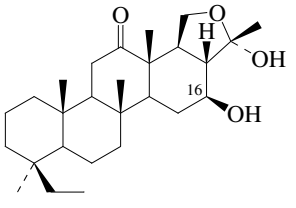
$C_{27}H_{44}O_4$ 432.642

Constit. of *Euplexaura anastomosans.* Solid.

Mp 75-76°. $[\alpha]_D^{25}$ -9.1 (c, 0.5 in MeOH).

Seo, Y. *et al., J. Nat. Prod.*, 1996, **59**, 1196-1199 (*isol, pmr, cmr*)

24,25-Epoxy-16,24-dihydroxy-20,24-dimethyl-12-scalaranone E-210



(16β,24α*OH*)-*form*

$C_{27}H_{44}O_4$ 432.642

(16β,24α*OH*)-*form*

16-Ac: ***Phyllohemiketal A***

[146453-11-4]

$C_{29}H_{46}O_5$ 474.679

Isol. from the sponge *Phyllospongia foliascens.* May be identical with Scalardysin B.

(16β,24ξ)-*form*

16-Ac: ***Scalardysin B***

[73731-34-7]

$C_{29}H_{46}O_5$ 474.679

Constit. of *Dysidea herbacea.*

24-Me ether, 16-Ac: ***Phylloketal***

[125990-23-0]

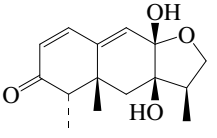
$C_{30}H_{48}O_5$ 488.706

Constit. of *Phyllospongia foliascens.* Needles (Me_2CO).

Mp 201-202°.

Kashman, Y. *et al., Tet. Lett.*, 1979, 3879 (*isol*)
Fu, X. *et al., Chin. Chem. Lett.*, 1991, **2**, 543 (*Phylloketal*)
Fu, X. *et al., Gaodeng Xuexiao Huaxue Xuebao*, 1991, **12**, 1486-1487; *CA*, **121**, 104452g (*Phyllohemiketal A*)

8,12-Epoxy-7,8-dihydroxy-1,9-eremophiladien-3-one E-211



$C_{15}H_{20}O_4$ 264.321

(4α,7β,8β*OH*,11β)-*form*

8-Me ether: ***Microsphaeropsisin***

[218292-48-9]

$C_{16}H_{22}O_4$ 278.347

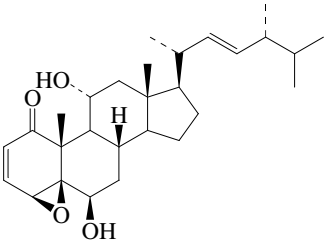
Metab. of the marine-derived *Microsphaeropsis incrustans.*

Powder.

Mp 152-154°. $[\alpha]_D^{20}$ -97.7 (c, 0.13 in $CHCl_3$). λ_{max} 223 (ϵ 2250); 280 (ϵ 8560) (EtOH).

Höller, U. *et al., J. Nat. Prod.*, 1999, **62**, 114-118 (*isol, pmr, cmr*)

4,5-Epoxy-6,11-dihydroxyergosta-2,22-dien-1-one E-212



$C_{28}H_{42}O_4$ 442.637

(4β,5β,6β,11α,22*E*)-*form*

Yonarasterol D

[263764-04-1]

Constit. of *Clavularia viridis.*

Amorph. solid. $[\alpha]_D^{25}$ -34 (c, 0.1 in $CHCl_3$). λ_{max} 231 (log ϵ 3.61) (EtOH).

22,23-Dihydro: 4,5-Epoxy-6,11-dihydroxyergost-2-en-1-one.

Yonarasterol E

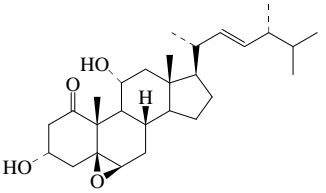
[263764-05-2]

$C_{28}H_{44}O_4$ 444.653

Constit. of *Clavularia viridis.* Amorph. solid. $[\alpha]_D^{25}$ -14.5 (c, 0.2 in $CHCl_3$). λ_{max} 232 (log ϵ 3.66) (EtOH).

Iwashima, M. *et al., Steroids*, 2000, **65**, 130-137 (*isol, pmr, cmr*)

5,6-Epoxy-3,11-dihydroxyergost-22-en-1-one E-213



(3α,5β,6β,11α,22*E*,24*R*)-*form*

$C_{28}H_{44}O_4$ 444.653

(3α,5β,6β,11α,22*E*,24*R*)-*form*

11-Ac: [180001-20-1]
$C_{30}H_{46}O_5$ 486.69
Constit. of *Clavularia viridis*. Amorph. solid. $[\alpha]_D$ -116.3 (c, 0.7 in $CHCl_3$).

22,23-Dihydro, 11-Ac: [180001-21-2]
$C_{30}H_{48}O_5$ 488.706
Constit. of *Clavularia viridis*. Amorph. solid. $[\alpha]_D$ -120.3 (c, 1.3 in $CHCl_3$).

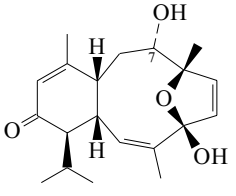
22,23-Dihydro, 24,28-didehydro, 11-Ac: [180001-19-8]
$C_{30}H_{46}O_5$ 486.69
Constit. of *Clavularia viridis*. Viscous oil. $[\alpha]_D$ -56.9 (c, 0.065 in $CHCl_3$).

(3β,5β,6β,11α,22*E*,24*R*)-*form*

Di-Ac: [180001-17-6]
$C_{32}H_{48}O_6$ 528.728
Constit. of *Clavularia viridis*. Needles (MeCN aq.).
Mp 175.5-177°. $[\alpha]_D$ -76 (c, 0.15 in $CHCl_3$).

22,23-Dihydro, di-Ac: [180001-18-7]
$C_{32}H_{50}O_6$ 530.743
Constit. of *Clavularia viridis*. Needles (MeCN aq.).
Mp 130.5-132°. $[\alpha]_D$ -78.5 (c, 0.27 in $CHCl_3$).
Watanabe, K. *et al., Steroids*, 1996, **61**, 439 (*isol, pmr, cmr, cryst struct*)

8,11-Epoxy-7,11-dihydroxy-3,9,12-eunicellatrien-2-one E-214



$C_{20}H_{28}O_4$ 332.439

(7α,8β,11β)-*form*

7-(3-Methyl-2-butenoyl): ***Valdivone A***
[152130-61-5]
$C_{25}H_{34}O_5$ 414.541
Constit. of *Alcyonium valdivae*. Shows antiinflammatory activity. Phosphatidase A2 inhibitor. Needles.
Mp 89-91°. $[\alpha]_D$ +94.4 (c, 0.34 in $CHCl_3$). λ_{max} 254 (ϵ 7650) ($CHCl_3$) (Berdy).

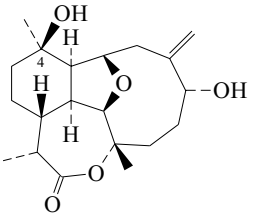
7-(3-Methylbutanoyl): ***Dihydrovaldivone A***
[152246-89-4]
$C_{25}H_{36}O_5$ 416.556
Constit. of *Alcyonium valdivae*. Shows antiinflammatory activity. Phosphatidase A2 inhibitor. Oil. λ_{max} 248 (ϵ 2270) ($CHCl_3$) (Berdy).

7-(Phenylacetyl): ***Valdivone B***
[152110-08-2]
$C_{28}H_{34}O_5$ 450.574
Constit. of *Alcyonium valdivae*. Shows antiinflammatory activity. Phosphatidase A2 inhibitor. Needles.
Mp 171-173°. $[\alpha]_D$ +79.4 (c, 0.57 in $CHCl_3$). λ_{max} 242 (ϵ 11600) ($CHCl_3$) (Berdy).

11-Me ether, 7-(3-methyl-2-butenoyl): ***4-O-Methylvaldivone A***
[152246-87-2]
$C_{26}H_{36}O_5$ 428.567
Constit. of *Alcyonium valdivae*. Oil.

11-Me ether, 7-(phenylacetyl): ***4-O-Methylvaldivone B***
[152246-88-3]
$C_{29}H_{36}O_5$ 464.6
Constit. of *Alcyonium valdivae*. Oil.
Lin, Y. *et al., Tetrahedron*, 1993, **49**, 7977 (*isol, pmr, cmr, activity*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)

6,13-Epoxy-4,9-dihydroxy-8(19)-eunicellen-16,12-olide E-215



$C_{20}H_{30}O_5$ 350.454

(4β,6β,9α,12α,13β,15α)-*form*

4-Ac: ***Briarellin K***
[503552-40-7]
$C_{22}H_{32}O_6$ 392.491
Constit. of *Briareum polyanthes*. Oil. $[\alpha]_D^{26}$ -14.9 (c, 1.2 in $CHCl_3$).

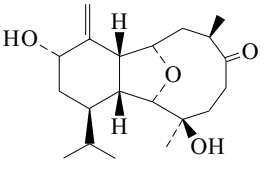
4-Butanoyl: ***Briarellin D***
[165171-24-4]
$C_{24}H_{36}O_6$ 420.545
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{30}$ -17.89 (c, 0.33 in $CHCl_3$).

4-Butanoyl, 9-Ac: ***Briarellin L***
[503552-43-0]
$C_{26}H_{38}O_7$ 462.582
Constit. of *Briareum polyanthes*. Oil. $[\alpha]_D^{26}$ -20.8 (c, 1.2 in $CHCl_3$).

9-Hydroperoxide, 4-Ac: ***Briarellin K hydroperoxide***
[503552-41-8]
$C_{22}H_{32}O_7$ 408.491
Constit. of *Briareum polyanthes*. Oil. $[\alpha]_D^{20}$ -25.6 (c, 1 in $CHCl_3$).

9-Hydroperoxide, 4-butanoyl: ***Briarellin D hydroperoxide***
[503552-42-9]
$C_{24}H_{36}O_7$ 436.544
Constit. of *Briareum polyanthes*. Oil. $[\alpha]_D^{20}$ -25.2 (c, 1 in $CHCl_3$).
Rodríguez, A.D. *et al., Tetrahedron*, 1995, **51**, 6869 (*Briarellin D*)
Ospina, C.A. *et al., J. Nat. Prod.*, 2003, **66**, 357-363 (*Briarellins K,L, hydroperoxides*)

6,13-Epoxy-3,12-dihydroxy-4(18)-eunicellen-9-one E-216

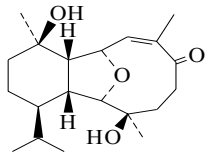


$C_{20}H_{32}O_4$ 336.47

(3α,6α,8β,12β,13α)-*form*

12-Butanoyl: ***Litophynin J***
[139579-23-0]
$C_{24}H_{38}O_5$ 406.561
Constit. of a *Litophyton* sp. Shows molluscidal and repellant activity. Needles.
Mp 120-121.5°. $[\alpha]_D^{20}$ +5.9 (c, 0.51 in $CHCl_3$).
Ochi, M. *et al., Chem. Lett.*, 1992, 155 (*isol, pmr, cmr, activity*)

6,13-Epoxy-4,12-dihydroxy-7-eunicellen-9-one E-217

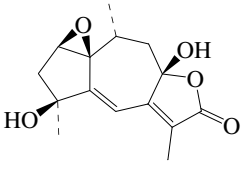


$C_{20}H_{32}O_4$ 336.47

(4β,6α,12β,13α)-*form*

Di-Ac: ***Palmonine E***
[151515-28-5]
$C_{24}H_{36}O_6$ 420.545
Constit. of *Eunicella verrucosa*. Cryst.
Mp 152-153°. $[\alpha]_D$ -17.25 (c, 0.4 in $CHCl_3$).
Ortega, M.J. *et al., Tetrahedron*, 1993, **49**, 7823 (*isol, pmr, cmr*)

1,2-Epoxy-4,8-dihydroxy-5,7(11)-guaiadien-12,8-olide E-218



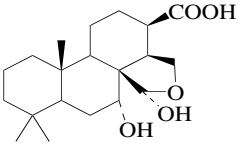
$C_{15}H_{18}O_5$ 278.304

(1β,2β,4β,8β,10α)-*form*

Americanolide H

8-Me ether: ***Methoxyamericanolide H***
[205507-16-0]
$C_{16}H_{20}O_5$ 292.331
Constit. of *Pseudopterogorgia americana*. Oil. $[\alpha]_D^{26}$ -39.7 (c, 1.3 in $CHCl_3$). λ_{max} 216 (ϵ 5030); 276 (ϵ 3420) (MeOH).
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1998, **61**, 451-455 (*isol, pmr, cmr*)

15,17-Epoxy-7,17-dihydroxy-16-isocopalanoic acid E-219



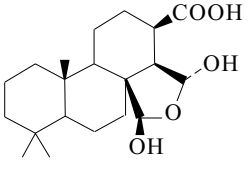
$C_{20}H_{32}O_5$ 352.47

(7α,13α*H*,14α*H*,17α)-*form*

17-Me ether, 7-Ac, Me ester: [194020-39-8]
$C_{24}H_{38}O_6$ 422.561
Constit. of *Cadlina luteomarginata*. Oil. $[\alpha]_D^{25}$ -5.5 ($CHCl_3$).
λ_{max} 248 (sh) (log ϵ 2.64); 252 (log ϵ 2.68) ($CHCl_3$).
Dumdei, E.J. *et al., Can. J. Chem.*, 1997, **75**, 773-789 (*isol, pmr, cmr*)

15,17-Epoxy-15,17-dihydroxy-16-isocopalanoic acid E-220

15,16-Dideoxy-15,17-dihydroxy-15,17-oxido-16-spongianoic acid



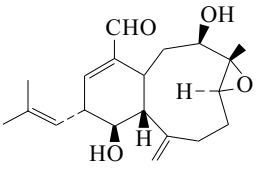
$C_{20}H_{32}O_5$ 352.47

(13α*H*,14α*H*,15α,17β)-*form*

Di-Ac, Me ester: Methyl 15α,17β-diacetoxy-15,16-dideoxy-15,17-oxido-16-spongianoate. Spongiane lactone 10
[109152-44-5]
$C_{25}H_{38}O_7$ 450.571
Constit. of *Ceratosoma brevicaudatum*. Oil.
Ksebati, M.B. *et al., J.O.C.*, 1987, **52**, 3766

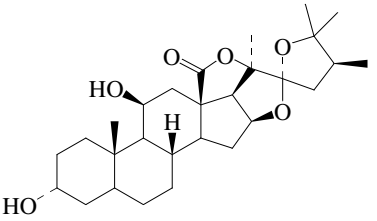
5,6-Epoxy-7,13-dihydroxy-2-methylene-12-(2-methyl-1-propenyl)-6-methylbicyclo[7.4.0]tridec-10-ene-10-carboxaldehyde E-221

[85228-00-8]



$C_{20}H_{28}O_4$ 332.439
Constit. of an *Efflatounaria* sp. Cryst. (EtOAc).
Mp 166-169°. $[\alpha]_D^{21}$ -63.6 (c, 0.28 in $CHCl_3$). λ_{max} 228 (ϵ 9000) (MeOH) (Derep).
Burns, K.P. *et al., Aust. J. Chem.*, 1983, **36**, 171 (*isol, cryst struct*)

22,25-Epoxy-3,11-dihydroxy-24-methylfurostan-18,20-olide E-222



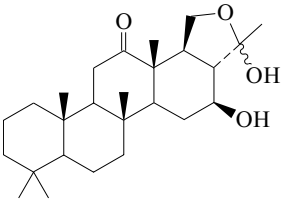
$C_{28}H_{42}O_6$ 474.636

(3α,5α,11β,20*R*,22*S*,24*S*)-*form* [467227-51-6]
Constit. of *Isis hippuris.*
Cryst. (MeOH aq.).
Mp 225-226°. $[\alpha]_D$ -22 (c, 0.85 in $CHCl_3$).

(3α,5α,11β,20*R*,22ξ,24ξ)-*form*

3-Ac: [79849-37-9]
$C_{30}H_{44}O_7$ 516.673
Constit. of *Isis hippuris.* Cryst.
Mp 260-262°. $[\alpha]_D$ -31 ($CHCl_3$).
Di-Ac: Mp 258-259°.
Higa, T. *et al., Tet. Lett.*, 1981, **29**, 2777-2780 (*3-Ac*)
Tanaka, J. *et al., Tetrahedron*, 2002, **58**, 6259-6266 (*isol, pmr, cmr, cryst struct*)
Chao, C.H. *et al., J. Nat. Prod.*, 2005, **68**, 880-885 (*cryst struct*)

24,25-Epoxy-16,24-dihydroxy-24-methyl-12-scalaranone E-223

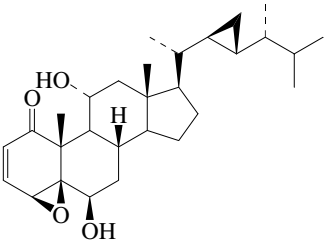


$C_{26}H_{42}O_4$ 418.615

16β-*form*

16-Ac: ***Scalardysin A***
[73723-39-4]
$C_{28}H_{44}O_5$ 460.653
Constit. of *Dysidea herbacea*.
Kashman, Y. *et al., Tet. Lett.*, 1979, 3879 (*isol*)

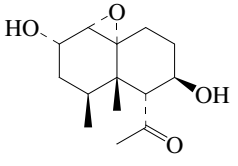
4,5-Epoxy-6,11-dihydroxy-33-norgorgost-2-en-1-one E-224



$C_{29}H_{44}O_4$ 456.664

(4β,5β,6β,11α,22*R*,23*R*,24*R*)-*form*
Yonarasterol F
[263764-06-3]
Constit. of *Clavularia viridis.*
Amorph. solid. $[\alpha]_D^{25}$ -8.3 (c, 0.06 in $CHCl_3$). λ_{max} 229 (log ϵ 3.72) (EtOH).
Iwashima, M. *et al., Steroids*, 2000, **65**, 130-137 (*isol, pmr, cmr*)

1,10-Epoxy-2,7-dihydroxy-13-nor-11-nardosinanone E-225



(1α,2α,6α,7β,10α)-*form*

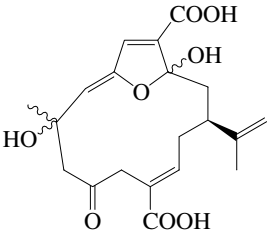
$C_{14}H_{22}O_4$ 254.325

(1α,2α,6α,7β,10α)-*form*
Laevinol F
[874384-39-1]
Constit. of *Lemnalia laevis.*
$[\alpha]_D^{25}$ -76 (c, 0.2 in $CHCl_3$).
2-Deoxy: 1,10-Epoxy-7-hydroxy-13-nor-11-nardosinanone. ***Laevinol H***
[874384-42-6]
$C_{14}H_{22}O_3$ 238.326
Constit. of *Lemnalia laevis.*
$[\alpha]_D^{25}$ -82 (c, 0.1 in $CHCl_3$).

(1α,2β,6α,7β,10α)-*form*
Laevinol G
[874384-41-5]
Constit. of *Lemnalia laevis.*
$[\alpha]_D^{25}$ -166 (c, 0.3 in $CHCl_3$).
7-Ketone: ***1,10-Epoxy-2-hydroxy-13-nor-7,11-nardosinanedione***
[148410-02-0]
$C_{14}H_{20}O_4$ 252.31
Constit. of *Lemnalia africana*. Yellow oil. $[\alpha]_D$ -307 (c, 1 in $CHCl_3$).

(1α,2β,6β,7β,10α)-*form*
7-Ketone: [148410-01-9]
$C_{14}H_{20}O_4$ 252.31
Constit. of *Lemnalia africana*. Yellow oil. $[\alpha]_D$ -78 (c, 0.3 in $CHCl_3$).
Jurek, Y. *et al., J. Nat. Prod.*, 1993, **56**, 508-513 (*7-ketones*)
El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 1749-1753 (*Laevinols*)

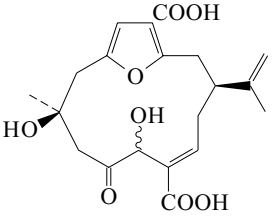
3,6-Epoxy-3,8-dihydroxy-10-oxo-4,6,12,15-cembratetraene-18,20-dioic acid E-226



$C_{20}H_{24}O_8$ 392.405

(3ξ,6*Z*,8ξ,12*E*)-*form*
3-Me ether, di-Me ester: ***Sethukarailin***
[226561-96-2]
$C_{23}H_{30}O_8$ 434.485
Constit. of *Sinularia maxima*. Pale yellow viscous liq. $[\alpha]_D^{25}$ -23.4 (c, 0.25 in $CHCl_3$). λ_{max} 240 (ϵ 7380); 295 (ϵ 6945) (MeOH).
Venkateswarlu, Y. *et al., J. Nat. Prod.*, 1999, **62**, 756-758 (*isol, pmr, cmr*)

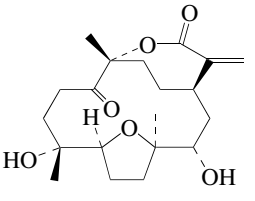
3,6-Epoxy-8,11-dihydroxy-10-oxo-3,5,12,15-cembratetraene-18,20-dioic acid E-227



$C_{20}H_{24}O_8$ 392.405

(8*S*,11ξ,12*E*)-*form*
Di-Me ester: [151554-89-1]
$C_{22}H_{28}O_8$ 420.458
Constit. of *Sinularia dissecta*. Needles (MeOH). Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 170-172°. $[\alpha]_D^{25}$ -8.7 (c, 0.12 in CH_2Cl_2). λ_{max} 216 (ϵ 6676); 245 (ϵ 3788) (MeOH) (Berdy).
Reddy, M.V.R. *et al., J. Nat. Prod.*, 1993, **56**, 970 (*isol, pmr, cmr*)

4,7-Epoxy-3,8-dihydroxy-11-oxo-15(17)-cembren-16,12-olide E-228

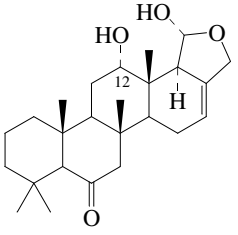


$C_{20}H_{30}O_6$ 366.453

(1*R*,3*S*,4*R*,7*S*,8*R*,12*R*)-*form*
Sinulariolone
[169238-13-5]
Constit. of *Sinularia flexibilis.*
Cryst. (Et_2O).
Mp 215-216°. $[\alpha]_D^{25}$ -15.8 (c, 0.63 in EtOH).

Guerrero, P.P. *et al., J. Nat. Prod.*, 1995, **58**, 1185-1191 (*isol, pmr, cmr, cryst struct*)

24,25-Epoxy-12,25-dihydroxy-16-scalaren-6-one E-229

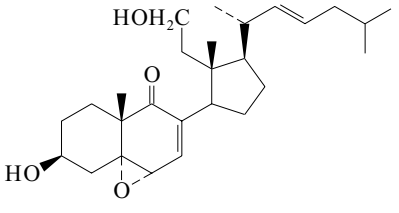


$C_{25}H_{38}O_4$ 402.573

(12α,25α)-*form*

12-Ac: ***6-Ketodeoxoscalarin***
[151109-54-5]
$C_{27}H_{40}O_5$ 444.61
Isol. from the mollusc *Hypselodoris orsini*.
$[\alpha]_D$ +12.6 (c, 0.15 in $CHCl_3$).
Cimino, G. *et al., Experientia*, 1993, **49**, 582-586 (*isol, pmr, cmr*)

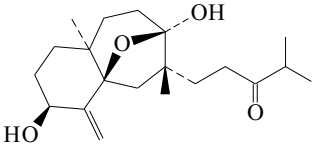
5,6-Epoxy-3,11-dihydroxy-9,11-secocholesta-7,22-dien-9-one E-230



$C_{27}H_{42}O_4$ 430.626

(3β,5α,6α,22*E*)-*form* [168982-43-2]
Constit. of *Dysidea fragilis* from the lagoon of Venice.
Aiello, A. *et al., Steroids*, 1995, **60**, 666-673 (*isol, pmr, cmr*)

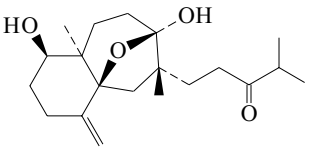
8,14-Epoxy-2,8-dihydroxy-8,9-seco-1(15)-dolasten-9-one E-231



$C_{20}H_{32}O_4$ 336.47
Mp 136.5-137.5°.

(2β,14β)-*form*
***Linearol*†**
[78095-12-2]
Constit. of *Dictyota linearis*.
Cryst.
Mp 136.5-137.5°. $[\alpha]_D$ -1.9 (c, 0.11 in $CHCl_3$).
Ochi, M. *et al., Chem. Comm.*, 1981, 100

8,14-Epoxy-4,8-dihydroxy-8,9-seco-1(15)-dolasten-9-one E-232



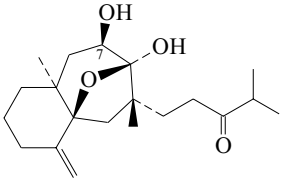
$C_{20}H_{32}O_4$ 336.47
$[\alpha]_D^{21}$ -52.1 ($CHCl_3$).

(4β,14β)-*form*
***Isolinearol*†**
[103772-44-7]
Constit. of *Dictyota cervicornis*.
Gum. $[\alpha]_D^{21}$ -52.1 ($CHCl_3$).

4-Ac: ***Isolinearol acetate***
[103772-45-8]
$C_{22}H_{34}O_5$ 378.508
From *Dictyota cervicornis*. Gum. $[\alpha]_D$ -50 ($CHCl_3$).

4-Ketone: 8,14-Epoxy-8-hydroxy-8,9-seco-1(15)-dolastene-4,9-dione. ***Dichotodione***
[625835-23-6]
Constit. of *Dictyota dichotoma*.
$[\alpha]_D^{24}$ -55.5 (c, 0.144 in $CHCl_3$).
Teixeira, V.L. *et al., J. Nat. Prod.*, 1986, **49**, 570
Ali, M.S. *et al., Z. Naturforsch., B*, 2003, **58**, 438-442 (*Dichotodione*)

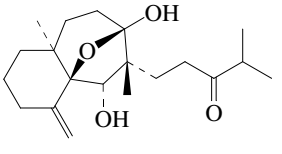
8,14-Epoxy-7,8-dihydroxy-8,9-seco-1(15)-dolasten-9-one E-233



$C_{20}H_{32}O_4$ 336.47

(7β,14β)-*form*
Cervicol
[103772-42-5]
Constit. of brown alga *Dictyota cervicornis*.
Pale-yellow gum (as 7-Ac). $[\alpha]_D^{25}$ -76.1 (c, 1.00 in $CHCl_3$) (7-Ac).
Teixeira, V.L. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 263

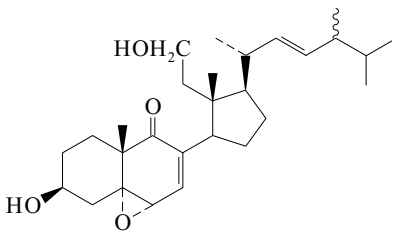
8,14-Epoxy-8,13-dihydroxy-8,9-seco-1(15)-dolasten-9-one E-234



$C_{20}H_{32}O_4$ 336.47

(13α,14β)-*form*
Dichotone
[625835-22-5]
Constit. of *Dictyota dichotoma*.
$[\alpha]_D^{24}$ -51.3 (c, 0.93 in $CHCl_3$).
Ali, M.S. *et al., Z. Naturforsch., B*, 2003, **58**, 438-442 (*isol, pmr, cmr*)

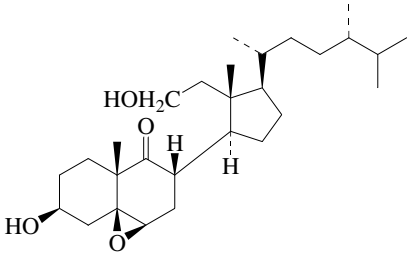
5,6-Epoxy-3,11-dihydroxy-9,11-secoergosta-7,22-dien-9-one E-235



$C_{28}H_{44}O_4$ 444.653

(3β,5α,6α,22*E*,24ξ)-*form* [168982-44-3]
Constit. of *Dysidea fragilis* from the lagoon of Venice.
Aiello, A. *et al., Steroids*, 1995, **60**, 666-673 (*isol, pmr, cmr*)

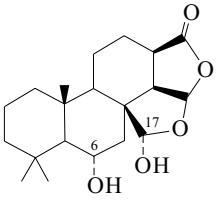
5,6-Epoxy-3,11-dihydroxy-9,11-secoergostan-9-one E-236
5,6-Epoxy-3,11-dihydroxy-24-methyl-9,11-secocholestan-9-one



$C_{28}H_{48}O_4$ 448.685

(3β,5β,6β,24*S*)-*form* [466690-55-1]
Constit. of *Pachyclavularia violacea*.
Amorph. solid. $[\alpha]_D^{25}$ -23.1 (c, 0.26 in CH_2Cl_2).
Anta, C. *et al., J. Nat. Prod.*, 2002, **65**, 1357-1359 (*isol, pmr, cmr*)

15,17-Epoxy-6,17-dihydroxy-16-spongianone E-237
6,17-Dihydroxy-15,17-oxido-16-spongianone

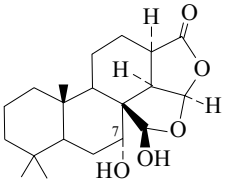


$C_{20}H_{30}O_5$ 350.454

(6α,17α)-*form*
Di-Ac: 6,17-Diacetoxy-15,17-oxido-16-spongianone. Spongiane lactone 4
[109152-40-1]
$C_{24}H_{34}O_7$ 434.528
Constit. of *Ceratosoma brevicaudatum*. Oil.
6-Butanoyl, 17-Ac: 17-Acetoxy-6-butanoyloxy-15,17-oxido-16-spongianone. Spongiane lactone 5
[109152-41-2]
$C_{26}H_{38}O_7$ 462.582
From *Ceratosoma brevicaudatum*. Oil.

(6α,17β)-*form*
6-Ac: 6-Acetoxy-17-hydroxy-15,17-oxido-16-spongianone. Spongiane lactone 3
[109181-98-8]
$C_{22}H_{32}O_6$ 392.491
From *Ceratosoma brevicaudatum*. Oil.
6-Butanoyl: 6-Butanoyloxy-17-hydroxy-15,17-oxido-16-spongianone. Spongiane lactone 2
[109181-97-7]
$C_{24}H_{36}O_6$ 420.545
From *Ceratosoma brevicaudatum*. Oil.
Ksebati, M.B. *et al., J.O.C.*, 1987, **52**, 3766,

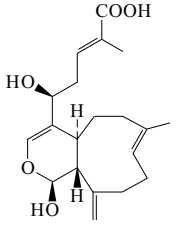
15,17-Epoxy-7,17-dihydroxy-16-spongianone E-238
7,17-Dihydroxy-15,17-oxido-16-spongianone



$C_{20}H_{30}O_5$ 350.454

(7α,17β)-*form* [96999-36-9]
Constit. of *Igernella notabilis*.
Cryst.
Mp 199-204°. $[\alpha]_D$ -21.7 (MeOH).
*7-Ac: **Aplyroseol 2***
[96999-35-8]
$C_{22}H_{32}O_6$ 392.491
From *Igernella notabilis*, *Chromodoris inopinata* and *Aplysilla rosea*. Cryst. or oil.
Mp 114-117°. $[\alpha]_D$ -35 ($CHCl_3$).
*7-Butanoyl: **Aplyroseol 1***
[97042-20-1]
$C_{24}H_{36}O_6$ 420.545
From *Igernella notabilis* and *Aplysilla rosea*. Cryst. (petrol).
Mp 197-198° (190-192°). $[\alpha]_D^{25}$ -52.8 (c, 2.86 in $CHCl_3$). $[\alpha]_D$ -37.2 ($CHCl_3$).
Schmitz, F.J. *et al., J.O.C.*, 1985, **50**, 2862
Karuso, P. *et al., Aust. J. Chem.*, 1986, **39**, 1629; 1643
De Silva, E.D. *et al., J. Nat. Prod.*, 1991, **54**, 993 (*Aplyroseol 2, isol*)
Abad, A. *et al., J.C.S. Perkin 1*, 1993, 1861 (*synth*)
Hambley, T.W. *et al., Aust. J. Chem.*, 1997, **50**, 391-394 (*Aplyroseol I, cryst struct, abs config*)

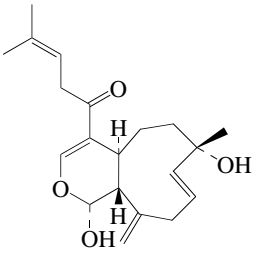
17,18-Epoxy-11,18-dihydroxy-1(19),6,10(17),13-xenicatetraen-15-oic acid E-239



$C_{20}H_{28}O_5$ 348.438

*Di-Ac, Me ester: **Acalycigorgin A***
[147318-39-6]
$C_{25}H_{34}O_7$ 446.539
Constit. of an *Acalycigorgia* sp. Oil. $[\alpha]_D^{20}$ +82.3 (c, 0.4 in $CHCl_3$). λ_{max} 219 (ε 10000) (MeOH) (Derep).
*6α,7α-Epoxide, di-Ac, Me ester: **Acalycigorgin B***
[147318-40-9]
$C_{25}H_{34}O_8$ 462.539
Constit. of an *Acalycigorgia* sp. Oil. $[\alpha]_D^{21}$ +70.8 (c, 0.13 in $CHCl_3$). λ_{max} 219 (ε 10000) (MeOH) (Derep).
Ochi, M. *et al., Heterocycles*, 1993, **36**, 41 (*isol, pmr, cmr*)

17,18-Epoxy-6,18-dihydroxy-1(19),7,10(17),13-xenicatetraen-11-one E-240

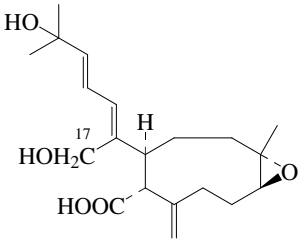


$C_{20}H_{28}O_4$ 332.439

(6α,7*E*,18α)-*form*

Di-Ac: ***Tsitsixenicin D***
[168075-14-7]
$C_{24}H_{32}O_6$ 416.513
Constit. of *Capnella thyrsoidea*. Oil. $[\alpha]_D^{21}$ -126 (c, 0.8 in $CHCl_3$).
Hooper, G.J. *et al., Tetrahedron*, 1995, **51**, 9973-9984 (*isol, pmr, cmr*)

6,7-Epoxy-14,17-dihydroxy-1(19),10,12-xenicatrien-18-oic acid E-241



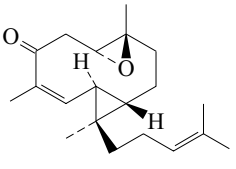
$C_{20}H_{30}O_5$ 350.454

(6α,7β)-*form*

17-Ac, Me ester: ***Florlide F***
[267417-28-7]
$C_{23}H_{34}O_6$ 406.518
Constit. of *Xenia florida*. Oil. $[\alpha]_D$ -117 (c, 0.05 in MeOH).
λ_{max} 242 (log ϵ 4.23) (MeOH).
Iwagawa, T. *et al., J. Nat. Prod.*, 2000, **63**, 468-472 (*isol, pmr, cmr*)

Epoxydilopholone E-242

[70142-89-1]

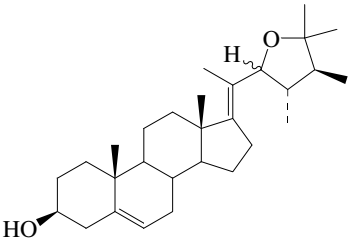


$C_{20}H_{30}O_2$ 302.456
Constit. of brown alga *Dilophus prolificans.* Oil. $[\alpha]_D^{20}$ +167 (c, 0.95 in $CHCl_3$).

Kazlauskas, R. *et al., Tet. Lett.*, 1978, 4155,

22,25-Epoxy-23,24-dimethylcholesta-5,17(20)-dien-3-ol E-243

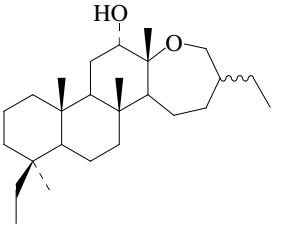
22,25-Epoxy-23-methylergost-5,17(20)-dien-3-ol



$C_{29}H_{46}O_2$ 426.681

(3β,17(20)*E*,22ξ,23*S*,24*S*)-*form* [157459-24-0]
Isol. from soft coral *Sinularia mayi*.
Kobayashi, M. *et al., CA*, 1993, **121**, 175533,

13,18-Epoxy-20,24-dimethyl-25-nor-13,18-seco-12-scalaranol E-244

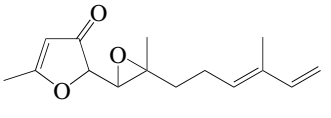


$C_{26}H_{46}O_2$ 390.648

(12α,17ξ)-*form* [757954-66-8]
Constit. of *Phyllospongia madagascarensis.*
Amorph. solid. $[\alpha]_D^{25}$ +35 (c, 0.02 in $CHCl_3$).
Ponomarenko, L.P. *et al., J. Nat. Prod.*, 2004, **67**, 1507-1510 (*isol, pmr, cmr*)

2-(1,2-Epoxy-2,6-dimethyl-5,7-octadienyl)-5-methyl-3(2*H*)-furanone E-245

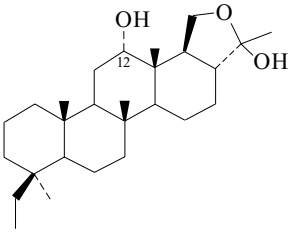
[181776-08-9]



$C_{15}H_{20}O_3$ 248.321
Constit. of *Lobophytum catalai*. Oil. $[\alpha]_D^{25}$ -1.1 (c, 0.85 in $CHCl_3$).
λ_{max} 226; 247 ($CHCl_3$).

Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 1001-1003; 1998, **37**, 267-274 (*isol, pmr, cmr*)

24,25-Epoxy-20,24-dimethyl-12,24-scalaranediol E-246

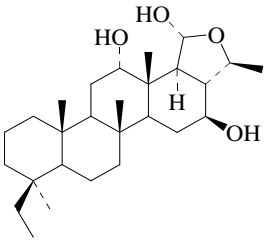


$C_{27}H_{46}O_3$ 418.659

12α-*form*

12-Ac: 12α-Acetoxy-24,25-epoxy-24-hydroxy-20,24-dimethylscalarane
[99617-43-3]
$C_{29}H_{48}O_4$ 460.696
Constit. of sponge *Carteriospongia foliascens*. Ichthyotoxin. Oil. $[\alpha]_D$ +65 (c, 0.61 in CH_2Cl_2).
Braekman, J.C. *et al., Tetrahedron*, 1985, **41**, 4603,

24,25-Epoxy-20,24-dimethyl-12,16,25-scalaranetriol E-247

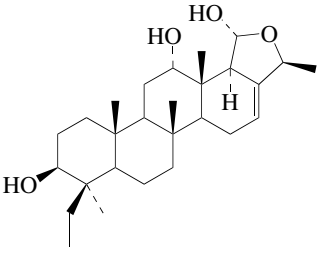


$C_{27}H_{46}O_4$ 434.658

(12α,16β,24α*H*,25α)-*form*

12-Ac: [478364-20-4]
$C_{29}H_{48}O_5$ 476.695
Constit. of a *Phyllospongia* sp. Amorph. solid. $[\alpha]_D^{23}$ +38 (c, 0.99 in $CHCl_3$).
Roy, M.C. *et al., J. Nat. Prod.*, 2002, **65**, 1838-1842 (*isol, pmr, cmr*)

24,25-Epoxy-20,24-dimethyl-16-scalarene-3,12,25-triol E-248



$C_{27}H_{44}O_4$ 432.642

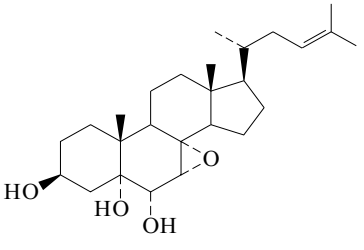
(3β,12α,24β,25α)-*form*

12-Ac: [173107-61-4]
$C_{29}H_{46}O_5$ 474.679
Constit. of a Indo-Pacific foliose sponge. Cryst. $[\alpha]_D$ +51.9 (c, 1.5 in CH_2Cl_2).

3-Ketone, 12-Ac: [173107-62-5]
$C_{29}H_{44}O_5$ 472.664
Constit. of a Indo-Pacific foliose sponge. Oil.
Jaspars, M. *et al., J. Nat. Prod.*, 1997, **60**, 556-561 (*isol, pmr, cmr, cryst struct*)

7,8-Epoxy-26,27-dinorergost-23-ene-3,5,6-triol E-249

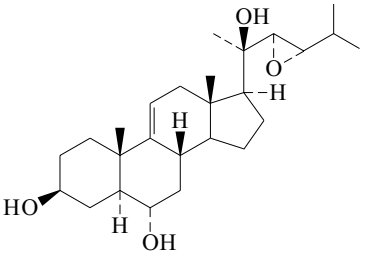
7,8-Epoxy-24-norcholest-23(25)-ene-3,5,6-triol



$C_{26}H_{42}O_4$ 418.615

(3β,5α,6α,7α,8α)-*form* [177856-27-8]
Constit. of *Acabaria undulata*.
Cryst.
Mp 184-185°.
Shin, J. *et al., J. Nat. Prod.*, 1996, **59**, 679-682 (*isol, pmr, cmr*)

22,23-Epoxy-26,27-dinorergost-9(11)-ene-3,6,20-triol E-250

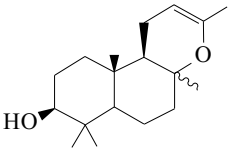


$C_{26}H_{42}O_4$ 418.615

(3β,5α,6α,20*R*,22*R*,23*S*)-*form*

6-O-[β-D-Quinovopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[β-D-quinovopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-β-D-quinovopyranoside], 3-sulfate: ***Asteroside B***
[115178-50-2]
$C_{55}H_{90}O_{28}S$ 1231.365
Constit. of *Asterias amurensis*.
$[\alpha]_D$ -9.2 (MeOH).
Riccio, R. *et al., J.C.S. Perkin 1*, 1988, 1337-1347 (*isol, pmr, cmr, ms*)

8,13-Epoxy-14,15-dinor-12-labden-3-ol E-251

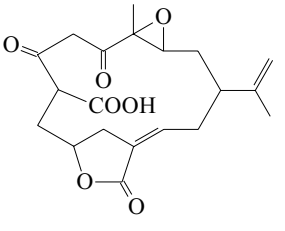


$C_{18}H_{30}O_2$ 278.434

(3β,8ξ)-*form*

Constit. of *Cystophora moniliformis*.
Viscous oil. $[\alpha]_D^{20}$ +6.2 (c, 1.3 in CH_2Cl_2).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 171

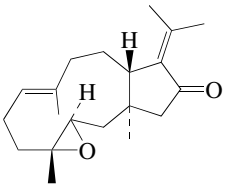
3,4-Epoxy-5,7-dioxo-12,15-cembradien-20,10-olid-19-oic acid E-252



$C_{20}H_{24}O_7$ 376.405

Me ester: ***Sinulariadione***
[154512-23-9]
$C_{21}H_{26}O_7$ 390.432
Constit. of a *Sinularia* sp. Cryst. (MeOH).
Mp 174-175°. $[\alpha]_D^{25}$ +20.7 (c, 0.86 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., Nat. Prod. Lett.*, 1993, **3**, 149 (*isol, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 463-465 (*isol, pmr, cmr*)

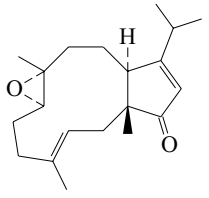
3,4-Epoxy-7,12(18)-dolabelladien-13-one E-253



$C_{20}H_{30}O_2$ 302.456

(3*R*,4*R*,7*E*)-*form*
Claenone
[112790-42-8]
Constit. of the soft coral *Clavularia* sp.
Needles (hexane/EtOAc). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 124-126°. $[\alpha]_D$ -50.9 (c, 1.2 in $CHCl_3$). λ_{max} 256 (ε 9060) (EtOH).
Mori, K. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2840-2852 (*isol, uv, ir, pmr, cmr*)
Miyaoka, H. *et al., Tet. Lett.*, 1998, **39**, 6503-6506 (*synth*)
Miyaoka, H, *et al., Tetrahedron*, 2003, **59**, 61-75 (*synth*)

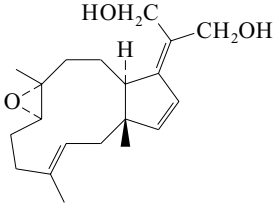
7,8-Epoxy-3,12-dolabelladien-14-one E-254



$C_{20}H_{30}O_2$ 302.456

(3*E*,7α,8α)-*form* [169211-81-8]
Constit. of *Eunicea tourneforti*.
Cryst.
Mp 134-136°. $[\alpha]_D^{24}$ +10 (c, 0.6 in $CHCl_3$). λ_{max} 250 (ε 7000) (MeOH) (Berdy).
Govindan, M. *et al., J. Nat. Prod.*, 1995, **58**, 1174 (*isol, pmr, cmr*)

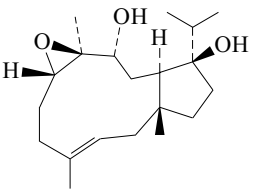
7,8-Epoxy-3,12(18),13-dolabellatriene-19,20-diol E-255



$C_{20}H_{30}O_3$ 318.455

(3*E*,7α,8α)-*form*
Di-Ac: [169211-82-9]
$C_{24}H_{34}O_5$ 402.53
Constit. of *Eunicea tourneforti*. Glass. $[\alpha]_D^{24}$ 0 (c, 0.1 in $CHCl_3$).
Govindan, M. *et al., J. Nat. Prod.*, 1995, **58**, 1174 (*isol, pmr, cmr*)

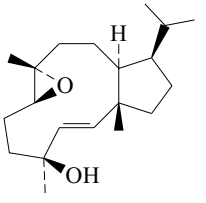
7,8-Epoxy-3-dolabellene-9,12-diol E-256



$C_{20}H_{34}O_3$ 322.487

(7α,8β,9α,12β)-*form* [160489-00-9]
Constit. of *Dictyota pardalis* f. *pseudohamata*.
Oil. $[\alpha]_D^{25}$ +51.5 (c, 0.26 in $CHCl_3$).
König, G.M. *et al., J. Nat. Prod.*, 1994, **57**, 1529 (*isol, pmr, cmr*)

7,8-Epoxy-2-dolabellen-4-ol E-257

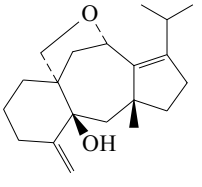


$C_{20}H_{34}O_2$ 306.487

(2*E*,4β,7β,8α)-*form*
Constit. of a *Dictyota* sp.
Oil. $[\alpha]_D$ +0.1 (c, 2.85 in $CHCl_3$).
Gallardo, A. *et al., Rev. Latinoam. Quim.*, 1988, **19**, 86 (*isol, pmr, cmr*)

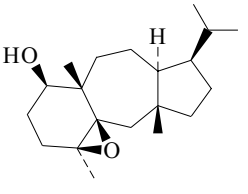
7,16-Epoxy-1(15),8-dolastadien-14-ol E-258

Dictinol
[133882-85-6]



$C_{20}H_{30}O_2$ 302.456
Metab. of *Dictyota indica*. Gum. $[\alpha]_D$ -40 (c, 0.05 in $CHCl_3$).
Ahmad, V.U. *et al., Phytochemistry*, 1991, **30**, 1015 (*isol, pmr, cmr*)

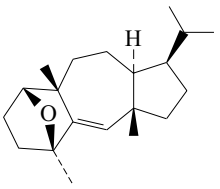
1,14-Epoxy-4-dolastanol E-259



$C_{20}H_{34}O_2$ 306.487

(1β,4β,14β)-*form*
Ac: 4-Acetoxy-1,14-epoxydolastane
$C_{22}H_{36}O_3$ 348.525
Constit. of a *Dictyota* sp. Cryst.
Mp 138-139°. $[\alpha]_D$ +8.6 (c, 0.88 in $CHCl_3$).
Gallardo, A. *et al., Rev. Latinoam. Quim.*, 1988, **19**, 86 (*isol, pmr, cmr, cryst struct*)

1,4-Epoxy-13-dolastene E-260



$C_{20}H_{32}O$ 288.472

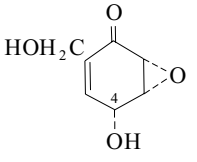
(1β,4β)-*form*

Constit. of a *Dictyota* sp.
Oil. $[\alpha]_D$ +10.5 (c, 0.4 in $CHCl_3$).

Gallardo, A. *et al., Rev. Latinoam. Quim.*, 1988, **19**, 86 (*isol, pmr, cmr*)

Epoxydon E-261

5-Hydroxy-3-(hydroxymethyl)-7-oxabicyclo[4.1.0]hept-3-en-2-one, 9CI. 5,6-Epoxy-4-hydroxy-2-hydroxymethyl-2-cyclohexen-1-one. Parasitenone. Phyllosinol. Sphaeropsidin
[5831-38-9]



(+)–*form*

$C_7H_8O_4$ 156.138

Struct. of Parasitenone revised in 2005.

(+)-*form* [24292-29-3]

Metab. of *Phoma* spp. and *Mycosphaerella ligulicola* and the marine *Aspergillus parasiticus.*
Cryst. (Me_2CO/Et_2O).
Mp 40-45°. $[\alpha]_D^{22}$ +93 (c, 0.29 in MeOH). λ_{max} 203 (log ϵ 3.72); 237 (log ϵ 3.68) (MeOH). λ_{max} 232 (sh) (ϵ 6670); 262 (ϵ 3440); 324 (sh) (ϵ 870) (EtOH/NaOH).

1′-Ac: [79516-80-6]
$C_9H_{10}O_5$ 198.175
Metab. of *Mycosphaerella ligulicola*. Needles ($CHCl_3$/MeOH).
Mp 60-62°. $[\alpha]_D^{23}$ +90.4 (c, 0.1 in EtOH).

Di-Ac:
Oil. $[\alpha]_D^{22}$ +48 (c, 0.5 in $CHCl_3$).

4-Epimer: ***Epiepoxydon***. *Isoepoxydon*
[67772-76-3]
Isolated from the crape myrtle, *Lagerstroemia indica*. Metab. of *Pestalotiopsis longiseta*.
Cryst. $[\alpha]_D^{24}$ +194 (c, 1.57 in EtOH). $[\alpha]_D^{25}$ +261 (c, 1 in MeOH).
Precursor of Patulin, P-124.

(±)-*form* [39910-94-6]

Cryst. (EtOAc). Mp 64-64.5°.

Di-Ac: [52194-63-5]
Oil. Sol. $CHCl_3$, MeOH.

4-Epimer: [62929-65-1]
Cryst. (EtOAc). Mp 78.5-79°.

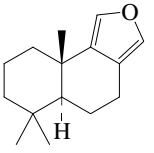
(ξ)-*form*

O-*(2-Hydroxy-6-methylbenzoyl):* ***Epoxydon 6-methylsalicylate***
$C_{15}H_{14}O_6$ 290.272
Prod. by *Phoma sorghina*. Phytotoxin.
Posn. of esterification not known.

[25163-24-0]

Closse, A. *et al., Helv. Chim. Acta*, 1966, **49**, 204 (*isol, ir, pmr, uv*)
Ichihara, A. *et al., Agric. Biol. Chem.*, 1974, **38**, 163; 1982, **46**, 1879 (*synth, ir, pmr, uv*)
Ichihara, A. *et al., Tet. Lett.*, 1976, 4741 (*synth*)
Nagasawa, H. *et al., Agric. Biol. Chem.*, 1978, **42**, 1303 (*isol, ir, ms, pmr*)
Sekiguchi, J. *et al., Biochem. J.*, 1979, 182; 445 (*isol*)
Chou, D.T.-W. *et al., J.A.C.S.*, 1980, **102**, 7987 (*synth*)
Assante, G. *et al., Phytopathol. Mediterr.*, 1980, **19**, 163 (*isol*)
Assante, G. *et al., Phytochemistry*, 1981, **20**, 1955 (*isol*)
Nagata, T. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 810 (*Epiepoxydon*)
Venkatasubbaiah, P. *et al., Mycologia*, 1992, **84**, 715-723 (*6-methylsalicylate*)
Kamikubo, T. *et al., Tet. Lett.*, 1996, **37**, 499 (*synth*)
Tachihara, T. *et al., Tetrahedron*, 2003, **59**, 1773-1780 (*Epiepoxydon, synth*)
Mehta, G. *et al., Tet. Lett.*, 2004, **45**, 7683-7687; 2005, **46**, 3373-3376 (*synth*)

11,12-Epoxy-8(12),9(11)-drimadiene E-262



5α-*form*

$C_{15}H_{22}O$ 218.338

5α-*form*

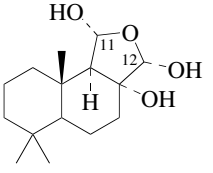
(+)-Euryfuran
Constit. of *Dysidea herbacea*.
Oil; fine needles.
Mp 26°. $[\alpha]_D$ +19 (c, 1.6 in $CHCl_3$). $[\alpha]_D^{20}$ +21 (c, 1.0 in CCl_4).

(*ent*-5α)-*form*

(-)-Euryfuran
[79895-94-6]
Constit. of the nudibranch *Hypselodoris* spp. and and *Spongia* sp.
Oil. $[\alpha]_D$ -24 (c, 0.5 in $CHCl_3$).

Dunlop, R.W. *et al., Aust. J. Chem.*, 1982, **35**, 95 (*isol, Dysidea*)
Hochlowski, J.E. *et al., J.O.C.*, 1982, **47**, 88 (*isol, marine organisms*)
Ley, S.V. *et al., J.C.S. Perkin 1*, 1983, 1379 (*synth*)
Grode, S.H. *et al., J. Nat. Prod.*, 1984, **47**, 76
Cortés, M. *et al., Bull. Soc. Chim. Belg.*, 1987, **96**, 631-632 (*synth, abs config*)
Nakano, T. *et al., J.C.S. Perkin 1*, 1987, 2137 (*synth*)
Baba, Y. *et al., Tetrahedron*, 1994, **50**, 5645 (*synth*)

11,12-Epoxy-8,11,12-drimanetriol E-263



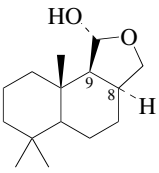
$C_{15}H_{26}O_4$ 270.368

(8α,11α,12α)-*form*

11-Me ether: 11,12-Epoxy-11-methoxy-8,12-drimanediol
[198423-23-3]
$C_{16}H_{28}O_4$ 284.395
Constit. of a *Dysidea* sp. Gum. $[\alpha]_D^{25}$ +2.8 (c, 0.2 in MeOH).

Paul, V.J. *et al., J. Nat. Prod.*, 1997, **60**, 1115-1120 (*isol, pmr, cmr*)

11,12-Epoxy-11-drimanol E-264



11α-*form*

$C_{15}H_{26}O_2$ 238.369

11α-*form*

Ac: [151751-76-7]
$C_{17}H_{28}O_3$ 280.406
Constit. of *Dysidea* sp. Oil. $[\alpha]_D$ -37.8 (c, 0.2 in $CHCl_3$).

11-Me ether:
$C_{16}H_{28}O_2$ 252.396
Constit. of a *Dysidea* sp. Oil. $[\alpha]_D^{25}$ -21.6 (c, 0.3 in MeOH).

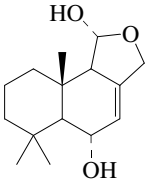
11β-*form* [151751-77-8]
Constit. of *Dysidea* sp.
Oil. $[\alpha]_D$ -46.8 (c, 0.43 in $CHCl_3$).

(8β*H*,11α)-*form*
Constit. of *Dysidea fusca*.
Oil. $[\alpha]_D$ -6 (c, 0.6 in $CHCl_3$).

11-Ketone (lactone): ***11,12-Drimanolide***
$C_{15}H_{24}O_2$ 236.353
Constit. of a *Dysidea* sp. Solid.
Mp 75-76°. $[\alpha]_D^{25}$ +14.4 (c, 0.3 in MeOH).

Butler, M.S. *et al., Aust. J. Chem.*, 1993, **46**, 1255 (*isol, pmr, cmr*)
Montagnac, A. *et al., J. Nat. Prod.*, 1996, **59**, 866 (*isol, pmr, cmr*)
Paul, V.J. *et al., J. Nat. Prod.*, 1997, **60**, 1115-1120 (*11,12-Drimanolide, Me ether*)

11,12-Epoxy-7-drimene-6,11-diol E-265

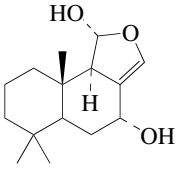


(6α,11α)-*form*

$C_{15}H_{24}O_3$ 252.353

(6α,11α)-*form*
Dendocarbin C
[350986-76-4]
Constit. of *Dendrodoris carbunculosa*.
Oil. $[\alpha]_D^{25}$ +26 (c, 0.06 in $CHCl_3$).
Sakio, Y. *et al., J. Nat. Prod.*, 2001, **64**, 726-731

11,12-Epoxy-8(12)-drimene-7,11-diol E-266

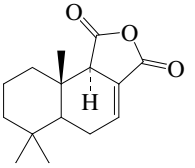


$C_{15}H_{24}O_3$ 252.353
Sol. MeOH, hexane; poorly sol. H_2O.

(7α,11*R*)-*form*
Di-Ac: ***Olepupuane***
[85356-02-1]
$C_{19}H_{28}O_5$ 336.427
Constit. of nudibranches *Dendrodoris grandiflora*, *Dendrodoris krebsii*, *Dendrodoris limbata*, *Dendrodoris nigra*, *Dendrodoris tuberclata*, *Doriopsilla albopunctata* and *Doriopsilla janaina*. Oil. $[\alpha]_D$ -83.3 (c, 0.54 in $CHCl_3$).
Okuda, R.K. *et al., J.O.C.*, 1983, **48**, 1866-1869 (*isol*)
Cimino, G. *et al., Tetrahedron*, 1985, **41**, 1093 (*isol*)
Cimino, G. *et al., J. Nat. Prod.*, 1988, **51**, 1010-1011 (*isol, pmr*)
Fontana, A. *et al., Tetrahedron*, 1999, **55**, 5937-5946 (*biosynth*)

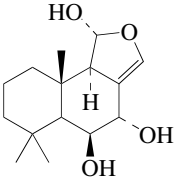
11,12-Epoxy-7-drimene-11,12-dione E-267

Dendocarbin H
[350986-81-1]



$C_{15}H_{20}O_3$ 248.321
Constit. of *Dendrodoris carbunculosa*. Oil. $[\alpha]_D^{25}$ -55 (c, 0.04 in $CHCl_3$).
Sakio, Y. *et al., J. Nat. Prod.*, 2001, **64**, 726-731 (*isol, pmr, cmr*)

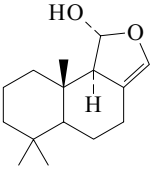
11,12-Epoxy-8(12)-drimene-6,7,11-triol E-268



$C_{15}H_{24}O_4$ 268.352

(6β,7α,11*R*)-*form*
Tri-Ac: ***6-Acetoxyolepupuane***
[97530-61-5]
$C_{21}H_{30}O_7$ 394.464
Constit. of nudibranch *Dendrodoris grandiflora*. Feeding deterrent against *Carassius auratus*. $[\alpha]_D$ -118.7 (c, 1.3 in $CHCl_3$).
Cimino, G. *et al., Tetrahedron*, 1985, **41**, 1093-1100 (*isol, pmr, cmr*)
Fontana, A. *et al., Tetrahedron*, 1999, **55**, 5937-5946 (*biosynth*)

11,12-Epoxy-8(12)-drimen-11-ol E-269



$C_{15}H_{24}O_2$ 236.353

(11α*OH*)-*form*
Found in the mollusc *Dendrodoris limbata* as a mixt. of C_{15}-C_{21} acyl esters.

Ac: ***7-Deacetoxyolepupuane***
[134822-40-5]
$C_{17}H_{26}O_3$ 278.391
Constit. of *Dendrodoris limbata*, *Dendrodoris grandiflora* and a *Dysidea* sp. Shows antimicrobial and antifungal activity; antifeedant; ichthyotoxin. Cryst. (CH_2Cl_2/hexane).
Mp 83-85°. $[\alpha]_D$ -166.7 (c, 0.104 in $CHCl_3$).

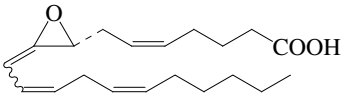
11ξ-*form* [78798-43-3]
Constit. of *Dysidea* sp. Antitumour agent. Oil.

[99603-90-4]

Cimino, G. *et al., Tet. Lett.*, 1981, **22**, 1271-1272 (*acyl esters, isol*)
Okuda, R.K. *et al., J.O.C.*, 1983, **48**, 1866 (*acyl esters, isol*)
Avila, C. *et al., Experientia*, 1991, **47**, 306 (*isol, pmr*)
Garson, M.J. *et al., J. Nat. Prod.*, 1992, **55**, 364-367 (*Ac, isol*)
Butler, M.-S. *et al., Aust. J. Chem.*, 1993, **46**, 1255 (*isol, pmr, cmr*)

Paul, V.J. *et al., J. Nat. Prod.*, 1997, **60**, 1115-1120 (*isol*)
Barrero, A.F. *et al., J. Nat. Prod.*, 1999, **62**, 1488-1491 (*synth, activity*)
Fontana, A. *et al., J.O.C.*, 2003, **68**, 2405-2409 (*biosynth*)

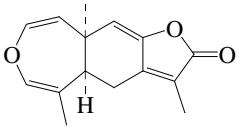
8,9-Epoxy-5,9,11,14-eicosatetraenoic acid E-270



$C_{20}H_{30}O_3$ 318.455

(5*Z*,8*R*,9ξ,11*Z*,14*Z*)-*form*
Isol. from the gorgonian *Plexaura homomalla*. Unstable intermed. in biosynth. of prostaglandins by the organism. λ_{max} 239 (hexane).
Brash, A.R. *et al., J.A.C.S.*, 1989, **111**, 1891-1892

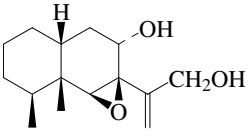
2,3-Epoxy-1,3,7(11),8-elematetraen-12,8-olide E-271



$C_{15}H_{16}O_3$ 244.29

(5α,10α)-*form*
Tubipolide F
[385793-36-2]
Constit. of *Tubipora musica*.
Oil. $[\alpha]_D^{25}$ -8.7 (c, 0.03 in $CHCl_3$). λ_{max} 246 (log ϵ 4.24) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 2001, **64**, 1430-1433 (*isol, pmr, cmr*)

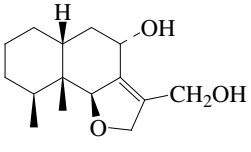
6,7-Epoxy-11(13)-eremophilene-8,12-diol E-272



$C_{15}H_{24}O_3$ 252.353

(6β,7β,8α,10β)-*form*
Peribysin A
Prod. by *Periconia byssoides* isol. from *Aplysia kurodai*.
Pale yellow oil. $[\alpha]_D$ -63.7 (c, 4.3 in EtOH). λ_{max} 233 (log ϵ 2.66) (EtOH).
Yamada, T. *et al., Org. Biomol. Chem.*, 2004, **2**, 2131-2135 (*isol, pmr, cmr*)
Yamada, T. *et al., J. Antibiot.*, 2005, **58**, 185-191 (*abs config*)

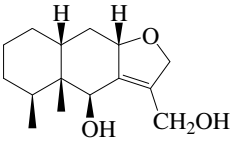
6,12-Epoxy-7(11)-eremophilene-8,13-diol E-273



$C_{15}H_{24}O_3$ 252.353

(6β,8α,10β)-*form*
Peribysin D
Prod. by *Periconia byssoides* isol. from *Aplysia kurodai*.
Pale yellow oil. $[\alpha]_D$ +4.6 (c, 0.1 in EtOH). Struct. revised in 2006.
λ_{max} 214 (log ϵ 3.56) (EtOH).
Yamada, T. *et al., Org. Biomol. Chem.*, 2004, **2**, 2131-2135 (*isol*)
Koshino, H. *et al., Tet. Lett.*, 2006, **47**, 4623-4626 (*struct*)

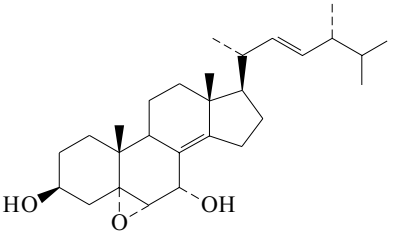
8,12-Epoxy-7(11)-eremophilene-6,13-diol E-274



$C_{15}H_{24}O_3$ 252.353

(6β,8α,10β)-*form*
Peribysin C
[763111-88-2]
Prod. by *Periconia byssoides* isol. from *Aplysia kurodai*.
Pale yellow oil. $[\alpha]_D$ +31.5 (c, 0.54 in EtOH). Struct. revised in 2006. λ_{max} 214 (log ϵ 3.58) (EtOH).
Yamada, T. *et al., Org. Biomol. Chem.*, 2004, **2**, 2131-2135 (*isol*)
Koshino, H. *et al., Tet. Lett.*, 2006, **47**, 4623-4626 (*struct*)

5,6-Epoxyergosta-8(14),22-diene-3,7-diol E-275
5,6-Epoxy-24-methylcholesta-8(14),22-diene-3,7-diol



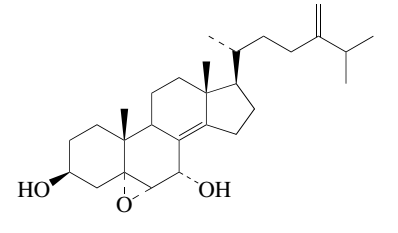
$C_{28}H_{44}O_3$ 428.654

(3β,5α,6α,7α,22*E*,24*R*)-*form* [22259-18-3]
[116150-66-4 (di-Ac)]
Constit. of *Arum italicum*.
$[\alpha]_D$ -83 (c, 0.9 in $CHCl_3$).

(3β,5α,6α,7β,22*E*,24*R*)-*form*
Constit. of *Grifola frondosa* (maitake).
Amorph. powder. $[\alpha]_D^{18}$ -52.4 (c, 0.2 in $CHCl_3$).

(3β,5α,6α,7α,22*E*,24ξ)-*form*
[148090-63-5 (di-Ac)]
Constit. of *Spongia officinalis.*
Cryst. (MeOH) (as di-Ac).
Mp 128-130° (di-Ac). $[\alpha]_D^{20}$ -125 (c, 0.12 in $CHCl_3$).
Della Greca, M. *et al., Nat. Prod. Lett.*, 1993, **2**, 27-32 (*isol, pmr, cmr*)
Migliuolo, A. *et al., Steroids*, 1993, **58**, 134-140 (*isol, pmr, cmr*)
Ishizuka, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1756-1760 (*isol, pmr, cmr*)
Yue, J.-M. *et al., Phytochemistry*, 2001, **56**, 801-806 (*isol, pmr, cmr*)

5,6-Epoxyergosta-8(14),24(28)-diene-3,7-diol E-276
5,6-Epoxy-24-methylenecholest-8(14)-ene-3,7-diol

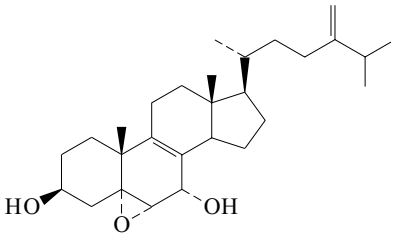


$C_{28}H_{44}O_3$ 428.654

(3β,5α,6α,7α)-*form*
Constit. of *Spongia officinalis.*
Di-Ac: [148010-40-6]
Cryst. (MeOH). Mp 161-163°. $[\alpha]_D^{20}$ -55.7 (c, 0.07 in $CHCl_3$).
Migliuolo, A. *et al., Steroids*, 1993, **58**, 134-140 (*isol, pmr, cmr*)

5,6-Epoxyergosta-8,24(28)-diene-3,7-diol E-277

5,6-Epoxy-24-methylenecholest-8-ene-3,7-diol



$C_{28}H_{44}O_3$ 428.654

(3β,5α,6α,7α)-*form*

Melithasterol D

[133883-10-0]

Constit. of *Melithaea ocracea* and *Spongia officinalis.*

Cryst. (MeOH). Mp 164-165°. $[\alpha]_D^{26}$ -59 (c, 0.54 in $CHCl_3$).

Di-Ac: [135574-61-7]

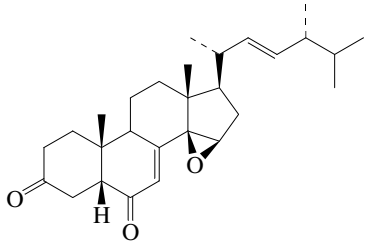
Cryst. (MeOH). Mp 175-177°. $[\alpha]_D^{20}$ -108 (c, 0.1 in $CHCl_3$).

Kobayashi, M. *et al., J.C.S. Perkin 1*, 1991, 1177 (*isol, pmr, cmr*)

Migliuolo, A. *et al., Steroids*, 1993, **58**, 134-140 (*isol, pmr, cmr*)

14,15-Epoxyergosta-7,22-diene-3,6-dione E-278

14,15-Epoxy-24-methylcholesta-7,22-diene-3,6-dione



$C_{28}H_{40}O_3$ 424.622

(14β,15β,22*E*,24*R*)-*form*

Gymnasterone B

[209169-58-4]

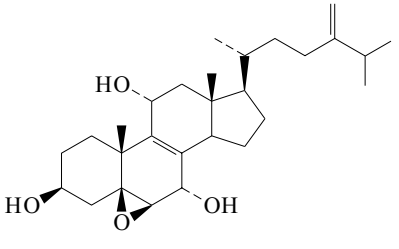
Constit. of *Gymnascella dankaliensis* isol. from the sponge *Halichondria japonica*. Antitumour agent. Powder. Mp 197-199°. $[\alpha]_D$ -76.3 (c, 0.76 in $CHCl_3$). λ_{max} 255 (log ϵ 4.13) (MeOH).

Amagata, T. *et al., Tet. Lett.*, 1998, **39**, 3773-3774 (*isol, pmr, cmr*)

Li, M. *et al., Tet. Lett.*, 2006, **47**, 3409-3412 (*synth, abs config*)

5,6-Epoxyergosta-8,24(28)-diene-3,7,11-triol, 9CI E-279

5,6-Epoxy-24-methylenecholest-8-ene-3,7,11-triol



$C_{28}H_{44}O_4$ 444.653

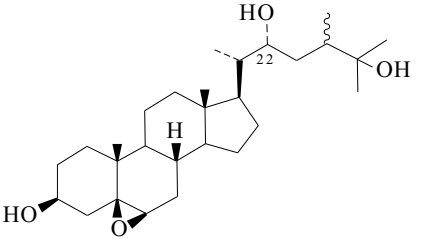
(3β,5β,6β,7α,11α)-*form* [133738-43-9]

Metab. of *Dysidea herbacea*. $[\alpha]_D$ -15 (c, 0.3 in $CHCl_3$) (Tri-Ac).

Isaacs, S. *et al., J. Nat. Prod.*, 1991, **54**, 83 (*isol, pmr, cmr*)

5,6-Epoxyergostane-3,22,25-triol, 9CI E-280

5,6-Epoxy-24-methylcholestane-3,22,25-triol



$C_{28}H_{48}O_4$ 448.685

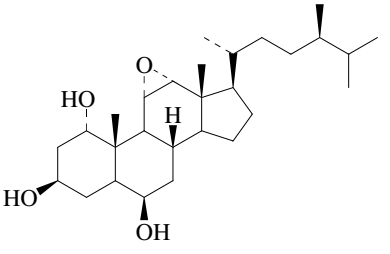
(3β,5β,6β,22*R*,24ξ)-*form* [80322-16-3]

Constit. of *Lobophytum depressum*. Amorph. solid. Mp 210-212°.

Carmely, S. *et al., Tetrahedron*, 1981, **37**, 2397-2403 (*isol*)

11,12-Epoxyergostane-1,3,6-triol E-281

11,12-Epoxy-24-methylcholestane-1,3,6-triol



$C_{28}H_{48}O_4$ 448.685

(1α,3β,5α,6β,11α,12α,24*R*)-*form* [253195-40-3]

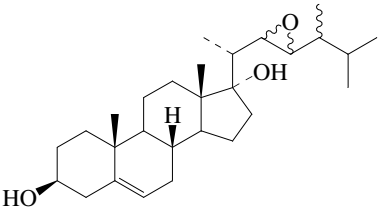
Constit. of *Sinularia dissecta*.

Tri-Ac: [253195-44-7]

Oil. $[\alpha]_D^{25}$ -36.3 (c, 0.6 in $CHCl_3$).

Ramesh, P. *et al., Steroids*, 1999, **64**, 785-789 (*isol, pmr, cmr*)

22,23-Epoxyergost-5-ene-3,17-diol E-282



$C_{28}H_{46}O_3$ 430.67

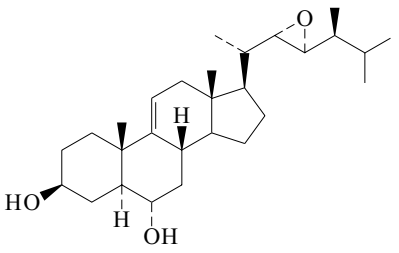
(3β,17α,22ξ,23ξ,24ξ)-*form* [675106-20-4]

Constit. of *Axinella* cf. *bidderi*. Powder.

Funel, C. *et al., J. Nat. Prod.*, 2004, **67**, 491-494 (*isol, pmr, cmr*)

22,23-Epoxyergost-9(11)-ene-3,6-diol E-283

22,23-Epoxy-24-methylcholest-9(11)-ene-3,6-diol



$C_{28}H_{46}O_3$ 430.67

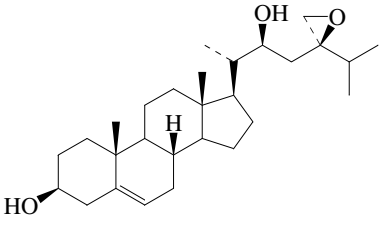
(3β,5α,6α,22*S*,23*S*,24*S*)-*form*

3-O-*β*-D-Glucuronopyranoside, 6-sulfate: ***Downeyoside D***
[174286-16-9]
$C_{34}H_{54}O_{12}S$ 686.859
Constit. of *Henricia downeyae*. $[\alpha]_D$ -23.3.

3-O-*[α*-L-*Arabinopyranosyl-(1→2)-β*-D-*glucuronopyranoside], 6-sulfate:* ***Downeyoside I***
[174286-21-6]
$C_{39}H_{62}O_{16}S$ 818.975
Constit. of *Henricia downeyae*. $[\alpha]_D$ -5.5.

Palagiano, E. *et al., J. Nat. Prod.*, 1996, **59**, 348 (*isol, pmr, cmr*)

24,28-Epoxyergost-5-ene-3,22-diol E-284



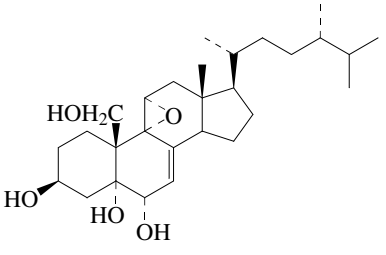
$C_{28}H_{46}O_3$ 430.67

(3β,22*S*,24*R*)-*form*

Muriceanol
[882400-85-3]
Constit. of a *Muricea* sp. Oil. $[\alpha]_D^{25}$ -9 (c, 0.51 in CH_2Cl_2).

Lorenzo, M. *et al., Eur. J. Org. Chem.*, 2006, 582-585

9,11-Epoxyergost-7-ene-3,5,6,19-tetrol E-285



$C_{28}H_{46}O_5$ 462.668

(3β,5α,6α,9α,11α,24*S*)-*form*

6-Ac: ***Dysideasterol D***
[851318-96-2]
$C_{30}H_{48}O_6$ 504.706
Constit. of a *Dysidea* sp. Powder. $[\alpha]_D^{20}$ +53 (c, 0.12 in $CHCl_3$).

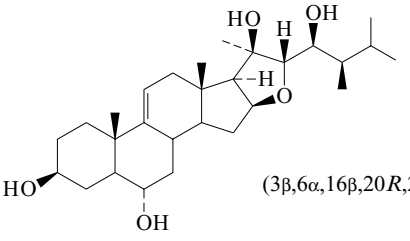
24,28-Didehydro: 9,11-Epoxyergosta-7,24(28)-diene-3,5,6,19-tetrol
$C_{28}H_{44}O_5$ 460.653

24,28-Didehydro, 6-Ac: ***Dysideasterol C***
[851318-95-1]
$C_{30}H_{46}O_6$ 502.69
Constit. of a *Dysidea* sp.

Huang, X.-C. *et al., Helv. Chim. Acta*, 2005, **88**, 281-289 (*Dysideasterols C and D*)

16,22-Epoxyergost-9(11)-ene-3,6,20,23-tetrol E-286

16,22-Epoxy-24-methylcholest-9(11)-ene-3,6,20,23-tetrol



(3β,6α,16β,20*R*,22*S*,23*S*,24*R*)–*form*

$C_{28}H_{46}O_5$ 462.668

(3β,6α,16β,20*R*,22*S*,23*S*,24*R*)-*form*

3-O-*β*-D-Glucuronopyranoside, 6-sulfate: ***Downeyoside A***
[170894-36-7]
$C_{34}H_{54}O_{14}S$ 718.858
Constit. of *Henricia downeyae*. Antifouling agent. Feeding deterrent.

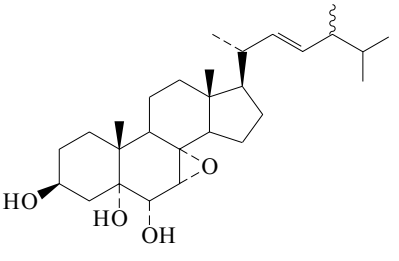
(3β,6α,16β,20*R*,22*S*,23*S*,24*S*)-*form*

3-O-*β*-D-Glucuronopyranoside, 6-sulfate: ***Downeyoside B***
[170894-37-8]
$C_{34}H_{54}O_{14}S$ 718.858
Constit. of *Henricia downeyae*.

Palagiano, E. *et al., Tetrahedron*, 1995, **51**, 12293

7,8-Epoxyergost-22-ene-3,5,6-triol E-287

7,8-Epoxy-24-methylcholest-22-ene-3,5,6-triol

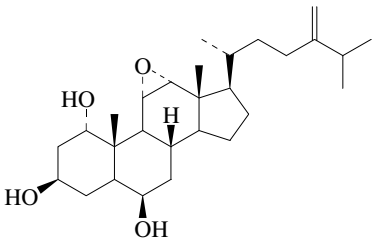


$C_{28}H_{46}O_4$ 446.669

(3β,5α,6α,7α,8α,22*E*,24ξ)-*form* [177856-26-7]
Constit. of *Acabaria undulata*.
Cryst.
Mp 187-188°. Error in struct. diag. in ref.

Shin, J. *et al., J. Nat. Prod.*, 1996, **59**, 679-682 (*isol, pmr, cmr*)

11,12-Epoxyergost-24(28)-ene-1,3,6-triol E-288



$C_{28}H_{46}O_4$ 446.669

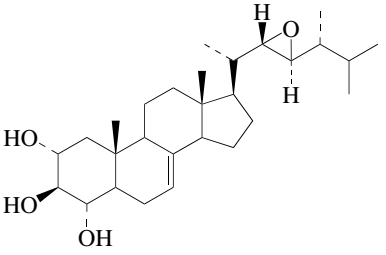
(1α,3β,5α,6β,11α,12α)-*form* [224577-38-2]
Constit. of *Sinularia dissecta*.

Tri-Ac: [224577-39-3]
$C_{34}H_{52}O_7$ 572.781
Cryst. Mp 102°. $[\alpha]_D$ -26 (c, 1 in $CHCl_3$).

Venkateswarlu, Y. *et al., Nat. Prod. Lett.*, 1999, **13**, 11-14; 229-232 (*isol, pmr, cmr*)

22,23-Epoxyergost-7-ene-2,3,4-triol E-289

22,23-Epoxy-24-methylcholest-7-ene-2,3,4-triol



$C_{28}H_{46}O_4$ 446.669

(2α,3β,4α,22*S*,23*S*,24*R*)-*form*

4-Sulfate: ***Acanthosterol sulfate F***
[215113-08-9]
$C_{28}H_{46}O_7S$ 526.733
Constit. of an *Acanthodendrilla* sp.
$[\alpha]_D^{25}$ +4.9 (c, 0.15 in MeOH).

4-Sulfate, 2-Ac: ***Acanthosterol sulfate I***
[215113-11-4]
$C_{30}H_{48}O_8S$ 568.77
Constit. of an *Acanthodendrilla* sp.
$[\alpha]_D^{25}$ -11 (c, 0.15 in MeOH).

4-Sulfate, 3-Ac: ***Acanthosterol sulfate D***
[215113-06-7]
$C_{30}H_{48}O_8S$ 568.77
Constit. of an *Acanthodendrilla* sp.
$[\alpha]_D^{25}$ +20 (c, 0.062 in MeOH).

(2α,3β,4α,22*S*,23*S*,24*S*)-*form*

4-Sulfate: ***Acanthosterol sulfate G***
[215113-09-0]
$C_{28}H_{46}O_7S$ 526.733
Constit. of an *Acanthodendrilla* sp.
$[\alpha]_D^{25}$ +4.9 (c, 0.15 in MeOH).

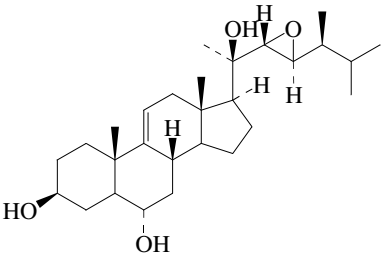
4-Sulfate, 2-Ac: ***Acanthosterol sulfate J***
[215113-12-5]
$C_{30}H_{48}O_8S$ 568.77
Constit. of an *Acanthodendrilla* sp.
$[\alpha]_D^{25}$ -25 (c, 0.092 in MeOH).

4-Sulfate, 3-Ac: ***Acanthosterol sulfate E***
[215113-07-8]
$C_{30}H_{48}O_8S$ 568.77
Constit. of an *Acanthodendrilla* sp.

Tsukamoto, S. *et al., J. Nat. Prod.*, 1998, **61**, 1374-1378 (*isol, pmr, cmr*)

22,23-Epoxyergost-9(11)-ene-3,6,20-triol E-290

22,23-Epoxy-24-methylcholest-9(11)-ene-3,6,20-triol



$C_{28}H_{46}O_4$ 446.669

(3β,5α,6α,20*R*,22*R*,23*S*,24*S*)-*form* [106521-61-3]
Sapogenin from *Asterina pectinifera*.
Amorph. powder.
Mp 202-206°. $[\alpha]_D$ +6.6 (c, 1.05 in $CHCl_3$).

3-O-*β*-D-*Glucuronopyranoside, 6-sulfate:* ***Downeyoside E***
[174286-17-0]
$C_{34}H_{54}O_{13}S$ 702.859
Constit. of *Henricia downeyae*.
$[\alpha]_D$ -14.7.

6-O-*[α*-L-*Arabinopyranosyl-(1→2)-β*-D-*glucopyranosyl-(1→4)-[6-deoxy-β*-D-*glucopyranosyl-(1→2)]-β*-D-*xylopyranosyl-(1→3)-6-deoxy-β*-D-*glucopyranoside], 3*-O-*sulfate:* ***Henricioside A***
[129393-27-7]
$C_{56}H_{92}O_{28}S$ 1245.392
Constit. of *Henricia laeviuscula*.

6-O-*[β*-D-*Fucopyranosyl-(1→2)-α*-L-*arabinopyranosyl-(1→4)-[6-deoxy-β*-D-*glucopyranosyl-(1→2)]-6-deoxy-β*-D-*glucopyranosyl-(1→3)-β*-D-*glucopyranoside], 3*-O-*sulfate:* ***Novaeguinoside II***
[849950-25-0]
$C_{57}H_{94}O_{28}S$ 1259.419
Constit. of the starfish *Culcita novaeguineae*. Cryst.
Mp 215-217°. $[\alpha]_D^{20}$ +3 (c, 0.132 in MeOH).

6-O-*[β*-D-*Fucopyranosyl-(1→2)-β*-D-*fucopyranosyl-(1→4)-[6-deoxy-β*-D-*glucopyranosyl-(1→2)]-6-deoxy-β*-D-*glucopyranosyl-(1→3)-β*-D-*glucopyranoside], 3*-O-*sulfate:* ***Novaeguinoside I***
[849950-23-8]
$C_{58}H_{96}O_{28}S$ 1273.446
Constit. of the starfish *Culcita novaeguineae*. Cryst.
Mp 217-219°. $[\alpha]_D^{20}$ +10 (c, 0.204 in MeOH).

6-O-*[β*-D-*Fucopyranosyl-(1→2)-6-deoxy-β*-D-*glucopyranosyl-(1→4)-[6-deoxy-β*-D-*glucopyranosyl-(1→2)]-6-deoxy-β*-D-*glucopyranosyl-(1→3)-β*-D-*glucopyranoside], 3*-O-*sulfate:* ***Regularoside A***
[99957-24-1]
$C_{58}H_{96}O_{28}S$ 1273.446
Constit. of *Halityle regularis*.
$[\alpha]_D$ +12.3 (c, 0.5 in MeOH) (as Na salt). CAS no. refers to Na salt.

6-O-*[6-Deoxy-β*-D-*glucopyranosyl-(1→2)-β*-D-*galactopyranosyl-(1→4)-[6-deoxy-β*-D-*glucopyranosyl-(1→2)]-β*-D-*xylopyranosyl-(1→3)-6-deoxy-β*-D-*glucopyranoside], 3*-O-*sulfate:* ***Ruberoside F***
[685561-54-0]
$C_{57}H_{94}O_{28}S$ 1259.419
Constit. of *Asterias rubens*.

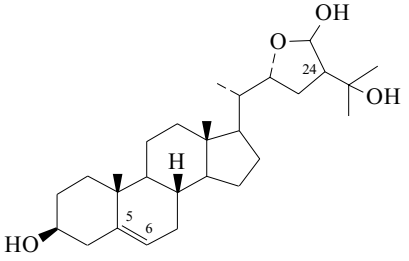
6-O-*[β*-D-*Fucopyranosyl-(1→4)-[α*-L-*arabinopyranosyl-(1→2)]-β*-D-*glucopyranosyl-(1→4)-[6-deoxy-β*-D-*glucopyranosyl-(1→2)]-β*-D-*xylopyranosyl-(1→3)-6-deoxy-β*-D-*glucopyranoside], 3*-O-*sulfate:* ***Patirioside A***
[128885-03-0]
$C_{62}H_{102}O_{32}S$ 1391.535
Constit. of *Patiria miniata*.
$[\alpha]_D$ +5.8 (MeOH).

6-O-[β-D-Galactopyranosyl-(1→4)-[β-D-fucopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-O-sulfate: ***Pectinioside B***
[106521-63-5]
$C_{63}H_{104}O_{33}S$ 1421.561
Constit. of *Asterina pectinifera*. Shows antihypertensive, sedative and hypnotic props. Needles.
Mp >300° dec. $[\alpha]_D$ +5.5 (c, 1.28 in H_2O). λ_{max} 207 (E1%/1cm 649) (MeOH/HCl) (Berdy).

Riccio, R. *et al., J. Nat. Prod.*, 1985, **48**, 756-765 (*Regularoside A*)
Noguchi, Y. *et al., Annalen*, 1987, 341-348 (*Pectinioside B*)
D'Auria, M.V. *et al., Gazz. Chim. Ital.*, 1990, **120**, 155-163 (*Henricioside A*)
D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1990, 1019-1023 (*Patirioside A*)
Palagiano, E. *et al., J. Nat. Prod.*, 1996, **59**, 348-354 (*Downeyoside E*)
Sandvoss, M. *et al., Magn. Reson. Chem.*, 2003, **41**, 949-954 (*Ruberoside F*)
Tang, H.-F. *et al., J. Nat. Prod.*, 2005, **68**, 337-341 (*Novaeguinosides I,II*)

22,28-Epoxyergost-5-ene-3,25,28-triol, 9CI E-291

22,28-Epoxy-24-methylcholest-5-ene-3,25,28-triol



$C_{28}H_{46}O_4$ 446.669

(3β,22*R*,24ξ)-*form*
Lobophytosterol
[80322-10-7]
Constit. of *Lobophytum depressum*.
Amorph. solid.
Mp 193-194.5°.

5β,6β-Epoxide: ***5,6:22,28-Diepoxyergostane-3,25,28-triol***.
5,6:22,28-Diepoxy-24-methylcholestane-3,25,28-triol
[77517-50-1]
$C_{28}H_{46}O_5$ 462.668
Constit. of *Lobophytum depressum*. Amorph. solid.
Mp 223-224.5°.

Carmely, S. *et al., Tetrahedron*, 1981, **37**, 2397-2403 (*isol*)

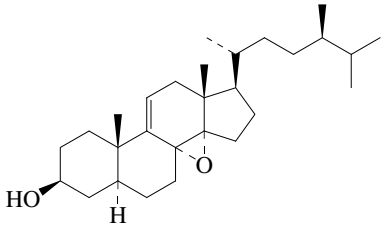
5,6-Epoxyergost-24(28)-en-3-ol E-292

5,6-Epoxy-24-methylenecholestan-3-ol
$C_{28}H_{46}O_2$ 414.67

(3β,5β,6β)-*form*
Constit. of *Haliclona oculata*.
$[\alpha]_D^{20}$ -0.3 (c, 0.75 in $CHCl_3$).

Findlay, J.A. *et al., Can. J. Chem.*, 1985, **63**, 2406

8,14-Epoxyergost-9(11)-en-3-ol E-293

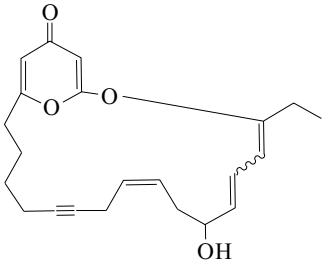


$C_{28}H_{46}O_2$ 414.67

(3β,5α,8α,14α,24*R*)-*form*
Me ether: 8,14-Epoxy-3-methoxyergost-9(11)-ene
[139765-34-7]
$C_{29}H_{48}O_2$ 428.697
Constit. of the sponge *Jereicopsis graphidiophora*.

D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*isol, pmr, ms*)

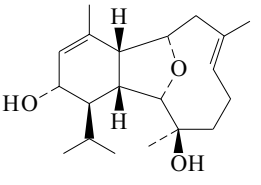
2,6-Epoxy-21-ethyl-17-hydroxy-1-oxacycloheneicosa-2,5,14,18,20-pentaen-11-yn-4-one E-294



$C_{22}H_{26}O_4$ 354.445
Metabolite of red alga *Phacelocarpus labillardieri*. λ_{max} 231 (ϵ 18000) (MeOH) (Derep).

Shin, J. *et al., Tet. Lett.*, 1986, **27**, 5189

6,13-Epoxy-3,8-eunicelladiene-2,12-diol E-295

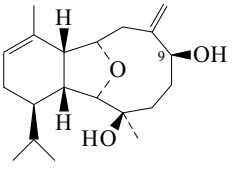


$C_{20}H_{32}O_3$ 320.471

(2α,6α,12β,13α)-*form*
Di-Ac: ***Calicophirin B***
[134381-17-2]
$C_{24}H_{36}O_5$ 404.545
Constit. of a *Calicogorgia* sp. and *Muricella* sp. Shows insecticidal and cytotoxic activities. Inhibits cAMP phosphodiesterase. Anti-inflammatory agent. Oil. $[\alpha]_D^{19}$ -106 (c, 0.46 in $CHCl_3$).

Ochi, M. *et al., Heterocycles*, 1991, **32**, 19 (*isol, pmr, cmr, activity*)
Seo, Y. *et al., J. Nat. Prod.*, 1997, **60**, 171-174 (*isol, activity*)
Park, Y.-H. *et al., Yakhak Hoeji*, 1997, **41**, 345-351 (*activity*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)

6,13-Epoxy-3,8(19)-eunicelladiene-9,12-diol E-296

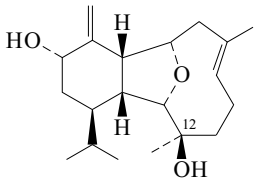


$C_{20}H_{32}O_3$ 320.471

(6α,9β,12β,13α)-*form*
9-Ac: [141257-48-9]
$C_{22}H_{34}O_4$ 362.508
Constit. of a *Cladiella* coral. Oil. $[\alpha]_D$ -132 (c, 0.13 in $CHCl_3$).

Uchio, Y. *et al., Tet. Lett.*, 1992, **33**, 1317 (*isol, pmr, cmr*)
MacMillan, D.W.C. *et al., J.A.C.S.*, 2001, **123**, 9033-9044 (*synth*)
Molander, G.A. *et al., J.A.C.S.*, 2004, **126**, 1642-1643 (*synth*)

6,13-Epoxy-4(18),8-eunicelladiene-3,12-diol E-297

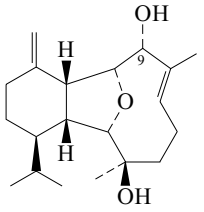


$C_{20}H_{32}O_3$ 320.471

(3α,6α,12β,13α)-*form*

12-Butanoyl: ***Litophynin C***
[118035-05-5]
$C_{24}H_{38}O_4$ 390.562
Constit. of a *Litophyton* sp. Exhibits insecticidal activity. Oil. $[\alpha]_D^{24}$ -2.3 (c, 0.9 in $CHCl_3$).
Ochi, M. *et al., Chem. Lett.*, 1987, 2207; 1988, 1661 (*isol, pmr, cmr, activity*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)

6,13-Epoxy-4(18),8-eunicelladiene-7,12-diol E-298

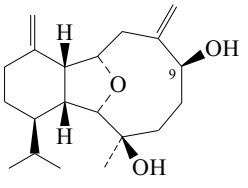


$C_{20}H_{32}O_3$ 320.471

(6α,7α,12β,13α)-*form*

Dibutanoyl: ***Litophynin B***
[112514-42-8]
$C_{28}H_{44}O_5$ 460.653
Constit. of *Litophyton* sp. Exhibits insecticide activity. Needles. Mp 99.5-100.5°. $[\alpha]_D^{20}$ -78.8 (c, 0.19 in EtOH).
Ochi, M. *et al., Chem. Lett.*, 1987, 2207 (*isol, pmr, cmr, activity*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)

6,13-Epoxy-4(18),8(19)-eunicelladiene-9,12-diol E-299



$C_{20}H_{32}O_3$ 320.471

(6α,9β,12β,13α)-*form*
Cladiellisin
[149182-75-2]
[153546-22-6]
Constit. of *Cladiella sphaeroides*, *Cladiella australis* and *Cladiella similis*.
Cryst.
Mp 215°. $[\alpha]_D^{23}$ -21.3 (c, 0.51 in $CHCl_3$). $[\alpha]_D^{26}$ +90 (c, 0.3 in $CHCl_3$).
12-Ac: [158831-74-4]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Cladiella australis*. Oil. $[\alpha]_D^{28}$ -58.8 (c, 0.17 in $CHCl_3$).

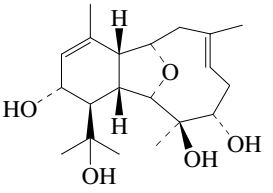
12-Butanoyl: ***Litophynin F***
[120484-78-8]
$C_{24}H_{38}O_4$ 390.562
Constit. of a *Litophyton* sp. Amorph. solid. $[\alpha]_D^{24}$ -9.4 (c, 0.43 in $CHCl_3$).

9-Ketone, 12-butanoyl: ***Litophynin G***
[120484-80-2]
$C_{24}H_{36}O_4$ 388.546
Constit. of a *Litophyton* sp. Cryst.
Mp 134-136°. $[\alpha]_D^{23}$ -26.1 (c, 0.11 in $CHCl_3$).

9-Hydroperoxide: ***Cladiellaperoxide***
$C_{20}H_{32}O_4$ 336.47
Constit. of *Cladiella sphaeroides*. Toxic to brine shrimp. Amorph. solid. $[\alpha]_D^{23}$ -27.8 (c, 0.42 in $CHCl_3$).

Ochi, M. *et al., Heterocycles*, 1991, **32**, 29 (*isol, pmr, cmr*)
Liu, J.K. *et al., Chin. Sci. Bull.*, 1992, **37**, 1627-1630 (*isol*)
Rao, D.S. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 198-199 (*Cladiella australis constit*)
Rao, C.B. *et al., J. Nat. Prod.*, 1994, **57**, 574 (*isol, pmr, cmr*)
Yamada, K. *et al., J. Nat. Prod.*, 1997, **60**, 393-396 (*Cladiellisin, Cladiellaperoxide*)

6,13-Epoxy-3,8-eunicelladiene-2,11,12,15-tetrol E-300

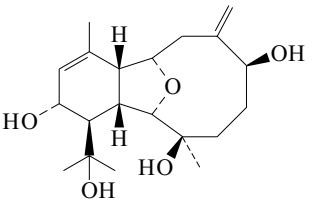


$C_{20}H_{32}O_5$ 352.47

(2α,6α,8*E*,11α,12β,13α)-*form*

2,11,15-Tri-Ac: ***Muricellin***
[309945-94-6]
$C_{26}H_{38}O_8$ 478.581
Constit. of *Muricella* sp. Oil. $[\alpha]_D^{25}$ -132 (c, 0.5 in $CHCl_3$).
Seo, Y. *et al., Nat. Prod. Lett.*, 2000, **14**, 197-203 (*isol, pmr, cmr*)

6,13-Epoxy-3,8(19)-eunicelladiene-2,9,12,15-tetrol E-301

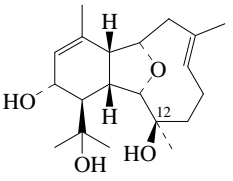


$C_{20}H_{32}O_5$ 352.47

(2α,6α,9β,12β,13α)-*form*

Tetra-Ac: ***Astrogorgin***
[126210-15-9]
$C_{28}H_{40}O_9$ 520.619
Metab. of gorgonian *Astrogorgia* sp. Also produced by *Muricella* sp. Cytotoxic agent. Antiinflammatory agent. Toxic to brine shrimp. Inhibits cell division in fertilised starfish eggs. cAMP inhibitor. Sol. MeOH, $CHCl_3$, Et_2O; poorly sol. H_2O. $[\alpha]_D$ -118 (c, 0.064 in $CHCl_3$).
Fusetani, N. *et al., Tet. Lett.*, 1989, **30**, 7079
Seo, Y. *et al., J. Nat. Prod.*, 1997, **60**, 171-174 (*activity, isol*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)
Crimmins, M.T. *et al., J.A.C.S.*, 2006, **128**, 1371-1378 (*synth*)

6,13-Epoxy-3,8-eunicelladiene-2,12,15-triol E-302



(2α,6α,8*E*,12β,13α)-*form*

$C_{20}H_{32}O_4$ 336.47

(2α,6α,8*E*,12β,13α)-*form*

Solid. Mp 88-89°. $[\alpha]_D$ -49.7 (c, 0.1 in $CHCl_3$).

Tri-Ac: ***Ophirin***

[74313-87-4]

$C_{26}H_{38}O_7$ 462.582

Constit. of *Muricella* spp., *Calicogorgia* sp. and an *Astrogorgia* sp. Inhibits cell division in fertilised starfish eggs. Toxic to brine shrimp. Inhibits cAMP phosphodiesterase. Cryst. Sol. MeOH, Et_2O, $CHCl_3$; poorly sol. H_2O.

Mp 133-134° (94-95°). $[\alpha]_D^{25}$ -119.7 (c, 1 in $CHCl_3$).

(2α,6α,8*Z*,12β,13α)-*form*

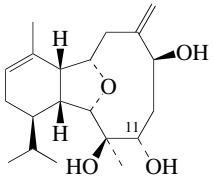
Tri-Ac: ***Ophirin B***

Constit. of *Muricella* spp.

Gum. $[\alpha]_D^{25}$ -35.3 (c, 0.1 in $CHCl_3$).

Kashman, Y. *et al., Tet. Lett.*, 1980, **21**, 879 (*isol, activity*)
Fusetani, N. *et al., Tet. Lett.*, 1989, 7079 (*isol, activity*)
Ochi, M. *et al., Heterocycles*, 1991, **32**, 19-23 (*isol*)
Seo, Y. *et al., J. Nat. Prod.*, 1997, **60**, 171 (*isol, pmr, cmr*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)
Crimmins, M.T. *et al., J.A.C.S.*, 2004, **126**, 10264-10266 (*synth*)
Crimmins, M.T. *et al., J.A.C.S.*, 2006, **128**, 1371-1378 (*synth*)

6,13-Epoxy-3,8(19)-eunicelladiene-9,11,12-triol E-303



$C_{20}H_{32}O_4$ 336.47

(6α,9β,11α,12β*OH*)-*form*

9-Hydroperoxide, 11-Ac: ***Alcyonin***

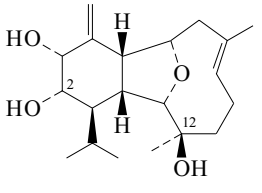
[115834-33-8]

$C_{22}H_{34}O_6$ 394.507

Constit. of the coelenterate *Sinularia flexibilis*. Cytotoxic agent. Struct. revised in 2003. Formerly assigned as 9-hydroxy.

Kusumi, T. *et al., Chem. Lett.*, 1988, 1077 (*isol, pmr, cmr*)
Corminboeuf, O. *et al., Org. Lett.*, 2003, **5**, 1543-1546 (*synth, struct*)

6,13-Epoxy-4(18),8-eunicelladiene-2,3,12-triol E-304



$C_{20}H_{32}O_4$ 336.47

(2α,3α,6α,12β,13α)-*form*

12-Butanoyl, 2,3-di-Ac: ***Litophynin D***

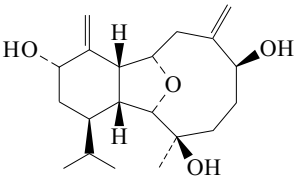
[120501-99-7]

$C_{28}H_{42}O_7$ 490.636

Constit. of a *Litophyton* sp. Toxic to brine shrimp. Oil. $[\alpha]_D^{22.5}$ -32.5 (c, 0.14 in $CHCl_3$).

Ochi, M. *et al., Chem. Lett.*, 1987, 2207; 1990, 2183 (*isol, pmr, cmr, activity*)

6,13-Epoxy-4(18),8(19)-eunicelladiene-3,9,12-triol E-305



$C_{20}H_{32}O_4$ 336.47

(3α,6α,9β,12β,13α)-*form*

12-Butanoyl: ***Litophynin H***

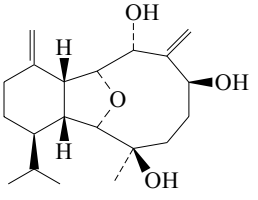
[135094-14-3]

$C_{24}H_{38}O_5$ 406.561

Constit. of a *Litophyton* sp. Exhibits ichthyotoxic and hemolytic activities. Amorph. solid. $[\alpha]_D^{20}$ +31.4 (c, 0.12 in $CHCl_3$).

Ochi, M. *et al., Heterocycles*, 1991, **32**, 29 (*isol, pmr, cmr*)
Miyamoto, T. *et al., J. Nat. Prod.*, 1994, **57**, 1212 (*isol, pmr, cmr, activity*)

6,13-Epoxy-4(18),8(19)-eunicelladiene-7,9,12-triol E-306



$C_{20}H_{32}O_4$ 336.47

(6α,7α,9β,12β,13α)-*form*

12-Butanoyl: ***Litophynol A***

[162831-73-4]

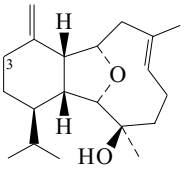
$C_{24}H_{38}O_5$ 406.561

Constit. of a *Litophyton* sp. Shows ichthyotoxic and hemolytic activities. Amorph. solid.

Mp 131-132°. $[\alpha]_D^{28}$ +19.2 (c, 1.1 in $CHCl_3$).

Miyamoto, T. *et al., J. Nat. Prod.*, 1994, **57**, 1212 (*isol, pmr, cmr, cryst struct, activity*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)

6,13-Epoxy-4(18),8-eunicelladien-12-ol E-307



$C_{20}H_{32}O_2$ 304.472

(6α,12β,13α)-*form*

Ac: ***Cladiellin***

[66873-35-6]

$C_{22}H_{34}O_3$ 346.509

Constit. of *Cladiella* spp. Antiinflammatory agent. cAMP phosphodiesterase inhibitor. Toxic to brine shrimp.

Butanoyl: ***Litophynin A***

[112500-87-5]

$C_{24}H_{38}O_3$ 374.562

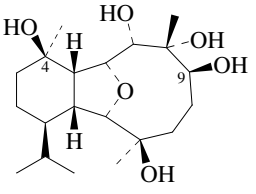
Constit. of a *Litophyton* sp. Insecticide. Oil. $[\alpha]_D^{20}$ -16.5 (c, 0.23 in EtOH).

Δ^3-Isomer: 6,13-Epoxy-3,8-eunicelladien-12-ol
[77390-37-5]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Cladiella* spp. Toxic to brine shrimp. Cryst. Mp 48-52°. $[\alpha]_D$ -22.7 (c, 0.3 in $CHCl_3$).

Δ^3-Isomer, Ac: [185613-31-4]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Muricella* spp. Toxic to brine shrimp. Solid. Mp 78-79°. $[\alpha]_D^{25}$ -34.7 (c, 0.5 in $CHCl_3$).

Kazlauskas, R. *et al., Tet. Lett.*, 1977, 4643-4646 (*isol, cryst struct*)
Hochlowski, J.E. *et al., Tet. Lett.*, 1980, **21**, 4055-4056 (*Δ^3-isomer, Δ^3-isomer Ac*)
Ochi, M. *et al., Chem. Lett.*, 1987, 2207-2210 (*Litophynin A, activity*)
Seo, Y. *et al., J. Nat. Prod.*, 1997, **60**, 171-174 (*isol, pmr, cmr*)

6,13-Epoxy-4,7,8,9,12-eunicellanepentol E-308

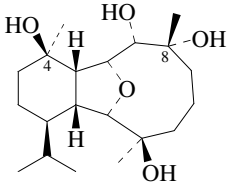


$C_{20}H_{36}O_6$ 372.501

(4β,6α,7α,8α,9β,12β,13α)-*form*

4,9-Di-Ac: ***Klyxumine A***
[845298-25-1]
$C_{24}H_{40}O_8$ 456.575
Constit. of *Klyxum flaccidum*. Oil. $[\alpha]_D^{25}$ +10.5 (c, 0.27 in Me_2CO).
Chill, L. *et al., J. Nat. Prod.*, 2005, **68**, 19-25 (*isol, pmr, cmr*)

6,13-Epoxy-4,7,8,12-eunicellanetetrol E-309

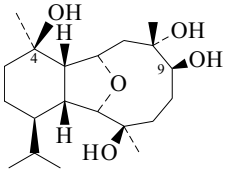


$C_{20}H_{36}O_5$ 356.501

(4β,6α,7α,8α,12β,13α)-*form*

4,8-Di-Ac: ***Klyxumine B***
[845298-26-2]
$C_{24}H_{40}O_7$ 440.576
Constit. of *Klyxum flaccidum*. Oil.
Chill, L. *et al., J. Nat. Prod.*, 2005, **68**, 19-25 (*isol, pmr, cmr*)

6,13-Epoxy-4,8,9,12-eunicellanetetrol E-310



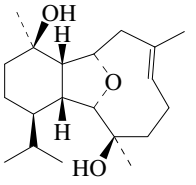
$C_{20}H_{36}O_5$ 356.501

(4β,6α,8α,9β,12β,13α)-*form*

9-Me ether, 12-Ac: ***Palmonine C***
[151484-82-1]
$C_{23}H_{40}O_6$ 412.565
Constit. of *Eunicella verrucosa*. Oil.

9-Me ether, 4,12-di-Ac: ***Palmonine A***
[151484-80-9]
$C_{25}H_{42}O_7$ 454.603
Constit. of *Eunicella verrucosa*. Oil. $[\alpha]_D$ +43.4 (c, 1.04 in $CHCl_3$).
Ortega, M.J. *et al., Tetrahedron*, 1993, **49**, 7823 (*isol, pmr, cmr*)

6,13-Epoxy-8-eunicellene-4,12-diol E-311



(4β,6α,8*E*,12β,13α)-*form*

$C_{20}H_{34}O_3$ 322.487

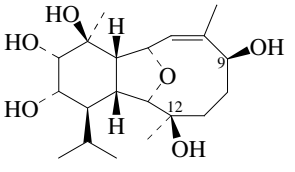
(4β,6α,8*E*,12β,13α)-*form*

Di-Ac: ***Acetoxycladiellin***
[66873-36-7]
$C_{24}H_{38}O_5$ 406.561
Constit. of *Cladiella* spp. Cryst. (pentane at -10°).

(4β,6α,8*Z*,13α)-*form*

Di-Ac:
$C_{24}H_{38}O_5$ 406.561
Constit. of *Eunicella cavolini*. Ichthyotoxic agent. Toxic to brine shrimp. Oil. $[\alpha]_D$ -15.6 (c, 1.4 in $CHCl_3$).
Kazlauskas, R. *et al., Tet. Lett.*, 1977, 4643
De Rosa, S. *et al., Nat. Prod. Lett.*, 1995, **7**, 259 (*isol, pmr, cmr*)

6,13-Epoxy-7-eunicellene-2,3,4,9,12-pentol E-312



$C_{20}H_{34}O_6$ 370.485

(2α,3α,4β,9β,12β)-*form*

2,3,4,9-Tetra-Ac: [296231-39-5]
$C_{28}H_{42}O_{10}$ 538.634
Constit. of *Eunicella cavolinii*.
$[\alpha]_D^{25}$ -24 (c, 0.1 in $CHCl_3$).

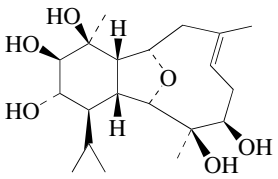
2,3,4,12-Tetra-Ac: [296231-40-8]
$C_{28}H_{42}O_{10}$ 538.634
Constit. of *Eunicella cavolinii*.
$[\alpha]_D^{25}$ -9 (c, 0.2 in $CHCl_3$).

Penta-Ac: [296231-38-4]
$C_{30}H_{44}O_{11}$ 580.671
Constit. of *Eunicella cavolinii*.
$[\alpha]_D$ +7 (c, 0.08 in $CHCl_3$).

9-Ketone: 6,13-Epoxy-2,3,4,12-tetrahydroxy-7-eunicellen-9-one
$C_{20}H_{32}O_6$ 368.469

9-Ketone, 2,3,4,12-tetra-Ac: [296231-41-9]
$C_{28}H_{40}O_{10}$ 536.618
Constit. of *Eunicella cavolinii*.
$[\alpha]_D^{25}$ -23 (c, 0.2 in $CHCl_3$).
Mancini, I. *et al., Helv. Chim. Acta*, 2000, **83**, 1561-1575 (*isol, pmr, cmr*)

6,13-Epoxy-8-eunicellene-2,3,4,11,12-pentol E-313

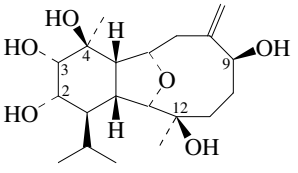


$C_{20}H_{34}O_6$ 370.485

(2α,3β,4β,8*E*,11β,12β)-*form*

2,12-Dibutanoyl, 3-Ac:
$C_{30}H_{48}O_9$ 552.704
Constit. of *Alcyonium molle*. Cryst. ($Et_2O/CHCl_3$).
Mp 174-175°. $[\alpha]_D^{20}$ -39 (c, 0.69 in $CHCl_3$).
Bowden, B.F. *et al., Aust. J. Chem.*, 1989, **42**, 665-673

6,13-Epoxy-8(19)-eunicellene-2,3,4,9,12-pentol E-314



$C_{20}H_{34}O_6$ 370.485

(2α,3α,4β,9β,12β)-*form*

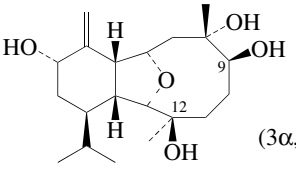
2,3,4,9-Tetra-Ac: [296231-36-2]
$C_{28}H_{42}O_{10}$ 538.634
Constit. of *Eunicella cavolinii*.
$[\alpha]_D^{25}$ -41 (c, 0.4 in $CHCl_3$).

Penta-Ac: [296231-35-1]
$C_{30}H_{44}O_{11}$ 580.671
Constit. of *Eunicella cavolinii*.
$[\alpha]_D^{25}$ -40 (c, 0.4 in $CHCl_3$).

9-Ketone: 6,13-Epoxy-2,3,4,12-tetrahydroxy-8(19)-eunicellen-9-one
$C_{20}H_{32}O_6$ 368.469

9-Ketone, 2,3,4,12-tetra-Ac: [296231-37-3]
$C_{28}H_{40}O_{10}$ 536.618
Constit. of *Eunicella cavolinii*.
$[\alpha]_D^{25}$ +16 (c, 0.4 in $CHCl_3$).
Mancini, I. *et al., Helv. Chim. Acta*, 2000, **83**, 1561-1575 (*isol, pmr, cmr*)

6,13-Epoxy-4(18)-eunicellene-3,8,9,12-tetrol E-315



(3α,6α,8α,9β,12β,13α)-*form*

$C_{20}H_{34}O_5$ 354.486

(3α,6α,8α,9β,12β,13α)-*form*

9-Butanoyl, 12-Ac: ***Australin B***
[863638-10-2]
$C_{26}H_{42}O_7$ 466.614
Constit. of *Cladiella australis*. Cryst.
Mp 137-139°. $[\alpha]_D^{25}$ -91 (c, 1.32 in $CHCl_3$).

(3α,6α,8β,9β,12β,13α)-*form*

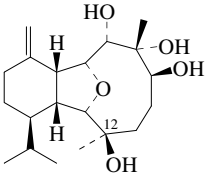
12-Butanoyl: ***Litophynin I***
[139579-22-9]
$C_{24}H_{40}O_6$ 424.576
Constit. of a *Litophyton* coral. Shows molluscicidal activity. Insecticide. Needles.
Mp 122.5-123.5°. $[\alpha]_D^{20}$ +45.2 (c, 0.58 in $CHCl_3$).

12-Butanoyl, 3-Ac: ***Litophynin I 3-acetate***
[162244-66-8]
$C_{26}H_{42}O_7$ 466.614
Constit. of a *Litophyton* sp. Ichthyotoxin. Haemolytic agent. Oil.
$[\alpha]_D$ +40 (c, 0.3 in $CHCl_3$).

12-Butanoyl, 9-Ac: ***Litophynin I 9-acetate***
$C_{26}H_{42}O_7$ 466.614
Constit. of a *Litophyton* sp. Ichthyotoxic. Oil. $[\alpha]_D^{27}$ +40.1 (c, 0.3 in $CHCl_3$).

Ochi, M. *et al., Chem. Lett.*, 1992, 155 (*Litophynin I, isol, activity*)
Miyamoto, T. *et al., J. Nat. Prod.*, 1994, **57**, 1212-1219 (*Litophynin I 3-Ac, Litophynin I 9-Ac, activity*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)
Ahmed, A.F. *et al., J. Nat. Prod.*, 2005, **68**, 1051-1055 (*Australin B*)

6,13-Epoxy-4(18)-eunicellene-7,8,9,12-tetrol E-316



(6α,7α,8α*OH*,9β,12β*OH*,13α)-*form*

$C_{20}H_{34}O_5$ 354.486

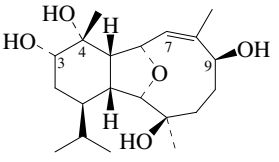
(6α,7α,8α*OH*,9β,12β*OH*,13α)-*form*

12-Butanoyl: ***Litophynol B***
[162831-74-5]
$C_{24}H_{40}O_6$ 424.576
Constit. of a *Litophyton* sp. Shows ichthyotoxic and hemolytic activities. Oil. $[\alpha]_D^{28}$ -17.6 (c, 3.1 in $CHCl_3$).

(6α,7β,8α*OH*,9β,12β*OH*,13α)-*form*
Sclerophytin D
[119456-13-2]
Isol. from *Sclerophytum capitalis*.
Gum. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O.
$[\alpha]_D$ -138 (c, 0.15 in $CHCl_3$).

12-Ac: ***Sclerophytin C***
[119456-12-1]
Constit. of *Sclerophytum capitalis* and *Cladiella australis*.
Cryst. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O.
Mp 94-95°. $[\alpha]_D^{28}$ -16.1 (c, 0.32 in $CHCl_3$).
Alam, M. *et al., J.O.C.*, 1989, **54**, 1896-1900 (*Sclerophytins*)
Rao, C.B. *et al., J. Nat. Prod.*, 1994, **57**, 574 (*Sclerophytin C, isol, pmr, cmr*)
Miyamoto, T. *et al., J. Nat. Prod.*, 1994, **57**, 1212-1219 (*Lytophynol B*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)
Friedrich, D. *et al., J. Nat. Prod.*, 2002, **65**, 126-130 (*bibl*)

6,13-Epoxy-7-eunicellene-3,4,9,12-tetrol E-317



(3α,4α,6α,9β,12β,13α)-*form*

$C_{20}H_{34}O_5$ 354.486

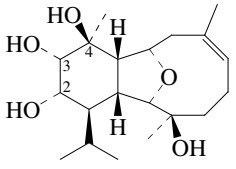
(3α,4α,6α,9β,12β,13α)-*form*

3,4,12-Tri-Ac: ***Labiatin E***
[226238-72-8]
$C_{26}H_{40}O_8$ 480.597
Constit. of *Eunicella labiata*. Oil. $[\alpha]_D^{25}$ +45.5 ($CHCl_3$). λ_{max} 233 (MeOH).

9-Ketone, 3,4,12-tri-Ac: ***Labiatin D***
[226238-70-6]
$C_{26}H_{38}O_8$ 478.581
Constit. of *Eunicella labiata*. Oil. $[\alpha]_D^{25}$ -21.3 ($CHCl_3$). λ_{max} 235 (MeOH).

(3α,4β,6α,9β,12β,13α)-*form*
Tetra-Ac: [296231-42-0]
$C_{28}H_{42}O_9$ 522.634
Constit. of *Eunicella singularis*.
Kakonikos, C. *et al., Nat. Prod. Lett.*, 1999, **13**, 89-95 (*isol, pmr, cmr*)
Mancini, I. *et al., Helv. Chim. Acta*, 2000, **83**, 1561-1575 (*Eunicella singularis constit*)

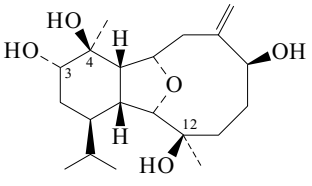
6,13-Epoxy-8-eunicellene-2,3,4,12-tetrol E-318



$C_{20}H_{34}O_5$ 354.486

(2α,3α,4β,8*Z*,12β)-*form*
2,3,4-Tri-Ac: [296231-32-8]
$C_{26}H_{40}O_8$ 480.597
Constit. of *Eunicella cavolinii*.
$[\alpha]_D^{25}$ +37 (c, 0.1 in $CHCl_3$).
Mancini, I. *et al., Helv. Chim. Acta*, 2000, **83**, 1561-1575 (*isol, pmr, cmr*)

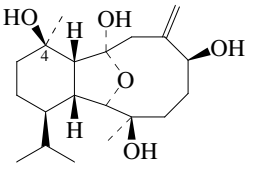
6,13-Epoxy-8(19)-eunicellene-3,4,9,12-tetrol E-319



$C_{20}H_{34}O_5$ 354.486

(3α,4β,6α,9β,12β,13α)-*form*
3,4,9-Tri-Ac: [174285-81-5]
$C_{26}H_{40}O_8$ 480.597
Constit. of *Eunicella singularis*.
$[\alpha]_D^{25}$ -13 (c, 0.2 in $CHCl_3$).
3,4,12-Tri-Ac: ***Labiatin C***
$C_{26}H_{40}O_8$ 480.597
Constit. of *Eunicella labiata*. Oil. $[\alpha]_D$ -6 (c, 0.4 in $CHCl_3$).
Tetra-Ac: ***Eunicellin***
[20589-51-9]
$C_{28}H_{42}O_9$ 522.634
Constit. of the gorgonian *Eunicella stricta*. Cryst. (Et_2O/petrol). Mp 186-188°.
9-Ketone, 3,4,12-tri-Ac: ***Labiatin B***
[174285-80-4]
$C_{26}H_{38}O_8$ 478.581
Constit. of *Eunicella labiata*. Oil. $[\alpha]_D$ +22.5 (c, 0.3 in $CHCl_3$). λ_{max} 219 (ϵ 15800) (MeOH) (Berdy).
Kennard, O. *et al., Tet. Lett.*, 1968, 2879-2884 (*Eunicellin, cryst struct*)
Roussis, V. *et al., Tetrahedron*, 1996, **52**, 2735-2742 (*Labiatins*)
Ortega, M.J. *et al., Tetrahedron*, 1997, **60**, 485-488 (*activity*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)
Mancini, I. *et al., Helv. Chim. Acta*, 2000, **83**, 1561-1575 (*Eunicella singularis constit*)

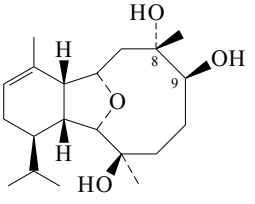
6,13-Epoxy-8(19)-eunicellene-4,6,9,12-tetrol E-320



$C_{20}H_{34}O_5$ 354.486

(4β,6α,9β,12β,13α)-*form*
4-Butanoyl, 9-Ac: ***Australin C***
[863638-11-3]
$C_{26}H_{42}O_7$ 466.614
Constit. of *Cladiella australis*. Oil. $[\alpha]_D^{25}$ +35 (c, 0.46 in $CHCl_3$).
Ahmed, A.F. *et al., J. Nat. Prod.*, 2005, **68**, 1051-1055 (*Australin C*)

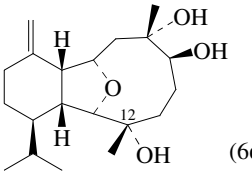
6,13-Epoxy-3-eunicellene-8,9,12-triol E-321



$C_{20}H_{34}O_4$ 338.486

(6α,8α,9β,12β,13α)-*form* [123012-55-5]
Metab. of *Cladiella* coral.
Prisms (CH_2Cl_2/hexane).
Mp 205.5-206°. $[\alpha]_D$ -16.1 (c, 0.75 in $CHCl_3$).
12-Ac:
$C_{22}H_{36}O_5$ 380.523
Constit. of a *Cladiella* coral. Oil. $[\alpha]_D$ -1.84 (c, 2.17 in $CHCl_3$).
3α,4α-Epoxide, 9,12-di-Ac:
$C_{24}H_{38}O_7$ 438.56
Constit. of a *Cladiella* sp. Amorph. solid. $[\alpha]_D$ -49.5 (c, 0.38 in $CHCl_3$).
Uchio, Y. *et al., Tet. Lett.*, 1989, **30**, 3331; 1992, **33**, 1317 (*isol, pmr, cmr, cryst struct*)
MacMillan, D.W.C. *et al., J.A.C.S.*, 2001, **123**, 9033-9044 (*synth*)
Gallou, F. *et al., Org. Lett.*, 2001, **3**, 135-137 (*synth*)

6,13-Epoxy-4(18)-eunicellene-8,9,12-triol E-322



(6α,8α*OH*,9β,12α*OH*,13α)-*form*

$C_{20}H_{34}O_4$ 338.486
The stereochem. of many of these derivs. was revised in 2002.

(6α,8α*OH*,9β,12α*OH*,13α)-*form*
Sclerophytin F
[66873-43-6]
Constit. of *Sclerophytum capitatis*.
Gum. Sol. MeOH; mod. sol. hexane; poorly sol. H_2O. $[\alpha]_D$ +55 (c, 0.2 in $CHCl_3$).
9-Ac: [153474-19-2]
$C_{22}H_{36}O_5$ 380.523
Constit. of *Cladiella australis*. Cryst.
Mp 68°. $[\alpha]_D^{26}$ +38 (c, 0.5 in $CHCl_3$).

12-Ac: ***Sclerophytin E***
[119456-14-3]
$C_{22}H_{36}O_5$ 380.523
Constit. of *Cladiella australis* and *Sclerophytum capitalis*. Gum. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D^{28}$ +10.4 (c, 0.48 in $CHCl_3$).

9-Butanoyl:
$C_{24}H_{40}O_5$ 408.577
Constit. of *Cladiella australis*. Oil. $[\alpha]_D^{28}$ +7.1 (c, 0.7 in $CHCl_3$).

12-Butanoyl: ***Litophynin E***
[132278-75-2]
$C_{24}H_{40}O_5$ 408.577
Constit. of *Litophyton* sp. Shows ichthyotoxic activity. Oil. $[\alpha]_D^{20}$ -13.1 (c, 0.21 in $CHCl_3$).

9-(3-Methylbutanoyl), 12-Ac: [405150-02-9]
$C_{27}H_{44}O_6$ 464.641
Constit. of *Cladiella australis*. Oil.

(6α,8α*OH*,9β,12β*OH*,13α)-*form*
Sclerophytin A
[117176-35-9]
Metab. of *Sclerophytum capitalis*.
Needles (C_6H_6). Sol. MeOH, hexane.
Mp 187°. Struct. revised in 2000.

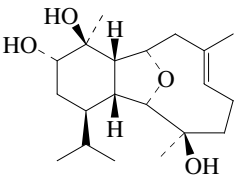
9-Ac: ***Sclerophytin B***
[117176-36-0]
$C_{22}H_{36}O_5$ 380.523
Metab. of *Sclerophytum capitalis*. Needles (Me_2CO). Sol. MeOH, hexane.
Mp 190-192°. Struct. revised in 2000.

9-Me ether: ***Sclerophytin A methyl ether***. *Sclerophytin F methyl ether (incorr.)*
[153229-17-5]
$C_{21}H_{36}O_4$ 352.513
Constit. of *Cladiella krempfi*. Cryst. (MeOH).
Mp 202-203°.

9-Et ether: ***Patagonicol***
[153415-47-5]
$C_{22}H_{38}O_4$ 366.54
Constit. of *Alcyonium patagonicum*. Cryst. (Me_2CO).
Mp 172.5-174°.

Sharma, P. *et al., J.C.S. Perkin 1*, 1988, 2537-2540 (*Sclerophytin A, Sclerophytin B*)
Alam, M. *et al., J.O.C.*, 1989, **54**, 1896-1900 (*Sclerophytin E, Sclerophytin F*)
Ochi, M. *et al., Chem. Lett.*, 1990, 2183-2186 (*Litophynin E*)
Su, J. *et al., J. Nat. Prod.*, 1993, **56**, 1601-1604 (*Patagonicol, cryst struct*)
Sarma, N.S. *et al., J. Nat. Prod.*, 1993, **56**, 1977-1980 (*Sclerophytin A methyl ether*)
Rao, D.S. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 198-199 (*Cladiella australis constit*)
Rao, C.B. *et al., J. Nat. Prod.*, 1994, **57**, 574-580 (*Cladiella australis constits*)
Miyamoto, T. *et al., J. Nat. Prod.*, 1994, **57**, 1212-1219 (*Litophynin E, activity*)
Overman, L.E. *et al., Org. Lett.*, 2000, **2**, 1879-1882 (*Sclerophytin A, synth*)
Bernardelli, P. *et al., J.A.C.S.*, 2001, **123**, 9021-9032 (*Sclerophytin A, synth*)
MacMillan, D.W.C. *et al., J.A.C.S.*, 2001, **123**, 9033-9044 (*Sclerophytin A, synth*)
Gallou, F. *et al., Org. Lett.*, 2001, **3**, 135-137 (*Sclerophytin A, synth*)
Friedrich, D. *et al., J. Nat. Prod.*, 2002, **65**, 126-130 (*struct*)

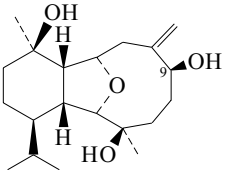
6,13-Epoxy-8-eunicellene-3,4,12-triol E-323



$C_{20}H_{34}O_4$ 338.486

(3α,4β,8*E*,12β)-*form*
Tri-Ac: [296231-33-9]
$C_{26}H_{40}O_7$ 464.598
Constit. of *Eunicella singularis*.
Mancini, I. *et al., Helv. Chim. Acta*, 2000, **83**, 1561-1575 (*isol, pmr, cmr*)

6,13-Epoxy-8(19)-eunicellene-4,9,12-triol E-324



$C_{20}H_{34}O_4$ 338.486

(4β,6α,9β,12β,13α)-*form*
Tri-Ac: ***Palmonine B***
[151484-81-0]
$C_{26}H_{40}O_7$ 464.598
Constit. of *Eunicella verrucosa*. Cytotoxic agent. Oil. $[\alpha]_D$ -35.8 (c, 1 in $CHCl_3$).

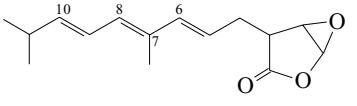
9-Ketone, di-Ac: ***Palmonine D***
[151484-83-2]
$C_{24}H_{36}O_6$ 420.545
Constit. of *Eunicella verrucosa*. Oil. $[\alpha]_D$ +7.3 (c, 0.7 in $CHCl_3$).

4,12-Di-Ac: ***Palmonine F***
$C_{24}H_{38}O_6$ 422.561
Constit. of *Eunicella verrucosa*. Oil. $[\alpha]_D^{25}$ -4.6 (c, 0.5 in $CHCl_3$).

Ortega, M.J. *et al., Tetrahedron*, 1993, **49**, 7823 (*isol, pmr, cmr*)
Ortega, M.-J. *et al., J. Nat. Prod.*, 1994, **57**, 1584 (*Palmonine F, Palmonine B, activity*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)

1,2-Epoxy-5,7,9-farnesatrien-15,1-olide E-325

4-(4,8-Dimethyl-2,4,6-nonatrienyl)-2,6-dioxabicyclo[3.1.0]hexan-3-one
[126030-33-9]



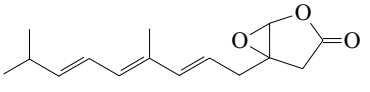
$C_{15}H_{20}O_3$ 248.321
Constit. of a *Euryspongia* sp. Cryst. (Et_2O/petrol).
Mp 50-51°. $[\alpha]_D$ -7 (c, 0.62 in $CHCl_3$).

7,8-Dihydro, Δ^6,Δ^{10}-isomer: 1,2-Epoxy-6,10-farnesadien-15,1-olide. ***Dictyodendrillin A***
Isol. from a *Dictyodendrilla* sp.
Oil. $[\alpha]_D$ +0.2 (c, 1.6 in $CHCl_3$). $[\alpha]_D$ -0.2 (c, 1.35 in MeOH).

Van Altena, I.A. *et al., Aust. J. Chem.*, 1989, **42**, 2181 (*isol, pmr, cmr*)
Tran, N.H. *et al., Aust. J. Chem.*, 1995, **48**, 1757 (*Dictyodendrillin A*)

3,15-Epoxy-5,7,9-farnesatrien-1,15-olide E-326

5-(4,8-Dimethyl-2,4,6-nonatrienyl)-2,6-dioxabicyclo[3.1.0]hexan-3-one
[126030-34-0]

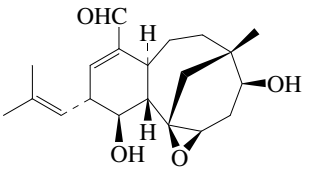


$C_{15}H_{20}O_3$ 248.321
Constit. of a *Euryspongia* sp. Unstable cryst. $[\alpha]_D$ -41 (c, 0.22 in $CHCl_3$).

Van Altena, I.A. *et al., Aust. J. Chem.*, 1989, **42**, 2181 (*isol, pmr, cmr*)

2-Epoxyfloridicin E-327

[267407-25-0]

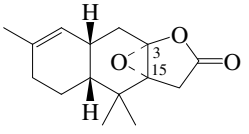


$C_{20}H_{28}O_4$ 332.439
Constit. of *Xenia florida*. Needles.
Mp 203-205°. $[\alpha]_D$ -36 (c, 0.09 in MeOH). λ_{max} 224 (log ϵ 4.18) (MeOH).

Iwagawa, T. *et al., J. Nat. Prod.*, 2000, **63**, 468-472 (*isol, pmr, cmr*)

α-Epoxyfurodysin lactone E-328

[103202-17-1]

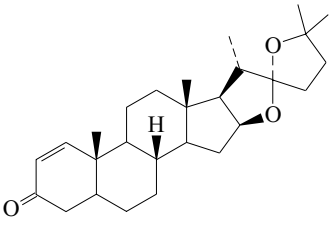


$C_{15}H_{20}O_3$ 248.321
Isol. from mollusc *Chromodoris funerea*.

3,15-Diepimer: ***β-Epoxyfurodysin lactone***
[103301-94-6]
$C_{15}H_{20}O_3$ 248.321
Isol. from mollusc *Chromodoris funerea*.

Carté, B. *et al., J.O.C.*, 1986, **51**, 3528-3532 (*isol, pmr*)

22,25-Epoxyfurost-1-en-3-one E-329

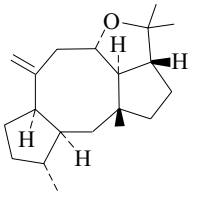


$C_{27}H_{40}O_3$ 412.611

(22*S*)-*form* [161776-72-3]
Constit. of *Alcyonium gracillimum*.
Cryst.
Mp 181-183°. $[\alpha]_D$ -20.7 (c, 0.5 in $CHCl_3$).

Seo, Y. *et al., Tetrahedron*, 1995, **51**, 2497 (*isol, pmr, cmr*)

9,8-Epoxy-7(17)-fusicoccene E-330



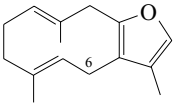
Absolute configuration

$C_{20}H_{32}O$ 288.472

9α-*form*
Epoxydictymene
[89002-20-0]
Constit. of brown alga *Dictyota dichotoma*.
Oil. $[\alpha]_D^{18}$ +78.1 (c, 0.9 in hexane).

Enoki, N. *et al., Tet. Lett.*, 1983, **24**, 4341-4342 (*Epoxydictymene, cryst struct*)
Jamison, T.F. *et al., J.A.C.S.*, 1994, **116**, 5505-5506 (*synth*)
Jamison, T.F. *et al., J.A.C.S.*, 1997, **119**, 4353-4363 (*synth*)
Paquette, L.A. *et al., J.A.C.S.*, 1997, **119**, 8438-8450 (*synth*)

8,12-Epoxy-1(10),4,7,11-germacratetraene E-331

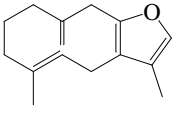


$C_{15}H_{20}O$ 216.322

(1(10)*E*,4*E*)-*form*
Furanodiene. *Isofuranodiene*
[19912-61-9]
Constit. of *Curcuma zedoaria* (zedoary) and *Stenocalyx michelii* (preferred genus name *Eugenia*). Isol. from gorgonians *Cespitularia* sp. and *Pseudopterogorgia* sp. Active against gram-positive bacteria and *Candida albicans*. Cryst.
Mp 66°. λ_{max} 220 (ϵ 11000) (EtOH).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1970, **18**, 752-755 (*isol, struct*)
Rücker, G. *et al., Phytochemistry*, 1971, **10**, 221 (*isol*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1980, **33**, 927-932 (*isol, pmr, cmr*)
Chan, W.R. *et al., Tetrahedron*, 1990, **46**, 1499-1502 (*isol, Pseudopterogorgia*)
Phan, M.G. *et al., Tap Chi Hoa Hoc*, 2000, **38**, 91-94 (*activity*)

8,12-Epoxy-4,7,10(15),11-germacratetraene E-332

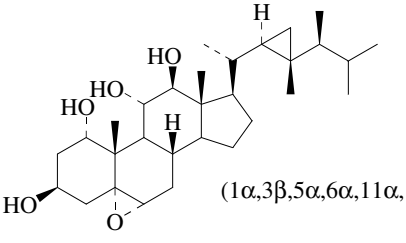


$C_{15}H_{20}O$ 216.322

(4*E*)-*form* [75222-51-4]
Constit. of *Clavularia inflata*.
Oil. λ_{max} 220 (ϵ 7000) (EtOH).

Bowden, B.F. *et al., Aust. J. Chem.*, 1980, **33**, 927-932 (*isol, pmr, cmr*)

5,6-Epoxygorgostane-1,3,11,12-tetrol E-333



(1α,3β,5α,6α,11α,12β,24*S*)-*form*

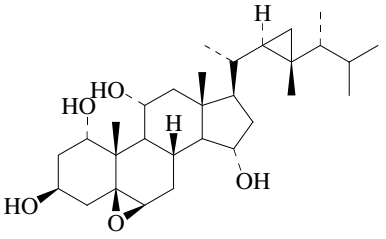
$C_{30}H_{50}O_5$ 490.722

(1α,3β,5α,6α,11α,12β,24*S*)-*form*
12-Ac: ***Isihippurol B***
[364599-48-4]
$C_{32}H_{52}O_6$ 532.759
Constit. of *Isis hippuris*. Amorph. powder. $[\alpha]_D^{25}$ +45.7 (c, 0.05 in MeOH).

(1α,3β,5β,6β,11α,12β)-*form*
12-Ac: [467227-42-5]
$C_{32}H_{52}O_6$ 532.759
Constit. of *Isis hippuris*. Amorph. solid. $[\alpha]_D$ -12.8 (c, 0.25 in $CHCl_3$).

Shen, Y.-C. *et al., Steroids*, 2001, **66**, 721-725 (*isol, pmr, cmr*)
Tanaka, J. *et al., Tetrahedron*, 2002, **58**, 6259-6266 (*isol, pmr, cmr*)

5,6-Epoxygorgostane-1,3,11,15-tetrol E-334

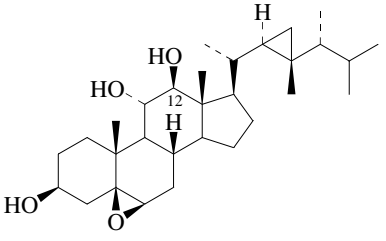


$C_{30}H_{50}O_5$ 490.722

(1α,3β,5β,6β,11α,15α)-*form*

11,15-Di-Ac: [467227-50-5]
$C_{34}H_{54}O_7$ 574.796
Constit. of *Isis hippuris*. Glass. $[\alpha]_D^{25}$ +32 (c, 0.04 in $CHCl_3$).
Tanaka, J. *et al., Tetrahedron*, 2002, **58**, 6259-6266 (*isol, pmr, cmr*)

5,6-Epoxygorgostane-3,11,12-triol E-335

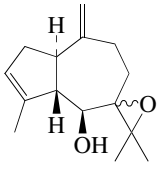


$C_{30}H_{50}O_4$ 474.723

(3β,5β,6β,11α,12β)-*form*

12-Ac: [467227-41-4]
$C_{32}H_{52}O_5$ 516.76
Constit. of *Isis hippuris*. Glass. $[\alpha]_D$ -8 (c, 0.23 in $CHCl_3$).
Tanaka, J. *et al., Tetrahedron*, 2002, **58**, 6259-6266 (*isol, pmr, cmr*)

7,11-Epoxy-3,10(14)-guaiadien-6-ol E-336



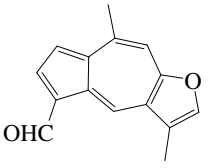
$C_{15}H_{22}O_2$ 234.338

(1α,5β,6β,7ξ)-*form* [160543-33-9]
Oil. $[\alpha]_D$ +84.1 (c, 0.82 in $CHCl_3$).

Ac:
$C_{17}H_{24}O_3$ 276.375
Constit. of *Nephthea chabroli*. Cryst. ($CHCl_3$/hexane).
Mp 178-180°. $[\alpha]_D$ +121 (c, 0.9 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 32-39 (*isol, pmr, cmr*)

8,12-Epoxy-1,3,5,7,9,11-guaiahexaen-15-al E-337

11-Formyllinderazulene (incorr.)
[835629-54-4]

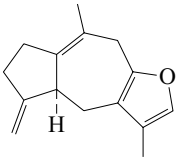


$C_{15}H_{12}O_2$ 224.259
Constit. of a *Paramuricea* sp. Pink solid.
Mp 136°. λ_{max} 215 (log ϵ 4.08); 260 (log ϵ 4.15); 293 (log ϵ 4.03); 316 (log ϵ 4.12); 332 (log ϵ 3.97); 395 (log ϵ 3.86) (MeOH).

15-Carboxylic acid: 8,12-Epoxy-1,3,5,7,9,11-guaiahexaen-15-oic acid
$C_{15}H_{12}O_3$ 240.258

15-Carboxylic acid, Me ester: 11-Carbomethoxylinderazulene (incorr.)
[835629-53-3]
$C_{16}H_{14}O_3$ 254.285
Constit. of a *Paramuricea* sp. Pink solid.
Mp 138-139°. λ_{max} 228 (log ϵ 4.05); 247 (log ϵ 4); 308 (log ϵ 4.3); 325 (log ϵ 4.07); 376 (log ϵ 3.8); 389 (log ϵ 3.92) (MeOH).
Reddy, N.S. *et al., J. Nat. Prod.*, 2005, **68**, 248-250 (*isol, pmr, cmr*)

8,12-Epoxy-1(10),4(15),7,11-guaiatetraene E-338

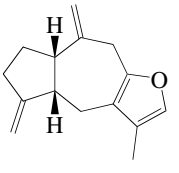


$C_{15}H_{18}O$ 214.307

5α-*form*

***Echinofuran*†**
Constit. of *Echinogorgia praelonga*.
Oil. $[\alpha]_D^{20}$ -91 (c, 0.138 in $CHCl_3$). Not registered in CA.
Tanaka, J.-I. *et al., J. Nat. Prod.*, 1992, **55**, 1522 (*isol, pmr, cmr*)
Yim, H.-K. *et al., Tetrahedron*, 2003, **59**, 1877-1884 (*synth*)

8,12-Epoxy-4(15),7,10(14),11-guaiatetraene E-339



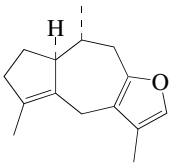
$C_{15}H_{18}O$ 214.307

(1β,5β)-*form*

Bebryazulene
[213818-05-4]
Constit. of *Bebryce grandicalyx*.
Oil. λ_{max} 230 (ϵ 5890); 279 (ϵ 1113) (MeOH).
Aknin, M. *et al., J. Nat. Prod.*, 1998, **61**, 1286-1287 (*isol, pmr, cmr*)

8,12-Epoxy-4,7,11-guaiatriene E-340

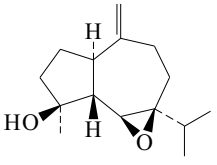
Furano-4-guaiene



$C_{15}H_{20}O$ 216.322

(1α,10α)-*form* [185014-59-9]
Constit. of *Pseudopterogorgia americana*.
Unstable yellow oil.
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 207-211 (*isol, pmr, cmr*)

6,7-Epoxy-10(14)-guaien-4-ol E-341



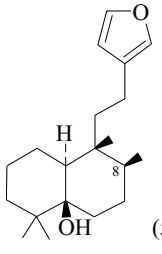
$C_{15}H_{24}O_2$ 236.353
Abs. config. revised in 1994.

(1α,4β,5β,6β,7β)-*form*
Orientalol C
[147511-74-8]
Constit. of *Alisma orientale* and *Nephthea chabrolii*.
Oil. $[\alpha]_D^{20}$ +2.5 (c, 0.56 in MeOH).

[147511-75-9, 290819-12-4]

Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2582; 1994, **42**, 1813 (*isol, pmr, cmr*)
Rao, M.R. *et al., J. Chem. Res., Synop.*, 2000, 245-247 (*isol, pmr, cmr*)

15,16-Epoxy-13(16),14-halimadien-5-ol E-342



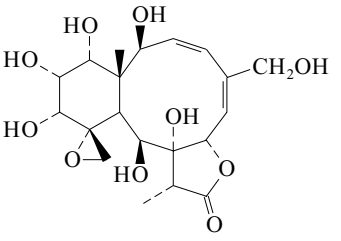
(5β,8α*H*)−*form*

$C_{20}H_{32}O_2$ 304.472

(5β,8α*H*)-*form*
Ambliol B
[76215-27-5]
Constit. of *Dysidea amblia*. Ichthyotoxin. Algicide. Oil. Sol. MeOH, $CHCl_3$, Et_2O; poorly sol. H_2O. $[\alpha]_D^{20}$ -3.4 (c, 1.5 in $CHCl_3$). λ_{max} 214 (ϵ 5260) (MeOH) (Berdy).

(5β,8β*H*)-*form*
Ambliol C
[93601-06-0]
From *Dysidea amblia*. Ichthyotoxin. Algicide. Cryst. (hexane). Sol. MeOH, $CHCl_3$, Et_2O; poorly sol. H_2O.
Mp 45-46°. $[\alpha]_D$ -37.8 (c, 2 in $CHCl_3$).
Walker, R.P. *et al., J.O.C.*, 1981, **46**, 1098; 1984, **49**, 5160 (*isol, struct*)
Piers, E. *et al., Chem. Comm.*, 1989, 1222 (*synth*)

11,20-Epoxy-2,8,9,12,13,14,16-heptahydroxy-3,5-briaradien-18,7-olide E-343



$C_{20}H_{28}O_{10}$ 428.435

2,9,13-Tri-Ac: ***Juncin Q***
[799804-61-8]
$C_{26}H_{34}O_{13}$ 554.547
Constit. of *Junceella juncea*. Powder. $[\alpha]_D$ -14 (c, 0.4 in Py). λ_{max} 274 (MeOH).

2,9,12,13,14-Penta-Ac: ***Juncenolide C***
[498556-53-9]
$C_{30}H_{38}O_{15}$ 638.621
Constit. of *Junceella juncea*. Amorph. solid. $[\alpha]_D^{25}$ -24.4 (c, 0.05 in CH_2Cl_2). λ_{max} 276 (log ϵ 2.5) (MeOH).

2,9,12,13,14-Penta-Ac, 16-Me ether: ***Juncenolide D***
[498556-54-0]
$C_{31}H_{40}O_{15}$ 652.648
Constit. of *Junceella juncea*. Amorph. solid. $[\alpha]_D^{25}$ -10.3 (c, 0.2 in CH_2Cl_2). λ_{max} 274 (log ϵ 2.54) (MeOH).

9,12,13,14,16-Penta-Ac: ***Gemmacolide F***
[134915-03-0]
$C_{30}H_{38}O_{15}$ 638.621
Constit. of *Junceella gemmacea*. Oil. $[\alpha]_D$ -3.8 (c, 0.32 in $CHCl_3$).

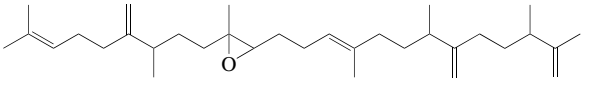
13-(2-Methylbutanoyl), 2,9,12,14,16-penta-Ac: ***Juncin I***
[524741-50-2]
$C_{35}H_{46}O_{16}$ 722.739
Constit. of *Junceella juncea*. Amorph. powder. $[\alpha]_D^{25}$ -40.6 (c, 0.48 in $CHCl_3$).

12,13-Bis(2-methylbutanoyl), 2,9,14,16-tetra-Ac: ***Juncin J***
[524741-51-3]
$C_{38}H_{52}O_{16}$ 764.819
Constit. of *Junceella juncea*. Amorph. powder. $[\alpha]_D^{25}$ -22.4 (c, 0.38 in $CHCl_3$).

He, H. *et al., Tetrahedron*, 1991, **47**, 3271 (*Gemmacolide F*)
Shen, Y.-C. *et al., J. Nat. Prod.*, 2003, **66**, 302-305 (*Juncenolides*)
Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 2003, **66**, 507-510 (*Juncins*)
Qi, S.-H. *et al., J. Nat. Prod.*, 2004, **67**, 1907-1910 (*Juncin Q*)

14,15-Epoxy-2,3,7,10,15,18,23-heptamethyl-6,19-dimethylene-1,10,22-tetracosatriene E-344

[188554-71-4]

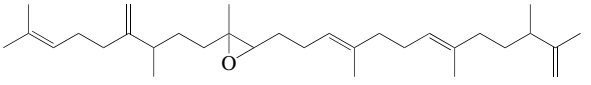


$C_{33}H_{56}O$ 468.805
Constit. of *Botryococcus braunii*.

Delahais, V. *et al., Phytochemistry*, 1997, **44**, 671-678 (*isol, pmr, cmr, ms*)

14,15-Epoxy-2,3,6,10,15,18,23-heptamethyl-19-methylene-1,6,10,22-tetracosatetraene E-345

[188554-70-3]



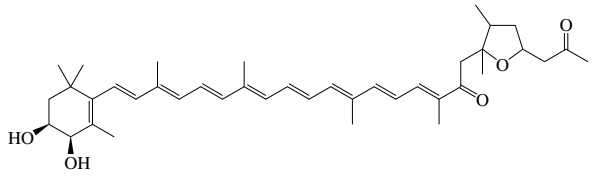
$C_{32}H_{54}O$ 454.778

Constit. of *Botryococcus braunii*.

Delahais, V. *et al., Phytochemistry*, 1997, **44**, 671-678 (*isol, pmr, cmr, ms*)

3′,6′-Epoxy-1′,2′,5′,6′,7′,8′-hexahydro-3,4-dihydroxy-6′-methyl-16′-nor-β,ϕ-carotene-1′,8′-dione E-346

[870188-34-4]

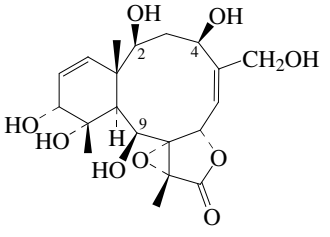


$C_{40}H_{56}O_5$ 616.879

Constit. of the oyster *Crassostrea gigas*. Red solid. λ_{max} 450; 470 (Et_2O).

Maoka, T. *et al., Chem. Pharm. Bull.*, 2005, **53**, 1207-1209 (*Crassostrea gigas constit*)

8,17-Epoxy-2,4,9,11,12,16-hexahydroxy-5,13-briaradien-18,7-olide E-347



$C_{20}H_{28}O_9$ 412.436

(2β,4β,5*E*,7α,8α,9β,11α,12α,17α)-*form*

4-Hexanoyl, 2,9-di-Ac: ***Briarlide M***

[845641-23-8]

$C_{30}H_{42}O_{12}$ 594.655

Constit. of a *Briareum* sp. Amorph. solid. $[\alpha]_D$ +52 (c, 0.06 in MeOH).

4-Octanoyl, 2,9-di-Ac: ***Violide N***

[299926-24-2]

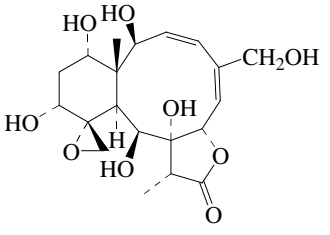
$C_{32}H_{46}O_{12}$ 622.708

Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ -2.3 (c, 0.1 in MeOH). λ_{max} 206 (log ϵ 3.85) (MeOH).

Iwagawa, T. *et al., Heterocycles*, 2000, **53**, 1789-1792 (*Violide N*)

Iwagawa, T. *et al., J. Nat. Prod.*, 2005, **68**, 31-35 (*Briarlide M*)

11,20-Epoxy-2,8,9,12,14,16-hexahydroxy-3,5-briaradien-18,7-olide E-348



$C_{20}H_{28}O_9$ 412.436

(2β,3*Z*,5*E*,7α,8α,9β,11α,12α,14α)-*form*

12,14-Bis(2-methylbutanoyl), 2,9,16-tri-Ac: ***Juncin K***

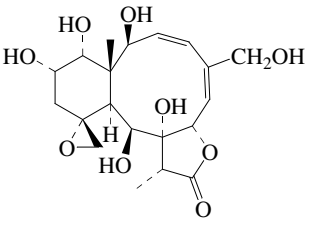
[524741-52-4]

$C_{36}H_{50}O_{14}$ 706.783

Constit. of *Junceella juncea*. Amorph. powder. $[\alpha]_D^{25}$ -61.7 (c, 0.06 in $CHCl_3$).

Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 2003, **66**, 507-510 (*isol, pmr, cmr*)

11,20-Epoxy-2,8,9,13,14,16-hexahydroxy-3,5-briaradien-18,7-olide E-349



$C_{20}H_{28}O_9$ 412.436

(2β,3*Z*,5*E*,7α,8α,9β,11α,13α,14α)-*form*

2,9,13,14-Tetra-Ac: ***Juncenolide B***

[498556-52-8]

$C_{28}H_{36}O_{13}$ 580.585

Constit. of *Junceella juncea*. Amorph. solid. $[\alpha]_D^{25}$ -12.4 (c, 0.4 in MeOH). λ_{max} 275 (log ϵ 2.52) (MeOH).

2-(3-Methylbutanoyl), 9,13,14-tri-Ac: ***Juncenolide E***

[680608-91-7]

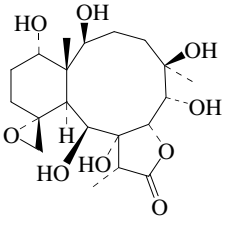
$C_{31}H_{42}O_{13}$ 622.665

Constit. of *Junceella juncea*. Amorph. solid. $[\alpha]_D^{25}$ -2.1 (c, 0.2 in CH_2Cl_2). λ_{max} 275 (log ϵ 3.45) (no solvent reported).

Shen, Y.-C. *et al., J. Chin. Chem. Soc. (Taipei)*, 2003, **50**, 1267-1270; *CA*, **140**, 335909v (*Juncenolide E*)

Shen, Y.-C. *et al., J. Nat. Prod.*, 2003, **66**, 302-305 (*isol, pmr, cmr*)

11,20-Epoxy-2,5,6,8,9,14-hexahydroxy-18,7-briaranolide E-350



$C_{20}H_{32}O_9$ 416.467

(2β,5β,6α,7α,8α,9β,11α,14α,17α)-*form*

2,9,14-Tri-Ac: ***Junceellolide L***

[881418-04-8]

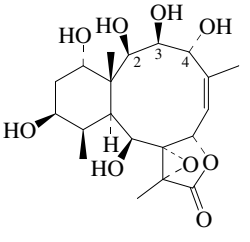
$C_{26}H_{38}O_{12}$ 542.579

Constit. of *Junceella fragilis*. Powder.

Mp 243-245°. $[\alpha]_D^{25}$ +43 (c, 0.7 in $CHCl_3$).

Sheu, J.-H. *et al., J. Nat. Prod.*, 2006, **69**, 269-273,

8,17-Epoxy-2,3,4,9,12,14-hexahydroxy-5-briaren-18,7-olide E-351



$C_{20}H_{30}O_9$ 414.452

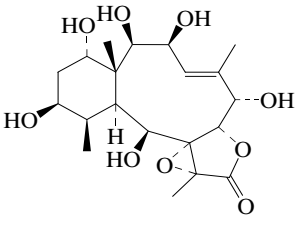
(2β,3β,4α,5*Z*,7α,8α,9β,12β,14α,17α)-*form*

4-Butanoyl, 2,9,14-tri-Ac: ***Briaexcavatolide P***
[383414-37-7]
$C_{30}H_{42}O_{13}$ 610.654
Constit. of *Briareum excavatum*. Cryst.
Mp 248-251°. $[\alpha]_D^{27}$ +167 (c, 1 in $CHCl_3$).

4-Butanoyl, 3,9,14-tri-Ac: ***Briaexcavatolide O***
[383414-36-6]
$C_{30}H_{42}O_{13}$ 610.654
Constit. of *Briareum excavatum*. Cryst.
Mp 281-284°. $[\alpha]_D^{27}$ +165 (c, 0.9 in $CHCl_3$).

4-Butanoyl, 2,9,12,14-tetra-Ac: ***Briaexcavatolide Q***
[383414-38-8]
$C_{32}H_{44}O_{14}$ 652.691
Constit. of *Briareum excavatum*. Powder.
Mp 204-206°. $[\alpha]_D^{27}$ +253 (c, 0.1 in $CHCl_3$).
Wu, S.-L. *et al., J. Nat. Prod.*, 2001, **64**, 1415-1420 (*isol, pmr, cmr, cryst struct*)

8,17-Epoxy-2,3,6,9,12,14-hexahydroxy-4-briaren-18,7-olide E-352

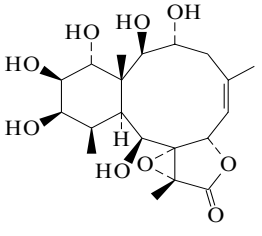


$C_{20}H_{30}O_9$ 414.452

(2β,3β,4*E*,6α,7α,8α,9β,12β,14α,17α)-*form*

2,3,9,14-Tetra-Ac: ***Fragilide A***
[732295-59-9]
$C_{28}H_{38}O_{13}$ 582.6
Constit. of *Junceella fragilis*. Powder.
Mp >300°. $[\alpha]_D^{25}$ +68.2 (c, 0.4 in $CHCl_3$).
Sung, P.-J. *et al., Bull. Chem. Soc. Jpn.*, 2004, **77**, 1229-1230 (*isol, pmr, cmr*)

8,17-Epoxy-2,3,9,12,13,14-hexahydroxy-5-briaren-18,7-olide E-353

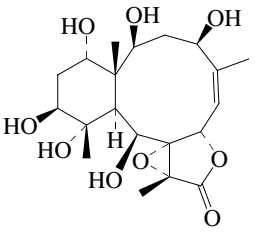


$C_{20}H_{30}O_9$ 414.452

(2β,3α,5*Z*,7α,8α,9β,12β,13β,15α,17α)-*form*

2,3,9,14-Tetra-Ac: ***Stecholide N***
[152340-01-7]
$C_{28}H_{38}O_{13}$ 582.6
Constit. of *Solenopodium excavatum*. Glass. $[\alpha]_D^{20}$ -53 (c, 0.2 in $CHCl_3$).
Schmitz, F.J. *et al., J. Nat. Prod.*, 1993, **56**, 1339 (*isol, pmr, cmr*)

8,17-Epoxy-2,4,9,11,12,14-hexahydroxy-5-briaren-18,7-olide E-354

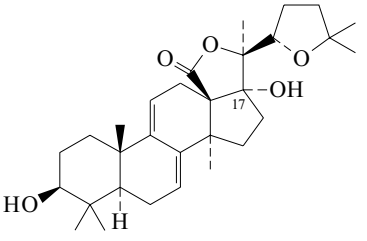


$C_{20}H_{30}O_9$ 414.452

(2β,4β,5*Z*,7α,8α,9β,11α,12β,14α,17α)-*form*

2,4,9,14-Tetra-Ac: ***Briaexcavatolide U***
[593279-01-7]
$C_{28}H_{38}O_{13}$ 582.6
Constit. of *Briareum excavatum*. Powder.
Mp 110-111°. $[\alpha]_D^{27}$ +48 (c, 0.1 in $CHCl_3$).
Wu, S.-L. *et al., J. Nat. Prod.*, 2003, **66**, 1252-1256 (*isol, pmr, cmr*)

22,25-Epoxyholosta-7,9(11)-diene-3,17-diol E-355



$C_{30}H_{44}O_5$ 484.675

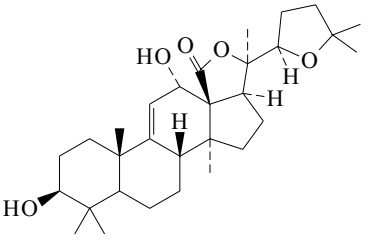
(3β,20*R*,22*R*)-*form*

22,25-Epoxyholothurinogenin. 22,25-Oxidoholothurinogenin
[6853-99-2]
Aglycone from *Holothuria polii* and *Holothuria atra*.
Cryst. (EtOAc).
Mp 315.2-315.8°. $[\alpha]_D^{25}$ -21.2 ($CHCl_3$).

3-Ac: Mp 289-290°. $[\alpha]_D$ +5.5 ($CHCl_3$). Artifact arising from rearrangements of genuine aglycones present in the glycoside mixture Holothurin A.

17-Deoxy: 22,25-Epoxyholosta-7,9(11)-dien-3-ol. 17-Deoxy-22,25-epoxyholothurinogenin
[6758-71-0]
Aglycone from *Holothuria polii*.
Cryst. (MeOH).
Mp 285.8-286.4°. $[\alpha]_D^{25}$ -9.3. Other genins were obt. by enzymic hydrol. of desulfated Holothurin A by Chanley, *et al.*
Chanley, J.D. *et al., Tetrahedron*, 1966, **22**, 1857; 1969, **25**, 1911
Habermehl, G. *et al., Annalen*, 1970, **731**, 53 (*isol*)
Delia, T.J. *et al., Toxicon*, 1977, **15**, 401 (*isol, struct*)

22,25-Epoxyholost-9(11)-ene-3,12-diol E-356



$C_{30}H_{46}O_5$ 486.69

(3β,12α,20*R*,22*R*)-*form*

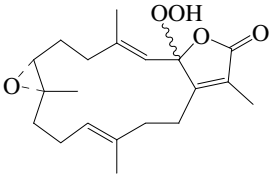
3-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Holothurinoside D***
[136024-80-1]
$C_{41}H_{64}O_{13}$ 764.949
Constit. of *Holothuria forskalii*. Antitumour and antiviral agent.
Cryst.
Mp 219-221°.

3-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Holothurin B_3***
[852469-37-5]
$C_{41}H_{64}O_{16}S$ 845.013
Constit. of *Holothuria polii*. Cryst.
Mp 245°. $[\alpha]_D^{20}$ -18 (c, 0.1 in Py).

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Holothurinoside C***
[136024-79-8]
$C_{54}H_{86}O_{23}$ 1103.26
Constit. of *Holothuria forskalii*. Antitumour and antiviral agent.
Cryst.
Mp 223-225°.

Rodriguez, J. *et al., Tetrahedron*, 1991, **47**, 4753-4762 (*isol, pmr, cmr*)
Silchenko, A.S. *et al., J. Nat. Prod.*, 2005, **68**, 564-567 (*Holothurin B_3*)

7,8-Epoxy-2-hydroperoxy-1(15),3,11-cembratrien-16,2-olide E-357

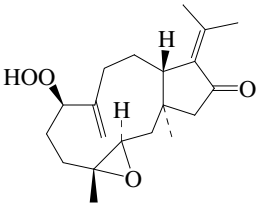


$C_{20}H_{28}O_5$ 348.438

(2ξ,3*E*,7*S*,8*S*,11*E*)-*form*
2-Hydroperoxysarcophine
[882302-75-2]
Constit. of *Lobophytum crassum*.
Cryst.
Mp 101-103°. $[\alpha]_D^{20}$ -153 (c, 1.15 in Me_2CO). λ_{max} 212 (log ϵ 1.11) (Me_2CO).

Yin, S.-W. *et al., Helv. Chim. Acta*, 2006, **89**, 567-572 (*2-Hydroperoxysarcophine*)

3,4-Epoxy-7-hydroperoxy-8(17),12(18)-dolabelladien-13-one E-358

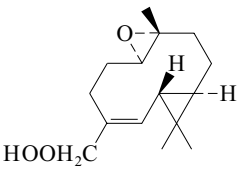


$C_{20}H_{30}O_4$ 334.455

(3*R*,4*R*,7*R*)-*form* [404913-77-5]
Constit. of a *Clavularia* sp.
Cryst. $[\alpha]_D^{25}$ +111.8 (c, 0.17 in $CHCl_3$).

Iguchi, K. *et al., Bull. Chem. Soc. Jpn.*, 2002, **75**, 131-136 (*isol, pmr, cmr, cryst struct*)

1,10-Epoxy-15-hydroperoxy-4-lepidozene E-359

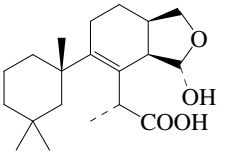


$C_{15}H_{24}O_3$ 252.353

(1α,4*E*,10α)-*form* [126979-95-1]
Constit. of *Anthopleura pacifica*.
Oil. $[\alpha]_D$ -143 (c, 0.12 in $CHCl_3$).

Zheng, G.-C. *et al., J.O.C.*, 1990, **55**, 3677 (*isol, pmr, cmr*)

15,16-Epoxy-15-hydroxy-8-aplysulphuren-17-oic acid E-360



$C_{20}H_{32}O_4$ 336.47

15α-*form*

Me ether: ***15,16-Epoxy-15-methoxy-8-aplysulphuren-17-oic acid***
[676348-93-9]
$C_{21}H_{34}O_4$ 350.497
Constit. of *Dendrilla membranosa*. Oil. $[\alpha]_D^{25}$ +12 (c, 0.25 in $CHCl_3$).

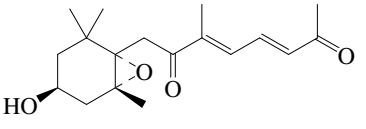
17→15 Lactone: ***15,16-Epoxy-8-aplysulphuren-17,15-olide***
[676348-94-0]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Dendrilla membranosa*. Oil.

15-Ketone (lactone), Me ester: ***Methyl 8-aplysulphuren-15,16-olid-17-oate***
[676348-92-8]
$C_{21}H_{32}O_4$ 348.481
Constit. of *Dendrilla membranosa*. Oil. $[\alpha]_D^{25}$ -30 (c, 0.1 in $CHCl_3$).

Díaz-Marrero, A.R. *et al., Tetrahedron*, 2004, **60**, 1073-1078 (*isol, pmr, cmr*)

5,6-Epoxy-3-hydroxy-13-apo-β-carotene-8,13-dione E-361

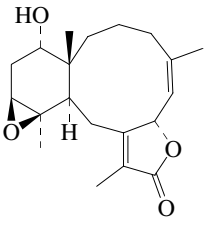
[835925-59-2]



$C_{18}H_{26}O_4$ 306.401
Constit. of *Scytosiphon lomentaria*. Yellow oil. $[\alpha]_D$ +34.1 (c, 0.02 in EtOH).

Mori, K. *et al., Mar. Drugs*, 2004, **2**, 63-72 (*isol, pmr, cmr*)

11,12-Epoxy-14-hydroxy-5,8(17)-briaradien-18,7-olide E-362

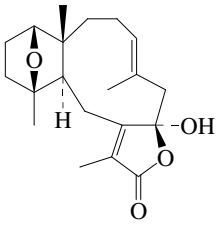


$C_{20}H_{28}O_4$ 332.439

(5*Z*,7α,11β,12β,14α)-*form*

14-Ac: ***Briviolide G***
[868526-14-1]
$C_{22}H_{30}O_5$ 374.476
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ -42 (c, 0.06 in MeOH). λ_{max} 219 (ϵ 13600) (no solvent reported).
Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 2083-2093 (*Briviolide G*)

11,14-Epoxy-7-hydroxy-4,8(17)-briaradien-18,7-olide E-363



(4*E*,7α*OH*,11β,14β)-*form*

$C_{20}H_{28}O_4$ 332.439

(4*E*,7α*OH*,11β,14β)-*form*

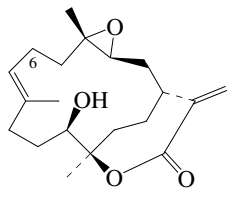
Pachyclavulariolide B
[325691-33-6]
Constit. of *Pachyclavularia violacea*.
Cryst. (C_6D_6).
Mp 152.3-154.6°. $[\alpha]_D$ +23.1 (c, 0.28 in MeOH).

Me ether: ***Pachyclavulariolide C***
[325691-34-7]
$C_{21}H_{30}O_4$ 346.466
Constit. of *Pachyclavularia violacea*. Amorph. solid. $[\alpha]_D$ +11.1 (c, 0.42 in MeOH).

(4*E*,7β*OH*,11β,14β)-*form*

Me ether: ***Pachyclavulariolide D***
[325691-35-8]
$C_{21}H_{30}O_4$ 346.466
Constit. of *Pachyclavularia violacea*. Amorph. solid. $[\alpha]_D$ +12.1 (c, 0.32 in MeOH).
Xu, L. *et al., Tetrahedron*, 2000, **56**, 9031-9037 (*isol, pmr, cmr, cryst struct*)

3,4-Epoxy-11-hydroxy-7,15(17)-cembradien-16,12-olide E-364



(1*R*,3*S*,4*S*,7*E*,11*R*,12*R*)-*form*

$C_{20}H_{30}O_4$ 334.455

(1*R*,3*S*,4*S*,7*E*,11*R*,12*R*)-*form*

11-Episinulariolide
[88643-48-5]
Constit. of *Sinularia flexibilis* and *Planaxis sulcatus*. Algicide.
Cryst.
Mp 166.5-168.5°. $[\alpha]_D$ +19.7 (c, 0.5 in MeOH).

Ac: ***11-Episinulariolide acetate***
$C_{22}H_{32}O_5$ 376.492
Constit. of *Sinularia flexibilis*. Cryst.
Mp 161-163°. $[\alpha]_D$ -25 (c, 3.7 in $CHCl_3$). λ_{max} 202 (ϵ 23990) (MeOH) (Berdy).

(1*R*,3*S*,4*S*,7*E*,11*S*,12*R*)-*form*

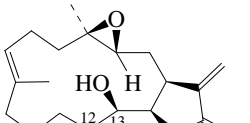
Sinulariolide
[56326-25-1]
Constit. of *Sinularia flexibilis* and *Sinularia capillosa*. Shows cytotoxic activity and inhibits gram-positive bacteria. Cryst. (C_6H_6).
Mp 170-173°. $[\alpha]_D$ +76 (c, 0.7 in MeOH). λ_{max} 212 (ϵ 5000) (MeOH) (Derep).

11-Ketone: 3,4-Epoxy-11-oxo-7,15(17)-cembradien-16,12-olide. ***11-Dehydrosinulariolide***
[62824-08-2]
Constit. of *Sinularia flexibilis*.
Cryst. (Et_2O).
Mp 120°. $[\alpha]_D$ +87 (EtOH).

6ξ-Hydroxy: 3,4-Epoxy-6,11-dihydroxy-7,15(17)-cembradien-16,12-olide. ***6-Hydroxysinulariolide***
[62824-07-1]
$C_{20}H_{30}O_5$ 350.454
Constit. of *Sinularia flexibilis*. Cryst. (Et_2O).
Mp 192-194°. $[\alpha]_D$ +54.5 (c, 0.45 in $CHCl_3$).

Tursch, B. *et al., Tetrahedron*, 1975, **31**, 129 (*isol, struct*)
Herin, M. *et al., Bull. Soc. Chim. Belg.*, 1976, **85**, 707 (*isol*)
Karlsson, R. *et al., Acta Cryst. B*, 1977, **33**, 2027-2031 (*Sinulariolide, cryst struct*)
Kashman, Y. *et al., Isr. J. Chem.*, 1977, **16**, 1-3 (*11-Episinulariolide acetate*)
Weinheimer, A.J. *et al., Tet. Lett.*, 1977, **18**, 2923-2926 (*abs config*)
Mori, K. *et al., Chem. Lett.*, 1983, 1515 (*isol*)
Sanduja, R. *et al., J. Nat. Prod.*, 1986, **49**, 718-719 (*11-Episinulariolide, isol*)
Michalek, K. *et al., J. Chem. Ecol.*, 1997, **23**, 259-273 (*activity*)
Aceret, T.L. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1998, **120**, 121-126; *CA*, **130**, 2118w (*Sinulariolide, isol, activity*)
Roulin Yang, J.S. *et al., J. Nat. Prod.*, 2000, **63**, 1543-1545 (*Sinulariolide, activity*)
Hsieh, P.-W. *et al., Nat. Prod. Res.*, 2003, **17**, 409-418 (*11-Episinulariolide acetate, cmr, cryst struct*)

3,4-Epoxy-13-hydroxy-7,15(17)-cembradien-16,14-olide E-365



(1*S*,3*R*,4*R*,7*E*,12*R*,13*R*,14*R*)-*form*

$C_{20}H_{30}O_4$ 334.455

(1*S*,3*R*,4*R*,7*E*,12*R*,13*R*,14*R*)-*form*

Ac: ***12-Epieupalmerin acetate***
[149343-53-3]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Eunicea succinea*. Oil. $[\alpha]_D^{25}$ +17.8 (c, 0.9 in $CHCl_3$). λ_{max} 242 (ϵ 660) (MeOH) (Berdy).

13-Ketone: ***12-Epieupalmerone****. Sarcophyocrassolide B. Sarcocrassolide B*
[149270-77-9]
[587873-85-6]
$C_{20}H_{28}O_4$ 332.439
Constit. of *Eunicea pinta* and *Sarcophyton crassocaule*. Cryst.
Mp 96-97° Mp 92°. $[\alpha]_D^{25}$ -25.9 (c, 1 in $CHCl_3$).

(1*S*,3*R*,4*R*,7*E*,12*R*,13*S*,14*R*)-*form*

12,13-Bisepieupalmerin. *12,13-Diepieupalmerin*
[92693-30-6]
Constit. of *Eunicea succinea*.
Cryst. (C_6H_6).
Mp 144-145°. $[\alpha]_D$ -158.8 (c, 1.57 in $CHCl_3$).

Ac: ***12,13-Bisepieupalmerin acetate***
[149343-52-2]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Eunicea succinea*. Oil. $[\alpha]_D^{27}$ -170 (c, 0.4 in $CHCl_3$). λ_{max} 242 (ϵ 1040) (MeOH) (Berdy).

*7*S,*8*R-*Epoxide:* ***12,13-Diepieupalmerin epoxide***
[200271-83-6]
$C_{20}H_{30}O_5$ 350.454
Constit. of *Eunicea succinea*. Oil. $[\alpha]_D^{25}$ -13.2 (c, 4.4 in $CHCl_3$). λ_{max} 208 (ϵ 11400) (MeOH).

13-Ketone: 3,4-Epoxy-13-oxo-7,15(17)-cembradien-16,14-olide.
Succinolide
[149404-02-4]
$C_{20}H_{28}O_4$ 332.439
Constit. of *Eunicea succinea*. Oil. $[\alpha]_D^{25}$ -7.5 (c, 0.8 in $CHCl_3$). Struct. revised in 2002. λ_{max} 214 (ϵ 5260) (MeOH) (Berdy).

(1*S*,3*R*,4*R*,7*E*,12*S*,13*R*,14*R*)-*form*

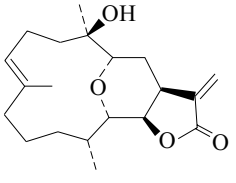
Eupalmerin
[52239-68-6]
Metab. of *Eunicea mammosa*.
Cryst.
Mp 148-149°. $[\alpha]_D^{27}$ -79.3 (c, 1.36 in $CHCl_3$). λ_{max} 242 (ϵ 831) ($CHCl_3$) (Berdy).

Ac: ***Eupalmerin acetate***
[37299-08-4]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Eunicea palmari*. Algicide. λ_{max} 210 (ϵ 10000) (MeOH) (Derep). λ_{max} 242 (ϵ 300) ($CHCl_3$) (Derep).

13-Ketone: ***Eupalmerone***
[149404-03-5]
Constit. of *Eunicea mammosa*.
Cryst.
Mp 159-160°.

Ealick, S.E. *et al., Acta Cryst. B*, 1975, **31**, 1618-1626 (*Eupalmerin acetate, cryst struct*)
Gopichand, Y. *et al., J. Nat. Prod.*, 1984, **47**, 607-614 (*12,13-Bisepieupalmerin*)
Fontán, L.A. *et al., J.O.C.*, 1990, **55**, 4956-4960 (*Eupalmerin acetate, pmr, cmr*)
Fontán, L.A. *et al., J. Nat. Prod.*, 1991, **54**, 298-301 (*Eupalmerin, isol*)
Rodríquez, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 564-570 (*Eunicea succinea constits, isol, pmr, cmr*)
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 1101-1113 (*Eupalmerone*)
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1998, **61**, 40-45 (*12,13-Diepieupalmerin epoxide*)
Shi, Y.-P. *et al., J. Nat. Prod.*, 2002, **65**, 1232-1241 (*12-Epieupalmerone, Succinolide, cryst struct*)
Xu, X.-H. *et al., Chin. J. Chem.*, 2003, **21**, 1506-1509 (*Sarcophyocrassolide B*)
Xu, X.H. *et al., Gaodeng Xuexiao Huaxue Xuebao*, 2003, **24**, 1023-1025; *CA*, **139**, 211011 (*Sarcocrassolide B*)

3,13-Epoxy-4-hydroxy-7,15(17)-cembradien-16,14-olide E-366



$C_{20}H_{30}O_4$ 334.455

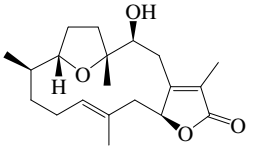
(1*S*,3*S*,4*R*,7*E*,12*R*,13*S*,14*R*)-*form*

Eunicin
[22551-45-7]
Constit. of the gorgonian *Eunicea mammosa*. Antibacterial and cytotoxic. Algicide. Cryst.
Mp 154-155.5°. $[\alpha]_D^{29}$ -95 (c, 2.0 in EtOH). λ_{max} 212 (ϵ 10000) (MeOH) (Derep).

Ac: [22465-64-1]
Cryst. Mp 157°.

Westheimer, A.J. *et al., Chem. Comm.*, 1968, 384 (*struct*)
Hossain, M.B. *et al., Chem. Comm.*, 1968, 385 (*struct, abs config*)
Gampe, R.T. *et al., J.A.C.S.*, 1984, **106**, 1823 (*cmr*)
Morales, G.A. *et al., Acta Cryst. C*, 1996, **52**, 1272 (*cryst struct*)

4,7-Epoxy-3-hydroxy-1(15),11-cembradien-16,14-olide E-367



(3*R**,4*S**,7*R**,8*S**,11*E*,14*R**)-*form*

$C_{20}H_{30}O_4$ 334.455

(3*R,4*S**,7R*,8*S**,11*E*,14*R**)-*form***

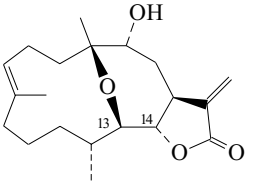
Pachyclavulariolide N
[551938-77-3]
Constit. of *Pachyclavularia violacea*.
Solid.
Mp 108-110°. $[\alpha]_D^{31}$ -26 (c, 0.23 in $CHCl_3$). λ_{max} 215 (ϵ 9585) (EtOH aq.).

(3*R,4*S**,7*R**,8*S**,11*Z*,14*R**)-*form***

Pachyclavulariolide O
[551938-78-4]
Constit. of *Pachyclavularia violacea*.
Gum. $[\alpha]_D^{26}$ -2 (c, 0.09 in $CHCl_3$). λ_{max} 210 (ϵ 8650) (EtOH aq.).

Sheu, J.-H. *et al., J. Nat. Prod.*, 2003, **66**, 662-666 (*isol, pmr, cmr*)

4,13-Epoxy-3-hydroxy-7,15(17)-cembradien-16,14-olide E-368



(1*S*,3*R*,4*S*,12*R*,13*R*,14*S*)–*form*

$C_{20}H_{30}O_4$ 334.455

(1*S*,3*R*,4*S*,12*R*,13*R*,14*S*)-*form*

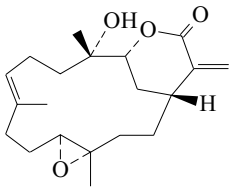
13α*H,*14β*H-Jeunicin
Constit. of the gorgonian *Eunicea mammosa*. Shows cytotoxic props. Cryst. Poorly sol. hexane.
Mp 147-147.5°. $[\alpha]_D^{20}$ -31.1 (c, 3.0 in $CHCl_3$).

(1*S*,3*R*,4*S*,12*R*,13*R*,14*R*)-*form*

Jeunicin
[28028-66-2]
Constit. *Eunicea mammosa* and *Planaxis sulcatus*. Cytotoxic. Cryst. Poorly sol. hexane.
Mp 139-141°. $[\alpha]_D^{27}$ +12.8 (c, 0.75 in $CHCl_3$).

Van der Helm, D. *et al., Acta Cryst. B*, 1976, **32**, 1558 (*cryst struct*)
Westheimer, A.J. *et al., Acta Cryst. B*, 1982, **38**, 580 (*cryst struct*)
Sanduja, R. *et al., J. Het. Chem.*, 1986, **23**, 529-535 (*isol, Planaxis*)

11,12-Epoxy-4-hydroxy-7,15(17)-cembradien-16,3-olide E-369



$C_{20}H_{30}O_4$ 334.455

(1*R*,3*R*,4*S*,7*E*,11*S*,12*S*)-*form*

Sinularin. *Flexibilide*
[65669-72-9]
Constit. of *Sinularia flexibilis* and *Sinularia capillosa*. Shows potent cytotoxic and antiinflammatory activity. Inhibits gram-positive bacteria. Cryst. (Et_2O).
Mp 150-152°. $[\alpha]_D^{21}$ -115 (c, 1 in $CHCl_3$). λ_{max} 212 (ϵ 5000) (MeOH) (Derep).

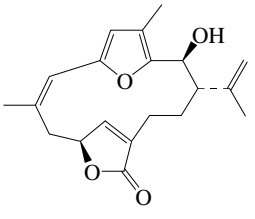
▶ JH5029600

15,17-Dihydro: 11,12-Epoxy-4-hydroxy-7-cembren-16,3-olide.
Dihydrosinularin. *Dihydroflexibilide*
[65669-71-8]
$C_{20}H_{32}O_4$ 336.47
Constit. of *Sinularia flexibilis* and mollusc *Planaxis sulcatus*.
Cryst. (toluene/hexane).
Mp 108-109°. $[\alpha]_D^{21}$ -44 (c, 1 in $CHCl_3$).

▶ Cytotoxic.

Weinheimer, A.J. *et al., Tet. Lett.*, 1977, 2923 (*Dihydrosinularin, cryst struct*)
Kazlauskas, R. *et al., Aust. J. Chem.*, 1978, **31**, 1817
Hossain, M.B. *et al., Acta Cryst. B*, 1979, **35**, 660 (*cryst struct*)
Sanduja, R. *et al., J. Nat. Prod.*, 1986, **49**, 718-719 (*Dihydrosinularin: isol*)
Aceret, T.L. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1998, **120**, 121-126 (*isol, activity*)
Yang, R.-L. *et al., Huaxue Xuebao*, 2000, **58**, 1186-1187 (*isol, activity*)
Yang, J.S. *et al., J. Nat. Prod.*, 2000, **63**, 1543-1545 (*activity*)
Lin, C.-W. *et al., Youji Huaxue*, 2001, **21**, 56-59 (*pmr, cmr*)

3,6-Epoxy-2-hydroxy-3,5,7,11,15-cembrapentaen-20,10-olide E-370



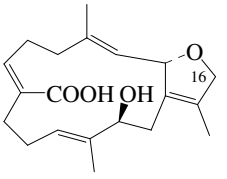
$C_{20}H_{24}O_4$ 328.407

(1*S*,2*S*,7*Z*,10*S*)-*form*

Bipinnatin J
[201742-79-2]
Constit. of *Pseudopterogorgia bipinnata*.
Cryst.
Mp 141-142° dec. $[\alpha]_D^{24}$ -125.4 (c, 1.65 in $CHCl_3$). λ_{max} 210 (ϵ 19800); 282 (ϵ 16600) (MeOH).

Rodriguez, A.D. *et al., J.O.C.*, 1998, **63**, 420-421 (*Bipinnatin J, cryst struct*)

2,16-Epoxy-13-hydroxy-1(15),3,7,11-cembratetraen-18-oic acid E-371



$C_{20}H_{28}O_4$ 332.439

(2*S*,3*E*,7*Z*,11*E*,13*S*)-*form*

Me ester: ***Sarcoglaucol***
[68299-89-8]
$C_{21}H_{30}O_4$ 346.466
Constit. of *Sarcophyton glaucum*. Ichthyotoxin. Cryst. (Et_2O).
Mp 150-152°. $[\alpha]_D^{22}$ +177 (c, 0.312 in MeOH). λ_{max} 206 (ϵ 26900) (MeOH) (Derep).

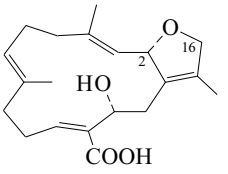
16-Oxo(lactone): 13-Hydroxy-1(15),3,7,11-cembratetraen-16,2-olid-18-oic acid

16-Oxo(lactone), Me ester: ***Sarcoglaucol-16-one***
[541509-69-7]
$C_{21}H_{28}O_5$ 360.449
Constit. of *Sarcophyton cherbonnieri*. Solid. $[\alpha]_D^{23}$ +119.8 (c, 0.26 in MeOH). λ_{max} 217 (ϵ 15260) (MeOH).

16-Oxo(lactone), 13-Ac, Me ester: ***16-Oxysarcoglaucol acetate***
[757954-41-9]
$C_{23}H_{30}O_6$ 402.486
Constit. of *Sarcophyton glaucum*. Oil. $[\alpha]_D^{25}$ +81 (c, 0.07 in $CHCl_3$).

Albericci, M. *et al., Bull. Soc. Chim. Belg.*, 1978, **87**, 487
Gross, H. *et al., Org. Biomol. Chem.*, 2003, **1**, 944-949 (*Sarcoglaucol-16-one*)
Feller, M. *et al., J. Nat. Prod.*, 2004, **67**, 1303-1308 (*16-Oxysarcoglaucol acetate*)
Gross, H. *et al., Org. Biomol. Chem.*, 2004, **2**, 1133-1138 (*abs config*)

2,16-Epoxy-13-hydroxy-1(15),3,7,11-cembratetraen-20-oic acid E-372



$C_{20}H_{28}O_4$ 332.439

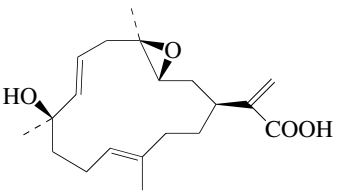
(2*S*,1(15)*Z*,3*E*,7*E*,11*Z*,13*R*)-*form*

Me ester:
$C_{21}H_{30}O_4$ 346.466
Constit. of a *Sarcophyton* sp. Cryst. (EtOAc/petrol).
Mp 141-142°. $[\alpha]_D^{23}$ +176 (c, 0.4 in $CHCl_3$). λ_{max} 206 (ϵ 26900) (MeOH) (Derep).

*16-Oxo, Me ester: Methyl 13*R*-hydroxy-1(15)Z,3*E*,7*E*,11Z-cembratetraen-16,25-olid-20-oate*
$C_{21}H_{28}O_5$ 360.449
Constit. of *Sarcophyton* sp. Oil. $[\alpha]_D^{20}$ +144 (c, 0.3 in $CHCl_3$). λ_{max} 207 (ϵ) (MeOH) (Derep).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 61

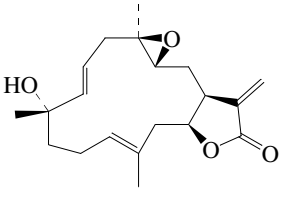
3,4-Epoxy-8-hydroxy-6,11,15(17)-cembratrien-16-oic acid E-373



$C_{20}H_{30}O_4$ 334.455

(1*S*,3*S*,4*R*,6*E*,8*R*,11*E*)-*form*
Uproeunioic acid
Me ester: ***Methyl uproeuniolate***
[198494-50-7]
$C_{21}H_{32}O_4$ 348.481
Constit. of *Eunicea succinea*. Oil. $[\alpha]_D^{25}$ -3.6 (c, 12.9 in $CHCl_3$).
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 1134-1138 (*isol, pmr, cmr*)

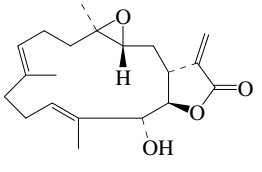
3,4-Epoxy-8-hydroxy-6,11,15(17)-cembratrien-16,14-olide E-374



$C_{20}H_{28}O_4$ 332.439

(1*S*,3*S*,4*R*,6*E*,8*S*,11*E*,14*S*)-*form*
Uproeuniolide
[200271-89-2]
Constit. of *Eunicea succinea*.
Oil. $[\alpha]_D^{25}$ -30.6 (c, 5 in $CHCl_3$). λ_{max} 212 (ϵ 3900) (MeOH).
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1998, **61**, 40-45 (*isol, pmr, cmr*)
Shi, Y.-P. *et al., J. Nat. Prod.*, 2002, **65**, 1232-1241 (*struct*)

3,4-Epoxy-13-hydroxy-7,11,15(17)-cembratrien-16,14-olide E-375



(1*R*,3*R*,4*S*,7*E*,11*E*,13*R*,14*R*)-*form*

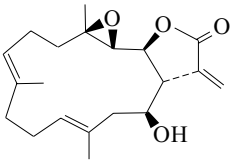
$C_{20}H_{28}O_4$ 332.439

(1*R*,3*R*,4*S*,7*E*,11*E*,13*R*,14*R*)-*form*
Sinularolide E
[852469-28-4]
Constit. of *Sinularia gibberosa*.
Oil. $[\alpha]_D^{25}$ -29.7 (c, 0.08 in $CHCl_3$).

(1*S*,3*R*,4*R*,7*E*,11*E*,13*R*,14*S*)-*form*
Ac: ***13-Acetoxysarcocrassolide***
[313674-27-0]
$C_{22}H_{30}O_5$ 374.476
Constit. of *Sarcophyton crassocaule*. Oil. $[\alpha]_D^{25}$ +56.6 (c, 0.19 in MeOH). λ_{max} 232 (log ϵ 4.2) (MeOH).

(1*S*,3*R*,4*R*,7*E*,11*E*,14*R*)-*form*
Ketone: 3,4-Epoxy-13-oxo-7,11,15(17)-cembratrien-16,14-olide.
Peunicin
[67034-32-6]
$C_{20}H_{26}O_4$ 330.423
Constit. of *Eunicea succinea*. Cryst. (EtOH).
Mp 175-178°. $[\alpha]_D^{24}$ +93.6 (c, 7.8 in $CHCl_3$).
Chang, C.Y. *et al., Acta Cryst. B*, 1980, **36**, 731-733 (*Peunicin, cryst struct*)
Duh, C.Y. *et al., J. Nat. Prod.*, 2000, **63**, 1634-1637 (*13-Acetoxysarcocrassolide*)
Li, G. *et al., J. Nat. Prod.*, 2005, **68**, 649-652 (*Sinularolide E*)

3,4-Epoxy-14-hydroxy-7,11,15(17)-cembratrien-16,2-olide E-376

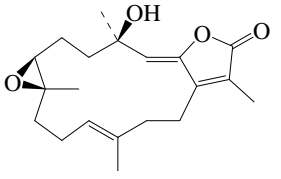


Absolute configuration

$C_{20}H_{28}O_4$ 332.439

(1*R*,2*S*,3*R*,4*R*,7*E*,11*E*,14*S*)-*form*
Constit. of *Lobophytum cristigalli*.
Cryst. (Et_2O/hexane).
Mp 136-137°. $[\alpha]_D$ -168 (c, 0.55 in $CHCl_3$).
Ac: ***Antibiotic Sch 56421***. *Sch 56421*
$C_{22}H_{30}O_5$ 374.476
From *Lobophytum cristigalli* and *Lobophytum denticulatum*.
Cytotoxic agent. Cryst.
Mp 146°. $[\alpha]_D$ -250 (c, 0.35 in $CHCl_3$). $[\alpha]_D$ -344 (MeOH).
Bowden, B.F. *et al., Aust. J. Chem.*, 1984, **37**, 545
Coval, S.J. *et al., Bioorg. Med. Chem. Lett.*, 1996, **6**, 909 (*Sch 56421, isol, pmr, cmr, cryst struct*)
Vanisree, M. *et al., J. Asian Nat. Prod. Res.*, 2000, **2**, 87-95 (*Ac*)

7,8-Epoxy-4-hydroxy-1(15),2,11-cembratrien-16,2-olide E-377



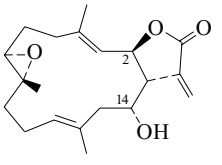
(2*Z*,4*R*,7*S*,8*S*,11*E*)-*form*

$C_{20}H_{28}O_4$ 332.439

(2*Z*,4*R*,7*S*,8*S*,11*E*)-*form* [214900-64-8]
Constit. of *Lobophytum crassum*.
Cryst.
Mp 101-102°. $[\alpha]_D^{25}$ -1.4 (c, 0.1 in $CHCl_3$). λ_{max} 247 (log ϵ 2.71); 287 (log ϵ 2.49); 295 (log ϵ 2.39) (MeOH).

(2*Z*,4*S*,7*S*,8*S*,11*E*)-*form* [214900-63-7]
Constit. of *Lobophytum crassum*.
Cryst.
Mp 106-108°. $[\alpha]_D^{25}$ -5 (c, 0.1 in $CHCl_3$). λ_{max} 247 (log ϵ 2.68); 289 (log ϵ 2.51); 298 (log ϵ 2.45) (MeOH).
Yin, S.W. *et al., Helv. Chim. Acta*, 2006, **89**, 567-572

7,8-Epoxy-14-hydroxy-3,11,15(17)-cembratrien-16,2-olide E-378



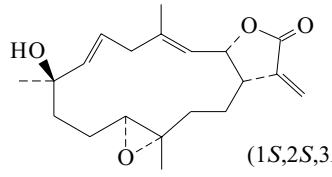
(1*R*,2*R*,3*E*,7*R*,8*R*,11*E*,14*R*)–*form*

$C_{20}H_{28}O_4$ 332.439
λ_{max} 205 (ϵ) (MeOH) (Derep).

(1*R*,2*R*,3*E*,7*R*,8*R*,11*E*,14*R*)-*form* [81575-72-6]
Constit. of a *Cespitularia* sp.
Cryst. (Et_2O/petrol).
Mp 146-151°. $[\alpha]_D^{22}$ -40.4 (c, 0.5 in MeOH).

(1*R*,2*S*,3*E*,7*R*,8*R*,11*E*,14*S*)-*form* [81601-86-7]
Constit. of a *Cespitularia* sp.
Oil. $[\alpha]_D$ -26.5 (c, 0.5 in MeOH).
Burns, K.P. *et al., Aust. J. Chem.*, 1982, **35**, 85-94

11,12-Epoxy-8-hydroxy-3,6,15(17)-cembratrien-16,2-olide E-379



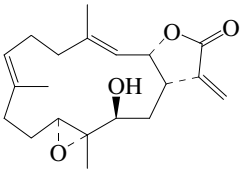
(1*S*,2*S*,3*E*,6*E*,8*R*,11*S*,12*S*)–*form*

$C_{20}H_{28}O_4$ 332.439

(1*S*,2*S*,3*E*,6*E*,8*R*,11*S*,12*S*)-*form*
Mayolide E
[157660-95-2]
Constit. of *Sinularia mayi*.
Oil. $[\alpha]_D$ +17 (c, 0.46 in Py).

(1*S*,2*S*,3*E*,6*E*,8*S*,11*S*,12*S*)-*form*
Mayolide B
[114728-07-3]
Constit. of *Sinularia mayi*.
Oil. $[\alpha]_D$ +35 (c, 1.07 in $CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 488 (*isol, pmr, cmr*)
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1993, 458 (*isol, pmr, cmr*)

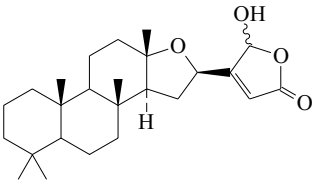
11,12-Epoxy-13-hydroxy-3,7,15(17)-cembratrien-16,2-olide E-380



$C_{20}H_{28}O_4$ 332.439

(1α,2α,3*E*,7*E*,11*S*,12*S*,13*S*)-*form*
Ac: ***Cembranolide A***
[75077-42-8]
$C_{22}H_{30}O_5$ 374.476
Constit. of *Lobophytum pauciflorum* and *Sinularia mayi*. Also (poss. a stereoisomer) from *Lobophytum chevalieri*. Cryst. (MeOH).
Mp 181-184°. $[\alpha]_D$ +50.5 (c, 0.30 in $CHCl_3$).
13-Ketone: 11,12-Epoxy-13-oxo-3,7,15(17)-cembratrien-16,2-olide. ***Cembranolide B***
[67240-43-1]
$C_{20}H_{26}O_4$ 330.423
Isol. from a *Lobophytum* sp. and from *Sinularia mayi*. Oil. $[\alpha]_D$ +1 (c, 0.83 in $CHCl_3$). $[\alpha]_D$ -5.8 (c, 0.11 in $CHCl_3$).
Bowden, B.F. *et al., Aust. J. Chem.*, 1978, **31**, 1303
Yamada, Y. *et al., Chem. Pharm. Bull.*, 1980, **28**, 2035
Kusumi, T. *et al., Tet. Lett.*, 1988, **29**, 4731-4734 (*isol, abs config, cryst struct*)
Li, R. *et al., Zhongguo Haiyang Yaowu*, 1989, **8**, 1-6; *CA*, **115**, 110911y (*isol*)

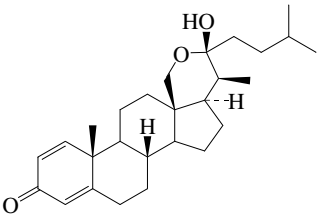
13,16-Epoxy-25-hydroxy-17-cheilanthen-19,25-olide E-381



$C_{25}H_{38}O_4$ 402.573

(13α,16*R*,25ξ)-*form*
Lintenolide C
[174063-81-1]
Constit. of *Cacospongia* cf. *linteiformis*. Antifeedant. Yellow solid. $[\alpha]_D^{25}$ +47 (c, 0.004 in $CHCl_3$).
[174063-82-2]
Carotenuto, A. *et al., Annalen*, 1996, 77-81 (*isol, pmr, cmr*)

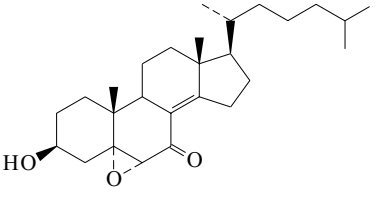
18,22-Epoxy-22-hydroxycholesta-1,4-dien-3-one E-382



$C_{27}H_{40}O_3$ 412.611

(22*R*)-*form*
Cladiellin A
[849904-88-7]
Constit. of a *Cladiella* sp.
Cryst.
Mp 169.5-171.5°. $[\alpha]_D^{20}$ +18.2 (c, 1 in MeOH).
Zhang, G.-W. *et al., Org. Lett.*, 2005, **7**, 991-994 (*Cladiellin A, cryst struct*)

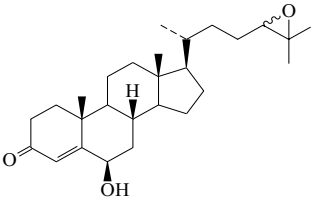
5,6-Epoxy-3-hydroxycholest-8(14)-en-7-one E-383



$C_{27}H_{42}O_3$ 414.627

(3β,5α,6α)-*form*
Constit. of *Oscarella lobularis*.
Aiello, A. *et al., J. Nat. Prod.*, 1990, **53**, 487 (*isol, pmr, cmr*)

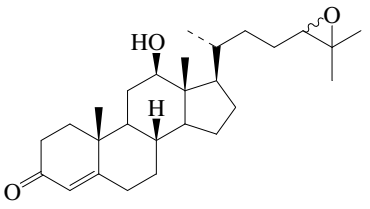
24,25-Epoxy-6-hydroxycholest-4-en-3-one E-384



$C_{27}H_{42}O_3$ 414.627

(6β,24ξ)-*form* [172377-50-3]
Constit. of *Galaxaura marginata*.
Powder.
Mp 205-208°.
Sheu, J.-H. *et al., J. Nat. Prod.*, 1996, **59**, 23 (*isol, pmr, cmr*)

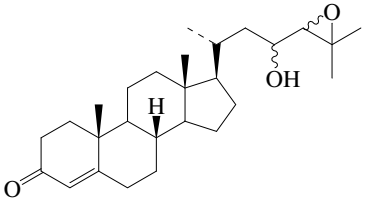
24,25-Epoxy-12-hydroxycholest-4-en-3-one E-385



$C_{27}H_{42}O_3$ 414.627

(12β,24ξ)-*form*
12-Ac: [745075-27-8]
$C_{29}H_{44}O_4$ 456.664
Constit. of *Dasystenella acanthina*. Amorph. powder. $[\alpha]_D^{25}$ +71.8 (c, 0.03 in $CHCl_3$). λ_{max} 239 (ϵ 16830) (MeOH).
Mellado, G.G. *et al., Steroids*, 2004, **69**, 291-299 (*isol, pmr, cmr*)

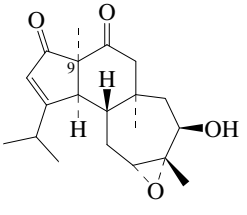
24,25-Epoxy-23-hydroxycholest-4-en-3-one E-386



$C_{27}H_{42}O_3$ 414.627

(23ξ,24ξ)-*form*
23-Ac: [745075-25-6]
$C_{29}H_{44}O_4$ 456.664
Constit. of *Dasystenella acanthina*. Amorph. powder. $[\alpha]_D^{25}$ +51.4 (c, 0.12 in $CHCl_3$). λ_{max} 239 (ϵ 10500) (MeOH).
Mellado, G.G. *et al., Steroids*, 2004, **69**, 291-299 (*isol, pmr, cmr*)

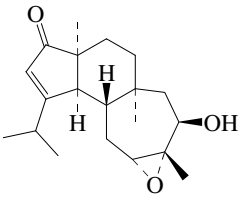
11,12-Epoxy-13-hydroxy-2-cyathene-1,8-dione E-387



$C_{20}H_{28}O_4$ 332.439

(9α,11α,12α,13β)-*form*
Cyanthiwigin N
[481643-49-6]
Constit. of *Myrmekioderma styx*.
Cryst. $[\alpha]_D$ -102 (c, 0.1 in MeOH). λ_{max} 236 (ϵ 7181) (MeOH).
13-Ketone: 11,12-Epoxy-2-cyathene-1,8,13-trione. ***Cyanthiwigin O***
[481643-50-9]
$C_{20}H_{26}O_4$ 330.423
Constit. of *Myrmekioderma styx*. Powder. $[\alpha]_D$ +90 (c, 0.08 in MeOH). λ_{max} 236 (ϵ 10228) (MeOH).
Peng, J. *et al., Tetrahedron*, 2002, **58**, 7809-7819 (*isol, pmr, cmr*)

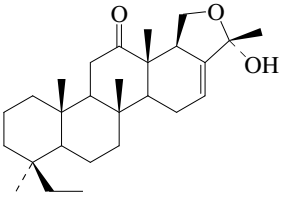
11,12-Epoxy-13-hydroxy-2-cyathen-1-one E-388



$C_{20}H_{30}O_3$ 318.455

(9α,13β)-*form*
Cyanthiwigin P
[481643-51-0]
Constit. of *Myrmekioderma styx*.
Powder. $[\alpha]_D$ +50 (c, 0.1 in MeOH). λ_{max} 238 (ϵ 6681) (MeOH).
13-Ketone: ***11,12-Epoxy-2-cyathene-1,13-dione. Cyanthiwigin Q***
[481643-52-1]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Myrmekioderma styx*. Powder. $[\alpha]_D$ +90 (c, 0.08 in MeOH). λ_{max} 236 (ϵ 10228) (MeOH).
Peng, J. *et al., Tetrahedron*, 2002, **58**, 7809-7819 (*isol, pmr, cmr*)

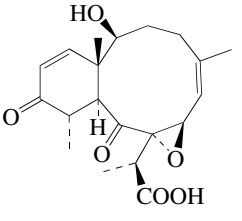
24,25-Epoxy-24-hydroxy-20,24-dimethyl-16-scalaren-12-one E-389



$C_{27}H_{42}O_3$ 414.627

24α-*form*
Phyllohemiketal B
[146396-24-9]
Isol. from sponge *Phyllospongia foliascens* from the South China sea.
Fu, X. *et al., Gaodeng Xuexiao Huaxue Xuebao*, 1991, **12**, 1486-1487; *CA*, **118**, 165465y (*isol, pmr, cmr*)

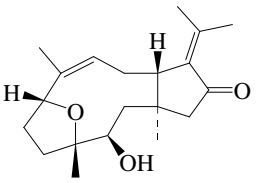
7,8-Epoxy-2-hydroxy-9,12-dioxo-5,13-briaradien-18-oic acid E-390



$C_{20}H_{26}O_6$ 362.422

2-Butanoyl, Me ester: Briareolate ester I
[180283-29-8]
$C_{25}H_{34}O_7$ 446.539
Constit. of *Briareum asbestinum*. Toxic to brine shrimp. Gum. $[\alpha]_D$ -113.2 (c, 0.22 in $CHCl_3$). λ_{max} 228 (ϵ 5012) (MeOH) (Berdy).
Mootoo, B.S. *et al., Tetrahedron*, 1996, **52**, 9953-9962 (*isol, pmr, cmr*)

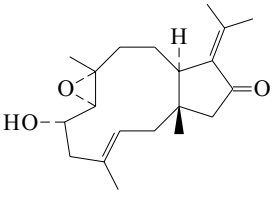
4,7-Epoxy-3-hydroxy-8,12(18)-dolabelladien-13-one E-391



$C_{20}H_{30}O_3$ 318.455

(3β,4α,7α,8*Z*)-*form*
Euniciniatin
[188635-58-7]
Constit. of *Eunicea laciniata*.
Cryst.
Rodriguez, A.D. *et al., Acta Cryst. C*, 1997, **53**, 311-313 (*isol, cryst struct*)

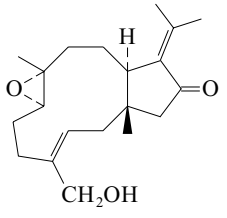
7,8-Epoxy-6-hydroxy-3,12(18)-dolabelladien-13-one E-392



$C_{20}H_{30}O_3$ 318.455

(3*E*,6α,7α,8α)-*form*
Ac: [169211-80-7]
$C_{22}H_{32}O_4$ 360.492
Constit. of *Eunicea tourneforti*. Solid. $[\alpha]_D^{24}$ +90 (c, 0.2 in $CHCl_3$).
Govindan, M. *et al., J. Nat. Prod.*, 1995, **58**, 1174 (*isol, pmr, cmr*)

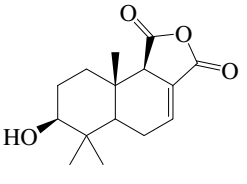
7,8-Epoxy-16-hydroxy-3,12(18)-dolabelladien-13-one E-393



$C_{20}H_{30}O_3$ 318.455

(3*Z*,7α,8α)-*form*
Ac: [169211-79-4]
$C_{22}H_{32}O_4$ 360.492
Constit. of *Eunicea tourneforti*. Glass. $[\alpha]_D^{24}$ +40 (c, 0.45 in $CHCl_3$).
λ_{max} 252 (ϵ 16000) (MeOH) (Berdy).
Govindan, M. *et al., J. Nat. Prod.*, 1995, **58**, 1174 (*isol, pmr, cmr*)

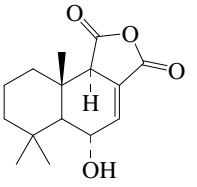
11,12-Epoxy-3-hydroxy-7-drimene-11,12-dione E-394



$C_{15}H_{20}O_4$ 264.321

3β-*form*
Dendocarbin E
[350986-78-6]
Constit. of *Dendrodoris carbunculosa*.
Oil. $[\alpha]_D^{25}$ -42 (c, 0.05 in $CHCl_3$).
Sakio, Y. *et al., J. Nat. Prod.*, 2001, **64**, 726-731 (*isol, pmr, cmr*)

11,12-Epoxy-6-hydroxy-7-drimene-11,12-dione E-395

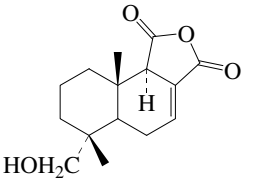


$C_{15}H_{20}O_4$ 264.321

6α-*form*
Dendocarbin G
[350986-80-0]
Constit. of *Dendrodoris carbunculosa*.
Oil. $[\alpha]_D^{25}$ -31 (c, 0.07 in $CHCl_3$).
Sakio, Y. *et al., J. Nat. Prod.*, 2001, **64**, 726-731 (*isol, pmr, cmr*)

11,12-Epoxy-13-hydroxy-7-drimene-11,12-dione E-396

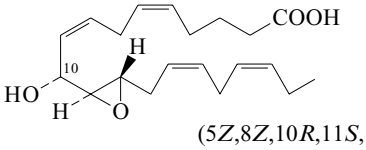
Dendocarbin F
[350986-79-7]



$C_{15}H_{20}O_4$ 264.321
Constit. of *Dendrodoris carbunculosa*. Oil. $[\alpha]_D^{25}$ -65 (c, 0.06 in $CHCl_3$).
Sakio, Y. *et al., J. Nat. Prod.*, 2001, **64**, 726-731 (*isol, pmr, cmr*)

11,12-Epoxy-10-hydroxy-5,8,14,17-eicosatetraenoic acid E-397

10-Hydroxy-10-[3-(2,5-octadienyl)oxiranyl]-5,8-decadienoic acid, 9CI. ***Hepoxilin B₄***
[103188-12-1]



(5*Z*,8*Z*,10*R*,11*S*,12*S*,14*Z*,17*Z*)–*form*

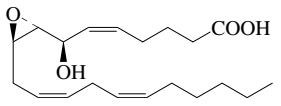
$C_{20}H_{30}O_4$ 334.455

(5*Z*,8*Z*,10*R*,11*S*,12*S*,14*Z*,17*Z*)-*form*
Isol. from the red alga *Murrayella periclados.*
Me ester: [157381-50-5]
$[\alpha]_D$ -47 (c, 0.27 in Me_2CO).

(5*Z*,8*Z*,10*S*,11*S*,12*S*,14*Z*,17*Z*)-*form*
Isol. from *Murrayella periclados.*
Me ester: [157340-25-5]
$[\alpha]_D$ +31 (c, 0.27 in Me_2CO).
Pace-Asciak, C.R. *et al., Prostaglandins, Leukotrienes Med.*, 1986, **22**, 1 (*synth*)
Hamberg, M. *et al., Lipids*, 1992, **27**, 1042 (*abs config*)
Bernart, M.W. *et al., Phytochemistry*, 1994, **36**, 1233 (*isol, pmr*)

8,9-Epoxy-7-hydroxy-5,11,14-eicosatrienoic acid E-398

7-Hydroxy-7-[3-(2,5-undecadienyl)oxiranyl]-5-heptenoic acid



(5*Z*,7*R**,8*R**,9*R**,11*Z*,14*Z*)-*form*

$C_{20}H_{32}O_4$ 336.47

(5*Z*,7*R,8*R**,9*R**,11*Z*,14*Z*)-*form*** [189082-71-1]

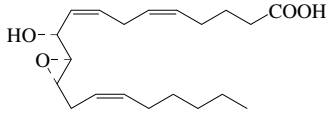
Me ester: [189082-72-2]
$C_{21}H_{34}O_4$ 350.497
Isol. from the red alga *Polyneura latissima*. Oil. $[\alpha]_D^{23}$ +70 (c, 0.07 in $CHCl_3$).

(5*Z*,7*R,8*S**,9*S**,11*Z*,14*Z*)-*form*** [189082-73-3]

Me ester: [189082-74-4]
Isol. from the red alga *Polyneura latissima*.
Oil. $[\alpha]_D^{23}$ -58 (c, 0.19 in $CHCl_3$).
Jiang, Z.-D. *et al., Lipids*, 1997, **32**, 231-235 (*isol, pmr, cmr, ms*)

11,12-Epoxy-10-hydroxy-5,8,14-eicosatrienoic acid E-399

10-Hydroxy-10-[3-(2-octenyl)oxiranyl]-5,8-decadienoic acid



(5*Z*,8*Z*,10*R*,11*S*,12*S*,14*Z*)-*form*

$C_{20}H_{32}O_4$ 336.47

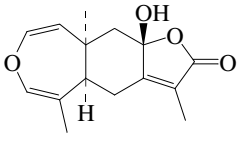
(5*Z*,8*Z*,10*R*,11*S*,12*S*,14*Z*)-*form*
Constit. of the red alga *Murrayella periclados*.
Me ester: $[\alpha]_D$ -68.2 (c, 0.5 in Me_2CO).

(5*Z*,8*Z*,10*S*,11*S*,12*S*,14*Z*)-*form*
Hepoxilin B. Hepoxilin B_3
[94161-10-1]
Constit. of *Murrayella periclados*. Metab. of arachidonic acid in mammalian blood platelets. Constit. of the algae *Platysiphonia miniata* and *Cottoniella filamentosa*. Insulin release enhancer. Active against gram-positive bacteria. Toxic to brine shrimp. Oil.
Me ester: [89461-47-2]
$[\alpha]_D$ +34.1 (c, 0.5 in Me_2CO).

[89461-48-3, 89461-49-4]

Pace-Asciak, C.R. *et al., J. Biol. Chem.*, 1983, **258**, 6835 (*synth*)
Corey, E.J. *et al., Tet. Lett.*, 1983, **24**, 4913 (*synth*)
Moghaddam, M.F. *et al., J. Biol. Chem.*, 1990, **265**, 6126-6131 (*isol, activity, Hepoxilin B_3*)
Wu, W.-L. *et al., J.C.S. Perkin 1*, 1992, 2705 (*synth, ir, pmr, ms*)
Wu, W.-L. *et al., J.O.C.*, 1993, **58**, 2760 (*synth, ir, pmr, ms*)
Vasiljeva, L.L. *et al., Tetrahedron*, 1993, **49**, 4099 (*synth*)
Bernart, M.W. *et al., Phytochemistry*, 1994, **36**, 1233 (*isol, pmr*)
Belosludtsev, Y.Y. *et al., Tet. Lett.*, 1994, **35**, 5327 (*synth*)
Melnikova, V.I. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1998, **47**, 1199-1208 (*synth*)

2,3-Epoxy-8-hydroxy-1,3,7(11)-elematrien-12,8-olide E-400

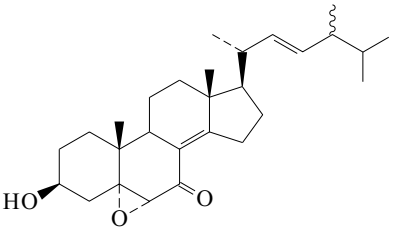


$C_{15}H_{18}O_4$ 262.305

(5α,8β*OH*,10α)-*form*
Tubipolide E
Constit. of *Tubipora musica*.
Oil. $[\alpha]_D^{25}$ +7 (c, 0.04 in $CHCl_3$). λ_{max} 242 (log ϵ 4.28) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 2001, **64**, 1430-1433 (*isol, pmr, cmr*)

5,6-Epoxy-3-hydroxyergosta-8(14),22-dien-7-one E-401

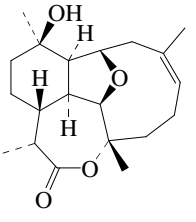
5,6-Epoxy-3-hydroxy-24-methylcholesta-8(14),22-dien-7-one



$C_{28}H_{42}O_3$ 426.638

(3β,5α,6α,24ξ)-*form*
Constit. of *Oscarella lobularis*.
Aiello, A. *et al., J. Nat. Prod.*, 1990, **53**, 487 (*isol, pmr, cmr*)

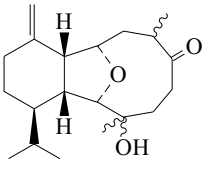
6,13-Epoxy-4-hydroxy-8-eunicellen-16,12-olide E-402



$C_{20}H_{30}O_4$ 334.455

(4β,6β,8*Z*,12α,13β,15α)-*form*
Ac: ***Briarellin J***
[503552-39-4]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Briareum polyanthes*. Semisolid. $[\alpha]_D^{26}$ -7.3 (c, 1.1 in $CHCl_3$).
Ospina, C.A. *et al., J. Nat. Prod.*, 2003, **66**, 357-363 (*isol, pmr, cmr*)

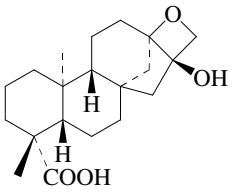
6,13-Epoxy-12-hydroxy-4(18)-eunicellen-9-one E-403



$C_{20}H_{32}O_3$ 320.471

(6α,8ξ,12ξ,13α)-*form*
12-Ac: [158831-75-5]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Cladiella australis*. Oil. $[\alpha]_D^{28}$ -8.5 (c, 0.97 in $CHCl_3$).
12-Ac, stereoisomer:
$C_{22}H_{34}O_4$ 362.508
Constit. of *Cladiella australis*. Oil. $[\alpha]_D^{28}$ -8.5 (c, 0.97 in $CHCl_3$).
Rao, C.B. *et al., J. Nat. Prod.*, 1994, **57**, 574 (*isol, pmr, cmr*)

13,17-Epoxy-16-hydroxy-19-kauranoic acid E-404

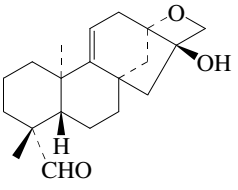


$C_{20}H_{30}O_4$ 334.455

(*ent*-16α)-*form*

Me ester: ***Ceriopsin F***
[554412-02-1]
$C_{21}H_{32}O_4$ 348.481
Constit. of *Ceriops decandra*. Cryst. (MeOH).
Mp 130-133°. $[\alpha]_D^{25}$ +40.2 (c, 0.4 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., Phytochemistry*, 2003, **62**, 1207-1211 (*isol, pmr, cmr*)

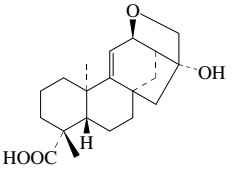
13,17-Epoxy-16-hydroxy-9(11)-kauren-19-al E-405



$C_{20}H_{28}O_3$ 316.439

(*ent*-16α)-*form* [873222-61-8]
Constit. of *Bruguiera sexangula* var. *rhynchopetala*.
Amorph. solid. $[\alpha]_D^{20}$ +123.8 (c, 0.17 in $CHCl_3$).
Bao, S. *et al., Helv. Chim. Acta*, 2005, **88**, 2757-2763 (*Bruguiera sexangula constit*)

12,17-Epoxy-16-hydroxy-9(11)-kauren-19-oic acid E-406

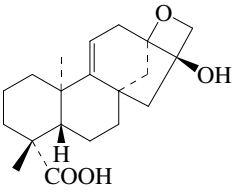


$C_{20}H_{28}O_4$ 332.439

(*ent*-12α,16β*OH*)-*form*

Me ester: ***Ceriopsin E***
[421546-80-7]
$C_{21}H_{30}O_4$ 346.466
Constit. of *Ceriops decandra*. Cryst. (EtOAc/hexane).
Mp 133-142°. $[\alpha]_D^{25}$ -59.2 (c, 1 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 2002, **65**, 592-594 (*isol, pmr, cmr, cryst struct*)

13,17-Epoxy-16-hydroxy-9(11)-kauren-19-oic acid E-407

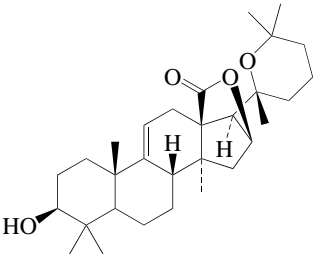


$C_{20}H_{28}O_4$ 332.439

(*ent*-16α)-*form*

Me ester: [238431-77-1]
$C_{21}H_{30}O_4$ 346.466
Constit. of *Bruguiera gymnorhiza*. Needles (C_6H_6/$CHCl_3$).
Mp 173°. $[\alpha]_D^{30}$ +22 (c, 0.1 in MeOH).
Subrahmanyan, C. *et al., Phytochemistry*, 1999, **51**, 83-90 (*isol, pmr, cmr*)

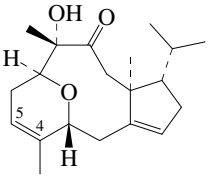
20,25-Epoxy-3-hydroxylanost-9(11)-en-18,16-olide E-408



$C_{30}H_{46}O_4$ 470.691

(3β,16β,20*R*)-*form*
Philinopgenin B
[851625-06-4]
Constit. of *Pentacta quadrangularis.*
Powder.
Mp 212.5-213.5°.
Zhang, S.-L. *et al., Mar. Drugs*, 2004, **2**, 185-191 (*Philinopgenin B*)

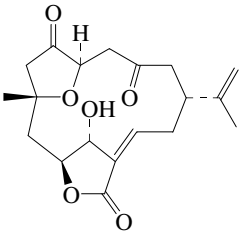
3,7-Epoxy-8-hydroxy-1(14),4-neodolabelladien-9-one E-409



$C_{20}H_{30}O_3$ 318.455

(3*R*,4*Z*,7*S*,8*S*,11*S*,12*S*)-*form*
4,5-Deoxyneodolabelline
[103197-41-7]
Constit. of *Cespitularia* spp.
Cryst.
Mp 116.5-117.5°. $[\alpha]_D$ +29 (c, 0.42 in $CHCl_3$).
4α,5α-Epoxide: 3,7:4,5-Diepoxy-8-hydroxy-1(14)-neodolabellen-9-one. ***Neodolabelline***
[94818-03-8]
Isol. from the soft coral *Clavularia koellikeri*.
Amorph. solid. $[\alpha]_D^{19}$ +53 ($CHCl_3$).
Kobayashi, M. *et al., Tet. Lett.*, 1984, **25**, 5543 (*cryst struct, Neodolabelline*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1986, **39**, 803 (*Deoxyneodolabelline*)
Williams, D.R. *et al., J.A.C.S.*, 2003, **125**, 1843-1850 (*synth*)

5,8-Epoxy-11-hydroxy-18-nor-3,6-dioxo-12,15-cembradien-20,10-olide E-410



(1*R*,5*R*,8*R*,10*S*,11*R*,12*Z*)-*form*

$C_{19}H_{24}O_6$ 348.395

(1*R*,5*R*,8*R*,10*S*,11*R*,12*Z*)-*form*
Sinuleptolide
[153379-85-2]
Constit. of a *Sinularia* sp.
Prisms (MeOH).
Mp 206-208°. $[\alpha]_D^{25}$ +57.5 (c, 0.27 in MeOH).

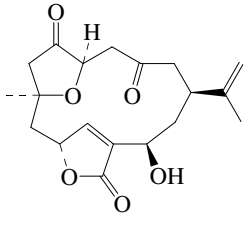
(1*R*,5*S*,8*R*,10*S*,11*R*,12*Z*)-*form*
5-Episinuleptolide
[153063-22-0]
Constit. of *Sinularia numerosa*, *Sinularia querciformis*, *Sinularia gardineri* and *Sinularia leptoclades*.
Cryst.
Mp 226-227° Mp 233-234°. $[\alpha]_D^{25}$ -119 (c, 0.16 in $CHCl_3$)
$[\alpha]_D^{20}$ -95.2 (c, 0.3 in MeOH). The 11α-epimer was prev. reported but was shown to be the same as this isomer.

(1*S*,5*R*,8*S*,10*R*,11*R*,12*Z*)-*form*
Constit. of *Sinularia inelegans*, *Sinularia polydactyla* and *Sinularia inexplicita*.
Cryst.
Mp 196-197°. $[\alpha]_D$ +3.8 (c, 0.004 in $CHCl_3$). λ_{max} 220 (ϵ 6025) (MeOH) (Berdy).

(1*S*,5*S*,8*R*,10*R*,11*S*,12*Z*)-*form*
Scabrolide E
[815587-55-4]
Constit. of *Sinularia scabra*.
Cryst.
Mp 225-226°. $[\alpha]_D^{27}$ -3.2 (c, 0.95 in $CHCl_3$).

(1*S*,5*S*,8*S*,10*R*,11*R*,12*Z*)-*form* [263260-91-9]
[263260-92-0]
Constit. of *Sinularia dissecta*.
Bowden, B.F. *et al., Aust. J. Chem.*, 1978, **31**, 2049-2056 (*5-Episinuleptolide, cryst struct*)
Duh, C.Y. *et al., CA*, 1993, **120**, 159198p (*isol*)
Shoji, N. *et al., J. Nat. Prod.*, 1993, **56**, 1651-1653 (*Sinuleptolide*)
El Sayed, K.A. *et al., J. Nat. Prod.*, 1996, **59**, 687-689 (*Sinuleptolide, 5-Episinuleptolide*)
Ramesh, P. *et al., J. Chem. Res., Synop.*, 2000, 48-50 (*Sinularia dissecta constit*)
Ahmed, A.F. *et al., Tetrahedron*, 2003, **59**, 7337-7344 (*isol*)
Ahmed, A.F. *et al., J. Nat. Prod.*, 2004, **67**, 2079-2082 (*Scabrolide E*)
Tseng, Y.-J. *et al., Org. Lett.*, 2005, **7**, 3813-3816 (*Sinuleptolide, 5-Episinuleptolide, abs config*)

5,8-Epoxy-13-hydroxy-18-nor-3,6-dioxo-11,15-cembradien-20,10-olide E-411



(1*S*,5*R*,8*S*,10*R*,13*R*)-*form*

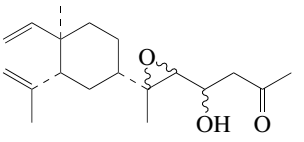
$C_{19}H_{24}O_6$ 348.395
Constit. of *Sinularia scabra*. Cryst.
Mp 81-82°. $[\alpha]_D^{29}$ -16.7 (c, 0.6 in $CHCl_3$).

(1*S*,5*R*,8*S*,10*R*,13*R*)-*form*
11β,12β-Epoxide: 5,8:11,12-Diepoxy-13-hydroxy-18-nor-3,6-dioxo-11,15-cembradien-20,10-olide. ***Scabrolide G***
[815587-57-6]
$C_{19}H_{24}O_7$ 364.394
Constit. of *Sinularia scabra*. Cryst.
Mp 180-182°. $[\alpha]_D^{27}$ +37.5 (c, 0.08 in $CHCl_3$).

(1*S*,5*S*,8*S*,10*R*,13*R*)-*form*
Me ether: 5,8-Epoxy-13-methoxy-18-nor-3,6-dioxo-11,15-cembradien-20,10-olide. ***Scabrolide C***
[479201-58-6]
$C_{20}H_{26}O_6$ 362.422
Constit. of *Sinularia scabra*. Cryst.
Mp 81-82°. $[\alpha]_D^{29}$ -16.7 (c, 0.6 in $CHCl_3$).
Sheu, J.-H. *et al., J. Nat. Prod.*, 2002, **65**, 1904-1908 (*Scabrolide C, isol, pmr, cmr*)
Ahmed, A.F. *et al., J. Nat. Prod.*, 2004, **67**, 2079-2082 (*Scabrolide G*)

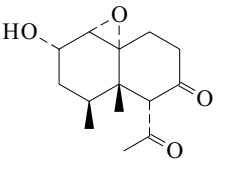
13,15-Epoxy-16-hydroxy-19-nor-8,10-lobadien-18-one E-412

[185336-75-8]



$C_{19}H_{30}O_3$ 306.444
Isol. from *Lobophytum microlobulatum*.
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 1294-1303 (*isol, ir, pmr, cmr*)

1,10-Epoxy-2-hydroxy-13-nor-7,11-nardosinanedione E-413

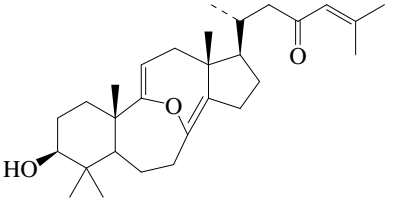


$C_{14}H_{20}O_4$ 252.31

(1α,2α,10α)-*form*
2-Hydroxylemnaliadione
[143705-30-0]
Constit. of *Parerythropodium fulvum fulvum*.
Oil. $[\alpha]_D$ -313 (c, 0.25 in CCl_4).
Ac: [143705-31-1]
$C_{16}H_{22}O_5$ 294.347
Constit. of *Parerythropodium fulvum fulvum*. Oil. $[\alpha]_D$ -244 (c, 0.1 in CH_2Cl_2).
Green, D. *et al., J. Nat. Prod.*, 1992, **55**, 1186-1196 (*isol, pmr, cmr*)

8,9-Epoxy-3-hydroxy-30-nor-8,9-secolanosta-9(11),8(14),24-trien-23-one E-414

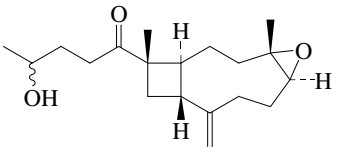
8,9-Epoxy-3-hydroxy-4,4-dimethyl-30-nor-8,9-secocholesta-9(11),8(14),24-trien-23-one



$C_{29}H_{44}O_3$ 440.665

3β-*form*
3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]: ***Sarasinoside M***
[865369-24-0]
$C_{62}H_{98}N_2O_{27}$ 1303.453
Constit. of *Melophlus sarassinorum*. Yellow amorph. solid.
$[\alpha]_D^{20}$ -7.6 (c, 0.5 in MeOH). λ_{max} 240 (MeOH).
Dai, H.-F. *et al., J. Nat. Prod.*, 2005, **68**, 1231-1237 (*Sarasinoside M*)

4,5-Epoxy-15-hydroxy-17-nor-8(19),13-xeniaphyl-ladien-12-one E-415

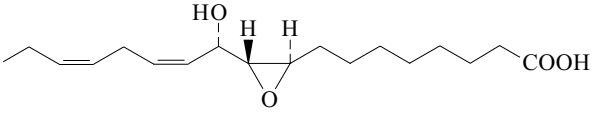


$C_{19}H_{30}O_3$ 306.444

(4*S*,5*S*,13*E*,15ξ)-*form*

Ac: ***Nanolobatin C***
[681145-47-1]
$C_{21}H_{32}O_4$ 348.481
Constit. of *Sinularia nanolobata*. Oil. $[\alpha]_D^{25}$ +21 (c, 0.92 in $CHCl_3$).
Ahmed, A.F. *et al., J. Nat. Prod.*, 2004, **67**, 592-597 (*isol, pmr, cmr*)

9,10-Epoxy-11-hydroxy-12,15-octadecadienoic acid E-416



$C_{18}H_{30}O_4$ 310.433

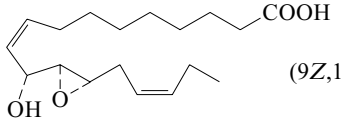
(9*R*,10*R*,11*S*,12*Z*,15*Z*)-*form*

Me ester: [147293-04-7]
$C_{19}H_{32}O_4$ 324.459
Isol. from the green alga *Acrosiphonia coalita*. Oil. $[\alpha]_D^{23}$ +46 (c, 0.28 in Me_2CO).

15,16-Dihydro, Me ester: [147383-01-5]
$C_{19}H_{34}O_4$ 326.475
Isol. from *Acrosiphonia coalita*. Light yellow oil. $[\alpha]_D^{25}$ +43 (c, 0.18 in Me_2CO).
Bernart, M.W. *et al., J. Nat. Prod.*, 1993, **56**, 245 (*isol, struct*)

12,13-Epoxy-11-hydroxy-9,15-octadecadienoic acid E-417

11-Hydroxy-1-[3-(2-pentenyl)oxiranyl]-9-undecenoic acid, 9CI



(9*Z*,11*R*,12*S*,13*S*,15*Z*)–*form*

$C_{18}H_{30}O_4$ 310.433

(9*Z*,11*R*,12*S*,13*S*,15*Z*)-*form* [106034-49-5]
Isol. from rice plants with rice blast disease (*Pyricularia oryzae*). Phytoalexin. Oil. $[\alpha]_D^{27}$ +40.3 (c, 1.2 in $CHCl_3$).
O-*(*p-*Bromobenzoyl):* $[\alpha]_D$ +26 (c, 0.493 in $CHCl_3$).

(9*Z*,11*S*,12*S*,13*S*,12*Z*)-*form* [105977-35-3]
Isol. from rice plants with rice blast disease (*Pyricularia oryzae*). Phytoalexin. Oil. $[\alpha]_D^{27}$ +65.2 (c, 0.8 in $CHCl_3$). $[\alpha]_D$ +65.2 ($CHCl_3$) (synthetic).
O-*(*p-*Bromobenzoyl):* $[\alpha]_D$ -41.2 (c, 0.131 in $CHCl_3$).

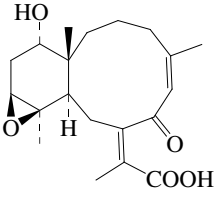
(9*Z*,11*R*,12*S*,13*S*,15*Z*)-*form*
$[\alpha]_D$ -54.2 ($CHCl_3$) (synthetic).
Me ester: [130931-06-5]
$C_{19}H_{32}O_4$ 324.459
Isol. from the green alga *Acrosiphonia coalita.*
$[\alpha]_D^{25}$ -48 (c, 0.63 in Me_2CO).

15,16-Dihydro, Me ester: Methyl 12,13-epoxy-11-hydroxy-9-octadecenoic acid
$C_{19}H_{34}O_4$ 326.475
Isol. from *Acrosiphonia coalita*.

[106034-56-4, 106034-57-5]

Kato, T. *et al., Chem. Comm.*, 1986, 743 (*isol, ms, pmr, abs config*)
Haynes, R.K. *et al., Chem. Comm.*, 1990, 1102 (*synth*)
Bernart, M.W. *et al., J. Nat. Prod.*, 1993, **56**, 245 (*isol*)
Wu, W. *et al., Tetrahedron*, 1993, **49**, 4665 (*synth*)
Honda, T. *et al., Heterocycles*, 1997, **46**, 137-140 (*synth*)
Honda, T. *et al., J.C.S. Perkin 1*, 1999, 23-29 (*synth, ir, pmr, cmr*)

11,12-Epoxy-14-hydroxy-7-oxo-5,8(17)-briaradien-18-oic acid E-418

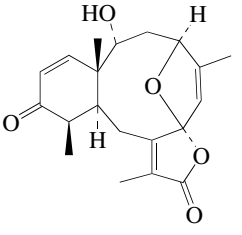


$C_{20}H_{28}O_5$ 348.438

(5*Z*,8(17)*Z*,11β,12β,14α)-*form*

14-Ac, Me ester: ***Briviolide I***
[868526-16-3]
$C_{23}H_{32}O_6$ 404.502
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ -122 (c, 0.04 in MeOH). Error in struct. diag. in ref. λ_{max} 224 (ε 9200) (MeOH).
Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 2083-2093 (*Briviolide I*)

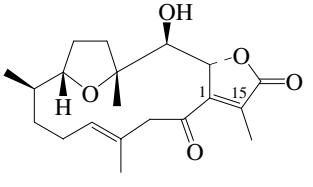
4,7-Epoxy-2-hydroxy-12-oxo-5,8(17),13-briara-trien-18,7-olide E-419



$C_{20}H_{24}O_5$ 344.407

Ac: [153977-16-3]
$C_{22}H_{26}O_6$ 386.444
Constit. of *Briareum asbestinum*. Amorph. powder.
Dookran, R. *et al., Tetrahedron*, 1994, **50**, 1983-1983 (*isol, pmr, cmr*)

4,7-Epoxy-3-hydroxy-14-oxo-1(15),11-cembradien-16,2-olide E-420



$C_{20}H_{28}O_5$ 348.438

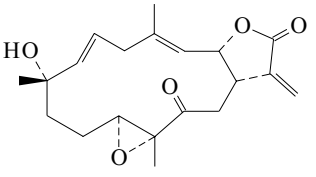
(2*R,3*S**,4*R**,7*R**,8*R**,11*E*)-*form***
Pachyclavulariolide P
[551938-79-5]
Constit. of *Pachyclavularia violacea*.

Solid.
Mp 133-135°. $[\alpha]_D^{30}$ +131 (c, 0.68 in $CHCl_3$). λ_{max} 219 (ϵ 8920) (EtOH aq.).

1β,15α-Dihydro: 4,7-Epoxy-3-hydroxy-14-oxo-11-cembren-16,2-olide. ***Pachyclavulariolide Q***
[551938-80-8]
$C_{20}H_{30}O_5$ 350.454
Constit. of *Pachyclavularia violacea*. Solid.
Mp 186-189°. $[\alpha]_D^{30}$ +28 (c, 0.05 in $CHCl_3$).

1β,15α-Dihydro, 15-hydroxy: 4,7-Epoxy-3,15-dihydroxy-14-oxo-11-cembren-16,2-olide. ***Pachyclavulariolide R***
[551938-81-9]
$C_{20}H_{30}O_6$ 366.453
Constit. of *Pachyclavularia violacea*. Solid.
Mp 204-205°. $[\alpha]_D^{31}$ -103 (c, 0.2 in $CHCl_3$).
Sheu, J.-H. *et al., J. Nat. Prod.*, 2003, **66**, 662-666 (*isol, pmr, cmr*)

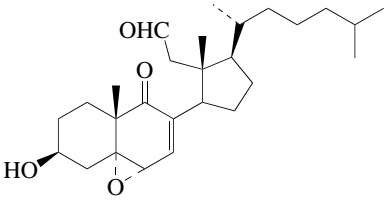
11,12-Epoxy-8-hydroxy-13-oxo-3,6,15(17)-cembratrien-16,2-olide E-421



$C_{20}H_{26}O_5$ 346.422

(1*S*,2*S*,3*E*,6*E*,8*S*,11*S*,12*R*)-*form*
Mayolide D
[114742-72-2]
Constit. of *Sinularia mayi*.
Oil. $[\alpha]_D$ +33 (c, 0.84 in $CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 488 (*isol, pmr, cmr*)
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1993, 458 (*struct*)

5,6-Epoxy-3-hydroxy-9-oxo-9,11-secocholest-7-en-11-al E-422

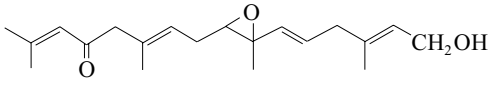


$C_{27}H_{42}O_4$ 430.626

(3β,5α,6α)-*form* [185801-44-9]
Constit. of *Spongia matamata*.
Needles.
Mp 171-173°. $[\alpha]_D$ -6.7 (c, 0.24 in $CHCl_3$). λ_{max} 260 (ϵ 3400) (CH_2Cl_2).
Lu, Q. *et al., J. Nat. Prod.*, 1997, **60**, 195-198 (*isol, pmr, cmr*)

7,8-Epoxy-1-hydroxy-2,5,10,14-phytatetraen-13-one E-423

7,8-Epoxy-1-hydroxy-3,7,11,15-tetramethyl-2,5,10,14-hexadecatetraen-13-one

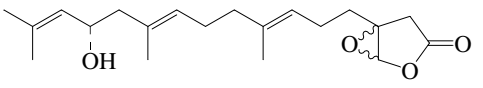


$C_{20}H_{30}O_3$ 318.455

(2*E*,5*E*,7ξ,8ξ,10*E*)-*form*
Constit. of *Bifurcaria bifurcata*.
Oil.
Combaut, G. *et al., Phytochemistry*, 1983, **22**, 1787

3,20-Epoxy-13-hydroxy-6,10,14-phytatrien-1,20-olide E-424

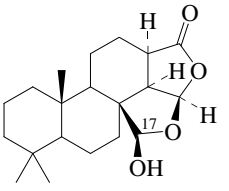
5-(10-Hydroxy-4,8,12-trimethyl-3,7,11-tridecatrienyl)-2,6-dioxabicyclo[3.1.0]hexan-3-one



$C_{20}H_{30}O_4$ 334.455

(3ξ,6*E*,10*E*,13*S*,20ξ)-*form* [260805-94-5]
Constit. of *Bifurcaria bifurcata*.
Oil. $[\alpha]_D^{25}$ -0.9 (c, 2.8 in CH_2Cl_2).
Culioli, G. *et al., Phytochemistry*, 1999, **52**, 1447-1454 (*isol, pmr, cmr*)

15,17-Epoxy-17-hydroxy-16-spongianone E-425



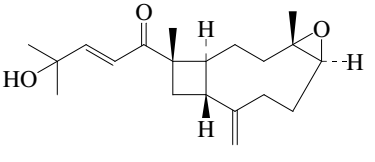
(15β,17*R*)-*form*

$C_{20}H_{30}O_4$ 334.455

(15β,17*R*)-*form*
Dendrillol 1
[106009-81-8]
Constit. of *Dendrilla rosea* and *Ceratosoma brevicaudatum*.
Cryst. (CH_2Cl_2/hexane).
Mp 229-231°. $[\alpha]_D^{20}$ -31.8 (c, 1 in $CHCl_3$).

(15β,17*S*)-*form*
Ac:
$C_{22}H_{32}O_5$ 376.492
Constit. of *Cadlina luteomarginata*. Oil.
Karuso, P. *et al., Aust. J. Chem.*, 1986, **39**, 1643 (*Dendrillol 1, cryst struct*)
Ksebati, M.B. *et al., J.O.C.*, 1987, **52**, 3766 (*isol*)
Abad, A. *et al., J.O.C.*, 1992, **57**, 6861 (*synth*)
Dumdei, E.J. *et al., Can. J. Chem.*, 1997, **75**, 773-789 (*isol, pmr, cmr*)
Arnó, M. *et al., J.O.C.*, 2003, **68**, 1242-1251 (*synth*)

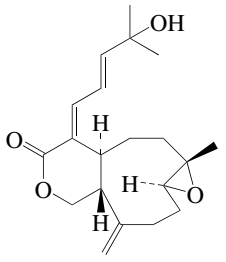
4,5-Epoxy-15-hydroxy-8(19),13-xeniaphylladien-12-one E-426



$C_{20}H_{30}O_3$ 318.455

(4*S*,5*S*,13*E*)-*form*
Nanolobatin B
[681145-46-0]
Constit. of *Sinularia nanolobata*.
Oil. $[\alpha]_D^{25}$ +66.7 (c, 0.6 in $CHCl_3$).
Ahmed, A.F. *et al., J. Nat. Prod.*, 2004, **67**, 592-597 (*isol, pmr, cmr*)

6,7-Epoxy-14-hydroxy-1(19),10,12-xenicatrien-17,18-olide E-427



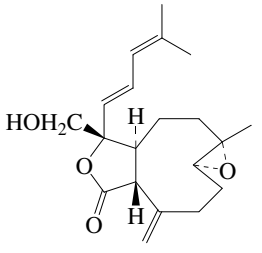
(6α,7β,10*E*,12*E*)-*form*

$C_{20}H_{28}O_4$ 332.439

(6α,7β,10*E*,12*E*)-*form*
Xeniolactone B
[861676-58-6]
Constit. of *Xenia florida* and *Xenia blumi*.
Oil. $[\alpha]_D^{25}$ +68 (c, 0.3 in CH_2Cl_2). $[\alpha]_D^{25}$ +28 (c, 0.3 in $CHCl_3$).
λ_{max} 235 (MeOH). λ_{max} 258 (log ϵ 3.9) (MeOH).

(6α,7β,10*Z*,12*E*)-*form* [866228-94-6]
Constit. of *Xenia blumi*.
$[\alpha]_D^{25}$ +26 (c, 0.2 in $CHCl_3$). λ_{max} 261 (log ϵ 3.9) (MeOH).
El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 1336-1340 (*Xenia blumi constits*)
Shen, Y.-C. *et al., Tet. Lett.*, 2005, **46**, 4793-4796 (*Xeniolactone B*)

6,7-Epoxy-17-hydroxy-1(19),11,13-xenicatrien-18,10-olide E-428



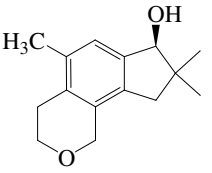
(6α,7α,10α,11*E*)-*form*

$C_{20}H_{28}O_4$ 332.439

(6α,7α,10α,11*E*)-*form*
Xeniolide H
[479067-65-7]
Constit. of *Xenia umbellata*.
Oil. $[\alpha]_D^{25}$ +16.3 (c, 0.46 in $CHCl_3$).
13ξ,14-Epoxide: 6,7:13,14-Diepoxy-17-hydroxy-1(19),11-xenicadien-18,10-olide. ***14,15-Epoxyxeniolide H***
[871483-40-8]
$C_{20}H_{28}O_5$ 348.438
Constit. of *Xenia umbellata*. Amorph. solid. $[\alpha]_D^{25}$ +26 (c, 0.2 in $CHCl_3$).
13ξ,14-Epoxide, 17-Ac: ***3-Acetyl-14,15-epoxyxeniolide H***
[871483-41-9]
$C_{22}H_{30}O_6$ 390.475
Constit. of *Xenia umbellata*. Amorph. solid. $[\alpha]_D^{25}$ +22 (c, 0.1 in $CHCl_3$).

(6α,7β,10ξ)-*form*
Florlide G
[267417-29-8]
Constit. of *Xenia florida*.
Oil. $[\alpha]_D$ -123 (c, 0.08 in MeOH). λ_{max} 245 (log ϵ 4.15) (MeOH).
Iwagawa, T. *et al., J. Nat. Prod.*, 2000, **63**, 468-472 (*isol, pmr, cmr*)
Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1882-1885 (*isol, pmr, cmr*)
El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2006, **69**, 338-341 (*13,14-epoxide derivs*)

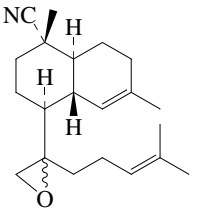
4,15-Epoxy-2,6,8-illudalatrien-10-ol E-429



$C_{15}H_{20}O_2$ 232.322

(*S*)-*form*
Alcyopterosin I
[288851-35-4]
Constit. of *Alcyonium paessleri*.
Cryst. (cyclohexane).
Mp 97-99°. $[\alpha]_D^{25}$ +6.16 (c, 2.59 in $CHCl_3$). λ_{max} 212 (log ϵ 3.17); 230 (log ϵ 3.65); 280 (log ϵ 2.98) (CH_2Cl_2).
Palermo, J.A. *et al., J.O.C.*, 2000, **65**, 4482-4486 (*isol, pmr, cmr*)

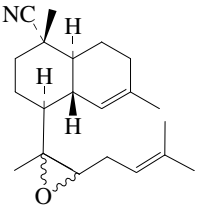
11,12-Epoxy-10-isocyano-4,15-bifloradiene E-430



$C_{21}H_{31}NO$ 313.482

(10α,11ξ)-*form* [287101-64-8]
Constit. of *Acanthella cavernosa*.
$[\alpha]_D$ +7.3 (c, 0.0011 in CH_2Cl_2).
Clark, R.J. *et al., Tetrahedron*, 2000, **56**, 3071-3076 (*isol, pmr, cmr*)

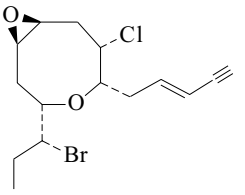
11,13-Epoxy-10-isocyano-4,15-bifloradiene E-431



$C_{21}H_{31}NO$ 313.482

(10α,11ξ,13ξ)-*form* [287101-63-7]
Constit. of *Acanthella cavernosa*.
$[\alpha]_D$ +17.3 (c, 0.0033 in CH_2Cl_2).
Clark, R.J. *et al., Tetrahedron*, 2000, **56**, 3071-3076 (*isol, pmr, cmr*)

Epoxyisodihydrorhodophytin E-432

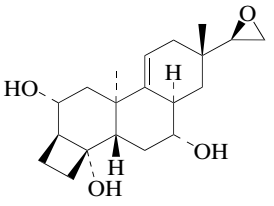


$C_{15}H_{20}BrClO_2$ 347.679
Constit. of *Laurencia obtusa*. Needles (hexane).

Mp 92-93°. $[\alpha]_D^{20}$ +23.7 (c, 0.815 in $CHCl_3$).

Imre, S. *et al., Z. Naturforsch., C*, 1987, **42**, 507

15,16-Epoxy-9(11)-isoparguerene-2,4,7-triol E-433



$C_{20}H_{30}O_4$ 334.455

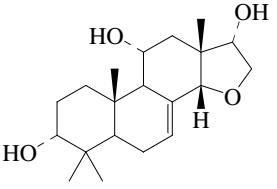
(ent*-2β,4β,7β,15*R*)-*form

2-Ac: [202870-59-5]
$C_{22}H_{32}O_5$ 376.492

Constit. of *Laurencia saitoi*. Oil. $[\alpha]_D^{27}$ -28.6 (c, 0.97 in $CHCl_3$).

Kurata, K. *et al., Phytochemistry*, 1998, **47**, 363-369 (*isol, pmr, cmr*)

14,16-Epoxy-7-isopimarene-3,11,15-triol E-434



$C_{20}H_{32}O_4$ 336.47

(3α,11α,15α)-form

Agallochaol D

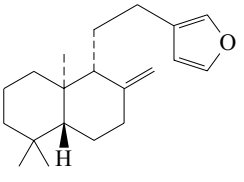
[862255-96-7]

Constit. of *Excoecaria agallocha*.

Oil. $[\alpha]_D^{20}$ +28 (c, 0.79 in MeOH/$CHCl_3$).

Wang, J.-D. *et al., Helv. Chim. Acta*, 2005, **88**, 979-985 (*Agallochaol D*)

15,16-Epoxy-8(17),13(16),14-labdatriene E-435



$C_{20}H_{30}O$ 286.456

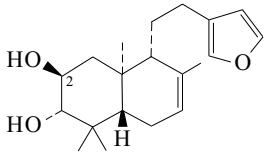
***ent*-form**

Constit. of *Blepharispermum zanguebaricum* and a *Cacospongia* sp.

Oil. $[\alpha]_D$ -22 (c, 0.14 in $CHCl_3$).

Zdero, C. *et al., Phytochemistry*, 1991, **30**, 3297 (*isol, pmr*)
Tasdemir, D. *et al., Tetrahedron*, 2000, **56**, 9025-9030 (*isol, cmr*)
Villamizar, J. *et al., J. Nat. Prod.*, 2003, **66**, 1623-1627 (*synth*)

15,16-Epoxy-7,13(16),14-labdatriene-2,3-diol E-436



$C_{20}H_{30}O_3$ 318.455

(ent*-2α,3β)-*form

Constit. of *Baccharis salicifolia*.

Oil. $[\alpha]_D^{24}$ -11 (c, 0.74 in $CHCl_3$).

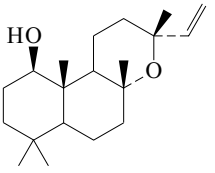
2-Ketone: 15,16-Epoxy-3-hydroxy-7,13(16),14-labdatrien-2-one.
Blanesin

$C_{20}H_{28}O_3$ 316.439

Constit. of *Raspaciona aculeata*. Amorph. powder. $[\alpha]_D^{20}$ -14.3 (c, 0.1 in $CHCl_3$).

Zdero, C. *et al., Phytochemistry*, 1986, **25**, 2841
Ciavatta, M.L. *et al., Tet. Lett.*, 1994, **35**, 7871 (*Blanesin*)

8,13-Epoxy-14-labden-1-ol E-437



$C_{20}H_{34}O_2$ 306.487

(1β,8α,13R)-form

1β-Hydroxymanoyl oxide. *Apiculol*

[152517-79-8]

Constit. of *Kyllinga erecta* and *Rhizophora apiculata*.

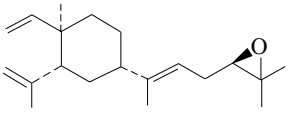
Cryst.

Mp 100° Mp 122°. $[\alpha]_D$ +3.3 (c, 0.27 in $CHCl_3$).

Mahmout, Y. *et al., Phytochemistry*, 1993, **34**, 865 (*isol, pmr, cmr*)
Saxena, E. *et al., Nat. Prod. Lett.*, 1994, **4**, 149 (*isol, pmr, cmr*)

17,18-Epoxy-8,10,13(15)-lobatriene E-438

[71593-05-0]



$C_{20}H_{32}O$ 288.472

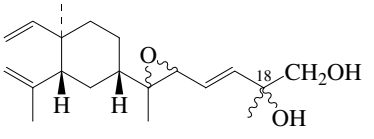
(17R)-form

Constit. of *Lobophytum* sp.

Yellow oil.

Dunlop, R.W. *et al., Aust. J. Chem.*, 1979, **32**, 1345

13,15-Epoxy-8,10,16-lobatriene-18,19-diol E-439



$C_{20}H_{32}O_3$ 320.471

Tentative struct.

18-Me ether: [161467-67-0]
$C_{21}H_{34}O_3$ 334.498

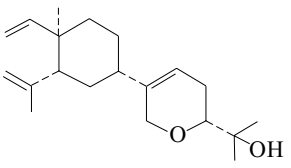
Isol. from a soft coral *Lobophytum* sp.

Raju, B.L. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 1033-1037 (*isol, pmr, cmr*)

14,17-Epoxy-8,10,13(15)-lobatrien-18-ol E-440

Lobatriene

[71593-06-1]



$C_{20}H_{32}O_2$ 304.472

Constit. of *Lobophytum* sp. Oil.

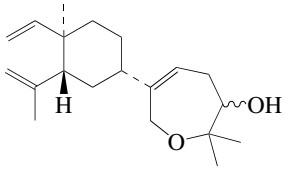
Ac: [203798-90-7]

$C_{22}H_{34}O_3$ 346.509

Constit. of *Lobophytum pauciflorum*. Yellow viscous oil. $[\alpha]_D$ +47.3 (c, 0.31 in $CHCl_3$). λ_{max} 199 (ϵ 4300) (hexane). λ_{max} 199 (ϵ 4300) (MeOH) (Berdy).

Dunlop, R.W. *et al., Aust. J. Chem.*, 1979, **32**, 1345 (*isol, struct*)
Kusumi, T. *et al., J.O.C.*, 1992, **57**, 1033 (*isol, pmr, cmr, abs config*)
Edrada, R.A. *et al., J. Nat. Prod.*, 1998, **61**, 358-361 (*acetate*)

14,18-Epoxy-8,10,13(15)-lobatrien-17-ol E-441



$C_{20}H_{32}O_2$ 304.472

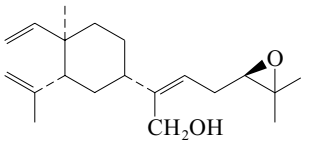
17ξ-*form* [203871-98-1]

Constit. of *Lobophytum pauciflorum*.

Viscous oil. λ_{max} 206 (ϵ 4350) (hexane). λ_{max} 206 (ϵ 4350) (MeOH) (Berdy).

Edrada, R.U. *et al., J. Nat. Prod.*, 1998, **61**, 358-361 (*isol, pmr, cmr*)

17,18-Epoxy-8,10,13(15)-lobatrien-14-ol E-442



$C_{20}H_{32}O_2$ 304.472

Ac: ***Acetoxylobaoxide***

[139579-32-1]

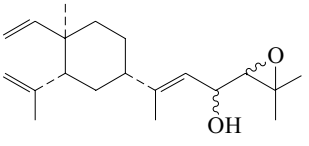
$C_{22}H_{34}O_3$ 346.509

Constit. of *Sinularia flexibilis*. Oil. $[\alpha]_D^{25}$ -3.3 (c, 0.06 in $CHCl_3$).

Hamada, T. *et al., Chem. Lett.*, 1992, 33 (*isol, pmr, cmr*)

17,18-Epoxy-8,10,13(15)-lobatrien-16-ol E-443

[150312-94-0]



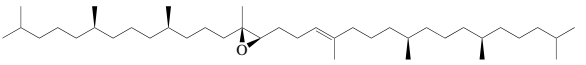
$C_{20}H_{32}O_2$ 304.472

Constit. of a *Lobophytum* sp. Oil. $[\alpha]_D$ +10.7 (c, 1.4 in $CHCl_3$).

Raju, B.L. *et al., J. Nat. Prod.*, 1993, **56**, 961 (*isol, pmr, cmr*)

Epoxylycopaene E-444

[188413-79-8]



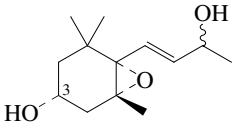
$C_{40}H_{78}O$ 575.056

Constit. of *Botryococcus braunii*. Oil. $[\alpha]_D$ -3.5 (c, 3.45 in heptane).

Delahais, V. *et al., Phytochemistry*, 1997, **44**, 671 (*isol, pmr, cmr, ms*)

5,6-Epoxy-7-megastigmene-3,9-diol E-445

5,6-Epoxy-3-hydroxy-β-ionol



(3α,5α,6α,7*E*,9ξ)-*form*

$C_{13}H_{22}O_3$ 226.315

(3β,5α,6α,7*E*,9*R*)-*form*

9-O-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]: ***Premnaionoside***

[272458-28-3]

$C_{24}H_{40}O_{12}$ 520.573

Constit. of *Acanthus ebracteatus* and *Premna subscandens*.

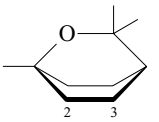
Amorph. powder. $[\alpha]_D^{19}$ -82.6 (c, 0.56 in MeOH).

Sudo, H. *et al., Chem. Pharm. Bull.*, 2000, **48**, 542-546 (*Premna subscandens glycosides*)
Kanchanapoom, T. *et al., Phytochemistry*, 2001, **58**, 811-817 (*Acanthus ebracteatus constit*)

1,8-Epoxy-*p*-menthane E-446

1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane, 9CI. ***1,8-Cineole*** *. Eucalyptol. Eucapur. Soledum. Terpane. Zineol. Cineole. Cyneol. Cajeputol. FEMA 3658*

[470-82-6]



$C_{10}H_{18}O$ 154.252

Occurs in eucalyptus, lavender, sage and many other oils. Detected in the Black Sea bryozoan *Conopeum seuratum*. Used in perfumery and flavour industries. Antiseptic agent. Inhalational expectorant (vet. use). Phytotoxin. Oil with camphoraceous odour.

Mp 1.5°. Bp 176-177°. n_D^{20} 1.4550. Log P 2.76 (calc).

▶ Flammable, fl. p. 50°. LD_{50} (rat, orl) 2480 mg/kg. Exp. reprod. effects (large dose). OS9275000

2,3-Didehydro: ***Dehydro-1,8-cineole****. 1,8-Epoxy-*p*-menth-2-ene*

[92760-25-3]

$C_{10}H_{16}O$ 152.236

Isol. from *Laurus nobilis* (bay laurel) oil and from the opisthonotal gland secretion of the mite *Caloglyphus rodriguezi*. Oil. Bp_{40} 78-80°. $[\alpha]_D^{20}$ -53 (c, 3 in EtOH). Props. refer to synthetic material. Opt. rotn. and abs. config. of nat. isolates not reported.

3-Oxo: 1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octan-2-one, 9CI. ***3-Oxo-1,8-cineole****. 1,8-Epoxy-*p*-menthan-3-one*

[101221-23-2]

$C_{10}H_{16}O_2$ 168.235

Constit. of *Paeonia albiflora* flowers.

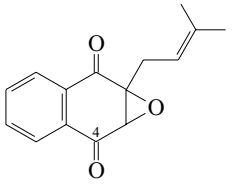
[58264-16-7, 63025-72-9, 66113-06-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 245C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 395A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 323D (*ir*)
Coxen, J.M. *et al., Chem. Ind. (London)*, 1968, **652**, (*synth*)

Achilladelis, B. *et al., Phytochemistry*, 1968, **7**, 1317 (*biosynth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 570 (*occur*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Hogg, J.W. *et al., Phytochemistry*, 1974, **13**, 868 (*Dehydrocineole, isol*)
Zenin, V.S. *et al., Khim. Prir. Soedin.*, 1975, **11**, 15; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 13 (*ir, anal*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Bondavalli, F. *et al., J.C.S. Perkin 1*, 1977, 430; 1978, 804 (*synth*)
Orsini, F. *et al., Gazz. Chim. Ital.*, 1980, **110**, 553 (*biosynth*)
Ayorinde, F.O. *et al., Tet. Lett.*, 1984, **25**, 3525 (*isol, synth, Dehydrocineole*)
Kumar, N. *et al., Phytochemistry*, 1986, **25**, 250 (*3-Oxocineole*)
Hadijeva, P. *et al., Z. Naturforsch., C*, 1987, **42**, 1019-1022 (*occur, Conopeum*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CAL000
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1354
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 113 (*rev*)
Brecknell, D.J. *et al., Aust. J. Chem.*, 1997, **50**, 35 (*synth*)
Rieder, C. *et al., Helv. Chim. Acta*, 2000, **83**, 2504-2513 (*biosynth*)
Bond, A.D. *et al., Aust. J. Chem.*, 2001, **54**, 683-684 (*cryst struct*)
Wise, M.L. *et al., J.A.C.S.*, 2002, **124**, 8546-8547 (*biosynth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAL000

2,3-Epoxy-2-(3-methyl-2-butenyl)-1,4-naphthalenedione E-447

[137492-06-9]

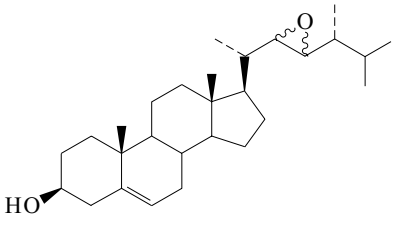


$C_{15}H_{14}O_3$ 242.274
Cytotoxic agent. Oil.

4-Di-Me acetal: ***2,3-Epoxy-4,4-dimethoxy-2-(3-methyl-2-butenyl)-1(2H)-naphthalenone***
[137414-54-1]
$C_{17}H_{20}O_4$ 288.343
Constit. of the brown alga *Landsburgia quercifolia*. Oil. Possible artifact.
Perry, N.B. *et al., J. Nat. Prod.*, 1991, **54**, 978 (*isol*)

22,23-Epoxy-24-methylcholest-5-en-3-ol E-448

22,23-Epoxy-5-ergosten-3-ol, 9CI

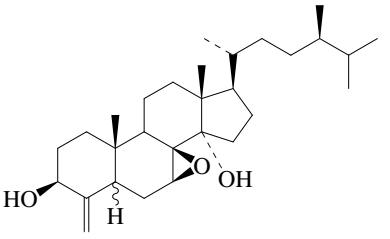


$C_{28}H_{46}O_2$ 414.67

(3β,22ξ,23ξ,24R)-form [89411-31-4]
Constit. of a sponge, *Hyrtios* sp.
Koch, P. *et al., Helv. Chim. Acta*, 1983, **66**, 2431

7,8-Epoxy-4-methyleneergostane-3,14-diol E-449

7,8-Epoxy-24-methyl-4-methylenecholestane-3,14-diol

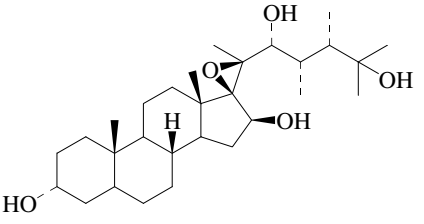


$C_{29}H_{48}O_3$ 444.696

(3β,5ξ,7β,8β,14α,24R)-form
O[14]*-Me: 7,8-Epoxy-14-methoxy-4-methyleneergostan-3-ol. 7,8-Epoxy-14-methoxy-24-methyl-4-methylenecholestan-3-ol*
$C_{30}H_{50}O_3$ 458.723
Constit. of *Theonella swinhoei.*
Sugo, Y. *et al., Steroids*, 1995, **60**, 738-742 (*isol, pmr, cmr*)

17,20-Epoxy-23-methylergostane-3,16,22,25-tetrol E-450

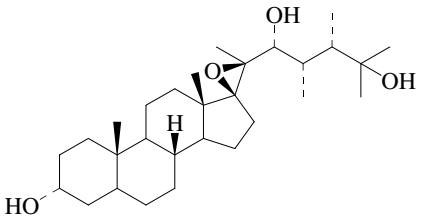
17,20-Epoxy-23,24-dimethylcholestane-3,16,22,25-tetrol



$C_{29}H_{50}O_5$ 478.711

(3α,5α,16β,17β,20S,22R,23S)-form
22-Ac: ***Hippuristerol F***
[868395-90-8]
$C_{31}H_{52}O_6$ 520.748
Constit. of *Isis hippuris.* Powder.
Mp 98-100°. $[\alpha]_D$ -1 (c, 2.44 in $CHCl_3$).
22,25-Di-Ac: ***Hippuristerol A***
[346423-96-9]
$C_{33}H_{54}O_7$ 562.785
Constit. of *Isis hippuris.* Powder. $[\alpha]_D^{25}$ +6.1 (c, 0.4 in $CHCl_3$).
16,22,25-Tri-Ac: ***Hippuristerol C***
[346423-97-0]
$C_{35}H_{56}O_8$ 604.823
Constit. of *Isis hippuris.* Powder. $[\alpha]_D^{30}$ +10.4 (c, 0.195 in $CHCl_3$).
3-Ketone, 22-Ac: ***Hippuristerone H***
[549528-41-8]
$C_{31}H_{50}O_6$ 518.732
Constit. of *Isis hippuris.* Powder.
Mp 122-124°. $[\alpha]_D$ +9 (c, 0.31 in $CHCl_3$).
3-Ketone, 22,25-di-Ac: ***Hippuristerone A***
[311311-30-5]
$C_{33}H_{52}O_7$ 560.77
Constit. of *Isis hippuris.* Cryst.
Mp 153-154°. $[\alpha]_D^{25}$ +17 (c, 0.5 in $CHCl_3$) (+1.36).
3-Ketone, 16,22,25-tri-Ac: ***Hippuristerone C***
[346423-98-1]
$C_{35}H_{54}O_8$ 602.807
Constit. of *Isis hippuris.* Powder. $[\alpha]_D^{28}$ +48.4 (c, 0.015 in $CHCl_3$).
Sheu, J.-H. *et al., Tet. Lett.*, 2000, **41**, 7885-7888 (*Hippuristerone A*)
González, N. *et al., Tetrahedron*, 2001, **57**, 3487-3497 (*Hippuristerol A, Hippuristerol C, Hippuristerone C*)
Sheu, J.-H. *et al., J. Nat. Prod.*, 2003, **66**, 917-921 (*Hippuristerone H*)
Chao, C.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1366-1370 (*Hippuristerol F*)

17,20-Epoxy-23-methylergostane-3,22,25-triol E-451



$C_{29}H_{50}O_4$ 462.712

(3α,5α,17β,20*S*,22*R*,23*S*)-*form*

22-Ac: ***Hippuristerol E***
[868395-88-4]
$C_{31}H_{52}O_5$ 504.749
Constit. of *Isis hippuris*. Powder.
Mp 134-136°. $[\alpha]_D$ +8 (c, 0.45 in $CHCl_3$).

22,25-Di-Ac: ***Hippuristerol B***
[346423-95-8]
$C_{33}H_{54}O_6$ 546.786
Constit. of *Isis hippuris*. Powder. $[\alpha]_D^{24}$ +2.3 (c, 0.225 in $CHCl_3$).

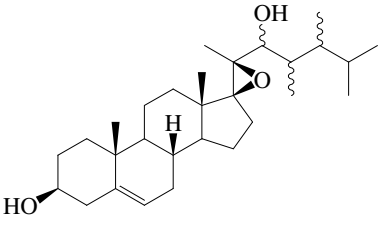
3-Ketone: 17,20-Epoxy-22,25-dihydroxy-23-methylergostan-3-one
$C_{29}H_{48}O_4$ 460.696

3-Ketone, 22-Ac: ***Hippuristerone I***
[343934-55-4]
$C_{31}H_{50}O_5$ 502.733
Constit. of *Isis hippuris*. Powder.
Mp 120-122°. $[\alpha]_D$ +12 (c, 0.36 in $CHCl_3$).

3-Ketone, 22,25-di-Ac: ***Hippuristerone B***
[346423-94-7]
$C_{33}H_{52}O_6$ 544.77
Constit. of *Isis hippuris*. Powder. $[\alpha]_D^{26}$ +8.7 (c, 0.765 in $CHCl_3$).
González, N. *et al., Tetrahedron*, 2001, **57**, 3487-3497 (*Hippuristerol B, Hippuristerone B*)
Sheu, J.-H. *et al., J. Nat. Prod.*, 2003, **66**, 917-921 (*Hippuristerone I*)
Chao, C.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1366-1370 (*Hippuristerol E*)

17,20-Epoxy-23-methylergost-5-ene-3,22-diol E-452

17,20-Epoxy-23,24-dimethylcholest-5-ene-3,22-diol

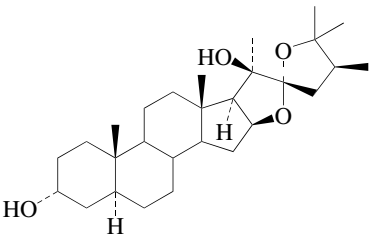


$C_{29}H_{48}O_3$ 444.696

(3β,17β,20*R*,22ξ,23ξ,24ξ)-*form*
Constit. of *Sarcophyton crassocaule*.
Needles. $[\alpha]_D^{25}$ -31.5 (c, 0.003 in $CHCl_3$).

Di-Ac: [253195-58-3]
$C_{33}H_{52}O_5$ 528.771
Constit. of *Sarcophyton crassocaule*. Oil. $[\alpha]_D^{25}$ -38 (c, 0.002 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 2000, **63**, 112-118 (*isol, pmr, cmr*)

22,25-Epoxy-24-methylfurostane-3,20-diol E-453

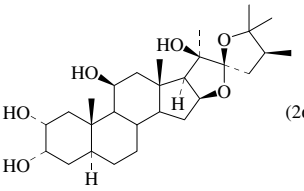


$C_{28}H_{46}O_4$ 446.669

(3α,5α,16β,20*R*,22*S*,24*S*)-*form*
11-Dehydroxy-22-epihippuristanol
[343934-53-2]
Constit. of *Isis hippuris*.
Powder. $[\alpha]_D^{26}$ -23.1 (c, 0.625 in $CHCl_3$).

3-Ketone: 22,25-Epoxy-20-hydroxy-24-methylfurostan-3-one.
11-Dehydroxy-22-epihippuristan-3-one
[343934-54-3]
$C_{28}H_{44}O_4$ 444.653
Constit. of *Isis hippuris*. Powder. $[\alpha]_D^{26}$ -41.5 (c, 0.03 in $CHCl_3$).
González, N. *et al., Tetrahedron*, 2001, **57**, 3487-3497

22,25-Epoxy-24-methylfurostane-2,3,11,20-tetrol E-454



(2α,3α,5α,11β,16β,20*R*,22*R*,24*S*)-*form*

$C_{28}H_{46}O_6$ 478.668

(2α,3α,5α,11β,16β,20*R*,22*R*,24*S*)-*form*
2α-Hydroxyhippuristanol
Constit. of *Isis hippuris*. Shows *in vivo* anticancer activity.
Amorph. solid. Poorly sol. hexane.

2-Ac: ***Hippurin 1***
[66536-82-1]
$C_{30}H_{48}O_7$ 520.705
Constit. of *Isis hippuris*. Cryst. (H_2O/petrol).
Mp 183-185°. $[\alpha]_D$ +36.2 (c, 1 in $CHCl_3$).

3-Ac: ***3-Acetyl-2-desacetylhippurin 1***
[117569-40-1]
$C_{30}H_{48}O_7$ 520.705
Constit. of *Isis hippuris*. Powder.
Mp >300°. $[\alpha]_D$ +27 (c, 0.3 in $CHCl_3$).

2,3,11-Tri-Ac: ***3,11-Diacetylhippurin 1***
$C_{34}H_{52}O_9$ 604.779
Constit. of *Isis hippuris*. Oil.

(2α,3α,5α,11β,16β,20*R*,22*S*,24*S*)-*form*
2-Desacetyl-22-epihippurin 1
Constit. of *Isis hippuris*.
Cryst.
Mp 260-261°.

2-Ac: ***22-Epihippurin 1***
[364344-14-9]
$C_{30}H_{48}O_7$ 520.705
Constit. of *Isis hippuris*. Cryst. (MeOH).
Mp 243-245°.

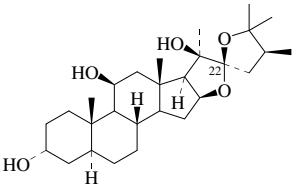
3-Ac: ***3-Acetyl-2-desacetyl-22-epihippurin 1***
[364344-15-0]
$C_{30}H_{48}O_7$ 520.705
Constit. of *Isis hippuris*. Cryst.
Mp 248-250°.

2,3-Di-Ac: ***3-Acetyl-22-epihippurin 1***
$C_{32}H_{50}O_8$ 562.742
Constit. of *Isis hippuris*. Cryst.
Mp 240-243°.

2,3,11-Tri-Ac: ***3,11-Diacetyl-22-epihippurin 1***
$C_{34}H_{52}O_9$ 604.779
Constit. of *Isis hippuris*. Needles.
Mp 178-180°.

Kazlauskas, R. *et al., Tet. Lett.*, 1977, **18**, 4439-4442 (*Hippurin 1, cryst struct*)
Higa, T. *et al., Chem. Lett.*, 1981, 1647-1650 (*22-Epihippurin 1, 2-Hydroxyhippuristanol*)
Rao, C.B. *et al., J. Nat. Prod.*, 1988, **51**, 954-958 (*Ac derivs*)
Chao, C.H. *et al., J. Nat. Prod.*, 2005, **68**, 880-885 (*3-Acetyl-2-desacetylhippurin 1*)

22,25-Epoxy-24-methylfurostane-3,11,20-triol E-455



(3α,5α,11β,16β,20*R*,22*R*,24*S*)-*form*

$C_{28}H_{46}O_5$ 462.668

(3α,5α,11β,16β,20*R*,22*R*,24*S*)-*form*
Hippuristanol
[80442-78-0]
Constit. of *Isis hippuris*. Shows anticancer activity. Cryst. (MeOH). Sol. MeOH, Et_2O; poorly sol. H_2O, hexane.
Mp 188-190°. C-22 config. revised in 1983.

(3α,5α,11β,16β,20*R*,22*S*,24*S*)-*form*
22-Epihippuristanol
[80442-79-1]
Constit. of *Isis hippuris*.
Cryst. (MeOH).
Mp 248-249°.

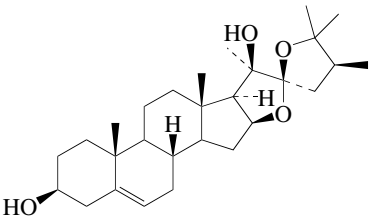
3-Ac: ***3-Acetyl-22-epihippuristanol***
[80442-82-6]
$C_{30}H_{48}O_6$ 504.706
Constit. of *Isis hippuris*. Powder. $[\alpha]_D^{27}$ -23.9 (c, 0.14 in $CHCl_3$).

3,11-Di-Ac: ***Hippurin 2***
[80442-84-8]
$C_{32}H_{50}O_7$ 546.743
Constit. of *Isis hippuris*. Cryst. (MeOH).
Mp 252-253°.

11-Ketone: 22,25-Epoxy-3,20-dihydroxy-24-methylfurostan-11-one. ***22-Epihippuristan-11-one***
[858950-55-7]
$C_{28}H_{44}O_5$ 460.653
Constit. of *Isis hippuris*. Powder.
Mp 165-167°. $[\alpha]_D$ +38 (c, 0.16 in $CHCl_3$).

Higa, T. *et al., Chem. Lett.*, 1981, 1647-1650 (*Hippuristanol, 22-Epihippuristanol*)
Martin, G.E. *et al., Steroids*, 1983, **41**, 637-642 (*config*)
Rao, C.B. *et al., J. Nat. Prod.*, 1988, **51**, 954-958 (*Ac derivs*)
Chao, C.H. *et al., J. Nat. Prod.*, 2005, **68**, 880-885 (*22-Epihippuristan-11-one*)

22,25-Epoxy-24-methylfurost-5-ene-3,20-diol E-456



$C_{28}H_{44}O_4$ 444.653

(3β,20β,22*R*,24*S*)-*form* [205503-43-1]
Constit. of *Sarcophyton crassocaule*.
Cryst.
Mp 198-200°. $[\alpha]_D^{25}$ -23.3 (c, 0.002 in $CHCl_3$).

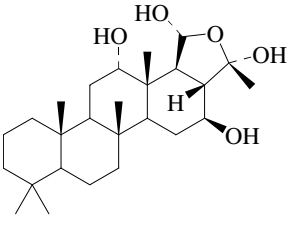
3-Ac: [205503-45-3]
$C_{30}H_{46}O_5$ 486.69
Constit. of *Sarcophyton crassocaule*. Oil. $[\alpha]_D^{25}$ -61.5 (c, 0.002 in $CHCl_3$).

(3β,20β,22*S*,24*S*)-*form* [205503-42-0]
Constit. of *Sarcophyton crassocaule*.
Cryst.
Mp 213-216°. $[\alpha]_D^{25}$ -38 (c, 0.001 in $CHCl_3$).

3-Ac: [205503-44-2]
$C_{30}H_{46}O_5$ 486.69
Constit. of *Sarcophyton crassocaule*. Cryst.
Mp 180-184°. $[\alpha]_D^{25}$ -74.4 (c, 0.002 in $CHCl_3$).

Anjaneyulu, A.S.R. *et al., J. Chem. Res., Synop.*, 1997, 450-451; *J. Chem. Res., Miniprint*, 1997, 2743-2757 (*isol, pmr, cmr*)

24,25-Epoxy-24-methyl-12,16,24,25-scalaranetetrol E-457



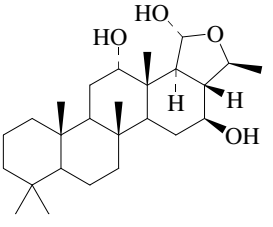
$C_{26}H_{44}O_5$ 436.631

(12α,16β,24α,25α)-*form*

24,25-Di-Me ether, 12-Ac: [478364-21-5]
$C_{30}H_{50}O_6$ 506.721
Constit. of a *Phyllospongia* sp. Cryst. (MeOH aq.).
Mp 170-171°. $[\alpha]_D^{23}$ +58 (c, 0.5 in $CHCl_3$).

Roy, M.C. *et al., J. Nat. Prod.*, 2002, **65**, 1838-1842 (*isol, pmr, cmr*)

24,25-Epoxy-24-methyl-12,16,25-scalaranetriol E-458

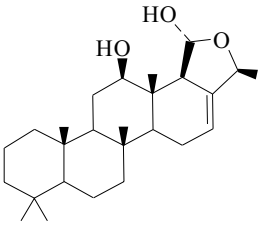


$C_{26}H_{44}O_4$ 420.631

(12α,16β,24α*H*,25α)-*form*

12-Ac: [478364-19-1]
$C_{28}H_{46}O_5$ 462.668
Constit. of a *Phyllospongia* sp. Amorph. solid.
Mp 128-130°. $[\alpha]_D^{23}$ +42 (c, 1.8 in $CHCl_3$).
Roy, M.C. *et al., J. Nat. Prod.*, 2002, **65**, 1838-1842 (*isol, pmr, cmr*)

24,25-Epoxy-24-methyl-16-scalarene-12,25-diol E-459

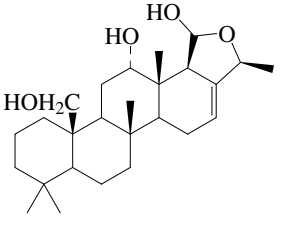


$C_{26}H_{42}O_3$ 402.616

(12β,25α)-*form*

12-Deacetyl-20-methyl-12-epideoxoscalarin
[85337-12-8]
Constit. of *Chromodoris sedna*.
Glass. Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane. $[\alpha]_D^{23}$ +4.2 (c, 0.33 in $CHCl_3$).
Hochlowski, J.E. *et al., J.O.C.*, 1983, **48**, 1738

24,25-Epoxy-24-methyl-16-scalarene-12,22,25-triol E-460



(12α,25ξ)-*form*

$C_{26}H_{42}O_4$ 418.615

(12α,25ξ)-*form*

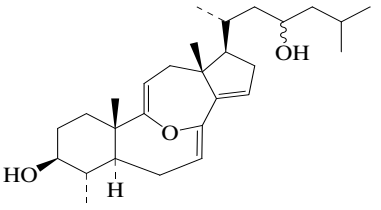
12-Ac: ***22-Hydroxy-24-methyldeoxoscalarin***
[85354-71-8]
$C_{28}H_{44}O_5$ 460.653
Constit. of *Chromodoris sedna*. Oil.

25-Me ether, 12-Ac:
$C_{29}H_{46}O_5$ 474.679
Constit. of *Phyllospongia dendyi*. Needles ($CHCl_3$/petrol).
Mp 200-201°. $[\alpha]_D^{25}$ +14.5 (c, 0.15 in $CHCl_3$).

(12β,25α)-*form*

22-Ac: [264254-87-7]
$C_{28}H_{44}O_5$ 460.653
Constit. of *Glossodoris sedna* and *Glossodoris dalli*. Oil. $[\alpha]_D$ -35.5 (c, 0.1 in $CHCl_3$).
Hochlowski, J.E. *et al., J.O.C.*, 1983, **48**, 1738-1740 (*12-Ac*)
Rao, C.B. *et al., Indian J. Chem., Sect. B*, 1993, **32**, 288 (*isol, pmr, cmr*)
Fontana, A. *et al., J. Nat. Prod.*, 2000, **63**, 527-530 (*Glossodoris sedna constit*)

8,9-Epoxy-4-methyl-8,9-secocholesta-7,9(11),14-triene-3,23-diol E-461

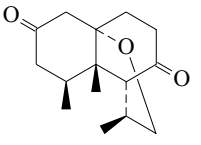


$C_{28}H_{44}O_3$ 428.654

(3β,4α,5α,23ξ)-*form*

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-galactopyranoside]:
Eryloside L†
[781648-14-4]
$C_{40}H_{64}O_{13}$ 752.938
Constit. of *Erylus lendenfeldi*. Amorph. powder. $[\alpha]_D^{20}$ +23 (c, 0.2 in MeOH). λ_{max} 202 (MeOH).
Fouad, M. *et al., ARKIVOC*, 2004, **xiii**, 17-27 (*isol, pmr, cmr*)

10,12-Epoxy-2,7-nardosinanedione E-462

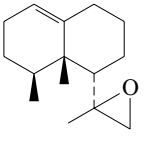


$C_{15}H_{22}O_3$ 250.337

(10α)-*form*

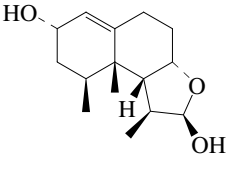
2,7-Nardosinoxanedione
Constit. of *Lemnalia africana*.
Semicrystalline. $[\alpha]_D$ +87 (c, 0.3 in $CHCl_3$).
Jurek, J. *et al., J. Nat. Prod.*, 1993, **56**, 508 (*isol, pmr, cmr*)

11,12-Epoxy-1(10)-nardosinene E-463



$C_{15}H_{24}O$ 220.354
Constit. of *Phyllogorgia dilatata*. Oil. $[\alpha]_D$ -62 (c, 1 in $CHCl_3$).
Kelecom, A. *et al., J. Nat. Prod.*, 1990, **53**, 750 (*isol*)

7,12-Epoxy-1(10)-nardosinene-2,12-diol E-464



(2α,4β,5β,6α,7α,11β,12β)-*form*

$C_{15}H_{24}O_3$ 252.353

(2α,4β,5β,6α,7α,11β,12β)-*form*

12-Me ether: ***Armatin D***
[745828-19-7]
$C_{16}H_{26}O_3$ 266.38
Constit. of *Nephthea armata*. Oil. $[\alpha]_D^{25}$ -178 (c, 0.1 in $CHCl_3$). λ_{max} 204 (log ϵ 3.6) (MeOH).

2-Ketone: 7,11-Epoxy-12-hydroxy-1(10)-nardosinen-2-one

2-Ketone, 12-Me ether: ***Armatin E***
[745828-20-0]
$C_{16}H_{24}O_3$ 264.364
Constit. of *Nephthea armata*. Amorph. solid. $[\alpha]_D^{25}$ -28 (c, 0.2 in $CHCl_3$). λ_{max} 239 (log ϵ 4.7) (MeOH).

2-Ketone, 12-ketone (lactone): 2-Oxo-1(10)-nardosinen-12,7-olide. 1(10)-Lemnalene-2,12-dione. ***Armatin F***
[745828-21-1]
$C_{15}H_{20}O_3$ 248.321
Constit. of *Nephthea armata*. Amorph. solid. $[\alpha]_D^{25}$ -11 (c, 0.2 in $CHCl_3$). λ_{max} 246 (log ϵ 4.3) (MeOH).

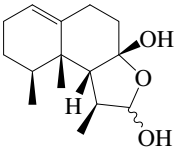
(2α,4β,5β,6α,7β,11β,12α)-*form*
Armatin A
[745828-16-4]
Constit. of *Nephthea armata*.
Amorph. solid. $[\alpha]_D^{25}$ -106 (c, 0.4 in $CHCl_3$). λ_{max} 205 (log ϵ 3.4) (MeOH).

12-Me ether: ***Armatin C***
[745828-18-6]
$C_{16}H_{26}O_3$ 266.38
Constit. of *Nephthea armata*. Amorph. solid. $[\alpha]_D^{25}$ -198 (c, 0.4 in $CHCl_3$). λ_{max} 209 (log ϵ 3.9) (MeOH).

12-Ketone (lactone): 2-Hydroxy-1(10)-nardosinen-12,7-olide. ***Armatin B***
[745828-17-5]
$C_{15}H_{22}O_3$ 250.337
Constit. of *Nephthea armata*. Amorph. solid. $[\alpha]_D^{25}$ -243 (c, 0.8 in $CHCl_3$). λ_{max} 207 (log ϵ 3.5) (MeOH).

(2β,4β,5β,6α,7α,11β,12β)-*form* [77209-64-4]
Constit. of *Lemnalia africana*.
Cryst.
Mp 129-131°. $[\alpha]_D$ -38 (c, 0.13 in $CHCl_3$).
Bowden, B.F. *et al., Aust. J. Chem.*, 1980, **33**, 2737-2747 (*Lemnalia africana constit*)
El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2004, **67**, 1455-1458 (*Nephthea armata constits*)

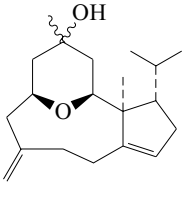
7,12-Epoxy-1(10)-nardosinene-7,12-diol E-465



$C_{15}H_{24}O_3$ 252.353

(7β*OH*,11α*H*,12ξ)-*form* [75222-54-7]
Constit. of *Paralemnalia thyrsoides.*
Cryst.
Mp 142-144°. $[\alpha]_D$ -70.3 (c, 0.2 in $CHCl_3$).
Bowden, B.F. *et al., Aust. J. Chem.*, 1980, **33**, 885-890 (*isol, pmr, cmr*)

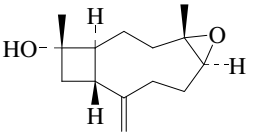
6,10-Epoxy-1(14),4(16)-neodolabelladien-8-ol E-466



$C_{20}H_{32}O_2$ 304.472

(6β,10β,8ξ)-*form*
Constit. of a *Lobophytum* coral.
Gum. $[\alpha]_D^{30}$ -66.7 (c, 0.15 in $CHCl_3$).
Subrahmanyam, C. *et al., Tetrahedron*, 1992, **48**, 3111 (*isol, pmr, cmr*)

6,7-Epoxy-13-nor-3(15)-caryophyllen-11-ol E-467

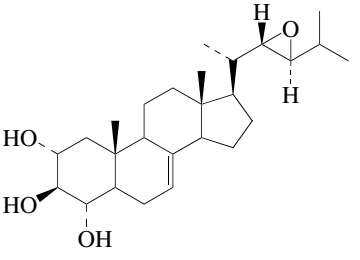


$C_{14}H_{22}O_2$ 222.327

(6*S*,7*S*,11α)-*form*
Nanonorcaryophyllene A
[681145-43-7]
Constit. of *Sinularia nanolobata*.
Oil. $[\alpha]_D^{25}$ +42.6 (c, 1.48 in $CHCl_3$).
Ahmed, A.F. *et al., J. Nat. Prod.*, 2004, **67**, 592-597 (*isol, pmr, cmr*)

22,23-Epoxy-24-norcholest-7-ene-2,3,4-triol E-468

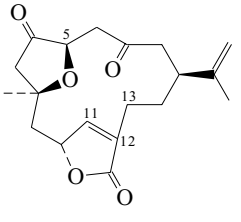
22,23-Epoxy-26,27-dinorergost-7-ene-2,3,4-triol



$C_{26}H_{42}O_4$ 418.615

(2α,3β,4α,22*S*,23*S*)-*form*
4-Sulfate: ***Acanthosterol sulfate A***
[215113-03-4]
$C_{26}H_{42}O_7S$ 498.68
Constit. of an *Acanthodendrilla* sp.
$[\alpha]_D^{25}$ -18 (c, 0.038 in MeOH).
Tsukamoto, S. *et al., J. Nat. Prod.*, 1998, **61**, 1374-1378 (*isol, pmr, cmr*)

5,8-Epoxy-18-nor-3,6-dioxo-11,15-cembradien-20,10-olide E-469



(1*S*,5*R*,8*S*,10*R*)–*form*

$C_{19}H_{24}O_5$ 332.396

(1*S*,5*R*,8*S*,10*R*)-*form*
Norcembrene
[100015-16-5]
Constit. of soft coral *Sinularia numerosa*.
Cryst.
Mp 138-140°. $[\alpha]_D$ -47 (c, 0.01 in $CHCl_3$).

11β,12β-Epoxide: ***5,8:11,12-Diepoxy-18-nor-3,6-dioxo-11,15-cembradien-20,10-olide***
$C_{19}H_{24}O_6$ 348.395
Constit. of *Sinularia inelegans*. Cryst.
Mp 176-177°. $[\alpha]_D$ -36 (c, 0.009 in $CHCl_3$).

(1*S*,5*S*,8*R*,10*R*)-*form*
Scabrolide F
[815587-56-5]
Constit. of *Sinularia scabra*.
Cryst.
Mp 119-120°. $[\alpha]_D^{27}$ -6.3 (c, 0.48 in $CHCl_3$).

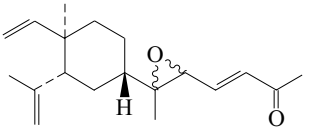
(1*S*,5*S*,8*S*,10*R*)-*form*
Isonorcembrene
[208259-79-4]
Constit. of *Sinularia erecta*.
Oil.

11β,12β-Epoxide: ***Leptocladolide B***
[605659-50-5]
$C_{19}H_{24}O_6$ 348.395
Constit. of *Sinularia leptoclados*. Cryst.
Mp 172-173°. $[\alpha]_D^{25}$ +10 (c, 0.24 in $CHCl_3$).

Sato, A. *et al., Tetrahedron*, 1985, **41**, 4303-4308 (*Sinularia numerosa constit, Sinularia inelegans constit, cryst struct*)
Rudi, A. *et al., J. Nat. Prod.*, 1998, **61**, 872-875 (*Isonorcembrene*)
Ahmed, A.F. *et al., Tetrahedron*, 2003, **59**, 7337-7344 (*Leptocladolide B*)
Ahmed, A.F. *et al., J. Nat. Prod.*, 2004, **67**, 2079-2082 (*Scabrolide F*)

13,15-Epoxy-20-nor-8,10,16-lobatrien-18-one E-470

[154473-65-1]

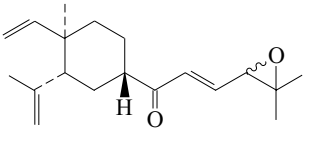


$C_{19}H_{28}O_2$ 288.429
Constit. of *Lobophytum pauciflorum*.
$[\alpha]_D^{25}$ +16.8 (c, 1 in $CHCl_3$).

Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1993, **32**, 1198 (*isol, pmr*)

17,18-Epoxy-14-nor-8,10,15-lobatrien-13-one E-471

[154473-66-2]

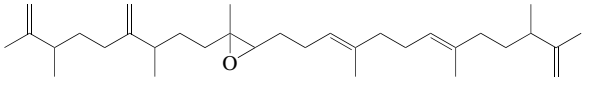


$C_{19}H_{28}O_2$ 288.429
Constit. of *Lobophytum pauciflorum*.
$[\alpha]_D^{25}$ +21.2 (c, 0.9 in $CHCl_3$).

Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1993, **32**, 1198 (*isol, pmr*)

14,15-Epoxy-2,3,6,10,15,18,22,23-octamethyl-19-methylene-1,6,10,23-tetracosatetraene E-472

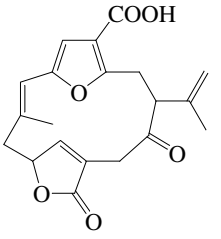
[188554-72-5]



$C_{33}H_{56}O$ 468.805
Constit. of *Botryococcus braunii*.

Delahais, V. *et al., Phytochemistry*, 1997, **44**, 671-678 (*isol, pmr, cmr, ms*)

3,6-Epoxy-14-oxo-3,5,7,11,15-cembrapentaen-20,10-olid-18-oic acid E-473

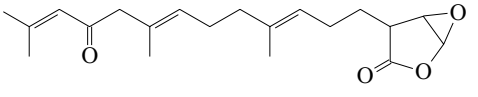


$C_{20}H_{20}O_6$ 356.374

(1ξ,7*E*,10ξ)-*form*
Me ester: ***Acerosolide***
[132235-61-1]
$C_{21}H_{22}O_6$ 370.401
Isol. from the gorgonian *Pseudopterogorgia acerosa* after methylation. Gum. $[\alpha]_D$ +35 (c, 0.43 in $CHCl_3$). Dec. on storage.
λ_{max} 253 (ε 6800) (no solvent reported).
Chan, W.R. *et al., J.O.C.*, 1991, **56**, 1773-1776 (*isol, uv, pmr, cmr, struct*)
Paquette, L.A. *et al., J.O.C.*, 1993, **58**, 165-169 (*synth*)

1,2-Epoxy-13-oxo-6,10,14-phytatrien-20,1-olide E-474

(4,8,12-Trimethyl-10-oxo-3,7,11-tridecatrienyl)-2,6-dioxabicyclo[3.1.0]hexan-3-one, 9CI



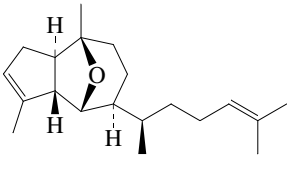
$C_{20}H_{28}O_4$ 332.439

(1ξ,2ξ,6*E*,10*E*)-*form*
Metab. of *Bifurcaria bifurcata*.

*13*S*-Alcohol: 1,2-Epoxy-13-hydroxy-6,10,14-phytatrien-20,1-olide.* ***Epoxyeleganolactone***
[165133-76-6]
$C_{20}H_{30}O_4$ 334.455
Constit. of *Bifurcaria bifurcata*. Oil. $[\alpha]_D^{25}$ -9.1 (c, 2.2 in CH_2Cl_2).

Hougaard, L. *et al., Phytochemistry*, 1991, **30**, 3049 (*isol, pmr, cmr*)
Valls, R. *et al., Phytochemistry*, 1995, **39**, 145 (*deriv*)
Li, J. *et al., Chin. Chem. Lett.*, 1997, **8**, 595-598 (*synth*)

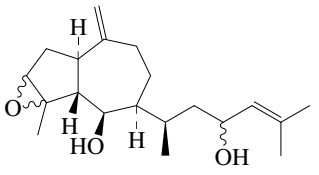
6,10-Epoxy-3,14-pachydictyadiene E-475



$C_{20}H_{32}O$ 288.472

(1α,5β,6β,10β,11*R*)-*form*
Dictyoxide†
[73542-75-3]
Constit. of *Dilophus ligulatus* and *Dictyota dichotoma*.
Oil. $[\alpha]_D$ +10.1 (c, 1 in $CHCl_3$).
Amico, V. *et al., Phytochemistry*, 1979, **18**, 1895-1897 (*isol, struct*)
Enoki, N. *et al., Chem. Lett.*, 1983, 1627-1630 (*isol*)

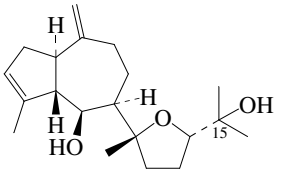
3,4-Epoxy-10(18),14-pachydictyadiene-6,13-diol E-476



$C_{20}H_{32}O_3$ 320.471

(1α,3ξ,4ξ,5β,6β,11*R*,13ξ)-*form*
3,4-Epoxy-13-hydroxypachydictyol A
[604807-32-1]
Constit. of *Dictyota dichotoma*.
Gedara, S.R. *et al., Z. Naturforsch., C*, 2003, **58**, 17-22 (*isol, pmr, cmr*)

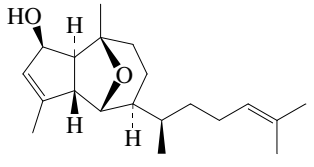
11,14-Epoxy-3,10(18)-pachydictyadiene-6,15-diol E-477



$C_{20}H_{32}O_3$ 320.471

(1α,5β,6β,11*R*,14*S*)-*form*
Deacetyldictyol H. *Deacetoxydictyol H (incorr.)*
[133585-93-0]
Constit. of *Dictyota divaricata*.
Oil. $[\alpha]_D^{25}$ +45.7 (c, 0.002 in $CHCl_3$).
15-Ac: ***Dictyol H***
[96627-35-9]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Dictyota dentata*. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{32}$ +7.1 (c, 1.7 in $CHCl_3$).
Alvarado, A.B. *et al., J. Nat. Prod.*, 1985, **48**, 132-134 (*Dictyol H, isol, struct*)
König, G.M. *et al., Tetrahedron*, 1991, **43**, 1399-1410 (*Deacetyldictyol H*)

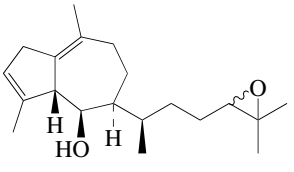
6,10-Epoxy-3,14-pachydictyadien-2-ol E-478



$C_{20}H_{32}O_2$ 304.472

(1α,2β,5β,6β,10β,11*R*)-*form*
2-Hydroxydictyoxide
Isol. from *Dictyota divaricata*.
Oil. $[\alpha]_D^{25}$ -37.8 (c, 0.09 in $CHCl_3$).
König, G.M. *et al., Tetrahedron*, 1991, **47**, 1399-1410 (*2-Hydroxydictyoxide*)

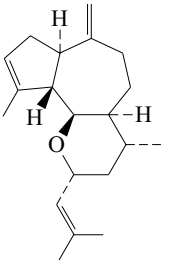
14,15-Epoxy-1(10),3-pachydictyadien-6-ol E-479



$C_{20}H_{32}O_2$ 304.472

(5β,6β,11*R*,14ξ)-*form*
Acutilol A
[182284-97-5]
Constit. of *Dictyota acutiloba*. Feeding deterrent. Oil. $[\alpha]_D^{25}$ +29.8 (c, 1.5 in $CHCl_3$). λ_{max} (MeOH) (Berdy).
Ac: ***Acutilol A acetate***
[182246-61-3]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Dictyota acutiloba*. Feeding deterrent. Oil. $[\alpha]_D^{25}$ +29.6 (c, 2 in $CHCl_3$). λ_{max} (MeOH) (Berdy).
Hardt, I.H. *et al., Phytochemistry*, 1996, **43**, 71-73 (*isol, pmr, cmr*)

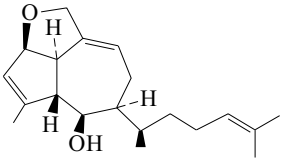
6,13-Epoxy-3,10(18),14-pachydictyatriene E-480



$C_{20}H_{30}O$ 286.456

(1α,5β,6β,11*R*,13*R*)-*form*
Dictyoxide A†
[93754-87-1]
Constit. of *Dictyota binghamiae*.
Oil. $[\alpha]_D^{21}$ -5.6 (c, 0.16 in $CHCl_3$).
Pathirana, C. *et al., Can. J. Chem.*, 1984, **62**, 1666-1671 (*isol, pmr, cmr*)

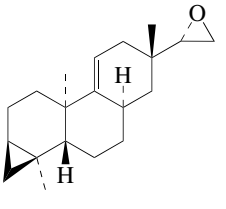
2,18-Epoxy-3,9,14-pachydictyatrien-6-ol E-481



$C_{20}H_{30}O_2$ 302.456

(1α,2β,5β,6β,11*R*)-*form*
Dictyol A
[61263-82-9]
Constit. of *Dictyota dichotoma* and *Aplysia depilans*.
Cryst. (hexane).
Mp 84-86°. $[\alpha]_D$ +79.6 ($CHCl_3$).
Fattorusso, E. *et al., Chem. Comm.*, 1976, 575-576 (*isol*)
Minale, L. *et al., Tet. Lett.*, 1976, 2711-2714 (*isol*)

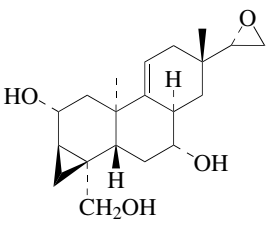
15,16-Epoxy-9(11)-parguerene E-482



$C_{20}H_{30}O$ 286.456

(ent*-15*R*)-*form [202870-60-8]
Constit. of *Laurencia saitoi*.
Oil. $[\alpha]_D^{26}$ -37.6 (c, 0.644 in $CHCl_3$).
Kurata, K. *et al., Phytochemistry*, 1998, **47**, 363-369 (*isol, pmr, cmr*)

15,16-Epoxy-9(11)-parguerene-2,7,19-triol E-483

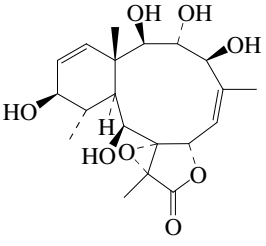


$C_{20}H_{30}O_4$ 334.455

(*ent*-2β,7β,15*R*)-*form*

2-Ac: [132342-74-6]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Laurencia saitoi*. Oil. $[\alpha]_D^{26}$ -49.9 (c, 1.11 in $CHCl_3$).
Takeda, S. *et al., Bull. Chem. Soc. Jpn.*, 1990, **63**, 3066 (*pmr*)
Kurata, K. *et al., Phytochemistry*, 1998, **47**, 363-369 (*isol*)

8,17-Epoxy-2,3,4,9,12-pentahydroxy-5,13-briaradien-18,7-olide E-484

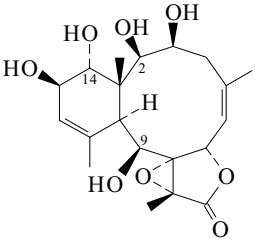


$C_{20}H_{28}O_8$ 396.436

(2β,3α,4β,5*Z*,7α,8α,9β,11α,12β,17α)-*form*

2,3,4,9-Tetra-Ac: ***Violide S***
[851723-73-4]
$C_{28}H_{36}O_{12}$ 564.585
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +51 (c, 0.11 in MeOH).
Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 607-617 (*Violide S*)

8,17-Epoxy-2,3,9,13,14-pentahydroxy-5,11-briaradien-18,7-olide E-485



$C_{20}H_{28}O_8$ 396.436

(2β,3β,5*Z*,7α,8α,9β,13β,14α,17α)-*form*

2,3,9,14-Tetra-Ac: ***Stecholide J***
[152339-97-4]
$C_{28}H_{36}O_{12}$ 564.585
Constit. of *Solenopodium excavatum*. Cryst.
Mp 204°. $[\alpha]_D^{20}$ -39.2 (c, 0.5 in $CHCl_3$).

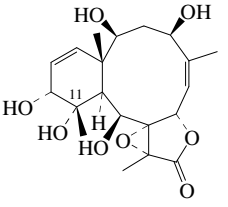
3-Butanoyl, 2,9,14-tri-Ac: ***Stecholide I***
[152339-96-3]
$C_{30}H_{40}O_{12}$ 592.639
Constit. of *Solenopodium excavatum*. Cryst. (MeOH).
Mp 116-118°. $[\alpha]_D^{20}$ -40.8 (c, 2.55 in $CHCl_3$).

11β,12β-Epoxide, 3-butanoyl, 2,9,14-tri-Ac: ***Stecholide M***
[152340-00-6]
$C_{30}H_{40}O_{13}$ 608.638
Constit. of *Solenopodium excavatum*. Cryst.
Mp 108°. $[\alpha]_D^{20}$ -62.6 (c, 0.26 in $CHCl_3$).

11β,12β-Epoxide, 2,3,9,14-tetra-Ac: ***Stecholide L***
[152339-99-6]
$C_{28}H_{36}O_{13}$ 580.585
Constit. of *Solenopodium excavatum*. Cryst.
Mp 148-150°. $[\alpha]_D^{20}$ -53.3 (c, 2.28 in $CHCl_3$).

11β,12β-Epoxide, 2,3,9,13,14-penta-Ac: ***Stecholide K***
[152339-98-5]
$C_{30}H_{38}O_{14}$ 622.622
Constit. of *Solenopodium excavatum*. Glass. $[\alpha]_D^{20}$ -58.5 (c, 0.39 in $CHCl_3$).
Schmitz, F.J. *et al., J. Nat. Prod.*, 1993, **56**, 1339 (*isol, pmr, cmr, cryst struct*)

8,17-Epoxy-2,4,9,11,12-pentahydroxy-5,13-briaradien-18,7-olide E-486



(2β,4β,5*Z*,7α,8α,9β,11α,12α,17α)-*form*

$C_{20}H_{28}O_8$ 396.436

(2β,4β,5*Z*,7α,8α,9β,11α,12α,17α)-*form*

2,4,9-Tri-Ac: [125239-52-3]
$C_{26}H_{34}O_{11}$ 522.548
Constit. of a *Briareum* sp. (DD6). Glass. $[\alpha]_D$ +4.7 (c, 0.66 in $CHCl_3$).

2,4,9,12-Tetra-Ac: ***Briarlide N***
[125239-53-4]
[845641-24-9]
$C_{28}H_{36}O_{12}$ 564.585
Constit. of a *Briareum* sp. (DD6). Glass or amorph. solid.
$[\alpha]_D$ -44.7 (c, 0.57 in $CHCl_3$). $[\alpha]_D$ -83 (c, 0.07 in MeOH).

4-Hexanoyl, 2,9-di-Ac: ***Violide I***
[243972-87-4]
$C_{30}H_{42}O_{11}$ 578.655
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ -3.1 (c, 0.13 in MeOH).
λ_{max} 205 (ϵ 7100) (MeOH).

4-Octanoyl, 2,9-di-Ac: ***Violide H***
[230647-96-8]
$C_{32}H_{46}O_{11}$ 606.709
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ -0.8 (c, 0.66 in MeOH).
λ_{max} 206 (ϵ 7600) (MeOH).

4-Octanoyl, 2,9,12-tri-Ac: ***Briarlide L***
[845641-22-7]
$C_{34}H_{48}O_{12}$ 648.746
Constit. of a *Briareum* sp. Amorph. solid. $[\alpha]_D$ -45 (c, 0.007 in MeOH).

(2β,4β,5*Z*,7α,8α,9β,11β,12α,17α)-*form*

2,4,9,12-Tetra-Ac: Constit. of a *Briareum* sp. (DD6).
Glass. $[\alpha]_D$ -73 (c, 0.27 in $CHCl_3$).

4-Propanoyl, 2,9,12-tri-Ac: ***Excavatolide Y***
[247921-84-2]
$C_{29}H_{38}O_{12}$ 578.612
Constit. of *Briareum excavatum*. Solid.
Mp 147-148°. $[\alpha]_D^{27}$ -71 (c, 0.4 in $CHCl_3$).

12-Butanoyl, 2,4,9-tri-Ac: ***Excavatolide X***
[247921-83-1]
$C_{30}H_{40}O_{12}$ 592.639

Constit. of *Briareum excavatum*. Solid.
Mp 189-190°. $[\alpha]_D^{27}$ -61 (c, 0.2 in $CHCl_3$).

(2β,4β,5*Z*,7α,8α,9β,11β,12β,17α)-*form*

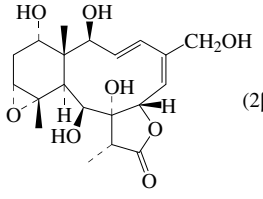
2,9,12-Tri-Ac: ***Briaexcavatolide S***
[593278-99-0]
$C_{26}H_{34}O_{11}$ 522.548
Constit. of *Briareum excavatum*. Powder.
Mp 227-229°. $[\alpha]_D^{27}$ -79 (c, 0.1 in Me_2CO).

12-Butanoyl, 2,9-di-Ac: ***Briaexcavatolide W***
[690267-90-4]
$C_{28}H_{38}O_{11}$ 550.602
Constit. of *Briareum excavatum*. Powder (EtOAc).
Mp 97.5-98.9°. $[\alpha]_D^{27}$ -129 (c, 0.24 in $CHCl_3$).

4-Octanoyl, 2,9-di-Ac: ***Violide R***
[851723-72-3]
$C_{32}H_{46}O_{11}$ 606.709
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +14 (c, 0.08 in MeOH).

Bowden, B.F. *et al., Aust. J. Chem.*, 1989, **42**, 1705 (*isol, pmr, cmr*)
Iwagawa, T. *et al., Heterocycles*, 1999, **51**, 1653-1659 (*Violides*)
Sheu, J.H. *et al., J. Nat. Prod.*, 1999, **62**, 1415-1420 (*Excavatolides*)
Wu, S.-L. *et al., J. Nat. Prod.*, 2003, **66**, 1252-1256 (*Briaexcavatolide S*)
Wu, S.-L. *et al., Heterocycles*, 2004, **63**, 895-898 (*Briaexcavatolide W*)
Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 607-617 (*Violide R*)
Iwagawa, T. *et al., J. Nat. Prod.*, 2005, **68**, 31-35 (*Briarlides L and N*)

11,12-Epoxy-2,8,9,14,16-pentahydroxy-3,5-briaradien-18,7-olide E-487



(2β,3*E*,5*E*,7α,8α,9β,11α,12α,14α)-*form*

$C_{20}H_{28}O_8$ 396.436

(2β,3*E*,5*E*,7α,8α,9β,11α,12α,14α)-*form*

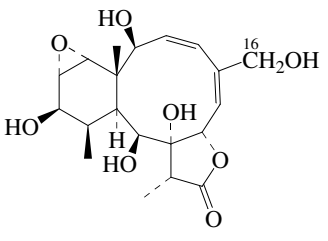
2,9,14,16-Tetra-Ac: [753001-77-3]
$C_{28}H_{36}O_{12}$ 564.585
Constit. of a *Pteroeides* sp. Solid. $[\alpha]_D^{26}$ -62 (c, 0.383 in $CHCl_3$).

(2β,3*Z*,5*E*,7α,8α,9α,11α,12α,14α)-*form*

2,9,14-Tri-Ac: ***Minabein 10***
[104993-15-9]
$C_{26}H_{34}O_{11}$ 522.548
Constit. of *Minabea* sp. Powder.
Mp 135-138°.

Ksebati, M.B. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 835-851 (*Minabein 10*)
Tanaka, C. *et al., J. Nat. Prod.*, 2004, **67**, 1368-1373 (*Pteroeides constit*)

13,14-Epoxy-2,8,9,12,16-pentahydroxy-3,5-briaradien-18,7-olide E-488



$C_{20}H_{28}O_8$ 396.436

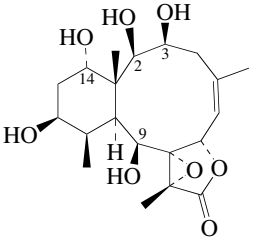
(2β,3*Z*,5*E*,7α,8α,9β,12β,13α,14α)-*form*

9,12-Di-Ac: ***Briaexcavatolide N***
[334831-92-4]
$C_{24}H_{32}O_{10}$ 480.511
Constit. of *Briareum excavatum*. Powder.
Mp 174-175°. $[\alpha]_D^{26}$ -23 (c, 0.2 in $CHCl_3$). λ_{max} 236 (log ϵ 3.94) (MeOH).

16-Deoxy,16-chloro, 9,12-di-Ac: ***Briaexcavatolide M***
[334831-91-3]
Constit. of *Briareum excavatum*.
Powder.
Mp 211-213°. $[\alpha]_D^{26}$ -29 (c, 0.1 in $CHCl_3$). λ_{max} 234 (log ϵ 3.97) (MeOH).

Sung, P.-J. *et al., J. Nat. Prod.*, 2001, **64**, 318-323 (*isol, pmr, cmr*)

8,17-Epoxy-2,3,9,12,14-pentahydroxy-5-briaren-18,7-olide E-489



$C_{20}H_{30}O_8$ 398.452

3,14-Di-Ac: ***Excavatolide M***
[221664-95-5]
$C_{24}H_{34}O_{10}$ 482.527
Constit. of *Briareum excavatum*. Solid.
Mp 219-221°. $[\alpha]_D^{26}$ +74 (c, 0.6 in $CHCl_3$).

3,9,14-Tri-Ac: ***Excavatolide D***
[205581-12-0]
$C_{26}H_{36}O_{11}$ 524.564
Constit. of *Briareum excavatum*. Cryst.
Mp 235-237°. $[\alpha]_D^{24}$ +32 (c, 0.38 in $CHCl_3$).

2,3,9,14-Tetra-Ac: ***Excavatolide C***
[205581-11-9]
$C_{28}H_{38}O_{12}$ 566.601
Constit. of *Briareum excavatum*. Cryst.
Mp 134-135°. $[\alpha]_D^{30}$ -13 (c, 0.18 in $CHCl_3$).

Penta-Ac: ***Excavatolide K***
[221664-93-3]
$C_{30}H_{40}O_{13}$ 608.638
Constit. of *Briareum excavatum*. Solid.
Mp 178-180°. $[\alpha]_D^{26}$ +35 (c, 0.7 in $CHCl_3$).

12-Propanoyl, 2,3,9,14-tetra-Ac: ***Excavatolide V***
[247921-81-9]
$C_{31}H_{42}O_{13}$ 622.665
Constit. of *Briareum excavatum*. Powder.
Mp 183-185°. $[\alpha]_D^{25}$ +40 (c, 0.6 in $CHCl_3$).

3-Butanoyl, 14-Ac: ***Briarenol A***
[876305-44-1]
$C_{26}H_{38}O_{10}$ 510.58
Constit. of a *Briareum* sp. Powder.
Mp 104-105°. $[\alpha]_D^{25}$ +21 (c, 1.2 in $CHCl_3$).

3-Butanoyl, 2,9,14-tri-Ac: ***Excavatolide B***
[205581-10-8]
$C_{30}H_{42}O_{12}$ 594.655
Constit. of *Briareum excavatum*. Cryst. (Me_2CO).
Mp 224-225°. $[\alpha]_D^{26}$ -23 (c, 0.09 in $CHCl_3$).

3-Butanoyl, 2,9,12,14-tetra-Ac: ***Excavatolide I***
[221664-91-1]
$C_{32}H_{44}O_{13}$ 636.692
Constit. of *Briareum excavatum*. Solid.
Mp 225-227°. $[\alpha]_D^{26}$ +23 (c, 1 in $CHCl_3$).

3-Butanoyl, 12-propanoyl, 2,9,14-tri-Ac: ***Excavatolide U***
[247921-80-8]
$C_{33}H_{46}O_{13}$ 650.719
Constit. of *Briareum excavatum*. Cryst.
Mp 169-170°. $[\alpha]_D^{25}$ +34 (c, 0.8 in $CHCl_3$).

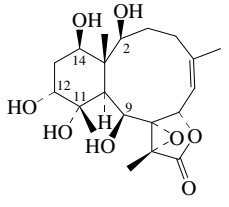
12-Butanoyl, 2,3,9,14-tetra-Ac: ***Excavatolide J***
[221664-92-2]
$C_{32}H_{44}O_{13}$ 636.692
Constit. of *Briareum excavatum*. Solid.
Mp 203-205°. $[\alpha]_D^{26}$ +38 (c, 0.6 in $CHCl_3$).

3,12-Dibutanoyl, 2,9,14-tri-Ac: ***Excavatolide H***
[221664-90-0]
$C_{34}H_{48}O_{13}$ 664.745
Constit. of *Briareum excavatum*. Solid.
Mp 189-190°. $[\alpha]_D^{27}$ +27 (c, 0.3 in $CHCl_3$).

12-Octanoyl, 3-butanoyl, 2,9,14-tri-Ac: ***Briaexcavatolide R***
[383414-39-9]
$C_{38}H_{56}O_{13}$ 720.853
Constit. of *Briareum excavatum*. Powder.
Mp 150-151°. $[\alpha]_D^{25}$ -39 (c, 0.8 in $CHCl_3$).

Sheu, J.-H. *et al., J. Nat. Prod.*, 1998, **61**, 602-608; 1999, **62**, 1415-1420 (*isol, pmr, cmr, cryst struct*)
Sung, P.-J. *et al., J. Nat. Prod.*, 1999, **62**, 457-465 (*Excavatolides H,I,J,K,M*)
Wu, S.-L. *et al., J. Nat. Prod.*, 2001, **64**, 1415-1420 (*Briaexcavatolide R*)
Sung, P.-J. *et al., Nat. Prod. Res.*, 2005, **19**, 689-694 (*Briarenol A*)

8,17-Epoxy-2,9,11,12,14-pentahydroxy-5-briaren-18,7-olide E-490



(2β,5*Z*,7α,8α,9β,11α,12α,14β)-*form*

$C_{20}H_{30}O_8$ 398.452

(2β,5*Z*,7α,8α,9β,11α,12α,14β)-*form*

2,9,14-Tri-Ac: ***Briareolide B***
[132750-54-0]
$C_{26}H_{36}O_{11}$ 524.564
Constit. of a *Briareum* sp. Antiinflammatory agent. Needles (Me_2CO/hexane).
Mp 249-250°.

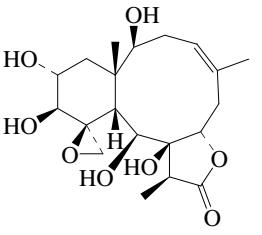
2-Butanoyl, 9,14-di-Ac: ***Briareolide A***
[132750-53-9]
$C_{28}H_{40}O_{11}$ 552.617
Constit. of a *Briareum* sp. Antiinflammatory agent. Needles (Me_2CO/hexane).
Mp 242-243°.

(2β,5*Z*,7α,8α,9β,11β,12α,14α)-*form*

12-Butanoyl, 2,14-di-Ac: ***Excavatolide Z***
[247921-85-3]
Constit. of *Briareum excavatum*.
Powder.
Mp 257-259°. $[\alpha]_D^{25}$ +22 (c, 0.5 in $CHCl_3$).

Pordesimo, E.O. *et al., J.O.C.*, 1991, **56**, 2344 (*Briareolides*)
Sheu, J.H. *et al., J. Nat. Prod.*, 1999, **62**, 1415-1420 (*Excavatolide Z*)

11,20-Epoxy-2,8,9,12,13-pentahydroxy-4-briaren-18,7-olide E-491



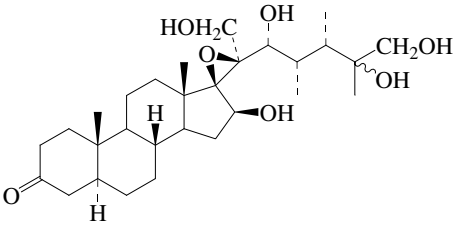
$C_{20}H_{30}O_8$ 398.452

(2β,4*Z*,7α,8β,9β,10β,11β,12β,13α)-*form*

13-(3-Methylbutanoyl), 2,9,12-tri-Ac: ***Juncenolide B***
[496953-48-1]
$C_{31}H_{44}O_{12}$ 608.681
Constit. of *Junceella juncea*.

Krishna, N. *et al., Asian J. Chem.*, 2003, **15**, 344-348; *CA*, **138**, 166835u (*isol, pmr, cmr*)

17,20-Epoxy-16,21,22,25,26-pentahydroxy-23-methylergostan-3-one E-492



$C_{29}H_{48}O_7$ 508.694

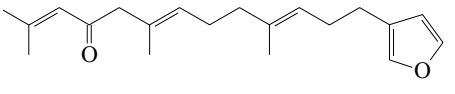
(5α,16β,17β,20*S*,22*R*,23*S*,24*S*,25ξ)-*form*

21,22,26-Tri-Ac: ***Hippuristerone J***
[868395-82-8]
$C_{35}H_{54}O_{10}$ 634.806
Constit. of *Isis hippuris*. Powder.
Mp 124-125°. $[\alpha]_D$ -5 (c, 0.32 in $CHCl_3$).

Chao, C.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1366-1370 (*Hippuristerone J*)

1,20-Epoxy-1,3(20),6,10,14-phytapentaen-13-one E-493

13-(3-Furanyl)-2,6,10-trimethyl-2,6,10-tridecatrien-4-one, 9CI.
(10-Oxo-4,8,12-trimethyl-3,7,11-tridecatrienyl)furan



$C_{20}H_{28}O_2$ 300.44

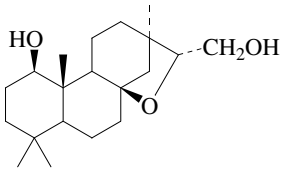
(6*E*,10*E*)-*form*

13-Oxoambliofuran
[137761-11-6]
Metab. of *Bifurcaria bifurcata*.

*13*S*-Alcohol: 1,20-Epoxy-1,3(20),6,10,14-phytapentaen-13-ol.* ***Bifurcane***
$C_{20}H_{30}O_2$ 302.456
Constit. of *Bifurcaria bifurcata*. Toxic to sea urchins. Oil.
$[\alpha]_D^{25}$ -7.6 (c, 9.5 in EtOH).

Hougaard, L. *et al., Phytochemistry*, 1991, **30**, 3049 (*isol, pmr, cmr*)
Valls, R. *et al., Phytochemistry*, 1995, **39**, 145 (*deriv*)

8,15-Epoxy-1,16-pimaranediol E-494

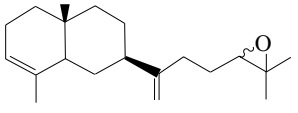


$C_{20}H_{34}O_3$ 322.487

(1β,8β,15*R*)-*form*
Ceriopsin D
[478175-21-2]
Constit. of *Ceriops decandra*.
Oil. $[\alpha]_D^{25}$ +50.6 (c, 1.5 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., Phytochemistry*, 2002, **60**, 777-782 (*isol, pmr, cmr*)

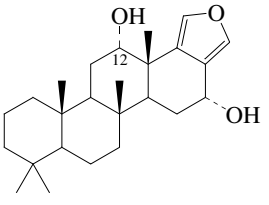
14,15-Epoxy-3,11(18)-prenyleudesmadiene E-495

[81575-71-5]



$C_{20}H_{32}O$ 288.472
Constit. of *Nephthea* sp. Oil. $[\alpha]_D^{20}$ -12.8 (c, 4.6 in CCl_4).
Poet, S.E. *et al., Aust. J. Chem.*, 1982, **35**, 77

24,25-Epoxy-17(24),18(25)-scalaradiene-12,16-diol E-496



(12α,16α)-*form*

$C_{25}H_{38}O_3$ 386.573

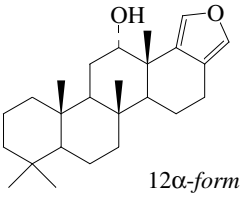
(12α,16α)-*form*
12-Ac: ***Isoscalarafuran B***
[152340-14-2]
$C_{27}H_{40}O_4$ 428.611
Constit. of *Spongia hispida*. Oil.

(12α,16β)-*form*
12-Ac: ***Isoscalarafuran A***
[152340-13-1]
$C_{27}H_{40}O_4$ 428.611
Constit. of *Spongia hispida*. Oil.

(12β,16α)-*form*
Sesterstatin 4
[214358-13-1]
Constit. of *Hyrtios erecta*.
Cryst. (MeCN aq.).
Mp 252-254°. $[\alpha]_D^{25}$ -10 (c, 0.09 in $CHCl_3$).
16-Ketone: 24,25-Epoxy-12-hydroxy-17(24),18(25)-scalaradien-16-one. ***Salmahyrtisol B***
[394248-42-1]
$C_{25}H_{36}O_3$ 384.558
Constit. of *Hyrtios erecta*. Amorph. solid. $[\alpha]_D$ +68 (c, 0.4 in CH_2Cl_2). λ_{max} 226 (log ϵ 2.13); 275 (log ϵ 2.41) (MeOH).

(12β,16β)-*form*
Sesterstatin 5
[214358-14-2]
Constit. of *Hyrtios erecta*.
Cryst. (CH_2Cl_2/MeOH).
Mp 245°. $[\alpha]_D^{25}$ +27 (c, 0.29 in $CHCl_3$). λ_{max} 219 (ϵ 4148) (MeOH).
16-Ac: ***Scalarafuran***
[62008-03-1]
$C_{27}H_{40}O_4$ 428.611
Isol. from *Spongia idia*. Cryst.
Mp 182°. $[\alpha]_D$ -19.8 (c, 0.9 in $CHCl_3$).
Walker, R.P. *et al., J.O.C.*, 1980, **45**, 4976 (*Scalarafuran*)
Davis, R. *et al., Aust. J. Chem.*, 1993, **46**, 1295 (*Isoscalarafurans*)
Pettit, G.R. *et al., Bioorg. Med. Chem. Lett.*, 1998, **8**, 2093-2098 (*Sesterstatins, cryst struct*)
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2002, **65**, 2-6 (*Salmahyrtisol B*)

24,25-Epoxy-17(24),18(25)-scalaradien-12-ol E-497



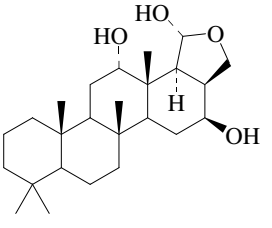
12α-*form*

$C_{25}H_{38}O_2$ 370.574

12α-*form*
Ac:
$C_{27}H_{40}O_3$ 412.611
Constit. of *Spongia officinalis*. Cryst. (hexane).
Mp 130-132°. $[\alpha]_D^{25}$ +68 (c, 0.5 in $CHCl_3$).

12β-*form*
16-Deacetoxyscalarafuran
[75283-88-4]
Constit. of a *Spongia* sp.
Oil. $[\alpha]_D^{25}$ -9.1 (c, 0.076 in $CHCl_3$). λ_{max} 222 (log ϵ 3.4) (MeOH).
De Guilio, A. *et al., J. Nat. Prod.*, 1989, **52**, 1258-1262 (*isol, pmr, cmr*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 2003, **66**, 438-440 (*16-Deacetoxyscalarafuran*)

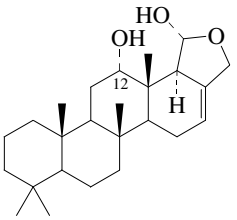
24,25-Epoxy-12,16,25-scalaranetriol E-498



$C_{25}H_{42}O_4$ 406.604

(12α,16β,25α)-*form*
12,16-Di-Ac: [508194-53-4]
$C_{29}H_{46}O_6$ 490.679
Constit. of *Cacospongia scalaris*. Oil. $[\alpha]_D$ -10 (c, 0.07 in CH_2Cl_2).
Tsoukatou, M. *et al., J. Nat. Prod.*, 2003, **66**, 444-446 (*isol, pmr, cmr*)

24,25-Epoxy-16-scalarene-12,25-diol E-499



(12α,25α)-*form*

$C_{25}H_{40}O_3$ 388.589

(12α,25α)-*form*

12-Ac: ***Deoxoscalarin***
[64825-80-5]
$C_{27}H_{42}O_4$ 430.626
Constit. of *Spongia officinalis*, *Glossodoris tricolor*, *Chromodoris funerea* and *Hypselodoris orsini*. Toxic to brine shrimp. Cryst. (CCl_4). Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 166-168°. $[\alpha]_D$ +42.5 (c, 1.1 in $CHCl_3$).

Di-Ac: ***Deoxoscalarin acetate***
$C_{29}H_{44}O_5$ 472.664
Constit. of *Spongia officinalis*. Cryst. (hexane).
Mp 165-168°. $[\alpha]_D^{25}$ +40 (c, 1.5 in $CHCl_3$). λ_{max} 221 (ϵ 4180) (MeOH) (Berdy).

(12β,25α)-*form* [208708-24-1]
Constit. of *Hyrtios erecta* and *Glossodoris atromarginata*.
Cryst.
Mp 218-220°. $[\alpha]_D^{25}$ +17.1 (c, 0.31 in $CHCl_3$). $[\alpha]_D$ +13.5 (c, 0.5 in $CHCl_3$). There are several differences in the cmr data of the two isolates.

12-Ac: ***12-Epideoxoscalarin***
[64825-83-8]
Constit. of *Spongia nitens*.
Cryst. (CCl_4).
Mp 166-168°. $[\alpha]_D$ +42.5 (c, 1.1 in $CHCl_3$).

12-Ketone: ***24,25-Epoxy-25-hydroxy-16-scalaren-12-one***
[247154-63-8]
$C_{25}H_{38}O_3$ 386.573
Constit. of *Glossodoris atromarginata* and *Spongia* sp. Powder. $[\alpha]_D$ +32.6 (c, 0.5 in $CHCl_3$).

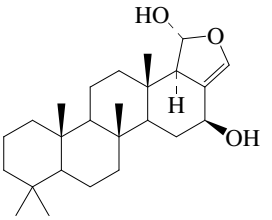
12-Ketone, 25-Ac: [823804-83-7]
$C_{27}H_{40}O_4$ 428.611
Constit. of *Glossodoris rufomarginata*. Oil. $[\alpha]_D$ +17.8 (c, 0.5 in $CHCl_3$).

(*ent*-12β,25α)-*form*

12-Ac: **ent-*12-Epideoxoscalarin***
$C_{27}H_{42}O_4$ 430.626
Constit. of *Spongia officinalis*.

Cimino, G. *et al., J.C.S. Perkin 1*, 1977, 1587 (*struct*)
Walker, R.P. *et al., J.O.C.*, 1980, **45**, 4976
Kernan, M.R. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1988, **89**, 275 (*isol*)
De Guilo, A. *et al., J. Nat. Prod.*, 1989, **52**, 1258-1262 (*Deoxoscalarin acetate, ent-12-Epideoxoscalarin*)
Cimino, G. *et al., Experientia*, 1993, **49**, 582-586 (*isol, Hypselodoris*)
Tsuchiya, N. *et al., J. Nat. Prod.*, 1998, **61**, 468-473 (*isol, pmr, cmr*)
Fontana, A. *et al., J. Nat. Prod.*, 1999, **62**, 1367-1370 (*Glossodoris atromarginata constits*)
Gavagnin, M. *et al., J. Nat. Prod.*, 2004, **67**, 2104-2107 (*Glossodoris rufomarginata constit*)

24,25-Epoxy-17(24)-scalarene-16,25-diol E-500

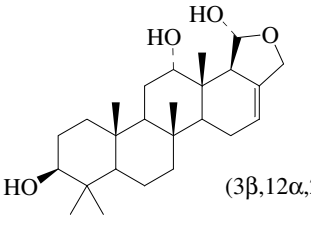


$C_{25}H_{40}O_3$ 388.589

(16β,18α*H*,25α)-*form*

Di-Ac: ***Hyrtiosin E***
[107748-95-8]
$C_{29}H_{44}O_5$ 472.664
Constit. of *Hyrtios erecta*. Powder. $[\alpha]_D^{20}$ -67.9 (c, 0.52 in $CHCl_3$).
Yu, Z.-G. *et al., Helv. Chim. Acta*, 2005, **88**, 1004-1009 (*Hyrtiosin E*)

24,25-Epoxy-16-scalarene-3,12,25-triol E-501



(3β,12α,25α)-*form*

$C_{25}H_{40}O_4$ 404.589

(3β,12α,25α)-*form*

3-Ketone, 12-Ac: ***Deoxoscalarin-3-one***
[154861-85-5]
$C_{27}H_{40}O_5$ 444.61
Constit. of *Chromodoris inornata*. Amorph. solid (MeOH).
Mp 65-67°. $[\alpha]_D^{23}$ +63.6 (c, 0.87 in $CHCl_3$).

(3β,12β,25α)-*form* [208708-23-0]
Condit. of *Hyrtios ereta*.
Cryst.
Mp 229-231°. $[\alpha]_D^{25}$ +11.4 (c, 0.56 in MeOH/$CHCl_3$).

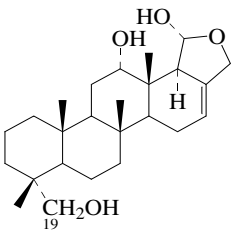
12-Ac: [208708-27-4]
$C_{27}H_{42}O_5$ 446.626
Constit. of *Hyrtios erecta*. Amorph. powder. $[\alpha]_D^{25}$ -10.5 (c, 1.51 in $CHCl_3$).

3-Ketone: 24,25-Epoxy-12,25-dihydroxy-16-scalaren-3-one. ***Salmahyrtisol C***
[208708-22-9]
$C_{25}H_{38}O_4$ 402.573
Constit. of *Hyrtios erecta*. Cryst.
Mp 195-196°. $[\alpha]_D^{25}$ +40.3 (c, 0.65 in $CHCl_3$).

3-Ketone, 12-Ac: ***12-Epideoxoscalarin-3-one***
[153144-79-7]
$C_{27}H_{40}O_5$ 444.61
Constit. of *Chromodoris inornata*. Amorph. solid (MeOH).
Mp 132-135°. $[\alpha]_D^{27}$ +10.2 (c, 0.1 in $CHCl_3$).

Tsuchiya, N. *et al., J. Nat. Prod.*, 1998, **61**, 468-473 (*isol, pmr, cmr, cryst struct*)
Miyamoto, T. *et al., Tetrahedron*, 1999, **55**, 9133-9142 (*3-ketone 12-Ac*)
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2002, **65**, 2-6 (*Salmahyrtisol C*)

24,25-Epoxy-16-scalarene-12,19,25-triol E-502



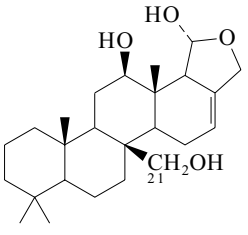
$C_{25}H_{40}O_4$ 404.589

(12α,25α)-*form*

12-Ac: ***21-Hydroxydeoxoscalarin***
[153144-80-0]
$C_{27}H_{42}O_5$ 446.626
Constit. of *Chromodoris inornata*. Amorph. solid (MeOH). Mp 121-122°. $[\alpha]_D^{25}$ +55.4 (c, 0.9 in $CHCl_3$). Two numbering systems in use.

12,19-Di-Ac: ***21-Acetoxydeoxoscalarin***
[153144-81-1]
$C_{29}H_{44}O_6$ 488.663
Constit. of *Chromodoris inornata*. Amorph. solid (MeOH). Mp 70-72°. $[\alpha]_D^{25}$ +60.6 (c, 0.9 in $CHCl_3$).
Miyamoto, T. *et al., Tetrahedron*, 1999, **55**, 9133-9142 (*isol, pmr, cmr*)

24,25-Epoxy-16-scalarene-12,21,25-triol E-503

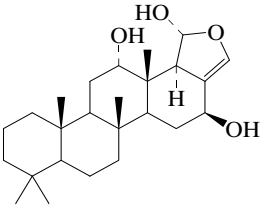


$C_{25}H_{40}O_4$ 404.589

(12β,25α)-*form*

21-Ac: ***21-Acetoxy-12-deacetyl-12-epideoxoscalarin***
$C_{27}H_{42}O_5$ 446.626
Constit. of *Hyatella intestinalis*. Waxy oil.
Karuso, P. *et al., J. Nat. Prod.*, 1989, **52**, 289 (*isol, pmr, cmr*)

24,25-Epoxy-17(24)-scalarene-12,16,25-triol E-504



(12α,16β,18α*H*,25α)-*form*

$C_{25}H_{40}O_4$ 404.589

(12α,16β,18α*H*,25α)-*form*

16,25-Di-Ac: ***12-Epiheteronemin***
[153630-94-5]
$C_{29}H_{44}O_6$ 488.663
Constit. of *Hyrtios erecta*. Cryst.
Mp 175°. $[\alpha]_D$ -35 (c, 0.01 in $CHCl_3$).

Tri-Ac: [107748-94-7]
$C_{31}H_{46}O_7$ 530.7
Constit. of *Hyrtios erecta*. Shows antiinflammatory props. Oil.

(12β,16β,18α*H*,25α)-*form*

25-Ac: ***Hyrtiosin D***
[862200-50-8]
$C_{27}H_{42}O_5$ 446.626
Constit. of *Hyrtios erecta*. Amorph. powder. $[\alpha]_D^{20}$ -16 (c, 0.16 in $CHCl_3$).

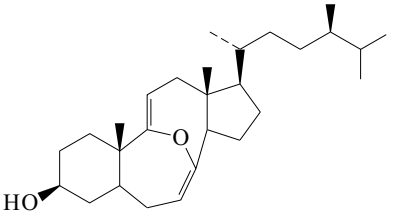
16,25-Di-Ac: ***Heteronemin***
[62008-04-2]
$C_{29}H_{44}O_6$ 488.663
Constit. of *Heteronema erecta*, *Leiosella idia*, *Hyrtios erecta*, *Cacospongia scalaris*, *Hyatella intestinalis* and *Spongia idia*. Toxic to brine shrimp and abalone larvae. Phospholipase A_2 inhibitor. Antiinflammatory. Cryst. (petrol).
Mp 182°. Struct. revised in 1977. λ_{max} 238 (ϵ 11600) (MeOH) (Berdy). λ_{max} 223 (ϵ 1400) (EtOH) (Berdy).

Tri-Ac: [107748-93-6]
Constit. of *Hyrtios erecta*.
Cryst.
Mp 211-212°. $[\alpha]_D$ -30 (c, 0.1 in $CHCl_3$).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1062A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 603A (*nmr*)
Kazlauskas, R. *et al., Tet. Lett.*, 1976, **30**, 2631-2634 (*Heteronemin, isol, struct*)
Kashman, Y. *et al., Tetrahedron*, 1977, **33**, 2997-2998 (*Heteronemin, cmr, stereochem*)
Walker, R.P. *et al., J.O.C.*, 1980, **45**, 4976-4979 (*Spongia idia constit*)
Crews, P. *et al., J. Nat. Prod.*, 1986, **40**, 1041-1052 (*tri-Ac derivs*)
Patil, A.D. *et al., Acta Cryst. C*, 1991, **47**, 1250-1253 (*Heteronemin, cryst struct*)
Bourguet-Kondracki, M.L. *et al., Tet. Lett.*, 1994, **35**, 109 (*12-Epiheteronemin*)
Yu, Z.-G. *et al., Helv. Chim. Acta*, 2005, **88**, 1004-1009 (*Hyrtiosin D*)

8,9-Epoxy-8,9-secoergosta-7,9(11)-dien-3-ol E-505

8,9-Epoxy-24-methyl-8,9-secocholesta-7,9(11)-dien-3-ol

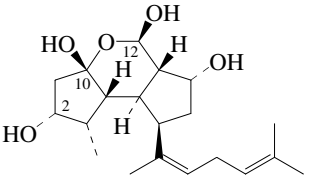


$C_{28}H_{46}O_2$ 414.67

(3β,24*R*)-*form*

Me ether: 8,9-Epoxy-3-methoxy-8,9-secoergosta-7,9(11)-diene.
Jereisterol A
[135474-09-09-8]
$C_{29}H_{48}O_2$ 428.697
Constit. of *Jereicopsis graphidiophora*.
D'Auria, M.V. *et al., Tet. Lett.*, 1991, **32**, 2149-2152 (*isol, pmr*)

10,12-Epoxy-4,10-seco-13(15),17-spatadiene-2,5,10,12-tetrol E-506



$C_{20}H_{32}O_5$ 352.47

(2*R*,5*R*,10*S*,12*R*,13(15)*Z*)-*form*

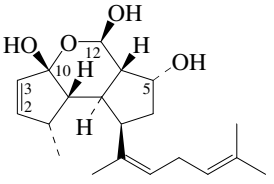
2,10,12-Tri-Me ether, 5-Ac: ***Secospatacetal C***
[243465-68-1]
$C_{25}H_{40}O_6$ 436.587
Constit. of *Dilophus okamurai*.

(2*S*,5*R*,10*S*,12*R*,13(15)*Z*)-*form*

2,10,12-Tri-Me ether, 5-Ac: ***Secospatacetal A***
[243465-66-9]
$C_{25}H_{40}O_6$ 436.587
Constit. of *Dilophus okamurai*.
$[\alpha]_D$ +85.6 (c, 0.1 in MeOH).

10,12-Di-Me ether, 2,5-di-Ac: ***Secospatacetal***
[243465-67-0]
$C_{26}H_{40}O_7$ 464.598
Constit. of *Dilophus okamurai*.
$[\alpha]_D$ +56.1 (c, 0.28 in MeOH).
Yamase, H. *et al., Chem. Pharm. Bull.*, 1999, **47**, 813-818 (*isol, pmr, cmr*)

10,12-Epoxy-4,10-seco-2,13(15),17-spatatriene-5,10,12-triol E-507



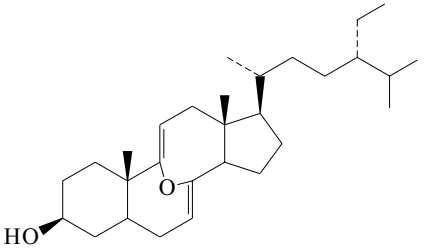
$C_{20}H_{30}O_4$ 334.455

(5*R*,10*S*,12*R*,13(15)*Z*)-*form*

10,12-Di-Me ether, 5-Ac: ***Secospatacetal D***
[243465-69-2]
$C_{24}H_{36}O_5$ 404.545
Constit. of *Dilophus okamurai*.

2,3-Dihydro, 10,12-di-Me ether, 5-Ac: ***Secospatacetal E***
[243465-70-5]
$C_{24}H_{38}O_5$ 406.561
Constit. of *Dilophus okamurai*.
$[\alpha]_D$ +59.4 (c, 0.13 in MeOH).
Yamase, H. *et al., Chem. Pharm. Bull.*, 1999, **47**, 813-818 (*isol, pmr, cmr*)

8,9-Epoxy-8,9-secostigmasta-7,9(11)-dien-3-ol E-508

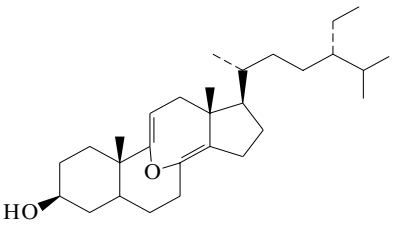


$C_{29}H_{48}O_2$ 428.697

(3β,24*S*)-*form*

Me ether: 8,9-Epoxy-3-methoxy-8,9-secostigmasta-7,9(11)-diene
[156352-63-5]
$C_{30}H_{50}O_2$ 442.724
Constit. of *Microscleroderma spirophora*.
Costantino, V. *et al., Steroids*, 1994, **59**, 181-184 (*isol, pmr, ms*)

8,9-Epoxy-8,9-secostigmasta-8(14),9(11)-dien-3-ol E-509

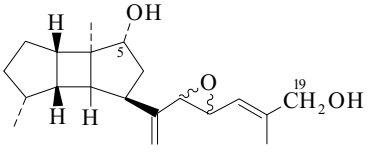


$C_{29}H_{48}O_2$ 428.697

(3β,24*S*)-*form*

Me ether: 8,9-Epoxy-3-methoxy-8,9-secostigmasta-8(14),9(11)-diene
[156352-64-6]
$C_{30}H_{50}O_2$ 442.724
Constit. of *Microscleroderma spirophora*.
Costantino, V. *et al., Steroids*, 1994, **59**, 181-184 (*isol, pmr, cmr*)

15,16-Epoxy-13,17-spatadiene-5,19-diol E-510

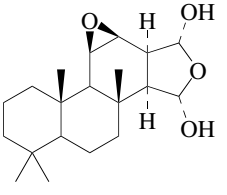


$C_{20}H_{30}O_3$ 318.455

(5*R*)-*form*

19-Ac: 19-Acetoxy-15,16-epoxy-13,17-spatadien-5α-ol
[111576-31-9]
$C_{22}H_{32}O_4$ 360.492
Constit. of *Stoechospermum marginatum*. Cryst. ($CHCl_3$/hexane).
Mp 130-132°. $[\alpha]_D$ +48.5 (c, 0.8 in $CHCl_3$).
Rao, C.B. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 79

11,12-Epoxy-15,16-spongianediol E-511



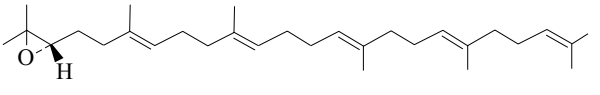
$C_{20}H_{32}O_4$ 336.47

(11β,12β,15α,16α)-*form*

Di-Ac: ***15,16-Diacetoxy-11,12-epoxyspongiane***
[178180-03-5]
$C_{24}H_{36}O_6$ 420.545
Constit. of *Chromodoris obsoleta*. Needles (MeOH).
Mp 154-157°. $[\alpha]_D^{26}$ -10.7 (c, 0.61 in $CHCl_3$).
Miyamoto, T. *et al., Tetrahedron*, 1996, **52**, 8187-8198 (*isol, pmr, cmr*)

2,3-Epoxysqualene E-512

2,3-Oxidosqualene. Squalene 2,3-epoxide
[7200-26-2]



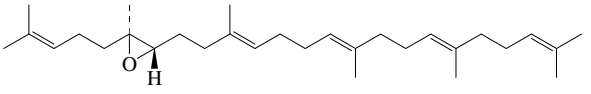
$C_{30}H_{50}O$ 426.724

(*S*)-*form*
Utilised in the biosynth. of triterpenes and steroids. Isol. from marine green alga *Caulerpa prolifera*.
Oil. $[\alpha]_D$ -1.7 (c, 1 in $CHCl_3$).

(±)-*form*
Oil.
v. Tamelen, E.E. *et al., J.A.C.S.*, 1966, **88**, 5937 (*synth*)
Benveniste, P. *et al., Tet. Lett.*, 1967, 3553 (*isol*)
Clayton, R.B. *et al., Proc. Int. Congr. Horm. Steroids, 3rd*, 1970, 82 (*rev*)
Dean, P.D.G. *et al., Steroidologia*, 1971, **2**, 143 (*rev*)
Shishibori, T. *et al., Chem. Lett.*, 1973, 1137 (*abs config*)
Yamada, S. *et al., Tet. Lett.*, 1976, 2561 (*synth*)
De Napoli, L. *et al., Tet. Lett.*, 1980, **21**, 2917-2918 (*isol*)
Corey, E.J. *et al., Tet. Lett.*, 1992, **33**, 2319; 1993, **34**, 5995 (*synth*)

6,7-Epoxysqualene E-513

6,7-Oxidosqualene. Squalene 6,7-epoxide

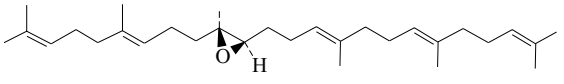


$C_{30}H_{50}O$ 426.724

(6*S*,7*S*)-*form* [82729-37-1]
Constit. of *Caulerpa prolifera*.
Oil. $[\alpha]_D^{20}$ -11.2 (c, 0.1 in $CHCl_3$).
[56882-06-5]
De Napoli, L. *et al., Phytochemistry*, 1982, **21**, 782-784 (*Caulera prolifera constit*)
Abad, J.-L. *et al., J.O.C.*, 1995, **60**, 3648-3656 (*synth, abs config*)

10,11-Epoxysqualene E-514

10,11-Oxidosqualene. Squalene 10,11-epoxide



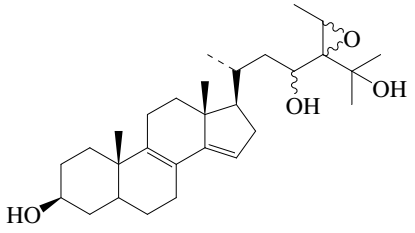
(10R,11R)–*form*

$C_{30}H_{50}O$ 426.724

(10*R*,11*R*)-*form*
Constit. of red alga *Laurencia okamurai*.
Oil. $[\alpha]_D^{25}$ +10.4 (c, 0.80 in $CHCl_3$).

(10*S*,11*S*)-*form* [60661-28-1]
Constit. of *Sclerotinia fructicola* and *Caulerpa prolifera*.
Oil. $[\alpha]_D^{20}$ -3.8 (c, 0.100 in $CHCl_3$).
Katayama, M. *et al., Tet. Lett.*, 1976, 1293 (*struct*)
De Napoli, L. *et al., Phytochemistry*, 1982, **21**, 782 (*config*)
Kigoshi, H. *et al., Tet. Lett.*, 1982, **23**, 5413 (*isol, synth*)
Kigoshi, H. *et al., Tetrahedron*, 1986, **42**, 3789 (*struct, synth*)
Abad, J.-L. *et al., J.O.C.*, 1995, **60**, 3648 (*synth, abs config*)

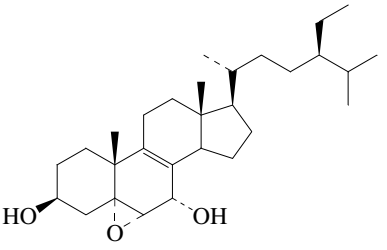
24,28-Epoxystigmasta-8,14-diene-3,23,25-triol E-515



$C_{29}H_{46}O_4$ 458.68

(3β,23ξ,24ξ,28ξ)-*form* [678185-30-3]
Constit. of *Vernonia colorata*.
Cryst. (MeOH). $[\alpha]_D^{25}$ +25 (c, 0.1 in MeOH). λ_{max} 236; 244; 252 (MeOH).
Cioffi, G. *et al., J. Nat. Prod.*, 2004, **67**, 389-394 (*isol, pmr, cmr*)

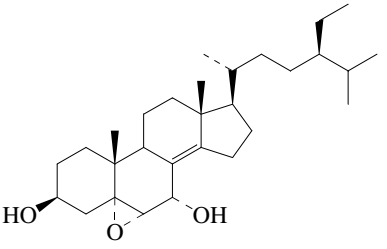
5,6-Epoxystigmast-8-ene-3,7-diol E-516



$C_{29}H_{48}O_3$ 444.696

(3β,5α,6α,7α,24*R*)-*form* [459832-66-7]
Constit. of *Polymastia tenax*.
Amorph. solid. $[\alpha]_D^{25}$ -47.3 (c, 0.175 in CH_2Cl_2).
Santafé, G. *et al., J. Nat. Prod.*, 2002, **65**, 1161-1164 (*isol, pmr, cmr*)

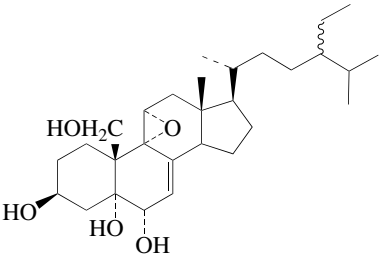
5,6-Epoxystigmast-8(14)-ene-3,7-diol E-517



$C_{29}H_{48}O_3$ 444.696

(3β,5α,6α,7α,24*R*)-*form* [459832-65-6]
Constit. of *Polymastia tenax*.
Amorph. solid. $[\alpha]_D^{25}$ -69 (c, 0.225 in CH_2Cl_2). λ_{max} 206 (log ϵ 3.96); 248 (log ϵ 3.92) (MeOH).
Santafé, G. *et al., J. Nat. Prod.*, 2002, **65**, 1161-1164 (*isol, pmr, cmr*)

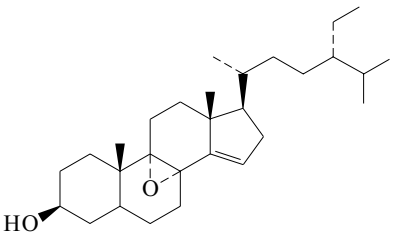
9,11-Epoxystigmast-7-ene-3,5,6,19-tetrol E-518



$C_{29}H_{48}O_5$ 476.695

(3β,5α,6α,9α,11α,24ξ)-*form*
6-Ac: ***Dysideasterol E***
[851318-97-3]
$C_{31}H_{50}O_6$ 518.732
Constit. of a *Dysidea* sp. Powder. $[\alpha]_D^{20}$ +30 (c, 0.16 in $CHCl_3$).
Huang, X.-C. *et al., Helv. Chim. Acta*, 2005, **88**, 281-289 (*Dysideasterol E*)

8,9-Epoxystigmast-14-en-3-ol E-519

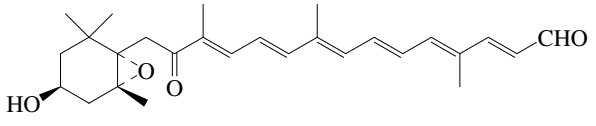


$C_{29}H_{48}O_2$ 428.697

(3β,8α,9α,24*S*)-*form*

Me ether: 8,9-Epoxy-3-methoxystigmast-14-ene
[156352-65-7]
$C_{30}H_{50}O_2$ 442.724
Constit. of *Microscleroderma spirophora*.
Costantino, V. *et al., Steroids*, 1994, **59**, 181-184 (*isol, pmr, cmr*)

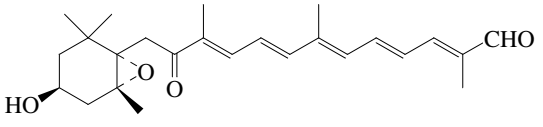
5,6-Epoxy-5,6,7,8-tetrahydro-3-hydroxy-8-oxo-10′-apo-β,ψ-carotenal E-520



$C_{27}H_{36}O_4$ 424.579

(3*S*,5*R*,6*S*)-*form*
Apo-10′-fucoxanthinal
[22488-62-6]
Constit. of *Phaeodactylum tricornutum*. λ_{max} 418 (log ϵ 4.62); 439 (log ϵ 4.6) (MeOH). λ_{max} 409 (Et_2O).
Shaw, B.A. *et al., Mar. Biol. (Berlin)*, 1995, **124**, 467-472 (*isol, pmr*)

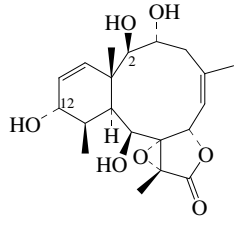
5,6-Epoxy-5,6,7,8-tetrahydro-3-hydroxy-8-oxo-12′-apo-β,ψ-carotenal E-521



$C_{25}H_{34}O_4$ 398.541

(3*S*,5*R*,6*S*)-*form*
Apo-12′-fucoxanthinal
[22488-61-5]
Constit. of *Phaeodactylum tricornutum*. λ_{max} 393 (log ϵ 4.53); 410 (log ϵ 4.51) (MeOH). λ_{max} 383 (Et_2O).
Shaw, B.A. *et al., Mar. Biol. (Berlin)*, 1995, **124**, 467-472 (*isol, pmr*)

8,17-Epoxy-2,3,9,12-tetrahydroxy-5,13-briaradien-18,7-olide E-522



(2β,3α,5*Z*,7α,8α,9β,12α,17α)-*form*

$C_{20}H_{28}O_7$ 380.437

(2β,3α,5*Z*,7α,8α,9β,12α,17α)-*form*

2,3-Di-Ac: ***Excavatolide N***
[247158-31-2]
$C_{24}H_{32}O_9$ 464.511
Constit. of *Briareum excavatum*. Cryst. ($CHCl_3$/petrol).
Mp 239-240°. $[\alpha]_D$ +22 (c, 0.05 in $CHCl_3$).

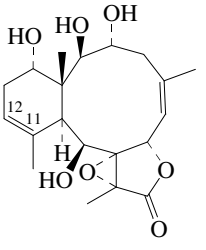
12-Ketone: 8,17-Epoxy-2,3,9-trihydroxy-12-oxo-5,13-briaradien-18,7-olide

12-Ketone, 2,3-di-Ac: ***Excavatolide Q***
[247158-40-3]
$C_{24}H_{30}O_9$ 462.496
Constit. of *Briareum excavatum*. Cryst. (EtOH).
Mp 212-214°. $[\alpha]_D$ -27 (c, 0.05 in $CHCl_3$).

(2β,3β,5*Z*,7α,8α,9β,12α,17α)-*form*

12-Ketone, tri-Ac: ***Briaexcavatolide A***
[256388-03-1]
$C_{26}H_{32}O_{10}$ 504.533
Constit. of *Briareum excavatum*. Powder.
Mp 85-87°. $[\alpha]_D^{25}$ -10 (c, 0.1 in $CHCl_3$). λ_{max} 222 (ϵ 5524) ($CHCl_3$).
Neve, J.E. *et al., Aust. J. Chem.*, 1999, **52**, 359-366 (*Excavatolides*)
Sheu, J.-H. *et al., Tetrahedron*, 1999, **55**, 14555-14564 (*Briaexcavatolide A*)

8,17-Epoxy-2,3,9,14-tetrahydroxy-5,11-briaradien-18,7-olide E-523



(2β,3α,5*Z*,7α,8α,9β,14α,17α)-*form*

$C_{20}H_{28}O_7$ 380.437

(2β,3α,5*Z*,7α,8α,9β,14α,17α)-*form*

3,9,14-Tri-Ac: ***Briarlide R***
[845641-28-3]
$C_{26}H_{34}O_{10}$ 506.549
Constit. of a *Briareum* sp. Amorph. solid. $[\alpha]_D$ +120 (c, 0.06 in MeOH).

(2β,3β,5*Z*,7α,8α,9β,14α,17α)-*form*

2,3,14-Tri-Ac: [125239-55-6]
$C_{26}H_{34}O_{10}$ 506.549
Constit. of *Briareum* sp. (DD6). Glass.

2,9,14-Tri-Ac: ***Briaranolide G***
[866087-91-4]
$C_{26}H_{34}O_{10}$ 506.549
Constit. of a *Briareum* sp. Amorph. solid. $[\alpha]_D^{25}$ +3 (c, 1 in $CHCl_3$).

2,3,9,14-Tetra-Ac: ***13-Dehydroxystecholide J***. *Briaranolide E*
[203051-07-4]
[866087-89-0]
$C_{28}H_{36}O_{11}$ 548.586
Constit. of a *Briareum* sp. Cryst.
Mp 183-187°. $[\alpha]_D$ -19.2 (c, 0.05 in CH_2Cl_2). $[\alpha]_D^{26}$ -26 (c, 1 in CH_2Cl_2). λ_{max} 230 (MeOH).

3-Butanoyl, 2,14-di-Ac: [125239-54-5]
$C_{28}H_{38}O_{10}$ 534.602
Constit. of a *Briareum* sp. (DD6). Glass. $[\alpha]_D$ -7.9 (c, 0.89 in $CHCl_3$).

3-Butanoyl, 2,9,14-tri-Ac: ***Briaranolide F***
[866087-90-3]
$C_{30}H_{40}O_{11}$ 576.639
Constit. of a *Briareum* sp. Cryst.
Mp 130-135°. $[\alpha]_D^{28}$ -50.3 (c, 1 in $CHCl_3$).

3-Butanoyl, 2-propanoyl, 9,14-di-Ac: ***Briaranolide H***
[866087-92-5]
$C_{31}H_{42}O_{11}$ 590.666
Constit. of a *Briareum* sp. Cryst.
Mp 207-210°. $[\alpha]_D^{26}$ -39.8 (c, 1 in $CHCl_3$).

11,12-Epoxide: 8,17:11,12-Diepoxy-2,3,9,14-tetrahydroxy-5-briaren-18,7-olide
$C_{20}H_{28}O_8$ 396.436

11β,12β-Epoxide, 2,3,14-tri-Ac: [125272-58-4]
$C_{26}H_{34}O_{11}$ 522.548
Constit. of a *Briareum* sp. (DD6). Cryst. (CH_2Cl_2/petrol).
Mp 238-240°. $[\alpha]_D$ +127 (c, 0.78 in $CHCl_3$).

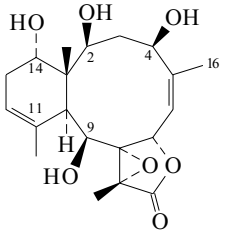
11β,12β-Epoxide, tetra-Ac: ***Excavatolide P***
[247158-37-8]
$C_{28}H_{36}O_{12}$ 564.585
Constit. of *Briareum excavatum*. Amorph. powder.
Mp 94-96°. $[\alpha]_D$ +27 (c, 0.05 in $CHCl_3$).

11β,12β-Epoxide, 2-butanoyl, 3,14-di-Ac: [125239-49-8]
$C_{28}H_{38}O_{11}$ 550.602
Constit. of a *Briareum* sp. (DD6). Cryst. (CH_2Cl_2/petrol).
Mp 172-173°. $[\alpha]_D$ +74 (c, 0.51 in $CHCl_3$).

[125280-15-1]

Bowden, B.F. *et al., Aust. J. Chem.*, 1989, **42**, 1705-1726 (*2,3,14-tri-Ac, 3-butanoyl-2,14-di-Ac, 11,12-epoxide-2,3,14-tri-Ac, 11,12-epoxide-2-butanoyl-3,14-di-Ac*)
Rodriguez, J. *et al., J. Nat. Prod.*, 1998, **61**, 313-317 (*tetra-Ac*)
Neve, J.E. *et al., Aust. J. Chem.*, 1999, **52**, 359-366 (*Excavatolide P*)
Iwagawa, T. *et al., J. Nat. Prod.*, 2005, **68**, 31-35 (*Briarlide R*)
Hoshino, A. *et al., J. Nat. Prod.*, 2005, **68**, 1328-1335 (*Briaranolides E-H*)

8,17-Epoxy-2,4,9,14-tetrahydroxy-5,11-briaradien-18,7-olide E-524



$C_{20}H_{28}O_7$ 380.437

2-Butanoyl, 4,9,14-tri-Ac: ***11,12-Deoxystecholide A acetate***
[138629-85-3]
$C_{30}H_{40}O_{11}$ 576.639
Isol. from *Solenopodium stechei.*

11β,12β-Epoxide, 2-butanoyl, 4,14-di-Ac: ***Stecholide A***
[138629-76-2]
$C_{28}H_{38}O_{11}$ 550.602
Constit. of *Solenopodium stechei*. Solid (Me_2CO/hexane).
Mp 113-115°. $[\alpha]_D$ +54.8 (c, 0.23 in $CHCl_3$).

11β,12β-Epoxide, 2-butanoyl, 4,9,14-tri-Ac: ***Stecholide A acetate***
[138629-77-3]
$C_{30}H_{40}O_{12}$ 592.639
Constit. of *Solenopodium stechei*. Cryst. (Et_2O).
Mp 179-182°. $[\alpha]_D$ +45.1 (c, 0.63 in $CHCl_3$).

11β,12β-Epoxide, 2-propanoyl, 4,14-di-Ac: ***Stecholide B***
[138629-78-4]
$C_{27}H_{36}O_{11}$ 536.575
Constit. of *Solenopodium stechei*. Cryst. (C_6H_6/hexane).
Mp 123-127°. $[\alpha]_D$ +89 (c, 0.09 in $CHCl_3$).

11β,12β-Epoxide, 2-propanoyl, 4,9,14-tri-Ac: ***Stecholide B acetate***
[138629-79-5]
$C_{29}H_{38}O_{12}$ 578.612
Constit. of *Solenopodium stechei*. Powder (Me_2CO/hexane).
Mp 247-249°. $[\alpha]_D$ +43.6 (c, 0.28 in $CHCl_3$).

11β,12β-Epoxide, 2,4,14-tri-Ac: ***Stecholide C***
[138629-80-8]
$C_{26}H_{34}O_{11}$ 522.548
Constit. of *Solenopodium stechei*. Powder (Me_2CO/hexane).
Mp 90-95°.

11β,12β-Epoxide, 2,4,9,14-tetra-Ac: ***Stecholide C acetate***
[138629-81-9]
$C_{28}H_{36}O_{12}$ 564.585
Constit. of *Solenopodium stechei*. Solid (Me_2CO/hexane).
Mp 251-253°. $[\alpha]_D$ +43.5 (c, 0.48 in $CHCl_3$).

11β,12β-Epoxide, 2-butanoyl, 9,14-di-Ac: ***Stecholide D***
[138629-86-4]
$C_{28}H_{38}O_{11}$ 550.602
Constit. of *Solenopodium stechei*. Solid (Me_2CO/hexane).
Mp 85-88°. $[\alpha]_D$ +11.7 (c, 0.36 in $CHCl_3$).

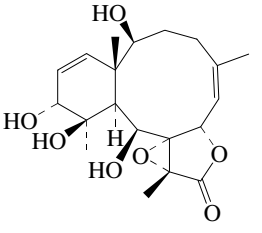
11β,12β-Epoxide, 2,4-dibutanoyl, 9,14-di-Ac: ***Stecholide D butyrate***
[138666-13-4]
$C_{32}H_{44}O_{12}$ 620.692
Constit. of *Solenopodium stechei.*

11β,12β-Epoxide, 16-acetoxy, 2-butanoyl, 4,9,14-tri-Ac: ***16-Acetoxystecholide A acetate***
[138629-82-0]
$C_{32}H_{42}O_{14}$ 650.675
Constit. of *Solenopodium stechei*. Cryst. (Et_2O).
Mp 90-95°. $[\alpha]_D$ +50.6 (c, 0.16 in $CHCl_3$).

11β,12β-Epoxide, 16-acetoxy, 2-propanoyl, 4,9,14-tri-Ac: ***16-Acetoxystecholide B acetate***
[138629-83-1]
$C_{31}H_{40}O_{14}$ 636.649
Constit. of *Solenopodium stechei*. Powder (Me_2CO/hexane).
Mp 229-231°. $[\alpha]_D$ +52.7 (c, 0.7 in $CHCl_3$).

11β,12β-Epoxide, 16-acetoxy, 2,4,9,14-tetra-Ac: ***16-Acetoxystecholide C acetate***
[138629-84-2]
$C_{30}H_{38}O_{14}$ 622.622
Constit. of *Solenopodium stechei*. Cryst. (Et_2O).
Mp 277-279°. $[\alpha]_D$ +36 (c, 0.18 in $CHCl_3$).
Bloor, S.J. *et al., J.O.C.*, 1992, **57**, 1205 (*isol, pmr, cmr*)

8,17-Epoxy-2,9,11,12-tetrahydroxy-5,13-briaradien-18,7-olide E-525

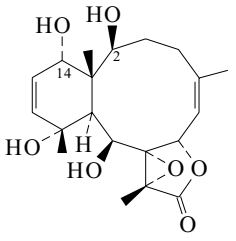


$C_{20}H_{28}O_7$ 380.437

2,9,12-Tri-Ac: ***Briaexcavatolide C***
[256388-05-3]
$C_{26}H_{34}O_{10}$ 506.549
Constit. of *Briareum excavatum*. Powder.
Mp 226-228°. $[\alpha]_D^{25}$ -96 (c, 0.4 in $CHCl_3$).

12-Butanoyl, 2,9-di-Ac: ***Briaexcavatolide B***
[256388-04-2]
$C_{28}H_{38}O_{10}$ 534.602
Constit. of *Briareum excavatum*. Powder.
Mp 219-221°. $[\alpha]_D^{25}$ -11 (c, 1 in $CHCl_3$).
Sheu, J.-H. *et al., Tetrahedron*, 1999, **55**, 14555-14564 (*isol, pmr, cmr*)

8,17-Epoxy-2,9,11,14-tetrahydroxy-5,12-briaradien-18,7-olide E-526

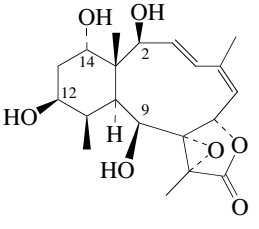


$C_{20}H_{28}O_7$ 380.437

2,9,14-Tri-Ac: ***2,9-Diacetyl-2-debutyrylstecholide H***
[203051-06-3]
$C_{26}H_{34}O_{10}$ 506.549
Constit. of a *Briareum* sp. Powder. $[\alpha]_D$ -69.8 (c, 0.05 in CH_2Cl_2).
λ_{max} 228 (MeOH).

2-Butanoyl, 14-Ac: ***Stecholide H***
[138629-92-2]
$C_{26}H_{36}O_9$ 492.565
Constit. of *Solenopodium stechei*. Powder.
Mp 84-88°. $[\alpha]_D$ -57.2 (c, 0.32 in $CHCl_3$).
Bloor, S.J. *et al., J.O.C.*, 1992, **57**, 1205 (*isol, pmr, cmr*)
Rodriguez, J. *et al., J. Nat. Prod.*, 1998, **61**, 313-317 (*tri-Ac*)

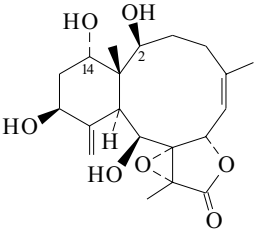
8,17-Epoxy-2,9,12,14-tetrahydroxy-3,5-briaradien-18,7-olide E-527



$C_{20}H_{28}O_7$ 380.437

12-Butanoyl, 2,9,14-tri-Ac: ***Excavatolide F***
[221664-88-6]
$C_{30}H_{40}O_{11}$ 576.639
Constit. of *Briareum excavatum*. Powder.
Mp 79-80°. $[\alpha]_D^{27}$ -28 (c, 1 in $CHCl_3$). λ_{max} 225 (ϵ 6610) (MeOH).
Sung, P.-J. *et al., J. Nat. Prod.*, 1999, **62**, 457-463 (*isol, pmr, cmr*)

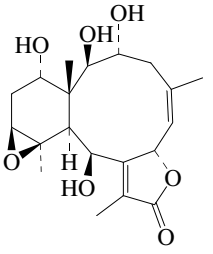
8,17-Epoxy-2,9,12,14-tetrahydroxy-5,11(20)-briaradien-18,7-olide E-528



$C_{20}H_{28}O_7$ 380.437
The abs. configs. of naturally occurring briaranes are not well established. A tentative assignment of the opposite abs. config. to that shown here was made for this compd. and one or two others by Bowden *et al* (1990) but for the time being they are shown with the opposite abs. config. for consistency with other briarane entries.

2,14-Di-Ac: 2,14-Diacetoxy-8,17-epoxy-9,12-dihydroxy-5,11(20)-briaradien-18,7-olide
[126636-52-0]
$C_{24}H_{32}O_9$ 464.511
Constit. of *Junceella gemmacea*. Oil. $[\alpha]_D$ +115.1 (c, 0.08 in $CHCl_3$).
Bowden, B.F. *et al., Aust. J. Chem.*, 1990, **43**, 151 (*isol, pmr, cmr*)

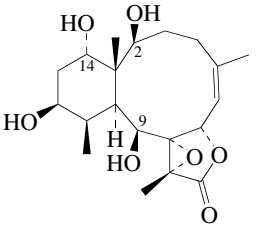
11,12-Epoxy-2,3,9,14-tetrahydroxy-5,8(17)-briaradien-18,7-olide E-529



$C_{20}H_{28}O_7$ 380.437

Tetra-Ac: ***Excavatolide S***
[247158-46-9]
$C_{28}H_{36}O_{11}$ 548.586
Constit. of *Briareum excavatum*. Cryst.
Mp 236-240°. $[\alpha]_D$ +87 (c, 0.04 in $CHCl_3$).
Neve, J.E. *et al., Aust. J. Chem.*, 1999, **52**, 359-366 (*isol, pmr, cmr*)

8,17-Epoxy-2,9,12,14-tetrahydroxy-5-briaren-18,7-olide E-530



$C_{20}H_{30}O_7$ 382.453

(2β,5*Z*,7α,8α,9β,11β,12β,14α,17α)-*form*

2,14-Di-Ac: ***Excavatolide E***
[205581-13-1]
$C_{24}H_{34}O_9$ 466.527
Constit. of *Briareum excavatum*. Cryst.
Mp 190-191°. $[\alpha]_D^{30}$ +53 (c, 0.14 in $CHCl_3$).

2,12,14-Tri-Ac: ***Excavatolide L***
[221664-94-4]
$C_{26}H_{36}O_{10}$ 508.564
Constit. of *Briareum excavatum*. Solid.
Mp 269-270°. $[\alpha]_D^{26}$ +28 (c, 0.5 in $CHCl_3$).

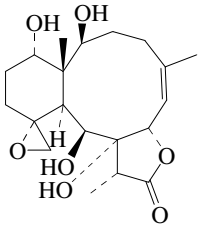
Tetra-Ac: ***Excavatolide G***
[221664-89-7]
$C_{28}H_{38}O_{11}$ 550.602
Constit. of *Briareum excavatum*. Powder.
Mp 219-220°. $[\alpha]_D^{27}$ +40 (c, 0.2 in $CHCl_3$).

12-Propanoyl, 2,14-di-Ac: ***Excavatolide W***
[247921-82-0]
$C_{27}H_{38}O_{10}$ 522.591
Constit. of *Briareum excavatum*. Amorph. solid.
Mp 222-224°. $[\alpha]_D^{25}$ +53 (c, 0.8 in $CHCl_3$).

12-Butanoyl, 2,14-di-Ac: ***Briaexcavatolide V***
[593279-02-8]
$C_{28}H_{40}O_{10}$ 536.618
Constit. of *Briareum excavatum*. Powder.
Mp 173-175°. $[\alpha]_D^{27}$ +49 (c, 1.8 in $CHCl_3$).

2-Butanoyl, 9,12,14-tri-Ac: [138629-90-0]
$C_{30}H_{42}O_{11}$ 578.655
Isol. from *Solenopodium stechei*. Oil. $[\alpha]_D$ +14.3 (c, 0.21 in $CHCl_3$).
Bloor, S.J. *et al., J.O.C.*, 1992, **57**, 1205 (*2-butanoyl tri-Ac*)
Sheu, J.-H. *et al., J. Nat. Prod.*, 1998, **61**, 602-608; 1999, **62**, 457-463; 1415-1420 (*Excavatolides*)
Wu, S.-L. *et al., J. Nat. Prod.*, 2003, **66**, 1252-1256 (*Briaexcavatolide V*)

11,20-Epoxy-2,8,9,14-tetrahydroxy-5-briaren-18,7-olide E-531



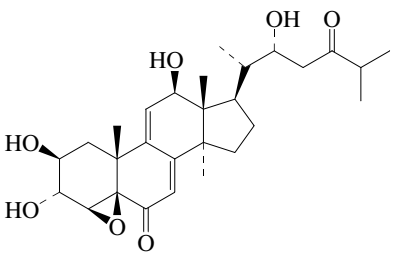
(2β,5*Z*,7α,8α,9β,11α,14α)-*form*

$C_{20}H_{30}O_7$ 382.453

(2β,5*Z*,7α,8α,9β,11α,14α)-*form*
2,9,14-Tri-Ac: ***Junceellolide K***
[881303-56-6]
$C_{26}H_{36}O_{10}$ 508.564
Constit. of *Junceella fragilis*. Powder.
Mp 265-268°. $[\alpha]_D^{25}$ -28 (c, 0.3 in $CHCl_3$).

(2β,5*Z*,7α,8α,9β,11β,14α)-*form*
2,9,14-Tri-Ac: ***11,20-Epoxy-4-deacetoxyjunceellolide D***
[221056-51-5]
$C_{26}H_{36}O_{10}$ 508.564
Constit. of *Junceella fragilis*. Powder. $[\alpha]_D^{22}$ -53.1 (c, 0.5 in CH_2Cl_2).
Struct. revised in 2006.
2-Propanoyl, 9,14-di-Ac: ***Junceellolide F***
[303963-52-2]
$C_{27}H_{38}O_{10}$ 522.591
Constit. of *Junceella fragilis*. Powder.
Mp 103-104°. $[\alpha]_D^{26}$ -127 (c, 0.6 in $CHCl_3$). Struct. revised in 2006.
5,6-Epoxide: 5,6:11,20-Diepoxy-2,8,9,14-tetrahydroxy-18,7-briaranolide
$C_{20}H_{30}O_8$ 398.452
5β,6β-Epoxide, 2,9,14-tri-Ac: ***Junceellolide J***
[881418-03-7]
$C_{26}H_{36}O_{11}$ 524.564
Constit. of *Junceella fragilis*. Cryst.
Mp 254-255°. $[\alpha]_D^{25}$ -82 (c, 0.7 in $CHCl_3$).
García, M. *et al., J. Nat. Prod.*, 1999, **62**, 257-260 (*11,20-Epoxy-4-deacetoxyjunceellolide D*)
Sung, P.-J. *et al., J. Nat. Prod.*, 2000, **63**, 1483-1487 (*Junceellolide F*)
Sheu, J.-H. *et al., J. Nat. Prod.*, 2006, **69**, 269-273 (*Junceellolides J and K, cryst struct*)

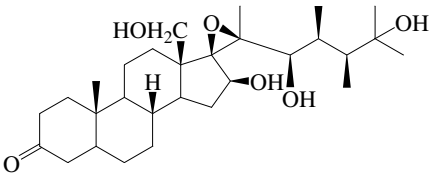
4,5-Epoxy-2,3,12,22-tetrahydroxy-14-methylcholesta-7,9(11)-diene-6,24-dione E-532



$C_{28}H_{40}O_7$ 488.62

(2β,3α,4β,5β,12β,22*R*)-*form* [347418-45-5]
Constit. of a *Xestospongia* sp.
Powder. λ_{max} 296 (MeOH).
Lerch, M.L. *et al., Tetrahedron*, 2001, **57**, 4091-4094 (*isol, pmr, cmr*)

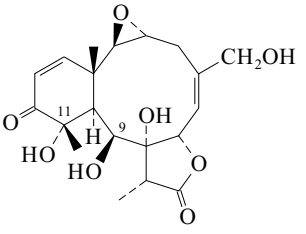
17,20-Epoxy-16,18,22,25-tetrahydroxy-23-methylergostan-3-one E-533



$C_{29}H_{48}O_6$ 492.695

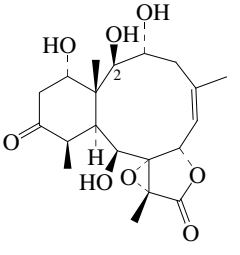
(16β,17β,20*S*,22*R*,23*S*,24*S*)-*form*
18,22-Di-Ac: ***Hippuristerone F***
[549528-39-4]
$C_{33}H_{52}O_8$ 576.769
Constit. of *Isis hippuris*. Powder.
Mp 125-127°. $[\alpha]_D$ -15 (c, 0.3 in $CHCl_3$).
18,22,25-Tri-Ac: ***Hippuristerone G***
[549528-40-7]
$C_{35}H_{54}O_9$ 618.806
Constit. of *Isis hippuris*. Powder.
Mp 113-114°. $[\alpha]_D$ +23 (c, 0.02 in $CHCl_3$).
Sheu, J.-H. *et al., J. Nat. Prod.*, 2003, **66**, 917-921 (*isol, pmr, cmr*)

2,3-Epoxy-8,9,11,16-tetrahydroxy-12-oxo-5,13-briaradien-18,7-olide E-534



$C_{20}H_{26}O_8$ 394.421
9,11-Di-Ac: ***Erythrolide H***
[132750-49-3]
$C_{24}H_{30}O_{10}$ 478.495
Constit. of *Erythropodium caribaeorum*. Foam.
9,11,16-Tri-Ac:
$C_{26}H_{32}O_{11}$ 520.532
Constit. of *Erythropodium caribaeorum*. Powder.
Pordesimo, E.O. *et al., J.O.C.*, 1991, **56**, 2344 (*isol, pmr, cmr*)
Maharaj, D. *et al., J. Nat. Prod.*, 1999, **62**, 313-314 (*9,11,16-Tri-Ac*)

8,17-Epoxy-2,3,9,14-tetrahydroxy-12-oxo-5-briaren-18,7-olide E-535

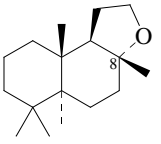


$C_{20}H_{28}O_8$ 396.436

2-Ac: ***Excavatolide T***
[247158-50-5]
$C_{22}H_{30}O_9$ 438.474
Constit. of *Briareum excavatum*. Amorph. powder.
Mp >250° dec. $[\alpha]_D$ +43 (c, 0.05 in $CHCl_3$).
Neve, J.E. *et al., Aust. J. Chem.*, 1999, **52**, 359-366 (*isol, pmr, cmr*)

8,12-Epoxy-13,14,15,16-tetranorlabdane E-536

*Dodecahydro-3*a*,6,6,9*a*-tetramethylnaphtho[2,1-*b*]furan, 9CI. 1,1,4*a*,6-Tetramethyl-5-ethyl-6,5-oxidodecahydronaphthalene. Norlabdane oxide*



8α-*form*

$C_{16}H_{28}O$ 236.397
Terpenoid numbering shown.

8α-*form*

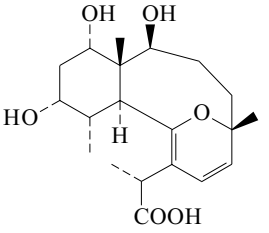
Ambrox. *Bicyclofarnesyl epoxide. Ambronide.* n-*Epoxide. Amberlyn. Ambroxan. FEMA 3471*
[6790-58-5]
Volatile constit. of Ambergris tincture. Obt. comly. by degradn. of natural 14-Labdene-8,13-diol. Important amber perfumery ingredient.
Cryst. (petrol).
Mp 75-76°. $[\alpha]_D$ -25 (c, 1 in $CHCl_3$) (>99%ee). The (+)-enantiomer has a much weaker odour.

8β-*form*

Isoambrox. Isoepoxide
[68365-88-8]
Mp 60°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 383A (*nmr*)
Stoll, M. *et al., Helv. Chim. Acta*, 1950, **33**, 1251; 1951, **34**, 1664 (*synth, config*)
Hinder, M. *et al., Helv. Chim. Acta*, 1953, **36**, 1995 (*synth, ir*)
Lucius, G. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1958, **291**, 57; *CA*, **52**, 14635e (*config*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1977, **60**, 2763-2766 (*Ambergris constit, synth*)
Torii, S. *et al., J.O.C.*, 1978, **43**, 4600 (*synth*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1985, **68**, 2022-2029 (*Ambrox*)
Gonzalez-Sierra, M. *et al., Heterocycles*, 1987, **26**, 2801 (*synth*)
Koyama, H. *et al., Tet. Lett.*, 1987, **28**, 2863 (*synth*)
Decorzaut, R. *et al., Tetrahedron*, 1987, **43**, 1871 (*synth*)
Büchi, G. *et al., Helv. Chim. Acta*, 1989, **72**, 996 (*synth, ir, pmr*)
Mori, K. *et al., Annalen*, 1990, 361 (*synth*)
Escher, S. *et al., Helv. Chim. Acta*, 1990, **73**, 1935
Snowden, R.L. *et al., Tet. Lett.*, 1991, **32**, 4119 (*synth*)
Martnes, P. *et al., Tet. Lett.*, 1993, **34**, 629 (*synth*)
Barrero, A.F. *et al., Tetrahedron*, 1993, **49**, 6251; 9325 (*synth*)
Barton, D.H.R. *et al., Tet. Lett.*, 1994, **35**, 5801 (*synth*)
Verstegen-Haaksma, A.A. *et al., Tetrahedron*, 1994, **50**, 10095 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 748
Barco, A. *et al., Tetrahedron*, 1995, **51**, 8333 (*synth*)
Barrero, A.F. *et al., J.O.C.*, 1996, **61**, 2215 (*synth*)
Tanimoto, H. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 1695 (*synth*)
Kutney, J.P. *et al., Can. J. Chem.*, 1997, **75**, 1136-1150 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2768-2769
Hashimoto, T. *et al., Heterocycles*, 1998, **49**, 315-326 (*synth*)
Zoretic, P.A. *et al., J.O.C.*, 1998, **63**, 4779-4785 (*synth*)
Koga, T. *et al., Tetrahedron: Asymmetry*, 1998, **93819-3823** (*synth*)
Moulines, J. *et al., Synth. Commun.*, 2001, **31**, 749-758 (*synth*)
Bolster, M.G. *et al., Tetrahedron*, 2001, **57**, 5657-5662 (*synth*)
Ishihara, K. *et al., J.A.C.S.*, 2002, **124**, 3647-3655 (*synth*)
Castro, J.M. *et al., Tetrahedron*, 2002, **58**, 5941-5949 (*synth*)
Moulines, J. *et al., Helv. Chim. Acta*, 2004, **87**, 2695-2705 (*synth*)
Barrero, A.F. *et al., Synth. Commun.*, 2004, **34**, 3631-3643 (*synth, ir, pmr, cmr, ms*)

5,9-Epoxy-2,12,14-trihydroxy-6,8-briaradien-18-oic acid E-537



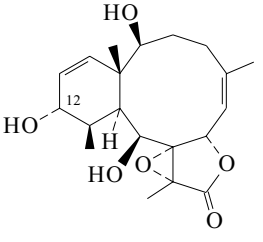
$C_{20}H_{30}O_6$ 366.453

2-Butanoyl, 14-Ac, Me ester: ***Briareolate ester B***
$C_{27}H_{40}O_8$ 492.608
Constit. of *Briareum asbestinum*. Cryst.
Mp 173-176°. $[\alpha]_D$ +154.7 (c, 0.21 in $CHCl_3$).

2-Butanoyl, 12,14-di-Ac, Me ester: ***Briareolate ester H***
$C_{29}H_{42}O_9$ 534.645
Constit. of *Briareum asbestinum*. Gum. $[\alpha]_D$ +127.3 (c, 0.27 in $CHCl_3$).

2,12-Dibutanoyl, 14-Ac, Me ester: ***Methyl briareolate***. *Briareolate ester A*
[146467-22-3]
$C_{31}H_{46}O_9$ 562.699
Constit. of *Briareum asbestinum*. Cryst.
Mp 165-167°. $[\alpha]_D$ +130.9 (c, 0.11 in $CHCl_3$).
Maharaj, D. *et al., Tet. Lett.*, 1992, **33**, 7761 (*isol, pmr, cmr, cryst struct*)
Dookran, R. *et al., Tetrahedron*, 1994, **50**, 1983 (*Briareolate esters A and B*)
Mootoo, B.S. *et al., Tetrahedron*, 1996, **52**, 9953 (*Briareolate ester H*)

8,17-Epoxy-2,9,12-trihydroxy-5,13-briaradien-18,7-olide E-538



(2β,5*Z*,7α,8α,9β,12α,17α)–*form*

$C_{20}H_{28}O_6$ 364.438

(2β,5*Z*,7α,8α,9β,12α,17α)-*form*

2,12-Di-Ac: [125272-59-5]
$C_{24}H_{32}O_8$ 448.512
Constit. of a *Briareum* sp. (DD6). Glass. $[\alpha]_D$ -44.9 (c, 0.31 in $CHCl_3$).

2-Butanoyl, 12-Ac: ***Stecholide G***
[138629-91-1]
$C_{26}H_{36}O_8$ 476.566
Constit. of *Solenopodium stechei*. Powder (Me_2CO/hexane).
Mp 58-60°. $[\alpha]_D$ -16.7 (c, 0.27 in $CHCl_3$).

12-Ketone: 8,17-Epoxy-2,9-dihydroxy-12-oxo-5,13-briaradien-18,7-olide. ***Briaexcavatolide D***
[256388-06-4]
$C_{20}H_{26}O_6$ 362.422
Constit. of *Briareum excavatum*. Powder.
Mp 217-219°. $[\alpha]_D^{25}$ -14 (c, 0.2 in $CHCl_3$). λ_{max} 224 (ϵ 6074) ($CHCl_3$).

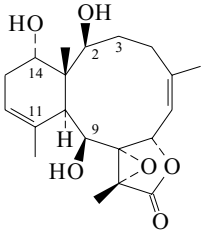
12-Ketone, 2-Ac: ***Briaexcavatolide T***
[593279-00-6]
$C_{22}H_{28}O_7$ 404.459
Isol. from *Briareum excavatum*. Powder.
Mp 195-197°. $[\alpha]_D^{27}$ +19 (c, 0.1 in $CHCl_3$). λ_{max} 221 (log ϵ 4.02) (MeOH).

12-Ketone, 2-butanoyl, 9-Ac: ***Briareolide I***
[132750-61-9]
$C_{26}H_{34}O_8$ 474.55
Isol. from a *Briareum* sp. Gum. λ_{max} 217 (ϵ 5610) (MeOH) (Derep).

Bowden, B.F. *et al., Aust. J. Chem.*, 1989, **42**, 1705-1743 (*2,12-di-Ac*)
Pordesino, E.O. *et al., J.O.C.*, 1991, **56**, 2344-2357 (*Briareolide I*)
Bloor, S.J. *et al., J.O.C.*, 1992, **57**, 1205-1216 (*Stecholide G*)
Sheu, J.-H. *et al., Tetrahedron*, 1999, **55**, 14555-14564 (*Briaexcavatolide D*)
Wu, S.L. *et al., J. Nat. Prod.*, 2003, **66**, 1252-1256 (*Briaexcavatolide T*)

8,17-Epoxy-2,9,14-trihydroxy-5,11-briaradien-18,7-olide E-539

Junceellolide H
[654646-03-4]



$C_{20}H_{28}O_6$ 364.438
Constit. of *Junceella fragilis*. Powder.
Mp 207-209°. $[\alpha]_D^{25}$ -22 (c, 0.8 in $CHCl_3$).

2,14-Di-Ac: 2,14-Diacetoxy-8,17-epoxy-9-hydroxy-5,11-briaradien-18,7-olide
[126610-17-1]
$C_{24}H_{32}O_8$ 448.512
Isol. from *Junceella gemmacea*. Cryst. (Et_2O).
Mp 240-241°. $[\alpha]_D$ +2.3 (c, 0.26 in $CHCl_3$). The opposite abs. config. to that shown has been tentively assigned: see note under 8,17-Epoxy-2,9,12,14-tetrahydroxy-5,11(20)-briaradien-18,7-olide, E-528. λ_{max} 230 (ϵ 7800) (MeOH) (Berdy).

Tri-Ac: ***Briareolide H***
[132750-60-8]
$C_{26}H_{34}O_9$ 490.549
Isol. from a *Briareum* sp. Gum.

2-Butanoyl, 14-Ac: ***11,12-Deoxystecholide E***
[138629-89-7]
$C_{26}H_{36}O_8$ 476.566
Constit. of *Solenopodium stechei*. Cryst. (C_6H_6/hexane).
Mp 71-74°. $[\alpha]_D$ +8.3 (c, 0.18 in $CHCl_3$).

11β,12β-Epoxide, 2,14-di-Ac: ***2β-Acetoxy-2-(debutanoyloxy)stecholide E***
$C_{24}H_{32}O_9$ 464.511
Constit. of *Briareum* sp. Cryst.
Mp 218-220°. $[\alpha]_D^{26}$ +27 (c, 1.2 in $CHCl_3$).

11β,12β-Epoxide, 2,9,14-tri-Ac: [203196-11-6]
$C_{26}H_{34}O_{10}$ 506.549
Constit. of a *Briareum* sp. Powder.

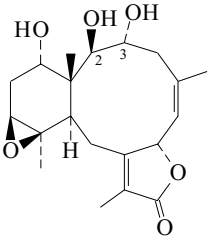
11β,12β-Epoxide, 2-propanoyl, 14-Ac: ***Stecholide F***
[138629-88-6]
$C_{25}H_{34}O_9$ 478.538
Constit. of *Solenopodium stechei*. Powder (Me_2CO/hexane).
Mp 100-103°. $[\alpha]_D$ +7.8 (c, 0.27 in $CHCl_3$).

11β,12β-Epoxide, 2-butanoyl, 14-Ac: ***Stecholide E***
[138629-87-5]
$C_{26}H_{36}O_9$ 492.565
Constit. of *Solenopodium stechei*. Powder (Me_2CO/hexane).
Mp 96-100°. $[\alpha]_D$ +10 (c, 0.36 in $CHCl_3$).

11β,12β-Epoxide, 2-butanoyl, 9,14-di-Ac: ***Stecholide E acetate***
[138749-83-4]
$C_{28}H_{38}O_{10}$ 534.602
Constit. of *Solenopodium stechei*. Cryst. (Et_2O).
Mp 123-125°. $[\alpha]_D$ -2.8 (c, 0.35 in $CHCl_3$).

Bowden, B.F. *et al., Aust. J. Chem.*, 1990, **43**, 151 (*isol, pmr, cmr*)
Pordesimo, E.O. *et al., J.O.C.*, 1991, **56**, 2344 (*isol, pmr, cmr*)
Bloor, S.J. *et al., J.O.C.*, 1992, **57**, 1205 (*isol, pmr, cmr*)
Sheu, J.-H. *et al., J. Nat. Prod.*, 1996, **59**, 935 (*isol, pmr, cmr*)
Rodríguez, J. *et al., J. Nat. Prod.*, 1998, **61**, 313-317 (*11,12-epoxy-tri-Ac*)
Sung, P.-J. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1429-1431 (*Junceellolide H*)

11,12-Epoxy-2,3,14-trihydroxy-5,8(17)-briaradien-18,7-olide E-540



$C_{20}H_{28}O_6$ 364.438

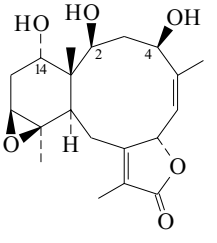
(2β,3α,7α,11β,12β,14α)-*form*

2-Butanoyl, 3,14-di-Ac: ***3,14-Diacetoxy-2-butanoyloxy-11,12-epoxy-5,8(17)-briaradien-18,7-olide***
[112781-23-4]
$C_{28}H_{38}O_9$ 518.603
Constit. of *Briareum steckei*. Glass. $[\alpha]_D$ +155 (c, 0.62 in $CHCl_3$).

Tri-Ac: 2,3,14-Triacetoxy-11,12-epoxy-5,8(17)-briaradien-18,7-olide
[125239-50-1]
$C_{26}H_{34}O_9$ 490.549
Constit. of a *Briareum* sp. (DD6). Glass. $[\alpha]_D$ +123 (c, 1.24 in $CHCl_3$).

Bowden, B.F. *et al., Aust. J. Chem.*, 1987, **40**, 2085; 1989, **42**, 1705

11,12-Epoxy-2,4,14-trihydroxy-5,8(17)-briaradien-18,7-olide E-541



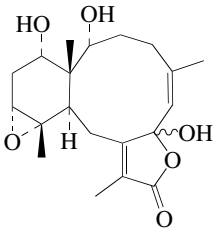
$C_{20}H_{28}O_6$ 364.438

2-Propanoyl, 4,14-di-Ac: 4,14-Diacetoxy-2-propanoyloxy-5,8(17)-briaradien-18,7-olide
[112781-26-7]
$C_{27}H_{36}O_9$ 504.576
Isol. from *Briareum steckei*.

2-Butanoyl, 4,14-di-Ac: 4,14-Diacetoxy-2-butanoyloxy-5,8(17)-briaradien-18,7-olide
[112781-25-6]
$C_{28}H_{38}O_9$ 518.603
Isol. from *Briareum steckei*.

Bowden, B.F. *et al., Aust. J. Chem.*, 1987, **40**, 2085

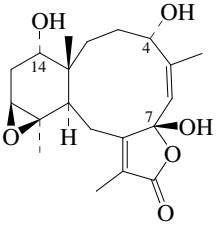
11,12-Epoxy-2,7,14-trihydroxy-5,8(17)-briaradien-18,7-olide E-542



$C_{20}H_{28}O_6$ 364.438

2,14-Di-Ac: [153977-17-4]
$C_{24}H_{32}O_8$ 448.512
Constit. of *Briareum asbestinum*. Gum. $[\alpha]_D$ -31.4 (c, 0.54 in $CHCl_3$).
Dookran, R. *et al., Tetrahedron*, 1994, **50**, 1983-1992 (*isol, pmr, cmr*)

11,12-Epoxy-4,7,14-trihydroxy-5,8(17)-briaradien-18,7-olide E-543



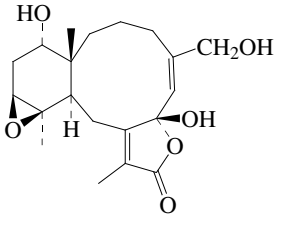
$C_{20}H_{28}O_6$ 364.438

4,14-Di-Ac:
$C_{24}H_{32}O_8$ 448.512
Constit. of a *Pachyclavularia* sp.

7,14-Di-Ac: [126394-97-6]
$C_{24}H_{32}O_8$ 448.512
Constit. of a *Pachyclavularia* sp.

Uchio, Y. *et al., Tennen Yuki Kagobutsu*, 1989, **31**, 548-553; *CA*, **112**, 175870s

11,12-Epoxy-7,14,16-trihydroxy-5,8(17)-briaradien-18,7-olide E-544

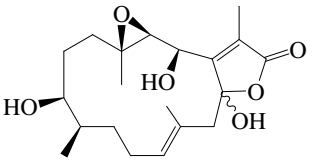


$C_{20}H_{28}O_6$ 364.438

(5*E*,7β*OH*,11β,12β,14α)-*form*

7-Me ether, 14-Ac: ***Briviolide H***
[868526-15-2]
$C_{23}H_{32}O_7$ 420.502
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +183 (c, 0.14 in MeOH). λ_{max} 230 (ϵ 9400) (MeOH).
Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 2083-2093 (*Briviolide H*)

3,4-Epoxy-2,7,14-trihydroxy-1(15),11-cembradien-16,14-olide E-545

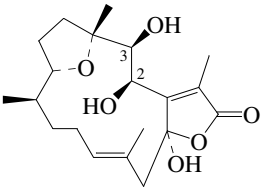


$C_{20}H_{30}O_6$ 366.453

(2*S,3*R**,4*R**,7*R**,8*S**,11*E*,14ξ)-*form***

14-Me ether, 7-octanoyl: ***Pachyclavulariolide F***
[325691-37-0]
$C_{29}H_{46}O_7$ 506.678
Constit. of *Pachyclavularia violacea*. Amorph. solid. $[\alpha]_D$ +32.1 (c, 1.22 in MeOH).
Xu, L. *et al., Tetrahedron*, 2000, **56**, 9031-9037 (*isol, pmr, cmr*)

4,7-Epoxy-2,3,14-trihydroxy-1(15),11-cembradien-16,14-olide E-546



$C_{20}H_{30}O_6$ 366.453

(2*R*,3*S*,4*R*,7*S*,8*R*,11*E*,14*S*)-*form*
Pachyclavulariolide L
[369632-01-9]
Constit. of *Pachyclavularia violacea*.
Solid.
Mp 194-196°. $[\alpha]_D^{29}$ +53 (c, 0.22 in $CHCl_3$). λ_{max} 220 (ϵ 5749) (EtOH aq.).

2,3-Di-Ac: ***Pachyclavulariolide E***
[325691-36-9]
$C_{24}H_{34}O_8$ 450.528
Constit. of *Pachyclavularia violacea*. Cryst.
Mp 150-152°. $[\alpha]_D$ -42 (c, 0.41 in $CHCl_3$). λ_{max} 203 (ϵ 17102) (EtOH aq.).

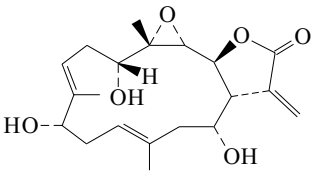
2-Butanoyl, 3-Ac: ***Pachyclavulariolide J***
[369631-99-2]
$C_{26}H_{38}O_8$ 478.581
Constit. of *Pachyclavularia violacea*. Oil. $[\alpha]_D^{25}$ -47 (c, 0.36 in $CHCl_3$). λ_{max} 207 (ϵ 4757) (EtOH aq.).

11β,12β-Epoxide: 4,7:11,12-Diepoxy-2,3,14-trihydroxy-1(15)-cembren-16,14-olide
$C_{20}H_{30}O_7$ 382.453

11β,12β-Epoxide, 2,3-di-Ac: ***Pachyclavulariolide M***
[551938-76-2]
$C_{24}H_{34}O_9$ 466.527
Constit. of *Pachyclavularia violacea*. Solid.
Mp 84-86°. $[\alpha]_D^{29}$ -14 (c, 0.15 in $CHCl_3$). λ_{max} 219 (ϵ 5680) (EtOH aq.).

Xu, L. *et al., Tetrahedron*, 2000, **56**, 9031-9037 (*Pachyclavulariolide E*)
Sheu, J.H. *et al., Tetrahedron*, 2001, **57**, 7639-7648 (*Pachyclavulariolides J,L, isol, pmr, cmr, cryst struct*)
Sheu, J.H. *et al., J. Nat. Prod.*, 2003, **66**, 662-666 (*Pachyclavulariolide M*)

3,4-Epoxy-5,9,14-trihydroxy-7,11,15(17)-cembratrien-16,2-olide E-547

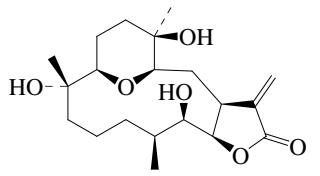


$C_{20}H_{28}O_6$ 364.438

(1*S*,2*R*,3*R*,4*S*,5*R*,7*E*,9*S*,11*E*,14*R*)-*form*

Tri-Ac: ***Crassolide***†
[66656-91-5]
$C_{26}H_{34}O_9$ 490.549
Constit. of *Lobophytum crassum* and *Lobophytum michaelae*. Amorph. solid. $[\alpha]_D$ -16 (c, 0.36 in $CHCl_3$). Stereochem. ambiguously drawn, not certain. λ_{max} 210 (ϵ 3200) (MeOH) (Berdy). λ_{max} 210 (ϵ 3200) (H_2O) (Berdy).
Tursch, B. *et al., Bull. Soc. Chim. Belg.*, 1978, **87**, 75
Wang, S.-K. *et al., J. Nat. Prod.*, 1992, **55**, 1430 (*isol, pmr, cmr*)

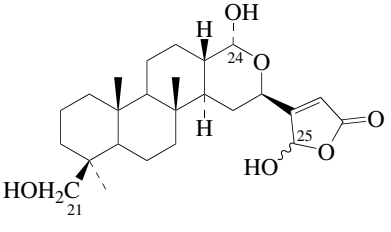
3,7-Epoxy-4,8,13-trihydroxy-15(17)-cembren-16,14-olide E-548



$C_{20}H_{32}O_6$ 368.469
Struct. revised in 2000.

(1*S*,3*R*,4*R*,7*R*,8*S*,12*S*,13*R*,14*R*)-*form*
Uprolide F
8,13-Di-Ac: ***Uprolide F diacetate***
[169217-45-2]
$C_{24}H_{36}O_8$ 452.544
Constit. of *Eunicea mammosa*. Oil. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{25}$ +146 (c, 0.7 in $CHCl_3$). λ_{max} 210 (ϵ 6900) (MeOH) (Berdy).
8-Me ether, 13-Ac: ***Uprolide G acetate***
[169217-46-3]
$C_{23}H_{36}O_7$ 424.533
Constit. of *Eunicea mammosa*. Oil. $[\alpha]_D^{25}$ +125 (c, 0.7 in $CHCl_3$).
Rodriguéz, A.D. *et al., J. Nat. Prod.*, 1995, **58**, 1209 (*isol, pmr, cmr*)
Rodriguéz, A.D. *et al., J.O.C.*, 2000, **65**, 7700-7702 (*struct*)

16,24-Epoxy-21,24,25-trihydroxy-17-cheilanthen-19,25-olide E-549

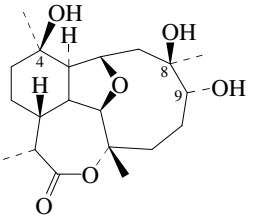


$C_{25}H_{38}O_6$ 434.572

(24α,25ξ)-*form*
21,24-Di-Ac: ***Petrosaspongiolide N***
[209408-72-0]
$C_{29}H_{42}O_8$ 518.646
Constit. of *Petrosaspongia nigra*. Amorph. solid. $[\alpha]_D$ -23 (c, 0.001 in $CHCl_3$). λ_{max} 224 (MeOH) (Berdy).

(24ξ,25ξ)-*form*
21-Ac: ***Petrosaspongiolide Q***
[209408-75-3]
$C_{27}H_{40}O_7$ 476.609
Constit. of *Petrosaspongia nigra*. Amorph. solid. $[\alpha]_D$ +5.8 (c, 0.001 in MeOH). λ_{max} 224 (MeOH) (Berdy).
Randazzo, A. *et al., J. Nat. Prod.*, 1998, **61**, 571-575 (*isol, pmr, cmr*)

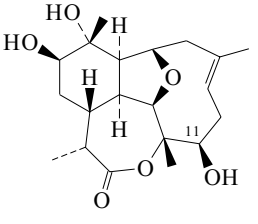
6,13-Epoxy-4,8,9-trihydroxy-16,12-eunicellanolide E-550



$C_{20}H_{32}O_6$ 368.469

(4β,6β,8β,9α,12α,13β,15α)-*form*
4-Ac: ***Briarellin M***
[503552-44-1]
$C_{22}H_{34}O_7$ 410.506
Constit. of *Briareum polyanthes*. Oil. $[\alpha]_D^{26}$ -14.5 (c, 1 in $CHCl_3$).
4-Butanoyl: ***Briarellin O***
[503552-46-3]
$C_{24}H_{38}O_7$ 438.56
Constit. of *Briareum polyanthes*. Oil. $[\alpha]_D^{26}$ -24.4 (c, 1.1 in $CHCl_3$).
9-Me ether, 4-Ac: ***Briarellin N***
[503552-45-2]
$C_{23}H_{36}O_7$ 424.533
Constit. of *Briareum polyanthes*. Oil. $[\alpha]_D^{20}$ -13.6 (c, 1.1 in $CHCl_3$).
9-Me ether, 4-butanoyl: ***Briarellin P***
[503552-47-4]
$C_{25}H_{40}O_7$ 452.587
Constit. of *Briareum polyanthes*. Oil. $[\alpha]_D^{26}$ -8.8 (c, 1.1 in $CHCl_3$).
Ospina, C.A. *et al., J. Nat. Prod.*, 2003, **66**, 357-363 (*isol, pmr, cmr*)

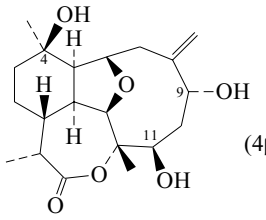
6,13-Epoxy-3,4,11-trihydroxy-8-eunicellen-16,12-olide E-551



$C_{20}H_{30}O_6$ 366.453

(3β,4α,6β,8*E*,11β,12α,13β)-*form*
11-Octanoyl: ***Briarellin H***
[171440-24-7]
$C_{28}H_{44}O_7$ 492.651
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{26}$ +10.1 (c, 2.8 in $CHCl_3$).
Rodríguez, A.D. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1853 (*isol, pmr, cmr*)

6,13-Epoxy-4,9,11-trihydroxy-8(19)-eunicellen-16,12-olide E-552



(4β,6β,9α,11β,12α,13β,15α)–*form*

$C_{20}H_{30}O_6$ 366.453

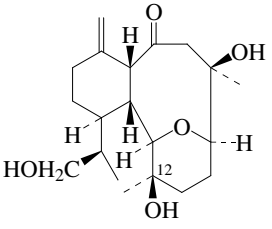
(4β,6β,9α,11β,12α,13β,15α)-*form*

11-Octanoyl: ***Briarellin B***
[165307-48-2]
$C_{28}H_{44}O_7$ 492.651
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{30}$ -7.89 (c, 5.7 in $CHCl_3$).

11-Octanoyl, 9-butanoyl: ***Briarellin C***
[165171-23-3]
$C_{32}H_{50}O_8$ 562.742
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{28}$ -29.75 (c, 11.8 in $CHCl_3$).

9-Hydroperoxide, 11-octanoyl: ***Briarellin A***
[165198-59-4]
$C_{28}H_{44}O_8$ 508.651
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{28}$ -25.24 (c, 14.9 in $CHCl_3$). Struct. revised in 2003. Formerly assigned as a deriv. of the triol.
Rodríguez, A.D. *et al., Tetrahedron*, 1995, **51**, 6869-6880 (*Briarellins A-C, isol, pmr, cmr*)
Ospina, C.A. *et al., J. Nat. Prod.*, 2003, **66**, 357-363 (*Briarellin A, struct*)

9,13-Epoxy-8,12,16-trihydroxy-4(18)-eunicellen-6-one E-553

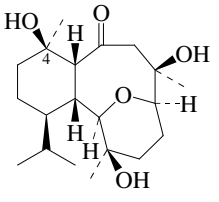


$C_{20}H_{32}O_5$ 352.47

(8β,12β,15*R*)-*form*

12-Butanoyl: ***Australin D***
[863638-12-4]
$C_{24}H_{38}O_6$ 422.561
Constit. of *Cladiella australis*. Oil. $[\alpha]_D^{25}$ -54 (c, 0.5 in $CHCl_3$).
Ahmed, A.F. *et al., J. Nat. Prod.*, 2005, **68**, 1051-1055 (*Australin D*)

9,13-Epoxy-4,8,12-trihydroxy-6-eunicellone E-554



Absolute Configuration

$C_{20}H_{34}O_5$ 354.486

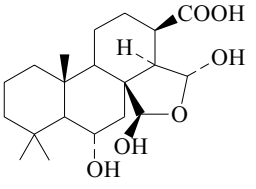
(4β,8β,12β)-*form*

4-Ac: ***Australin A***
[863638-09-9]
$C_{22}H_{36}O_6$ 396.523
Constit. of *Cladiella australis*. Oil. $[\alpha]_D^{25}$ -60 (c, 0.58 in $CHCl_3$).

Tri-Ac: ***Labiatin A***
[174232-50-9]
$C_{26}H_{40}O_8$ 480.597
Constit. of *Eunicella labiata*. Oil. $[\alpha]_D$ +17.3 (c, 0.8 in $CHCl_3$).
Roussis, V. *et al., Tetrahedron*, 1996, **52**, 2735-2742 (*Labiatin A*)
Ahmed, A.F. *et al., J. Nat. Prod.*, 2005, **68**, 1051-1055 (*Australin A*)

15,17-Epoxy-6,15,17-trihydroxy-16-isocopalanoic acid E-555

15,16-Dideoxy-6,15,17-trihydroxy-15,17-oxido-16-spongianoic acid



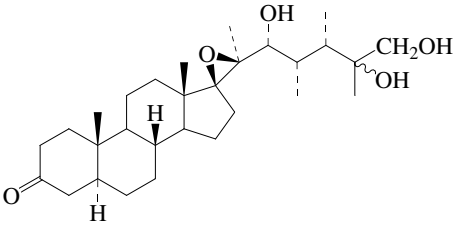
$C_{20}H_{32}O_6$ 368.469

(6α,13α*H*,14α*H*,15α,17β)-*form*

Tri-Ac, Me ester: Spongiane lactone 8
[109181-99-9]
$C_{27}H_{40}O_9$ 508.608
Isol. from *Ceratosoma brevicaudatum*. Oil.

6-Butanoyl,15,17-di-Ac, Me ester: Spongiane lactone 9
[109152-43-4]
$C_{29}H_{44}O_9$ 536.661
From *Ceratosoma brevicaudatum*. Oil.
Ksebati, M.B. *et al., J.O.C.*, 1987, **52**, 3766

17,20-Epoxy-22,25,26-trihydroxy-23-methylergostan-3-one E-556

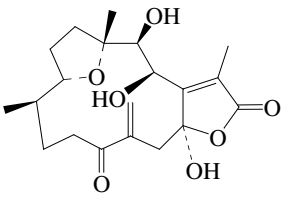


$C_{29}H_{48}O_5$ 476.695

(5α,17β,20*S*,22*R*,23*S*,24*S*,25ξ)-*form*

22,26-Di-Ac: ***Hippuristerone K***
[868395-84-0]
$C_{33}H_{52}O_7$ 560.77
Constit. of *Isis hippuris*. Powder.
Mp 103-105°. $[\alpha]_D$ +8 (c, 1.56 in $CHCl_3$).
Chao, C.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1366-1370 (*Hippuristerone K*)

4,7-Epoxy-2,3,14-trihydroxy-11-oxo-1(15),12(20)-cembradien-16,14-olide E-557

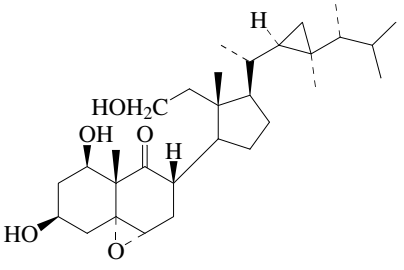


$C_{20}H_{28}O_7$ 380.437

(2*R,3*S**,4*R**,7*S**,8*R**,14*S**)-*form***

2,3-Di-Ac: ***Pachyclavulariolide K***
[369632-00-8]
$C_{24}H_{32}O_9$ 464.511
Constit. of *Pachyclavularia violacea*. Solid.
Mp 175-177°. $[\alpha]_D^{28}$ -47 (c, 0.41 in $CHCl_3$). λ_{max} 217 (ϵ 8821) (EtOH aq.).
Sheu, J.-H. *et al., Tetrahedron*, 2001, **57**, 7639-7648 (*isol, pmr, cmr*)

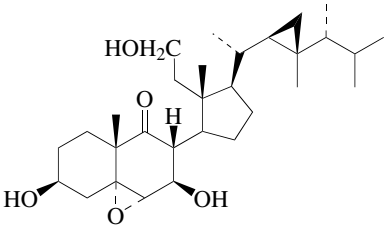
5,6-Epoxy-1,3,11-trihydroxy-9,11-secogorgostan-9-one E-558



$C_{30}H_{50}O_5$ 490.722

(1β,3β,5α,6α)-*form* [298199-94-7]
Constit. of *Pseudopterogorgia americana*.
Gum.
Naz, S. *et al., Tet. Lett.*, 2000, **41**, 6035-6040 (*isol, pmr, cmr*)

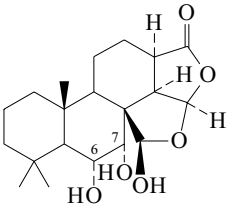
5,6-Epoxy-3,7,11-trihydroxy-9,11-secogorgostan-9-one E-559



$C_{30}H_{50}O_5$ 490.722

(3β,5α,6α,7β)-*form* [207918-95-4]
Constit. of a *Lobophytum* sp.
Oil. $[\alpha]_D$ +33.3 (c, 0.1 in $CHCl_3$).
Morris, L.A. *et al., J. Nat. Prod.*, 1998, **61**, 538-541 (*isol, pmr, cmr*)

15,17-Epoxy-6,7,17-trihydroxy-16-spongianone E-560



$C_{20}H_{30}O_6$ 366.453

(6α,7α,17β)-*form*

6,7-Di-Ac: ***Dendrillol 2***
[106009-82-9]
$C_{24}H_{34}O_8$ 450.528
Isol. from *Dendrilla rosea*. Glass.

6-Butanoyl: ***Aplyroseol 5***
[100814-66-2]
$C_{24}H_{36}O_7$ 436.544
From *Aplysilla rosea*. Tyrosine kinase inhibitor. Cryst. (EtOAc).
Mp 214-217°. $[\alpha]_D^{25}$ -3.4 (c, 2.55 in $CHCl_3$).

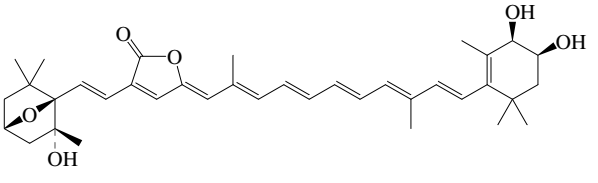
7-Butanoyl: ***Aplyroseol 3***
[100814-64-0]
$C_{24}H_{36}O_7$ 436.544
From *Aplysilla rosea*. Cryst. (EtOAc/petrol).
Mp 214-215°. $[\alpha]_D^{25}$ -0.6 (c, 1.32 in $CHCl_3$).

6-Butanoyl, 7-Ac: ***Aplyroseol 6***
[106009-79-4]
$C_{26}H_{38}O_8$ 478.581
From *Aplysilla rosea*. Tyrosine kinase inhibitor. Glass.
Mp 133-135°. $[\alpha]_D^{25}$ -10.9 (c, 2.43 in $CHCl_3$).

7-Butanoyl, 6-Ac: ***Aplyroseol 4***
[106009-78-3]
$C_{26}H_{38}O_8$ 478.581
From *Aplysilla rosea*. Glass.
Mp 125-127°.
Karuso, P. *et al., Aust. J. Chem.*, 1986, **39**, 1629; 1643
Molinski, T.F. *et al., J.O.C.*, 1986, **51**, 1144-1146 (*7-butanoyl*)

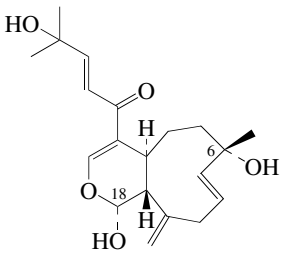
3,6-Epoxy-3′,4′,5-trihydroxy-12′,13′,20′-trinor-β,β-caroten-19,11-olide E-561

[870095-34-4]



$C_{37}H_{48}O_6$ 588.783
Constit. of the oyster *Crassostrea gigas*. Red solid. λ_{max} 455; 475 (Et_2O).
Maoka, T. *et al., Chem. Pharm. Bull.*, 2005, **53**, 1207-1209

17,18-Epoxy-6,14,18-trihydroxy-1(19),7,10(17),12-xenicatetraen-11-one E-562



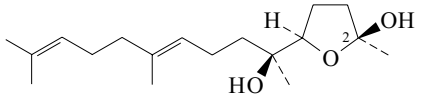
$C_{20}H_{28}O_5$ 348.438

(6α,7*E*,12*E*,18α)-*form*

6,18-Di-Ac: ***Tsitsixenicin C***
[168075-13-6]
$C_{24}H_{32}O_7$ 432.513
Constit. of *Capnella thyrsoidea*. Oil. $[\alpha]_D^{21}$ -138.9 (c, 0.6 in $CHCl_3$).
Hooper, G.J. *et al., Tetrahedron*, 1995, **51**, 9973-9984 (*isol, pmr, cmr*)

2,5-Epoxy-6,10,14-trimethyl-9,13-pentadecadiene-2,6-diol E-563

α-(4,8-Dimethyl-3,7-nonadienyl)tetrahydro-5-hydroxy-α,5-dimethyl-2-furanmethanol

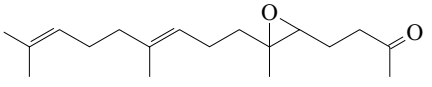


$C_{18}H_{32}O_3$ 296.449

2-Me ether: 2-(5-Methoxy-5-methyltetrahydro-2-furanyl)-6,10-dimethyl-5,9-undecadien-2-ol
[115028-54-1]
$C_{19}H_{34}O_3$ 310.476
Constit. of *Cystophora moniliformis*. Oil. $[\alpha]_D$ +11 (c, 1.3 in $CHCl_3$).
van Altena, I.A. *et al., Aust. J. Chem.*, 1988, **41**, 49

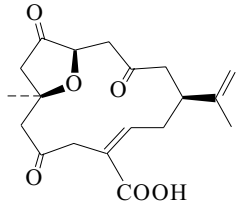
5,6-Epoxy-6,10,14-trimethyl-9,13-pentadecadien-2-one E-564

4-[3-(4,8-Dimethyl-3,7-nonadienyl)-3-methyloxiranyl]-2-butanone, 9CI
[115028-53-0]



$C_{18}H_{30}O_2$ 278.434
Constit. of *Cystophora moniliformis*. Unstable oil.
van Altena, I.A. *et al., Aust. J. Chem.*, 1988, **41**, 49

5,8-Epoxy-3,6,10-trioxo-18-norcembra-12,15-dien-20-oic acid E-565

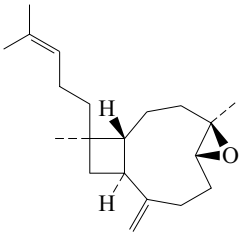


$C_{19}H_{24}O_6$ 348.395

Me ester: Methyl 5,8-epoxy-3,6,10-trioxo-18-norcembra-12,15-dien-20-oate
[99957-26-3]
$C_{20}H_{26}O_6$ 362.422
Constit. of *Sinularia querciformis* and *Sinularia polydactyla*. Cryst. Mp 183-185°. $[\alpha]_D$ -77 (c, 1.36 in $CHCl_3$).
Sato, A. *et al., Tetrahedron*, 1985, **41**, 4303
Duh, C.Y. *et al., CA*, 1993, **120**, 159198p (*isol*)

4,5-Epoxy-8(19),14-xeniaphylladiene E-566

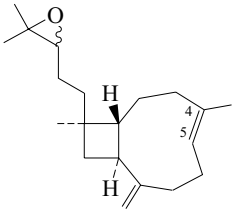
[153363-15-6]



$C_{20}H_{32}O$ 288.472
Constit. of a *Cespitularia* sp. Oil. $[\alpha]_D^{22}$ +2.7 (c, 0.07 in $CHCl_3$).
König, G.M. *et al., J. Nat. Prod.*, 1993, **56**, 2198 (*isol, pmr, cmr*)

14,15-Epoxy-4,8(19)-xeniaphylladiene E-567

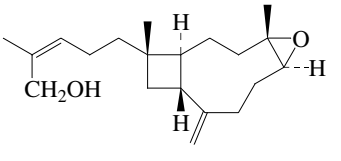
Xeniaphyllene-14,15-oxide



$C_{20}H_{32}O$ 288.472
Constit. of *Nephthea chabrolii* and of *Xenia lilielae*. Oil. $[\alpha]_D$ -2 (c, 0.24 in $CHCl_3$).

4β,5β-Epoxide: 4,5:14,15-Diepoxy-8(19)-xeniaphyllene. ***Xeniaphyllene dioxide***
$C_{20}H_{32}O_2$ 304.472
Isol. from *Xenia lilielae*. Oil. $[\alpha]_D^{25}$ +21 (c, 3.4 in $CHCl_3$).
Ahond, A. *et al., Aust. J. Chem.*, 1981, **34**, 2657 (*isol, struct*)
Groweiss, A. *et al., Tetrahedron*, 1983, **20**, 3385 (*isol, ms, cmr, config*)

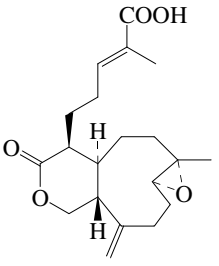
4,5-Epoxy-8(19),14-xeniaphylladien-16-ol E-568



$C_{20}H_{32}O_2$ 304.472

(4*S*,5*S*,14*Z*)-*form*
Nanolobatin A
[681145-45-9]
Constit. of *Sinularia nanolobata*.
Oil. $[\alpha]_D^{25}$ +15 (c, 1.6 in $CHCl_3$).
Ahmed, A.F. *et al., J. Nat. Prod.*, 2004, **67**, 592-597 (*isol, pmr, cmr*)

6,7-Epoxy-1(19),13-xenicadien-17,18-olid-15-oic acid E-569

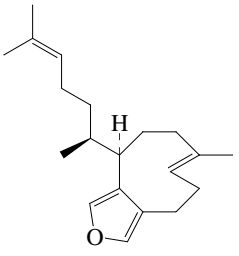


$C_{20}H_{28}O_5$ 348.438

(6α,7α,10α*H*,13*E*)-*form*

Me ester: ***Acalycixeniolide H***
[340156-16-3]
$C_{21}H_{30}O_5$ 362.465
Constit. of *Acalycigorgia inermis*. Amorph. solid.
Mp 162-164°. $[\alpha]_D$ +156.5 (c, 0.11 in MeOH). λ_{max} 216 (log ϵ 3.92) (MeOH).
Rho, J.-R. *et al., J. Nat. Prod.*, 2001, **64**, 540-543 (*isol, pmr, cmr*)

18,19-Epoxy-1(19),2(18),6,13-xenicatetraene E-570



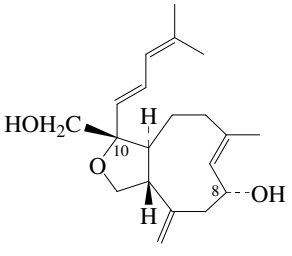
6*E-form*

$C_{20}H_{30}O$ 286.456

6*E-form*
Dictyofuran T
[87760-99-4]
Constit. of brown alga *Dictyota dichotoma*.
Oil. $[\alpha]_D^{25}$ +101 (c, 0.77 in cyclohexane).

6*Z-form*
Dictyofuran C
[87734-69-8]
Constit. of *Dictyota dichotoma*.
Oil. $[\alpha]_D^{25}$ +59.1 (c, 1.22 in cyclohexane).
Enoki, N. *et al., Chem. Lett.*, 1983, 1399

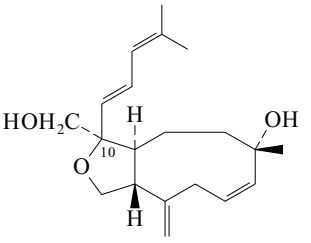
10,18-Epoxy-1(19),6,11,13-xenicatetraene-8,17-diol E-571



$C_{20}H_{30}O_3$ 318.455

(2β,3α,6*E*,8α,10*R*)-*form*
Xeniaoxolane
[308339-16-4]
Constit. of a *Xenia* sp.
Oil. $[\alpha]_D^{25}$ -140 (c, 0.2 in $CHCl_3$). λ_{max} 242 (ϵ 18300) (MeOH).
Miyaoka, H. *et al., Tetrahedron*, 2000, **56**, 7737-7740 (*isol, pmr, cmr, abs config*)

10,18-Epoxy-1(19),7,11,13-xenicatetraene-6,17-diol E-572



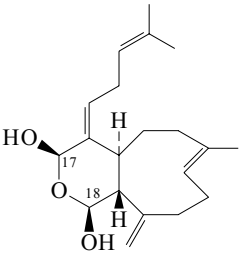
(6α,7*Z*,10α,11*E*)–*form*

$C_{20}H_{30}O_3$ 318.455

(6α,7*Z*,10α,11*E*)-*form*
Xeniaether B
[169869-80-1]
Constit. of *Xenia* spp.
Oil. $[\alpha]_D^{27}$ -75 (c, 0.09 in MeOH).

(6α,7*Z*,10β,11*E*)-*form*
Xeniaether A
[167172-86-3]
Constit. of *Xenia* spp.
Oil. $[\alpha]_D^{27}$ +135.7 (c, 0.07 in MeOH).
17-Hexadecanoyl: ***Xeniaether G***
[182806-33-3]
$C_{36}H_{60}O_4$ 556.868
Constit. of a *Xenia* sp. Oil. $[\alpha]_D$ +41.5 (c, 0.13 in MeOH).
17-Octadecanoyl: ***Xeniaether F***
[182806-31-1]
$C_{38}H_{64}O_4$ 584.921
Constit. of a *Xenia* sp. Oil. $[\alpha]_D$ +45.7 (c, 0.13 in MeOH). λ_{max} 240 (ϵ 13700) (no solvent reported).
17-Nonadecanoyl: ***Xeniaether H***
[182806-34-4]
$C_{39}H_{66}O_4$ 598.948
Constit. of a *Xenia* sp. Oil. $[\alpha]_D$ +80 (c, 0.05 in MeOH). λ_{max} 240 (ϵ 19600) (no solvent reported).
Iwagawa, T. *et al., Tetrahedron*, 1995, **51**, 11111; 1996, **52**, 13121-13128 (*isol, pmr, cmr, struct*)

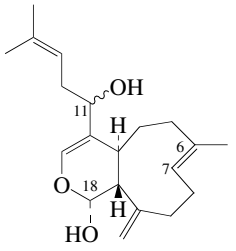
17,18-Epoxy-1(19),6,10,13-xenicatetraene-17,18-diol E-573



$C_{20}H_{30}O_3$ 318.455

(10*E*,17β,18β)-*form*
17-Me ether, 18-Ac: ***Acalycigorgin D***
[153660-21-0]
$C_{23}H_{34}O_4$ 374.519
Constit. of *Acalycigorgia* sp. Oil. $[\alpha]_D^{21}$ -51.3 (c, 0.18 in $CHCl_3$).
Ochi, M. *et al., Heterocycles*, 1994, **38**, 151-158 (*isol, pmr, cmr*)

17,18-Epoxy-1(19),6,10(17),13-xenicatetraene-11,18-diol E-574



$C_{20}H_{30}O_3$ 318.455

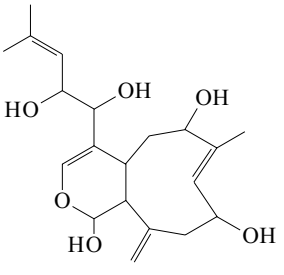
(11ξ,18α)-*form*

Di-Ac: ***Tsitsixenicin A***
[168113-67-5]
$C_{24}H_{34}O_5$ 402.53
Constit. of *Capnella thyrsoidea*. Yellow oil. $[\alpha]_D^{17}$ -64 (c, 0.9 in $CHCl_3$). λ_{max} 208 (ϵ 6800); 274 (ϵ 1790) (MeOH) (Berdy).

6α,7α-Epoxide, di-Ac: ***Tsitsixenicin B***
[168113-66-4]
$C_{24}H_{34}O_6$ 418.529
Constit. of *Capnella thyrsoidea*. Superoxide production inhibitor. Oil. $[\alpha]_D^{21}$ -38 (c, 0.49 in $CHCl_3$).

Hooper, G.J. *et al., Tetrahedron*, 1995, **51**, 9973-9984 (*isol, pmr, cmr*)

17,18-Epoxy-1(19),6,10(17),13-xenicatetraene-5,8,11,12,18-pentol E-575

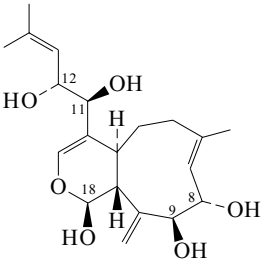


$C_{20}H_{30}O_6$ 366.453

11,12,18-Tri-Ac: ***9-Deacetyl-6-hydroxyxenicin***
$C_{26}H_{36}O_9$ 492.565
Constit. of *Xenia membranacea*. Amorph.

Almourabit, A. *et al., J. Nat. Prod.*, 1990, **53**, 894 (*isol, pmr*)

17,18-Epoxy-1(19),6,10(17),13-xenicatetraene-8,9,11,12,18-pentol E-576

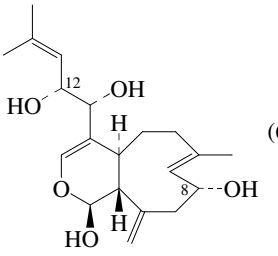


$C_{20}H_{30}O_6$ 366.453

12-Benzoyl, 8,11,18-tri-Ac: ***Antheliatin***
[172335-14-7]
$C_{33}H_{40}O_{10}$ 596.673
Constit. of *Anthelia glauca*. Cryst. (MeOH). Sol. MeOH, EtOAc, $CHCl_3$.
Mp 165°. $[\alpha]_D$ +3.5 (c, 1.2 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 1995, **58**, 1581 (*isol, pmr, cmr, cryst struct*)

17,18-Epoxy-1(19),6,10(17),13-xenicatetraene-8,11,12,18-tetrol E-577



(6*E*,8α,11*R*,12*R*,18β)-*form*

$C_{20}H_{30}O_5$ 350.454

(6*E*,8α,11*R*,12*R*,18β)-*form*

11,12,18-Tri-Ac:
$C_{26}H_{36}O_8$ 476.566
Constit. of *Anthelia glauca*. Oil.

Tetra-Ac: ***Xenicin***
[64504-52-5]
$C_{28}H_{38}O_9$ 518.603
Constit. of *Xenia elongata*. Cryst.
Mp 141.5-142.3°. $[\alpha]_D^{23.5}$ -36.7 (c, 0.6 in $CHCl_3$).

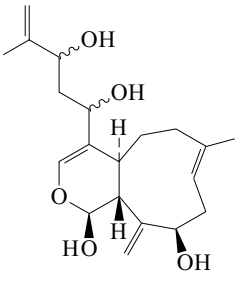
8-Acetoacetyl, 11,12,18-tri-Ac: [114933-24-3]
$C_{30}H_{40}O_{10}$ 560.64
Constit. of *Anthelia glauca*. Oil.

(6*E*,8α,11*R*,12*S*,18β)-*form*

11,12,18-Tri-Ac: ***9-Deacetyl-13-epixenicin***. *13-Epi-9-deacetylxenicin*
[71093-23-7]
$C_{26}H_{36}O_8$ 476.566
Constit. of *Xenia novae-britanniae* and *Asterospicularia laurae.*
Cryst. (hexane/Me_2CO).
Mp 150-151° (142-143°). $[\alpha]_D$ +51 (c, 0.11 in CH_2Cl_2) (+44).
λ_{max} 214 (ϵ 6600) (MeOH).

Vanderah, D.J. *et al., J.A.C.S.*, 1977, **99**, 5780-5784 (*Xenicin*)
Braekman, J.C. *et al., Bull. Soc. Chim. Belg.*, 1979, **88**, 71-77 (*13-Epi-9-deacetylxenicin, cryst struct*)
Green, D. *et al., Tet. Lett.*, 1988, **29**, 1605-1608 (*Anthelia glauca constits*)
Bowden, B.F. *et al., Mar. Drugs*, 2003, **1**, 18-26 (*Asterospicularia laurae constit*)

17,18-Epoxy-1(19),6,10(17),14-xenicatetraene-9,11,13,18-tetrol E-578



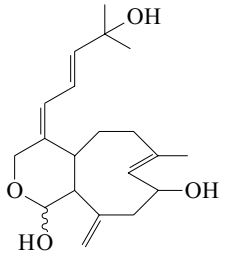
$C_{20}H_{30}O_5$ 350.454

11,13,18-Tri-Ac: ***Zahavin B***
[172335-16-9]
$C_{26}H_{36}O_8$ 476.566
Constit. of *Alcyonium aureum* and *Anthelia glauca*. Viscous oil. Sol. MeOH, EtOAc, $CHCl_3$. $[\alpha]_D^{20}$ +4.8 (c, 0.7 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 1995, **58**, 1581 (*isol, pmr, cmr*)

17,18-Epoxy-1(19),6,10,12-xenicatetraene-8,14,19-triol E-579

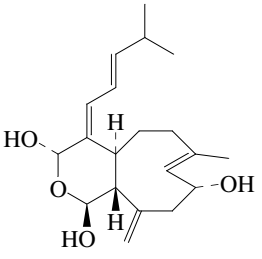
Xenialactol
[74175-99-8]



$C_{20}H_{30}O_4$ 334.455
Constit. of *Xenia* spp. Oil. $[\alpha]_D^{25}$ -90 (c, 1.9 in $CHCl_3$). λ_{max} 242 (ϵ 15900) (MeOH) (Derep).

Kashman, Y. *et al., J.O.C.*, 1980, **45**, 3814

17,18-Epoxy-1(19),6,10,12-xenicatetraene-8,17,18-triol E-580

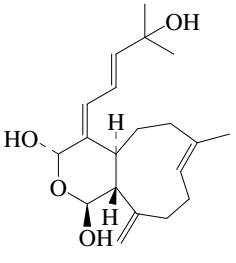


$C_{20}H_{30}O_4$ 334.455

(6*E*,8α,10*E*,12*E*,17α,18β)-*form*

17,18-Di-Me ether: ***Umbellacin G***
[871483-39-5]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Xenia umbellata*. Amorph. solid. $[\alpha]_D^{25}$ +36 (c, 0.3 in $CHCl_3$). λ_{max} 224 (log ϵ 3.8) (MeOH).
El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2006, **69**, 338-341 (*Umbellacin G*)

17,18-Epoxy-1(19),6,10,12-xenicatetraene-14,17,18-triol E-581

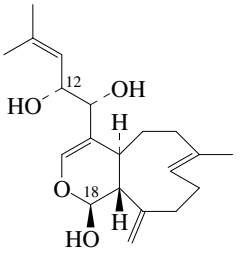


$C_{20}H_{30}O_4$ 334.455

(6*E*,10*E*,12*E*,17α,18β)-*form*

17,18-Di-Me ether: 17,18-Epoxy-17,18-dimethoxy-1(19),6,10,12-xenicatetraen-14-ol. ***Xenibecin***
[479067-64-6]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Xenia umbellata*. Oil. $[\alpha]_D^{25}$ -18.2 (c, 0.24 in $CHCl_3$). λ_{max} 218 (log ϵ 3.96) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1882-1885 (*isol, pmr, cmr*)

17,18-Epoxy-1(19),6,10(17),13-xenicatetraene-11,12,18-triol E-582



(6*E*,11*R*,12*R*,18β)-*form*

$C_{20}H_{30}O_4$ 334.455

(6*E*,11*R*,12*R*,18β)-*form*

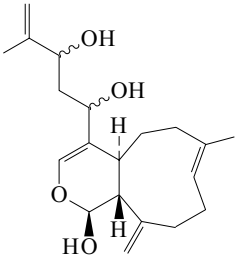
Tri-Ac: ***8-Deacetoxyxenicin****. 9-Deacetoxyxenicin*
[82490-36-6]
$C_{26}H_{36}O_7$ 460.566
Isol. from *Xenia crassa*. Cryst. (Et_2O/petrol).
Mp 120-122°. $[\alpha]_D$ +26.2 (c, 0.15 in $CHCl_3$). λ_{max} 209 (ϵ 12100) (EtOH).

(6*E*,11*R*,12*S*,18β)-*form*

Tri-Ac: ***9-Deacetoxy-13-epixenicin****. 13-Epi-9-deacetoxyxenicin*
[725740-07-8]
$C_{26}H_{36}O_7$ 460.566
Isol. from the soft coral *Asterospicularia laurae*. Prisms (hexane).
Mp 86-87°. $[\alpha]_D$ +63 (c, 0.06 in $CHCl_3$).

6S,7S-Epoxide, tri-Ac: [866228-95-7]
$C_{26}H_{36}O_8$ 476.566
Constit. of *Xenia blumi*. Oil. $[\alpha]_D^{25}$ +35 (c, 0.6 in $CHCl_3$). λ_{max} 233 (log ϵ 3.5) (MeOH).
Bowden, B.F. *et al., Aust. J. Chem.*, 1982, **35**, 997-1002 (*Xenia crassa constit*)
Bowden, B.F. *et al., Mar. Drugs*, 2003, **1**, 18-26 (*Asterospicularia laurae constit*)
El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 1336-1340 (*Xenia blumi constit*)

17,18-Epoxy-1(19),6,10(17),14-xenicatetraene-11,13,18-triol E-583

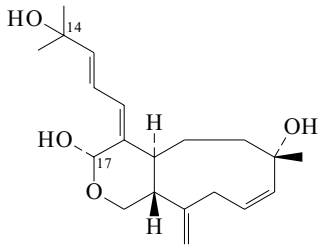


$C_{20}H_{30}O_4$ 334.455

Tri-Ac: ***Zahavin A***
[172335-15-8]
$C_{26}H_{36}O_7$ 460.566
Constit. of *Alcyonium aureum* and *Anthelia glauca*. Antiinflammatory agent. Superoxide release inhibitor. Viscous oil. Sol. MeOH, $CHCl_3$, EtOAc. $[\alpha]_D^{20}$ +7.3 (c, 1.8 in $CHCl_3$).

6α,7α-Epoxide, tri-Ac: ***6,7-Epoxyzahavin A****. 7,8-Epoxyzahavin A*
$C_{26}H_{36}O_8$ 476.566
Constit. of *Eleutherobia aurea*. Oil. $[\alpha]_D^{21}$ +121.7 (c, 0.34 in $CHCl_3$). Two numbering systems in use.
Rudi, A. *et al., J. Nat. Prod.*, 1995, **58**, 1581 (*Zahavin A*)
Hooper, G.J. *et al., J. Nat. Prod.*, 1997, **60**, 889-893 (*7,8-Epoxyzahavin A*)

17,18-Epoxy-1(19),7,10,12-xenicatetraene-6,14,17-triol E-584



$C_{20}H_{30}O_4$ 334.455

(6α,7*Z*,10*Z*,12*E*,17α)-*form*

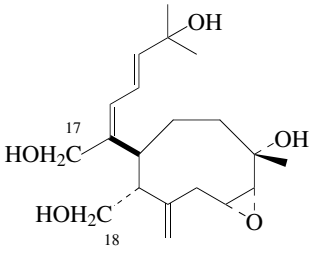
17-Me ether: [169529-96-8]
$C_{21}H_{32}O_4$ 348.481
Constit. of *Xenia* spp. Oil. $[\alpha]_D^{27}$ -93 (c, 0.08 in MeOH).

14,17-Di-Me ether: 17,18-Epoxy-14,17-dimethoxy-1(19),7,10,12-xenicatetraen-6-ol
[169337-61-5]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Xenia* spp. Oil. $[\alpha]_D^{27}$ -82.9 (c, 0.1 in MeOH).

14-Deoxy, 17-Me ether: 17,18-Epoxy-17-methoxy-1(19),7,10,12-xenicatetraen-6-ol
[169337-60-4]
$C_{21}H_{32}O_3$ 332.482
Constit. of *Xenia* spp. Oil. $[\alpha]_D^{27}$ -76.3 (c, 0.07 in MeOH).

14-Deoxy, 17-ketone (lactone): 6-Hydroxy-1(19),7,10,12-xenicatetraen-17,18-olide. ***Isoxeniatine B***
[169626-20-4]
$C_{20}H_{28}O_3$ 316.439
Isol. from *Xenia* spp. Oil. $[\alpha]_D^{27}$ +433 (c, 0.007 in MeOH).
Iwagawa, T. *et al., Tetrahedron*, 1995, **51**, 11111 (*isol, pmr, cmr*)

7,8-Epoxy-1(19),10,12-xenicatriene-6,14,17,18-tetrol E-585



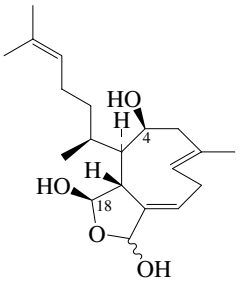
$C_{20}H_{32}O_5$ 352.47

(6α,7α,8α)-*form*

17-Octadecanoyl, 18-Ac: ***Azamilide H***
[178802-79-4]
$C_{40}H_{68}O_7$ 660.973
Constit. of a *Xenia* sp. Oil. $[\alpha]_D$ -62 (c, 0.1 in MeOH).

17-Hexadecanoyl, 18-Ac: ***Azamilide I***
[178802-80-7]
$C_{38}H_{64}O_7$ 632.919
Constit. of a *Xenia* sp. Oil. $[\alpha]_D$ -29 (c, 0.07 in MeOH).
Iwagawa, T. *et al., Heterocycles*, 1996, **43**, 1271-1277 (*isol, pmr, cmr*)

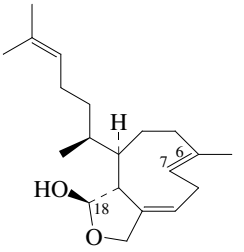
18,19-Epoxy-1(9),6,13-xenicatriene-4,18,19-triol E-586



$C_{20}H_{32}O_4$ 336.47

18,19-Di-Me ether, 4-Ac: ***Dictyodiacetal***
[84164-84-1]
$C_{24}H_{38}O_5$ 406.561
Constit. of *Dictyota dichotoma*.
$[\alpha]_D^{19}$ -113 (c, 0.5 in $CHCl_3$). Possible artifact.
Enoki, N. *et al., Chem. Lett.*, 1982, 1749-1752

18,19-Epoxy-1(9),6,13-xenicatrien-18-ol E-587



18β-*form*

$C_{20}H_{32}O_2$ 304.472

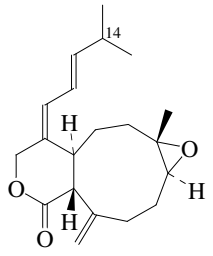
18β-*form*
Isodictyohemiacetal
[84236-21-5]
Constit. of marine alga *Dictyota dichotoma*.
Oil. $[\alpha]_D^{19}$ -50.2 (c, 0.23 in $CHCl_3$).

Me ether: ***Isodictyoacetal***
[89199-92-8]
$C_{21}H_{34}O_2$ 318.498
Constit. of *Pachydictyon coriaceum*.
$[\alpha]_D$ -7.7 (c, 0.75 in $CHCl_3$).

*(6*R*,7*R*)-Epoxide: 6,7:18,19-Diepoxy-1(9),13-xenicadien-18-ol.* ***6,7-Epoxyisodictyohemiacetal***
[130825-78-4]
$C_{20}H_{32}O_3$ 320.471
Isol. from *Glossophora kunthii*. Cryst.
Mp 90-92°. $[\alpha]_D$ +6.81 (c, 0.88 in $CHCl_3$).

18ξ-*form* [81575-23-7]
Isol. from *Dictyota prolificans.*
Foam. $[\alpha]_D^{22}$ -38 (c, 1 in $CHCl_3$).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 121-128 (*Dictyota prolificans constit*)
Enoki, N. *et al., Chem. Lett.*, 1982, 1749-1752 (*Isodictyohemiacetal*)
Ishitsuka, M. *et al., Chem. Lett.*, 1984, 151-154 (*Isodictyoacetal*)
Norte, M. *et al., Tetrahedron*, 1990, **46**, 6125-6132 (*6,7-Epoxyisodictyohemiacetal*)

6,7-Epoxy-1(19),10,12-xenicatrien-18,17-olide E-588



$C_{20}H_{28}O_3$ 316.439

(6α,7β,10*E*,12*E*)-*form*
Florlide D
[132922-85-1]
Constit. of *Xenia florida*.
Needles.
Mp 178°. $[\alpha]_D$ +178 (c, 0.09 in MeOH). λ_{max} 246 (log ϵ 4.11) (MeOH). λ_{max} 246 (ϵ 12880) (MeOH) (Berdy).

14-Hydroxy: 6,7-Epoxy-14-hydroxy-1(19),10,12-xenicatrien-18,17-olide. ***Florlide C***
[132943-56-7]
$C_{20}H_{28}O_4$ 332.439
Constit. of *Xenia florida*. Amorph. solid. $[\alpha]_D$ +173 (c, 0.09 in MeOH). λ_{max} 245 (log ϵ 4.24) (MeOH). λ_{max} 245 (ϵ 17380) (MeOH) (Berdy).

14-Hydroperoxy: 6,7-Epoxy-14-hydroperoxy-1(19),10,12-xenicatrien-18,17-olide. ***Florlide E***
[132922-86-2]
$C_{20}H_{28}O_5$ 348.438
Constit. of *Xenia florida*. Amorph. solid. $[\alpha]_D$ +157 (c, 0.07 in MeOH). λ_{max} 251 (log ϵ 3.94) (MeOH). λ_{max} 251 (ϵ 8710) (MeOH) (Berdy).

Iwagawa, T. *et al., J. Nat. Prod.*, 1998, **61**, 1513-1515 (*isol, pmr, cmr*)

Equinatoxins E-589

[54578-46-0]
Proteins, MW approx. 19500. Isol. from the venom of the sea anemone *Actinia equina*. Neurotoxins. Show antitumour activity.
▶ LD_{50} (mus, ivn) 0.33 mg/kg.

Equinatoxin I [115966-05-7]

Equinatoxin II [107852-47-1]
Comprises 2 nearly equimolar isoforms each with 179 amino acid residues and no cysteines; one isoform is identical to one isoform of Tenebrosin C.

Equinatoxin III [115966-06-8]

Equinatoxin V
Contains 179 amino acid residues.
[146836-98-8, 146836-99-9]

Ferlan, I. *et al., Toxicon*, 1974, **12**, 57-61; 63-68 (*isol*)
Macek, P. *et al., Toxicon*, 1988, **26**, 445-451 (*isol*)
Komatsu, S. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2873-2875 (*isol*)
Belmonte, G. *et al., Biochim. Biophys. Acta*, 1994, **1192**, 197-204 (*Equinatoxin II, struct*)
Pungercar, J. *et al., Biochim. Biophys. Acta*, 1997, **1341**, 105-107 (*Equinatoxin V, isol, struct*)
Athanasiadis, A. *et al., Structure (Cambridge, Mass.)*, 2001, **9**, 341-346 (*cryst struct*)
Anderluh, G. *et al., Toxicon*, 2002, **40**, 111-124 (*rev*)

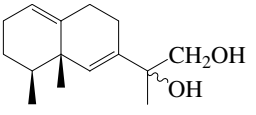
Erabutoxin E-590

[59536-69-5]
Peptide complex. Three Erabutoxins, designated Erabutoxin A, B and C, have been isolated. Each comprises a single chain of 62 amino-acid residues with 4 intramolecular disulfide bridges. Erabutoxin B differs from Erabutoxin A in one amino-acid residue. Erabutoxin C differs from erabutoxin B in a further residue. Isol. from the venom of the sea snake *Laticauda senifasciata*.
▶ KD8005000

[9083-23-2, 11091-63-7, 11091-64-8, 11094-61-4, 37357-76-9, 115203-87-7]

Tamiya, N. *et al., Biochem. J.*, 1966, **99**, 624-630; 1972, **130**, 547-555 (*isol*)
Bourne, P.E. *et al., Eur. J. Biochem.*, 1985, **153**, 521 (*struct*)
Corfield, P.W.R. *et al., J. Biol. Chem.*, 1989, **264**, 9239-9242 (*cryst struct, Erabutoxin A*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ECX000

1(10),6-Eremophiladiene-11,12-diol E-591



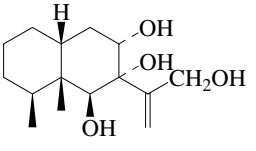
$C_{15}H_{24}O_2$ 236.353

(11ξ)-*form* [80322-52-7]
Constit. of *Lemnalia africana*.
Oil. $[\alpha]_D$ -133 (c, 1.32 in $CHCl_3$).

Di-Ac: ***Paralemnolin C***
[870152-42-4]
$C_{19}H_{28}O_4$ 320.428
Constit. of *Paralemnalia thyrsoides*. Oil. $[\alpha]_D^{25}$ -142 (c, 1.08 in $CHCl_3$).

Izac, R.R. *et al., Tetrahedron*, 1981, **37**, 2569-2573 (*Lemnalia africana constit*)
Huang, H.-C. *et al., Tet. Lett.*, 2005, **46**, 7711-7714 (*Paralemnolin C*)

11(13)-Eremophilene-6,7,8,12-tetrol E-592



(6β,7α*OH*,8α)-*form*

$C_{15}H_{26}O_4$ 270.368

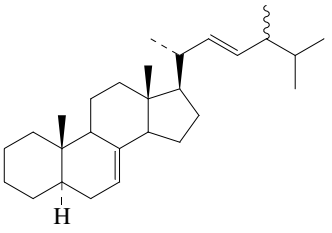
(6β,7α*OH*,8α)-*form*
Peribysin G
[858682-15-2]
Prod. by the marine-derived *Periconia byssoides* OUPS-N133.
Cell-adhesion inhibitor. Needles (hexane/CH_2Cl_2).
Mp 187-189°. $[\alpha]_D^{22}$ -1.3 (c, 0.1 in EtOH). λ_{max} 205 (log ϵ 2.25) (EtOH).

(6β,7β*OH*,8α)-*form*
Peribysin F
[859509-61-8]
Prod. by *Periconia byssoides* OUPS-N133. Cell-adhesion inhibitor. Pale yellow oil. $[\alpha]_D^{22}$ -21.5 (c, 0.1 in EtOH). λ_{max} 205 (log ϵ 3.41) (EtOH).

Yamada, T. *et al., J. Antibiot.*, 2005, **58**, 185-191 (*isol, pmr, cmr*)

Ergosta-7,22-diene E-593

24-Methylcholesta-7,22-diene

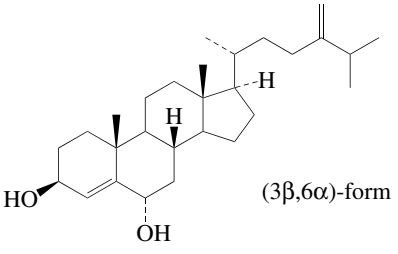


$C_{28}H_{46}$

(5α,22*E*,24ξ)-*form* [117142-13-9]
Isol. from the sponge *Agelas dispar*.
Carballeira, N.M. *et al., Biochem. Syst. Ecol.*, 1988, **16**, 421-424 (*isol*)

Ergosta-4,24(28)-diene-3,6-diol E-594

24-Methylenecholest-4-ene-3,6-diol



(3β,6α)-form

$C_{28}H_{46}O_2$ 414.67

(3β,6α)-*form*

3-Ketone: [851610-88-3]
$C_{28}H_{44}O_2$ 412.654
Constit. of *Iotrochota birotulana*. Cryst.
Mp 152-155°. $[\alpha]_D^{20}$ +74 (c, 0.62 in MeOH). Genus name given, apparently incorrectly, as Iotrichoto. λ_{max} 245 (MeOH).

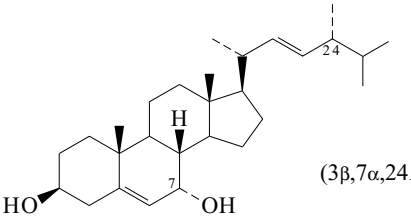
(3β,6β)-*form* [157469-40-4]
Constit. of *Alcyonium patagonicum*.
Needles (Me_2CO).
Mp 236-237°. $[\alpha]_D$ +20.5 (c, 0.15 in MeOH).

3-Ketone: ***6-Hydroxyergosta-4,24(28)-dien-3-one***
[851610-86-1]
$C_{28}H_{44}O_2$ 412.654
Constit. of *Iotrochota birotulata*. Cryst.
Mp 193-195°. $[\alpha]_D^{20}$ +56 (c, 0.32 in MeOH). λ_{max} 245 (MeOH).

Diketone: ***Ergosta-4,24(28)-diene-3,6-dione***. *24-Methylenecholest-4-ene-3,6-dione*
[59048-87-2]
$C_{28}H_{42}O_2$ 410.639
Isol. from the sponge *Geodia cydonium*. Cryst. (MeOH).
Mp 130-132°. λ_{max} 250 (ϵ 12300) (MeOH).
Migliuolo, A. *et al., J. Nat. Prod.*, 1990, **53**, 1262-1266; 1991, **54**, 371 (*diketone*)
Zeng, L. *et al., J. Nat. Prod.*, 1995, **58**, 296-298 (*isol, pmr, cmr*)
Cui, J.-G. *et al., Steroids*, 2001, **66**, 33-38 (*synth*)
Lin, H. *et al., Acta Cryst. C*, 2005, **61**, o1959-o1960 (*cryst struct*)
Li, L.-Y. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 115-120 (*3-ketones*)

Ergosta-5,22-diene-3,7-diol E-595

24-Methylcholesta-5,22-diene-3,7-diol



(3β,7α,24*R*)–*form*

$C_{28}H_{46}O_2$ 414.67

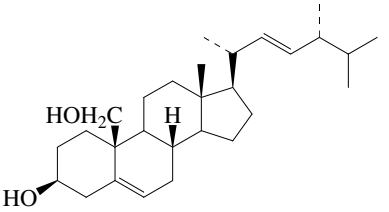
(3β,7α,24*R*)-*form* [145163-99-1]
Constit. of *Cliona copiosa*.

(3β,7α,24*S*)-*form* [145164-00-7]
Constit. of *Cliona copiosa*.

(3β,7β,24*R*)-*form* [69511-20-2]
Constit. of *Cliona copiosa*.

(3β,7β,24*S*)-*form* [99210-83-0]
Constit. of *Cliona copiosa* and *Haliclona oculata*.
$[\alpha]_D^{20}$ -87.1 (c, 0.66 in $CHCl_3$).
Findlay, J.A. *et al., Can. J. Chem.*, 1985, **63**, 2406 (*isol, pmr, ms*)
Notaro, G. *et al., J. Nat. Prod.*, 1992, **55**, 1588 (*isol, pmr, ms*)

Ergosta-5,22-diene-3,19-diol E-596



(3β,22*E*,24*R*)-*form*

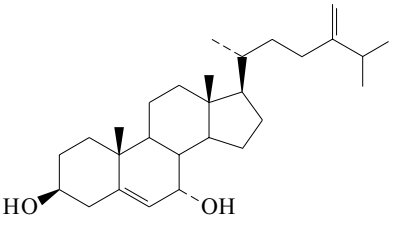
$C_{28}H_{46}O_2$ 414.67

(3β,22*E*,24*R*)-*form*
Acanthovagasteroid D
[815586-50-6]
Constit. of the gorgonian *Acanthogorgia vagae*.
Amorph. powder. $[\alpha]_D^{20}$ -21.6 (c, 0.05 in $CHCl_3$).

(3β,22*E*,24*S*)-*form*
Acanthovagasteroid C
[815586-49-3]
Constit. of *Acanthogorgia vagae*.
Amorph. powder. $[\alpha]_D^{20}$ -47.6 (c, 0.08 in $CHCl_3$).
Zhang, W. *et al., J. Nat. Prod.*, 2004, **67**, 2083-2085 (*isol, pmr, cmr*)

Ergosta-5,24(28)-diene-3,7-diol E-597

24-Methylenecholest-5-ene-3,7-diol



(3β,7α)–*form*

$C_{28}H_{46}O_2$ 414.67

(3β,7α)-*form* [99081-81-9]
Constit. of *Entandrophragma utile*, *Pseudobersama mossambicensis*, *Dysoxylum malabaricum* and *Stelodoryx chlorophylla*.
Cryst.
Mp 194-195° (MeOH). $[\alpha]_D$ -88 (c, 0.21 in $CHCl_3$). The compds. previously assigned this struct. from *Haliclona oculata* have been shown to be incorrect.

24ξ,28-Epoxide: 24,28-Epoxyergost-5-ene-3,7-diol
[145223-65-0]
$C_{28}H_{46}O_3$ 430.67
Constit. of *Pseudobersama mossambicensis*. Amorph. solid.
$[\alpha]_D^{20}$ -37 (c, 0.27 in $CHCl_3$).

7-Me ether: 7-Methoxyergosta-5,24(28)-dien-3-ol
[160316-62-1]
$C_{29}H_{48}O_2$ 428.697
Constit. of *Entandrophragma cylindricum*. Cryst.
Mp 198°. $[\alpha]_D$ -48 (c, 0.1 in Me_2CO).

(3β,7β)-*form* [99081-79-5]
Constit. of *Stelodoryx chlorophylla*.

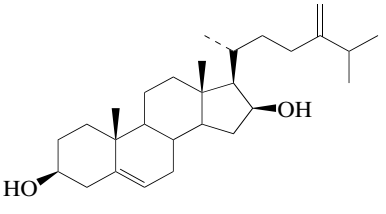
3-Sulfate, 7-Ac: ***Annasterol sulfate***
[160632-47-3]
$C_{30}H_{48}O_6S$ 536.772
Constit. of *Poecillastra laminaris*. Glucanase inhibitor. Cryst.
Mp 149-150°. $[\alpha]_D$ +28.6 (c, 0.35 in MeOH). CAS no. refers to Na salt.

5β,6β-Epoxide: ***5,6-Epoxyergost-24(28)-ene-3,7-diol****. 5,6-Epoxy-24-methylenecholestane-3,7-diol*
[395070-88-9]
$C_{28}H_{46}O_3$ 430.67
Constit. of *Plexaurella grisea*. Amorph. solid. $[\alpha]_D$ +48.9 (c, 0.09 in MeOH).

Findlay, J.A. *et al., Can. J. Chem.*, 1985, **63**, 2406-2410 (*Haliclona oculata constits*)
Garcia, J. *et al., J. Nat. Prod.*, 1991, **54**, 136-142 (*Entandrophragma utile constit*)
Gunatilaka, A.A.L. *et al., J. Nat. Prod.*, 1992, **55**, 1648-1654 (*24ξ,28-epoxide*)
De Riccardis, F. *et al., J. Nat. Prod.*, 1993, **56**, 282-287 (*Stelodoryx chlorophylla constits*)
Ngokam, D. *et al., Bull. Chem. Soc. Ethiop.*, 1994, **8**, 15-20; *CA*, **122**, 76570u (*7-Me ether*)
Heltzel, C.E. *et al., J. Nat. Prod.*, 1994, **57**, 620-628 (*synth, activity*)
Makarieva, T.N. *et al., Tet. Lett.*, 1995, **36**, 129-132 (*Annasterol sulfate*)
Govindachari, T.R. *et al., Phytochemistry*, 1997, **44**, 153-155 (*3β,7α-form, isol, pmr, cmr*)
Rueda, A. *et al., Steroids*, 2001, **66**, 897-904 (*5,6-epoxide*)

Ergosta-5,24(28)-diene-3,16-diol E-598

24-Methylenecholest-5-ene-3,16-diol



$C_{28}H_{46}O_2$ 414.67

(3β,16β)-*form* [146117-87-5]
Constit. of a *Sinularia* sp.
Needles.
Mp 154-156°. $[\alpha]_D$ +8.5 (c, 4.4 in $CHCl_3$).

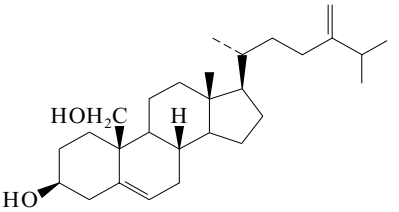
3-O-α-L-Fucopyranoside: [132214-23-4]
$C_{34}H_{56}O_6$ 560.813
Constit. of the soft corals *Cladiella* sp., *Lobophytum microlobulatum* and *Sinularia gibberosa*. Needles ($CHCl_3$/MeOH).
Mp 248-251°. $[\alpha]_D^{27}$ -122 (c, 1 in Py).

16-Ketone: ***3-Hydroxyergosta-5,24(28)-dien-16-one****. 3-Hydroxy-24-methylenecholest-5-en-16-one*
[224784-48-9]
$C_{28}H_{44}O_2$ 412.654
Constit. of *Cystophora brownii*. Cryst.
Mp 247-251°. $[\alpha]_D$ -49 (c, 0.42 in $CHCl_3$).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2400-2403; 1992, **40**, 2845-2846 (*isol, pmr, cmr, fucoside*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 45-48; 819-825; 2001, **40**, 405-409 (*fucoside, isol, pmr, cmr*)
Bian, B. *et al., Aust. J. Chem.*, 1998, **51**, 1157-1165 (*16-ketone*)

Ergosta-5,24(28)-diene-3,19-diol E-599

24-Methylenecholest-5-ene-3,19-diol



$C_{28}H_{46}O_2$ 414.67

3β-*form*
Litosterol
[126026-57-1]
Constit. of *Litophyton viridis*. Cryst. Mp 147.5-150°. $[\alpha]_D$ -25.8 (c, 0.24 in $CHCl_3$).

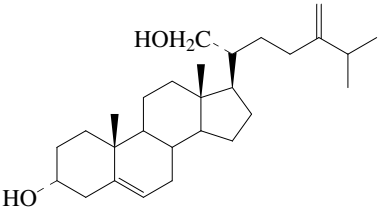
5β,6β-Epoxide: 5,6-Epoxyergost-24(28)-diene-3,19-diol. ***5,6-Epoxylitosterol***
[126026-58-2]
$C_{28}H_{46}O_3$ 430.67
Constit. of *Litophyton viridis*. Cryst. Mp 179-183°. $[\alpha]_D$ +3.8 (c, 0.26 in $CHCl_3$).

5β,6β-Epoxide, 19-Ac: ***Armatinol A***
[745828-22-2]
$C_{30}H_{48}O_4$ 472.707
Constit. of *Nephthea armata*. Amorph. solid. $[\alpha]_D^{25}$ -6.2 (c, 0.4 in $CHCl_3$). λ_{max} 206 (log ϵ 3.5) (MeOH).

Iguchi, K. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2553 (*Liosterol, Epoxylitosterol*)
El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2004, **67**, 1455-1458 (*Armatinol A*)

Ergosta-5,24(28)-diene-3,21-diol E-600

24-Methylenecholest-5-ene-3,21-diol



3α-*form*

$C_{28}H_{46}O_2$ 414.67

3α-*form*

3,21-Disulfate: [100942-75-4]
$C_{28}H_{46}O_8S_2$ 574.799
Constit. of the ophiuroid *Ophioderma longicaudum*. Isol. as di-Na salt to which CAS no. refers.

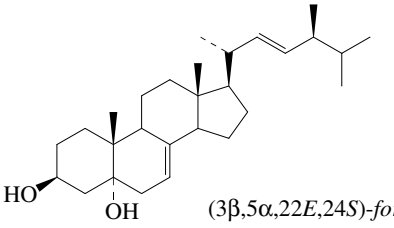
3β-*form* [95062-29-6]
Cryst. (EtOH). Mp 139-141°. $[\alpha]_D$ -23.8 (c, 2 in MeOH).

3,21-Disulfate: [95062-43-4]
Isol. from the starfish *Euretaster insignis*. CAS no. refers to di-Na salt.

D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1984, 2277-2282 (*3β-form*)
Riccio, R. *et al., Tetrahedron*, 1985, **41**, 6041-6046 (*3α-form*)

Ergosta-7,22-diene-3,5-diol E-601

24-Methylcholesta-7,22-diene-3,5-diol



(3β,5α,22*E*,24*S*)-*form*

$C_{28}H_{46}O_2$ 414.67

(3β,5α,22*E*,24*S*)-*form* [211358-70-2]
Cryst. Mp 133-135°. $[\alpha]_D$ -22.

3-O-β-D-Xylopyranoside: [211358-65-5]
$C_{33}H_{54}O_6$ 546.786
Constit. of *Synapta muculata*. Cryst.
Mp 233-235°. $[\alpha]_D^{28}$ +10.5 (c, 0.2 in MeOH).

(3α,5α,22*E*24ξ)-*form*
Cryst. (EtOAc). Mp 196-198°. $[\alpha]_D$ -1 (c, 1.7 in $CHCl_3$).

3-Ac: [63121-06-2]
Mp 153-155°. $[\alpha]_D$ -22 (c, 1.3 in $CHCl_3$).

(3β,5α,22*E*,24ξ)-*form* [14050-62-5]
Plates (EtOAc). Mp 231-234°. $[\alpha]_D$ +2.

3-Ac: [60045-90-1]
Needles (EtOAc). Mp 230-232° (228°). $[\alpha]_D$ +2 ($CHCl_3$).

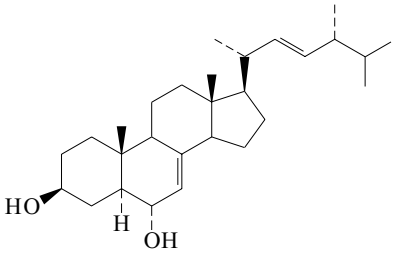
Di-Ac:
Needles (MeOH). Mp 158.5-161°. $[\alpha]_D$ +51 ($CHCl_3$).

[20649-78-9]

Dalton, F. *et al., J.C.S.*, 1961, 1880-1884; 1963, 4068-4075 (*synth, ir*)
Akhtar, M. *et al., Biochem. J.*, 1968, **108**, 527-531 (*synth*)
Kumar, S.V.A.S.P. *et al., J. Chem. Res., Synop.*, 1998, 404-405 (*isol, pmr, cmr*)

Ergosta-7,22-diene-3,6-diol E-602

24-Methylcholesta-7,22-diene-3,6-diol
[118574-73-5, 118574-74-6]



$C_{28}H_{46}O_2$ 414.67

(3β,5α,6α,22*E*,24*R*)-*form* [124649-09-8]
Constit. of *Spongionella gracilis*. Cryst. (MeOH/petrol). Mp 206-208°.

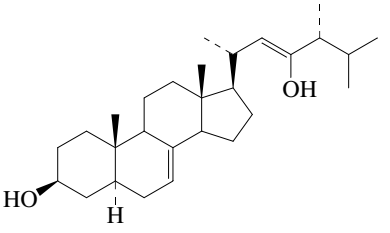
3,6-Diketone: Ergosta-7,22-diene-3,6-dione. ***Cyathisterone***
[159813-67-9]
$C_{28}H_{42}O_2$ 410.639
Constit. of *Calvatia cyathiformis*. Cryst. (hexane).
Mp 200-203°. $[\alpha]_D^{25}$ +12 (c, 0.17 in $CHCl_3$).

(3β,5α,6α,22*E*,24*S*)-*form*
*Campesta-7,22*E*-diene-3β,6α-diol*
[124649-10-1]
Constit. of *Spongionella gracilis*. Cryst. (MeOH/petrol). Mp 196-198°.

Madaio, A. *et al., J. Nat. Prod.*, 1989, **52**, 952-961 (*isol, pmr*)
Kawahara, N. *et al., Phytochemistry*, 1994, **37**, 213-215 (*Cyathisterone*)

Ergosta-7,22-diene-3,23-diol E-603

3-Hydroxyergost-7-en-23-one



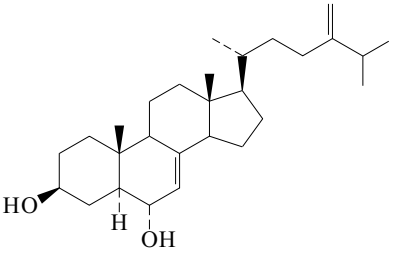
$C_{28}H_{46}O_2$ 414.67
Enol.

(3β,22*Z*,24*R*)-*form*

23-Sulfate: ***Arenicolsterol A***
[865139-51-1]
$C_{28}H_{46}O_5S$ 494.734
Constit. of *Arenicola cristata*. Glass.
Mp 169-171°. $[\alpha]_D^{20}$ +7.8 (c, 0.28 in MeOH). λ_{max} 250 (MeOH).
Chen, B. *et al., Chin. J. Chem.*, 2005, **23**, 599-602; *CA*, **143**, 322303e (*Arenicolsterol A*)

Ergosta-7,24(28)-diene-3,6-diol, 9CI E-604

24-Methylenecholest-7-ene-3,6-diol

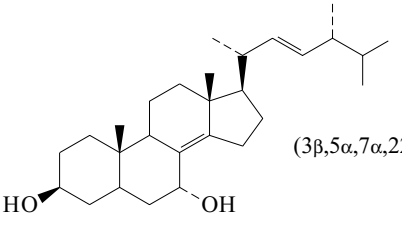


$C_{28}H_{46}O_2$ 414.67

(3β,5α,6α)-*form* [106534-44-5]
Constit. of *Spongionella gracilis.*
Piccialli, V. *et al., J. Nat. Prod.*, 1986, **49**, 779

Ergosta-8(14),22-diene-3,7-diol E-605

24-Methylcholesta-8(14),22-diene-3,7-diol



(3β,5α,7α,22*E*,24*R*)–*form*

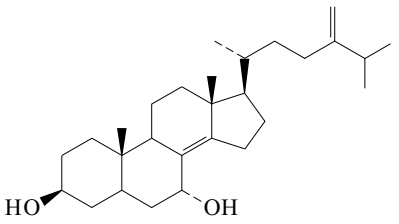
$C_{28}H_{46}O_2$ 414.67

(3β,5α,7α,22*E*,24*R*)-*form* [141859-98-5]
Constit. of *Pellina semitubulosa.*

(3β,5α,7α,22*E*,24*S*)-*form* [141902-00-3]
Constit. of *Pellina semitubulosa.*
Notaro, G. *et al., J. Nat. Prod.*, 1992, **55**, 773 (*isol, pmr*)

Ergosta-8(14),24(28)-diene-3,7-diol E-606

24-Methylenecholest-8(14)-ene-3,7-diol

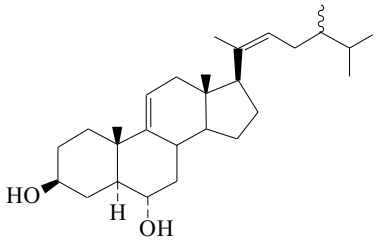


$C_{28}H_{46}O_2$ 414.67

(3β,5α,7α)-*form* [141859-99-6]
Constit. of *Pellina semitubulosa*.
Notaro, G. *et al., J. Nat. Prod.*, 1992, **55**, 773 (*isol, pmr, cmr*)

Ergosta-9(11),20(22)-diene-3,6-diol E-607

24-Methylcholesta-9(11),20(22)-diene-3,6-diol

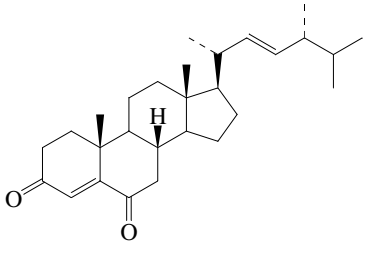


$C_{28}H_{46}O_2$ 414.67

(3β,5α,6α,24ξ)-*form* [37926-44-6]
Minor constit. of *Acanthaster planci*.
Sheikh, Y.M. *et al., Tet. Lett.*, 1972, 3721

Ergosta-4,22-diene-3,6-dione E-608

24-Methylcholesta-4,22-diene-3,6-dione



(22*E*,24*R*)-*form*

$C_{28}H_{42}O_2$ 410.639

(22*E*,24*R*)-*form* [131467-00-0]
Isol. from the sponge *Geodia cydonium*. λ_{max} 250 (ε 12300) (MeOH).

(22*E*,24*S*)-*form* [131565-70-3]
Isol. from *Geodia cydonium*. λ_{max} 250 (ε 12500) (MeOH).
Migliuolo, A. *et al., J. Nat. Prod.*, 1990, **53**, 1262-1266; 1991, **54**, 371 (*isol, pmr, ms*)

Ergosta-7,22-diene-2,3,5,6,9,11,19-heptol E-609

24-Methylcholesta-7,22-diene-2,3,5,6,9,11,19-heptol

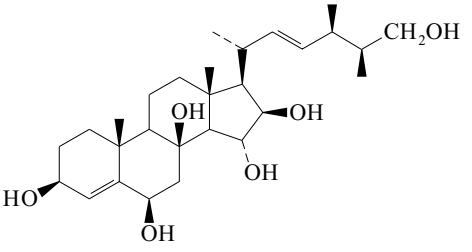
$C_{28}H_{46}O_7$ 494.667

(2α,3β,5α,6β,11α,24*S*)-*form* [114395-65-2]
Isol. from *Dysidea etheria*. Cryst. Mp 260-270° dec. $[\alpha]_D^{25}$ -24.4 (c, 1.2 in EtOH).

11-Ac: 11-Acetoxy-24-methylcholesta-7,22-diene-2α,3β,5α,6β,9α,19-hexol
[114395-66-3]
$C_{30}H_{48}O_8$ 536.704
Isol. from *Dysidea etheria*. Cryst. Mp 213°. $[\alpha]_D^{25}$ -32.2 (c, 1 in EtOH).
West, R.R. *et al., J.O.C.*, 1988, **53**, 2782-2787 (*Dysidea etheria constit*)

Ergosta-4,22-diene-3,6,8,15,16,26-hexol E-610

24-Methylcholesta-4,22-diene-3,6,8,15,16,26-hexol

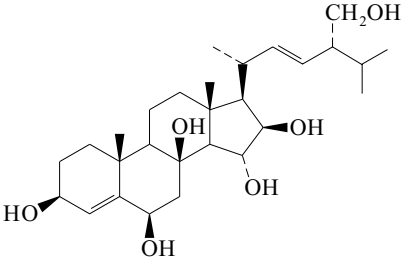


$C_{28}H_{46}O_6$ 478.668

(3β,6β,8β,15α,16β,22*E*,24*R*,25*S*)-*form*
3-O-*(2*-O-*Methyl-β-D-xylopyranoside):* [174158-29-3]
$C_{34}H_{56}O_{10}$ 624.81
Constit. of *Henricia downeyae*. Incorr. named in CAS.
3-O-*(2*-O-*Methyl-β-D-xylopyranoside), 15-sulfate:* ***Echinasteroside A***
[98166-57-5]
$C_{34}H_{56}O_{13}S$ 704.875
Constit. of *Echinaster sepositus*, *Echinaster brasiliensis* and *Henricia laeviuscola*. CAS no. refers to Na salt.
3-O-*(2,3-Di*-O-*methyl-β-D-xylopyranoside):* ***Henricioside H_2***
[168433-92-9]
$C_{35}H_{58}O_{10}$ 638.837
Constit. of a *Henricia* sp. Amorph. $[\alpha]_D$ -24.7 (c, 1.15 in MeOH).
Zollo, F. *et al., Gazz. Chim. Ital.*, 1985, **115**, 303
D'Auria, M.V. *et al., Gazz. Chim. Ital.*, 1990, **120**, 155-163 (*Henricioside H_2*)
Kicha, A.A. *et al., Khim. Prir. Soedin.*, 1993, **29**, 249; *Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 206 (*Henricioside H_2, isol, pmr, cmr*)
Palagiano, E. *et al., J. Nat. Prod.*, 1996, **59**, 348-354 (*isol*)
Ivanchina, N.V. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2004, **53**, 2639-2642 (*Henricioside H_2, abs config*)

Ergosta-4,22-diene-3,6,8,15,16,28-hexol E-611

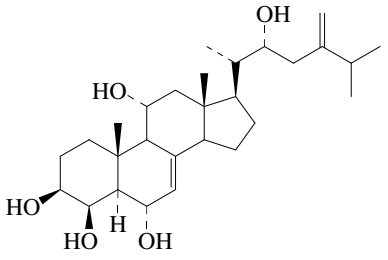
24-(Hydroxymethyl)cholesta-4,22-diene-3,6,8,15,16-pentol



$C_{28}H_{46}O_6$ 478.668

(3β,6β,8β,15α,16β,22*E*,24*R*)-*form*
3-O-*[2*-O-*Methyl-β-D-xylopyranoside], 15-sulfate:* ***Laeviuscoloside D***
[129369-37-5]
$C_{34}H_{56}O_{13}S$ 704.875
Constit. of *Henricia laeviuscola*.
D'Auria, M.V. *et al., Gazz. Chim. Ital.*, 1990, **120**, 155-163 (*isol, pmr, cmr*)

Ergosta-7,24(28)-diene-3,4,6,11,22-pentol E-612

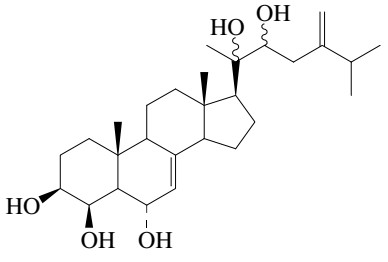


$C_{28}H_{46}O_5$ 462.668

(3β,4β,5α,6α,11α,22*R*)-*form*

3,4,6-Tri-Ac: ***Agosterol A₄***
[235791-43-2]
$C_{34}H_{52}O_8$ 588.78
Constit. of a *Spongia* sp.
$[\alpha]_D$ +17.5 (c, 0.9 in $CHCl_3$).
Aoki, S. *et al., Tetrahedron*, 1999, **55**, 13965-13972 (*isol, pmr, cmr*)

Ergosta-7,24(28)-diene-3,4,6,20,22-pentol E-613



$C_{28}H_{46}O_5$ 462.668

(3β,4β,5α,6α,20ξ,22ξ)-*form*

4,6-Di-Ac: ***Agosterol C₇***
[603113-62-8]
$C_{32}H_{50}O_7$ 546.743
Constit. of *Acanthodendrilla* sp.
$[\alpha]_D^{25}$ +34.2 (c, 0.336 in $CHCl_3$).
Tsukamoto, S. *et al., J. Nat. Prod.*, 2003, **66**, 1181-1185 (*isol, pmr, cmr*)

Ergosta-7,24(28)-diene-3,5,6,9,11-pentol E-614

24-Methylenecholest-7-ene-3,5,6,9,11-pentol
$C_{28}H_{46}O_5$ 462.668

(3β,5α,6α,9α,11α)-*form*

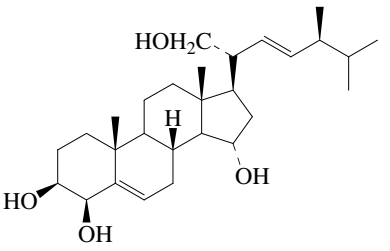
6-Ac: [133738-41-7]
$C_{30}H_{48}O_6$ 504.706
Metab. of *Dysidea herbacea*.
3,6,11-tri-Ac: $[\alpha]_D$ +9 (c, 0.3 in $CHCl_3$).

(3β,5α,6β,9α,11α)-*form*

6-Ac: [133738-42-8]
Metab. of *Dysidea herbacea*.
3,6,11-tri-Ac: $[\alpha]_D$ -80 (c, 0.6 in $CHCl_3$).
Isaacs, S. *et al., J. Nat. Prod.*, 1991, **54**, 83 (*isol, pmr, cmr*)

Ergosta-5,22-diene-3,4,15,21-tetrol E-615

24-Methylcholesta-5,22-diene-3,4,15,21-tetrol



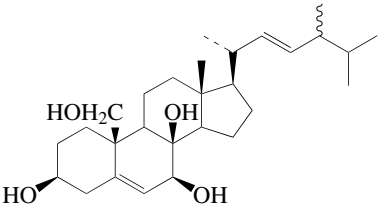
$C_{28}H_{46}O_4$ 446.669

(3β,4β,15α,22*E*,24*S*)-*form*

3-O-*[α-D-Galactopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→4)]-β-D-glucopyranoside]:* ***Mycaloside A***
[405520-37-8]
$C_{51}H_{84}O_{23}$ 1065.211
Constit. of *Mycale laxissima*. Cryst.
Mp 217-220°. $[\alpha]_D^{25}$ -23 (c, 0.5 in MeOH).

3-O-*[α-D-Galactopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→4)]-6*-O-*acetyl-β-D-glucopyranoside]:* ***Mycaloside D***
[593280-53-6]
$C_{53}H_{86}O_{24}$ 1107.248
Constit. of *Mycale laxissima*. Solid.
Mp 209-213°. $[\alpha]_D^{25}$ -32.2 (c, 0.6 in MeOH).
Kalinovsky, A.I. *et al., Tet. Lett.*, 2002, **43**, 523-525 (*Mycaloside A*)
Antonov, A.S. *et al., J. Nat. Prod.*, 2003, **66**, 1082-1088 (*Mycaloside D*)

Ergosta-5,22-diene-3,7,8,19-tetrol E-616



$C_{28}H_{46}O_4$ 446.669

(3β,7β,8β,22*E*,24ξ)-*form*
Stylisterol B
[848132-36-5]
Constit. of a *Stylissa* sp.
Powder.
Mp 189-192°. $[\alpha]_D^{25}$ -11.1 (c, 0.5 in MeOH).
Mitome, H. *et al., Steroids*, 2005, **70**, 63-70 (*Stylisterol B*)

Ergosta-5,24(28)-diene-1,3,11,18-tetrol E-617

24-Methylenecholest-5-ene-1,3,11,18-tetrol
$C_{28}H_{46}O_4$ 446.669

(1α,3β,11α)-*form* [97190-34-6]
[862261-40-3]
Constit. of *Sinularia dissecta*.
Amorph. solid. $[\alpha]_D^{20}$ -5 (c, 0.24 in MeOH).
18-Ac: [97190-31-3]
$C_{30}H_{48}O_5$ 488.706
Constit. of *Sinularia dissecta*.
18-Aldehyde: ***1,3,11-Trihydroxyergosta-5,24(28)-dien-18-al***
[97190-43-7]
$C_{28}H_{44}O_4$ 444.653
From *Sinularia dissecta*.

18-Carboxylic acid: ***1,3,11-Trihydroxyergosta-5,24(28)-dien-18-oic acid***
[97210-36-1]
$C_{28}H_{44}O_5$ 460.653
From *Sinularia dissecta*.

18-Carboxylic acid, 3-Ac: ***Sinulabasterol***
[153698-90-9]
$C_{30}H_{46}O_6$ 502.69
Isol. from soft coral *Sinularia abrupta*. Powerful antihistaminic agent. Amorph. powder. $[\alpha]_D^{25}$ -17.6 (c, 0.27 in $CHCl_3$).

5α,6-Dihydro, 18-Ac: [97190-38-0]
$C_{30}H_{50}O_5$ 490.722
From *Sinularia dissecta*.

5α,6-Dihydro, 18-aldehyde: ***1,3,11-Trihydroxyergost-24(28)-en-18-al***
[97190-46-0]
$C_{28}H_{46}O_4$ 446.669
From *Sinularia dissecta*.

5α,6-Dihydro, 18-carboxylic acid: 1,3,11-Trihydroxyergost-24(28)-en-18-oic acid
[97190-42-6]
$C_{28}H_{46}O_5$ 462.668
From *Sinularia dissecta*.

24S,28-Dihydro: ***Ergost-5-ene-1,3,11,18-tetrol***
[862261-38-9]
$C_{28}H_{48}O_4$ 448.685
Constit. of *Sinularia dissecta*. Amorph. powder. $[\alpha]_D^{20}$ -30 (c, 0.09 in MeOH).

24S,28-Dihydro, 18-carboxylic acid, 3-Ac: [862261-37-8]
$C_{30}H_{48}O_6$ 504.706
Constit. of *Sinularia dissecta*. Gum. $[\alpha]_D^{20}$ -42 (c, 0.14 in MeOH).

24,28-Dihydro, 18-Ac: [97190-36-8]
$C_{30}H_{50}O_5$ 490.722
From *Sinularia dissecta*.

24,28-Dihydro, 18-aldehyde: 1,3,11-Trihydroxyergost-5-en-18-al
[97190-44-8]
$C_{28}H_{46}O_4$ 446.669
From *Sinularia dissecta*.

24R,28-Dihydro, 22,23-didehydro, 18-Ac: [97190-37-9]
$C_{30}H_{48}O_5$ 488.706
From *Sinularia dissecta*.

Jagodzinska, B.M. *et al., J.O.C.*, 1985, **50**, 2988-2992 (*Sinularia dissecta constits*)
Shoji, N. *et al., J. Pharm. Sci.*, 1994, **83**, 761-762 (*Sinulabasterol*)
Jin, P. *et al., Steroids*, 2005, **70**, 487-493 (*Sinularia dissecta constits*)

Ergosta-5,24(28)-diene-2,3,4,7-tetrol E-618

$C_{28}H_{46}O_4$ 446.669

(2α,3β,4β,7α)-*form*

4-O-β-D-Galactopyranosyl, 7-O-(4-O-acetyl-β-D-xylopyranosyl): ***Pachastrelloside A***
[129744-13-4]
$C_{41}H_{66}O_{14}$ 782.964
Constit. of sponge *Pachastrella* sp. Powder.
Mp 165-167°.

(2α,3β,4β,7β)-*form*

4-O-[β-D-Galactopyranosyl-(1→2)-β-D-xylopyranoside]: ***Wondosterol A***
[252023-82-8]
$C_{39}H_{64}O_{13}$ 740.927
Constit. of an association of sponges *Jaspis* sp. and *Poecillastra* sp. Amorph. solid. $[\alpha]_D^{23}$ +38.4 (c, 1.2 in MeOH).

Hirota, M. *et al., Tet. Lett.*, 1990, **31**, 3321-3324 (*isol, struct*)
Ryu, G. *et al., Tetrahedron*, 1999, **55**, 13171-13178 (*Wondosterol A*)

Ergosta-5,24(28)-diene-2,3,15,18-tetrol E-619

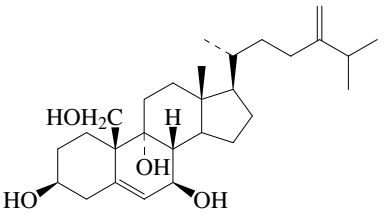
24-Methylenecholest-5-ene-2,3,15,18-tetrol
$C_{28}H_{46}O_4$ 446.669

(2α,3α,15β)-*form*

2,15,18-Tri Ac: 2α,15β,18-Triacetoxy-24-methylenecholest-5-en-3-ol
[99957-33-2]
$C_{34}H_{52}O_7$ 572.781
Constit. of *Eudendrium glomeratum*. Cryst. (MeOH).
Mp 185-187°. $[\alpha]_D^{26}$ +21 (c, 0.04 in $CHCl_3$).
Fattorusso, E. *et al., J. Nat. Prod.*, 1985, **48**, 784

Ergosta-5,24(28)-diene-3,7,9,19-tetrol E-620

24-Methylenecholest-5-ene-3,7,9,19-tetrol



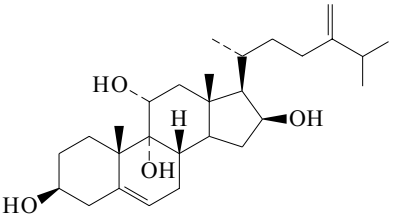
$C_{28}H_{46}O_4$ 446.669

(3β,7β,9α)-*form* [250143-36-3]
Constit. of *Nephthea chabroli*.

Tetra-Ac:
Oil. $[\alpha]_D^{25}$ -42 (c, 0.8 in $CHCl_3$).
Rao, M.R. *et al., J. Nat. Prod.*, 1999, **62**, 1584-1585 (*isol, pmr, cmr*)

Ergosta-5,24(28)-diene-3,9,11,16-tetrol E-621

24-Methylenecholest-5-ene-3,9,11,16-tetrol



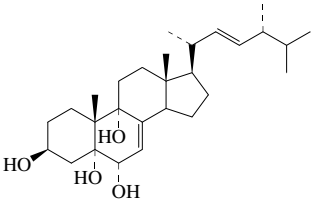
$C_{28}H_{46}O_4$ 446.669

(3β,9α,11α,16β)-*form*

3-O-α-L-Fucopyranoside: [155850-90-1]
$C_{34}H_{56}O_8$ 592.812
Constit. of *Sinularia gibberosa*. Cryst.
Mp 217-220°. $[\alpha]_D$ -35 (c, 0.84 in Py).
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1994, 140 (*isol, pmr, cmr*)

Ergosta-7,22-diene-3,5,6,9-tetrol, 9CI E-622

24-Methylcholesta-7,22-diene-3,5,6,9-tetrol



(3β,5α,6α,9α,22*E*,24*R*)-*form*

$C_{28}H_{46}O_4$ 446.669

(3β,5α,6α,9α,22*E*,24*R*)-*form* [211486-15-6]
Constit. of edible mushrooms including *Lentinus edodes* (shiitake), *Flammulina velutipes* (enokitake), *Hypsizygus marmoreus* (buna-shimeji), *Pleurotus ostreatus* (tree oyster) and *Pholiota nameko* (nameko).
Amorph. powder. $[\alpha]_D^{24}$ -28.8 (c, 0.1 in $CHCl_3$).

22,23-Dihydro, 6-ketone: ***3,5,9-Trihydroxyergost-7-en-6-one****. 3,5,9-Trihydroxy-24-methylcholest-7-en-6-one*
[211486-13-4]
$C_{28}H_{46}O_4$ 446.669
Isol. from the fungi *Lentinus edodes* (shiitake), *Hypsizygus marmoreus* (bunashimeji), *Pleurotus ostreatus* (tree oyster) and *Pholiota nameko* (nameko). Amorph. powder. $[\alpha]_D^{28}$ -21.5 (c, 0.09 in $CHCl_3$). Has 24*S*-config. (change of Cahn-Ingold-Prelog priorities). λ_{max} 236 (log ϵ 3.8) (MeOH).

(3β,5α,6α,9α,22*E*,24ξ)-*form*
6-O-*Sulfate:* [168982-46-5]
$C_{28}H_{46}O_7S$ 526.733
Constit. of *Dysidea fragilis* from the Venice lagoon.
22,23-Dihydro, 6-O-*sulfate:* [168982-47-6]
$C_{28}H_{48}O_7S$ 528.749
Constit of *Dysidea fragilis.*

(3β,5α,6β,9α,22*E*,24*R*)-*form* [88191-06-4]
Metab. of *Polyporus versicolor*, *Agaricus blazei* and *Lactarius volemus.*
Cryst. Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 225-227°. $[\alpha]_D$ -141 (c, 0.032 in Py).
3-O-*β*-D-*Glucopyranoside:*
$C_{34}H_{56}O_9$ 608.811
Isol. from *Pleurotus ostreatus* (tree oyster). Amorph. powder.
Mp 275-277°. $[\alpha]_D^{20}$ -90.6 (c, 0.36 in MeOH).
6-Me ether: ***6-Methoxyergosta-7,22-diene-3,5,9-triol***
[88191-15-5]
$C_{29}H_{48}O_4$ 460.696
Metab. of *Polyporus versicolor.* Cryst. Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 178-180°. $[\alpha]_D$ -117 (c, 0.75 in $CHCl_3$).
6-Ketone: ***3,5,9-Trihydroxyergosta-7,22-dien-6-one****. 3,5,9-Trihydroxy-24-methylcholesta-7,22-dien-6-one*
[88191-14-4]
$C_{28}H_{44}O_4$ 444.653
Metab. of *Polyporus versicolor.* Cryst.
Mp 225-228°. $[\alpha]_D$ -64 (c, 0.056 in $CHCl_3$).

(3β,5α,6β,9α,22*E*,24*S*)-*form* [133161-20-3]
Constit. of *Spongia officinalis.* Prod. by *Russula rosacea.*
Cryst. (MeOH aq.).
Mp 252-254°. $[\alpha]_D^{25}$ -25 (c, 0.08 in MeOH).
22,23-Dihydro: ***Ergost-7-ene-3,5,6,9-tetrol***
[243449-56-1]
$C_{28}H_{48}O_4$ 448.685
Constit. of *Amanita virgineoides.* Amorph. powder.
Valisolalao, J. *et al., Tetrahedron*, 1983, **39**, 2779-2785 (*Polyporus versicolor metabs*)
Migliuolo, A. *et al., J. Nat. Prod.*, 1990, **53**, 1414-1424 (*Spongia officinalis metab, isol, pmr, cmr*)
Aiello, A. *et al., Steroids*, 1995, **60**, 666-673 (*6-sulfates, isol, pmr, cmr*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1998, **46**, 944-950; 1999, **47**, 847-851 (*mushroom constits*)
Yue, J.-M. *et al., Phytochemistry*, 2001, **56**, 801-806 (*isol, pmr, cmr, ms*)
Zhan, Z.-J. *et al., Acta Bot. Sin.*, 2003, **45**, 753-756 (*Pleurotus ostreatus glucoside*)

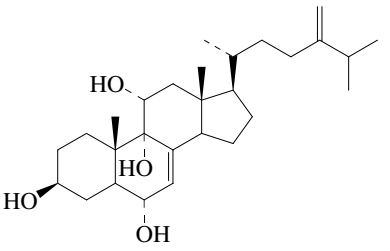
Ergosta-7,24(28)-diene-3,5,6,9-tetrol, 9CI E-623

24-Methylenecholest-7-ene-3,5,6,9-tetrol
$C_{28}H_{46}O_4$ 446.669

(3β,5α,6β,9α)-*form* [133056-66-3]
Constit. of *Spongia officinalis.*
$[\alpha]_D^{25}$ -57.1 (c, 0.14 in MeOH).
Migliuolo, A. *et al., J. Nat. Prod.*, 1990, **53**, 1414 (*isol, pmr, cmr*)

Ergosta-7,24(28)-diene-3,6,9,11-tetrol E-624

24-Methylenecholest-7-ene-3,6,9,11-tetrol

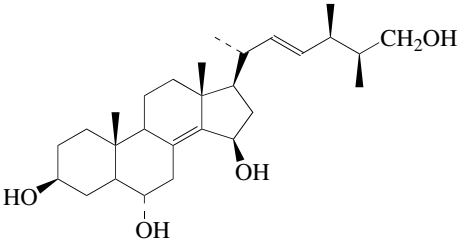


$C_{28}H_{46}O_4$ 446.669

(3β,6α,9α,11α)-*form* [153506-96-8]
Isol. from *Sinularia hirta.*
Mp 212-215°. Incorrect name in CA.
Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 144-147 (*isol, pmr*)

Ergosta-8(14),22-diene-3,6,15,26-tetrol E-625

24-Methylcholesta-8(14),22-diene-3,6,15,26-tetrol

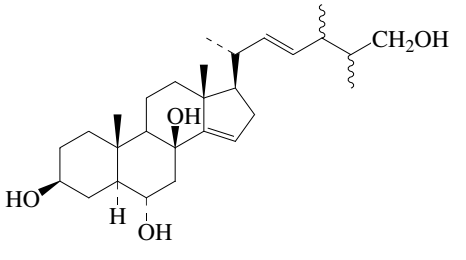


$C_{28}H_{46}O_4$ 446.669

(3β,6α,15β,22*E*,24*R*,25*S*)-*form* [194935-37-0]
Constit. of *Acodontaster conspicuus.*
$[\alpha]_D$ -2.5 (c, 1 in MeOH).
26-O-*[2*-O-*Methyl-β*-D-*xylopyranosyl-(1→2)-β*-D-*xylopyranoside]:* ***Acodontasteroside H***
[195063-95-7]
$C_{39}H_{64}O_{12}$ 724.927
Constit. of *Acodontaster conspicuus.*
$[\alpha]_D$ -21.7 (c, 1 in MeOH).
De Marino, S. *et al., J. Nat. Prod.*, 1997, **60**, 959-966 (*isol, pmr, cmr*)

Ergosta-14,22-diene-3,6,8,26-tetrol E-626

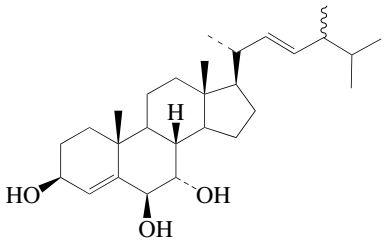
24-Methylcholesta-14,22-diene-3,6,8,26-tetrol



$C_{28}H_{46}O_4$ 446.669

(3β,5α,6α,8β,22*E*,24ξ,25ξ)-*form*
26-O-*(3*-O-*Methyl-β*-D-*glucopyranoside):* ***Crossasteroside P₃***
[128631-20-9]
$C_{35}H_{58}O_9$ 622.838
Isol. from starfish *Crossaster papposus.* Amorph. $[\alpha]_{Hg}$ +16.3 (c, 0.4 in MeOH).
Kicha, A.A. *et al., Khim. Prir. Soedin.*, 1990, 218-221; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 175-177

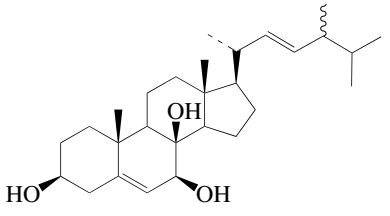
Ergosta-4,22-diene-3,6,7-triol E-627



$C_{28}H_{46}O_3$ 430.67

(3β,6β,7α,22*E*,24ξ)-*form*
Stylisterol C
[848132-37-6]
Constit. of a *Stylissa* sp.
Powder.
Mp 248-251°. $[\alpha]_D^{26}$ -26.3 (c, 1.4 in MeOH).
Mitome, H. *et al., Steroids*, 2005, **70**, 63-70 (*Stylisterol C*)

Ergosta-5,22-diene-3,7,8-triol E-628



$C_{28}H_{46}O_3$ 430.67

(3β,7β,8β,22*E*,24ξ)-*form*
Stylisterol A
[848132-35-4]
Constit. of a *Stylissa* sp.
Powder.
Mp 160-162°. $[\alpha]_D^{25}$ -59.4 (c, 3.5 in MeOH).
Mitome, H. *et al., Steroids*, 2005, **70**, 63-70 (*Stylisterol A*)

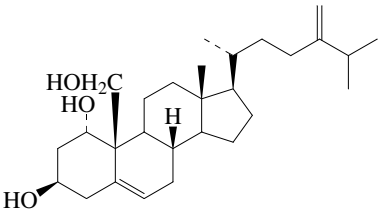
Ergosta-5,24(28)-diene-1,3,11-triol E-629

24-Methylenecholest-5-ene-1,3,11-triol
$C_{28}H_{46}O_3$ 430.67

(1α,3β,11α)-*form* [95513-57-8]
Constit. of *Sinularia dissecta*.
Cryst.
Mp 161-162°.
11-Ac: [95513-65-8]
$C_{30}H_{48}O_4$ 472.707
From *Sinularia dissecta*.
5α,6-Dihydro: Ergost-24(28)-ene-1,3,11-triol. 24-Methylenecholestane-1,3,11-triol
[95513-66-9]
$C_{28}H_{48}O_3$ 432.685
From *Sinularia dissecta*. Cryst.
Mp 185-186°.
Jagodzinska, B.M. *et al., J.O.C.*, 1985, **50**, 1435-1439 (*isol, pmr, ms*)

Ergosta-5,24(28)-diene-1,3,19-triol E-630

24-Methylenecholest-5-ene-1,3,19-triol

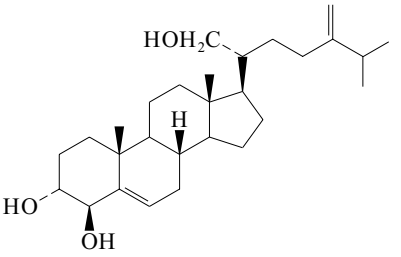


$C_{28}H_{46}O_3$ 430.67

(1α,3β)-*form* [250143-35-2]
Constit. of *Nephthea chabroli*.
Tri-Ac:
Oil. $[\alpha]_D^{25}$ +2 (c, 0.5 in $CHCl_3$).
Rao, M.R. *et al., J. Nat. Prod.*, 1999, **62**, 1584-1585 (*isol, pmr, cmr*)

Ergosta-5,24(28)-diene-3,4,21-triol E-631

24-Methylenecholest-5-ene-3,4,21-triol

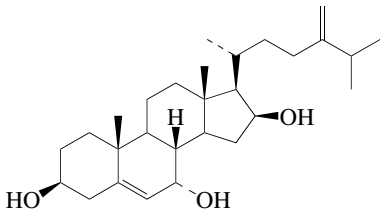


$C_{28}H_{46}O_3$ 430.67

(3α,4β)-*form*
3,21-Disulfate: [162830-23-1]
$C_{28}H_{46}O_9S_2$ 590.798
Constit. of *Ophiotrix fragilis* and *Ophiura texturata*.
$[\alpha]_D$ -14.
D'Auria, M.V. *et al., J. Nat. Prod.*, 1995, **58**, 189-196 (*3,21-disulfate, isol, pmr*)

Ergosta-5,24(28)-diene-3,7,16-triol E-632

24-Methylenecholest-5-ene-3,7,16-triol



(3β,7α,16β)-*form*

$C_{28}H_{46}O_3$ 430.67

(3β,7α,16β)-*form* [289054-34-8]
3-O-α-L-*Fucopyranoside:* [132237-35-5]
$C_{34}H_{56}O_7$ 576.812
Constit. of *Sinularia gibberosa* and *Lobophytum microlobulatum*.
Needles (MeOH).
Mp 241-243°. $[\alpha]_D^{21}$ -114 (c, 0.3 in EtOH).

(3β,7β,16β)-*form* [155850-88-7]
Constit. of *Sinularia gibberosa*. Also isol. from *Amoora yunnanensis*.
Cryst.
Mp 213-215°. $[\alpha]_D$ +63 (c, 0.32 in Py).

3-O-α-L-*Fucopyranoside:* [132214-24-5]
Constit. of *Sinularia gibberosa*.
Needles (MeOH).
Mp 255-257°. $[\alpha]_D^{27}$ -52 (c, 0.6 in Py).

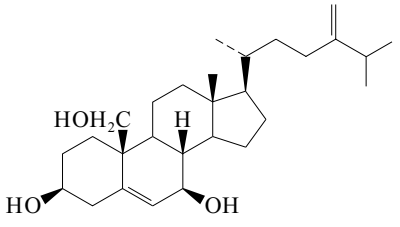
3-O-α-L-*Fucopyranoside, 7-Ac:* [151564-02-2]
$C_{36}H_{58}O_8$ 618.849
Constit. of a *Sinularia* sp. Cryst. (MeOH).
Mp 180-181°. $[\alpha]_D^{25}$ +11.32 (c, 2.5 in $CHCl_3$).

3-O-*(4*-O-*Acetyl*-α-L-*fucopyranoside):* [124561-20-2]
$C_{36}H_{58}O_8$ 618.849
Constit. of *Sinularia crispa* and *Sinularia gibberosa*. Needles (MeOH aq.).
Mp 172.5-173°. $[\alpha]_D^{28}$ -6.3 (c, 5.26 in $CHCl_3$).

Tillekaratne, L.M.V. *et al., J. Nat. Prod.*, 1989, **52**, 1143-1145 (*4-acetylfucoside*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2400 (*isol, struct*)
Subrahmanyam, C. *et al., Indian J. Chem., Sect. B*, 1993, **32**, 1093 (*derivs*)
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1994, 140 (*isol, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 45-48; 819 (*fucosides, isol*)
Vanisree, M. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 394-396 (*isol, cmr*)

Ergosta-5,24(28)-diene-3,7,19-triol E-633

24-Methylenecholest-5-ene-3,7,19-triol



$C_{28}H_{46}O_3$ 430.67

(3β,7β)-*form*
Nephalsterol B
[61737-96-0]
Constit. of *Litophyton arboreum*, *Litophyton viridis*, *Nephthea erecta* and *Nephthea albida*.
Flakes (Me_2CO).
Mp 160-162°.

7-Ac: ***Nephalsterol C***
[61737-97-1]
$C_{30}H_{48}O_4$ 472.707
Constit. of *Nephthea albida*.

19-Ac: [871117-79-2]
$C_{30}H_{48}O_4$ 472.707
Constit. of a *Sinularia* sp. Oil. $[\alpha]_D^{20}$ -22.4 (c, 0.1 in $CHCl_3$).

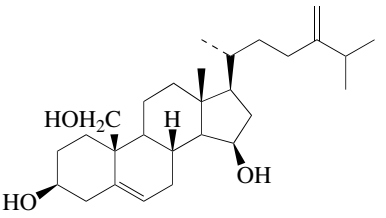
7,19-Di-Ac: [871117-80-5]
$C_{32}H_{50}O_5$ 514.744
Constit. of a *Sinularia* sp. Oil. $[\alpha]_D^{20}$ -5.38 (c. 0.08 in $CHCl_3$).

7-Ketone: ***3,19-Dihydroxyergosta-5,24(28)-dien-7-one****. 3,19-Dihydroxy-24-methylenecholest-5-en-7-one*
[211555-03-2]
$C_{28}H_{44}O_3$ 428.654
Constit. of *Nephthea erecta*. Prisms.
Mp 165-167°. $[\alpha]_D^{25}$ -19.1 (c, 0.13 in MeOH). λ_{max} 241 (log ϵ 4.56) (MeOH).

Bortolotto, M. *et al., Steroids*, 1976, **28**, 461-466 (*isol*)
Losman, D. *et al., Acta Cryst. B*, 1978, **34**, 2586-2589 (*cryst struct*)
Liu, J. *et al., CA*, 1992, **117**, 230410x; 230411y (*Nephalsterol*)
Li, R. *et al., Steroids*, 1994, **59**, 503-505 (*isol, pmr, cmr*)
Duh, C.-Y. *et al., J. Nat. Prod.*, 1998, **61**, 1022-1024 (*7-ketone*)
Lu, W.G. *et al., Chin. Chem. Lett.*, 2005, **16**, 604-606 (*synth*)
Jia, R. *et al., Nat. Prod. Res.*, 2005, **19**, 789-794 (*19-Ac, 7,19-di-Ac*)

Ergosta-5,24(28)-diene-3,15,19-triol E-634

24-Methylenecholest-5-ene-3,15,19-triol



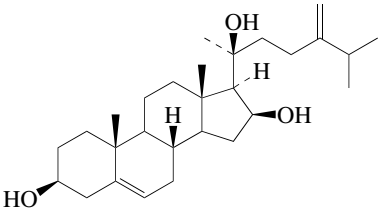
$C_{28}H_{46}O_3$ 430.67

(3β,15β)-*form* [211555-02-1]
Constit. of *Nephthea erecta*.
Prisms.
Mp 204-205°. $[\alpha]_D^{25}$ -28.8 (c, 0.34 in MeOH). λ_{max} 208 (log ϵ 4.4) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 1998, **61**, 1022-1024 (*isol, pmr, cmr*)

Ergosta-5,24(28)-diene-3,16,20-triol E-635

24-Methylenecholest-5-ene-3,16,20-triol



$C_{28}H_{46}O_3$ 430.67

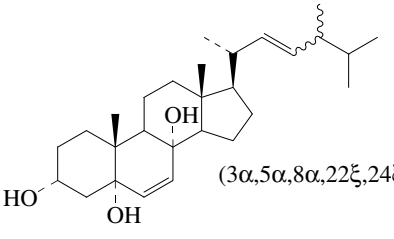
(3β,16β,20*S*)-*form* [224784-47-8]
Cryst. Mp 102-104°. $[\alpha]_D$ -12.5 (c, 0.64 in $CHCl_3$).

16-Ketone: ***3,20-Dihydroxyergosta-5,24(28)-dien-16-one****. 3,20-Dihydroxy-24-methylenecholest-5-en-16-one*
[224784-46-7]
$C_{28}H_{44}O_3$ 428.654
Constit. of *Cystophora brownii*. Cryst.
Mp 117-118°. $[\alpha]_D$ -177 (c, 0.52 in $CHCl_3$).

Bian, B. *et al., Aust. J. Chem.*, 1998, **51**, 1157-1165 (*isol, pmr, cmr*)

Ergosta-6,22-diene-3,5,8-triol E-636

24-Methylcholesta-6,22-diene-3,5,8-triol
[76420-88-7]



(3α,5α,8α,22ξ,24ξ)-*form*

$C_{28}H_{46}O_3$ 430.67

(3α,5α,8α,22ξ,24ξ)-*form*
Cryst. (EtOAc). Mp 178-181°. $[\alpha]_D$ -23 (c, 1.7 in $CHCl_3$).

(3β,5α,8α,22*E*,24ξ)-*form* [7001-69-6]
Constit. of *Adenophora stenanthina* ssp. *xifengensis*.
Cryst. (petrol/Me_2CO).
Mp 178-180°. $[\alpha]_D$ -2.1 (c, 1 in $CHCl_3$). $[\alpha]_D$ -16.8 (Py).

(3β,5β,8β,22*E*,24ξ)-*form* [288847-52-9]
Constit. of *Gyroporus castaneus* (chestnut bolete).

(5ξ,8ξ,22*E*,24ξ)-*form*

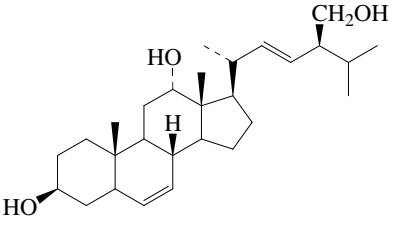
3-Ketone: ***5,8-Dihydroxyergosta-6,22-dien-3-one***
[870535-11-8]
$C_{28}H_{44}O_3$ 428.654
Constit. of *Laurencia cartilaginea*.

[40691-24-5]

Clayton, R.B. *et al., J.C.S.*, 1953, 2015-2021 (*synth*)
Dalton, F. *et al., J.C.S.*, 1961, 1880-1884 (*synth*)
Dannenberg, H. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1965, **342**, 199-213 (*synth*)
Hou, Z.-F. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 293-296 (*isol, ir, pmr, cmr, ms*)
Wan, H. *et al., Tianran Chanwu Yanjiu Yu Kaifa*, 1999, **11**, 18-21; *CA*, **133**, 190274c (*Gyroporus castaneus constit*)
Yang, X.-Y. *et al., Guangpu Shiyanshi*, 2005, **22**, 12-16; *CA*, **144**, 19295p (*Laurencia cartilaginea constit*)

Ergosta-6,22-diene-3,12,28-triol E-637

24-Hydroxymethylcholesta-6,22-diene-3,12-diol



$C_{28}H_{46}O_3$ 430.67

(3β,12α,22*E*,24*S*)-*form*

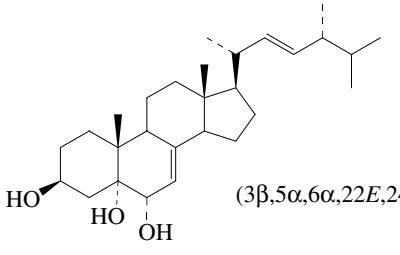
Petromyzosterol

3,28-Disulfate: ***Petromyzosterol disulfate***
[871543-68-9]
$C_{28}H_{46}O_9S_2$ 590.798
Pheromone of the sea lamprey (*Petromyzon marinus*).

Sorensen, P.W. *et al., Nat. Chem. Biol.*, 2005, **1**, 324-328

Ergosta-7,22-diene-3,5,6-triol E-638

24-Methylcholesta-7,22-diene-3,5,6-triol



(3β,5α,6α,22*E*,24*R*)-*form*

$C_{28}H_{46}O_3$ 430.67

(3β,5α,6β,22*E*,24*R*)-*form*

Cerevisterol
[516-37-0]
Isol. from *Agaricus blazei*, *Amanita phalloides*, *Ganoderma lucidum*, *Fusarium moniliforme* and *Myriapora truncata*; also from soft coral *Sinularia* sp. and sponge *Spongionella gracilis*. HIV protease inhibitor. Cryst. (MeOH).
Mp 254-256°. $[\alpha]_D^{21}$ -79.9 (c, 1.35 in Py).

6-Ac: [260062-88-2]
$C_{30}H_{48}O_4$ 472.707
Prod. by an unidentified *Colletotrichum* sp. Needles.
Mp 89-90°.

6-Phenylacetyl: [260062-90-6]
$C_{36}H_{52}O_4$ 548.804
Prod. by an unidentified *Colletotrichum* sp. Gum.

6-Me ether: 6-Methoxyergosta-7,22-diene-3,5-diol
[126060-09-1]
$C_{29}H_{48}O_3$ 444.696
Isol. from the fungus *Ganoderma lucidum* and the sponge *Dictyonella incisa*. Sol. MeOH, C_6H_6; poorly sol. H_2O.

(3β,5α,6β,22*E*,24*S*)-*form* [100761-25-9]
Isol. from *Russula rosacea*, *Dictyonella incisa*, *Heliometra glacialis maxima*, *Gymnocrinus richeri*, *Myriapora truncata* and *Spongionella gracilis*.
Cryst. (MeOH).
Mp 245-247°.

(3β,5α,6β,22*E*,24ξ)-*form*

6-Ketone: [135637-20-6]
Isol. from *Oscarella lobularis*. May be identical with the *G. frondosa* isolate above.

Serebryakov, E.P. *et al., Tetrahedron*, 1970, **26**, 5215-5223 (*Cerevisterol, isol*)
Cafieri, F. *et al., J. Nat. Prod.*, 1985, **48**, 944-947 (*Myriapora truncata constits*)
Piccialli, V. *et al., J. Nat. Prod.*, 1987, **50**, 915-920 (*Spongionella gracilis constits*)
Kawagishi, H. *et al., Phytochemistry*, 1988, **27**, 2777-2779 (*Cerevisterol, isol, pmr, cmr*)
Ciminiello, P. *et al., J.A.C.S.*, 1990, **112**, 3505-3509 (*Dictyonella incisa constits*)
Aiello, A. *et al., Steroids*, 1991, **56**, 337-340 (*isol, pmr, ketone*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1993, **41**, 87-89 (*cmr*)
Ishizuka, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1756-1760 (*6-ketone*)
Anjaneyulu, A.S.R. *et al., J.C.S. Perkin 1*, 1997, 959-962 (*Cerevisterol*)
Abate, D. *et al., Phytochemistry*, 1997, **44**, 1443-1448 (*Cerevisterol, pmr, cmr*)
Jinming, G. *et al., Steroids*, 2001, **66**, 771-775 (*Cerevisterol, pmr, cmr, Tuberoside*)

Ergosta-7,24(28)-diene-3,5,6-triol, 9CI E-639

24-Methylenecholest-7-ene-3,5,6-triol
$C_{28}H_{46}O_3$ 430.67

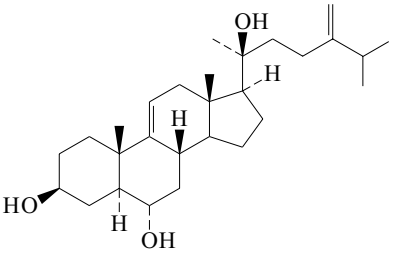
(3β,5α,6β)-*form* [112058-04-5]
Constit. of *Patinopecten yessoensis* and *Spongionella gracilis*.
Cryst. (MeOH).
Mp 244-246°. $[\alpha]_D$ -26 (MeOH).

6-Ketone: 3,5-Dihydroxyergosta-7,24(28)-dien-6-one. 3,5-Dihydroxy-24-methylenecholest-7-en-6-one
$C_{28}H_{44}O_3$ 428.654
Isol. from *Oscarella lobularis*.

Piccialli, V. *et al., J. Nat. Prod.*, 1987, **50**, 915 (*isol*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1988, **51**, 1098-1103 (*isol, pmr, cmr*)
Aiello, A. *et al., Steroids*, 1991, **56**, 337 (*isol, pmr, ketone*)

Ergosta-9(11),24(28)-diene-3,6,20-triol E-640

Ergosta-9(11),24(24^1)-diene-3,6,20-triol. 24-Methylenecholest-9(11)-ene-3,6,20-triol



$C_{28}H_{46}O_3$ 430.67

(3β,5α,6α,20*S*)-*form*

6-O-[6-Deoxy-β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate: ***Asteroside D***

[115178-51-3]
$C_{57}H_{94}O_{27}S$ 1243.419
Constit. of *Asterias amurensis*.
$[\alpha]_D$ +5 (MeOH).

6-O-[β-D-Galactopyranosyl-(1→3)-β-D-fucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate: ***Asteriidoside B***
[214976-30-4]
$C_{63}H_{104}O_{31}S$ 1389.562
Constit. of a starfish (Asteriidae).
$[\alpha]_D$ +9.2 (c, 1 in MeOH).

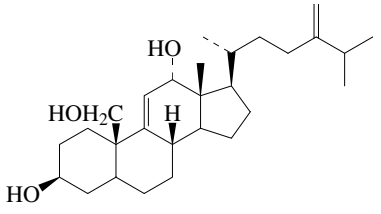
*6-O-[β-D-Galactopyranosyl-(1→3)-α-L-arabinopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-*O*-sulfate:* ***Asteriidoside D***
[214976-57-5]
$C_{62}H_{102}O_{31}S$ 1375.535
Constit. of a starfish (Asteriidae).
$[\alpha]_D$ +7.7 (c, 1 in MeOH).

*6-O-[6-Deoxy-β-D-glucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-*O*-sulfate:* ***Ruberoside C***
[270249-49-5]
$C_{57}H_{94}O_{26}S$ 1227.42
Constit. of *Asterias rubens*.

Riccio, R. *et al., J.C.S. Perkin 1*, 1988, 1337-1347 (*isol, pmr, cmr, ms*)
De Marino, S. *et al., J. Nat. Prod.*, 1998, **61**, 1319-1327 (*Asteriidosides*)
Sandvoss, M. *et al., Eur. J. Org. Chem.*, 2000, 1253-1262 (*Ruberoside C*)

Ergosta-9(11),24(28)-diene-3,12,19-triol E-641

24-Methylenecholest-9(11)-ene-3,12,19-triol



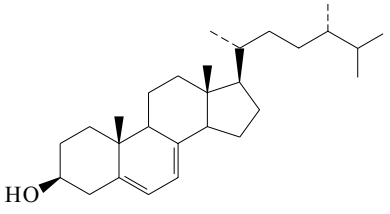
$C_{28}H_{46}O_3$ 430.67

(3β,12α)-*form* [623167-70-4]
Constit. of *Nephthea chabroli*.
Cryst.
Mp 163-164°. $[\alpha]_D^{25}$ -141.9 (c, 0.031 in MeOH).

Zhang, W. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1009-1011 (*isol, pmr, cmr*)

Ergosta-5,7-dien-3-ol E-642

24-Methylcholesta-5,7-dien-3-ol



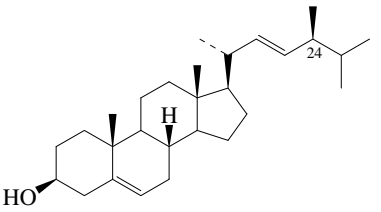
$C_{28}H_{46}O$ 398.671

(3β,24*S*)-*form*
22,23-Dihydroergosterol. *Provitamin D_4*
[516-79-0]
Constit. of *Saccharomyces cerevisiae*. Also from lipids of *Claviceps purpurea*, seed oil of *Vitis vinifera* (wine grape) and from *Polyporus* spp. Minor component of the lipids of a marine unicellular green alga.
Cryst. + H_2O (EtOAc/MeOH).
Mp 152-153°. $[\alpha]_D$ -128.7 (c, 0.4 in $CHCl_3$).

Barton, D.H.R. *et al., J.C.S. Perkin 1*, 1974, 1326; 1976, 821 (*isol, synth*)
Kircher, H.W. *et al., Lipids*, 1975, **10**, 517 (*synth*)
Brynjolffssen, J. *et al., J.C.S. Perkin 1*, 1976, 826 (*synth*)
Mercer, E.I. *et al., Phytochemistry*, 1976, **15**, 283 (*biosynth*)
Curry, D.J. *et al., J.C.S. Perkin 1*, 1977, 822 (*synth*)
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*occur, alga*)

Ergosta-5,22-dien-3-ol E-643

24-Methylcholesta-5,22-dien-3-ol



(3β,22*E*,24*R*)-*form*

$C_{28}H_{46}O$ 398.671

(3β,22*E*,24*R*)-*form*
Brassicasterol
[474-67-9]
[2638-57-5]
Constit. of *Brassica rapa* oil and of various marine organisms, incl. sponges, lipids of a marine unicellar alga and clam *Placopecten magellanicus*.
Cryst.
Mp 157-158° (148°). $[\alpha]_D^{19}$ -39.4. $[\alpha]_D^{19}$ -54 ($CHCl_3$). Prob. identical with Shakosterol isol. from a mollusc.

*3-*O*-Sulfate:* [151890-96-9]
$C_{28}H_{46}O_4S$ 478.735
Constit. of *Eupentacta fraudatrix*.

*3-*O*-β-D-Xylopyranoside:* [151890-81-2]
$C_{33}H_{54}O_5$ 530.787
Constit. of *Eupentacta fraudatrix*.

Me ether: 3-Methoxyergosta-5,22-diene
[139894-62-5]
$C_{29}H_{48}O$ 412.698
Constit. of *Jereicopsis graphidiophora*.

3-Ketone: Ergosta-5,22-dien-3-one. 24-Methylcholesta-5,22-dien-3-one. ***Brassicasterone***
[13963-13-8]
$C_{28}H_{44}O$ 396.655
Isol. from *Salvia multicaulis*. Prod. by oxidn. of Brassicasterol (see Ergosta-5,22-dien-3-ol, E-643). Cryst. (EtOAc).
Mp 150-151° (129-131°). $[\alpha]_D$ +46 (c, 0.6 in $CHCl_3$).

3-Ketone, 2,4-dinitrophenylhydrazone:
Red cryst. Mp 242-243°.

(3β,22*E*,24*S*)-*form*
Crinosterol. *Campesta-5,22-dien-3-ol. 24-Epibrassicasterol*
[17472-78-5]
Constit. of a crinoid (*Comatula* sp.), sponges *Jaspis stellifera*, *Phaeodactylum tricornutum* and *Chlorella ellipsoidea* and in *Patinopecten yessoensis*. Present in lipids of a marine unicellar alga.
Cryst. (MeOH or Me_2CO).
Mp 147-148°. $[\alpha]_D^{26}$ -47.2.

Me ether: [61586-00-3]
[139894-62-5]
Constit. of *Jereicopsis graphidiophora*.

(3β,22*E*,24ξ)-*form* [2638-57-5]
Constit. of *Pseudostichopus trachus*, *Synapta maculata*, *Echinaster sepositus*, *Petrosia ficiformis* and many other marine organisms.

*3-*O*-Sulfate:* [80677-77-6]
Constit. of *Asterias rubens*, *Echinus esculentus*, *Echinocardium cordatum*, *Antedon bifida* and *Ophiocomina nigra*.

Formyl: [848137-18-8]
$C_{29}H_{46}O_2$ 426.681
Constit. of a *Dendronephthya* sp. Amorph. solid. $[\alpha]_D^{25}$ -15.4 (c, 0.85 in $CHCl_3$).

Barton, D.H.R. *et al., J.C.S.*, 1949, 1771 (*3-ketone, synth*)
Daglish, A.F. *et al., J.C.S.*, 1954, 2627 (*3-ketone, synth*)
Shepherd, D.A. *et al., J.A.C.S.*, 1955, **77**, 1212 (*3-ketone, synth*)
Garrett, E.R. *et al., J.A.C.S.*, 1956, **78**, 3340 (*3-ketone, synth*)
Halkes, S.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1965, **84**, 889 (*pmr*)
Bolker, H.I. *et al., Nature (London)*, 1967, **213**, 905 (*isol*)
Rubinstein, I. *et al., Phytochemistry*, 1974, **13**, 485; 1976, **15**, 195 (*isol, pmr*)
Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*isol, sponges, ms*)
Sheikh, Y.M. *et al., Steroids*, 1975, **26**, 129 (*synth*)
Kobayashi, M. *et al., Steroids*, 1975, **26**, 605 (*isol*)
Adler, J.H. *et al., Lipids*, 1976, **11**, 634 (*biosynth*)
Tsai, L.B. *et al., Phytochemistry*, 1976, **15**, 1131 (*biosynth*)
Wright, J.L.C. *et al., Can. J. Chem.*, 1978, **56**, 1898 (*cmr*)
Theobald, N. *et al., J.A.C.S.*, 1978, **100**, 7677 (*isol*)
De Simone, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **66**, 351-357 (*24ξ-form, occur*)
Khalil, M.W. *et al., Steroids*, 1980, **35**, 707-719 (*24ξ-form, occur*)
Lang, R.W. *et al., Helv. Chim. Acta*, 1982, **65**, 407 (*synth*)
Goodfellow, R.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **76**, 575-578 (*sulfate*)
Anastasia, M. *et al., J.C.S. Perkin 1*, 1983, 379; 2365 (*synth*)
Seo, S. *et al., Chem. Comm.*, 1984, 1174 (*biosynth*)
Takatsuto, S. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2001 (*3-ketone, synth*)
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*occur, alga*)
Veares, M.P. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1988, **90**, 25-28 (*sulfate*)
Klimashina, M.M. *et al., Izv. Akad. Nauk Gruz. SSR, Ser. Biol.*, 1989, 429 (*3-ketone, synth*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*3-Methoxyergostadiene*)
KhripachV.A. *et al., Khim. Prir. Soedin.*, 1992, **28**, 90; *Chem. Nat. Compd. (Engl. Transl.)*, 1992, **28**, 74 (*synth*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Ulubelen, A. *et al., Phytochemistry*, 1997, **47**, 895-897 (*Brassicasterone*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*24ξ-form, occur*)
Li, G. *et al., Steroids*, 2005, **70**, 13-18 (*formyl*)

Ergosta-5,24-dien-3-ol E-644

24-Methylcholesta-5,24-dien-3-ol

$C_{28}H_{46}O$ 398.671

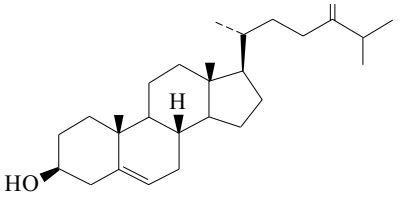
3β-*form* [20780-41-0]
Isol. from the sponges *Cliona chilensis* and *Xestospongia muta*. Also from *Lobophytum strictum*. Constit. of *Withania somnifera* and *Physalis peruviana*.
Cryst. (MeOH).
Mp 141.5-142.5°. $[\alpha]_D$ -46.7 ($CHCl_3$).

[70209-35-7, 70267-01-5]

Nair, M.G. *et al., Tet. Lett.*, 1971, 2513 (*synth*)
Lockley, W.J.S. *et al., Tet. Lett.*, 1974, 3773 (*isol*)
Massey, I.J. *et al., J.O.C.*, 1979, **44**, 2448 (*synth, ms*)
Li, H. *et al., J.O.C.*, 1982, **47**, 4298 (*synth, pmr*)
Parameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 1089-1090 (*isol*)
Fleury, B.G. *et al., Phytochemistry*, 1994, **37**, 1447-1449 (*isol, ms*)

Ergosta-5,24(28)-dien-3-ol E-645

24-Methylenecholest-5-en-3-ol



$C_{28}H_{46}O$ 398.671

3β-*form*
24-Methylenecholesterol. ***Ostreasterol***. *Chalinasterol*. *Oestreasterol*. *Campestadienol*
[474-63-5]
Constit. of many marine organisms, such as *Eupentacta fraudatrix*, *Holothuria nobilis*, *Synapta maculata*, *Echinus esculentus*, *Echinocardium cordatum*, *Antedon bifida*, *Ophiocomina nigra*. Isol. from plant pollens, e.g. *Pyrus malus*, *Hypochoeris radicata* and from a soft coral, *Sinularia* sp. Major sterol of green algae. Cytotoxic. Cryst.
Mp 142-143°. $[\alpha]_D^{20}$ -43.6 ($CHCl_3$).

3-O-*Sulfate:* [65645-02-5]
[151890-97-0]
$C_{28}H_{46}O_4S$ 478.735
Constit. of *Nitzschia alba*, *Psolus fabricii*, *Euretaster insignis*, *Echinus esculentus*, *Echinocardium cordatum*, *Antedon bifida*, *Ophiocomina nigra* and *Eupentacta fraudatrix*.

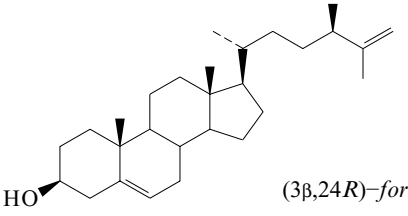
3-O-*β-D-Xylopyranoside:* [151890-82-3]
$C_{33}H_{54}O_5$ 530.787
Constit. of *Eupentacta fraudatrix*.

Nonadecanoyl:
$C_{47}H_{82}O_2$ 679.164
Constit. of the red alga *Ceratodictyon spongiosum* which contains the symbiotic sponge *Sigmadocia symbiotica*. Powder. Mp 74-76°. $[\alpha]_D^{25}$ -14.5 (c, 0.2 in $CHCl_3$).

Bergmann, W. *et al., Annalen*, 1957, **603**, 36-43 (*struct, ir*)
Devys, M. *et al., CA*, 1966, **64**, 10084g (*isol*)
Idler, D.R. *et al., Comp. Biochem. Physiol., A: Comp. Physiol.*, 1971, **38**, 581 (*isol*)
Popplestone, C.R. *et al., Phytochemistry*, 1973, **12**, 1131 (*isol*)
Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*isol, pmr, ms*)
Adler, G. *et al., Phytochemistry*, 1975, **14**, 723 (*biosynth*)
Bu'lock, J.D. *et al., Phytochemistry*, 1975, **15**, 1249 (*biosynth*)
Heble, M.R. *et al., Phytochemistry*, 1976, **15**, 681 (*biosynth*)
Anderson, R. *et al., Biochim. Biophys. Acta*, 1978, **528**, 89-106 (*sulfate*)
Goodfellow, R.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **76**, 575-578 (*sulfate, occur*)
D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1984, 2277-2282 (*sulfate, isol*)
Anastasia, M. *et al., J.C.S. Perkin 1*, 1985, 595-599 (*synth*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1997, **45**, 224-226 (*cmr, biosynth*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*occur*)
Sheu, J.-H. *et al., J. Chin. Chem. Soc. (Taipei)*, 1999, **46**, 253-257 (*isol, activity*)
Volkman, J.K. *et al., Phytochemistry*, 1999, **52**, 659-668 (*occur, dinoflagellates*)
Lo, J.-M. *et al., J. Chin. Chem. Soc. (Taipei)*, 2001, **48**, 821-826 (*nonadecanoate*)

Ergosta-5,25-dien-3-ol, 9CI E-646

24-Methylcholesta-5,25-dien-3-ol



(3β,24*R*)–*form*

$C_{28}H_{46}O$ 398.671

(3β,24*R*)-*form*
24-Epicodisterol. *Campesta-5,25-dien-3-ol*
[71486-08-3]
Constit. of *Verongia cauliformis* and *Jaspis stellifera*.

(3β,24*S*)-*form*
Codisterol
[52936-69-3]
Constit. of *Codium bursa*, *Codium fragile*, *Ajuga reptans*, *Cucurbita maxima* and also from *Verongia cauliformis*.

Cryst. (EtOH).
Mp 148-150°.

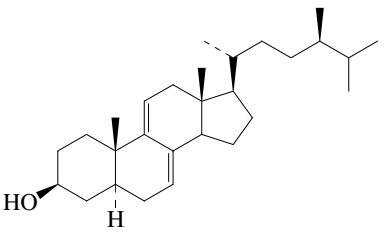
Ac: [52936-70-6]
Cryst. Mp 118-121°.

[69349-82-2]

Rubinstein, I. *et al., Phytochemistry*, 1974, **13**, 481-484 (*isol, pmr*)
Djerassi, C. *et al., Helv. Chim. Acta*, 1979, **62**, 1210-1216; 1310-1318 (*isol*)
Djerassi, C. *et al., J.O.C.*, 1982, **47**, 4298-4303; 1983, **48**, 4472-4479 (*pmr, ms*)
Romeo, G. *et al., J. Nat. Prod.*, 1983, **46**, 187-189 (*isol, pmr*)
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*occur, alga*)
Garg, V.K. *et al., Phytochemistry*, 1984, **23**, 2925-2929 (*isol, pmr, ms*)
Stoilov, I.L. *et al., Tetrahedron*, 1987, **43**, 2213-2222 (*biosynth*)
Cho, J.-H. *et al., J.O.C.*, 1988, **53**, 3466-3469 (*biosynth*)
Yagi, T. *et al., Phytochemistry*, 1996, **41**, 1057-1064 (*biosynth*)

Ergosta-7,9(11)-dien-3-ol E-647

24-Methylcholesta-7,9(11)-dien-3-ol



$C_{28}H_{46}O$ 398.671

(3β,5α,24*R*)-*form*

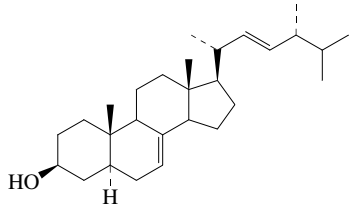
Me ether: 3-Methoxyergosta-7,9(11)-diene
[139765-30-3]
$C_{29}H_{48}O$ 412.698
Constit. of the sponge *Jereicopsis graphidiophora*.

9α,11α-Epoxide, Me ether: 9,11-Epoxy-3-methoxyergost-7-ene
[139765-33-6]
$C_{29}H_{48}O_2$ 428.697
Constit. of *Jereicopsis graphidiophora*.

D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*isol, pmr, ms*)

Ergosta-7,22-dien-3-ol E-648

24-Methylcholesta-7,22-dien-3-ol
[96391-64-9]



(3β,5α,22*E*,24*R*)-*form*

$C_{28}H_{46}O$ 398.671

(3β,5α,22*E*,24*R*)-*form*

Stellasterol
[2465-11-4]
[17608-76-3]
Constit. of wood-rotting fungi, *Ganoderma applanatum* and *Sarcodon asparatus*.
Cryst. (CH_2Cl_2/MeOH).
Mp 159.5-161°. $[\alpha]_D$ -17.8 ($CHCl_3$).

3-O-*Sulfate:* [152005-19-1]
$C_{28}H_{46}O_4S$ 478.735
Constit. of *Eupentacta fraudatrix*.

3-O-*β*-D-*Xylopyranoside:* [74185-11-8]
$C_{33}H_{54}O_5$ 530.787
Constit. of *Eupentacta fraudatrix*.

(3β,5α,22*E*,24*S*)-*form*

α-Dihydroergosterol. *Campesta-7,22*E*-dien-3β-ol*
[50364-22-2]
[17608-76-3]
Isol. from yeasts and fungi, e.g. *Coriolus sanguineus, Polyporus* spp. and *Luidia ludwigi*.
Cryst. (MeOH).
Mp 173.5-174°. $[\alpha]_D$ -23.4.

3-O-β-D-*Glucopyranoside:* [121379-48-4]
$C_{34}H_{56}O_6$ 560.813
Isol. from *Tylopilus neofelleus*. Needles (MeOH).
Mp 272-274°. $[\alpha]_D^{22}$ +31.1 (c, 0.9 in Py).

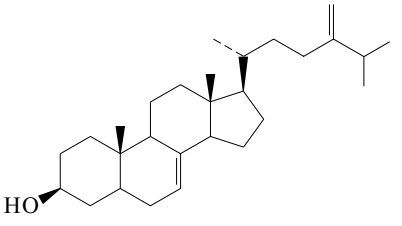
(3β,5α,22*E*,24ξ)-*form* [60426-59-7]
Constit. of *Cucumaria* sp., *Eupentacta fraudatrix*, *Bathyplotes natans*, *Holothuria nobilis*, *Holothuria scabra*, *Coelastrum cambricum*, *Asterias rubens*, *Marthasterias glacialis*, *Henricia sanguinolenta* and *Cucumaria lactea*.

3-O-*Sulfate:* [88357-79-3]
Constit. of *Asterias rubens*, *Marthasterias glacialis*, *Henricia sanguinolenta* and *Cucumaria lactea*.

Arthur, H.R. *et al., J.C.S.*, 1958, 2603-2605 (*synth*)
Pettit, G.R. *et al., J.O.C.*, 1962, **27**, 2696-2700 (*α-Dihydroergosterol*)
Bélanger, P. *et al., Can. J. Chem.*, 1973, **51**, 3294-3298 (*biosynth*)
Kobayashi, M. *et al., Tetrahedron*, 1973, **29**, 1193-1196 (*Stellasterol*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195-200 (*pmr*)
Goodfellow, R.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **76**, 575-578 (*sulfate, occur*)
Lu, W. *et al., Chem. Pharm. Bull.*, 1985, **33**, 5083-5087 (*α-Dihydroergosterol*)
Veares, M.P. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1988, **90**, 25-28 (*sulfate*)
Takaishi, Y. *et al., Phytochemistry*, 1989, **28**, 945-947 (*glucoside*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Keller, A.C. *et al., Phytochemistry*, 1996, **41**, 1041-1046 (*cmr*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*3β,5α,22E,24ξ-form, occur*)

Ergosta-7,24(28)-dien-3-ol E-649

24-Methylenecholest-7-en-3-ol



$C_{28}H_{46}O$ 398.671

(3β,5α)-*form*

Episterol
[474-68-0]
Constit. of yeasts, *Polizoa opuntia*, *Neurospora crassa* and *Asterias amurensis*. Also present in lichens. Minor component of the lipids of a marine unicellular green alga. Isol. from *Cucumaria* sp., *Eupentacta fraudatrix*, *Bathyplotes natans* and *Trochostoma orientale*.
Cryst. (MeOH).
Mp 127.5-128.5° (150-151°). $[\alpha]_D$ +4.4 (c, 2.3 in $CHCl_3$) (-5).

3-O-*Sulfate:* [151891-07-5]
$C_{28}H_{46}O_4S$ 478.735
Constit. of *Eupentacta fraudatrix*.

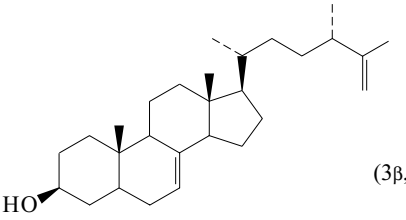
3-O-*β*-D-*Xylopyranoside:* [74185-13-0]
$C_{33}H_{54}O_5$ 530.787
Constit. of *Eupentacta fraudatrix*.

Barton, D.H.R. *et al., J.C.S.*, 1945, 813-819; 1946, 512-522 (*struct*)
Kobayashi, M. *et al., Tetrahedron*, 1973, **29**, 1193-1196 (*isol*)
Renaud, R. *et al., Phytochemistry*, 1976, **15**, 977-979 (*isol*)
Kokke, W.C.M.C. *et al., J.O.C.*, 1985, **49**, 3742-3752 (*occur, alga*)

Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Palermo, J.A. *et al., Steroids*, 1996, **61**, 2-6 (*occur*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **128**, 337-347 (*occur*)
Takatsuto, S. *et al., Nihon Yukagakkaishi*, 1999, **48**, 37-40; *CA*, **130**, 220260c (*synth*)

Ergosta-7,25-dien-3-ol E-650

24-Methylcholesta-7,25-dien-3-ol



(3β,5α,24*S*)–*form*

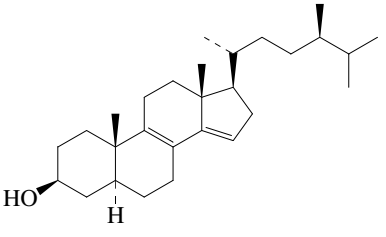
$C_{28}H_{46}O$ 398.671

(3β,5α,24*S*)-*form*
25-Dehydrofungisterol
[95043-18-8]
Isol. from seeds of *Cucurbita maxima* and the alga *Prototheca wickerhamii*.

(3β,5α,24ξ)-*form* [91811-31-3]
Isol. from the copepod *Calanus helgolandicus.*
Prahl, F.G. *et al., J. Mar. Biol. Assoc. U.K.*, 1984, **64**, 317; 1986, **66**, 1
Garg, V.K. *et al., Phytochemistry*, 1984, **23**, 2919; 1986, **25**, 2591
Norton, R.A. *et al., Lipids*, 1991, **26**, 247 (*isol*)

Ergosta-8,14-dien-3-ol E-651

24-Methylcholesta-8,14-dien-3-ol



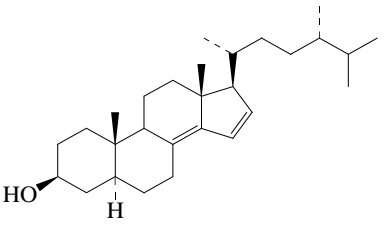
$C_{28}H_{46}O$ 398.671

(3β,5α,24*R*)-*form*
Ignosterol
[23839-47-6]
Constit. of *Chlorella* spp. Prod. by various fungi and yeasts incl. *Candida albicans* and *Saccharomyces cerevisiae.*

Me ether: 3-Methoxyergosta-8,14-diene
[139765-28-9]
$C_{29}H_{48}O$ 412.698
Constit. of the sponge *Jereicopsis graphidiophora*.
Loeffler, R.S.T. *et al., Phytochemistry*, 1990, **29**, 3423-3429 (*isol*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*3-Methoxyergostadiene*)

Ergosta-8(14),15-dien-3-ol E-652

24-Methylcholesta-8(14),15-dien-3-ol

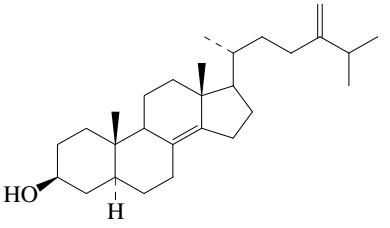


$C_{28}H_{46}O$ 398.671

(3β,5α,24*S*)-*form* [90195-43-0]
Minor component of the lipids of a marine unicellular green alga.
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*isol, pmr*)

Ergosta-8(14),24(28)-dien-3-ol E-653

24-Methylenecholest-8(14)-en-3-ol

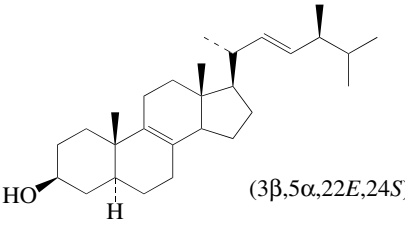


$C_{28}H_{46}O$ 398.671

(3β,5α)-*form*
Trace constit. of the lipids of a marine unicellular green alga.
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*isol*)

Ergosta-8,22-dien-3-ol E-654

24-Methylcholesta-8,22-dien-3-ol



(3β,5α,22*E*,24*S*)-*form*

$C_{28}H_{46}O$ 398.671

(3β,5α,22*E*,24*S*)-*form* [85798-13-6]
Constit. of the sponge *Axinella cannabina*.

(3β,5α,22ξ,24*R*)-*form* [6673-68-3]
Constit. of the sponge *Pachychalina* sp.

(3β,5ξ,22*E*,24*R*)-*form* [36904-77-5]
Constit. of *Neurospora crassa.*
Renaud, R.L. *et al., Lipids*, 1978, **13**, 56-58 (*isol, Neurospora*)
Pierce, A.M. *et al., Can. J. Biochem.*, 1979, **57**, 112-116 (*biosynth*)
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol, Axinella, pmr, ms*)
Zeng, Z. *et al., CA*, 1996, **125**, 190994x (*isol, Pachychalina*)

Ergosta-8,24(28)-dien-3-ol E-655

24-Methylenecholest-8-en-3-ol

$C_{28}H_{46}O$ 398.671

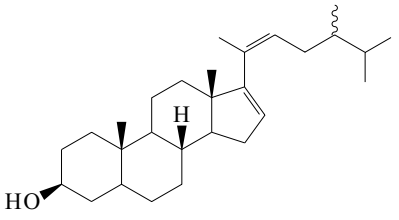
(3β,5α)-*form*
Fecosterol. *Faecosterol*
[516-86-9]

Constit. of *Lobaria* spp. and *Saccharomyces cerevisiae*. Minor component of the lipids of a marine unicellular green alga.
Cryst. (Me_2CO).
Mp 126-130°. $[\alpha]_D$ +44.8 ($CHCl_3$).

Barton, D.H.R. *et al., J.C.S. Perkin 1*, 1972, 513 (*isol*)
Safe, S. *et al., Phytochemistry*, 1975, **14**, 1821 (*isol*)
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*occur, alga*)
Tong, Y. *et al., Tet. Lett.*, 1997, **38**, 6115-6118 (*biosynth*)

Ergosta-16,20(22)-dien-3-ol E-656

24-Methylcholesta-16,20(22)-dien-3-ol



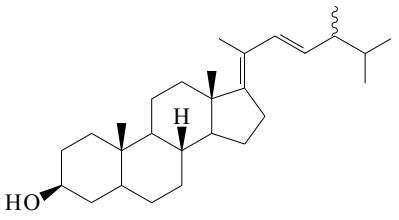
$C_{28}H_{46}O$ 398.671

(3β,24ξ)-*form* [144686-41-9]
Constit. of a *Virgularia* sp.
Needles (MeOH).
Mp 140-142°. $[\alpha]_D^{25}$ -3.66 (c, 1.31 in $CHCl_3$).

Anjaneyulu, A.S.R. *et al., J. Indian Chem. Soc.*, 1992, **69**, 150 (*isol, pmr*)

Ergosta-17(20),22-dien-3-ol E-657

24-Methylcholesta-17(20),22-dien-3-ol



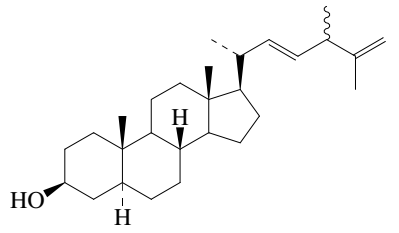
$C_{28}H_{46}O$ 398.671

(3β,24ξ)-*form* [144686-42-0]
Constit. of *Virgularia* sp.
Needles (MeOH).
Mp 190-192°. $[\alpha]_D^{25}$ +45.58 (c, 1.8 in $CHCl_3$).

Anjaneyulu, A.S.R. *et al., J. Indian Chem. Soc.*, 1992, **69**, 150 (*isol, pmr*)

Ergosta-22,25-dien-3-ol E-658

24-Methylcholesta-22,25-dien-3-ol



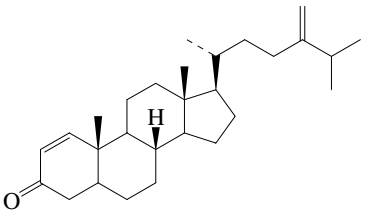
$C_{28}H_{46}O$ 398.671

(3β,5α,22*E*,24ξ)-*form*
O-*Sulfate:* [211427-00-8]
$C_{28}H_{46}O_4S$ 478.735
Constit. of the sea cucumber *Holothuria* sp.

Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 262-266

Ergosta-1,24(28)-dien-3-one E-659

24-Methylenecholest-1-en-3-one. ***Dendronesterone B***
[771534-37-3]

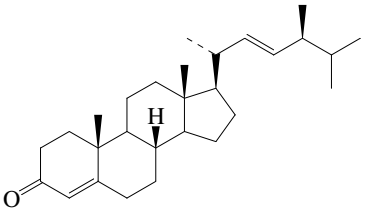


$C_{28}H_{44}O$ 396.655
Constit. of *Dendronephthya gigantea*. Solid. $[\alpha]_D^{25}$ +18 (c, 0.1 in $CHCl_3$). λ_{max} 222 (log ϵ 3.56) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2004, **67**, 1650-1653 (*isol, pmr, cmr*)

Ergosta-4,22-dien-3-one E-660

24-Methylcholesta-4,22-dien-3-one
[4030-92-6 (*R-form*)]



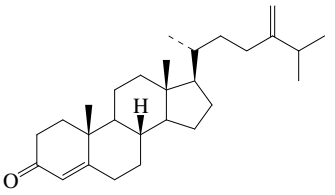
$C_{28}H_{44}O$ 396.655

(22*E*,24*S*)-*form* [55780-27-3]
Constit. of the sponge *Stelletta clarella* and the tunicate *Ascidia nigra*.
Mp 128-129°. $[\alpha]_D^{20}$ +44.6 ($CHCl_3$).

Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*Stelletta clarella constit*)
Tam, T.F. *et al., Steroids*, 1982, **40**, 433-453 (*Ascidia nigra constit*)

Ergosta-4,24(28)-dien-3-one E-661

24-Methylenecholest-4-en-3-one
[55688-44-3]

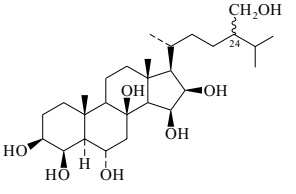


$C_{28}H_{44}O$ 396.655
Isol. from sponges *Geodia cydonium* and *Stelletta clarella*.
Mp 115° (111-113°). $[\alpha]_D^{20}$ +89.1.

Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*isol, ms*)
Migliuolo, A. *et al., J. Nat. Prod.*, 1990, **53**, 1262-1266 (*isol*)

Ergostane-3,4,6,8,15,16,28-heptol E-662

24-(Hydroxymethyl)cholestane-3,4,6,8,15,16-hexol



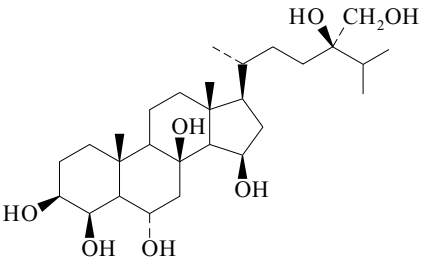
$C_{28}H_{50}O_7$ 498.699

(3β,4β,5α,6α,15β,16β,24ξ)-*form*

28-O-*[2,4-Di*-O-*methyl-β-*D*-xylopyranosyl-(1→2)-α-*L*-arabinofuranoside]:* ***Culcitoside C₂***
[107041-31-6]
$C_{40}H_{70}O_{15}$ 790.984
Isol. from the starfish *Culcita novaeguineae.*
Mp 226-228°. $[\alpha]_D^{20}$ -18 (c, 0.1 in EtOH).
Kicha, A.A. *et al., Khim. Prir. Soedin.*, 1986, **22**, 592; *Chem. Nat. Compd. (Engl. Transl.)*, 557,

Ergostane-3,4,6,8,15,24,28-heptol E-663

24-(Hydroxymethyl)cholestane-3,4,6,8,15,24-hexol

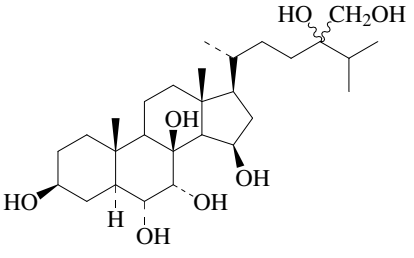


$C_{28}H_{50}O_7$ 498.699

(3β,4β,5α,6α,8β,15β,24*R*)-*form*

24-O-α-*L*-*Arabinofuranoside:* ***Antarcticoside N***
[181034-84-4]
$C_{33}H_{58}O_{11}$ 630.815
Constit. of an Antarctic starfish (Echinasteridae).
$[\alpha]_D$ -11 (MeOH).
Iorizzi, M. *et al., Tetrahedron*, 1996, **52**, 10997-11012 (*isol, pmr, cmr*)

Ergostane-3,6,7,8,15,24,28-heptol E-664



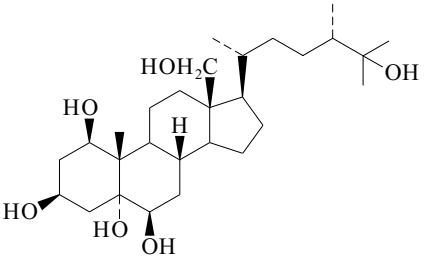
$C_{28}H_{50}O_7$ 498.699

(3β,5α,6α,7α,15β,24ξ)-*form*

28-O-*(5-Methyl-β-*D*-galactofuranoside):* ***Indicoside A***†
[109575-71-5]
$C_{35}H_{62}O_{12}$ 674.868
Metabolite of starfish *Astropecten indicus.* Glass. $[\alpha]_D$ -69.4 (c, 1 in MeOH).
Riccio, R. *et al., Tet. Lett.*, 1987, **28**, 2291-2294 (*isol, pmr*)

Ergostane-1,3,5,6,18,25-hexol E-665

24-Methylcholestane-1,3,5,6,18,25-hexol

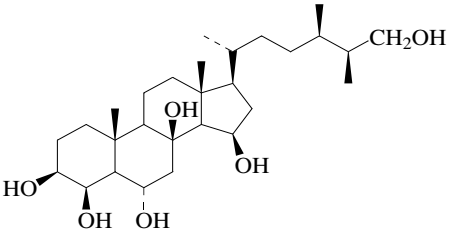


$C_{28}H_{50}O_6$ 482.699

(1β,3β,5α,6β,24*S*)-*form*

25-Ac: [142780-38-9]
$C_{30}H_{52}O_7$ 524.737
Constit. of *Sarcophyton subviride.*
Raja, B.L. *et al., J. Nat. Prod.*, 1992, **55**, 904 (*isol, pmr, cmr*)

Ergostane-3,4,6,8,15,26-hexol E-666

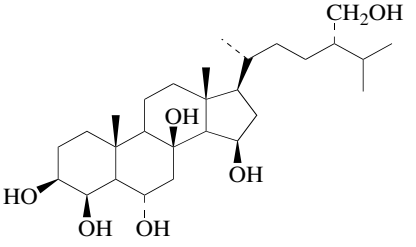


$C_{28}H_{50}O_6$ 482.699

(3β,4β,5α,6α,8β,15β,24*R*,25*S*)-*form*

Certonardosterol M
[517900-61-7]
Constit. of *Certonardoa semiregularis.*
Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2003, **66**, 384-391 (*isol, pmr, cmr*)

Ergostane-3,4,6,8,15,28-hexol E-667



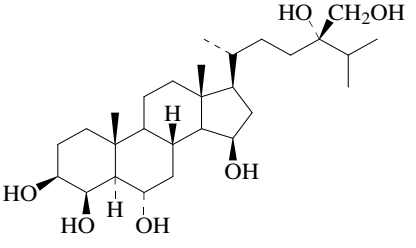
$C_{28}H_{50}O_6$ 482.699

(3β,4β,5α,6α,8β,15β,24*S*)-*form*

28-O-*[2,4-Di*-O-*methyl-β-*D*-xylopyranosyl-(1→2)-α-*L*-arabinofuranoside]:* ***Culcitoside C₆***
[138207-51-9]
$C_{40}H_{70}O_{14}$ 774.985
Constit. of *Culcita novaeguineae.*
$[\alpha]_D$ -23.2 (c, 0.1 in MeOH).

28-O-*[2,4-Di*-O-*methyl-β-*D*-xylopyranosyl-(1→2)-α-*L*-arabinofuranoside], 6-sulfate:* ***Culcitoside C₇***
[138192-13-9]
$C_{40}H_{70}O_{17}S$ 855.049
Constit. of *Culcita novaeguineae.*
$[\alpha]_D$ -17.7 (c, 0.1 in MeOH).
Iorizzi, M. *et al., J. Nat. Prod.*, 1991, **54**, 1254-1264 (*Culcitosides*)

Ergostane-3,4,6,15,24,28-hexol E-668

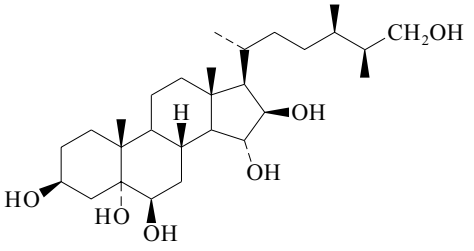


$C_{28}H_{50}O_6$ 482.699

(3β,4β,5α,6α,15β,24*S*)-*form*
Certonardosterol B₄
[781646-87-5]
Constit. of *Certonardoa semiregularis.*
Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 1654-1660 (*isol, pmr, cmr*)

Ergostane-3,5,6,15,16,26-hexol E-669

24-Methylcholestane-3,5,6,15,16,26-hexol



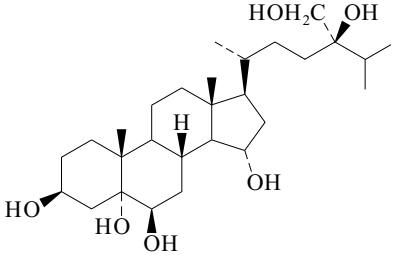
$C_{28}H_{50}O_6$ 482.699

(3β,5α,6β,15α,16β,24*R*,25*S*)-*form*
26-Sulfate: [165815-79-2]
$C_{28}H_{50}O_9S$ 562.764
Constit. of *Luidia clathrata.*
$[\alpha]_D$ +22.6.

(3β,5α,6β,15α,16β,24*S*,25*R*)-*form* [221163-00-4]
Constit. of *Luidiaster dawsoni.*
Iorizzi, M. *et al., J. Nat. Prod.*, 1995, **58**, 653-671 (*26-sulfate*)
Kicha, A.A. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1998, **47**, 2032-2033 (*Luidiaster dawsoni constit*)

Ergostane-3,5,6,15,24,28-hexol E-670

24-(Hydroxymethyl)cholestane-3,5,6,15,24-pentol



$C_{28}H_{50}O_6$ 482.699

(3β,5α,6β,15α,24*R*)-*form*
28-Sulfate: [165815-83-8]
$C_{28}H_{50}O_9S$ 562.764
Constit. of *Luidia clathrata.*
$[\alpha]_D$ +17.
Iorizzi, M. *et al., J. Nat. Prod.*, 1995, **58**, 653-671 (*isol, pmr, cmr*)

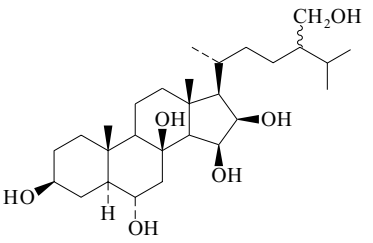
Ergostane-3,6,8,15,16,26-hexol, 9CI E-671

24-Methylcholestane-3,6,8,15,16,26-hexol
$C_{28}H_{50}O_6$ 482.699

(3β,6α,15α,16β,25ξ)-*form* [93368-89-9]
Constit. of *Protoreaster nodosus.*
Cryst. (MeOH).
Mp 253-256°. $[\alpha]_D$ +27.8 (c, 0.8 in MeOH).
Minale, L. *et al., J. Nat. Prod.*, 1984, **47**, 790-795

Ergostane-3,6,8,15,16,28-hexol E-672

24-(Hydroxymethyl)cholestane-3,6,8,15,16-pentol

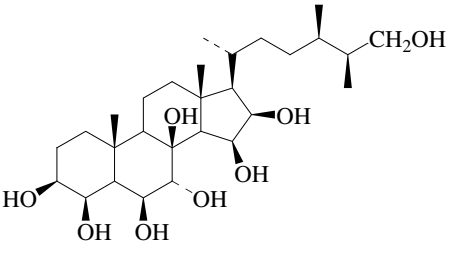


$C_{28}H_{50}O_6$ 482.699

(3β,5α,6α,15β,16β,24ξ)-*form*
*28-*O*-[2,4-Di-*O*-methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside]:* ***Culcitoside C₃***
[107041-32-7]
$C_{40}H_{70}O_{14}$ 774.985
Isol. from the starfish *Culcita novaeguineae.*
Mp 228-230°. $[\alpha]_D^{20}$ -19.1 (c, 0.17 in EtOH).
Kicha, A.A. *et al., Khim. Prir. Soedin.*, 1986, **22**, 592; *Chem. Nat. Compd. (Engl. Transl.)*, 557,

Ergostane-3,4,6,7,8,15,16,26-octol E-673

24-Methylcholestane-3,4,6,7,8,15,16,26-octol



$C_{28}H_{50}O_8$ 514.698

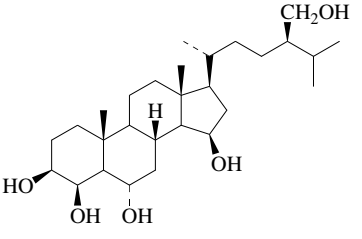
(3β,4β,5α,6β,7α,15β,16β,24*R*,25*S*)-*form*
Constit. of *Solaster borealis.*
Iorizzi, M. *et al., J. Nat. Prod.*, 1992, **55**, 866-877 (*isol, pmr, cmr, ms*)

Ergostane-1,3,5,6,25-pentol E-674

24-Methylcholestane-1,3,5,6,25-pentol
$C_{28}H_{50}O_5$ 466.7

(1β,3β,5α,6β,24*S*)-*form*
Cryst. (MeOH aq.). Mp 266.5-269°. $[\alpha]_D$ -18.2 (c, 1.02 in MeOH).
25-Ac: [72534-11-3]
$C_{30}H_{52}O_6$ 508.737
Constit. of *Sarcophyton glaucum* and a *Lobophytum* sp. Needles ($MeOH/Me_2CO$).
Mp 266-270°. $[\alpha]_D$ -14 (c, 1.13 in MeOH).
Kobayashi, M. *et al., Steroids*, 1979, **34**, 285 (*isol, pmr, ms*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1848 (*cmr*)
Raju, B.L. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 1033-1037 (*isol*)

Ergostane-3,4,6,15,28-pentol E-675



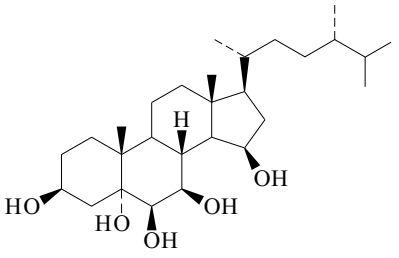
$C_{28}H_{50}O_5$ 466.7

(3β,4β,6α,15β,24*R*)-*form*

*28-*O*-(4-*O*-Methyl-β-*D*-xylopyranoside):* ***Certonardoside H_2***
[681226-41-5]
$C_{34}H_{60}O_9$ 612.843
Constit. of *Certonardoa semiregularis*. Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 584-591 (*isol, pmr, cmr*)

Ergostane-3,5,6,7,15-pentol E-676

24-Methylcholestane-3,5,6,7,15-pentol

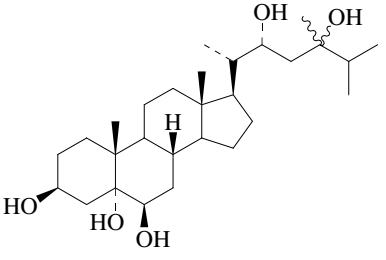


$C_{28}H_{50}O_5$ 466.7

(3β,5α,6β,7β,15β,24*S*)-*form* [147170-09-0]
Constit. of *Lobophytum crassum*.
Needles.
Mp 212-215°. $[\alpha]_D$ +16 (c, 0.5 in Py).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1993, **41**, 87 (*isol, pmr, cmr*)

Ergostane-3,5,6,22,24-pentol E-677

24-Methylcholestane-3,5,6,22,24-pentol



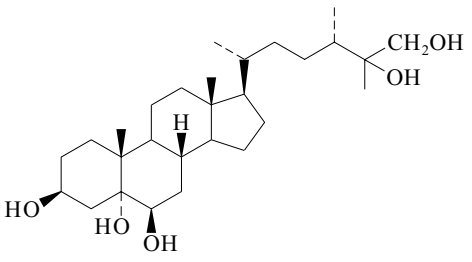
$C_{28}H_{50}O_5$ 466.7

(3β,5α,6β,22*R*,24ξ)-*form*

6-Ac: [96736-31-1]
$C_{30}H_{52}O_6$ 508.737
Isol. from the soft coral *Asterospicularia randalli*. Powder (Me_2CO/hexane).
Mp 144-146°. $[\alpha]_D^{25}$ -29.2 (c, 0.31 in $CHCl_3$).
Ksebati, M.B. *et al., Steroids*, 1984, **43**, 639-649 (*isol*)
Litvinovskaya, R.P. *et al., Zh. Org. Khim.*, 1996, **32**, 741-745 (*config*)

Ergostane-3,5,6,25,26-pentol, 9CI E-678

24-Methylcholestane-3,5,6,25,26-pentol



$C_{28}H_{50}O_5$ 466.7

(3β,5α,6β,24*S*,25ξ)-*form* [89026-28-8]
Constit. of soft coral *Sarcophyton glaucum*.
Cryst. (Me_2CO/hexane).
Mp 262-264°. $[\alpha]_D$ -14 (c, 1.4 in MeOH).

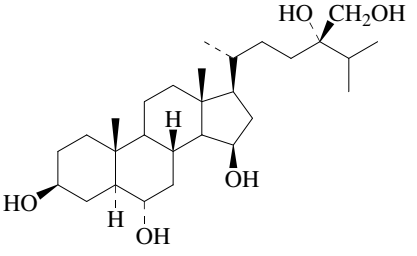
25-Ac:
$C_{30}H_{52}O_6$ 508.737
Constit. of *Sarcophyton subviride*.

25,26-Di-Ac: [719294-67-4]
$C_{32}H_{54}O_7$ 550.774
Constit. of *Sarcophyton glaucum*. Gum. $[\alpha]_D^{30}$ -3 (c, 0.1 in $CHCl_3$).

26-Decanoyl: [719294-66-3]
$C_{38}H_{68}O_6$ 620.952
Constit. of *Sarcophyton glaucum*. Gum. $[\alpha]_D^{30}$ -11.2 (c, 0.1 in $CHCl_3$).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 4127
Raja, B.L. *et al., J. Nat. Prod.*, 1992, **55**, 904 (*25-Ac*)
Wang, G.-H. *et al., J. Chin. Chem. Soc. (Taipei)*, 2004, **51**, 217-220; *CA*, **141**, 103422y (*Sarcophyton glaucum constits*)

Ergostane-3,6,15,24,28-pentol E-679



$C_{28}H_{50}O_5$ 466.7

(3β,5α,6α,15β,24*S*)-*form*
Certonardosterol D_5
[781646-88-6]
Constit. of *Certonardoa semiregularis*.
Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 1654-1660 (*isol, pmr, cmr*)

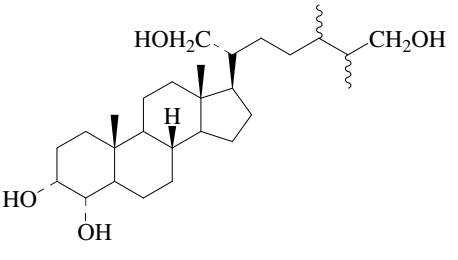
Ergostane-1,3,5,6-tetrol E-680

24-Methylcholestane-1,3,5,6-tetrol
[72534-13-5]
$C_{28}H_{50}O_4$ 450.701

(1β,3β,5α,6β,24*S*)-*form* [87727-70-6]
Constit. of soft coral *Sarcophyton glaucum* and a *Lobophytum* sp.
Cryst. (MeOH/Me_2CO).
Mp 273-275.5°. $[\alpha]_D$ -13.2 (c, 1.14 in MeOH).
Yamada, Y. *et al., Chem. Pharm. Bull.*, 1980, **28**, 473
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1848 (*config*)
Raju, B.L. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 1033-1037 (*isol*)

Ergostane-3,4,21,26-tetrol E-681

24-Methylcholestane-3,4,21,26-tetrol

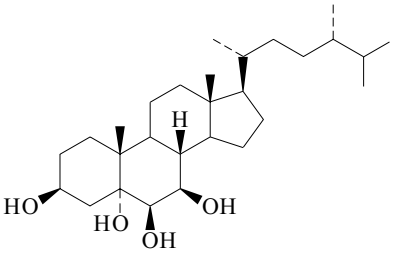


$C_{28}H_{50}O_4$ 450.701

(3α,4α,5β,24ξ,25ξ)-*form*

3,21-Disulfate: [116407-18-2]
$C_{28}H_{50}O_{10}S_2$ 610.829
Isol. from the Pacific ophiuroid *Ophiolepis superba*.
$[\alpha]_D$ +31.5 (MeOH) (as di-Na salt).
D'Auria, M.V. *et al., J.O.C.*, 1989, **54**, 234-239 (*isol, pmr, cmr, struct*)

Ergostane-3,5,6,7-tetrol E-682



$C_{28}H_{50}O_4$ 450.701

(3β,5α,6β,7β,24*S*)-*form* [80525-48-0]
Constit. of *Lobophytum crassum, Anthelia glauca* and a *Xenia* sp. Needles.
Mp 212-215°. $[\alpha]_D$ +16 (c, 0.5 in Py).

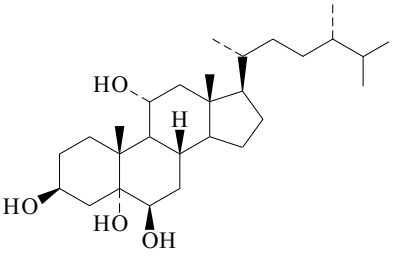
7-Ac: ***Xeniasterol B***
[107168-58-1]
$C_{30}H_{52}O_5$ 492.738
Isol. from a soft coral *Xenia* sp. Needles (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 218-220°. $[\alpha]_D^{22}$ +50 (c, 1 in Py).

24,28-Didehydro: ***Ergost-24(28)-ene-3,5,6,7-tetrol****. 24-Methylene-cholestane-3,5,6,7-tetrol*
[395070-89-0]
$C_{28}H_{48}O_4$ 448.685
Constit. of *Plexaurella grisea*. Amorph. solid. $[\alpha]_D$ +30 (c, 0.12 in MeOH).

Sjöstrand, U. *et al., Steroids*, 1981, **38**, 347 (*isol*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4590 (*isol*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1993, **41**, 87 (*isol, pmr, cmr*)
Rueda, A. *et al., Steroids*, 2001, **66**, 897-904 (*didehydro*)

Ergostane-3,5,6,11-tetrol E-683

24-Methylcholestane-3,5,6,11-tetrol



$C_{28}H_{50}O_4$ 450.701

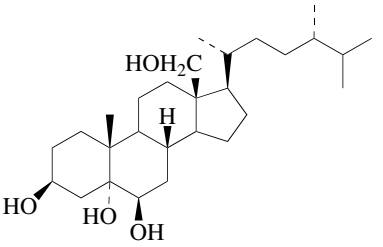
(3β,5α,6β,11α,24*S*)-*form*
Sarcoaldesterol B
[180313-85-3]
Constit. of a *Sarcophyton* sp.
Semisolid. $[\alpha]_D^{25}$ -23.6 (c, 1.5 in MeOH).

11-Ac: [195061-87-1]
$C_{30}H_{52}O_5$ 492.738
Constit. of *Lobophytum* cf. *pauciflorum*. Oil. $[\alpha]_D$ -38.8 (c, 1 in $CHCl_3$).

Umeyama, A. *et al., J. Nat. Prod.*, 1996, **59**, 894-895 (*isol, pmr, cmr*)
Lu, Q. *et al., Nat. Prod. Lett.*, 1997, **10**, 231-237 (*11-Ac*)

Ergostane-3,5,6,18-tetrol E-684

24-Methylcholestane-3,5,6,18-tetrol



$C_{28}H_{50}O_4$ 450.701

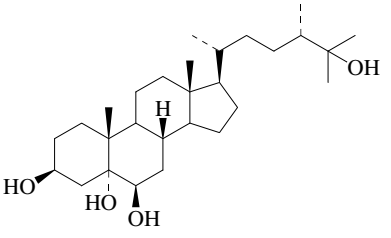
(3β,5α,6β,24*S*)-*form* [198273-65-3]
Constit. of *Lobophytum crassum*.

3,6,18-Tri-Ac:
$C_{34}H_{56}O_7$ 576.812
Viscous liq. $[\alpha]_D$ -23 (c, 0.2 in $CHCl_3$).

Venkateswarlu, Y. *et al., J. Nat. Prod.*, 1997, **60**, 1301-1302 (*isol, pmr, cmr*)

Ergostane-3,5,6,25-tetrol E-685

24-Methylcholestane-3,5,6,25-tetrol
[53866-44-7]



(3β,5α,6β,24*S*)-*form*

$C_{28}H_{50}O_4$ 450.701

(3β,5α,6β,24*S*)-*form*
Constit. of *Lobophytum pauciflorum*.
Cryst. (MeOH).
Mp 255-256°. $[\alpha]_D^{20}$ -21 (c, 0.3 in EtOH).

25-Ac: [53866-36-7]
$C_{30}H_{52}O_5$ 492.738
From *Lobophytum pauciflorum, Sarcophyton glaucum* and *Sarcophyton elegans*. Cryst.
Mp 237-237.5°. $[\alpha]_D$ -17.4 (c, 1.8 in $CHCl_3$).

3,6,25-Tri-Ac: [142797-30-6]
$C_{34}H_{56}O_7$ 576.812
Constit. of a *Lobophytum* sp. Cryst.
Mp 175-177°. $[\alpha]_D$ -51.7 (c, 0.97 in MeOH).

(3β,5β,6α,24*S*)-*form* [129518-76-9]
Constit. of *Lobophytum* sp. and *Sinularia* sp.
Mp 226-227°. $[\alpha]_D^{29}$ +16 (c, 0.5 in MeOH).

(3β,5α,6β,24ξ)-*form*

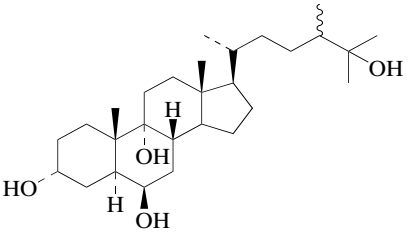
25-Ac: Constit. of *Lobophytum mirabile*. Also from *Sclerophytum* sp.
Cryst.
Mp 226°. $[\alpha]_D$ -17 (c, 0.25 in EtOH).

Kobayashi, M. *et al., Steroids*, 1979, **34**, 285 (*isol*)
Yamada, Y. *et al., Chem. Pharm. Bull.*, 1980, **28**, 473
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1848; 1990, **38**, 1724 (*isol, pmr, cmr, ms*)
Rao, C.B. *et al., Indian J. Chem., Sect. B*, 1990, **29**, 588-589 (*25-Ac, isol, Sclerophytum*)
Sheu, J.H. *et al., J. Chin. Chem. Soc. (Taipei)*, 1991, **38**, 397 (*isol, pmr, cmr*)
Shi, L. *et al., Jiegou Huaxue*, 1991, **10**, 204-208 (*cryst struct*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 1294 (*isol, ir, pmr*)
Anjaneyulu, A.S.R. *et al., J.C.S. Perkin 1*, 1997, 959 (*isol, pmr*)

Anjaneyulu, A.S.R. *et al., Tetrahedron*, 1997, **53**, 9301-9312 (*pmr, cmr*)
Radhika, P. *et al., Nat. Prod. Res.*, 2004, **18**, 575-579 (*tri-Ac*)

Ergostane-3,6,9,25-tetrol E-686

24-Methylcholestane-3,6,9,25-tetrol

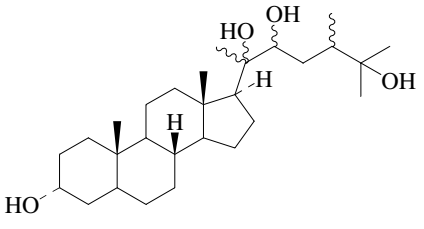


$C_{28}H_{50}O_4$ 450.701

(3α,5α,6β,24ξ)-*form*

25-Ac: ***Sartortuosterol A***
[110325-83-2]
$C_{30}H_{52}O_5$ 492.738
Isol. from the soft coral *Sarcophyton tortuosum*. Cryst. Mp 227-229°. $[\alpha]_D^{20}$ +48.
Su, J. *et al., Steroids*, 1986, **48**, 233-238 (*isol, ir, pmr, ms*)

Ergostane-3,20,22,25-tetrol E-687



$C_{28}H_{50}O_4$ 450.701

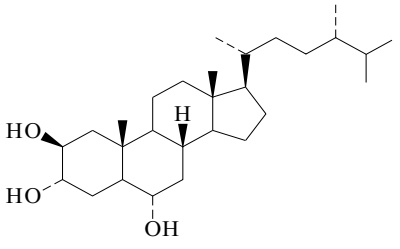
(3α,5α,20ξ,22ξ,24ξ)-*form*

22,25-Di-Ac: ***Hippuristerol D***
[346423-99-2]
$C_{32}H_{54}O_6$ 534.775
Constit. of *Isis hippuris*. Powder. $[\alpha]_D^{27}$ +3.7 (c, 0.175 in $CHCl_3$).

3-Ketone, 22,25-di-Ac: ***Hippuristerone D***
[346424-00-8]
$C_{32}H_{52}O_6$ 532.759
Constit. of *Isis hippuris*. Powder. $[\alpha]_D^{23}$ +7.38 (c, 0.38 in $CHCl_3$).
González, N. *et al., Tetrahedron*, 2001, **57**, 3487-3497 (*isol, pmr, cmr*)

Ergostane-2,3,6-triol E-688

24-Methylcholestane-2,3,6-triol



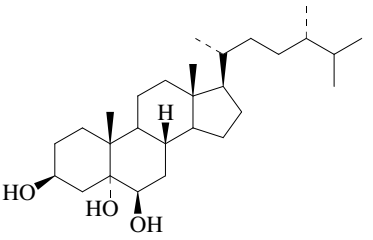
$C_{28}H_{50}O_3$ 434.701

(2β,3α,5α,6α,24*S*)-*form*

Tri-O-*sulfate:* ***Halistanol sulfate G***
[154205-19-3]
$C_{28}H_{50}O_{12}S_3$ 674.894
Constit. of sponge *Pseudaxinyssa digitata*.
Bifulco, G. *et al., J. Nat. Prod.*, 1994, **57**, 164-167 (*isol, pmr, cmr*)

Ergostane-3,5,6-triol E-689

24-Methylenecholestane-3,5,6-triol
[76036-11-8]



(3β,5α,6β,24*S*)-*form*

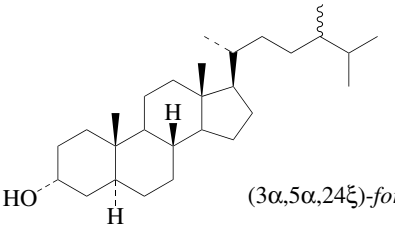
$C_{28}H_{50}O_3$ 434.701

(3β,5α,6β,24*S*)-*form* [62504-61-4]
Constit. of *Plexaurella grisea*.

(3β,5α,6β,24ξ)-*form* [59048-79-2]
Constit. of *Sinularia dissecta*.
Bortolotto, M. *et al., Bull. Soc. Chim. Belg.*, 1976, **85**, 27-34 (*Sinularia dissecta constit*)
Pruna, L. *et al., Pharmazie*, 1984, **39**, 117-120 (*Plexaurella grisea constit*)

Ergostan-3-ol E-690

24-Methylcholestan-3-ol
[122353-29-1]



(3α,5α,24ξ)-*form*

$C_{28}H_{50}O$ 402.702

(3α,5α,24ξ)-*form* [98463-66-2]
Constit. of the marine sponge *Esperiopsis edwardii*.

(3α,5β,24*R*)-*form* [70095-92-0]
Constit. of human faeces.

(3α,5β,24ξ)-*form* [106454-90-4]
Occurs in sewage sludge.

(3β,5α,24*R*)-*form*
Chalinastanol
[474-60-2]
Constit. of various sponges incl. *Haliclona flavescens* and *Phakellia aruensis*. Also from *Ascidia nigra*, *Euretaster insignis*, *Zooxanthella microadriatica*, *Posidonia oceanica*, *Cymodocea nodosa*, tubers of *Cyperus esculentus*, *Costus spiralis*, *Poa huecu* and many other spp. both terrestrial and marine. Also isol. from human faeces.
Cryst. (EtOH).
Mp 146-147°. $[\alpha]_D$ +32.6 ($CHCl_3$).

(3β,5α,24*S*)-*form*
Ergostanol. *γ-Ergostanol*
[6538-02-9]
Constit. of coffee and of pot marigold (*Calendula officinalis*), *Cerastium alpinum*, tobacco cell cultures and many other spp.
Cryst. ($MeOH/Et_2O$).
Mp 144-145°. $[\alpha]_D$ +15.94 ($CHCl_3$).

(3β,5α,24ξ)-*form* [17105-72-5]
Isol. from clam *Patinopecten yessoensis*. Constit. of *Holothuria nobilis*, *Pseudostichopus trachus*, *Ciona intestinalis*, *Charonia tritonis*, *Gigartina skottsbergii* and many other marine organisms.

3-O-*Sulfate:* [80677-68-5]
$C_{28}H_{50}O_4S$ 482.767
Constit. of *Parathyona* sp. and *Psolus fabricii*.

3-O-*β*-D-*Xylopyranoside:* [74185-14-1]
$C_{33}H_{58}O_5$ 534.818
Constit. of *Eupentacta fraudatrix*.

(3β,5β,24*R*)-*form* [33947-18-1]
Isol. from human faeces.

(3β,5β,24*S*)-*form*
Coprocampesterol
[35799-12-3]
Isol. from human faeces.

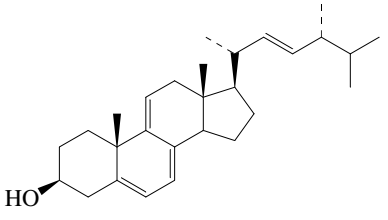
(3β,5β,24ξ)-*form* [66036-55-3]
Minor sterol from sponge *Petrosia ficiformis*, prob. as endobacterial metab. Constit. of human faeces.

[50298-91-4, 83861-56-7]

Karrer, P. *et al., Helv. Chim. Acta*, 1951, **34**, 832-834 (*isol*)
Nagasampagi, B.A. *et al., Phytochemistry*, 1971, **10**, 1101-1107 (*isol*)
Adler, G. *et al., Phytochemistry*, 1975, **14**, 627-631 (*isol*)
Kobayashi, M. *et al., Steroids*, 1975, **26**, 605 (*isol, Patinopecten*)
Orcutt, D.M. *et al., CA*, 1978, **89**, 143615 (*3α,5β,24ξ-form, occur*)
Wright, J.L.C. *et al., Can. J. Chem.*, 1978, **56**, 1898-1903 (*cmr*)
Teshima, S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1979, **64**, 225-228 (*3β,5α,24ξ-form, occur*)
Gupta, K.C. *et al., J. Nat. Prod.*, 1979, **42**, 307-308 (*3β,5α,24ξ-form, occur*)
Smetanina, O.F. *et al., Khim. Prir. Soedin.*, 1981, 585-588 (*3β,5α,24ξ-form, sulfate, occur*)
Bohlin, L. *et al., Phytochemistry*, 1981, **20**, 2397-2401 (*isol*)
Tam Ha, T.B. *et al., Steroids*, 1982, **40**, 433-453 (*isol*)
Arca, M. *et al., J. Lipid Res.*, 1983, **24**, 332-335 (*glc*)
Yan, M. *et al., Zhiwu Xuebao (Acta Bot. Sin.)*, 1983, **25**, 254-263; *CA*, **99**, 174437 (*3β,5α,24R-form, occur*)
D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1984, 2277-2282 (*isol*)
Sica, D. *et al., Phytochemistry*, 1984, **23**, 2609-2611 (*3β,5α,24R-form, occur*)
Jackson, E.M. *et al., J. Leukocyte Biol.*, 1985, **26**, 893-897 (*occur*)
Goad, L.J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **84**, 189-196 (*3β,5α,24ξ-form, sulfate, occur*)
Seidel, S.B. *et al., Steroids*, 1986, **47**, 49-62 (*3β,5β,24ξ-form, occur*)
Seldes, A.M. *et al., Tetrahedron*, 1988, **44**, 1359-1362 (*3α,5α,24ξ-form, isol*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Nguyen, D.-K. *et al., CA*, 1995, **122**, 273196 (*3α,5β,24ξ-form, occur*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*3β,5α,24ξ-form, occur*)
Batta, A.K. *et al., J. Lipid Res.*, 1999, **40**, 1148-1154 (*3β,5β,24ξ-form, glc, occur*)

Ergosta-5,7,9(11),22-tetraen-3-ol E-691

24-Methylcholesta-5,7,9(11),22-tetraen-3-ol



(3β,22*E*,24*R*)-*form*

$C_{28}H_{42}O$ 394.639

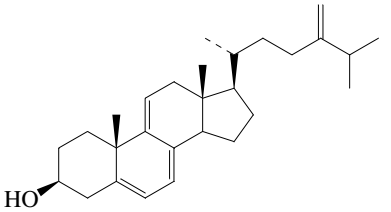
(3β,22*E*,24*R*)-*form* [516-85-8]
Constit. of the sponges *Axinella cannabina* and *Biemna fortis*.
Cryst. (MeOH).
Mp 145-147°. $[\alpha]_D^{20}$ +147 ($CHCl_3$).

(3β,22*E*,24*S*)-*form* [85798-12-5]
Constit. of *Axinella cannabina* and the green alga *Chlorella vulgaris*.

Delseth, C. *et al., Helv. Chim. Acta*, 1979, **62**, 2037-2045 (*isol, Biemna*)
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol, Axinella*)
Akihisa, T. *et al., Phytochemistry*, 1992, **31**, 1769-1772 (*isol, Chlorella*)

Ergosta-5,7,9(11),24(28)-tetraen-3-ol E-692

24-Methylenecholesta-5,7,9(11)-trien-3-ol



$C_{28}H_{42}O$ 394.639

3β-*form* [85733-71-7]
Constit. of the sponge *Axinella cannabina*.
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-151 (*isol, pmr, ms*)

Ergosta-5,7,22,25-tetraen-3-ol E-693

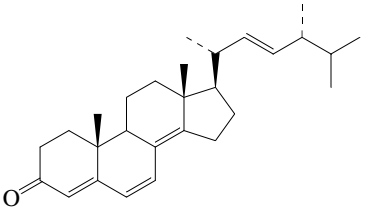
24-Methylcholesta-5,7,22,25-tetraen-3-ol
$C_{28}H_{42}O$ 394.639

(3β,22*E*,24*S*)-*form*
Protothecasterol. *25-Dehydroergosterol*
[119147-12-5]
Isol. from the algae *Dictylostelium discoideum, Prototheca wickerhamii* and the sponge *Ciocalypta* sp.

John, V. *et al., J.O.C.*, 1989, **54**, 1642-1647 (*isol*)
Nes, W.D. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1990, **87**, 7565 (*isol*)
Norton, R.A. *et al., Lipids*, 1991, **26**, 247 (*isol*)

Ergosta-4,6,8(14),22-tetraen-3-one E-694

24-Methylcholesta-4,6,8(14),22-tetraen-3-one



(22*E*,24*R*)-*form*

$C_{28}H_{40}O$ 392.623

(22*E*,24*R*)-*form* [19254-69-4]
Constit. of *Fomes officinalis*, *Alternaria alternata, Scleroderma polyrhizum* and *Acremonium coenophialum*. Detected in fruiting bodies of more than 100 fungal spp. Isol. from the sponge *Dysidea herbacea*. Phytotoxin. Yellow plates (MeOH).
Mp 114-115°. $[\alpha]_D^{24}$ +610 (c, 1.1 in $CHCl_3$).

(22*E*,24*S*)-*form* [142796-29-0]
Isol. from *Dysidea herbacea*.
Oil.

Barton, D.H.R. *et al., J.C.S.*, 1951, 468 (*synth*)
Schulte, K.E. *et al., Tet. Lett.*, 1968, 4763 (*isol*)
White, J.D. *et al., Bioorg. Chem.*, 1973, **2**, 163 (*biosynth*)
Seitz, L.M. *et al., J. Agric. Food Chem.*, 1977, **25**, 838 (*isol*)
Emke, A. *et al., J.C.S. Perkin 1*, 1977, 820 (*synth*)
Gonzalez, A.G. *et al., Phytochemistry*, 1983, **22**, 1049 (*isol*)
Barton, D.H.R. *et al., Bull. Soc. Chim. Fr.*, 1985, 849 (*synth*)
Davis, N.D. *et al., J. Agric. Food Chem.*, 1986, **34**, 105 (*isol*)
Tsantrizos, Y.S. *et al., Can. J. Chem.*, 1992, **70**, 158-164 (*synth, pmr, cmr, cryst struct*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 72-74 (*isol, Dysidea*)
Tanaka, N. *et al., Chem. Pharm. Bull.*, 1996, **44**, 843 (*occur, props*)

Ergosta-4,6,8(14),24(28)-tetraen-3-one E-695

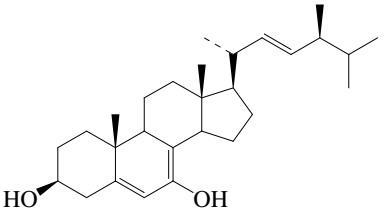
24-Methylenecholesta-4,6,8(14)-trien-3-one
[142755-13-3]
$C_{28}H_{40}O$ 392.623
Constit. of the sponge *Dysidea herbacea*. Oil.

24ξ,28-Dihydro: Ergosta-4,6,8(14)-trien-3-one
[142796-30-3]
$C_{28}H_{42}O$ 394.639
Constit. of *Dysidea herbacea*. Oil.

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 72-74 (*isol, pmr, cmr*)

Ergosta-5,7,22-triene-3,7-diol E-696

24-Methylcholesta-5,7,22-triene-3,7-diol



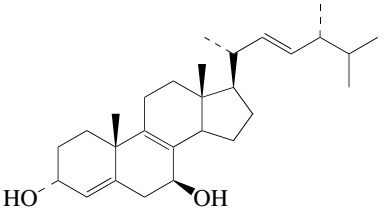
$C_{28}H_{44}O_2$ 412.654

(3β,22*E*)-*form*
7-Hydroxyergosterol
[158822-76-5]
Isol. from the marine-derived fungus *Lignincola laevis*.
Amorph. solid.

Abraham, S.P. *et al., Pure Appl. Chem.*, 1994, **66**, 2391-2394 (*isol, pmr*)

Ergosta-4,8,22-triene-3,7-diol E-697

24-Methylcholesta-4,8,22-triene-3,7-diol



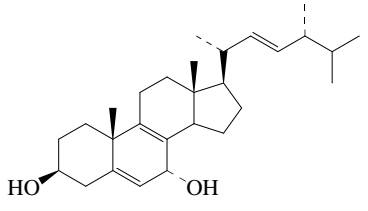
$C_{28}H_{44}O_2$ 412.654

(3α,7β,22*E*,24*R*)-*form* [179189-02-7]
Isol. from the marine sponge *Suberites carnosus*.
Solid.
Mp 155-160°. Incorrectly given as 7α-isomer in CA.

Mishra, P.D. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 806-809 (*isol, ir, pmr, ms*)

Ergosta-5,8,22-triene-3,7-diol E-698

24-Methylcholesta-5,8,22-triene-3,7-diol



(3β,7α,22*E*,24*R*)-*form*

$C_{28}H_{44}O_2$ 412.654

(3β,7α,22*E*,24*R*)-*form*
5α,6α:8α,9α-Diepoxide: ***5,6:8,9-Diepoxyergost-22-ene-3,7-diol***.
5,6:8,9-Diepoxy-24-methylcholest-22-ene-3,7-diol
[243449-51-6]
$C_{28}H_{44}O_4$ 444.653
Isol. from several mushroom spp. incl. *Amanita pantheria* and *Hypsizygus marmoreus* (bunashimeji). Amorph. powder. $[\alpha]_D$ -53.6 (c, 0.06 in $CHCl_3$).

(3β,7α,22*E*,24*S*)-*form*
5α,6α-Epoxide: 5,6-Epoxyergosta-8,22-diene-3,7-diol. ***Melithasterol B***
[16250-61-6]
$C_{28}H_{44}O_3$ 428.654
Constit. of *Melithaea ocracea* and *Arum italicum*, also from *Spongia officinalis*. Cryst. (MeOH).
Mp 184.5-186° (174-175°). $[\alpha]_D^{20}$ -51 (c, 0.76 in $CHCl_3$).
5α,6α-Epoxide, di-Ac: [148022-38-2]
Cryst. (MeOH). Mp 150-152°. $[\alpha]_D$ -86.

(3β,7β,22*E*,24*R*)-*form*
5α,6α-Epoxide: [243449-53-8]
$C_{28}H_{44}O_3$ 428.654
Constit. of *Tricholoma portentosum*. Amorph. powder. $[\alpha]_D^{26}$ -37 (c, 0.05 in $CHCl_3$).
5α,6α:8α,9α-Diepoxide: [243449-52-7]
Isol. from *Amanita pantheria* and *Hypsizygus marmoreus* (bunashimeji).
Amorph. powder. $[\alpha]_D^{20}$ -17.2 (c, 0.06 in $CHCl_3$).

Petzoldt, K. *et al., Annalen*, 1969, **724**, 194 (*Melithasterol B*)
Kobayashi, M. *et al., J.C.S. Perkin 1*, 1991, 1177 (*isol, pmr, cmr, Melithasterol B*)
Della Greca, M. *et al., Nat. Prod. Lett.*, 1993, **2**, 27 (*isol, pmr, cmr, Melithasterol B*)
Migliuolo, A. *et al., Steroids*, 1993, **58**, 134-140 (*isol, pmr, cmr, Melithasterol B*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1999, **47**, 847-851 (*diepoxides*)
Yue, J.-M. *et al., Phytochemistry*, 2001, **56**, 801-806 (*isol, pmr, cmr*)

Ergosta-5,22,24(28)-triene-3,7-diol E-699

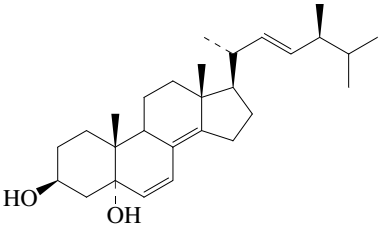
24-Methylenecholesta-5,22-diene-3,7-diol
$C_{28}H_{44}O_2$ 412.654

(3β,7β)-*form*
Constit. of *Haliclona oculata*.
$[\alpha]_D^{20}$ -87.1 (c, 0.66 in $CHCl_3$).

Findlay, J.A. *et al., Can. J. Chem.*, 1985, **63**, 2406

Ergosta-6,8(14),22-triene-3,5-diol E-700

24-Methylcholesta-6,8(14),22-triene-3,5-diol



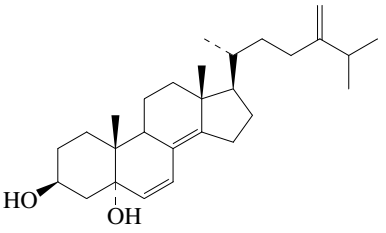
$C_{28}H_{44}O_2$ 412.654

(3β,5α,22*E*,24*S*)-*form*
5-Me ether: 5-Methoxyergosta-6,8(14),22-trien-3-ol
[85748-12-5]
$C_{29}H_{46}O_2$ 426.681
Constit. of the sponge *Axinella cannabina*.

Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol, pmr, ms*)

Ergosta-6,8(14),24(28)-triene-3,5-diol E-701

24-Methylenecholesta-6,8(14)-diene-3,5-diol



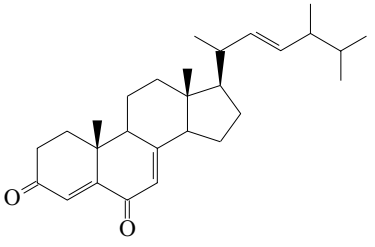
$C_{28}H_{44}O_2$ 412.654

(3β,5α)-*form*

5-Me ether: 5-Methoxyergosta-6,8(14),24(28)-trien-3-ol
[85748-13-6]
$C_{29}H_{46}O_2$ 426.681
Constit. of sponge *Axinella cannabina*.
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol, pmr, ms*)

Ergosta-4,7,22-triene-3,6-dione, 9CI E-702

Ganodosterone. *6-Ketoergosterone*
[19698-66-9]

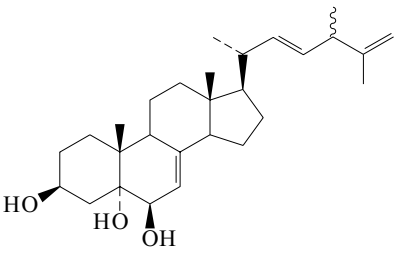


$C_{28}H_{40}O_2$ 408.623
Isol. from the sponge *Rhaphidostyla incisa* and the fungus *Ganoderma lucidum* (reishi). Cryst.
Mp 156-159° dec Mp 176-177°. Genus name given as Raphidostila, apparently incorrectly.

Malhotra, S.K. *et al., J.A.C.S.*, 1968, **90**, 6565-6566 (*synth*)
Malorni, A. *et al., Nouv. J. Chim.*, 1978, **2**, 351-354 (*isol, synth*)
Hirotani, M. *et al., Phytochemistry*, 1987, **26**, 2797-2803 (*isol, pmr*)
Kovganko, N.V. *et al., Khim. Prir. Soedin.*, 1999, **35**, 354-358; *Chem. Nat. Compd. (Engl. Transl.)*, 1999, **35**, 320-323 (*synth*)

Ergosta-7,22,25-triene-3,5,6-triol E-703

24-Methylcholesta-7,22,25-triene-3,5,6-triol



$C_{28}H_{44}O_3$ 428.654

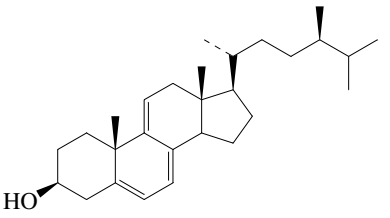
(3β,5α,6β,22*E*,24ξ)-*form*

Biemnasterol
[153229-20-0]
Constit. of a *Biemna* sp.
Cryst.
Mp 241-242°. $[\alpha]_D^{19}$ -7.6 (c, 0.43 in MeOH). λ_{max} 204 (ϵ 12700) (MeOH) (Berdy).

Zeng, C.-M. *et al., J. Nat. Prod.*, 1993, **56**, 2016 (*isol, pmr, cmr*)

Ergosta-5,7,9(11)-trien-3-ol E-704

24-Methylcholesta-5,7,9(11)-trien-3-ol
[24662-95-1, 95840-25-8]

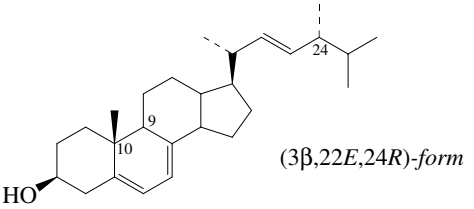


$C_{28}H_{44}O$ 396.655

(3β,24*R*)-*form* [85761-58-6]
Constit. of the sponge *Axinella cannabina*.
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-151 (*isol, pmr, ms*)

Ergosta-5,7,22-trien-3-ol E-705

24-Methylcholesta-5,7,22-trien-3-ol



(3β,22*E*,24*R*)-*form*

$C_{28}H_{44}O$ 396.655

(3β,22*E*,24*R*)-*form*

Ergosterol. *Ergosterin*. *Provitamin D_2*. *Ertron*
[57-87-4]
Occurs in yeast and fungi. The main fungal steroid. Also found in small amts. in higher plant prods., e.g. palm oil. Founf in marine fungi and the green alga *Bryopsis pennata*. Indicator of fungal contamination, esp. in cereals.
Small hydrated plates (EtOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 168° (165°). $[\alpha]_D$ -133 ($CHCl_3$). Log P 9.01 (uncertain value) (calc). λ_{max} 280 (MeOH) (Berdy). λ_{max} 262; 271; 282; 293 (EtOH) (Berdy).

3-Sulfate: [53216-04-9]
$C_{28}H_{44}O_4S$ 476.719
Mp 186° (as Na salt).

3-O-β-D-Galactopyranoside:
$C_{34}H_{54}O_6$ 558.797
Mp 204-205° (as 2′,3′,4′-tri-Ac, Me ester). $[\alpha]_D^{25}$ -27.9 ($CHCl_3$). Synthetic.

Ac: [2418-45-3]
$C_{30}H_{46}O_2$ 438.692
Plates (Et_2O/EtOH). Mp 175-176°.

Tetradecanoyl: Ergosteryl myristate
[23637-23-2]
$C_{42}H_{70}O_2$ 607.014
Isol. from an unidentified marine algicolous fungus, isolate MF001.

Hexadecanoyl: Ergosteryl palmitate
[3992-98-1]
$C_{44}H_{74}O_2$ 635.067
Isol. from microorganisms, *Penicillium* spp. and *Aspergillus itaconicus*. Cryst.
Mp 107-108°. $[\alpha]_D^{20}$ -57 ($CHCl_3$).

Benzoyl: [5035-30-3]
$C_{35}H_{48}O_2$ 500.763
Mp 168°. $[\alpha]_D$ -68.

Me ether: 3-Methoxyergosta-5,7,22-triene
[72007-94-4]
$C_{29}H_{46}O$ 410.682
Mp 151-152°.

5α,6α-Epoxide: 5,6-Epoxyergosta-7,22-dien-3-ol
[23637-31-2]
$C_{28}H_{44}O_2$ 412.654
Constit. of *Cordyceps sinensis.*

5ξ,6ξ-Epoxide: [216302-95-3]
Constit. of *Armillaria mellea* (honey mushroom).
Cryst.
Mp 229-231°. Stereochem. at C5 and C6 not clear from ref.

(3β,9α,22*E*,24*R*)-*form*
Isopyrocalciferol
[474-70-4]
Cryst. (EtOH). Mp 112-120°. $[\alpha]_D$ +332 ($CHCl_3$).

(3β,10α,22*E*,24*R*)-*form*
Pyrocalciferol
[128-27-8]
Isol. from dried mycelia of *Penicillium notatum.*
Needles (MeOH).
Mp 94-95°. $[\alpha]_D^{20}$ +502 (EtOH).

(3β,9β,10α,22*E*,24*R*)-*form*
Lumisterol
[474-69-1]
Initial prod. of uv irrad. of Ergosterol.
Cryst. (Me_2O/MeOH).
Mp 118°. $[\alpha]_D^{18}$ +197 ($CHCl_3$).

Ac: [3957-39-9]
Needles (Me_2CO/MeOH). Mp 100°. $[\alpha]_D^{18}$ +142 ($CHCl_3$).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1049C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 570B (*nmr*)
Heilbron, I.M. *et al., J.C.S.*, 1935, 1221-1223; 1937, 411-414; 1938, 869-876 (*synth, struct, Lumisterol*)
Sell, H.M. *et al., J. Biol. Chem.*, 1938, **125**, 235-240 (*Ergosterol galactoside*)
Kennedy, T. *et al., J.C.S.*, 1939, 250-253 (*struct*)
Angeletti, A. *et al., CA*, 1955, **49**, 7639 (*isol, Pyrocalciferol*)
Castells, J. *et al., J.C.S.*, 1959, 1159-1168 (*Lumisterol, Pyrocalciferol, synth, stereochem*)
Westerhof, P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1961, **80**, 1048-1056 (*synth, Pyrocalciferol*)
Jones, E.R.H. *et al., J.C.S.*, 1965, 2054-2063 (*Lumisterol, Pyrocalciferol, synth*)
Jacobs, H.J.C. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1965, **84**, 932-941 (*ord*)
Kirk Jr., P.W. *et al., Phytochemistry*, 1970, **9**, 595-597 (*Marine fungi constit*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 2060 (*occur*)
Fryberg, M. *et al., J.A.C.S.*, 1973, **95**, 5747-5757 (*Ergosterol, biosynth*)
de Kok, A.J. *et al., Acta Cryst. B*, 1974, **30**, 1695-1701 (*cryst struct, Lumisterol*)
Hull, S.E. *et al., Acta Cryst. B*, 1976, **32**, 2370-2373 (*cryst struct, Ergosterol*)
Mercer, E.I. *et al., Phytochemistry*, 1976, **15**, 283-286 (*biosynth*)
Adler, J.H. *et al., Lipids*, 1977, **12**, 364-366 (*pmr, struct*)
Smith, W.B. *et al., Org. Magn. Reson.*, 1977, **9**, 644-648 (*cmr*)
Kirk, D.N. *et al., J.C.S. Perkin 2*, 1990, 1567-1594 (*pmr*)
Young, J.C. *et al., J. Agric. Food Chem.*, 1993, **41**, 577-581; 1995, **43**, 2904-2910 (*Ergosterol, detn*)
Zhou, W. *et al., Tet. Lett.*, 1996, **37**, 1339-1342; 2000, **41**, 2791-2796 (*biosynth*)
Shi, L. *et al., Chem. Res. Chin. Univ.*, 1998, **14**, 270-272; *CA*, **130**, 22611e (*epoxide*)
Lee, D.I. *et al., Nat. Prod. Sci.*, 1999, **5**, 93-96; 154 (*tetradecanoyl*)
Aliya, R. *et al., Pak. J. Mar. Biol.*, 1999, **5**, 65-76 (*Bryopsis pennata constit*)
Bok, J.W. *et al., Phytochemistry*, 1999, **51**, 891-898 (*5,6-epoxide*)

Ergosta-5,8,22-trien-3-ol E-706

24-Methylcholesta-5,8,22-trien-3-ol
$C_{28}H_{44}O$ 396.655

(3β,22*E*,24*R*)-*form*
Lichesterol
[50657-31-3]
Constit. of the lichen *Xanthoria parietina* and the marine green alga *Bryopsis pennata*.
Cryst. (Et_2O/MeOH).
Mp 114-115°. $[\alpha]_D^{25}$ -26.6 (c, 0.3 in $CHCl_3$).

Ac: Mp 125-126°.

Lenton, J.R. *et al., Phytochemistry*, 1973, **12**, 1135-1140 (*Xanthoria parientina*)
Saddiqui, S. *et al., Pak. J. Pharm. Sci.*, 1994, **7**, 73-82 (*Bryopsis pennata constit*)

Ergosta-5,22,25-trien-3-ol E-707

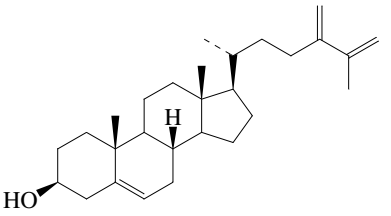
24-Methylcholesta-5,22,25-trien-3-ol
$C_{28}H_{44}O$ 396.655

(3β,22*E*,24*S*)-*form* [80525-49-1]
Constit. of sponges *Baicalospongia bacilifera* and *Pseudaxinella lunaecharta*. Also from *Sarcophyton glaucum*. Constit. of *Clerodendrum fragrans* and *Clerodendrum scandens.*
Cryst. (MeOH).
Mp 135-136.5°. $[\alpha]_D$ -47 (c, 0.89 in $CHCl_3$).

Sjöstrand, U. *et al., Steroids*, 1981, **38**, 355-364 (*isol, Pseudaxinella*)
Kobayashi, M. *et al., Steroids*, 1982, **40**, 209-221 (*isol, pmr, ms*)
Akihisa, T. *et al., Phytochemistry*, 1988, **27**, 241-244 (*isol, pmr, ms*)
Makarieva, T.N. *et al., J. Nat. Prod.*, 1991, **54**, 953-958 (*isol*)

Ergosta-5,24(28),25-trien-3-ol E-708

24-Methylenecholesta-5,25-dien-3-ol



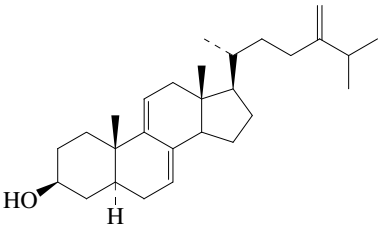
$C_{28}H_{44}O$ 396.655

3β-*form* [102607-76-1]
Isol. from the soft coral *Sinularia gyrosa*.

Gebreyesus, T. *et al., Steroids*, 1985, **45**, 447-452 (*isol, pmr, struct*)

Ergosta-7,9(11),24(28)-trien-3-ol E-709

24-Methylenecholesta-7,9(11)-dien-3-ol



$C_{28}H_{44}O$ 396.655

(3β,5α)-*form* [84223-03-0]
Constit. of the sponge *Haliclona flavescens.*

Zielinski, J. *et al., Steroids*, 1982, **39**, 675-680 (*isol, pmr, ms*)

Ergosta-8,14,22-trien-3-ol E-710

24-Methylcholesta-8,14,22-trien-3-ol
$C_{28}H_{44}O$ 396.655

(3β,5α,22*E*,24*R*)-*form*
Ergosterol B_1
[516-88-1]
Constit. of the marine green alga *Bryopsis pennata*.
Prisms (MeOH).
Mp 144-145° (140.5-141°). $[\alpha]_D$ -47 ($CHCl_3$).

Ac: [71242-49-4]
Cryst. (EtOAc). Mp 148.5-150° (143-144°). $[\alpha]_D^{25}$ -58.2 (c, 1 in $CHCl_3$).

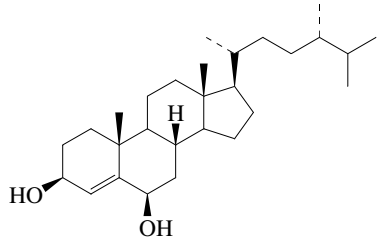
(3β,5β,22*E*,24*R*)-*form* [73679-06-8]
Isol. from *Aspergillus niger*.
Cryst. (MeOH).
Mp 144-145°. $[\alpha]_D$ -47.

[69610-91-9]

Windaus, A. *et al., Annalen*, 1931, **488**, 91 (*synth*)
Fieser, M. *et al., J.A.C.S.*, 1952, **74**, 5397
Andrieux, J. *et al., J.C.S. Perkin 1*, 1977, 359 (*synth*)
Kaneko, C. *et al., Chem. Pharm. Bull.*, 1978, **26**, 3582 (*synth*)
Bhat, H.K. *et al., J. Indian Chem. Soc.*, 1979, **56**, 934-935 (*Aspergillus niger metab*)
Dolle, R.E. *et al., J.O.C.*, 1988, **53**, 1563 (*synth, struct, bibl*)
Dolle, R.E. *et al., Tet. Lett.*, 1988, **29**, 1581 (*synth*)
Siddiqui, S. *et al., Pak. J. Pharm. Sci.*, 1994, **7**, 73-82 (*Bryopsis pennata constit*)

Ergost-4-ene-3,6-diol E-711

24-Methylcholest-4-ene-3,6-diol



(3β,6β,24*S*)-*form*

$C_{28}H_{48}O_2$ 416.686

(3β,6β,24*S*)-*form* [160324-94-7]
Constit. of *Rumphella aggregata*.
Cryst.
Mp 242-245°. $[\alpha]_D$ 0 (c, 0.42 in Py).

3,6-Diketone: ***Ergost-4-ene-3,6-dione***. *24-Methylcholest-4-ene-3,6-dione*
[50868-50-3]
$C_{28}H_{44}O_2$ 412.654
Isol. from *Glycine max* (soybean) and *Stephania cepharantha*. No phys. props. reported.

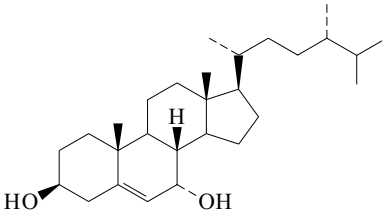
(24*R*)-*form*

3,6-Diketone: [85081-02-3]
Isol. from the stems of *Phoenix dactylifera* (date).
Cryst. (MeOH).
Mp 162-163°.

Itokawa, H. *et al., Chem. Pharm. Bull.*, 1973, **21**, 1386 (*diketone*)
Weber, N. *et al., Phytochemistry*, 1977, **16**, 1849 (*diketone*)
Fernandez, M.I. *et al., Phytochemistry*, 1983, **22**, 2087 (*diketone*)
Anjaneyula, V. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 78 (*isol, pmr, cmr*)

Ergost-5-ene-3,7-diol E-712

24-Methylcholest-5-ene-3,7-diol



$C_{28}H_{48}O_2$ 416.686

(3β,7α,24*R*)-*form*
7α-Hydroxycampesterol
Constit. of *Euphorbia fischeriana*.

7-Ketone: ***3-Hydroxyergost-5-en-7-one***
$C_{28}H_{46}O_2$ 414.67
Constit. of *Euphorbia fischeriana*, *Patinigera megalanica* and *Cyttaria jakowii*.

(3β,7α,24*S*)-*form* [71486-05-0]
Constit. of *Sclerophytum* sp.
Needles.
Mp 210-212°. $[\alpha]_D$ -75 (c, 0.38 in $CHCl_3$).

7-Ketone: Constit. of *Cyttaria johowii* and *Patinigera megalanica*.
Cryst.
Mp 140-142°. $[\alpha]_D^{27}$ -81 (c, 0.5 in $CHCl_3$). λ_{max} 235 (MeOH).

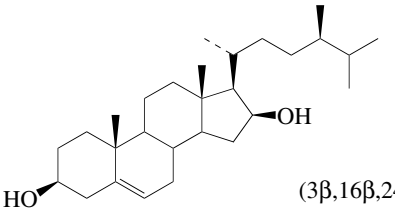
(3β,7β,24*R*)-*form*
7β-Hydroxycampesterol
Constit. of *Euphorbia fischeriana*.

(3β,7β,24*S*)-*form* [71486-04-9]
Constit. of a *Lobophytum* sp.
Cryst.
Mp 211-213°. $[\alpha]_D^{28}$ -64.1 (c, 0.05 in $CHCl_3$).

Cheng, K.-C. *et al., J. Chem. Res., Synop.*, 1979, 84 (*synth*)
Schroeder, G. *et al., Phytochemistry*, 1980, **19**, 2213-2215 (*isol, struct*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1993, **41**, 87 (*isol, pmr, cmr*)
Abraham, W.R. *et al., Phytochemistry*, 1994, **36**, 459-461 (*7-ketones*)
Lu, W. *et al., Steroids*, 2004, **69**, 803-808 (*synth*)
Muralidhar, P. *et al., Chem. Pharm. Bull.*, 2005, **53**, 168-171 (*Lobophytum constit*)

Ergost-5-ene-3,16-diol E-713

24-Methylcholest-5-ene-3,16-diol



(3β,16β,24*R*)-*form*

$C_{28}H_{48}O_2$ 416.686

(3β,16β,24*R*)-*form*
Constit. of *Cladiella krempfi*.
Cryst. (MeOH).
Mp 165-166°. There is confusion in the lit. regarding the C-24 config. . It is probable that the 24*R*- isomer has not been isolated.

(3β,16β,24*S*)-*form*
[161536-24-9]
Isol. from the soft coral *Cladiella krempfi*.
Needles (MeOH).
Mp 168-170°. $[\alpha]_D^{27}$ -35 (c, 0.8 in $CHCl_3$).

3-O-α-L-*Fucopyranoside:* [179883-53-5]
$C_{34}H_{58}O_6$ 562.829
Constit. of the soft coral *Sinularia gibberosa*. Needles ($CHCl_3$/MeOH).
Mp 235-238°. $[\alpha]_D^{27}$ -74 (c, 0.5 in Py).

Sarma, N.S. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 264-266 (*isol, pmr, ms*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 819 (*isol, pmr, cmr, ms*)

Ergost-5-ene-3,25-diol, 9CI E-714

24-Methylcholest-5-ene-3,25-diol

$C_{28}H_{48}O_2$ 416.686

(3β,24*S*)-*form* [56362-42-6]
Constit. of the corals *Sarcophyton glaucum* and *Nephthea* sp.
Cryst. (EtOAc).
Mp 185.5-187.5°. $[\alpha]_D$ -50.3 (c, 0.95 in $CHCl_3$). Earlier isol. with undetermined 24-config. from a soft coral, with phys. props. similar to those given for the (3β,24*S*)-isomer.

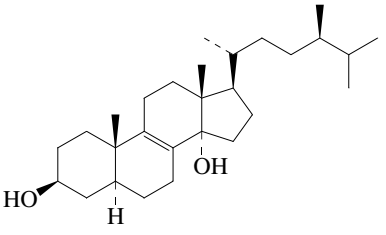
3-O-*β*-D-*Arabinopyranoside:* [178064-41-0]
$C_{33}H_{56}O_6$ 548.802
Constit. of *Sinularia grandilobata*. Cryst.
Mp 262-265°.

3-O-*α*-L-*Fucopyranoside:* [243668-12-4]
$C_{34}H_{58}O_6$ 562.829
Constit. of *Sinularia gravis*. Cryst. ($CHCl_3$/MeOH).
Mp 266-268°. $[\alpha]_D^{25}$ -90 (c, 0.5 in MeOH).

Engelbrecht, J.P. *et al., Steroids*, 1972, **20**, 121-126 (*isol*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1848
Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1992, **31**, 708; 1996, **35**, 757; 1999, **38**, 357-360 (*isol, pmr, cmr, glycosides*)

Ergost-8-ene-3,14-diol E-715

24-Methylcholest-8-ene-3,14-diol



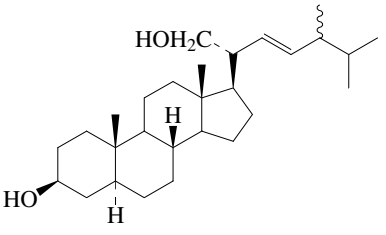
$C_{28}H_{48}O_2$ 416.686

(3β,5α,14α,24*R*)-*form*

3-Me ether: 3-Methoxyergost-8-en-14-ol
[139765-37-0]
$C_{29}H_{50}O_2$ 430.713
Constit. of the sponge *Jereicopsis graphidiophora*.
D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*isol, pmr, cmr, ms*)

Ergost-22-ene-3,21-diol E-716

24-Methylcholest-22-ene-3,21-diol



$C_{28}H_{48}O_2$ 416.686

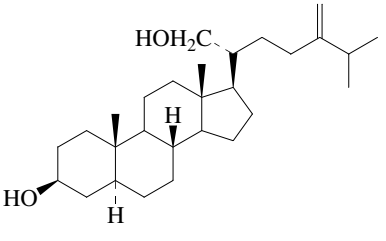
(3β,5α,22*E*,24ξ)-*form* [95062-31-0]
Constit. of *Euretaster insignis*.

Disulfate: [95062-44-5]
$C_{28}H_{48}O_8S_2$ 576.814
Constit. of *Euretaster insignis*.

D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1984, 2277-2282 (*isol, pmr, ms*)

Ergost-24(28)-ene-3,21-diol E-717

24-Methylenecholestane-3,21-diol



$C_{28}H_{48}O_2$ 416.686

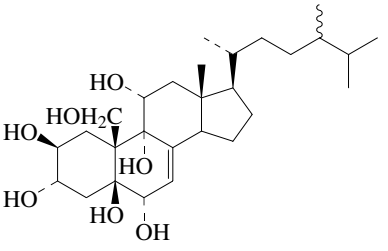
(3β,5α)-*form* [95062-30-9]
Constit. of *Euretaster insignis*.

Di-O-*sulfate:* [95062-42-3]
$C_{28}H_{48}O_8S_2$ 576.814
Constit. of *Euretaster insignis*.

D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1984, 2277-2282 (*isol, pmr, ms*)

Ergost-7-ene-2,3,5,6,9,11,19-heptol E-718

24-Methylcholest-7-ene-2,3,5,6,9,11,19-heptol



$C_{28}H_{48}O_7$ 496.683

(2β,3α,5β,6α,9α,11α,21ξ)-*form* [120711-49-1]
Isol. from sponge *Dysidea etheria*.
Mp 240-260°. $[\alpha]_D^{25}$ +18.2 (c, 0.28 in EtOH).
West, R.R. *et al., J.O.C.*, 1989, **54**, 3234-3236

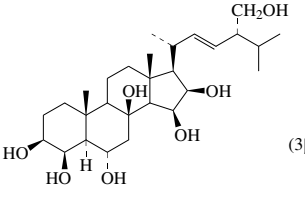
Ergost-22-ene-3,4,6,8,15,16,26-heptol, 9CI E-719

24-Methylcholest-22-ene-3,4,6,8,15,16,26-heptol
$C_{28}H_{48}O_7$ 496.683

(3β,4β,6α,15α,16β,22*E*)-*form* [93368-90-2]
Constit. of *Protoreaster nodosus*.
Cryst. (MeOH).
Mp 185-188°. $[\alpha]_D$ +20 (c, 0.4 in MeOH).
Minale, L. *et al., J. Nat. Prod.*, 1984, **47**, 790-795

Ergost-22-ene-3,4,6,8,15,16,28-heptol E-720

24-Hydroxymethylcholest-22-ene-3,4,6,8,15,16-hexol



(3β,4β,5α,6α,8β,15β,16β,22*E*,24*R*)-*form*

$C_{28}H_{48}O_7$ 496.683

(3β,4β,5α,6α,8β,15β,16β,22*E*,24*R*)-*form*

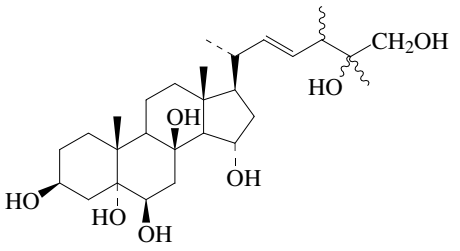
28-O-*[3*-O-*Methyl-β*-D-*xylopyranosyl-(1→4)-3*-O-*methyl-β*-D-*xylopyranoside]:* ***Milleporoside B***
[887141-47-1]
$C_{40}H_{68}O_{15}$ 788.968
Constit. of *Fromia milleporella*. Amorph. solid. $[\alpha]_D^{20}$ -16.6 (c, 0.12 in MeOH).

(3β,4β,5α,6α,8β,15β,16β,22*E*,24ξ)-*form*

28-O-*[2*-O-*Methyl-β*-D-*xylopyranosyl-(1→2)-β*-D-*galactofuranoside]:* ***Ceramasteroside C_1***
[192325-53-4]
$C_{40}H_{68}O_{16}$ 804.968
Constit. of *Ceramaster patagonicus*.
$[\alpha]_D$ -26.7 (c, 0.7 in MeOH).

Kicha, A.A. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1997, **46**, 186-191 (*Ceramasteroside C_1*)
Levina, E.V. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2006, **32**, 84-88 (*Milleporoside B*)

Ergost-22-ene-3,5,6,8,15,25,26-heptol E-721



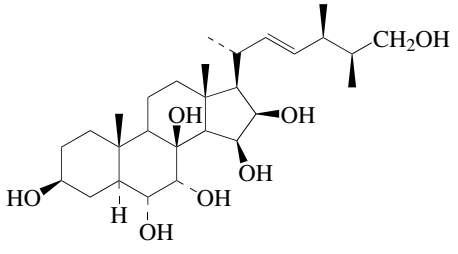
$C_{28}H_{48}O_7$ 496.683

(3β,5α,6β,8β,15α,22*E*,24ξ,25ξ)-*form*

26-O-*Sulfate:* [874351-59-4]
$C_{28}H_{48}O_{10}S$ 576.747
Constit. of *Ctenodiscus crispatus.* Amorph. $[\alpha]_D$ +11.8 (c, 0.1 in MeOH).
Kicha, A.A. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2005, **54**, 1266-1271

Ergost-22-ene-3,6,7,8,15,16,26-heptol E-722

24-Methylcholest-22-ene-3,6,7,8,15,16,26-heptol



$C_{28}H_{48}O_7$ 496.683

(3β,5α,6α,7α,15β,16β,22*E*,24*R*,25*S*)-*form*

3-O-*β-D-Xylopyranoside, 26-sulfate:* ***Coscinasteroside A***
[105404-85-1]
$C_{33}H_{56}O_{14}S$ 708.863
Constit. of *Coscinasterias tenuispina.*
$[\alpha]_D$ -1.4 (MeOH) (as Na salt). Incorrect structure given in CA. (Missing OH at C-15). CAS number refers to Na salt.
Riccio, R. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 869-893 (*isol, pmr, cmr, ms*)

Ergost-24(28)-ene-3,4,6,8,15,16,26-heptol E-723

24-Methylenecholestane-3,4,6,8,15,16,26-heptol

$C_{28}H_{48}O_7$ 496.683

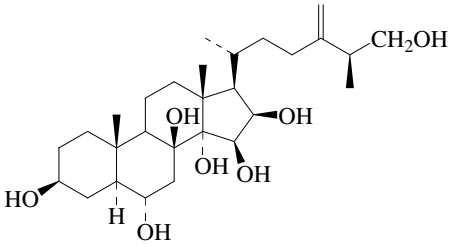
(3β,4β,5α,6α,8β,15β,16β,25*S*)-*form* [138169-03-6]
Constit. of *Culcita novaeguineae.*
$[\alpha]_D$ -10.4 (c, 0.1 in MeOH).

(3β,4β,5α,6β,15α,16β,25*R*)-*form*

3-O-*(2*-O-*Methyl-β-D-xylopyranoside):* ***Thromidioside***
[117585-44-1]
$C_{34}H_{58}O_{11}$ 642.826
Isol. from the starfish *Thromidia catalai.*
$[\alpha]_D$ +10 (c, 0.2 in MeOH).
Riccio, R. *et al., J. Nat. Prod.*, 1988, **51**, 1003-1005 (*Thromidioside, isol, pmr, cmr*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1991, **54**, 1254-1264 (*Culcita novaeguineae constit*)

Ergost-24(28)-ene-3,6,8,14,15,16,26-heptol E-724

24-Methylenecholestane-3,6,8,14,15,16,26-heptol

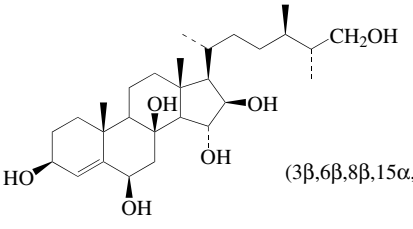


$C_{28}H_{48}O_7$ 496.683

(3β,5α,6α,15β,16β,25*S*)-*form* [128855-10-7]
Constit. of *Dermasterias imbricata.*
$[\alpha]_D$ +30.5 (c, 0.5 in MeOH).
Bruno, I. *et al., J. Nat. Prod.*, 1990, **53**, 366-374 (*isol, pmr, cmr*)

Ergost-4-ene-3,6,8,15,16,26-hexol E-725

24-Methylcholest-4-ene-3,6,8,15,16,26-hexol



(3β,6β,8β,15α,16β,24*R*,25*R*)-*form*

$C_{28}H_{48}O_6$ 480.684

(3β,6β,8β,15α,16β,24*R*,25*R*)-*form*

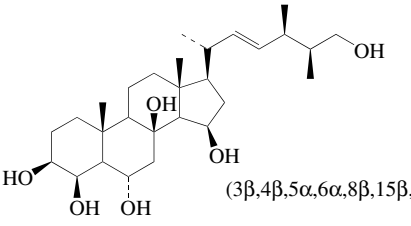
3-(2,3-Di-O-*methyl-β-D-xylopyranoside):* ***Henricioside H₃***
[168433-93-0]
$C_{35}H_{60}O_{10}$ 640.853
Constit. of a *Henricia* sp. Amorph. $[\alpha]_D$ -23.8 (c, 2.1 in MeOH).

(3β,6β,8β,15α,16β,24*R*,25*S*)-*form*

3-O-*(2,3-Di*-O-*methyl-β-D-xylopyranoside):* ***Asperoside A***
[877175-38-7]
$C_{35}H_{60}O_{10}$ 640.853
Constit. of *Henricia aspera*. Cryst.
Mp 98-99.5°. $[\alpha]_D^{20}$ -14 (c, 0.1 in MeOH).
Kicha, A.A. *et al., Khim. Prir. Soedin.*, 1993, **29**, 249; *Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 206 (*Henricioside H₃*)
Ivanchina, N.V. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2004, **53**, 2639-2642 (*abs config*)
Levina, E.V. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2005, **31**, 467-474 (*Asperoside A*)

Ergost-22-ene-3,4,6,8,15,26-hexol E-726

24-Methylcholest-22-ene-3,4,6,8,15,26-hexol



(3β,4β,5α,6α,8β,15β,22*E*,24*R*,25*S*)-*form*

$C_{28}H_{48}O_6$ 480.684

(3β,4β,5α,6α,8β,15β,22*E*,24*R*,25*S*)-*form*

Certonardosterol A_2

[681240-64-2]

Constit. of *Certonardoa semiregularis.*

Cryst. $[\alpha]_D^{21}$ +23.8 (c, 0.15 in MeOH).

26-O-*(3*-O-*Methyl-β-D-glucopyranoside), 6-sulfate:* ***Antarcticoside O***

[181034-85-5]

$C_{35}H_{60}O_{14}S$ 736.917

Constit. of an Antarctic starfish (Echinasteridae).

$[\alpha]_D$ +10.7 (MeOH).

26-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Acodontasteroside E***

$C_{39}H_{66}O_{14}$ 758.942

Constit. of *Acodontaster conspicuus.*

26-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-β-D-xylopyranoside], 6-sulfate:* ***Halityloside I***

[102040-08-4]

$C_{39}H_{66}O_{17}S$ 839.006

Constit. of *Halityle regularis*, *Acodontaster conspicuus* and *Nardoa gomophia*.

26-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-3*-O-*sulfo-β-D-xylopyranoside]:* ***Certonardoside D***

[476437-78-2]

$C_{39}H_{66}O_{17}S$ 839.006

Constit. of *Certonardoa semiregularis.* Cryst. $[\alpha]_D^{21}$ -20.2 (c, 0.6 in MeOH).

26-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→2)-β-D-galactofuranoside], 6-sulfate:* ***Antarcticoside P***

[181034-88-8]

$C_{41}H_{70}O_{18}S$ 883.059

Constit. of an Antarctic starfish.

$[\alpha]_D$ -15.5 (MeOH).

(3β,4β,5α,6α,8β,15β,22*E*,24ξ,25ξ)-*form*

26-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-β-D-galactofuranoside]:* ***Ceramasteroside C_4***

[192325-56-7]

$C_{40}H_{68}O_{15}$ 788.968

Constit. of *Ceramaster patagonicus.*

$[\alpha]_D$ -24.8 (c, 0.4 in MeOH).

(3β,4β,5α,6β,8β,15α,22*E*,24*R*,25*S*)-*form*

3-O-*(2,4-Di*-O-*methyl-β-D-xylopyranoside):* ***Asperoside B***

[877175-39-8]

$C_{35}H_{60}O_{10}$ 640.853

Constit. of *Henricia aspera*.

$[\alpha]_D^{20}$ -16 (c, 0.1 in MeOH).

3-O-*(2,3,4-Tri*-O-*methyl-β-D-xylopyranoside):* ***Sanguinoside C***

[639850-38-7]

$C_{36}H_{62}O_{10}$ 654.88

Constit. of *Henricia sanguinolenta*. Cryst. (MeOH).

Mp 178-179.5°. $[\alpha]_D^{20}$ -13 (c, 0.1 in EtOH).

Iorizzi, M. *et al., J. Nat. Prod.*, 1986, **49**, 67-78 (*Halityloside I*)

Iorizzi, M. *et al., Tetrahedron*, 1996, **52**, 10997-11012 (*Antarctic starfish constits*)

De Marino, S. *et al., J. Nat. Prod.*, 1997, **60**, 959-966 (*Acodontasteroside E*)

Kicha, A.A. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1997, **46**, 186-191 (*Ceramasteroside C_4*)

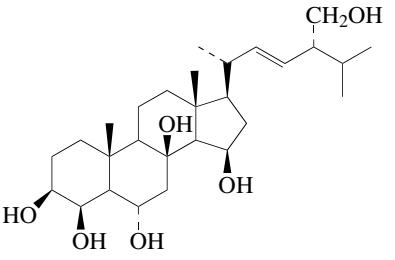
Wang, W. *et al., J. Nat. Prod.*, 2002, **65**, 1649-1656 (*Certonardoside D*)

Levina, E.V. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2003, **52**, 1623-1628; 2005, **31**, 467-474 (*Sanguinoside C, Asperoside B*)

Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 584-591 (*Certonardosterol A_2*)

Ergost-22-ene-3,4,6,8,15,28-hexol E-727

24-Methylcholest-22-ene-3,4,6,8,15,28-hexol



$C_{28}H_{48}O_6$ 480.684

(3β,4β,6α,8β,15β,22*E*,24*R*)-*form*

28-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-β-D-galactofuranoside], 6-sulfate:* ***Acodontasteroside A***

[195061-54-2]

$C_{40}H_{68}O_{18}S$ 869.032

Constit. of *Acodontaster conspicuus.*

$[\alpha]_D$ -8 (c,1 in MeOH).

28-O-*[2,4-Dimethyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside], 6-sulfate: Δ^{22E}-Culcitoside C_7*

[151507-65-2]

$C_{40}H_{68}O_{17}S$ 853.033

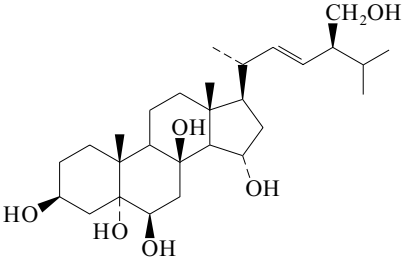
Isol. from starfish *Nardoa tuberculata.*

Bruno, I. *et al., J. Nat. Prod.*, 1993, **56**, 1057-1064 (*Δ^{22E}-Culcitoside C_7*)

De Marino, S. *et al., J. Nat. Prod.*, 1997, **60**, 959-966 (*Acodontasteroside A*)

Ergost-22-ene-3,5,6,8,15,28-hexol E-728

24-(Hydroxymethyl)cholest-22-ene-3,5,6,8,15-pentol



$C_{28}H_{48}O_6$ 480.684

(3β,5α,6β,8β,15α,24*S*)-*form*

28-Sulfate: [160538-73-8]

$C_{28}H_{48}O_9S$ 560.748

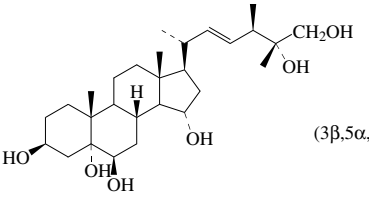
Constit. of *Styracaster caroli.*

$[\alpha]_D$ +2.5 (MeOH).

Iorizzi, M. *et al., J. Nat. Prod.*, 1994, **57**, 1361-1373 (*isol, pmr, cmr*)

Ergost-22-ene-3,5,6,15,25,26-hexol E-729

24-Methylcholest-22-ene-3,5,6,15,25,26-hexol



(3β,5α,6β,15α,22*E*,24*R*,25*R*)-*form*

$C_{28}H_{48}O_6$ 480.684

(3β,5α,6β,15α,22*E*,24*R*,25*R*)-*form*

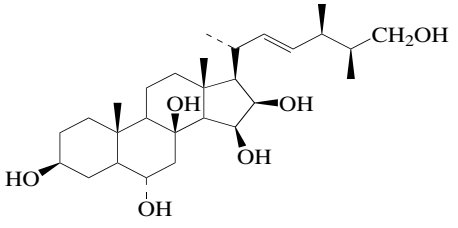
Amorph. $[\alpha]_D$ +22.7 (c, 0.9 in MeOH).

26-Sulfate: [874184-98-2]
$C_{28}H_{48}O_9S$ 560.748
Constit. of *Ctenodiscus crispatus*. Amorph. $[\alpha]_D$ +12.9 (c, 0.3 in MeOH).

(3β,5α,6β,15α,22*E*,24*R,25*S**)-*form***
26-Sulfate: [874351-57-2]
Constit. of *Ctenodiscus crispatus*.
Amorph. $[\alpha]_D$ +12.4 (c, 0.5 in MeOH).

(3β,5α,6β,15β,22*E*,24*R,25*R**)-*form*** [160538-70-5]
Constit. of *Styracaster caroli*.
$[\alpha]_D$ -10.6 (MeOH).
Kicha, A.A. *et al., Izv. Akad. Nauk, Ser. Khim.*, 1994, **43**, 1821; *Russ. Chem. Bull. (Engl. Transl.)*, 1994, **43**, 1726 (*isol, pmr, cmr*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1994, **57**, 1361-1373 (*isol, pmr, cmr*)
Kicha, A.A. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2005, **54**, 1266-1271 (*Ctenodiscus crispatus constits*)

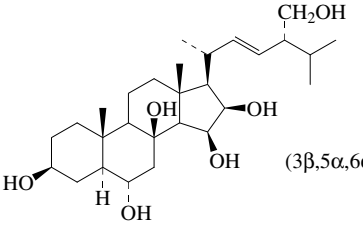
Ergost-22-ene-3,6,8,15,16,26-hexol E-730



$C_{28}H_{48}O_6$ 480.684

(3β,5α,6α,8β,15β,16β,22*E*,24*R*,25*S*)-*form*
3,26-Di-O-*β*-D-*xylopyranoside:* ***Asteriidoside G***
[214976-62-2]
$C_{38}H_{64}O_{14}$ 744.915
Constit. of a starfish (Asteriidae).
$[\alpha]_D$ -17.9 (c, 1 in MeOH).
De Marino, S. *et al., J. Nat. Prod.*, 1998, **61**, 1319-1327 (*isol, pmr, cmr*)

Ergost-22-ene-3,6,8,15,16,28-hexol E-731



(3β,5α,6α,15β,16β,22*E*,24*R*)-*form*

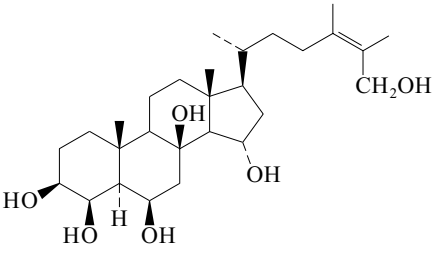
$C_{28}H_{48}O_6$ 480.684

(3β,5α,6α,15β,16β,22*E*,24*R*)-*form*
28-O-*(6*-O-*Sulfo-β*-D-*glucopyranoside):* ***Pisasteroside A***
[123154-33-6]
$C_{34}H_{58}O_{14}S$ 722.89
Isol. from the starfishes *Pisaster giganteus*, *Distolasterias nipon*, *Pisaster brevispinnus*, and *Pisaster ochraceus*.
$[\alpha]_D$ +4 (c, 0.8 in MeOH) (as Na salt).

(3β,5α,6α,15β,16β,22*E*,24ξ)-*form*
28-O-*(4*-O-*Sulfo-β*-D-*glucopyranoside):* ***Coscinasteroside C***
[105377-96-6]
$C_{34}H_{58}O_{14}S$ 722.89
Constit. of *Coscinasterias tenuispina*.
$[\alpha]_D$ +3.6 (MeOH) (as Na salt). CAS no. refers to Na salt.
28-O-*[2*-O-*Methyl-β*-D-*xylopyranosyl-(1→2)-β*-D-*galactofuranoside]:* ***Ceramasteroside C₃***
[192325-55-6]
$C_{40}H_{68}O_{15}$ 788.968
Constit. of *Ceramaster patagonicus*.
$[\alpha]_D$ -25.1 (c, 0.7 in MeOH).
28-O-*[2,4-Di*-O-*methyl-β*-D-*xylopyranosyl-(1→2)-β*-D-*galactofuranoside]:* ***Ceramasteroside C₂***
[192325-54-5]
$C_{41}H_{70}O_{15}$ 802.995
Constit. of *Ceramaster patagonicus*.
$[\alpha]_D$ -22 (c, 0.5 in MeOH).

(3β,5α,6β,8β,15α,22*E*,24*R*)-*form*
3-[2-O-*Methyl-β*-D-*xylopyranoside], 15-sulfate:* ***Laeviuscoloside C***
[129369-36-4]
$C_{34}H_{58}O_{13}S$ 706.89
Constit. of *Henricia laeviuscola*.
$[\alpha]_D$ +12.
Riccio, R. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 869-893 (*Coscinasteroside C*)
Zollo, F. *et al., J. Nat. Prod.*, 1989, **52**, 693-700 (*Pisasteroside A*)
D'Auria, M.V. *et al., Gazz. Chim. Ital.*, 1990, **120**, 155-163 (*Laeviuscoloside C*)
Kicha, A.A. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1997, **46**, 186-191 (*Ceramasterosides*)

Ergost-24-ene-3,4,6,8,15,26-hexol E-732

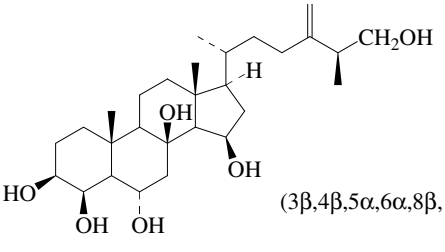


$C_{28}H_{48}O_6$ 480.684

(3β,4β,5α,6β,15α,24*Z*)-*form*
3-O-*(2*-O-*Methyl-β*-D-*arabinofuranoside), 26*-O-*α*-L-*arabinofuranoside:* ***Forbeside K***
[134985-04-9]
$C_{39}H_{66}O_{14}$ 758.942
Isol. from the starfish *Asterias forbesi*. Powder.
Mp 221° dec. $[\alpha]_D$ -9.2 (c, 0.6 in H_2O).
Findlay, J.A. *et al., J. Nat. Prod.*, 1991, **54**, 428

Ergost-24(28)-ene-3,4,6,8,15,26-hexol E-733

24-Methylenecholestane-3,4,6,8,15,26-hexol



(3β,4β,5α,6α,8β,15β,25*S*)-*form*

$C_{28}H_{48}O_6$ 480.684

(3β,4β,5α,6α,8β,15β,25*S*)-*form*
Certonardosterol A
[517900-49-1]
Constit. of *Certonardoa semiregularis*.
Cryst. $[\alpha]_D^{21}$ +16 (c, 0.23 in MeOH).
15-Ketone: 3,4,6,8,26-Pentahydroxyergost-24(28)-en-15-one. ***Certonardosterol Q₁***
[781646-76-2]
$C_{28}H_{46}O_6$ 478.668
Constit. of *Certonardoa semiregularis*. Cryst.

(3β,4β,5α,6α,8β,15β,25ξ)-*form*

26-O-*(3*-O-*Methyl-β-D-xylopyranoside):* ***Antarcticoside K***
[181034-81-1]
$C_{34}H_{58}O_{10}$ 626.826
Constit. of an Antarctic starfish.
$[\alpha]_D$ -10 (MeOH).

26-O-*(3*-O-*Methyl-4-sulfo-β-D-xylopyranoside):* ***Antarcticoside J***
[181034-80-0]
$C_{34}H_{58}O_{13}S$ 706.89
Constit. of an Antarctic starfish (Echinasteridae).
$[\alpha]_D$ -4.5 (MeOH).

26-O-*[4*-O-*Methyl-β-D-xylopyranosyl-(1→2)-arabinofuranoside]:* ***Antarcticoside M***
[181034-83-3]
$C_{39}H_{66}O_{14}$ 758.942
Constit. of an Antarctic starfish.
$[\alpha]_D$ -17 (MeOH).

26-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Acodontasteroside G***
[195062-63-6]
$C_{39}H_{66}O_{14}$ 758.942
Constit. of *Acodontaster conspicuus.*
$[\alpha]_D$ -14.4 (c, 1 in MeOH).

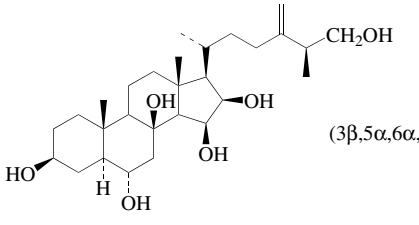
26-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-3*-O-*sulfo-β-D-xylopyranoside]:* ***Certonardoside A***
[476437-72-6]
$C_{39}H_{66}O_{17}S$ 839.006
Constit. of *Certonardoa semiregularis.* Cryst. $[\alpha]_D^{21}$ -19.5 (c, 0.41 in MeOH).

26-O-*[4*-O-*Methyl-β-D-xylopyranosyl-(1→2)-β-D-galactofuranoside]:* ***Antarcticoside L***
[181034-82-2]
$C_{40}H_{68}O_{15}$ 788.968
Constit. of an Antarctic starfish.
$[\alpha]_D$ -30.7 (MeOH).

Iorizzi, M. *et al., Tetrahedron*, 1996, **52**, 10997-11012 (*Antarctic starfish constits*)
De Marino, S. *et al., J. Nat. Prod.*, 1997, **60**, 959-966 (*Acodontasteroside G*)
Wang, W. *et al., J. Nat. Prod.*, 2002, **65**, 1649-1656 (*Certonardoside A*)
Wang, W. *et al., J. Nat. Prod.*, 2003, **66**, 384-391 (*Certonardosterol A*)
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 1654-1660 (*Certonardosterol Q_1*)

Ergost-24(28)-ene-3,6,8,15,16,26-hexol E-734

24-Methylenecholestane-3,6,8,15,16,26-hexol



(3β,5α,6α,15β,16β,25*S*)-*form*

$C_{28}H_{48}O_6$ 480.684

(3β,5α,6α,15β,16β,25*S*)-*form* [128946-38-3]
Constit. of *Dermasterias imbricata*.
$[\alpha]_D$ +35 (c, 0.5 in MeOH).

(3β,5α,6β,15α,16β,25*R*)-*form* [112076-57-0]
Constit. of the starfish *Sphaerodiscus placenta* and an Antarctic starfish.
$[\alpha]_D$ +11.7 (c, 0.5 in MeOH).

3-O-*(2*-O-*Methyl-β-D-xylopyranoside):* [100007-33-8]
$C_{34}H_{58}O_{10}$ 626.826
Constit. of *Poraster superbus.*
$[\alpha]_D$ -67 (MeOH).

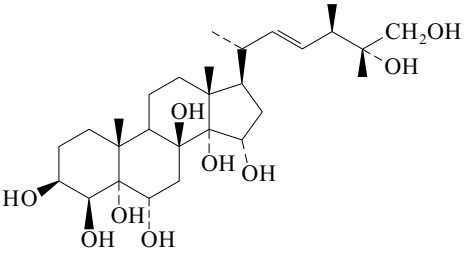
(3β,5α,6β,8β,15β,16β,25*S*)-*form*

26-[2-O-*Methyl-β-D-xylopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Culcitoside C_8***
[138169-02-5]
$C_{39}H_{66}O_{14}$ 758.942
Constit. of the starfish *Culcita novaeguineae.*
$[\alpha]_D$ -1.4 (MeOH).

Riccio, R. *et al., Gazz. Chim. Ital.*, 1985, **115**, 505-509 (*2-methylxyloside*)
Zollo, F. *et al., J. Nat. Prod.*, 1987, **50**, 794-799 (*Sphaerodiscus placenta constit*)
Bruno, I. *et al., J. Nat. Prod.*, 1990, **53**, 366-374 (*Dermasterias constit*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1991, **54**, 1254-1264 (*Culcitoside C_8*)
Iorizzi, M. *et al., Tetrahedron*, 1996, **52**, 10997-11012 (*Antarctic starfish constit*)

Ergost-22-ene-3,4,5,6,8,14,15,25,26-nonol E-735

24-Methylcholest-22-ene-3,4,5,6,8,14,15,25,26-nonol

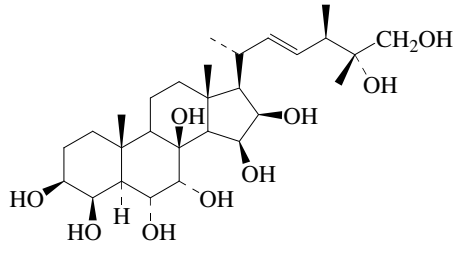


$C_{28}H_{48}O_9$ 528.682

(3β,4β,5α,6α,15α,22*E*,24*R*,25*R*)-*form*
Campest-22-ene-3,4,5,6,8,14,15,25,26-nonol
[123049-95-6]
Metab. of *Archaster typicus.*
Cryst. (MeOH).
Mp 288-290°. $[\alpha]_D$ +33.3 (c, 1 in MeOH).
Riccio, R. *et al., J.C.S. Perkin 1*, 1989, 823-826 (*isol, pmr, cmr*)

Ergost-22-ene-3,4,6,7,8,15,16,25,26-nonol E-736

24-Methylcholest-22-ene-3,4,6,7,8,15,16,25,26-nonol

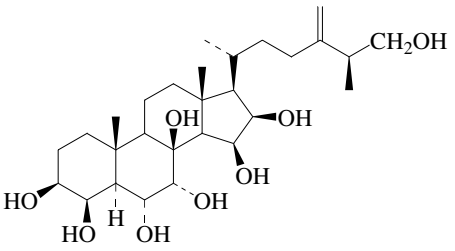


$C_{28}H_{48}O_9$ 528.682

(3β,4β,5α,6α,7α,15β,16β,22*E*,24*R*,25*R*)-*form*
6-Sulfate: [128269-49-8]
$C_{28}H_{48}O_{12}S$ 608.746
Constit. of *Patiria miniata*.
$[\alpha]_D$ +22.9 (c, 0.5 in MeOH).
D'Auria, M.V. *et al., J. Nat. Prod.*, 1990, **53**, 94-101 (*isol, pmr*)

Ergost-24(28)-ene-3,4,6,7,8,15,16,26-octol E-737

24-Methylenecholestane-3,4,6,7,8,15,16,26-octol

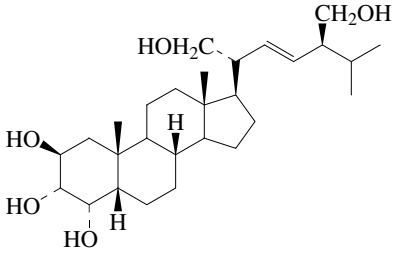


$C_{28}H_{48}O_8$ 512.682

(3β,4β,5α,6α,7α,15β,16β,25*S*)-*form* [128201-24-1]
Constit. of *Astropecten scoparius* and *Patiria miniata*.
$[\alpha]_D$ +8.5 (MeOH).
D'Auria, M.V. *et al., J. Nat. Prod.*, 1990, **53**, 94-101 (*Patiria miniata constit*)
iorizzi, M. *et al., J. Nat. Prod.*, 1990, **53**, 1225-1233 (*Astropecten scoparius constit*)

Ergost-22-ene-2,3,4,21,28-pentol E-738

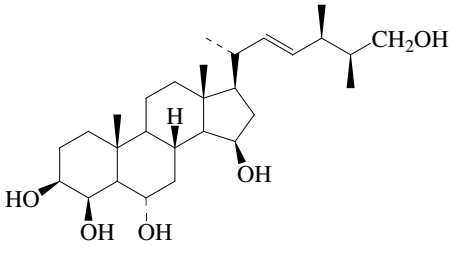
24-Hydroxymethylcholest-22-ene-2,3,4,21-tetrol



$C_{28}H_{48}O_5$ 464.684

(2β,3α,4α,5β,22*E*,24*S*)-*form* [116407-27-3]
3,21-Disulfate: [116407-22-8]
$C_{28}H_{48}O_{11}S_2$ 624.813
Isol. from the Pacific ophiuroid *Ophiolepis superba*.
$[\alpha]_D$ +22.3 (MeOH) (as di-Na salt).
D'Auria, M.V. *et al., J.O.C.*, 1989, **54**, 234-239 (*isol, pmr, cmr, synth*)

Ergost-22-ene-3,4,6,15,26-pentol E-739

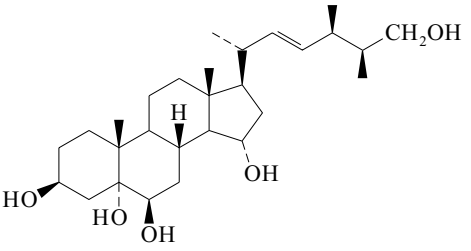


$C_{28}H_{48}O_5$ 464.684

(3β,4β,6α,15β,22*E*,24*R*,25*S*)-*form*
Certonardosterol C₂
[681240-63-1]
Constit. of *Certonardoa semiregularis.*
Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 584-591 (*isol, pmr, cmr*)

Ergost-22-ene-3,5,6,15,26-pentol E-740

24-Methylcholest-22-ene-3,5,6,15,26-pentol

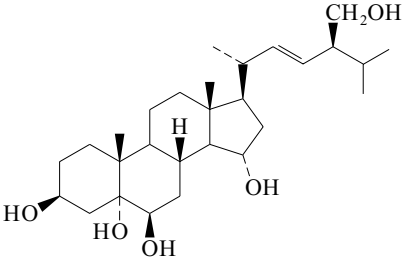


$C_{28}H_{48}O_5$ 464.684

(3β,5α,6β,15α,22*E*,24*R*,25*S*)-*form*
26-Sulfate: [165815-81-6]
$C_{28}H_{48}O_8S$ 544.748
Constit. of *Luidia clathrata*.
$[\alpha]_D$ +24.3.
Iorizzi, M. *et al., J. Nat. Prod.*, 1995, **58**, 653-671 (*isol, pmr, cmr*)

Ergost-22-ene-3,5,6,15,28-pentol E-741

24-(Hydroxymethyl)cholest-22-ene-3,5,6,15-tetrol

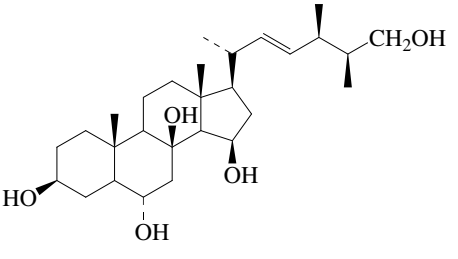


$C_{28}H_{48}O_5$ 464.684

(3β,5α,6β,15α,22*E*,24*S*)-*form*
28-Sulfate: [165815-82-7]
$C_{28}H_{48}O_8S$ 544.748
Constit. of *Luidia clathrata*.
$[\alpha]_D$ +5.4.
Iorizzi, M. *et al., J. Nat. Prod.*, 1995, **58**, 653-671 (*isol, pmr, cmr*)

Ergost-22-ene-3,6,8,15,26-pentol E-742

24-Methylcholest-22-ene-3,6,8,15,26-pentol



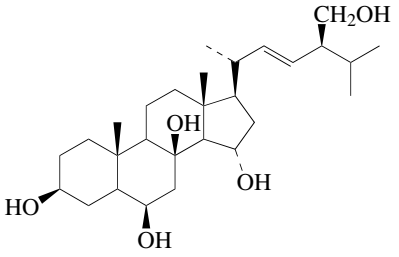
$C_{28}H_{48}O_5$ 464.684

(3β,6α,8β,15β,22*E*,24*R*,25*S*)-*form*
Certonardosterol B₂
[681240-62-0]
Constit. of *Certonardoa semiregularis.*
Cryst.
26-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-3*-O-*sulfo-β-D-xylopyranoside]:* ***Certonardoside E***
[476437-80-6]
$C_{39}H_{66}O_{16}S$ 823.007

Constit. of *Certonardoa semiregularis*. Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2002, **65**, 1649-1656 (*Certonardoside E*)
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 584-591 (*Certonardosterol B_2*)

Ergost-22-ene-3,6,8,15,28-pentol E-743

24-Hydroxymethylcholest-22-ene-3,6,8,15-tetrol



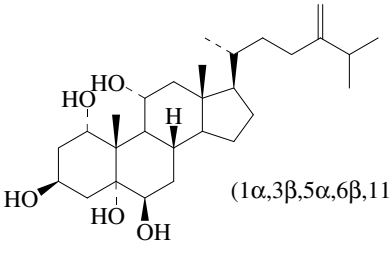
$C_{28}H_{48}O_5$ 464.684

(3β,5α,6β,8β,15α,22*E*,24*S*)-*form*

3-O-*β*-D-*Xylopyranoside, 28-sulfate:* ***Asteriidoside L***
[214976-65-5]
$C_{33}H_{56}O_{12}S$ 676.864
Constit. of a starfish (Asteriidae).
$[\alpha]_D$ +5.7 (c, 1 in MeOH).
De Marino, S. *et al., J. Nat. Prod.*, 1998, **61**, 1319-1327 (*isol, pmr, cmr*)

Ergost-24(28)-ene-1,3,5,6,11-pentol E-744

24-Methylenecholestane-1,3,5,6,11-pentol



(1α,3β,5α,6β,11α)-*form*

$C_{28}H_{48}O_5$ 464.684

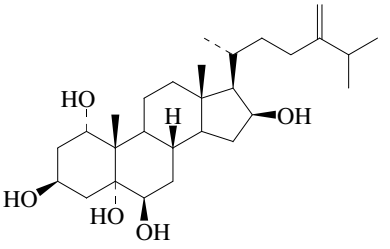
(1α,3β,5α,6β,11α)-*form* [156461-09-5]
Constit. of *Sinularia dissecta*.
Needles.
Mp 236-238°. $[\alpha]_D$ -4 (c, 1.6 in Py).
11-Ac: [156461-10-8]
$C_{30}H_{50}O_6$ 506.721
Constit. of *Sinularia dissecta*. Viscous oil. $[\alpha]_D$ -22 (c, 0.42 in Py).

(1β,3β,5α,6α,11α)-*form* [253195-39-0]
Constit. of *Sinularia dissecta*.
1,3,6,11-Tetra-Ac: [253195-43-6]
$C_{36}H_{56}O_9$ 632.833
Cryst. Mp 146-148°. $[\alpha]_D^{25}$ -12 (c, 0.2 in $CHCl_3$).

(1β,3β,5α,6β,11α)-*form* [253195-38-9]
Constit. of *Sinularia dissecta*.
1,3,6,11-Tetra-Ac: [253195-42-5]
$C_{36}H_{56}O_9$ 632.833
Cryst. Mp 196-198°. $[\alpha]_D^{25}$ -20 (c, 0.5 in $CHCl_3$).
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1994, 180 (*isol, pmr, cmr*)
Ramesh, P. *et al., Steroids*, 1999, **64**, 785-789 (*isol, pmr, cmr*)

Ergost-24(28)-ene-1,3,5,6,16-pentol E-745

24-Methylenecholestane-1,3,5,6,16-pentol

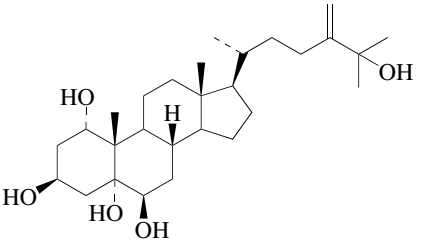


$C_{28}H_{48}O_5$ 464.684

(1α,3β,5α,6β,16β)-*form* [146117-86-4]
Isol. from a *Sinularia* sp. from the Andaman islands.
Solid.
Mp 268-271°. $[\alpha]_D$ -8 (c, 1.92 in Py).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2845-2846 (*isol, pmr*)

Ergost-24(28)-ene-1,3,5,6,25-pentol E-746

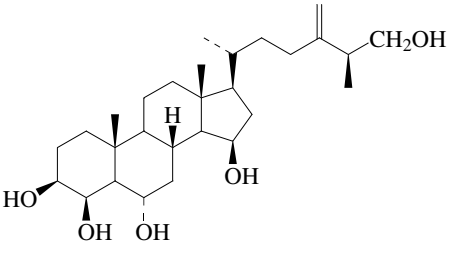
24-Methylenecholestane-1,3,5,6,25-pentol



$C_{28}H_{48}O_5$ 464.684

(1α,3β,5α,6β)-*form*
Constit. of *Sinularia microclavata*.
Cryst.
Mp 268-270°. $[\alpha]_D^{22.5}$ -4.4 (c, 0.023 in EtOH).
Li, R. *et al., Steroids*, 1992, **57**, 3 (*isol, pmr, cmr*)

Ergost-24(28)-ene-3,4,6,15,26-pentol E-747

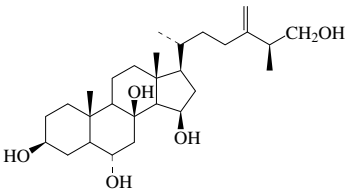


$C_{28}H_{48}O_5$ 464.684

(3β,4β,5α,6α,15β,25*S*)-*form*
Certonardosterol B
[517900-50-4]
Constit. of *Certonardoa semiregularis*.
Cryst. $[\alpha]_D^{21}$ -9.1 (c, 0.15 in MeOH).
Wang, W. *et al., J. Nat. Prod.*, 2003, **66**, 384-391 (*isol, pmr, cmr*)

Ergost-24(28)-ene-3,6,8,15,26-pentol E-748

24-Methylenecholestane-3,6,8,15,26-pentol



(3β,5α,6α,8β,15β,25*S*)-*form*

$C_{28}H_{48}O_5$ 464.684

(3β,6α,8β,15β,25*S*)-*form*
Certonardosterol C
[517900-51-5]
Constit. of *Certonardoa semiregularis.*
Cryst.

(3β,6α,8β,15β,25ξ)-*form*
*26-*O*-[2-*O*-Methyl-β-D-xylopyranosyl-(1→2)-3-*O*-sulfo-β-D-xylopyranoside]:* ***Certonardoside C***
[476437-76-0]
$C_{39}H_{66}O_{16}S$ 823.007
Constit. of *Certonardoa semiregularis.* Cryst. $[\alpha]_D^{21}$ -23.6 (c, 0.13 in MeOH).
Wang, W. *et al., J. Nat. Prod.*, 2002, **65**, 1649-1656; 2003, **66**, 384-391 (*isol, pmr, cmr*)

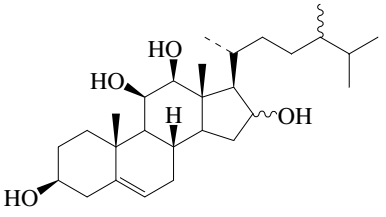
Ergost-24(28)-ene-3,6,15,16,26-pentol E-749

24-Methylenecholestane-3,6,15,16,26-pentol

$C_{28}H_{48}O_5$ 464.684

(3β,5α,6β,15α,16β,25*R*)-*form* [112058-07-8]
Constit. of the starfish *Sphaerodiscus placenta.*
$[\alpha]_D$ +28.1 (c, 1 in MeOH).
Zollo, F. *et al., J. Nat. Prod.*, 1987, **50**, 794-799 (*Sphaerodiscus placenta constit*)

Ergost-5-ene-3,11,12,16-tetrol E-750



$C_{28}H_{48}O_4$ 448.685

(3β,11β,12β,16ξ,24ξ)-*form*
11-Ac: [495380-48-8]
$C_{30}H_{50}O_5$ 490.722
Constit. of *Capnella lacertiliensis.* Oil. $[\alpha]_D^{22}$ -50 (c, 0.01 in $CHCl_3$).
12-Ac: [495380-47-7]
$C_{30}H_{50}O_5$ 490.722
Constit. of *Capnella lacertiliensis.* Oil. $[\alpha]_D^{22}$ -49 (c, 0.01 in $CHCl_3$).
Wright, A.D. *et al., J. Nat. Prod.*, 2003, **66**, 157-160 (*isol, pmr, cmr*)

Ergost-5-ene-3,22,25,28-tetrol E-751

24-Methylcholest-5-ene-3,22,25,28-tetrol. 24-Hydroxymethylcholest-5-ene-3,22,25-triol

$C_{28}H_{48}O_4$ 448.685

(3β,22*R*,24ξ)-*form*
Depresosterol
[77517-54-5]
Constit. of *Lobophytum depressum.*
Amorph. solid.
Mp 198-201°.

3-Ac: ***Sardisterol***
[351343-69-6]
$C_{30}H_{50}O_5$ 490.722
Constit. of *Sarcophyton digitatum.* Needles (EtOAc/hexane).
Mp 252-254°. $[\alpha]_D$ -6 (c, 0.02 in EtOH).

5β,6β-Epoxide: ***5,6-Epoxyergostane-3,22,25,28-tetrol***
[80322-17-4]
$C_{28}H_{48}O_5$ 464.684
Constit. of *Lobophytum depressum.* Amorph. solid.
Mp 228-229°.

28-Aldehyde: ***3,22,25-Trihydroxyergost-5-en-28-al***
$C_{28}H_{46}O_4$ 446.669
Constit. of *Lobophytum depressum.* Exists as 28→22 hemiacetal.

28-Aldehyde, 5β,6β-epoxide: ***5,6-Epoxy-3,22,25-trihydroxyergostan-28-al***
$C_{28}H_{46}O_5$ 462.668
Constit. of *Lobophytum depressum.*

Kashman, Y.S. *et al., Tet. Lett.*, 1980, **21**, 4939-4942 (*isol, epoxide, struct*)
Carmely, S. *et al., Tetrahedron*, 1981, **37**, 2397-2403 (*isol*)
Nakamura, E. *et al., J.A.C.S.*, 1985, **107**, 2138-2141 (*synth, config*)
Su, J.Y. *et al., Chin. J. Chem.*, 2001, **19**, 515-517 (*Sardisterol*)

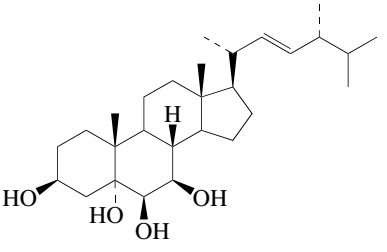
Ergost-7-ene-3,5,6,25-tetrol E-752

24-Methylcholest-7-ene-3,5,6,25-tetrol

$C_{28}H_{48}O_4$ 448.685

(3β,5α,6β,24*S*)-*form*
25-Ac: [133883-17-7]
$C_{30}H_{50}O_5$ 490.722
Constit. of *Sclerophytum* spp. Cryst.
Mp 225-230°. $[\alpha]_D^{29}$ -30 (c, 0.2 in $CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 297 (*isol, pmr, cmr*)

Ergost-22-ene-3,5,6,7-tetrol E-753



$C_{28}H_{48}O_4$ 448.685

(3β,5α,6β,7β,22*E*,24*S*)-*form*
7-Ac: ***Xeniasterol A***
[107168-57-0]
$C_{30}H_{50}O_5$ 490.722
Isol. from soft coral *Xenia* sp. Needles (EtOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 208-209°. $[\alpha]_D^{20}$ +12 (c, 0.6 in Py).
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4590-4596 (*isol, pmr, cmr*)
Ishizuka, *et al., Chem. Pharm. Bull.*, 1997, **45**, 1756-1760 (*7-ketone*)

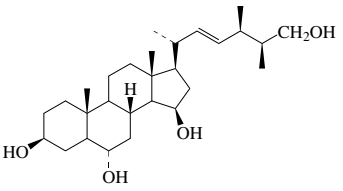
Ergost-22-ene-3,5,6,25-tetrol E-754

24-Methylcholest-22-ene-3,5,6,25-tetrol

$C_{28}H_{48}O_4$ 448.685

(3β,5α,6β,24*S*)-*form* [133883-18-8]
Constit. of *Sclerophytum* spp.
Cryst.
Mp 244°. $[\alpha]_D^{29}$ -20 (c, 0.84 in Py).
25-Ac:
$C_{30}H_{50}O_5$ 490.722
Constit. of *Sclerophytum* spp. Cryst.
Mp 241-244°. $[\alpha]_D^{29}$ -20 (c, 0.84 in Py).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 297 (*isol, pmr, cmr*)

Ergost-22-ene-3,6,15,26-tetrol E-755



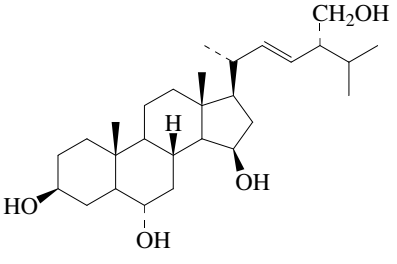
(3β,6α,15β,22*E*,24*R*,25*S*)-*form*

$C_{28}H_{48}O_4$ 448.685

(3β,6α,15β,22*E*,24*R*,25*S*)-*form*
Certonardosterol D₄
[681240-61-9]
Constit. of *Certonardoa semiregularis*.
Cryst.

(3β,6β,15α,22*E*,24*R*,25*S*)-*form*
Certonardosterol E₃
[681240-60-8]
Constit. of *Certonardoa semiregularis*.
Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 584-591 (*isol, pmr, cmr*)

Ergost-22-ene-3,6,15,28-tetrol E-756



$C_{28}H_{48}O_4$ 448.685

(3β,6α,22*E*,24*R*)-*form*
Certonardosterol D₂
[681240-54-0]
Constit. of *Certonardoa semiregularis*.
Cryst.

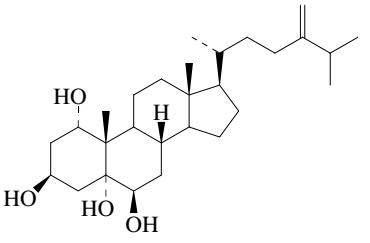
*28-*O*-[2,4-Di-*O*-methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside]:* ***Certonardoside B₃***
[681227-53-2]
$C_{40}H_{68}O_{12}$ 740.97
Constit. of *Certonardoa semiregularis*. Cryst.

22,23-Dihydro: Ergostane-3,6,15,28-tetrol
$C_{28}H_{50}O_4$ 450.701

*22,23-Dihydro, 28-*O*-[2,4-di-*O*-methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside]:* ***Certonardoside B₂***
[681227-03-2]
$C_{40}H_{70}O_{12}$ 742.986
Constit. of *Certonardoa semiregularis*. Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 584-591 (*isol, pmr, cmr*)

Ergost-24(28)-ene-1,3,5,6-tetrol E-757

24-Methylenecholestane-1,3,5,6-tetrol
[73700-29-5]



(1α,3β,5α,6β)-*form*

$C_{28}H_{48}O_4$ 448.685

(1α,3β,5α,6β)-*form*
Numersterol A
[124596-64-1]
Constit. of *Sinularia microclavata* and *Sinularia numerosa*.
Cryst. (EtOH or MeOH).
Mp 297-299° (268-270°). $[\alpha]_D^{22.5}$ +15 (c, 0.02 in EtOH). $[\alpha]_D^{25}$ +4.5 (c, 0.33 in MeOH).

6-Ketone: ***1,3,5-Trihydroxyergost-24(28)-en-6-one****. 1,3,5-Trihydroxy-24-methylenecholestan-6-one*
$C_{28}H_{46}O_4$ 446.669
Constit. of *Sinularia microclavata*. Cryst.
Mp 268-270°. $[\alpha]_D^{22.5}$ -4.4 (c, 0.023 in EtOH).

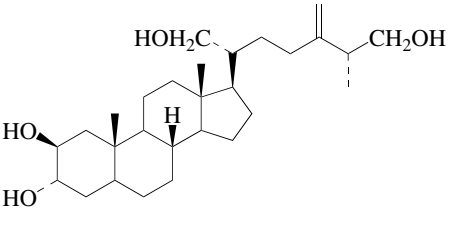
(1β,3β,5α,6β)-*form*
Constit. of *Lobophytum pauciflorum*.
Amorph. solid. $[\alpha]_D^{20}$ -3 (c, 0.14 in EtOH).

(1α,3β,5β)-*form*

6-Ketone: ***Gibberoketosterol***
[607388-87-4]
$C_{28}H_{46}O_4$ 446.669
Constit. of *Sinularia gibberosa*. Cryst. (EtOAc).
Mp 140-141°. $[\alpha]_D^{25}$ -0.7 (c, 0.38 in $CHCl_3$).
Yamada, Y. *et al., Chem. Pharm. Bull.*, 1980, **28**, 473
Su, J. *et al., J. Nat. Prod.*, 1989, **52**, 934 (*isol, pmr, cmr, cryst struct*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2845-2846 (*isol, pmr, cmr*)
Li, R. *et al., Steroids*, 1992, **57**, 3 (*isol, pmr, cmr*)
Ahmed, A.F. *et al., Steroids*, 2003, **68**, 377-381 (*Gibberoketosterol*)

Ergost-24(28)-ene-2,3,21,26-tetrol E-758

24-Methylenecholestane-2,3,21,26-tetrol



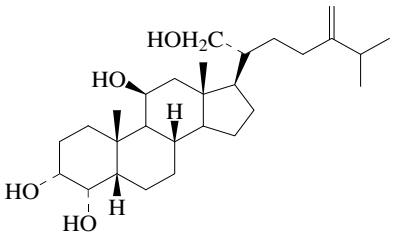
$C_{28}H_{48}O_4$ 448.685

(2β,3α,25*R*)-*form*

3,21-Disulfate: [214129-61-0]
$C_{28}H_{48}O_{10}S_2$ 608.813
Constit. of *Pteraster tesselatus*. Cryst. (MeOH).
Mp 178-179.5°. $[\alpha]_D^{20}$ +1.78 (c, 11.8 in MeOH).
Levina, E.V. *et al., J. Nat. Prod.*, 1998, **61**, 1423-1426 (*isol, pmr, cmr*)

Ergost-24(28)-ene-3,4,11,21-tetrol E-759

24-Methylenecholestane-3,4,11,21-tetrol



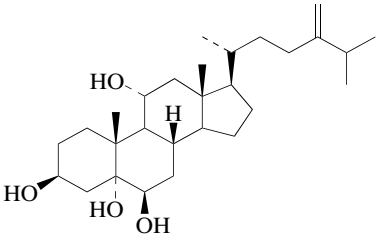
$C_{28}H_{48}O_4$ 448.685

(3α,4α,5β,11β)-*form* [109152-38-7]

3,21-Disulfate: [109152-32-1]
$C_{28}H_{48}O_{10}S_2$ 608.813
Constit. of *Ophioplocus januarii*.
$[\alpha]_D$ +15.8.
D'Auria, M.V. *et al., J.O.C.*, 1987, **52**, 3947-3953 (*isol, pmr*)
Roccatagliata, A.J. *et al., J. Nat. Prod.*, 1996, **59**, 887-889 (*isol*)

Ergost-24(28)-ene-3,5,6,11-tetrol E-760

24-Methylenecholestane-3,5,6,11-tetrol



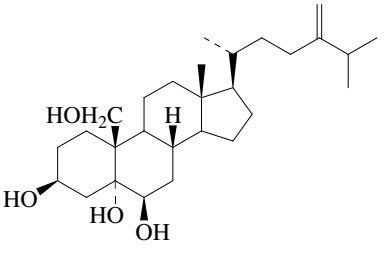
$C_{28}H_{48}O_4$ 448.685

(3β,5α,6β,11α)-*form*

11-Ac: [195061-86-0]
$C_{30}H_{50}O_5$ 490.722
Constit. of *Lobophytum* cf. *pauciflorum*. Oil. $[\alpha]_D$ -37.5 (c, 0.53 in $CHCl_3$).
Lu, Q. *et al., Nat. Prod. Lett.*, 1997, **10**, 231-237 (*isol, pmr, cmr*)

Ergost-24(28)-ene-3,5,6,19-tetrol E-761

24-Methylenecholestane-3,5,6,19-tetrol



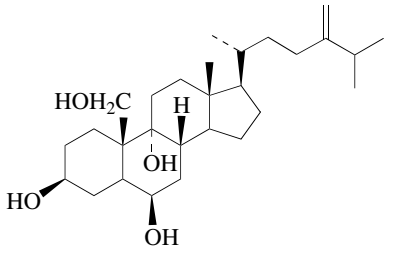
$C_{28}H_{48}O_4$ 448.685

(3β,5α,6β)-*form*
Nephalsterol A
[142754-97-0]
Isol. from the soft coral *Nephthea albida* and *Nephthea tiexieral verseveldt*.
Needles.
Mp 242-243°.

19-Ac: ***Armatinol B***
[745828-23-3]
$C_{30}H_{50}O_5$ 490.722
Constit. of *Nephthea armata*. Oil. $[\alpha]_D^{25}$ -4.4 (c, 0.6 in $CHCl_3$).
λ_{max} 206 (log ϵ 3.9) (MeOH).
Zeng, L. *et al., CA*, 1992, **117**, 87078n
El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2004, **67**, 1455-1458 (*Armatinol B*)
Lu, W. *et al., Steroids*, 2004, **69**, 445-449 (*synth*)

Ergost-24(28)-ene-3,6,9,19-tetrol E-762

24-Methylenecholestane-3,6,9,19-tetrol

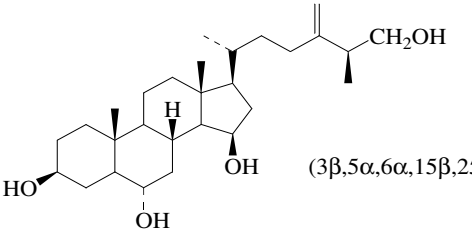


$C_{28}H_{48}O_4$ 448.685

(3β,5α,6β)-*form* [255829-10-8]
Constit. of *Sinularia inexplicata* and *Nephthea brassica*.
Cryst. (Me_2CO).
Mp 237-238°. $[\alpha]_D^{20}$ +25 (c, 0.053 in MeOH).
Liu, Q. *et al., CA*, 1999, **132**, 105500 (*isol*)
Xu, S.H. *et al., Chin. Chem. Lett.*, 2000, **11**, 531-534 (*isol, pmr, cmr*)

Ergost-24(28)-ene-3,6,15,26-tetrol E-763

24-Methylenecholestane-3,6,15,26-tetrol



(3β,5α,6α,15β,25*S*)-*form*

$C_{28}H_{48}O_4$ 448.685

(3β,5α,6α,15β,25*S*)-*form*
Certonardosterol D
[517900-52-6]
Constit. of *Certonardoa semiregularis.*
Cryst.

(3β,5α,6α,15β,25ξ)-*form*
26-O-[2-O-Methyl-β-D-xylopyranosyl-(1→2)-3-O-sulfo-β-D-xylopyranoside]: ***Certonardoside B***
[476437-74-8]
$C_{39}H_{66}O_{15}S$ 807.007
Constit. of *Certonardoa semiregularis.* Cryst.

(3β,5α,6β,15α,25*S*)-*form*
Certonardosterol E
[517900-53-7]
Constit. of *Certonardoa semiregularis.*
Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2002, **65**, 1649-1656; 2003, **66**, 384-391 (*isol, pmr, cmr*)

Ergost-25-ene-1,3,5,6-tetrol E-764

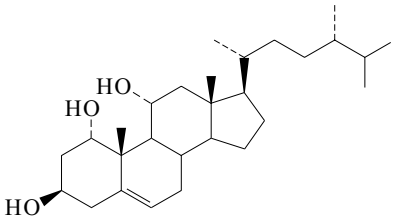
24-Methylcholest-25-ene-1,3,5,6-tetrol

$C_{28}H_{48}O_4$ 448.685

(1β,3β,5α,6β,24*S*)-*form* [142780-36-7]
Constit. of *Sarcophyton subviride.*
Raja, B.L. *et al., J. Nat. Prod.*, 1992, **55**, 904 (*isol, pmr, cmr*)

Ergost-5-ene-1,3,11-triol E-765

24-Methylcholest-5-ene-1,3,11-triol



$C_{28}H_{48}O_3$ 432.685

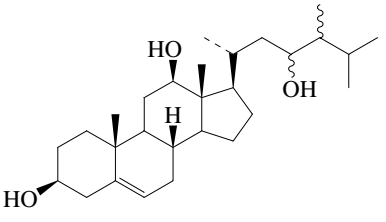
(1α,3β,11α,24*R*)-*form*

Campest-5-ene-1,3,11-triol
[95513-61-4]
Constit. of *Sinularia dissecta* and *Lobophytum catalai*.

*22,23-Didehydro(*E-*):* ***Ergosta-5,22-dien-1,3,11-triol***. *24-Methylcholesta-5,22-dien-1,3,11-triol*
[95513-62-5]
$C_{28}H_{46}O_3$ 430.67
Constit. of *Sinularia dissecta*.
Jagodzinska, B.M. *et al., J.O.C.*, 1985, **50**, 1435-1439 (*isol, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 267-274 (*isol*)

Ergost-5-ene-3,12,23-triol E-766

24-Methylcholest-5-ene-3,12,23-triol



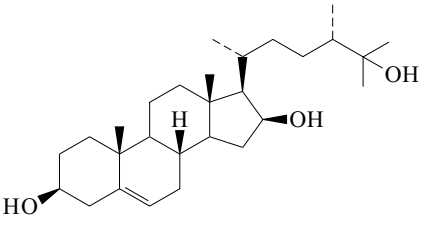
$C_{28}H_{48}O_3$ 432.685

(3β,12β,23ξ,24ξ)-*form*

12-Ac: [495380-46-6]
$C_{30}H_{50}O_4$ 474.723
Constit. of *Capnella lacertiliensis*. Oil. $[\alpha]_D^{22}$ -50 (c, 0.01 in $CHCl_3$).
Wright, A.D. *et al., J. Nat. Prod.*, 2002, **66**, 157-160 (*isol, pmr, cmr*)

Ergost-5-ene-3,16,25-triol E-767

24-Methylcholest-5-ene-3,16,25-triol



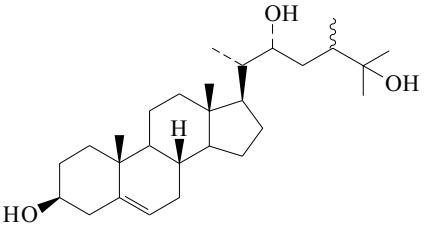
$C_{28}H_{48}O_3$ 432.685

(3β,16β,24*S*)-*form*

3-O-α-L-*Fucopyranoside:* [155850-89-8]
$C_{34}H_{58}O_7$ 578.828
Constit. of *Sinularia gibberosa*. Cryst.
Mp 250-255°. $[\alpha]_D$ -48 (c, 0.56 in Py). Incorrectly named in ref.
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1994, 140 (*isol, pmr, cmr*)

Ergost-5-ene-3,22,25-triol E-768

24-Methylcholest-5-ene-3,22,25-triol

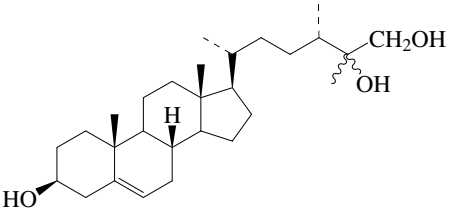


$C_{28}H_{48}O_3$ 432.685

(3β,22*R*,24ξ)-*form* [144466-07-9]
Constit. of a *Lobophytum* sp.
Cryst.
Mp 232-233°. $[\alpha]_D^{25}$ -15 (c, 0.8 in $CHCl_3$).
Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1992, **31**, 708 (*isol, pmr, cmr*)

Ergost-5-ene-3,25,26-triol E-769

24-Methylcholest-5-ene-3,25,26-triol



$C_{28}H_{48}O_3$ 432.685

(3β,24*S*,25ξ)-*form* [129409-60-5]
Isol. from soft corals *Sclerophytum* spp.
Cryst. (MeOH).
Mp 230-234°. $[\alpha]_D^{24}$ 0 (c, 0.03 in MeOH).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1724-1726 (*isol, pmr, struct*)

Ergost-7-ene-3,5,6-triol, 9CI E-770

24-Methylcholest-7-ene-3,5,6-triol
$C_{28}H_{48}O_3$ 432.685

(3β,5α,6β,24*S*)-*form* [53866-39-0]
Constit. of *Patinopecten yessoensis*.
$[\alpha]_D$ -10 (MeOH).

6-Ketone: ***3,5-Dihydroxyergost-7-en-6-one***
[449166-00-1]
$C_{28}H_{46}O_3$ 430.67
Constit. of the edible mushroom *Pleurotus eryngii*. Amorph. solid.
$[\alpha]_D^{30}$ +28.6 (c, 0.04 in MeOH).

(3β,5α,6α,24ξ)-*form*

Isol. from *Hippospongia communis*, *Spongia officinalis*, *Patinopecten yessoensis* and *Ircinia variabilis*.
Iorizzi, M. *et al., J. Nat. Prod.*, 1988, **51**, 1098 (*isol, pmr*)
Madaio, A. *et al., J. Nat. Prod.*, 1989, **52**, 952 (*isol, pmr*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 2002, **50**, 551-553 (*6-ketone*)

Ergost-22-ene-2,3,6-triol E-771

24-Methylcholest-22-ene-2,3,6-triol
$C_{28}H_{48}O_3$ 432.685

(2β,3α,5α,6α,22*E*,24ξ)-*form*

Tri-O-*sulfate:* ***Halistanol sulfate A***
[143049-12-1]
$C_{28}H_{48}O_{12}S_3$ 672.878

Constit. of an *Epipolasis* sp. Thrombin inhibitor. $[\alpha]_D^{21}$ +16.4 (c, 1 in MeOH). Isol. as tri-Na salt.

Kanazawa, S. *et al., Tetrahedron*, 1992, **48**, 5467-5472 (*isol, pmr, cmr*)

Ergost-22-ene-3,5,6-triol E-772

24-Methylcholest-22-ene-3,5,6-triol

$C_{28}H_{48}O_3$ 432.685

(3β,5α,6β,22*E*,24*R*)-*form*

Constit. of *Cliona copiosa*.

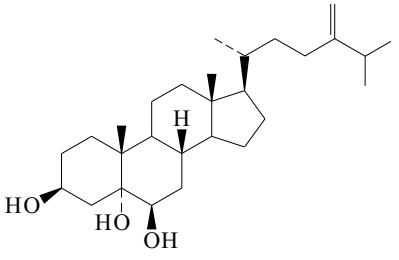
(3β,5α,6α,22*E*,24*S*)-*form*

Constit. of *Cliona copiosa*.

Notaro, G. *et al., J. Nat. Prod.*, 1991, **54**, 1570 (*isol, pmr*)

Ergost-24(28)-ene-3,5,6-triol E-773

24-Methylenecholestane-3,5,6-triol



$C_{28}H_{48}O_3$ 432.685

(3β,5α,6β)-*form* [59048-81-6]

Constit. of *Sinularia dissecta* and *Lobophytum catalai*.

Needles.

Mp 241-242°. $[\alpha]_D$ -4 (c, 0.26 in Py).

3-Ketone: 5,6-Dihydroxyergost-24(28)-en-3-one. 5,6-Dihydroxy-24-methylenecholestan-3-one

[90267-91-7]

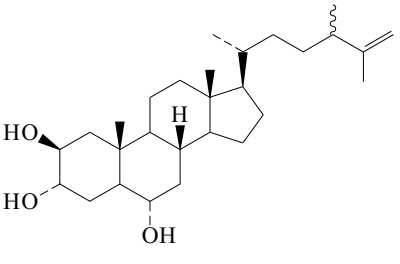
$C_{28}H_{46}O_3$ 430.67

Constit. of *Plexaurella grisea*.

Bartolotto, M. *et al., Bull. Soc. Chim. Belg.*, 1976, **85**, 27 (*isol*)
Pruna, L. *et al., Pharmazie*, 1984, **39**, 117-120 (*3-ketone*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1993, **41**, 87 (*isol, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 267-274 (*isol, pmr*)

Ergost-25-ene-2,3,6-triol E-774

24-Methylcholest-25-ene-2,3,6-triol



$C_{28}H_{48}O_3$ 432.685

(2β,3α,5α,6α,24ξ)-*form*

Tri-O-*sulfate:* ***Halistanol sulfate H***

[154205-20-6]

$C_{28}H_{48}O_{12}S_3$ 672.878

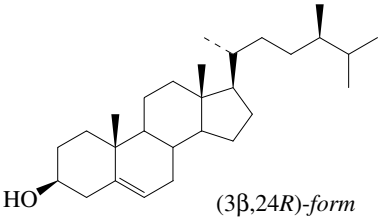
Constit. of sponge *Pseudaxinyssa digitata*.

Bifulco, G. *et al., J. Nat. Prod.*, 1994, **57**, 164-167 (*isol, pmr, cmr*)

Ergost-5-en-3-ol, 9CI E-775

24-Methylcholest-5-en-3-ol

[290299-12-6]



(3β,24*R*)-*form*

$C_{28}H_{48}O$ 400.687

(3β,24*R*)-*form*

Campesterol. *Mieyajunsu A. EB 82A*

[474-62-4]

[4651-51-8, 23929-42-2]

Constit. of rapeseed oil (*Brassica napa*), soybean oil (*Glycine max*) and wheatgerm oil (*Triticum* spp.). Found in virtually all plant oils. Also from *Bugula neritina* and the basidiomycete *Psalliota campestris*. Occurs in many marine organisms such as *Placopecten magellanicus*, *Posidonia oceanica*, *Cymodocea nodosa*, *Axinella cannabina*, *Phakellia aruensis*, *Ophioderma longicaudum* and *Nereis succinea*.

Cryst. (Me_2CO).

Mp 157-158°. $[\alpha]_D^{23}$ -33 ($CHCl_3$).

O-*β-D-Arabinopyranoside:* [475150-21-1]

$C_{33}H_{56}O_5$ 532.802

Constit. of a *Lobophytum* sp.

O-*Sulfate:* [24815-92-7]

$C_{28}H_{48}O_4S$ 480.751

Isol. from *Manduca sexta*, *Ophioderma longicaudum* and *Euretaster insignis*.

(3β,24*S*)-*form*

Dihydrobrassicasterol

[4651-51-8, 23929-42-2]

Occurs in lipids of *Chlorella ellipsoidea* and in *Physalis peruviana* (Cape gooseberry). Present in lipids of a marine unicellular alga. Major sterol of soft coral *Sarcophyton glaucum* and in *Placopecten magellanicus*.

Needles (Me_2CO).

Mp 157-158°. $[\alpha]_D^{24}$ -46.3 (c, 1.2 in $CHCl_3$).

3-O-*Sulfate:* [151890-98-1]

$C_{28}H_{48}O_4S$ 480.751

Constit. of *Eupentacta fraudatrix*.

3-O-*β-D-Xylopyranoside:* [151890-83-4]

$C_{33}H_{56}O_5$ 532.802

Constit. of *Eupentacta fraudatrix*.

(3β,24ξ)-*form* [23929-42-2]

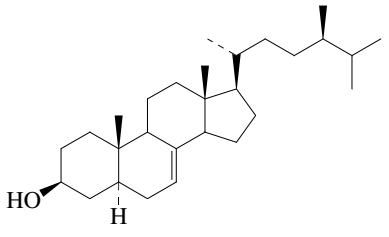
Widespread in terrestrial and marine spp. Constit. of *Holothuria scabra*, *Pseudostichopus trachus*, *Synapta maculata*, *Ahnfeltsia tobuchiensis*, *Macoma balthica*, *Mytilus edulis*, *Cardium glaucum*, *Myra arenaria*, *Gonyaulax polygramma*, *Panax ginseng* and *Panax quinquefolium*.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 567B (*nmr*)
Fernholz, E. *et al., J.A.C.S.*, 1940, **62**, 3346-3348 (*struct*)
Thompson, M.J. *et al., Steroids*, 1965, **5**, 745-752 (*synth*)
Fedeli, E. *et al., J. Am. Oil Chem. Soc.*, 1966, **43**, 254-256 (*occur*)
Tarzia, G. *et al., Gazz. Chim. Ital.*, 1967, **97**, 102-108 (*Campesterol, synth*)
Idler, D.R. *et al., Comp. Biochem. Physiol., A: Comp. Physiol.*, 1971, **38**, 581 (*isol, Placopecten magellicanus constits*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 2053 (*occur*)
Thompson, M.J. *et al., Phytochemistry*, 1972, **11**, 1781-1790 (*pmr*)
Lenton, J.R. *et al., Phytochemistry*, 1975, **14**, 1523-1528 (*biosynth*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195-200 (*cmr*)
Kobayashi, M. *et al., Steroids*, 1979, **34**, 273-284 (*Dihydrobrassicasterol, isol*)
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*Campesterol, Dihydrobrassicasterol, occur*)

Uomori, A. *et al., Chem. Comm.*, 1984, 1176-1177 (*biosynth*)
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*occur, alga*)
Volkman, J.K. *et al., Lipids*, 1984, **19**, 457-465 (*24ξ-form, occur*)
Sica, D. *et al., Phytochemistry*, 1984, **23**, 2609-2611 (*Campesterol, Dihydrobrassicasterol, occur*)
Jarzebski, A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **81**, 989-991 (*24ξ-form, occur*)
Smetania, O.F. *et al., Khim. Prir. Soedin.*, 1985, 576-577; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 545-547 (*Ahnfeltsia tobuchiensis constit*)
Riccio, R. *et al., Tetrahedron*, 1985, **41**, 6041-6046 (*Campesterol, sulfate, occur*)
Matsumoto, T. *et al., J. Am. Oil Chem. Soc.*, 1986, **63**, 544-546 (*24ξ-form, occur*)
Seo, S. *et al., J.C.S. Perkin 1*, 1992, 569-572 (*biosynth*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Zeeck, E. *et al., Steroids*, 1994, **59**, 341-344 (*Campesterol, occur*)
Yamada, J. *et al., Tetrahedron*, 1997, **53**, 877-884 (*biosynth*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*24ξ-form, occur*)
Kerr, R.G. *et al., J. Nat. Prod.*, 1999, **62**, 468-470 (*Bugula neritina constit, isol*)
Nasu, K. *et al., Phytochemistry*, 2000, **54**, 381-385 (*biosynth*)
Kuang, Y.-Y. *et al., Zhongshan Daxue Xuebao Ziran Kexueban*, 2002, **41**, 64-67; *CA*, **137**, 366688q (*arabinoside*)

Ergost-7-en-3-ol E-776

24-Methylcholest-7-en-3-ol
[116179-22-7]



(3β,5α,24*R*)-*form*

$C_{28}H_{48}O$ 400.687

(3β,5α,24*R*)-*form*
Campest-7-en-3-ol
[20304-54-5]
Isol. from seeds of *Nicotiana tabacum* and from *Trichosanthes kirilowii*.

Me ether: 3-Methoxyergost-7-ene
[139974-75-7]
$C_{29}H_{50}O$ 414.713
Constit. of *Jereicopsis graphidiophora*.

Methoxymethyl ether: [172303-91-2]
$C_{30}H_{52}O_2$ 444.74
Constit. of *Scleritoderma* sp. cf. *paccardi*. Cytotoxic agent. Gum. $[\alpha]_D^{24}$ +240 (c, 0.03 in CH_2Cl_2).

3-Ketone: ***Ergost-7-en-3-one***
[20817-92-9]
$C_{28}H_{46}O$ 398.671
Metab. of *Fomes fomentarius.*

(3β,5α,24*S*)-*form*
Fungisterol. *γ-Ergostenol*
[516-78-9]
Isol. from *Axinella cannabina* and other sponges, from *Chlorella ellipsoidea*, *Suillus sibiricus* and from higher fungi. Also from *Penicillium chrysogenum* and the lichen *Parmelia furfuracea*.
Immunopotentiator, anticomplementary agent, immunohaemolysis inhibitor. Cryst. (EtOH).
Mp 152°. $[\alpha]_D$ -0.2 ($CHCl_3$).

3-O-*Sulfate:* [152202-32-9]
$C_{28}H_{48}O_4S$ 480.751
Constit. of *Eupentacta fraudatrix*.

3-O-*β-D-Xylopyranoside:* [74185-07-2]
$C_{33}H_{56}O_5$ 532.802
Constit. of *Eupentacta fraudatrix*.

(3β,5α,24ξ)-*form*
Stellastenol
[41398-70-3]
[17105-75-8 (3β,24ξ-form), 37248-42-3 (3β,5α,20ξ,24ξ-form)]
Constit. of *Asterina pectinifera*, *Asterias amurensis*, *Luidia quinaria*, *Astropecten scoparius*, *Astropecten polycanthus*, *Coscinasterias acutispina*, *Eupentacta fraudatrix*, *Holothuria scabra*, *Patiria pectinifera*, *Cucumaria* sp., *Cucurbita moschata* seed oil, seeds of *Amaranthus* sp., seeds of *Echinochloa frumentacae*, wheat and buckwheat flour and many other spp.

3-O-*Sulfate:* [80677-74-3]
[152202-32-9, 275827-68-4]
Constit. of *Parathyona* sp., *Psolus fabricii* and *Eupentacta fraudatrix*.

[26047-31-4]

Wieland, H. *et al., Annalen*, 1941, **548**, 270-283 (*Fungisterol*)
Fryberg, M. *et al., Biochem. Biophys. Res. Commun.*, 1972, **48**, 593-597 (*biosynth*)
Matsuno, T. *et al., CA*, 1972, **77**, 85903j (*Stellastenol*)
Patterson, G.W. *et al., Phytochemistry*, 1974, **13**, 191-194 (*Fungisterol, isol*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195-200 (*pmr*)
Teshima, S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1979, **64**, 225-228 (*occur*)
Behari, M. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 926-927 (*isol*)
Goodfellow, R.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **76**, 575-578
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol*)
Goad, L.J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **84**, 189-196 (*3β,5α,24ξ-form, sulfate, occur*)
Frega, N. *et al., J. Am. Oil Chem. Soc.*, 1991, **68**, 29-33 (*isol, tobacco*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*Me ether*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Gunasekera, S.P. *et al., J. Nat. Prod.*, 1996, **59**, 161-162 (*methoxymethyl ether*)
Rodriguez, J.B. *et al., Lipids*, 1996, **31**, 1205-1208 (*3β,5α,24ξ-form, occur*)
Roccatagliata, A.J. *et al., CA*, 1997, **127**, 305544 (*isol*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*occur*)
Friebe, A. *et al., Phytochemistry*, 1999, **52**, 1607-1610 (*occur*)
Narumi, Y. *et al., CA*, 2000, **133**, 40555 (*3β,5α,24ξ-form, occur*)
Rösecke, J. *et al., Phytochemistry*, 2000, **54**, 603-610 (*ketone*)
Ponomarenko, L.P. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2001, **128**, 53-62 (*occur*)
Tanaka, T. *et al., J. Oleo Sci.*, 2001, **50**, 201-205 (*3β,5α,24ξ-form, occur*)

Ergost-8-en-3-ol E-777

24-Methylcholest-8-en-3-ol
$C_{28}H_{48}O$ 400.687

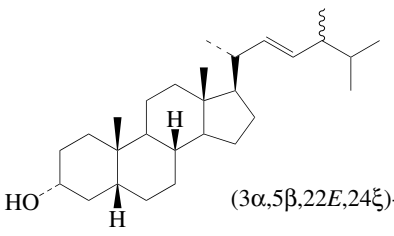
(3β,5α,24*R*)-*form* [5259-28-9]
Constit. of yeast.
Cryst.
Mp 155°. $[\alpha]_D$ +39.

Me ether: ***3-Methoxyergost-8-ene***
[139765-29-0]
$C_{29}H_{50}O$ 414.713
Constit. of *Jereicopsis graphidiophora* and *Microscleroderma spirophora*.

Barton, D.H.R. *et al., J.C.S.*, 1949, 214 (*synth*)
Barton, D.H.R. *et al., J.C.S. Perkin 1*, 1975, 88 (*biosynth*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*Me ether*)
Costantino, V. *et al., Steroids*, 1994, **59**, 181-184 (*Me ether*)

Ergost-22-en-3-ol E-778

24-Methylcholest-22-en-3-ol
[36422-25-0]



(3α,5β,22*E*,24ξ)-*form*

$C_{28}H_{48}O$ 400.687

(3α,5β,22*E*,24ξ)-*form*
Isol. from sponge *Petrosia ficiformis*, prob. as an endobacterial metab.

(3β,5α,22*E*,24*R*)-*form*
Neospongosterol. *22-Dehydrocampestanol*. *Spongesterol*
[59905-70-3]
Occurs in various sponges such as *Euretaster insignis* and *Stichopus japonicus*.
Cryst. (MeOH).
Mp 153°. $[\alpha]_D^{24}$ +10 ($CHCl_3$).

3-O-*β-D-Xylopyranoside:* [74185-04-9]
$C_{33}H_{56}O_5$ 532.802
Constit. of *Eupentacta fraudatrix*.

(3β,5α,22*E*,24*S*)-*form* [5813-65-0]
Constit. of *Petrosia hebes*, *Ascidia nigra*, *Euretaster insignis* and the Black Sea sponge *Haliclona flavescens*.

(3β,5α,22*E*,24ξ)-*form* [59905-70-3]
Constit. of *Echinaster sepositus*, *Chondrilla nucula*, *Jaspis stellifera*, *Pseudostichopus trachus*, *Holothuria nobilis*, *Holothuria scabra*, *Trochostoma orientale*, *Bathyplotes natans* and many other marine organisms.

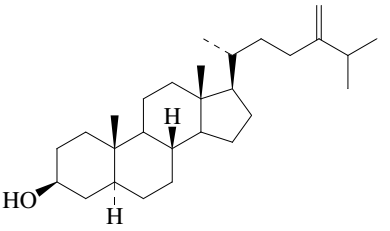
O-*Sulfate:*
$C_{28}H_{48}O_4S$ 480.751
Isol. from the crinoid *Gymnocrinus richeri*.

(3β,5β,22*E*,24ξ)-*form*
Isol. from sponge *Petrosia ficiformis*, prob. as an endobacterial metab.

Bergmann, W. *et al., J.O.C.*, 1945, **10**, 570-579 (*Spongosterol, isol*)
Tori, K. *et al., Chem. Pharm. Bull.*, 1963, **11**, 956-959 (*pmr*)
Eudman, T.R. *et al., Tetrahedron*, 1972, **28**, 5163-5173 (*Neospongosterol, isol, ms*)
De Simone, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **66**, 351-357 (*Echinaster sepositus constit*)
Bohlin, L. *et al., Steroids*, 1980, **35**, 295-304 (*24ξ-form, occur*)
Khalil, M. *et al., Steroids*, 1980, **35**, 707-719 (*24R-form, 24S-form, isol*)
Tam Ha, T.B. *et al., Steroids*, 1982, **40**, 433-453 (*24S-form, isol*)
D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1984, 2277-2282 (*24R-form, 24S-form, isol*)
Seidel, S.B. *et al., Steroids*, 1986, **47**, 49-62 (*3α,5β,22E,24ξ-form, 3β,5β,22E,24ξ-form*)
Cho, J.H. *et al., J.C.S. Perkin 1*, 1987, 1307-1318 (*isol*)
De Riccardis, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **100**, 647-651 (*Gymnocrinus richeri sulfate*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constit*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*24ξ-form, occur*)

Ergost-24(28)-en-3-ol E-779

24-Methylenecholestan-3-ol



(3β,5α)-*form*

$C_{28}H_{48}O$ 400.687

(3β,5α)-*form* [39832-31-0]
Constit. of buckwheat, *Axinella cannabina*, *Holothuria nobilis*, *Holothuria scabra*, *Trochostoma orientale*, *Crassostrea virginica*, *Ascidia nigris*, *Suberites carnosus*, *Ciona intestalis*, *Hymeniacidon perleve* and many other marine organisms.
Cryst. (MeOH).
Mp 110-115°.

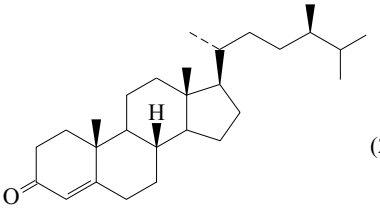
3-O-*Sulfate:* [104048-17-1]
[151891-02-0 (Na salt)]
$C_{28}H_{48}O_4S$ 480.751
Constit. of *Eupentacta fraudatrix* and *Psolus fabricii*.

3-O-*β-D-Xylopyranoside:* [74185-12-9]
$C_{33}H_{56}O_5$ 532.802
Constit. of *Eupentacta fraudatrix*.

(3β,5β)-*form* [84871-09-0]
Constit. of the tunicate *Ascidia nigra*.

Erdman, T.R. *et al., Tetrahedron*, 1972, **28**, 5163-5173 (*isol*)
Sucrow, W. *et al., Chem. Ber.*, 1976, **109**, 2884-2889 (*synth*)
Gupta, K.C. *et al., J. Nat. Prod.*, 1979, **42**, 307-308 (*isol*)
Sica, D. *et al., Gazz. Chim. Ital.*, 1980, **110**, 147-150 (*isol*)
Teshima, S. *et al., Lipids*, 1980, **15**, 1004-1011 (*sulfate, occur*)
Tam Ha, T.B. *et al., Steroids*, 1982, **40**, 433-453 (*Ascidia nigra constit, isol*)
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol*)
Goad, L.J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **84**, 189-196 (*sulfate, occur*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*occur*)
Tanaka, T. *et al., CA*, 2001, **134**, 323474 (*occur*)

Ergost-4-en-3-one E-780



(24*R*)–*form*

$C_{28}H_{46}O$ 398.671

(24*R*)-*form*
4-Campesten-3-one
[22260-46-4]
Isol. from *Cannabis sativa*, *Catharanthus pusillus*, *Melia azedarach*, *Metasequoia glyptostroboides*, *Phoenix dactylifera* (date) and *Pinus monticola*.
Cryst. (Et_2O/EtOH).
Mp 86-87°. $[\alpha]_D^{25}$ +77.5 ($CHCl_3$).

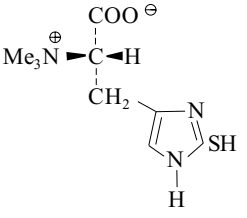
(24*S*)-*form* [51014-22-3]
Isol. from *Glycine max* (soybean) and *Stephania cepharantha* and from the dinoflagellate *Pyrocystis lunula*.

[61949-21-1]

Hayashi, S. *et al., Chem. Pharm. Bull.*, 1969, **17**, 163 (*isol*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1973, **21**, 3186 (*isol*)
Slatkin, D.J. *et al., Phytochemistry*, 1975, **14**, 580 (*isol*)
Smith, A.G. *et al., Biomed. Mass Spectrom.*, 1976, **3**, 81 (*synth, ms*)
Weber, N. *et al., Phytochemistry*, 1977, **16**, 1849 (*isol*)
Schulte, K.E. *et al., Planta Med.*, 1979, **35**, 76 (*isol*)
Subramanian, P.S. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 331 (*isol*)
Conner, A.H. *et al., Phytochemistry*, 1980, **19**, 1121 (*isol*)
Kokke, W.C.M.C. *et al., Steroids*, 1982, **40**, 307 (*isol*)
Fernandez, M.I. *et al., Phytochemistry*, 1983, **22**, 2087 (*isol*)

Ergothioneine E-781

α-Carboxy-2,3-dihydro-N,N,N-*trimethyl-2-thioxo-1*H-*imidazole-4-ethanaminium hydroxide inner salt, 9CI. 2-Mercaptohistidine trimethylbetaine. Thiolhistidine trimethylbetaine. Thioneine. Thiasine. Sympectothione*
[497-30-3]



$C_9H_{15}N_3O_2S$ 229.302
Present in blood, semen and various mammalian tissues, principally liver and kidneys. Also prod. by a variety of plants and microbes. Cryst. + $2H_2O$.
Mp 290° dec. $[\alpha]_D^{20}$ +116.5 (H_2O).

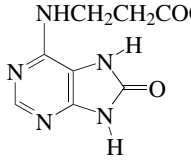
S-*(2-Amino-2-carboxyethyl),* S-*oxide:* [53252-98-5]
$C_{12}H_{20}N_4O_5S$ 332.38
Isol. from the fungi *Clitocybe acromelalga* and *Neurospora crassa*. Amorph. hygroscopic powder.
Mp 188-190° dec. $[\alpha]_D^{24}$ +74.7 (c, 0.5 in H_2O).

S-*(2-Hydroxyethyl):* ***Sclerothionine***
[19833-41-1]
$C_{11}H_{19}N_3O_3S$ 273.355
Isol. from *Sclerotinia libertiana*. Rhombic prisms (EtOH/Me_2CO).
Mp 218-223° dec. $[\alpha]_D^{24}$ +7.4 (c, 2 in H_2O).

Heath, H. *et al., J.C.S.*, 1951, 2215 (*synth*)
Genghof, D.S. *et al., J. Bacteriol.*, 1964, **87**, 852 (*biosynth*)
Crossland, J. *et al., Nature (London)*, 1964, **203**, 1388
Matsuo, M. *et al., Agric. Biol. Chem.*, 1967, **31**, 353; 1968, **32**, 605; 611 (*Sclerothionine*)
Ishikawa, Y. *et al., J. Biol. Chem.*, 1974, **249**, 4420 (*deriv*)
Sugihara, A. *et al., Acta Cryst. B*, 1976, **32**, 181 (*cryst struct*)
Motohashi, N. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1737 (*nmr*)
Nicholson, J.R. *et al., Biochem. J.*, 1983, **211**, 605 (*pmr*)

Erinacean E-782

N-*(7,8-Dihydro-8-oxo*-H-*purin-6-yl)-β-alanine, 9CI.* N^6-*β-Alanyl-8-oxoadenine*
[161212-38-0]

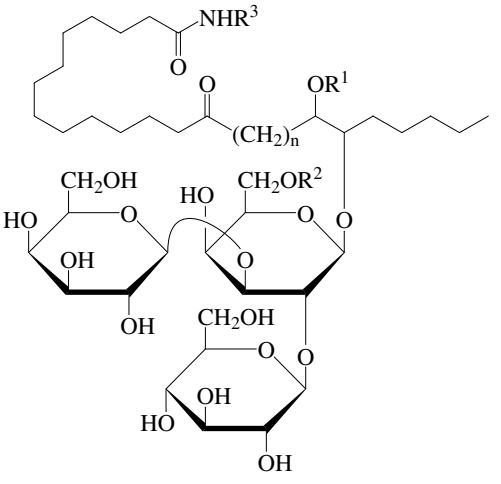


$C_8H_9N_5O_3$ 223.191
Isol. from the sponge *Isodictya erinacea*. Amorph. powder.
λ_{max} 272 (ϵ 8444) (MeOH).

Moon, B. *et al., J. Nat. Prod.*, 1998, **61**, 116-118 (*isol*)

Erylusamine TA E-783

[178063-82-6]

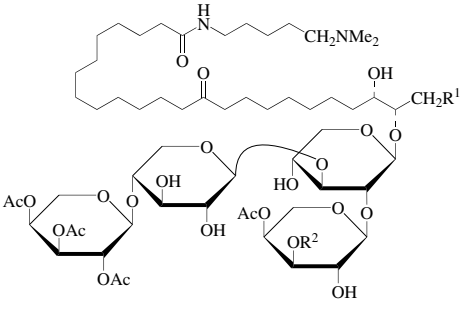


R^1 = H, R^2 = Ac, R^3 = -$(CH_2)_5NMe_2$, n = 6

$C_{54}H_{100}N_2O_{20}$ 1097.385
Glycolipid. Isol. from the marine sponge *Erylus* cf. *lendenfeldi* (tentative identification). Oil. $[\alpha]_D^{25}$ +2.8 (c, 2.9 in MeOH).

Goobes, R. *et al., Tetrahedron*, 1996, **52**, 7921-7928 (*isol, ir, pmr, cmr*)

Erylusamines A-E E-784



Absolute Configuration

Erylusamine A R^1 = -CH_2CH_3, R^2 = H
B R^1 = -$CH(CH_3)_2$, R^2 = H
C R^1 = -$CH(CH_3)_2$, R^2 = Ac
D R^1 = -$CH_2CH_2CH_3$, R^2 = Ac
E R^1 = -$CH_2CH_2CH_2CH_3$, R^2 = Ac

Glycolipid complex. Isol. from the marine sponge *Erylus placenta*. Interleukin-6 receptor antagonists.

Erylusamine A [155029-28-0]
$C_{61}H_{106}N_2O_{24}$ 1251.507
Oil. $[\alpha]_D^{20}$ -3.5 (c, 0.1 in MeOH).

Erylusamine B [150150-46-2]
$C_{62}H_{108}N_2O_{24}$ 1265.534
Cytokinin. Gum. $[\alpha]_D^{20}$ -5.5 (c, 0.2 in MeOH).

Erylusamine C [155029-29-1]
$C_{64}H_{110}N_2O_{25}$ 1307.571
Oil. $[\alpha]_D^{20}$ -9.6 (c, 0.3 in MeOH).

Erylusamine D [155029-30-4]
$C_{64}H_{110}N_2O_{25}$ 1307.571
Oil. $[\alpha]_D^{20}$ -6 (c, 0.1 in MeOH).

Erylusamine E [155029-31-5]

$C_{65}H_{112}N_2O_{25}$ 1321.598

Oil. $[\alpha]_D^{20}$ -8 (c, 0.2 in MeOH).

Fusetani, N. *et al., Tet. Lett.*, 1993, **34**, 4067-4070 (*isol, ir, pmr, cmr, ms*)
Sata, N. *et al., Tetrahedron*, 1994, **50**, 1105-1110 (*isol, ir, pmr, cmr, ms*)

Erylusidine E-785

[178063-84-8]

As Erylusamine TA, E-783 with

R^1 = -$COCH_2CH(CH_3)_2$, R^2 = H, R^3 = -$(CH_2)_4NHC(NH_2)$=NH, n = 7

$C_{56}H_{104}N_4O_{20}$ 1153.452

Isol. from the marine sponge *Erylus* cf. *lendenfeldi* (tentative identification). Oil. $[\alpha]_D^{25}$ -4.1 (c, 4.7 in MeOH).

Goobes, R. *et al., Tetrahedron*, 1996, **52**, 7921-7928 (*isol, ir, pmr, cmr*)

Erylusine E-786

[178063-83-7]

As Erylusamine TA, E-783 with

R^1 = H, R^2 = Ac, R^3 = -$(CH_2)_3N(Me)(CH_2)_4NMe_2$, n = 6

$C_{57}H_{107}N_3O_{20}$ 1154.48

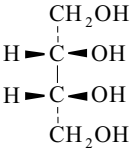
Glycolipid. Isol. from the marine sponge *Erylus* cf. *lendenfeldi* (tentative identification). Oil. $[\alpha]_D^{25}$ +1.9 (c, 4.3 in MeOH).

Goobes, R. *et al., Tetrahedron*, 1996, **52**, 7921-7928 (*isol, ir, pmr, cmr*)

Erythritol, 9CI, 8CI E-787

(R,S)-1,2,3,4-Butanetetrol, 9CI, 8CI. Mesoerythritol. Phycitol. Erythroglucin

[149-32-6]



$C_4H_{10}O_4$ 122.121

Opt. inactive (*meso*-): some derivs. may be chiral (see for example 5-Hydroxy-2-phenyl-1,3-dioxane-4-methanol). Found in a variety of algae, lichens and fungi. Prod. by *Protococcus vulgaris*, *Trentepohlia iolithus* and *Aspergillus terreus*. Bulk sweetener with good taste props. Also thickener, stabiliser, humectant, etc. in food. Shows vasodilatory props. Cryst. (MeOH).

Mp 121.5°. Bp 329-331° Bp_{200} 294-296°. Sweetness ca. 0.7 × sucrose.

▶KF2000000

Tetrakis(4-hydroxybenzoyl): ***Kelletinin I***

[87697-99-2]

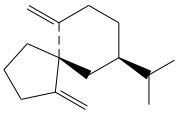
$C_{32}H_{26}O_{12}$ 602.55

Metab. of the marine molluscs *Kelletia kelletii* and *Buccinulum corneum*. Antibacterial, cytotoxic. Inhibitor of DNA polymerase and reverse transcriptase. Sol. MeOH, bases, Et_2O; poorly sol. H_2O. λ_{max} 258 (ϵ 63100) (EtOH/HCl) (Derep). λ_{max} 301 (ϵ 100000) (EtOH/NaOH) (Derep). λ_{max} 258 (ϵ 50100) (EtOH) (Derep).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 184C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 287A (*nmr*)
Trenner, N.R. *et al., J.A.C.S.*, 1949, **71**, 2352 (*synth*)
Jeanes, A. *et al., J.O.C.*, 1955, **20**, 1565 (*synth*)
Sonogashira, K. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 2616 (*synth, ir*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 144 (*occur*)
Ceccarelli, C. *et al., Acta Cryst. B*, 1980, **36**, 3079 (*cryst struct*)
Angyal, S.J. *et al., Carbohydr. Res.*, 1980, **84**, 201 (*cmr*)
Tymiak, A.A. *et al., J.A.C.S.*, 1983, **105**, 7396-7401 (*Kelletinin*)
Hawkes, G.E. *et al., J.C.S. Perkin 2*, 1984, 2073 (*pmr, conformn*)
Ciminiello, P. *et al., Gazz. Chim. Ital.*, 1988, **118**, 105 (*Kelletinin I*)
Orlando, P. *et al., Experientia*, 1991, **47**, 64 (*Kelletinin I*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1020
Rozenberg, M. *et al., Carbohydr. Res.*, 1999, **315**, 85-97 (*ir, Raman*)

Erythrodiene E-788

[138613-24-8]



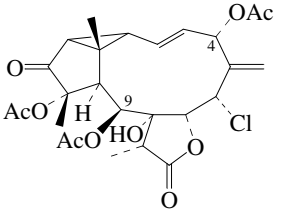
$C_{15}H_{24}$ 204.355

Constit. of *Erythropodium caribaeorum*. Oil. $[\alpha]_D$ -30.8 (c, 0.24 in $CHCl_3$).

Pathirana, C. *et al., Tet. Lett.*, 1993, **34**, 3371-3372 (*isol, pmr, cmr, cryst struct*)
Tokunaga, Y. *et al., J.C.S. Perkin 1*, 1997, 189-190 (*(±)-form, synth*)
Srikrishna, A. *et al., Tetrahedron*, 1997, **53**, 1439 (*synth*)
Oppolzer, W. *et al., Tet. Lett.*, 1998, **39**, 5019-5022 (*synth*)
Sattelkau, T. *et al., Tet. Lett.*, 1998, **39**, 9647-9648 (*synth*)
Oppolzer, W. *et al., Helv. Chim. Acta*, 2001, **84**, 416-430 (*synth*)
Deng, K. *et al., Org. Lett.*, 2005, **7**, 3637-3640 (*synth*)
Lachia, M. *et al., Org. Lett.*, 2005, **7**, 4103-4106 (*synth*)

Erythrolide A E-789

[89999-14-4]



$C_{26}H_{31}ClO_{10}$ 538.978

Constit. of *Erythropodium caribaeorum*. Antifeedant. Powder. λ_{max} 231 (ϵ 9000) (MeOH) (Derep).

O^4*-De-Ac:* ***Erythrolide V***

[91933-57-2]

$C_{24}H_{29}ClO_9$ 496.94

Constit. of *Erythropodium caribaorum*. Amorph. solid. $[\alpha]_D^{25}$ -38. λ_{max} 215 (ϵ 8500) (MeOH).

O^9*-De-Ac, 9-(acetoxyacetyl):* ***Erythrolide L***

[410096-42-3]

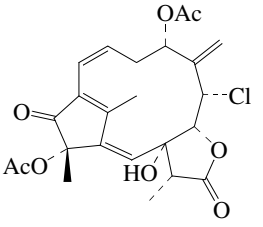
$C_{28}H_{33}ClO_{12}$ 597.014

Constit. of *Erythropodium caribaeorum*. Gum. $[\alpha]_D^{25}$ -62.9 (c, 0.35 in $CHCl_3$). λ_{max} 216 (log ϵ 3.94) (MeOH).

Look, S.A. *et al., J.A.C.S.*, 1984, **106**, 5026 (*isol, cryst struct*)
Pordesimo, E.O. *et al., J.O.C.*, 1991, **56**, 2344 (*isol, pmr*)
Dookran, R. *et al., J. Nat. Prod.*, 1993, **56**, 1051 (*pmr, cmr*)
Banjoo, D. *et al., J. Nat. Prod.*, 2002, **65**, 314-318 (*Erythrolide L*)
Taglialatela-Scafati, O. *et al., Eur. J. Org. Chem.*, 2003, 3515-3523 (*Erythrolide V*)

Erythrolide K E-790

[205191-85-1]

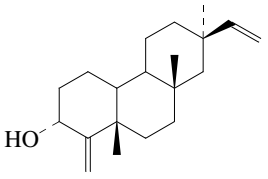


$C_{24}H_{27}ClO_8$ 478.925

Constit. of *Erythropodium caribaeorum*. Cryst.
Mp 220°. $[\alpha]_D^{25}$ -50 (c, 0.4 in $CHCl_3$). λ_{max} 208 (log ϵ 3.93) (MeOH).

Banjoo, D. *et al., Tet. Lett.*, 1998, **39**, 1469-1472 (*isol, pmr, cmr, cryst struct, synth*)
Banjoo, D. *et al., J. Nat. Prod.*, 2002, **65**, 314-318 (*isol*)

4(18),15-Erythroxyladien-3-ol E-791



3α-*form*

$C_{20}H_{32}O$ 288.472

3α-form
Givotin B
[717917-45-8]
Constit. of *Givotia madagascariensis*.
Oil.

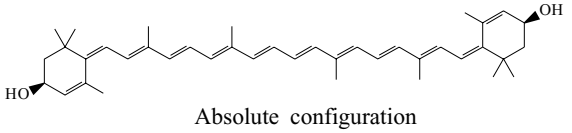
(ent-3α,4α)-*form*
3-Ketone: 4(18),15-Erythroxyladien-3-one. 4(18),15-Dolabradien-3-one. ***Tagalsin E***
[862588-83-8]
$C_{20}H_{30}O$ 286.456
Constit. of the mangrove *Ceriops tagal*. Yellow solid.
Mp 73-75°. $[\alpha]_D^{25}$ +7.85 (c, 0.07 in $CHCl_3$).

4β,18-Epoxide: 4,18-Epoxy-15-erythroxylen-3-ol. 4,18-Epoxy-15-dolabren-3-ol. ***Tagalsin D***
[862588-82-7]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Ceriops tagal*. Solid.
Mp 64-66°. $[\alpha]_D^{25}$ +38.4 (c, 0.074 in $CHCl_3$).

Krebs, H.C. *et al., Z. Naturforsch., B*, 2004, **59**, 58-62 (*Givotin B*)
Zhang, Y. *et al., Phytochemistry*, 2005, **66**, 1465-1471 (*Tagalsins D and E*)

Eschscholtzxanthin E-792

Retrodehydrozeaxanthin. Eschscholtziaxanthin
[472-75-3]



Absolute configuration

$C_{40}H_{54}O_2$ 566.865
Constit. of *Eschscholtzia californica*. Red cryst. (Me_2CO).
Mp 185-186°.

Monoketone: ***Eschscholtzxanthone***
[3484-59-1]
$C_{40}H_{52}O_2$ 564.85
Isol. from *Taxus baccata* and *Eschscholtzia californica*. Cryst. (C_6H_6/MeOH).
Mp 150-153°.

Diketone: ***Rhodoxanthin***. *Thujorhodin*
[116-30-3]
$C_{40}H_{50}O_2$ 562.834
Isol. from green alga *Chlorella* and the fish *Tilapia* spp. Found in higher plants, e.g. *Taxus baccata, Agathis australis, Potamogeton* spp. Blue-black cryst. (C_6H_6/MeOH).
Mp 219°.

Bodea, C. *et al., Annalen*, 1963, **666**, 189 (*ir*)
Bodea, C. *et al., Rev. Roum. Chim.*, 1964, **9**, 517; 839 (*Eschscholtzxanthone*)
Iwata, I. *et al., Agric. Biol. Chem.*, 1966, **25**, 377 (*isol*)
Williams, R.J.H. *et al., Biochim. Biophys. Acta*, 1966, **124**, 200 (*biosynth*)
Nicoara, E. *et al., Annalen*, 1966, **697**, 201
Mayer, H. *et al., Helv. Chim. Acta*, 1967, **50**, 1606 (*synth*)
Joesen, H. *et al., Acta Chem. Scand.*, 1972, **26**, 2185 (*pmr*)
Andrewes, A.G. *et al., Phytochemistry*, 1979, **18**, 303 (*abs config*)
Widmer, E. *et al., Helv. Chim. Acta*, 1982, **65**, 944; 958 (*synth*)

1,2-Ethanediol, 9CI E-793

Ethylene glycol, 8CI. Fridex. Glycol. Norkool. Zorex
[107-21-1]
$HOCH_2CH_2OH$
$C_2H_6O_2$ 62.068
Present in bound form (15%) in the lipids of the starfish *Distolasterias nipon*. Important component of antifreeze and hydraulic brake fluids. Used as solvent, stabiliser and softening agent. Also used in manuf. of explosives, waxes, fibres etc. Monomer and comonomer used in the manuf. of alkyd resins, polyurethanes, polyesters, esp. poly(ethylene terephthalate), and many other polymeric systems. Used in resin curing processes. Dissolves NaOH and KOH. Reagent for ethylene ketal prep. Important industrial chemical, 30th in order of volume for USA in 1994 (production 2.77 million tons/year). Colourless, viscous liq. with sweet taste. Misc. H_2O, EtOH, MeOH, Me_2CO, AcOH, Py. Immisc. $CHCl_3$, CCl_4, Et_2O, C_6H_6, CS_2, petrol. d_4^{20} 1.11. Mp -15.6°. Bp 197° Bp_3 70°. n_D^{20} 1.9310. pK_a 15.4 (25°).
▶ Fl. p. 111°, autoignition temp. 398°. Human systemic effects by ingestion and inhalation. Affects CNS and kidney function. Skin, eye and mucous membrane irritant. LD_{50} (rat, orl) 4700 mg/kg. Exp. reprod. and teratogenic effects (large doses). OES: long-term 10 mg m^{-3} (particulate); long-term 60 mg m^{-3}; short-term 125 mg m^{-3} (vapour). KW2975000

O-*(1Z,9Z-Octadecadienyl),* O′*-octadecanoyl: 1-(1,9-Octadecadienyloxy)-2-stearoyloxyethane*
[32453-42-2]
$C_{38}H_{72}O_3$ 576.985
Major component of starfish *Distolasterias nipon* lipids.

Vaver, V.A. *et al., Khim. Prir. Soedin.*, 1970, **6**, 657-664; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 673-678 (*Distolasterias nipon constit*)

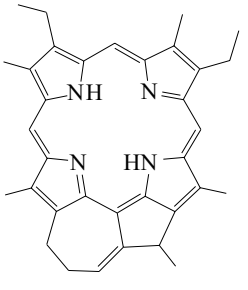
S,S′-Ethanediylcarbonodithioic acid E-794

S,S-*Dithiodimethylenethioacetic acid*
$HOC(S)SCH_2CH_2SC(S)OH \Leftrightarrow HSC(O)SCH_2CH_2SC(O)SH$
$C_4H_6O_2S_4$ 214.354

O,O-*Bis(2-methylpropyl) ester:* S,S′*-1,2-Ethanediyl* O,O-*bis(2-methylpropyl)carbonodithioate, 9CI. Ethylene bis(isobutylxanthate). Ethylene diisobutylxanthate*
[1787-00-4]
$C_{12}H_{22}O_2S_4$ 326.569
Isol. from the green alga *Dictyosphaeria favulosa*. Cryst.
Mp 47° (40-42°). Compds. of this type have been patented as oil additives and its occurrence as a natural product is therefore questionable (possible contaminant).

Khalikov, R.K. *et al., CA*, 1964, **61**, 1675e (*synth*)
Venkateswarlu, Y. *et al., Tet. Lett.*, 1993, **34**, 3633 (*isol, cryst struct*)

13,15-Ethano-3,8-diethyl-2,7,12,18,13[1]-pentamethyl-13[2],17-prop-13[2](17[3])-enoporphyrin E-795



$C_{34}H_{36}N_4$ 500.685
Isol. from marine Serpiano oil shale as Vanadium complex.

Chicarelli, M.I. *et al., Tet. Lett.*, 1986, **27**, 4653 (*isol, pmr, uv*)

1-Ethoxy-1-hydroperoxyethane E-796

(1-Ethoxyethyl) hydroperoxide. ***Mozukutoxin A***

[18321-53-4]

$H_3CCH(OEt)OOH$

$C_4H_{10}O_3$ 106.121

Isol. from various ascidians incl. *Cladosiphon okamuranus*, *Halocynthia roretzi* and *Styela plicata*. Oil. Given incorrect struct. in earliest ref. Possible artifact.

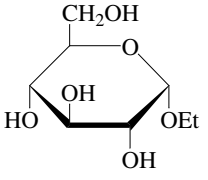
▶ Highly toxic. LD_{50} 250 mg/Kg (mice). Explosive.

[138343-26-7]

Nakamura, A. *et al., Tet. Lett.*, 1991, **32**, 4355-4358 (*isol*)
Anthoni, U. *et al., Tet. Lett.*, 1991, **32**, 7303-7304 (*struct*)

Ethyl glucoside, 8CI E-797

[27214-60-4]



α–D-Pyranose-*form*

$C_8H_{16}O_6$ 208.211

α-D-Pyranose-*form* [19467-01-7]

Isol. from the marine mollusc *Cryptochiton stelleri*.
Mp 114°. $[\alpha]_D^{26}$ +152 (H_2O).

Kapustina, I.I. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 109-110 (*Cryptochiton stelleri constit*)

Ethylamine, 8CI E-798

Ethanamine, 9CI

[75-04-7]

$H_3CCH_2NH_2$

C_2H_7N 45.084

Manuf. by catalytic amination of ethanol with ammonia. Prod. by marine algae, *Clostridium* spp., *Candida albicans, Brevibacterium linens* and *Streptococcus lactis*. Used in manuf. of resins, rubber, herbicides, etc. Flammable gas with ammoniacal odour. Misc. EtOH, Et_2O, H_2O, salted out by NaOH.
Fp -80. Bp 16.6°. pK_a 10.7.

▶ Extremely flammable, fl. p. 50 (rat, orl) 400 mg/kg. LD_{50} (rbt, skn) 390 mg/kg. OES: long-term 10 ppm. KH2100000

Hydrochloride: [557-66-4]
Cryst. (EtOH aq.). Sol. H_2O, EtOH; sl. sol. $CHCl_3$, Me_2CO; prac. insol. Et_2O.

▶ KR7600000

Hydrobromide: [593-55-5]
Needles or plates (EtOH). Mp 159.5°.

Hydroiodide: [506-58-1]
Hygroscopic needles (H_2O). Sol. H_2O, EtOH, spar. sol. Et_2O, $CHCl_3$. Mp 188.5°.

N-*Ac:* See *N*-Ethylacetamide in *The Combined Chemical Dictionary.*

N-*Methanesulfonyl:* See Methanesulfonic acid in *The Combined Chemical Dictionary.*

N-*(4-Methylbenzenesulfonyl):* See 4-Methylbenzenesulfonamide in *The Combined Chemical Dictionary.*

N,N-*Bis(4-methylbenzenesulfonylmethyl):* [4542-70-5]
$C_{18}H_{23}NO_4S_2$ 381.516
Cryst. Mp 114-115°.

[16999-99-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 279D; 364D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 449B; 449C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 364B (*ir*)
Helferich, B. *et al., Ber.*, 1940, **73**, 1131 (*methanesulfonyl*)
Watt, G.W. *et al., J.A.C.S.*, 1947, **69**, 836 (*synth*)
Bredereck, H. *et al., Chem. Ber.*, 1954, **87**, 129 (*ditosyl*)
Lerch, B. *et al., Z. Naturforsch., B*, 1966, **21**, 216 (*occur*)
Laughlin, R.G. *et al., J.A.C.S.*, 1967, **89**, 4268 (*methanesulfonyl*)
Steiner, M. *et al., Planta*, 1968, **79**, 113 (*isol*)
Ger. Pat., 1969, 1 929 295; *CA*, **72**, 66412 (*methanesulfonyl*)
Gallant, R.W. *et al., Hydrocarbon Process.*, 1969, **48**, 143 (*rev, bibl, props*)
Neurath, G.B. *et al., Food Cosmet. Toxicol.*, 1979, **15**, 275 (*isol*)
Wagner, W. *et al., Int. J. Mass Spectrom. Ion Phys.*, 1980, **36**, 125 (*ms*)
Faure, R. *et al., Org. Magn. Reson.*, 1980, **14**, 20 (*cmr*)
Altona, C. *et al., Magn. Reson. Chem.*, 1989, **27**, 564 (*pmr*)
Wolff, H. *et al., Spectrochim. Acta A*, 1991, **47**, 165 (*conformn, ir*)
, 1990, 95
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 585
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EFU400; EFW000

2-Ethylbutanal, 9CI E-799

2-Ethylbutyraldehyde, 8CI. Diethylacetaldehyde. FEMA 2426

[97-96-1]

$(H_3CCH_2)_2CHCHO$

$C_6H_{12}O$ 100.16

Occurs in melon, maize, scallops and other biol. sources. Liq. d^{20} 0.81.
Mp -89°. Bp 117-119°.

▶ Highly flammable, fl. p. 21°. Skin irritant. LD_{50} (rat, orl) 3980 mg/kg. ES2625000

2,4-Dinitrophenylhydrazone: [14086-21-6]
Orange plates (petrol). Mp 94.5-95° (129-130°, 137°).

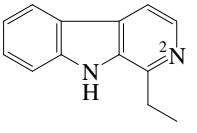
Semicarbazone: [33861-38-0]
Prisms (C_6H_6/petrol). Mp 97.5-99.5°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 466D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 728C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 552C (*ir*)
Brunner, H. *et al., J.C.S.*, 1937, 1039 (*synth, derivs*)
Wiechert, K. *et al., Z. Chem.*, 1967, **7**, 229 (*synth*)
Pallaud, R. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1971, **273**, 418 (*synth*)
Sultanov, N.T. *et al., CA*, 1972, **77**, 4817 (*synth*)
Mueller, E. *et al., Chem. Ber.*, 1975, **108**, 1475 (*derivs*)
Cornils, B. *et al., Chem.-Ztg.*, 1977, **101**, 107 (*rev, bibl*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 221
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 955-956
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DHI000

1-Ethyl-β-carboline E-800

*1-Ethyl-9*H*-pyrido[3,4-*b*]indole, 9CI*

[20127-61-1]



$C_{13}H_{12}N_2$ 196.251

Alkaloid from the roots of *Hannoa klaineana* (Simaroubaceae) and the bryozoan *Cribricellina cribraria*. Also from *Costaticella hastata*. Whitish-yellow needles (MeOH/$CHCl_3$).
Mp 202-203° (synthetic) (194-195°).

2-N-*Oxide:* ***1-Ethyl-β-carboline-2*N*-oxide***

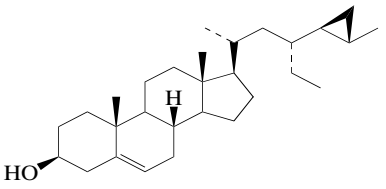
[90686-26-3]

$C_{13}H_{12}N_2O$ 212.251

Alkaloid from the roots of *Hannoa klaineana* (Simaroubaceae). Whitish-yellow needles (MeOH/$CHCl_3$).

Lumonadio, L. *et al., Phytochemistry*, 1984, **23**, 453-455 (*isol, uv, ir, pmr, ms, struct*)
Blackman, A.J. *et al., J. Nat. Prod.*, 1987, **50**, 494-496 (*isol, Costaticella*)
Rocca, P. *et al., Tetrahedron*, 1993, **49**, 3325-3342 (*synth, cmr*)
Ivanov, I. *et al., Heterocycles*, 2005, **65**, 2483-2492 (*synth, pmr*)

23-Ethyl-24,26-cyclocholest-5-en-3-ol E-801

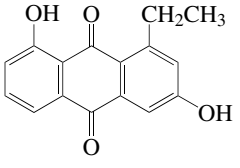


$C_{29}H_{48}O$ 412.698

(3β,23*R*,24*S*,25*R*)-*form* [114247-95-9]
Cryst. (MeCN). Mp 135-136°. $[\alpha]_D^{20}$ -40.5.

(3β,23*R*,24*S*,25*S*)-*form*
Hebesterol
[114174-00-4]
Isol. from *Petrosia hebes*.
Cryst. (MeCN).
Mp 133-134°. $[\alpha]_D^{20}$ -2.1 ($CHCl_3$).
Cho, J.-H. *et al., J.C.S. Perkin 1*, 1987, 1307-1318 (*isol, pmr, ms*)

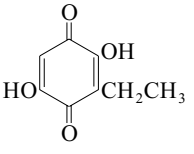
1-Ethyl-3,8-dihydroxyanthraquinone E-802
1-Ethyl-3,8-dihydroxy-9,10-anthracenedione



$C_{16}H_{12}O_4$ 268.268

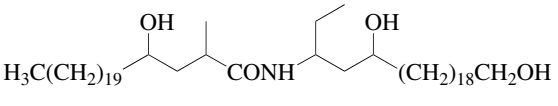
3-O-*(2,6-Dideoxy-β-D*-arabino-*hexopyranoside)*: ***Halawanone D***
[213547-28-5]
$C_{22}H_{22}O_7$ 398.412
Prod. by a marine-derived *Streptomyces* sp.
Ford, P.W. *et al., J. Nat. Prod.*, 1998, **61**, 1232-1236 (*isol*)

3-Ethyl-2,5-dihydroxy-1,4-benzoquinone E-803
3-Ethyl-2,5-dihydroxy-2,5-cyclohexadiene-1,4-dione
[13379-21-0]



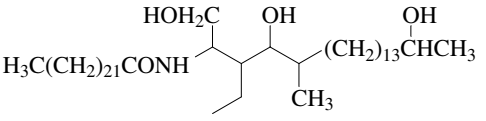
$C_8H_8O_4$ 168.149
Isol. from spines of *Echinothrix diadema*. Orange prisms (C_6H_6).
Mp 130-145° subl.
Moore, R.E. *et al., J.O.C.*, 1966, **31**, 3645 (*isol, uv, ir, pmr, synth*)
Dallacker, F. *et al., Chem. Ber.*, 1972, **105**, 614 (*synth*)

***N*-(1-Ethyl-3,22-dihydroxydocosyl)-4-hydroxy-2-methyltetracosanamide, 9CI** E-804
[150677-70-6]



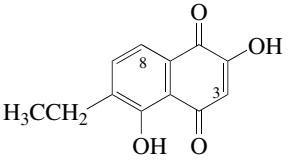
$C_{49}H_{99}NO_4$ 766.325
Sphingolipid isol. from a marine sponge.
Mp 138-140°.
Fu, J. *et al., CA*, 1993, **119**, 199887y; 1994, **120**, 102478a (*isol*)

***N*-[2-Ethyl-3,18-dihydroxy-1-(hydroxymethyl)-4-methylnonadecyl]tricosamide, 9CI** E-805
[152764-56-2]



$C_{46}H_{93}NO_4$ 724.245
Sphingolipid. Isol. from a marine sponge.
Mp 92-93°.
Fu, J. *et al., CA*, 1994, **120**, 102478a; **121**, 31379b (*isol*)

6-Ethyl-2,5-dihydroxy-1,4-naphthoquinone E-806
6-Ethyl-2-hydroxyjuglone
[13378-87-5]

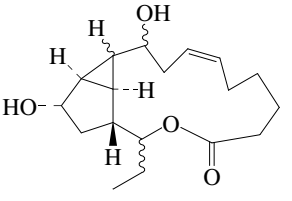


$C_{12}H_{10}O_4$ 218.209
Isol. from *Echinothrix calamaris*. Orange prisms (C_6H_6).
Mp 219-220°. λ_{max} 237 (ε 8190); 291 (ε 10300); 418 (sh) (ε 3460); 432 (ε 3870); 455 (sh) (ε 3120) ($CHCl_3$).

8-Hydroxy: 6-Ethyl-2,5,8-trihydroxy-1,4-naphthoquinone. 6-Ethyl-2-hydroxynaphthazarin
[13378-88-6]
$C_{12}H_{10}O_5$ 234.208
Isol. from *Echinothrix calamaris*. Brown cryst. (C_6H_6).
Mp 204-204.5°. λ_{max} 302 (ε 8560); 479 (sh) (ε 5160); 505 (ε 6300); 530 (ε 4150); 544 (ε 4230) ($CHCl_3$).

3,7-Dihydroxy: 6-Ethyl-2,3,5,7-tetrahydroxy-1,4-naphthoquinone. 6-Ethyl-2,3,7-trihydroxyjuglone
[13378-99-9]
$C_{12}H_{10}O_6$ 250.207
Isol. from *Echinothrix calamaris* and *Echinothrix diadema*. Brick-red needles ($CHCl_3$).
Mp 265-269° (with dec. and subl.). λ_{max} 270 (ε 21900); 330 (ε 10600); 417 (ε 3740); 485 (sh) (ε 1510) ($CHCl_3$).
Moore, R.E. *et al., J.O.C.*, 1966, **31**, 3638; 3645; 3650 (*isol, uv, pmr, ms*)

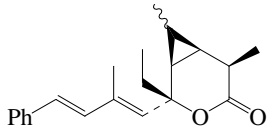
2-Ethyl-12,15-dihydroxy-3-oxabicyclo[11.3.1.0^{14,17}]hexadec-9-en-4-one E-807



$C_{18}H_{28}O_4$ 308.417
Oxylipin. Isol. from the brown alga *Eisenia bicyclis*. Oil. $[\alpha]_D^{20}$ +12 (c, 0.08 in $CHCl_3$).
Kousaka, K. *et al., J. Nat. Prod.*, 2003, **66**, 1318-1323 (*isol, pmr, cmr*)

2-Ethyl-5,7-dimethyl-2-(2-methyl-4-phenyl-1,3-butadienyl)-3-oxabicyclo[4.1.0]heptan-4-one, 9CI E-808

[70941-32-1]

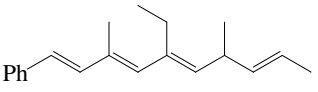


$C_{21}H_{26}O_2$ 310.435

Isol. from *Plakortis halichondrioides*. λ_{max} 219 (ϵ 17000); 289 (ϵ 33000); 306 (ϵ 19400) (hexane).

Ravi, B.N. *et al., J.O.C.*, 1979, **44**, 3109-3113 (*isol, pmr, cmr*)

5-Ethyl-3,7-dimethyl-1-phenyl-1,3,5,8-decatetraene E-809



(1*E*,3*E*,5*E*,8*E*)-*form*

$C_{20}H_{26}$ 266.425

(1*E*,3*E*,5*E*,8*E*)-*form* [70941-36-5]

Constit. of *Plakortis halichondrioides*. λ_{max} 302 (ϵ 32000) (hexane).

(1*E*,3*E*,5*E*,8*Z*)-*form* [70981-88-3]

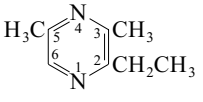
Constit. of *Plakortis halichondrioides*. λ_{max} 295 (ϵ 32000); 311 (ϵ 34500) (hexane).

Ravi, B.N. *et al., J.O.C.*, 1979, **44**, 3109-3113 (*isol, pmr, cmr*)

2-Ethyl-3,5-dimethylpyrazine E-810

FEMA 3150

[13925-07-0]



$C_8H_{12}N_2$ 136.196

Isol. from an arctic marine bacterium. Isol. from coffee aroma. Also present in raw asparagus, wheat bread, other breads, smoked fatty fish, roast chicken, roast beef, lamb and mutton liver, black tea, hydrolysed soy protein and other foods. Organoleptic agent. Flavouring agent. Bp_{19} 80-81° Bp_8 64-66°. n_D^{22} 1.4975.

▶ UQ3155000

Klein, B. *et al., J.A.C.S.*, 1951, **73**, 2949 (*synth*)
Goldman, I.M. *et al., Helv. Chim. Acta*, 1967, **50**, 694
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 968-969 (*use, occur*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol*)

3-Ethyl-2,5-dimethylpyrazine E-811

[13360-65-1]

$C_8H_{12}N_2$ 136.196

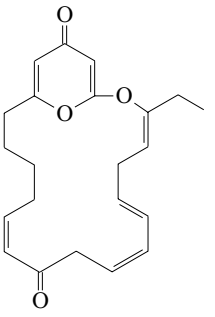
Pheromone of various ant spp. Isol. from various marine bacteria and from coffee. Organoleptic agent with nutty roasted odour. Bp 180.5° Bp_{11} 72-73°. n_D^{24} 1.4945.

Goldman, I.M. *et al., Helv. Chim. Acta*, 1967, **50**, 694
Gelas, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1968, **266**, 625 (*synth, uv, ir, pmr*)
Ohta, A. *et al., Heterocycles*, 1987, **26**, 2449 (*synth*)
Buechi, G. *et al., J.O.C.*, 1991, **56**, 2605 (*synth*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol*)
Dickschat, J.S. *et al., Eur. J. Org. Chem.*, 2005, 4141-4153 (*isol*)

3-Ethyl-2,22-dioxabicyclo[16.3.1]docosa-3,6,8,12,18,21-hexaene-11,20-dione, 9CI E-812

2,6-Epoxy-21-ethyl-1-oxa-2,5,11,15,17,20-cycloheneicosahexaene-4,13-dione

[167871-27-4]



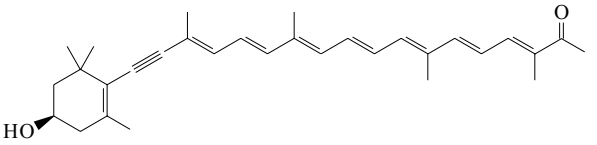
$C_{22}H_{26}O_4$ 354.445

Constit. of the red alga *Phacelocarpus peperocarpos* (*Phacelocarpus labillardieri*). Unstable yellow oil. λ_{max} 236 (ϵ 3600) (EtOH).

Murray, L. *et al., Aust. J. Chem.*, 1995, **48**, 1485-1489 (*isol, pmr, cmr, ir*)

3-Ethyl-2,19-dioxabicyclo[16.3.1]docosa-3,6,9,18(22),21-pentaen-12-yn-20-one, 9CI E-813

[106001-28-9]



$C_{22}H_{26}O_3$ 338.446

Authors' numbering shown. Metab. of red alga *Phacelocarpus labillardieri*. λ_{max} 243 (ϵ 12400) (MeOH) (Derep). λ_{max} 282 (ϵ 7650) (MeOH) (Derep).

19,20-Dihydro, 2,19-dibromo: 4,21-Dibromo-3-ethyl-2,19-dioxabicyclo[16.3.1]docosa-6,9,18(22),21-tetraen-12-yn-20-one, 9CI

[106009-90-9]

$C_{22}H_{26}Br_2O_3$ 498.254

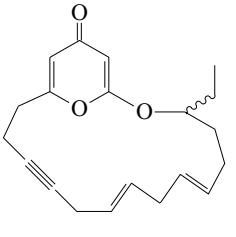
Metab. of *Phacelocarpus labillardieri*. λ_{max} 268 (ϵ 6610) (MeOH) (Derep). λ_{max} 304 (ϵ 7350) (MeOH) (Derep). λ_{max} 304 (MeOH) (Berdy).

Shin, J. *et al., Tet. Lett.*, 1986, **27**, 5189

3-Ethyl-2,20-dioxabicyclo[14.3.1]eicosa-3,6,9,16,19-pentaen-12-yn-18-one, 9CI E-814

19-Ethyl-2,6-epoxy-1-oxacyclononadeca-2,5,12,15,18-pentaen-9-yn-4-one

[81575-26-0]

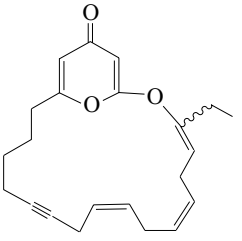


$C_{20}H_{22}O_3$ 310.392

Isol. from the red alga *Phacelocarpus labillardieri*. λ_{max} 245 (ϵ 13800) (MeOH) (Derep).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 113 (*ms, pmr, cmr*)

21-Ethyl-2,6-epoxy-1-oxa-2,5,14,17,20-cycloheneicosapentaen-11-yn-4-one E-815

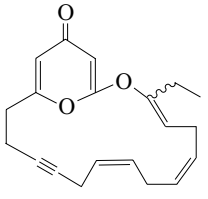


$C_{22}H_{26}O_3$ 338.446

(14*Z*,17*Z*,20*Z*)-*form*
Constit. of red alga *Phacelocarpus labillardieri*.
Pale-yellow oil.

(14*Z*,17*Z*,20*E*)-*form*
Metab. of *Phacelocarpus labillardieri*.
Kazlauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 113 (*ms, pmr, struct*)
Shin, J. *et al., Tet. Lett.*, 1986, **27**, 5189 (*struct*)

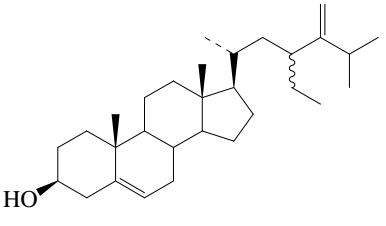
19-Ethyl-2,6-epoxy-1-oxa-2,5,12,15,18-cyclononadecapentaen-9-yn-4-one E-816



$C_{20}H_{22}O_3$ 310.392

(12*Z*,15*Z*)-*form*
Constit. of *Phacelocarpus labillardieri*.
Oil.
Kazlauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 113

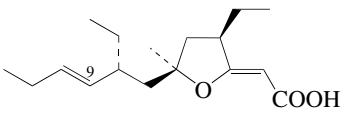
23-Ethylergosta-5,24(28)-dien-3-ol, 9CI E-817
[119944-26-2, 119944-27-3]



$C_{30}H_{50}O$ 426.724

(3β,23ξ)-*form*
Sipalosterol A
[82154-21-0]
Isol. from the chinese soft coral, *Sinularia sipalosa*.
Long, K. *et al., CA*, 1982, **97**, 21004x; 21005y (*isol*)
Giner, J.-L. *et al., J.O.C.*, 1989, **54**, 2117-2125 (*synth, pmr, ms*)

[3-Ethyl-5-(2-ethyl-3-hexenyl)tetrahydro-5-methyl-2-furanylidene]acetic acid E-818
3,6-Epoxy-4,8-diethyl-6-methyl-2,9-dodecadienoic acid



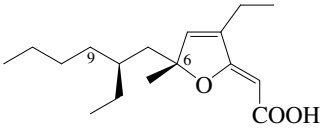
Absolute Configuration

$C_{17}H_{28}O_3$ 280.406

Me ester:
$C_{18}H_{30}O_3$ 294.433
Isol. from *Plakortis simplex*. Oil. $[\alpha]_D^{25}$ +20 (c, 0.001 in $CHCl_3$).

9,10-Dihydro, Me ester: Methyl 3,6-epoxy-4,8-diethyl-6-methyl-2-dodecenoate
$C_{18}H_{32}O_3$ 296.449
Isol. from *Plakortis simplex*. Oil. $[\alpha]_D^{25}$ +5 (c, 0.001 in $CHCl_3$).
Cafieri, F. *et al., Tetrahedron*, 1999, **55**, 7045-7056 (*isol, pmr, cmr, ms*)

[3-Ethyl-5-(2-ethylhexyl)-5-methyl-2(5*H*)-furanylidene]acetic acid E-819
3,6-Epoxy-4,8-diethyl-6-methyl-2,4-dodecadienoic acid

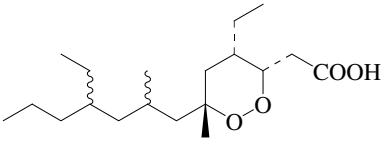


$C_{17}H_{28}O_3$ 280.406
Lower homologue of [3,5-Diethyl-5-(2-ethylhexyl)-2(5*H*)-furanylidene]acetic acid, D-496.

(2*Z*,6*R*,8*S*)-*form*
Me ester:
$C_{18}H_{30}O_3$ 294.433
Isol. from *Plakortis angulospiculatus*. Oil. $[\alpha]_D$ -182.6 (c, 0.01 in MeOH). $[\alpha]_D$ -86.6 (c, 0.01 in $CHCl_3$).

*9,10-Didehydro(*E-*), Me ester:*
$C_{18}H_{28}O_3$ 292.417
Isol. from *Plakortis angulospiculatus*. Oil. $[\alpha]_D$ -440.8 (c, 0.01 in MeOH). $[\alpha]_D$ -205.4 (c, 0.01 in $CHCl_3$).
Epifanio, R. de A. *et al., J. Braz. Chem. Soc.*, 2005, **16**, 1367-1371 (*isol, pmr, cmr, ms*)

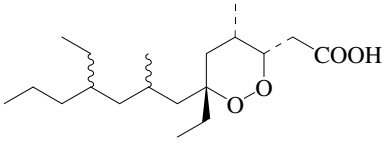
4-Ethyl-6-(4-ethyl-2-methylheptyl)-6-methyl-1,2-dioxan-3-acetic acid E-820
3,6-Epidioxy-4,10-diethyl-6,8-dimethyltridecanoic acid. ***14,18-Dinorplakortide Q***



$C_{19}H_{36}O_4$ 328.491
Isol. from *Plakortis zyggompha*.
Berrué, F. *et al., Tetrahedron*, 2005, **61**, 11843-11849 (*isol, pmr, cmr*)

6-Ethyl-6-(4-ethyl-2-methylheptyl)-4-methyl-1,2-dioxan-3-acetic acid E-821

3,6-Epidioxy-6,10-diethyl-4,8-dimethyltridecanoic acid. ***14,16-Dinorplakortide Q***

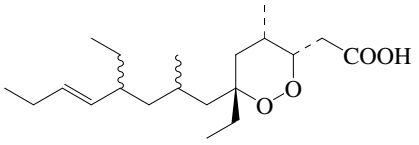


$C_{19}H_{36}O_4$ 328.491
Isol. from *Plakortis zyggompha*.

Berrué, F. *et al., Tetrahedron*, 2005, **61**, 11843-11849 (*isol, pmr, cmr*)

6-Ethyl-6-(4-ethyl-2-methyl-5-octenyl)-4-methyl-1,2-dioxan-3-acetic acid E-822

3,6-Epidioxy-6,10-diethyl-4,8-dimethyl-11-tetradecenoic acid. ***11,12-Didehydro-16-norplakortide Q***

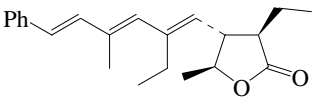


$C_{20}H_{36}O_4$ 340.502
Isol. from the sponge *Plakortis zyggompha*. Oil (as Me ester).

Berrué, F. *et al., Tetrahedron*, 2005, **61**, 11843-11849 (*isol, pmr, cmr*)

3-Ethyl-4-(2-ethyl-4-methyl-6-phenyl-1,3,5-hexatrienyl)dihydro-5-methyl-2(3*H*)-furanone E-823

[70941-34-3]



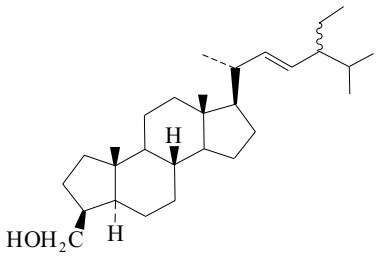
$C_{22}H_{28}O_2$ 324.462
Constit. of *Plakortis halichondrioides.*

Ravi, B.N. *et al., J.O.C.*, 1979, **44**, 3109-3113 (*isol, pmr*)

24-Ethyl-3-hydroxymethyl-A-norcholest-22-ene E-824

3-Hydroxymethyl-A-norstigmast-22-ene. A-Norstigmast-22-ene-3-methanol, 9CI

[74036-41-2]



$C_{29}H_{50}O$ 414.713

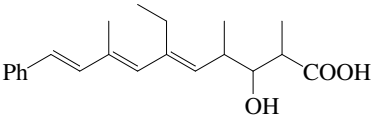
(3β,5α,22*E*,24ξ)-*form* [55081-42-0]
[83730-42-1]
Constit. of sponges *Axinella verrucosa*, *Hymeniacidon aldis* and *Acanthella aurantiaca*.

Ac: [55081-48-6]
Cryst. (MeOH). Mp 104-106°. $[\alpha]_D$ +12 (c, 1.65 in $CHCl_3$).

22,23-Dihydro, Ac:
Needles (MeOH). Mp 90-91°. $[\alpha]_D^{17}$ +28 (c, 0.1 in MeOH).

Minale, L. *et al., J.C.S. Perkin 1*, 1974, 2380-2384
Bohlin, L. *et al., J.O.C.*, 1982, **47**, 5309-5314 (*isol*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2321

6-Ethyl-3-hydroxy-2,4,8-trimethyl-10-phenyl-5,7,9-decatrienoic acid E-825

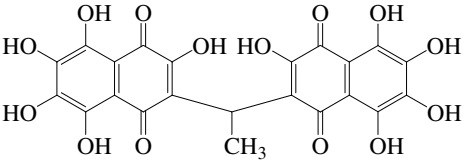


$C_{21}H_{28}O_3$ 328.45

Me ester: [70941-35-4]
$C_{22}H_{30}O_3$ 342.477
Isol. from *Plakortis halichondroides.* λ_{max} 305 (ϵ 33000) (hexane).
Ravi, B.N. *et al., J.O.C.*, 1979, **44**, 3109-3113 (*isol, pmr, cmr*)

2,2′-Ethylidenebis[3,5,6,7,8-pentahydroxy-1,4-naphthoquinone], 8CI E-826

[32013-74-4]

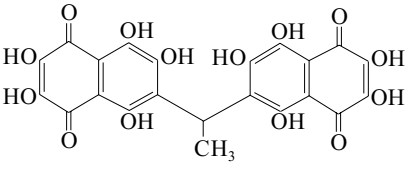


$C_{22}H_{14}O_{14}$ 502.344
Isol. from *Spatangus purpureus* and *Strongylocentrotus drobachiensis.* Red needles (MeOH aq.).
Mp 155-157°. λ_{max} 262 (log ϵ 4.55); 344 (log ϵ 4.14); 470 (log ϵ 4.07); 487 (log ϵ 4.13); 526 (log ϵ 4.03) (EtOH).

Mathieson, J.W. *et al., J.C.S.(C)*, 1971, 153-160 (*isol, ir, pmr, uv, synth*)
Kol'tsova, E.A. *et al., Khim. Prir. Soedin.*, 1978, 438-441; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 371-374 (*isol, uv, synth*)

6,6′-Ethylidenebis[2,3,5,7,8-pentahydroxy-1,4-naphthoquinone] E-827

3,3′-Ethylidenebis[2,6,7-trihydroxynaphthazarin]



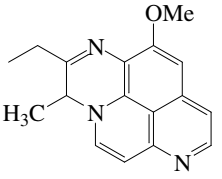
$C_{22}H_{14}O_{14}$ 502.344
Isol. from the sea urchins *Strongylocentrotus intermedius* and *Strongylocentrotus dröebachiensis.* Subl. without melting at 285-290°.

Hexa-Me ether: Mp 162°.

Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1976, **12**, 439; *Chem. Nat. Compd. (Engl. Transl.)*, 1976, **12**, 387
Kol'tsova, E.A. *et al., Khim. Prir. Soedin.*, 1978, **14**, 438; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 371

2-Ethyl-11-methoxy-3-methyl-3*H*-[1,6]naphthyridino[6,5,4-*def*]quinoxaline, 9CI E-828

[599173-39-4]



$C_{17}H_{17}N_3O$ 279.341

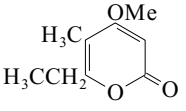
Alkaloid from a *Xestospongia* sp. Orange gum. λ_{max} 208 (ϵ 7400); 225 (ϵ 6590); 237 (ϵ 7390); 251 (ϵ 5550); 261 (ϵ 4400); 272 (ϵ 3470); 360 (ϵ 1970) (EtOH).

Calcul, L. *et al., Tetrahedron*, 2003, **59**, 6539-6544 (*isol, pmr, cmr*)

6-Ethyl-4-methoxy-5-methyl-2*H*-pyran-2-one E-829

Nectriapyrone B

[94632-40-3]

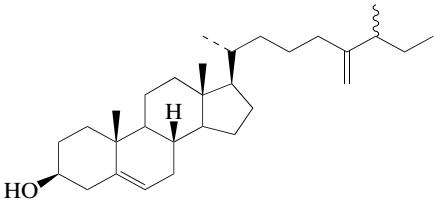


$C_9H_{12}O_3$ 168.192

Prod. by a fungus *Pleiochaeta* sp. from a marine sponge. Mp 82° (synthetic).

Effenberger, F. *et al., Chem. Ber.*, 1984, **117**, 3270 (*synth, pmr*)
Abrell, L.M. *et al., Tet. Lett.*, 1994, **35**, 9159 (*isol, pmr, cmr*)

26-Ethyl-26-methylcholesta-5,25(27)-dien-3-ol E-830



$C_{30}H_{50}O$ 426.724

(3β,26ξ)-*form*

Rhabdasterol

[206757-12-2]

Constit. of *Rhabdastrella globostellata*.

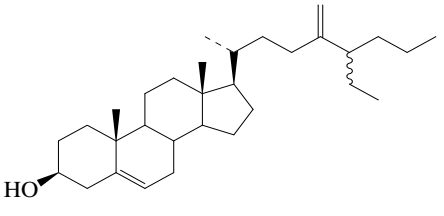
Cryst.

Mp 128-130°. $[\alpha]_D^{25}$ -27.4 (c, 0.042 in MeOH).

Rao, Z.-G. *et al., Gaodeng Xuexiao Huaxue Xuebao*, 1998, **19**, 406-407; *CA*, **128**, 306433g (*isol, pmr, cmr*)
Deng, S. *et al., Zhongguo Haiyang Yaowu*, 1999, **18**, 1-3; *CA*, **133**, 86885s (*isol, pmr, cmr*)

26-Ethyl-27-methyl-24-methylenecholest-5-en-3-ol E-831

26-Ethyl-27-methylergosta-5,24(28)-dien-3-ol



$C_{31}H_{52}O$ 440.751

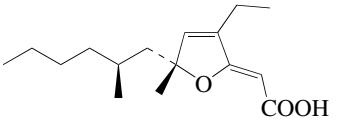
(3β,25ξ)-*form* [158237-68-4]

Isol. from *Nephthea albida*.

Fu, J. *et al., CA*, 1994, **121**, 226700

[3-Ethyl-5-methyl-5-(2-methylhexyl)-2(5*H*)-furanylidene]acetic acid E-832

3,6-Epoxy-4-ethyl-6,8-dimethyl-2,4-dodecadienoic acid



$C_{16}H_{26}O_3$ 266.38

(2*Z*,6*R*,8*S*)-*form*

Me ester: [206443-28-9]

$C_{17}H_{28}O_3$ 280.406

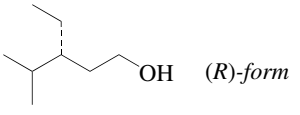
Isol. from the sponge *Plakortis* aff. *angulospiculatus*. Oil. $[\alpha]_D$ -129 (c, 0.5 in $CHCl_3$). λ_{max} 283 (ϵ 9400) (MeOH).

Compagnone, R.S. *et al., Tetrahedron*, 1998, **54**, 3057-3068 (*isol, ir, pmr, cmr, ms*)

3-Ethyl-4-methyl-1-pentanol, 9CI E-833

3-Isopropyl-1-pentanol

[38514-13-5]



$C_8H_{18}O$ 130.23

(*R*)-*form* [100431-82-1]

Liq. Bp_{36} 125-135°. $[\alpha]_D^{25}$ +6.9 (c, 5 in $CHCl_3$).

O-*Sulfate:*

$C_8H_{18}O_4S$ 210.294

Isol. from the sponge *Ptilocaulis spiculifer*.

$[\alpha]_D^{25}$ +0.5 (c, 0.01 in MeOH) (with Dakaramine, D-21 as counter ion).

(*S*)-*form* [100431-87-6]

Liq. Bp_{27} 125-130°. $[\alpha]_D$ -6.8 (c, 13 in $CHCl_3$).

(ξ)-*form*

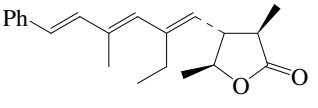
Occurs in *Formica rufa* and *Formica polyctenal*.

[111767-89-6]

Francke, W. *et al., Z. Naturforsch., C*, 1985, **40**, 661-664 (*ξ-form, occur*)
Nicotra, F. *et al., J.O.C.*, 1986, **51**, 1272-1276 (*synth, pmr*)
Enders, D. *et al., Tetrahedron*, 1986, **42**, 2235 (*synth, ir, pmr, cmr*)
Diop, M. *et al., J. Nat. Prod.*, 1996, **59**, 271-272 (*isol, sulfate*)
Schiendorfer, M. *et al., Synthesis*, 2005, 2701-2712 (*S-form, synth*)

4-(2-Ethyl-4-methyl-6-phenyl-1,3,5-hexatrienyl)dihydro-3,5-dimethyl-2(3*H*)-furanone E-834

[70941-33-2]



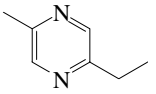
$C_{21}H_{26}O_2$ 310.435

Constit. of *Plakortis halichondrioides*. λ_{max} 227 (ϵ 13100); 301 (ϵ 38000) (hexane).

Ravi, B.N. *et al., J.O.C.*, 1979, **44**, 3109-3113 (*isol, pmr, cmr*)

2-Ethyl-5-methylpyrazine, 9CI, 8CI E-835

FEMA 3154
[13360-64-0]

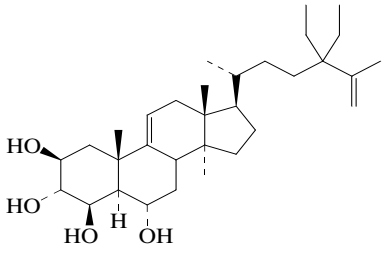


Found in roast peanuts, roast filberts, cooked beef, cooked lamb, coffee beans, cocoa butter, roast barley and other foodstuffs. Prod. by various marine bacteria. Used in food flavouring. Bp_{56} 79-80°. n_D^{25} 1.4925. Odour threshold 100 ppb in H_2O.

Goldman, I.M. *et al., Helv. Chim. Acta*, 1967, **50**, 694
U.S. Pat., 1976, 3 952 026; *CA*, **71**, 90131m (*manuf, uses*)
Shibamoto, T. *et al., J. Agric. Food Chem.*, 1979, **27**, 1027 (*formn*)
Milic, B.L. *et al., Food Chem.*, 1984, **13**, 165 (*gc*)
Dickschat, J.S. *et al., Eur. J. Org. Chem.*, 2005, 4141-4153 (*isol*)

24-Ethyl-14-methylstigmasta-9(11),25-diene-2,3,4,6-tetrol E-836

24,24-Diethyl-14-methylcholesta-9(11),25-diene-2,3,4,6-tetrol



$C_{32}H_{54}O_4$ 502.776

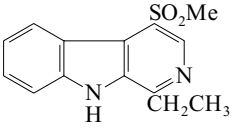
(2β,3α,4β,5α,6α,14α)-*form*

2,3,6-Tri-O-*sulfate:* ***Antibiotic Sch 575867***. *Sch 575867*
$C_{32}H_{54}O_{13}S_3$ 742.969
Isol. from a deep water sponge of the family Astroscleridae. Antifungal agent. Gum (as tri-Na salt).

Yang, S.-W. *et al., J. Antibiot.*, 2003, **56**, 186-189 (*isol, pmr, cmr*)

1-Ethyl-4-methylsulfonyl-β-carboline E-837

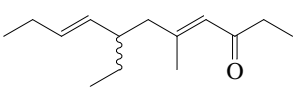
*1-Ethyl-4-(methylsulfonyl)-9*H*-pyrido[3,4-*b*]indole, 9CI*
[138683-70-2]



$C_{14}H_{14}N_2O_2S$ 274.343
Alkaloid from the marine bryozoan *Cribricellina cribraria*. Pale green oil. λ_{max} 213 (ϵ 2690); 250 (ϵ 1950); 258 (ϵ 2090); 299 (ϵ 871); 304 (ϵ 1070); 350 (ϵ 417) (MeOH) (Derep).

Prinsep, M.R. *et al., J. Nat. Prod.*, 1991, **54**, 1068 (*isol, uv, ir, pmr, cmr, ms, struct*)

7-Ethyl-5-methyl-4,8-undecadien-3-one E-838



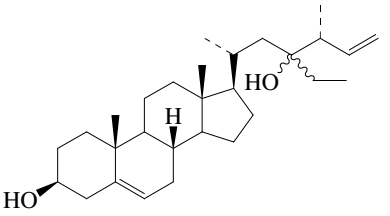
$C_{14}H_{24}O$ 208.343

(4*E*,7ξ,8*E*)-*form* [66984-56-3]
Isol. from *Plakortis halichondrioides*.
$[\alpha]_D^{20}$ +17 (c, 1.4 in $CHCl_3$). λ_{max} 237 (ϵ 18900) (MeOH).

Higgs, M.D. *et al., J.O.C.*, 1978, **43**, 3454-3457 (*isol, pmr, cmr*)

23-Ethyl-27-norergosta-5,25-diene-3,23-diol E-839

23-Ethyl-24-methyl-27-norcholesta-5,25-diene-3,23-diol



$C_{29}H_{48}O_2$ 428.697

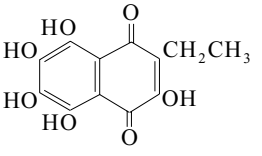
(3β,23ξ,24*R*)-*form* [273928-43-1]
Constit. of *Petrosia testudinaria*.

3-Ac: [273397-56-1]
$C_{31}H_{50}O_3$ 470.734
Cryst. Mp 102°. $[\alpha]_D^{25}$ -26 (c, 1 in $CHCl_3$).

Reddy, N.S. *et al., Nat. Prod. Lett.*, 1999, **14**, 131-134 (*isol, pmr, cmr*)

2-Ethyl-3,5,6,7,8-pentahydroxy-1,4-naphthoquinone E-840

2-Ethyl-3,5,6,7,8-pentahydroxy-1,4-naphthalenedione, 9CI. ***Echinochrome A***
[517-82-8]



$C_{12}H_{10}O_7$ 266.207
Potentially tautomeric with the 6-ethyl tautomer. Isol. from the sea urchins *Arbacia pustulosa*, *Echinothrix* spp. and *Scaphechinus miribilis*. Present as the prosthetic group of a high-molecular-weight complex which acts as a spermatozoa activating and agglutinating agent. Dark-red needles (toluene). Sol. MeOH, Me_2CO, bases, Et_2O; fairly sol. $CHCl_3$; poorly sol. hexane, H_2O.
Mp 220°. λ_{max} 260 (ϵ 21000); 343 (ϵ 9800); 470 (ϵ 7600); 530 (ϵ 4560) (EtOH) (Berdy).

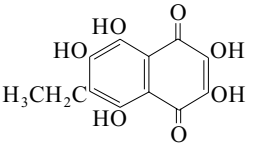
3,6,7-Tri-Me ether:
$C_{15}H_{16}O_7$ 308.287
Red needles. Mp 129-130°.

[1471-96-1]

Lederer, E. *et al., C. R. Hebd. Seances Acad. Sci.*, 1939, **208**, 1939 (*isol*)
Kuhn, R. *et al., Ber.*, 1942, **75**, 407
Wallenfels, K. *et al., Ber.*, 1942, **75**, 413
Goodwin, T.W. *et al., Experientia*, 1951, **7**, 375
Moore, R.E. *et al., J.O.C.*, 1966, **31**, 3645 (*synth*)
Peña-Cabrera, E. *et al., J.O.C.*, 2002, **67**, 1689-1691 (*synth, pmr, cmr*)
Mischenko, N.P. *et al., J. Nat. Prod.*, 2005, **68**, 1390-1393 (*isol, pmr, cmr*)

6-Ethyl-2,3,5,7,8-pentahydroxy-1,4-naphthoquinone E-841

6-Ethyl-2,3,5,7,8-pentahydroxy-1,4-naphthalenedione, 9CI.
6-Ethyl-2,3,7-trihydroxynaphthazarin
[1471-96-1]



$C_{12}H_{10}O_7$ 266.207

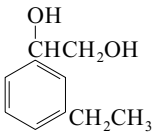
Pigment from spines of *Diadema antillarum* and *Spatangus purpureus*. Red needles.
Mp 216-217° (222-223°).

2-Me ether: [32013-73-3]
$C_{13}H_{12}O_7$ 280.234
Pigment of spines of *Diadema antillarum*. Deep red prisms (Et_2O/hexane).
Mp 202-204°.

3-Me ether: [15257-36-0]
$C_{13}H_{12}O_7$ 280.234
Pigment of spines of *Diadema antillarum*. Deep red prisms (Et_2O/hexane).
Mp 179-184°.

Millott, N. *et al., Proc. Zool. Soc. London*, 1957, **129**, 263 (*isol*)
Moore, R.E. *et al., Tetrahedron*, 1967, **23**, 3271-3305 (*synth*)
Mathieson, J.W. *et al., J.C.S.(C)*, 1971, 153-160 (*isol*)

1-(3-Ethylphenyl)-1,2-ethanediol **E-842**



$C_{10}H_{14}O_2$ 166.219

Dibenzoyl: [157403-32-2]
$C_{24}H_{22}O_4$ 374.435
Isol. from the starfish *Pteraster militaris*.

Yayli, N. *et al., Turk. J. Chem.*, 1993, **17**, 208; *CA*, **121**, 157326a (*isol, synth, struct*)

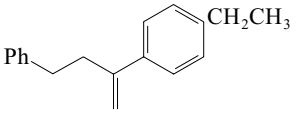
1-(4-Ethylphenyl)-1,2-ethanediol **E-843**

$C_{10}H_{14}O_2$ 166.219

Dibenzoyl: [157403-33-3]
$C_{24}H_{22}O_4$ 374.435
Constit. of the starfish *Pteraster militaris*.

Yayli, N. *et al., Turk. J. Chem.*, 1993, **17**, 208; *CA*, **121**, 157326a (*isol, synth, struct*)

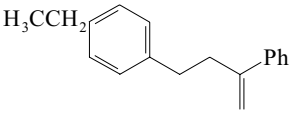
2-(4-Ethylphenyl)-4-phenyl-1-butene **E-844**
1-Ethyl-4-(1-methylene-3-phenylpropyl)benzene, 9CI
[156186-41-3]



$C_{18}H_{20}$ 236.356
Constit. of the starfish *Pteraster militaris*.

Yayli, N. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 556 (*isol, pmr, cmr*)

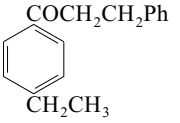
4-(4-Ethylphenyl)-2-phenyl-1-butene **E-845**
1-Ethyl-4-(3-phenyl-3-butenyl)benzene, 9CI
[156186-39-9]



$C_{18}H_{20}$ 236.356
Constit. of the starfish *Pteraster militaris*.

Yayli, N. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 556 (*isol, pmr, cmr*)

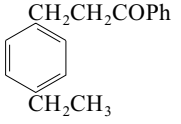
1-(4-Ethylphenyl)-3-phenyl-1-propanone **E-846**
[43008-74-8]



$C_{17}H_{18}O$ 238.329
Constit. of the starfish *Pteraster militaris*.
Mp 62-63°. Bp_{38} 195°.

Kursanov, D.N. *et al., Synthesis*, 1973, 420 (*synth, pmr*)
Yayli, N. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 556 (*isol*)

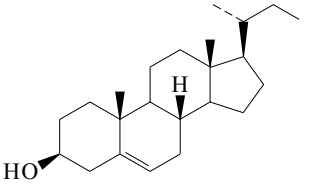
3-(4-Ethylphenyl)-1-phenyl-1-propanone **E-847**
[156186-40-2]



$C_{17}H_{18}O$ 238.329
Constit. of the starfish *Pteraster militaris*.

Yayli, N. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 556 (*isol*)

20-Ethylpregn-5-en-3-ol **E-848**
24,25,26,27-Tetranorcholest-5-en-3-ol. 24-Norchol-5-en-3-ol

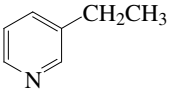


$C_{23}H_{38}O$ 330.553

3β-*form* [27460-32-8]
Constit. of *Polizoa opuntia* and sponge *Damiriana hawaiiana*.

Delseth, C. *et al., Helv. Chim. Acta*, 1979, **61**, 1470-1476 (*isol, Damiriana*)
Palermo, J.A. *et al., Steroids*, 1996, **61**, 2-6 (*isol, Polizoa, pmr, synth*)

3-Ethylpyridine **E-849**
FEMA 3394
[536-78-7]



C_7H_9N 107.155
Found in black tea and raw fish. Flavouring ingredient. Liq. with a tobacco flavour. Sl. sol. H_2O, sol. EtOH, Et_2O. d^0 0.95. Bp 162-165°. n_D^{20} 1.5020. pK_a 5.56 (25°).

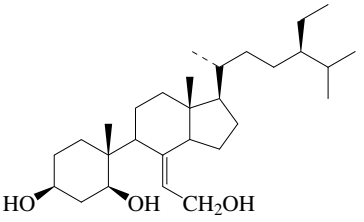
Picrate: Mp 128-130°.

N-*Oxide:* [14906-62-8]
C_7H_9NO 123.154
Bp_4 100°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 735C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 244C (*nmr*)
Mijajima, G. *et al., Chem. Pharm. Bull.*, 1972, **20**, 429 (*cmr*)
Ferles, M. *et al., Coll. Czech. Chem. Comm.*, 1973, **38**, 611 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 266

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1038
Bremner, D.H. *et al., Synth. Commun.*, 1997, **27**, 1535-1542 (*N-oxide*)

24-Ethyl-5,6-secocholest-7-ene-3,5,6-triol E-850



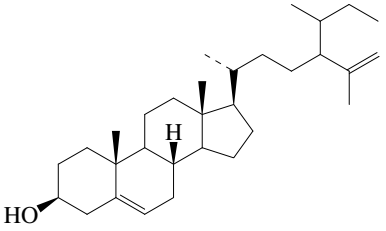
(3β,5β,7*Z*,24*R*)-*form*

$C_{29}H_{52}O_3$ 448.728

(3β,5β,7*Z*,24*R*)-*form*
5,6-Secostigmast-7-ene-3,5,6-triol
Constit. of *Hippospongia communis*.

(3β,5β,7*Z*,24*S*)-*form*
5,6-Secoporiferast-7-ene-3,5,6-triol
Constit. of *Hippospongia communis*.
Madaio, A. *et al., J. Nat. Prod.*, 1990, **53**, 565 (*isol, pmr, ms*)

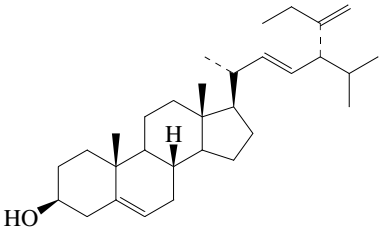
28-Ethylstigmasta-5,25-dien-3-ol E-851



$C_{31}H_{52}O$ 440.751

3β-*form* [365541-68-0]
Constit. of *Axinyssa aplysinoides*.
Liang, L. *et al., Zhongguo Haiyang Yaowu*, 2001, **20**, 1-4; *CA*, **135**, 301204t (*isol, pmr, cmr*)

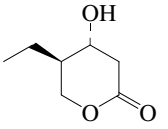
28-Ethylstigmasta-5,22,28-trien-3-ol E-852



$C_{31}H_{50}O$ 438.735

(3β,22*E*,24*R*)-*form*
Ophirasterol
[710324-96-2]
Constit. of *Topsentia ophiraphidites*.
Cryst.
Mp 133.5-137°. $[\alpha]_D^{25}$ -78.3 (c, 0.35 in $CHCl_3$).
Calderón, G.J. *et al., Steroids*, 2004, **69**, 93-100 (*isol, pmr, cmr*)

5-Ethyltetrahydro-4-hydroxy-2*H*-pyran-2-one E-853



(4*R*,5*R*)-*form*

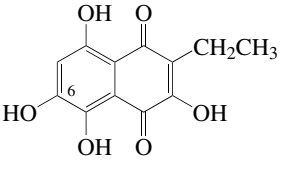
$C_7H_{12}O_3$ 144.17

(4*R*,5*R*)-*form*
Simplactone B
Isol. from the sponge *Plakortis simplex*. Cytotoxic agent.
Amorph. solid. $[\alpha]_D^{25}$ -6 (c, 0.001 in $CHCl_3$).

(4*R*,5*S*)-*form*
Simplactone A
Isol. from *Plakortis simplex*. Cytotoxic agent. Amorph. solid.
$[\alpha]_D^{25}$ -3 (c, 0.002 in $CHCl_3$).
Cafieri, F. *et al., Tetrahedron*, 1999, **55**, 13831-13840

2-Ethyl-3,5,6,8-tetrahydroxy-1,4-naphthoquinone, 8CI E-854

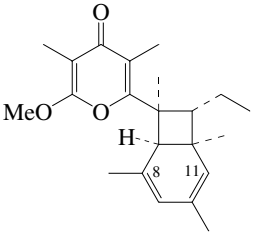
2-Ethyl-3,6-dihydroxynaphthazarin. 3-Ethyl-2,7-dihydroxynaphthazarin. 2-Ethyl-3,5,6,8-tetrahydroxy-1,4-naphthalenedione
[13378-91-1]



$C_{12}H_{10}O_6$ 250.207
Constit. of *Cetraria islandica* var. *polaris* and the sea urchins *Echinothrix* spp. Dark red needles (MeOH).
Mp 190-192° (182-185°). λ_{max} 232 (log ϵ 4.16); 268 (log ϵ 3.86); 318 (log ϵ 3.69); 442 (sh) (log ϵ 3.31); 479 (sh) (log ϵ 3.42); 511 (log ϵ 3.49); 551 (sh) (log ϵ 3.33) (MeOH).

6-Me ether: 2-Ethyl-3,5,8-trihydroxy-6-methoxy-1,4-naphthoquinone. ***Cristazarin***
[15254-99-6]
$C_{13}H_{12}O_6$ 264.234
Constit. of the lichen *Cladonia cristatella*. Red needles (Me_2CO).
Mp 154-157°. λ_{max} 316 (log ϵ 3.86); 506 (log ϵ 3.83) (MeOH).
Moore, R.E. *et al., J.O.C.*, 1966, **31**, 3638-3645; 3645-3650 (*synth, isol*)
Yamamoto, Y. *et al., Phytochemistry*, 1996, **43**, 1239-1242 (*Cristazarin*)
Stepanenko, L.S. *et al., Phytochemistry*, 1997, **46**, 565-568 (*isol, uv, ir, pmr, cmr, ms*)
Chai, C.L.L. *et al., J.O.C.*, 2006, **71**, 992-1001 (*synth*)

2-[8-Ethyl-1,3,5,7-tetramethylbicyclo[4.2.0]octa-2,4-dien-7-yl]-6-methoxy-3,5-dimethyl-4*H*-pyran-4-one E-855



$C_{22}H_{30}O_3$ 342.477
Isol. from the sacoglossan *Placobranchus ocellatus*.
$[\alpha]_D$ +9.5 (c, 0.06 in $CHCl_3$). λ_{max} 260 (ϵ 12100) (MeOH).

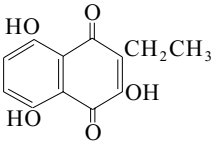
8,11-Epidioxide:
$C_{22}H_{30}O_5$ 374.476

Isol. from *Placobranchus ocellatus.*
$[\alpha]_D$ +5 (c, 0.08 in $CHCl_3$). Possible artifact. λ_{max} 275 (ϵ 11600) (MeOH).

Manzo, E. *et al., Tet. Lett.*, 2005, **46**, 465-468 (*isol, pmr, cmr*)

2-Ethyl-3,5,8-trihydroxy-1,4-naphthoquinone E-856

2-Ethyl-3,5,8-trihydroxy-1,4-naphthalenedione, 9CI



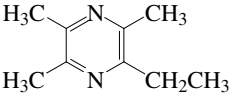
$C_{12}H_{10}O_5$ 234.208
Pigment from the ovaries of *Arbacia* spp. Red rods (EtOH aq. or petrol).
Mp 187°.

5,8-Di-Me ether:
$C_{14}H_{14}O_5$ 262.262
Orange-red cryst. (Et_2O). Mp 156°.

Wallenfels, K. *et al., Ber.*, 1942, **75**, 785 (*synth*)
Brunner, O. *et al., Monatsh. Chem.*, 1947, **77**, 251 (*synth*)

Ethyltrimethylpyrazine E-857

[17398-16-2]

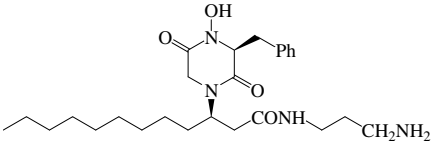


$C_9H_{14}N_2$ 150.223
Prod. by various marine bacteria.

Marion, J.P. *et al., Chimia*, 1967, **21**, 510-511; *CA*, **68**, 78249m (*synth*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol*)
Dickschat, J.S. *et al., Eur. J. Org. Chem.*, 2005, 4141-4153 (*isol*)

Etzionin E-858

[123794-29-6]



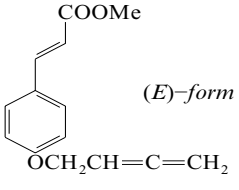
Absolute Configuration

$C_{26}H_{42}N_4O_4$ 474.642
Isol. from *Didemnum rodriguesi*. Exhibits cytotoxic and antifungal activity. Foaming oil. λ_{max} 260 (ϵ 1300) (MeOH) (Derep).

N,O-*Di-Ac:*
Foaming oil. $[\alpha]_D$ +14 (c, 0.1 in MeOH). Relatively unstable. Dec. slowly on standing for several days to give the mono-*N*-Ac.

Hirsch, S. *et al., Tet. Lett.*, 1989, **30**, 4291 (*isol, uv, ir, pmr, cmr, ms, struct*)
Vaz, E. *et al., Tetrahedron: Asymmetry*, 2003, **14**, 1935-1942 (*abs config*)

Eucalyptene E-859



(*E*)–*form*

$C_{14}H_{14}O_3$ 230.263

(*E*)-*form*

Eucalyptene A
[149064-39-1]
Metab. of *Clitocybe eucalyptorum* and *Xylaria* sp. No. 2508. Antifungal agent. Cryst. (hexane).
Mp 68°. λ_{max} 204 (ϵ 12050); 220 (ϵ 10950); 302 (ϵ 19060) (EtOH) (Berdy).

Parent acid: 4-(2,3-Butadienyloxy)cinnamic acid
$C_{13}H_{12}O_3$ 216.236
Metab. of a marine derived *Xylaria* sp. No. 2508. Cryst.
Mp 151-152°.

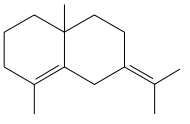
(*Z*)-*form*

Eucalyptene B
[149064-40-4]
Metab. of *Clitocybe eucalyptorum*. Antifungal agent. Oil.

Arnone, A. *et al., Phytochemistry*, 1993, **32**, 1279-1281 (*isol, esters*)
Lin, Y. *et al., Tet. Lett.*, 2001, **42**, 449-451 (*Xylaria constits*)

4,7(11)-Eudesmadiene E-860

4,7(11)-Selinadiene



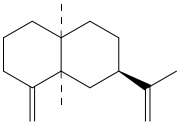
$C_{15}H_{24}$ 204.355
Constit. of *Laurencia nidifica*. Unstable oil. $[\alpha]_D^{24}$ +34 (c, 0.9 in $CHCl_3$).

[95343-73-0]

Sun, H.H. *et al., J.O.C.*, 1978, **43**, 1613
Banerjee, A.K. *et al., J. Chem. Res., Synop.*, 1984, 284 (*synth*)

4(15),11-Eudesmadiene E-861

4(15),11-Selinadiene



(5α,7β,10α)-*form*

$C_{15}H_{24}$ 204.355

(5α,7β,10α)-*form*

β-Helmiscapene
[66141-12-6]
Isol. from *Scapania undulata* and *Helminthosporium sativum*.
Oil.

(5α,7β,10β)-*form*

β-Selinene. *Cyperene II*
[17066-67-0]
Constit. of celery oil. Also from *Cyperus rotundus* (nutgrass) and *Humulus lupulus* (hops).
Oil. Bp_6 121-122°. $[\alpha]_D$ +61.

(5β,7α,10α)-*form*

ent-*β-Selinene*
[473-12-1]
Constit. of the essential oils of *Libanotis transcaucasica* and *Seseli indicum* and the liverwort *Tylimanthus tenellus.* Also from the gorgonian *Eunicea mammosa*.
Oil. $Bp_{1.5}$ 70-115° (lit. gives a pressure range). $[\alpha]_D$ -46 (c, 10 in $CHCl_3$).

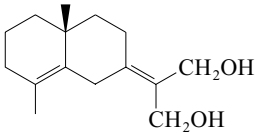
(5β,7β,10α)-*form* [29868-52-8]
Constit. of *Aristolochia indica.*
Oil. $Bp_{0.3}$ 80-85°. $[\alpha]_D$ -71.63 (c, 4.61 in $CHCl_3$).

(5β,7β,10β)-*form* [83434-35-9]
Constit. of the defence secretion of *Amitermes excellens.*

Trivedi, B. *et al., Coll. Czech. Chem. Comm.*, 1964, **29**, 1675 (*isol*)
Marshall, J.A. *et al., J.O.C.*, 1966, **31**, 2933 (*synth*)
Dixit, S.M. *et al., Chem. Ind. (London)*, 1967, 1256 (*isol*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1968, **45**, 1033 (*synth*)
Stevens, K.L. *et al., J.O.C.*, 1971, **36**, 2422 (*synth*)
Govindachari, T.R. *et al., Indian J. Chem., Sect. B*, 1973, **11**, 971 (*isol, struct*)
Andersen, N.H. *et al., Phytochemistry*, 1977, **16**, 1731 (*β-Helmiscapene*)
Naya, Y. *et al., Tet. Lett.*, 1982, **23**, 3047 (*isol*)
Wijnberg, J.B.P.A. *et al., J.O.C.*, 1983, **48**, 4380 (*synth*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 2860 (*β-Selinene, pmr, cmr*)
Caine, D. *et al., J.O.C.*, 1988, **53**, 4124 (*synth*)
Williams, H.J. *et al., Phytochemistry*, 1995, **40**, 1633 (*pmr, cmr, ms*)
Morita, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1603 (*synth*)
Raharivelomanana, P. *et al., Phytochemistry*, 1998, **47**, 1085-1088 (*cmr*)
Toyota, M. *et al., Chem. Pharm. Bull.*, 2004, **52**, 481-484 (*Tylimanthus tenellus constit*)

4,7(11)-Eudesmadiene-12,13-diol E-862

4,7(11)-Selinadiene-12,13-diol

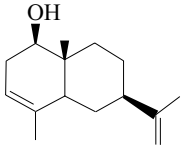


$C_{15}H_{24}O_2$ 236.353

Di-Ac: ***Coralloidin D***
[110299-95-1]
$C_{19}H_{28}O_4$ 320.428
Constit. of *Alcyonium coralloides*. Oil. $[\alpha]_D^{20}$ -14.1 (c, 0.227 in EtOH).
D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1987, **70**, 612

3,11-Eudesmadien-1-ol E-863

3,11-Selinadien-1-ol

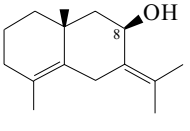


$C_{15}H_{24}O$ 220.354

1β-*form*
α-Dictyopterol
Constit. of *Dictyopteris divaricata*.
Oil.
Kurosawa, E. *et al., Bull. Chem. Soc. Jpn.*, 1966, **39**, 2509 (*isol, struct*)
Taber, D.F. *et al., J.O.C.*, 1995, **60**, 5537 (*synth*)

4,7(11)-Eudesmadien-8-ol E-864

4,7(11)-Selinadien-8-ol

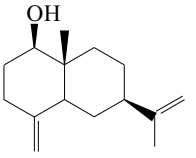


$C_{15}H_{24}O$ 220.354

8β-*form* [97530-58-0]
Constit. of soft coral *Nephthea* sp.
Cryst.
Mp 59-60°. $[\alpha]_D$ -10.
8-Ketone: ***4,7(11)-Eudesmadien-8-one***
[97530-59-1]
$C_{15}H_{22}O$ 218.338
Constit. of *Nephthea* sp. Oil. $[\alpha]_D$ +99.
Coll, J.C. *et al., Tetrahedron*, 1985, **41**, 1085

4(15),11-Eudesmadien-1-ol E-865

4(15),11-Selinadien-1-ol

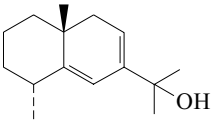


$C_{15}H_{24}O$ 220.354

1β-*form*
β-Dictyopterol
[87332-43-2]
Constit. of *Dictyopteris divaricata* and *Chrysanthemum morifolium*.
Cryst.
Mp 71-73°. $[\alpha]_D^{17}$ +18.9 (c, 0.75 in MeOH).
1-Ketone: 4(15),11-Eudesmadien-1-one. ***Dictyopterone***
$C_{15}H_{22}O$ 218.338
From *Dictyopteris divaricata*. Oil. $[\alpha]_D^{21}$ -12.5 (c, 2.16 in CCl_4).
Kurosawa, E. *et al., Bull. Chem. Soc. Jpn.*, 1966, **39**, 2509 (*isol, struct*)
Wijnberg, J.B.P.A. *et al., J.O.C.*, 1983, **48**, 4380 (*synth*)
Hu, L. *et al., Phytochemistry*, 1997, **44**, 1287 (*isol, pmr, cmr*)

5,7-Eudesmadien-11-ol E-866

5,7-Selinadien-11-ol

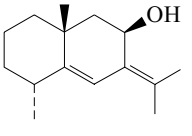


$C_{15}H_{24}O$ 220.354

(4α,10β)-*form*
Ac: ***Coralloidin E***
[110299-96-2]
$C_{17}H_{26}O_2$ 262.391
Constit. of *Alcyonium coralloides*. Cryst.
Mp 55°. $[\alpha]_D^{20}$ +305 (c, 0.09 in EtOH).
D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1987, **70**, 612

5,7(11)-Eudesmadien-8-ol E-867

5,7(11)-Selinadien-8-ol

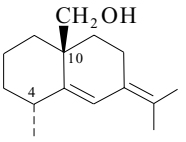


$C_{15}H_{24}O$ 220.354

8β-*form*
Oil. $[\alpha]_D^{20}$ +262 (c, 0.07 in cyclohexane).
Ac: ***Coralloidin A***
[105708-62-1]
$C_{17}H_{26}O_2$ 262.391
Constit. of *Alcyonium coralloides*. Oil. $[\alpha]_D^{20}$ +225 (c, 0.08 in cyclohexane).
Guerriero, A. *et al., J. Nat. Prod.*, 1986, **49**, 608

5,7(11)-Eudesmadien-14-ol E-868

5,7(11)-Selinadien-14-ol



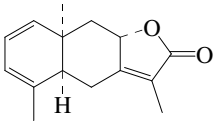
$C_{15}H_{24}O$ 220.354

(4α,10β)-*form* [110299-97-3]
Oil. $[\alpha]_D^{20}$ -172.9 (c, 0.14 in EtOH).

Ac: ***Coralloidin C***
[110299-91-7]
$C_{17}H_{26}O_2$ 262.391
Constit. of *Alcyonium coralloides*. Oil. $[\alpha]_D$ -168.7 (c, 0.34 in $CHCl_3$).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1987, **70**, 612

1,3,7(11)-Eudesmatrien-12,8-olide E-869

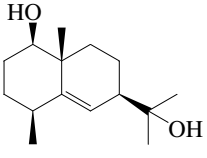


$C_{15}H_{18}O_2$ 230.306

(5α,10α)-*form*
Tubipolide B
[385793-33-9]
Constit. of *Tubipora musica*.
Oil. $[\alpha]_D^{25}$ -51.6 (c, 0.02 in $CHCl_3$). λ_{max} 225 (log ϵ 4.2); 266 (log ϵ 3.12) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2001, **64**, 1430-1433 (*isol, pmr, cmr*)

5-Eudesmene-1,11-diol E-870



1β-*form*

$C_{15}H_{26}O_2$ 238.369

1β-*form*
11-Ac: ***Junceol A***
[366788-43-4]
$C_{17}H_{28}O_3$ 280.406
Constit. of *Virgularia juncea*. Oil. $[\alpha]_D^{25}$ -1 (c, 0.1 in $CHCl_3$).

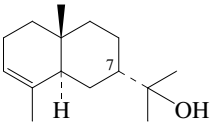
(1β,7β*H*)-*form* [87261-77-6]
Constit. of *Adelanthus lindenbergianus*.
Oil. $[\alpha]_D^{20}$ -21.5 (c, 0.6 in $CHCl_3$).

11-Me ether: 11-Methoxy-5-eudesmen-1-ol
[87279-31-0]
$C_{16}H_{28}O_2$ 252.396
Constit. of *Adelanthus lindenbergianus*. Oil. $[\alpha]_D^{20}$ -53.6 (c, 0.606 in $CHCl_3$).

Chen, S.-P. *et al., J. Nat. Prod.*, 2001, **64**, 1241-1242 (*isol, pmr, cmr*)
Bläs, B. *et al., Phytochemistry*, 2004, **65**, 127-137 (*Adelanthus lindenbergianus constit*)

3-Eudesmen-11-ol E-871

3-Selinen-11-ol



(5α,7α,10β)-*form*

$C_{15}H_{26}O$ 222.37

(5α,7α,10β)-*form*
7-Epi-α-eudesmol
[123123-38-6]
Constit. of *Amyris balsamifera* oil.
Oil.

(5α,7β,10β)-*form*
α-Eudesmol. *Selinelol*
[473-16-5]
Occurs with 4(15)-Eudesmen-11-ol in various eucalyptus oils and in the liverwort *Porella perrottetiana*.
Cryst. by subl.
Mp 87-89°. Bp_{10} 156°. $[\alpha]_D$ -8 (c, 1 in $CHCl_3$). Earlier samples were contaminated with 4(15)-Eudesmen-11-ol which has a large positive $[\alpha]_D$.

O-*(6-*O*-Tigloyl-β-*D*-glucopyranoside):* [125205-85-8]
$C_{26}H_{42}O_7$ 466.614
Constit. of *Pegolettia oxydonta*. Oil.

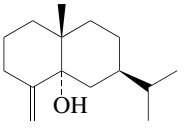
O-*[6-*O*-(3-Methylbutanoyl)-β-*D*-glucopyranoside]:* [125205-86-9]
$C_{26}H_{44}O_7$ 468.629
Constit. of *Pegolettia oxydonta*. Oil.

[51317-08-9, 69686-15-3]

McQuillan, F.J. *et al., J.C.S.*, 1956, 2973-2978 (*α-Eudesmol, isol, struct*)
Humber, D.C. *et al., Tet. Lett.*, 1966, 4985-4987 (*synth*)
Kutney, J.P. *et al., Can. J. Chem.*, 1984, **62**, 1407-1409 (*synth*)
Schwartz, M.A. *et al., J.O.C.*, 1985, **50**, 1359-1365 (*synth*)
Van Beek, T.A. *et al., Phytochemistry*, 1989, **28**, 1909-1911 (*7-Epi-α-eudesmol, isol*)
Zdero, C. *et al., Phytochemistry*, 1989, **28**, 1949-1953 (*glucosides*)
Raharivelomanana, P. *et al., Phytochemistry*, 1998, **47**, 1085-1088 (*cmr*)
Frey, B. *et al., Eur. J. Org. Chem.*, 1999, 1385-1394 (*synth*)
Toyota, M. *et al., Phytochemistry*, 1999, **52**, 689-694 (*synth, abs config*)

4(15)-Eudesmen-5-ol E-872

4(15)-Selinen-5-ol



5α-*form*

$C_{15}H_{26}O$ 222.37

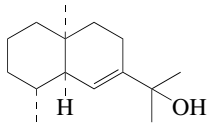
5α-*form* [70387-51-8]
Constit. of *Laurencia nipponica* and *Senecio rhyncholaenus*.
Oil. $[\alpha]_D$ +97.2 (c, 3 in $CHCl_3$).

(*ent*-5α)-*form* [352457-24-0]
Constit. of Haitian vetiver oil.

Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1763-1767 (*isol, pmr*)
Suzuki, M. *et al., Phytochemistry*, 1985, **24**, 2011
Weyerstahl, P. *et al., Flavour Fragrance J.*, 2000, **15**, 395-412 (*Vetiver oil constit*)

6-Eudesmen-11-ol E-873

6-Selinen-11-ol



(4α,5α,10α)-*form*

$C_{15}H_{26}O$ 222.37

(4α,5α,10α)-*form*

Constit. of Vetiver oil.
Oil. $[\alpha]_D$ -67 (c, 0.19 in $CHCl_3$).

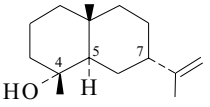
(4β,5α,10β)-*form*

Constit. of *Laurencia nipponica*.
Cryst. (MeOH).
Mp 49-50°. $[\alpha]_D^{20}$ +5.1 (c, 0.83 in $CHCl_3$).

Fukuzawa, A. *et al., Phytochemistry*, 1990, **29**, 2337 (*isol, pmr, cmr*)
Weyerstahl, P. *et al., Liebigs Ann./Recl.*, 1997, 1783-1787 (*isol, pmr, cmr, synth*)

11-Eudesmen-4-ol E-874

11-Selinen-4-ol



(4α,5α,7α,10β)–*form*

$C_{15}H_{26}O$ 222.37

(4α,5α,7α,10β)-*form*
Isointermedeol
[71963-78-5]
Constit. of *Cymbopogon flexuosus* (East Indian lemongrass).
Solid.
Mp 40-41°. $[\alpha]_D$ +2 (c, 3.3 in MeOH).

(4α,5α,7β,10β)-*form*
Kongol
[16641-47-7]
Constit. of essential oil of *Podocarpus dacrydioides*, *Nephthea brassica* and Japanese valerian. Cytotoxic to P388 and KB cell lines. Cryst.
Mp 94-96°. $[\alpha]_D^{20}$ -18.

4-O-*[3*-O-*Tigloyl-β-D-fucopyranoside]:*
$C_{26}H_{42}O_6$ 450.614
Constit. of *Pittosporum pentandrum*.

4-O-*[3-Methyl-2-butenoyl-(→3)-β-D-fucopyranoside]:*
$C_{26}H_{42}O_6$ 450.614
Constit. of *Pittosporum pentandrum*.

4-Ac: [249587-30-2]
$C_{17}H_{28}O_2$ 264.407
Constit. of *Nephthea brassica*. Oil. $[\alpha]_D^{25}$ -41.6 (c, 0.45 in $CHCl_3$).

Me ether: ***4-Methoxy-11-eudesmene***
[95360-08-0]
$C_{16}H_{28}O$ 236.397
Constit. of *Abies firma*. Oil. $[\alpha]_D$ -11.8.

(4α,5β,7β,10β)-*form*
Amiteol
[83378-02-3]
Constit. of the defence secretion of *Amitermes excellens*.
Oil. $[\alpha]_D^{24}$ +8 ($CHCl_3$).

(4β,5α,7β,10β)-*form*
Neointermedeol
[5945-72-2]
Constit. of *Bothriochloa intermedia*.
Oil. $Bp_{0.5}$ 85-87°. $[\alpha]_D^{25}$ +7.5 (c, 2.6 in EtOH).

(4β,5β,7β,10α)-*form*
Intermedeol. *Paradisiol*
[6168-59-8]
Constit. of *Bothriochloa intermedia* and *Citrus* spp. Shows cytotoxic activity. Cryst.
Mp 47-48°. $[\alpha]_D^{35}$ +10.7 (c, 0.957 in EtOH).

4-O-*β-D-Fucopyranoside:*
$C_{21}H_{36}O_5$ 368.512
Constit. of *Carthamus lanatus*. Cryst. (CH_2Cl_2/Et_2O).
Mp 179°. $[\alpha]_D^{22}$ -13.6 (c, 0.32 in $CHCl_3$).

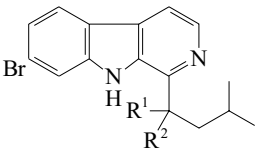
4-O-*[2*S-*Methylbutanoyl-(→2)-β-D-fucopyranoside]:*
$C_{26}H_{44}O_6$ 452.63
Constit. of *Carthamus lanatus*. Cryst.
Mp 86-88°. $[\alpha]_D^{22}$ -10.9 (c, 0.73 in $CHCl_3$).

[41664-11-3]

Corbett, R.E. *et al., Tet. Lett.*, 1967, 1009 (*Kongol*)
Chetty, G.L. *et al., Tet. Lett.*, 1968, 3223 (*synth, struct*)
Hoffmann, J.W. *et al., Tet. Lett.*, 1973, 751 (*Neointermedeol*)
Hoffmann, J.W. *et al., J.O.C.*, 1976, **41**, 3705 (*synth*)
Zalkow, V.B. *et al., J.O.C.*, 1976, **41**, 3710 (*synth*)
Thappa, R.K. *et al., Phytochemistry*, 1979, **18**, 671 (*Isointermedeol*)
Naya, Y. *et al., Tet. Lett.*, 1982, **23**, 3047 (*Amiteol*)
Kaneko, N. *et al., Phytochemistry*, 1985, **24**, 185-186 (*Methoxyeudesmene*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 2860 (*Intermedeol, pmr*)
Kawamata, T. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 3770 (*synth*)
San Feliciano, A. *et al., Phytochemistry*, 1990, **29**, 3204 (*deriv*)
Kesselmans, R.P.W. *et al., J.O.C.*, 1991, **56**, 7237 (*synth*)
Wassmuth-Wagner, I. *et al., Planta Med.*, 1995, **61**, 196 (*pmr, cmr*)
Ragasa, C.Y. *et al., Phytochemistry*, 1997, **45**, 545 (*glycosides*)
Raharivelomanana, P. *et al., Phytochemistry*, 1998, **47**, 1085-1088 (*cmr, ms*)
Sakar, M.K. *et al., Fitoterapia*, 1999, **70**, 103-105 (*Intermedeol, pmr, cmr*)
Duh, C.-Y. *et al., J. Nat. Prod.*, 1999, **62**, 1518-1521 (*Nephthea brassica constit, isol, activity*)
Park, H.-J. *et al., Planta Med.*, 2000, **66**, 783-784 (*Intermedeol, activity*)
Dachriyanus, A. *et al., Acta Cryst. C*, 2004, **60**, o503-o504 (*cryst struct*)

Eudistalbin A E-875

*7-Bromo-α-(2-methylpropyl)-9*H-*pyrido[3,4-*b*]indole-1-methanamine, 9CI*
[142755-07-5]



$R^1 = H$, $R^2 = NH_2$

$C_{16}H_{18}BrN_3$ 332.242
Alkaloid from the marine tunicate *Eudistoma album*. Exhibits cytotoxicity *in vitro* against KB human buccal carcinoma. Amorph. Sol. MeOH. $[\alpha]_D$ -10 (c, 0.1 in MeOH). λ_{max} 220 (sh); 240 (ε 45400); 290 (sh); 295 (ε 23200); 338 (ε 5790); 350 (ε 5790) (MeOH) (Derep). λ_{max} 240 (ε 45386); 295 (ε 23157); 338 (ε 5789); 350 (ε 5789) (MeOH) (Berdy).

Adesanya, S.A. *et al., J. Nat. Prod.*, 1992, **55**, 525-527 (*isol, uv, ir, pmr, cmr, ms, struct*)

Eudistalbin B E-876

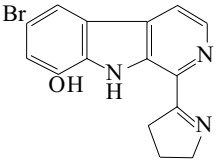
*1-(7-Bromo-9*H-*pyrido[3,4-*b*]-indol-1-yl)-3-methyl-1-butanone, 9CI*
[142755-08-6]
As Eudistalbin A, E-875 with
$R^1R^2 = O$

$C_{16}H_{15}BrN_2O$ 331.211
Alkaloid from the marine tunicate *Eudistoma album*. Amorph. Sol. MeOH. λ_{max} 210 (sh); 224 (ε 28400); 245 (ε 11700); 285 (ε 14700); 310 (ε 8120); 376 (ε 4730) (MeOH) (Derep).

Adesanya, S.A. *et al., J. Nat. Prod.*, 1992, **55**, 525-527 (*isol, uv, ir, pmr, ms, struct*)

Eudistomidin A E-877

*6-Bromo-1-(3,4-dihydro-2*H*-pyrrol-5-yl)-9*H*-pyrido[3,4-*b*]indol-8-ol, 9CI*
[102673-53-0]

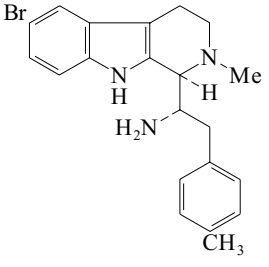


$C_{15}H_{12}BrN_3O$ 330.183
Alkaloid from the Okinawan tunicate *Eudistoma glaucus*. Calmodulin antagonist. Yellow solid.
Mp 225-230° dec Mp 260-270° dec Mp 265-280° dec. λ_{max} 222 (ϵ 33000); 254 (ϵ 17000); 371 (ϵ 5500) (MeOH) (Derep).

Kobayashi, J. *et al., Tet. Lett.*, 1986, **27**, 1191-1194 (*isol, uv, ir, pmr, cmr, ms, struct*)
Murakami, Y. *et al., Tet. Lett.*, 1989, **30**, 2099-2100 (*synth*)

Eudistomidin B E-878

*6-Bromo-2,3,4,9-tetrahydro-2-methyl-α-[(4-methylphenyl)-methyl]-1*H*-pyrido[3,4-*b*]indole-1-methanamine, 9CI*
[125443-66-5]

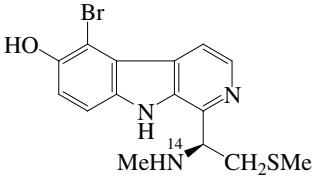


$C_{21}H_{24}BrN_3$ 398.345
Alkaloid from the marine tunicate *Eudistoma glaucus*. Cytotoxic. Activates rabbit heart muscle actomyosin ATPase. Yellow foam.
Mp 81-83°. $[\alpha]_D^{22}$ -54 (c, 0.2 in MeOH). $[\alpha]_D$ -76.4 (c, 0.3 in $CHCl_3$). λ_{max} 231 (ϵ 26900); 291 (ϵ 6300) (MeOH) (Derep).

Kobayashi, J. *et al., J.O.C.*, 1990, **55**, 3666-3670 (*isol, pmr, cmr, struct*)

Eudistomidin C E-879

*5-Bromo-1-[1-(methylamino)-2-(methylthio)ethyl]-9*H*-pyrido[3,4-*b*]indol-6-ol, 9CI*
[125422-17-5]



Absolute Configuration

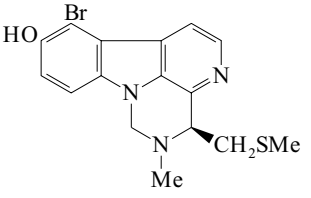
$C_{15}H_{16}BrN_3OS$ 366.281
Alkaloid from the marine tunicate *Eudistoma glaucus*. Cytotoxic. Exhibits calmodulin antagonistic activity. Yellow solid.
Mp 120-122°. $[\alpha]_D^{22}$ +15.6 (c, 0.2 in MeOH). λ_{max} 218 (ϵ 21300); 236 (ϵ 23700); 253 (sh) (ϵ); 287 (sh) (ϵ); 298 (ϵ 13100); 368 (ϵ 3800) (MeOH) (Derep).

N^{14}*-Me:* **N^{14}-*Methyleudistomidin C***
[380614-19-7]
$C_{16}H_{18}BrN_3OS$ 380.308
Alkaloid from *Eudistoma gilboverde*. Cytotoxic. Yellowish gum.
$[\alpha]_D$ +12.9 (c, 0.07 in MeOH). λ_{max} 216 (log ϵ 4.28); 234 (log ϵ 4.16); 252 (log ϵ 4.06); 287 (sh) (log ϵ 3.77); 298 (log ϵ 3.93); 369 (log ϵ 3.22) (EtOH).

Kobayashi, J. *et al., J.O.C.*, 1990, **55**, 3666-3670 (*isol, pmr, cmr, struct*)
Rashid, M.A. *et al., J. Nat. Prod.*, 2001, **64**, 1454-1456 (*N^{14}-Methyleudistomidin C*)

Eudistomidin F E-880

*7-Bromo-2,3-dihydro-2-methyl-3-[(methylthio)methyl]-1*H*-2,4,10*b*-triazafluoranthen-8-ol, 9CI*
[136094-36-5]



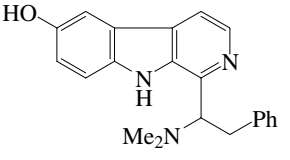
$C_{16}H_{16}BrN_3OS$ 378.292
Alkaloid from the marine tunicate *Eudistoma glaucus*. Amorph. $[\alpha]_D^{26}$ +16 (c, 0.1 in MeOH). Stereochem. not confirmed. λ_{max} 220 (ϵ 19000); 237 (ϵ 18000); 300 (ϵ 11000) (MeOH) (Derep). λ_{max} 218 (ϵ 18000); 237 (ϵ 17000); 300 (ϵ 10000) (MeOH) (Berdy).

S-*Oxide:* ***Eudistomidin E***
[136094-35-4]
$C_{16}H_{16}BrN_3O_2S$ 394.291
Alkaloid from the marine tunicate *Eudistoma glaucus*. Amorph. $[\alpha]_D^{24}$ +19 (c, 0.1 in MeOH). λ_{max} 220 (ϵ 19000); 237 (ϵ 18000); 300 (ϵ 11000) (MeOH) (Derep).

Murata, O. *et al., Tet. Lett.*, 1991, **32**, 3539-3542 (*isol, pmr, cmr, struct*)

Eudistomin X E-881

*1-(1-Dimethylamino-2-phenylethyl)-9*H*-pyrido[3,4-*b*]indol-6-ol*



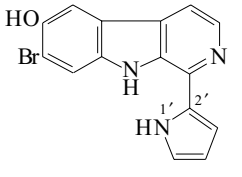
$C_{21}H_{21}N_3O$ 331.416

(ξ)-*form* [492463-46-4]
Alkaloid from the marine tunicate *Eudistoma* sp.
Amorph. brown powder. $[\alpha]_D^{20}$ -7 (c, 0.49 in MeOH). λ_{max} 201; 234; 251; 298; 373 (MeOH).

Schupp, P. *et al., J. Nat. Prod.*, 2003, **66**, 272-275 (*isol, pmr, cmr, ms*)

Eudistomin A E-882

*7-Bromo-1-(1*H*-pyrrol-2-yl)-9*H*-pyrido[3,4-*b*]indol-6-ol, 9CI. 7-Bromo-6-hydroxy-1-(2-pyrrolyl)-β-carboline*
[88704-36-3]



$C_{15}H_{10}BrN_3O$ 328.167
Alkaloid from the Caribbean tunicate *Eudistoma olivaceum*. Modestly active against viruses, gram-positive bacteria and yeasts. Yellow oil. λ_{max} 210 (ϵ 17600); 229 (sh); 258 (ϵ 13600); 272 (sh); 285 (sh); 326 (ϵ 11600); 373 (ϵ 6400); 389 (sh) (MeOH) (Derep).

*Debromo: 1-(1*H*-Pyrrol-2-yl)-9*H*-pyrido[3,4-*b*]indol-6-ol, 9CI. 6-Hydroxy-1-(2-pyrrolyl)-β-carboline.* ***Eudistomin M***
[88704-39-6]
$C_{15}H_{11}N_3O$ 249.271
Alkaloid from the tunicate *Eudistoma olivaceum*. Antiviral agent.

ATPase stimulant used as biochem. tool in study of muscular contraction. Yellow prisms ($CHCl_3$/MeOH).
Mp 225-227° (synthetic). λ_{max} 210 (ϵ 24000); 231 (ϵ 16500); 253 (ϵ 18000); 266 (sh) (ϵ 12700); 276 (sh) (ϵ 9900); 289 (sh) (ϵ 6800); 321 (ϵ 17100); 371 (ϵ 9900); 384 (ϵ 9800) (MeOH) (Derep).

*$\Delta^{1'}$-Isomer, 3′,4′-dihydro: 7-Bromo-1-(3,4-dihydro-2*H*-pyrrol-5-yl)-9*H*-pyrido[3,4-*b*]indol-6-ol, 9CI.* ***Eudistomin P***
[88704-48-7]
$C_{15}H_{12}BrN_3O$ 330.183
Found in *Eudistoma olivaceum*. Modestly active against gram-positive bacteria and yeasts. Sol. MeOH, $CHCl_3$, toluene; poorly sol. H_2O.
Mp 128-130°. λ_{max} 201 (sh); 216 (ϵ 28100); 249 (ϵ 11800); 300 (ϵ 13400); 318 (sh); 372 (ϵ 4600); 381 (ϵ 4800) (MeOH) (Derep). λ_{max} 216 (ϵ 28100); 249 (ϵ 11800); 300 (ϵ 10700); 372 (ϵ 4600); 381 (ϵ 4800) (hexane) (Berdy).

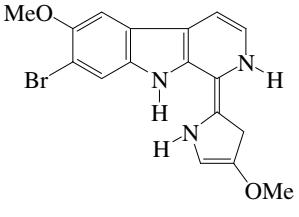
*$\Delta^{1'}$-Isomer, 3′,4′-dihydro, deoxy: 7-Bromo-1-(3,4-dihydro-2*H*-pyrrol-5-yl)-9*H*-pyrido[3,4-*b*]indole, 9CI.* ***Eudistomin G***
[88704-43-2]
$C_{15}H_{12}BrN_3$ 314.184
Found in *Eudistoma olivaceum*. Antiviral agent. Needles (CH_2Cl_2). Sol. MeOH, toluene, $CHCl_3$; poorly sol. H_2O.
Mp 204-206°. λ_{max} 220 (ϵ 36900); 238 (ϵ 17600); 284 (ϵ 18200); 297 (sh) (ϵ 10400); 370 (ϵ 7900) (MeOH) (Derep). λ_{max} 203 (ϵ 19000); 219 (ϵ 21500); 250 (ϵ 10000); 282 (ϵ 11700); 299 (ϵ 8700); 307 (ϵ 8400); 346 (ϵ 5100); 362 (ϵ 7600) (hexane) (Berdy).

$\Delta^{1'}$-Isomer, 3′,4′-dihydro, debromo: 6-Hydroxy-1-(1-pyrrolin-2-yl)-β-carboline. ***Eudistomin Q***
[88704-49-8]
$C_{15}H_{13}N_3O$ 251.287
Found in *Eudistoma olivaceum*. Modestly active against gram-positive bacteria. Sol. MeOH, $CHCl_3$, toluene; poorly sol. H_2O.
Mp 120-125°. λ_{max} 216 (ϵ 23500); 250 (ϵ 8700); 295 (ϵ 9600); 382 (ϵ 2900) (MeOH) (Derep). λ_{max} 214 (ϵ 19900); 288 (ϵ 8000); 348 (ϵ 2500); 362 (ϵ 2500) (hexane) (Berdy).

Kobayashi, J. *et al., J.A.C.S.*, 1984, **106**, 1526-1528 (*Eudistomins M,P,G,Q, isol, pmr, struct*)
Rinehart, K.L. *et al., J.A.C.S.*, 1987, **109**, 3378-3387 (*Eudistomins M,P,G,Q, isol, struct, props*)
Hino, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2596-2600 (*Eudistomins M,P, synth*)
Wasserman, H.H. *et al., Tet. Lett.*, 1989, **30**, 7117-7120 (*Eudistomin M, synth*)
Ohizumi, Y. *et al., J. Pharmacol. Exp. Ther.*, 1998, **285**, 381-389 (*Eudistomin M, use*)

Eudistomin B E-883

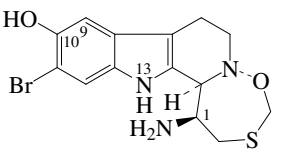
[96426-92-5]



$C_{17}H_{16}BrN_3O_2$ 374.236
Alkaloid antibiotic. Found in the Caribbean tunicate *Eudistoma olivaceum*. Shows activity against viruses, bacteria and yeasts.
Rinehart, K.L. *et al., J.A.C.S.*, 1987, **109**, 3378-3387 (*isol, struct, props*)

Eudistomin C E-884

*1-Amino-11-bromo-1,2,7,8,13,13*b*-hexahydro[1,6,2]oxathiazepino[2′,3′:1,2]pyrido[3,4-*b*]indol-10-ol, 9CI*
[88704-50-1]



Absolute Configuration

$C_{14}H_{16}BrN_3O_2S$ 370.269
Stereochem. of N–O bond revised in 1987. CA numbering shown. Alkaloid from the Caribbean tunicate *Eudistoma olivaceum* and the New Zealand ascidian *Ritterella sigillinoides*. Potent antiviral agent. Pale-yellow oil. $[\alpha]_D^{25}$ -52 (c, 0.4 in MeOH). Eudistomins C, E, F, K and L are the most potent of the group. λ_{max} 226 (ϵ 23400); 287 (ϵ 8000) (MeOH) (Derep).

N-*Methoxycarbonyl:* ***Eudistomin F***
[96426-93-6]
$C_{16}H_{18}BrN_3O_4S$ 428.306
Found in *Eudistoma olivaceum*. Potent antiviral agent. Oil. Sol. MeOH, $CHCl_3$, toluene; poorly sol. H_2O, hexane. λ_{max} 226 (ϵ 23400); 287 (ϵ 8000) (MeOH) (Derep). λ_{max} 225 (ϵ 10800); 276; 287 (ϵ 4100) (MeOH) (Berdy).

Deoxy: ***Eudistomin K***
[88704-52-3]
$C_{14}H_{16}BrN_3OS$ 354.27
From *Eudistoma olivaceum* and from the New Zealand ascidian *Ritterella sigillinoides*. Potent antiviral agent. Oil. Sol. MeOH, toluene, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -102 (c, 0.2 in MeOH). λ_{max} 230 (ϵ 11900); 237 (sh) (ϵ); 284 (ϵ 3470); 293 (ϵ); 301 (ϵ) (EtOH) (Derep). λ_{max} 226; 229 (ϵ 17000); 284 (ϵ 4000); 287 (MeOH) (Berdy).

Deoxy, S*-oxide (α-):* ***Eudistomin K sulfoxide***
[115276-12-5]
$C_{14}H_{16}BrN_3O_2S$ 370.269
Isol. from *Ritterella sigillinoides*. Shows antiviral props. Light yellow oil. $[\alpha]_D^{25}$ -3.3 (c, 0.09 in MeOH). λ_{max} 230 (ϵ 11900); 237 (sh) (ϵ); 284 (ϵ 3470); 293 (ϵ); 301 (ϵ) (EtOH) (Derep). λ_{max} 229 (ϵ 11920); 284 (ϵ 3470) (MeOH) (Berdy).

Debromo, 9-bromo: ***Eudistomin E***
[88704-51-2]
$C_{14}H_{16}BrN_3O_2S$ 370.269
Alkaloid from the Caribbean tunicate *Eudistoma olivaceum*. Potent antiviral agent. Pale-yellow oil. Sol. MeOH, $CHCl_3$, toluene; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -18 (c, 0.1 in MeOH). λ_{max} 226 (ϵ 23400); 287 (ϵ 8000) (MeOH) (Derep). λ_{max} 226 (ϵ 18600); 282 (ϵ 6700); 287 (MeOH) (Berdy).

*Debromo, 9-bromo, 1-*N*-Me:* N^{10}*-Methyleudistomin E.* ***Eudistomin V***†
[230636-55-2]
$C_{15}H_{18}BrN_3O_2S$ 384.296
Isol. from *Eudistoma olivaceum*. Not to be confused with, 7-Bromo.

Deoxy, debromo: ***Debromoeudistomin K***
[110597-53-0]
$C_{14}H_{17}N_3OS$ 275.374
From *Ritterella sigillinoides*. Sol. MeOH, EtOAc, Me_2CO, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ -58.3 (c, 0.06 in MeOH). λ_{max} 223 (ϵ 11500); 272 (ϵ 2900); 285 (ϵ 17270); 375 (ϵ 15870) (MeOH) (Berdy).

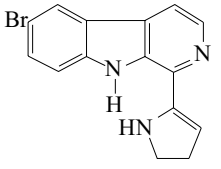
Deoxy, debromo, 10-bromo: ***Eudistomin L***
[88704-55-6]
$C_{14}H_{16}BrN_3OS$ 354.27
Alkaloid from the Caribbean tunicate *Eudistoma olivaceum*. Potent antiviral agent. Sol. MeOH, $CHCl_3$, toluene; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -77 (c, 0.2 in MeOH). Stereochem. of N–O bond revised in 1987. λ_{max} 230 (ϵ 11900); 237 (sh) (ϵ); 284 (ϵ 3470); 293 (ϵ); 301 (ϵ) (EtOH) (Derep). λ_{max} 226 (ϵ 26600); 288 (ϵ 6100) (MeOH) (Berdy).

Deoxy, debromo, 10-bromo, 1-N-*Ac:* N-*Acetyleudistomin L*
[123492-40-0]
$C_{16}H_{18}BrN_3O_2S$ 396.307
Amorph. solid. Mp 193.5-195.5°.

Rinehart, K.L. *et al., J.A.C.S.*, 1984, **106**, 1524-1526; 1987, **109**, 3378-3387 (*isol, uv, pmr, struct, Eudistomins E,F,K*)
Eur. Pat., 1985, 133 000; *CA*, **102**, 226023 (*isol, props*)
Blunt, J.W. *et al., Tet. Lett.*, 1987, **28**, 1825-1826 (*Eudistomins F,K, pmr, cmr, stereochem*)
Lake, R.J. *et al., Tet. Lett.*, 1988, **29**, 2255-2256; 4971-4972 (*Eudsitomin K S-oxide, Eudistomin K, cryst struct, abs config*)
Lake, R.J. *et al., Aust. J. Chem.*, 1989, **42**, 1201-1206 (*Debromoeudistomin K*)
Still, I.W.J. *et al., Tet. Lett.*, 1989, **30**, 1041-1044 (*N-Acetyleudistomin L, synth, pmr, cmr, ms*)
Liu, J.-J. *et al., Heterocycles*, 1990, **31**, 229-231 (*Eudistomin F, synth*)
Ibanez-Calero, S. *et al., CA*, 1999, **131**, 100027f (*N-Methyleudistomin E*)
Liu, J.-J. *et al., J.C.S. Perkin 1*, 2000, 3477-3486; 3487-3494 (*Eudistomins C,E,F,K,L, synth*)
Yamashita, T. *et al., J.A.C.S.*, 2005, **66**, 15038-15039 (*synth*)

Eudistomin H E-885

*6-Bromo-1-(3,4-dihydro-2*H*-pyrrol-5-yl)-9*H*-pyrido[3,4-*b*]indole, 9CI. 6-Bromo-1-(1-pyrrolin-2-yl)-β-carboline*
[88704-44-3]



$C_{15}H_{12}BrN_3$ 314.184
Alkaloid from the Caribbean tunicate *Eudistoma olivaceum*. Shows mod. activity against yeasts and viruses. Powder. Sol. MeOH, $CHCl_3$, toluene; poorly sol. H_2O.
Mp 140-142°. λ_{max} 220 (ε 36900); 238 (ε 17600); 284 (ε 18200); 297 (sh) (ε 10400); 370 (ε 7900) (MeOH) (Derep). λ_{max} 221 (ε 18300); 286 (ε 8300); 371 (ε 3000) (MeOH) (Berdy). λ_{max} 203 (ε 24700); 221 (ε 34200); 250 (ε 12400); 258 (ε 10000); 286 (ε 17000); 306 (ε 9400); 369 (ε 8400) (hexane) (Berdy).

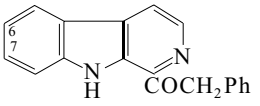
Debromo: ***Eudistomin I****. 1-(3,4-Dihydro-2*H*-pyrrol-5-yl)-9*H*-pyrido[3,4-*b*]indole, 9CI. 1-(1-Pyrrolin-2-yl)-β-carboline*
[88704-45-4]
$C_{15}H_{13}N_3$ 235.288
Found in *Eudistoma olivaceum*. Modestly active against gram-positive bacteria and viruses. Powder. Sol. MeOH, toluene, $CHCl_3$; poorly sol. H_2O.
Mp 153-155°. λ_{max} 227 (ε 14500); 282 (ε 11300); 368 (ε 5700) (CH_2Cl_2) (Derep). λ_{max} 216 (ε 24400); 247 (ε 3500); 277 (ε 14100); 298 (ε 7800); 366 (ε 9200) (MeOH) (Derep). λ_{max} 215 (ε 13800); 238 (ε 8500); 280 (ε 7000); 368 (ε 2800) (MeOH) (Berdy). λ_{max} 217 (ε 23800); 249 (ε 6500); 256 (ε 6000); 279 (ε 10700); 293 (ε 4700); 365 (ε 7000) (hexane) (Berdy).

7-Bromo: ***Eudistomin V***†
[211427-62-2]
$C_{15}H_{11}Br_2N_3$ 393.08
Alkaloid from the tunicate *Pseudodistoma aureum*. Yellow gum. λ_{max} 224 (ε 30000); 290 (ε 16000); 311 (ε 11900); 371 (ε 6300) (MeOH).

Kobayashi, J. *et al., J.A.C.S.*, 1984, **106**, 1526-1528 (*Eudistomin I, isol, struct*)
Rinehart, K.L. *et al., J.A.C.S.*, 1987, **109**, 3378-3387 (*isol, struct, props, rev*)
Hino, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2596-2600 (*Eudistomins H and I, synth*)
Van Wagenen, B.C. *et al., Tet. Lett.*, 1989, **30**, 3605-3608 (*Eudistomin I, synth*)
Wasserman, H.H. *et al., Tet. Lett.*, 1989, **30**, 7117-7120 (*Eudistomin I, synth*)
McNulty, J. *et al., J.C.S. Perkin 1*, 1994, 1329-1337 (*synth*)
Shen, G.Q. *et al., Tet. Lett.*, 1994, **35**, 1141-1144; 4923-4926 (*biosynth*)
Davis, R.A. *et al., J. Nat. Prod.*, 1998, **61**, 959-960 (*Eudistomin V*)

Eudistomin T E-886

*2-Phenyl-1-(9*H*-pyrido[3,4-*b*]indol-1-yl)ethanone, 9CI. 1-Phenylacetyl-β-carboline*
[108335-05-3]



$C_{19}H_{14}N_2O$ 286.332
Alkaloid from the marine tunicate *Eudistoma olivaceum*. Yellow cryst. (MeOH).
Mp 160-161°. λ_{max} 227 (ε 24100); 280 (ε 56100); 380 (ε 7000) (no solvent reported) (Derep). λ_{max} 227 (ε 39900); 292 (ε 21400); 379 (ε 7600) (CH_2Cl_2) (Derep).

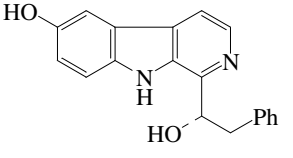
6-Bromo: ***Eudistomin S***
[108335-04-2]
$C_{19}H_{13}BrN_2O$ 365.228
Alkaloid from *Eudistoma olivaceum*. Yellow cryst. (MeOH).
Mp 168°. λ_{max} 227 (ε 24100); 280 (ε 56100); 380 (ε 7000) (no solvent reported) (Derep). λ_{max} 227 (ε 39900); 292 (ε 21400); 379 (ε 7600) (CH_2Cl_2) (Derep).

7-Bromo: ***Eudistomin R***
[108335-03-1]
$C_{19}H_{13}BrN_2O$ 365.228
Alkaloid from *Eudistoma olivaceum*. λ_{max} 227 (ε 24100); 280 (ε 56100); 380 (ε 7000) (no solvent reported) (Derep). λ_{max} 227 (ε 39900); 292 (ε 21400); 379 (ε 7600) (CH_2Cl_2) (Derep).

Kinzer, K.F. *et al., Tet. Lett.*, 1987, **28**, 925-926 (*uv, ir, pmr, ms, struct*)
Still, I.W.J. *et al., Heterocycles*, 1989, **29**, 2057 (*synth, cmr, Eudistomins S and T*)
Wasserman, H.H. *et al., Tet. Lett.*, 1989, **30**, 7117 (*synth*)
Bracher, F. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1994, **327**, 121 (*synth*)
McNulty, J. *et al., J.C.S. Perkin 1*, 1994, 1329 (*synth*)
Rocca, P. *et al., Synth. Commun.*, 1995, **25**, 3373 (*synth*)
Molina, P. *et al., Tet. Lett.*, 1996, **37**, 9353 (*synth, Eudistomin S, Eudistomin T*)

Eudistomin W E-887

*1-(1-Hydroxy-2-phenylethyl)-9*H*-pyrido[3,4-*b*]indol-6-ol. 6-Hydroxy-α-phenylmethyl-9*H*-pyrido[3,4-*b*]indole-1-methanol, 9CI*



(*S*)-*form*

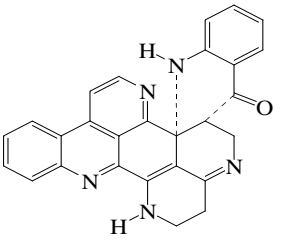
$C_{19}H_{16}N_2O_2$ 304.348

(*S*)-*form* [492463-95-3]
Alkaloid from the marine tunicate *Eudistoma* sp.
Amorph. brown powder. $[\alpha]_D^{20}$ -23 (c, 0.24 in MeOH). λ_{max} 208; 234; 266; 308; 405 (MeOH).

Schupp, P. *et al., J. Nat. Prod.*, 2003, **66**, 272-275 (*isol, pmr, cmr, ms*)

Eudistone A E-888

[135340-00-0]



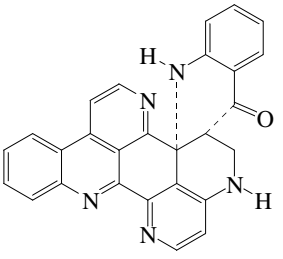
$C_{27}H_{19}N_5O$ 429.48

Alkaloid from the tunicate *Eudistoma* sp. Amorph. yellow powder. λ_{max} 210 (ϵ 44800); 238 (ϵ 48500); 260 (sh) (ϵ 24700); 323 (ϵ 15300); 338 (ϵ 15500); 359 (sh) (ϵ 13100); 395 (ϵ 10600) (MeOH) (Derep).

He, H.-Y. *et al., J.O.C.*, 1991, **56**, 5369-5371 (*isol, uv, ir, cd, pmr, cmr, struct*)

Eudistone B E-889

[135340-01-1]



$C_{27}H_{17}N_5O$ 427.464
Alkaloid from the tunicate *Eudistoma* sp. Amorph. powder. $[\alpha]_D$ -177.8 (c, 0.036 in MeOH). λ_{max} 204 (ϵ 45700); 239 (ϵ 47400); 259 (ϵ 39600); 324 (ϵ 14700) (MeOH) (Derep).

He, H.-Y. *et al., J.O.C.*, 1991, **56**, 5369-5371 (*isol, uv, ir, cd, pmr, cmr, struct*)

Eufauserase, BAN, INN E-890

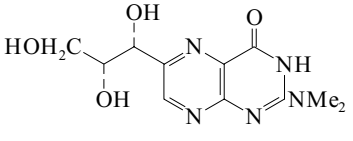
PHM 101

A purified extract from *Euphausia superba* (Euphausia Extract, BAN) contains serine proteases with a MW range of 20-40 kDA. Isol. from *Euphausia superba* (Antarctic krill). Broad-spectrum, monocomponent serine-protease enzyme. Used for debridement of necrotic tissue.

Pat. Coop. Treaty (WIPO), 1996, (*Phairson Medical*)96 24 371; *CA*, **125**, 265989k (*activity*)
Mekkes, J.R. *et al., Int. J. Biochem. Cell Biol.*, 1997, **29**, 703-706 (*pharmacol*)
Pat. Coop. Treaty (WIPO), 1998, (*Phairson Medical*)98 08 863; *CA*, **128**, 227064j (*cloning*)

Euglenapterin E-891

*2-Dimethylamino-6-(1,2,3-trihydroxypropyl)-4(3*H*)-pteridinone*
[73789-39-6]



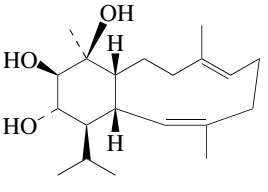
$C_{11}H_{15}N_5O_4$ 281.271
Found in the alga *Euglena gracilis*. Yellow cryst. (H_2O). Mp 200°. Occurs with 3′-*O*-phosphate and 2′,3′-cyclic phosphate. All show yellow fluorescence.

[73789-45-4]

Elstner, E. *et al., Arch. Biochem. Biophys.*, 1976, **173**, 614 (*isol*)
Jacobi, P.A. *et al., J.O.C.*, 1981, **46**, 5416 (*synth*)
Böhme, M. *et al., Annalen*, 1986, 1705 (*isol, cryst struct, uv, cd, pmr, synth*)

8,12-Eunicelladiene-2,3,4-triol E-892

2,6-Cladielladiene-11,12,13-triol



$C_{20}H_{34}O_3$ 322.487

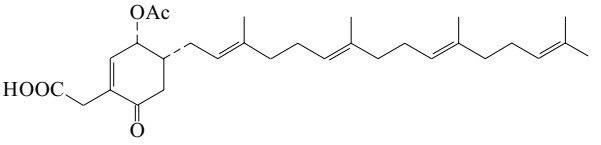
(2α,3β,4β,8*E*,12*Z*)-*form*

2,3-Di-Ac: [189818-92-6]
$C_{24}H_{38}O_5$ 406.561
Constit. of *Eunicella labiata*. Amorph. powder. $[\alpha]_D^{25}$ -18.3 (c, 0.4 in $CHCl_3$).

Ortega, M.J. *et al., J. Nat. Prod.*, 1997, **60**, 485-487 (*isol, pmr, cmr*)

Eunicenone B E-893

[152340-71-1]



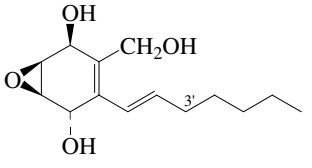
$C_{30}H_{44}O_5$ 484.675
Constit. of a *Eunicea* sp. Oil. $[\alpha]_D$ +101 (c, 0.8 in $CHCl_3$).

O-*De-Ac, Me ester:* ***Eunicenone A***
[152340-70-0]
$C_{29}H_{44}O_4$ 456.664
Constit. of a *Eunicea* sp. Oil. $[\alpha]_D$ +39.8 (c, 1.3 in $CHCl_3$).

Shin, J. *et al., Tetrahedron*, 1993, **49**, 9277 (*isol, pmr, cmr, cd*)
Lee, T. W. *et al., J.A.C.S.*, 2001, **123**, 1872-1877 (*synth*)

Eupenoxide E-894

3-(1-Heptenyl)-4-(hydroxymethyl)-7-oxabicyclo[4.1.0]hept-3-ene-2,5-diol, 9CI
[89773-19-3]



Absolute Configuration

$C_{14}H_{22}O_4$ 254.325
Abs. config. revised in 2004. Isol. from *Eupenicillium* sp. and a marine-derived *Phoma* sp. (CNC-651). Antifungal agent. λ_{max} 241 (EtOH) (Derep).

*3′,4′-Didehydro(*E*-): 3-(1,3-Heptadienyl)-4-(hydroxymethyl)-7-oxabicyclo[4.1.0]hept-3-ene-2,5-diol.* ***Phomoxide***
$C_{14}H_{20}O_4$ 252.31
Isol. from a marine-derived *Phoma* sp. (strain CNC-651). Amorph. powder. $[\alpha]_D$ -20 (c, 0.05 in MeOH). λ_{max} 203 (log ϵ 3.45); 230 (log ϵ 3.18); 275 (log ϵ 2.81) (MeOH).

Duke, R.K. *et al., J.O.C.*, 1984, **49**, 1898-1904 (*Eupenoxide*)
Liu, Z. *et al., Phytochemistry*, 2003, **64**, 571-574 (*Phomoxide*)
Mehta, G. *et al., Org. Lett.*, 2004, **6**, 2389-2392 (*synth, abs config*)

Euplomone E-895

[118337-10-3]

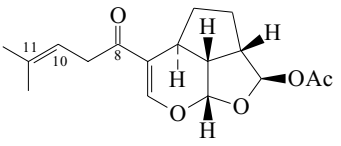
Peptide complex. The amino-acid sequences of 5 euplomones have been determined. Isol. from the ciliated protozoa *Euplotes raikovi*. Pheromones.

[104625-79-8, 120852-74-6, 120852-76-8, 129979-00-6]

Raffioni, S. *et al., J. Biol. Chem.*, 1988, **263**, 18152 (*struct*)
Raffioni, S. *et al., Biochemistry*, 1989, **28**, 5250 (*struct*)
Bradshaw, R.A. *et al., ACS Symp. Ser.*, 1990, **434**, 163 (*isol, struct*)
Anderson, D. *et al., J. Mol. Biol.*, 1990, **216**, 1 (*struct*)
Raffioni, S. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1992, **89**, 2071 (*isol, struct*)

Euplotin B E-896

[148000-40-2]



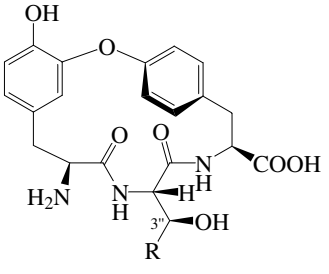
$C_{17}H_{22}O_5$ 306.358
Constit. of *Euplotes crassus*.

10,11-Dihydro: ***Euplotin A***
[148000-15-1]
$C_{17}H_{24}O_5$ 308.374
Constit. of *Euplotes crassus*. Cytotoxic agent.

8-Deoxo: ***Euplotin C***
[154512-15-9]
$C_{17}H_{24}O_4$ 292.374
Constit. of *Euplotes crassus*. Cytotoxic to ciliates.

Guella, G. *et al., J.C.S. Perkin 1*, 1994, 161 (*isol, pmr, cmr*)
Aungst, R.A. *et al., J.A.C.S.*, 2001, **123**, 9455-9456 (*Euplotin A, synth*)

Eurypamide A E-897



R = -CH(OH)CH_2NHC(=NH)NH_2 (*S*-)

$C_{24}H_{30}N_6O_8$ 530.536
Cyclic peptide. abs. config. revised in 2004. Constit. of the sponge *Microciona eurypa*. Powder.
Mp 171-175°. $[\alpha]_D$ -21.5 (c, 0.2 in MeOH). λ_{max} 203 (ϵ 45000); 231 (sh) (ϵ 9670); 271 (ϵ 2450); 278 (sh) (ϵ 2380) (MeOH).

Rami Reddy, M.V. *et al., Tetrahedron*, 1998, **54**, 10649-10656 (*isol, uv, ir, pmr, cmr, ms*)
Ito, M. *et al., Tetrahedron*, 2004, **60**, 5623-5634 (*synth, abs config*)

Eurypamide B E-898

As Eurypamide A, E-897 with
R = CH_3

$C_{22}H_{25}N_3O_7$ 443.455
Cyclic peptide. Constit. of the sponge *Microciona eurypa*.

3′′-Epimer: ***Eurypamide D***
$C_{22}H_{25}N_3O_7$ 443.455
From *Microciona eurypa*.

Rami Reddy, M.V. *et al., Tetrahedron*, 1998, **54**, 10649-10656 (*isol*)
Ito, M. *et al., Tetrahedron*, 2004, **60**, 5623-5634 (*synth*)

Eurypamide C E-899

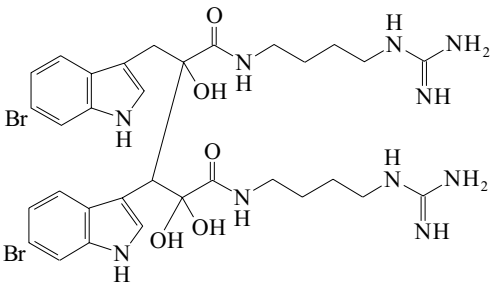
As Eurypamide A, E-897 with
R = H

$C_{21}H_{23}N_3O_7$ 429.429
Cyclic peptide. Constit. of the sponge *Microciona eurypa*.

Rami Reddy, M.V. *et al., Tetrahedron*, 1998, **54**, 10649-10656 (*isol*)

Eusynstyelamide E-900

[157878-21-2]

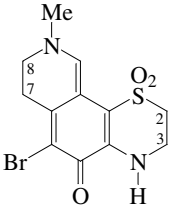


$C_{32}H_{42}Br_2N_{10}O_5$ 806.556
Highly modified tryptophan-arginine dipeptide dimer. Metab. from the ascidian *Eusynstyela misakiensis*.

Swersey, J.C. *et al., J. Nat. Prod.*, 1994, **57**, 842 (*isol, uv, ir, pmr, cmr, ms, struct*)

Euthyroideone A E-901

[219566-39-9]



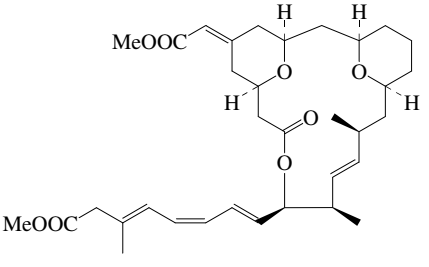
$C_{12}H_{13}BrN_2O_3S$ 345.216
Alkaloid from the bryozoan *Euthyroides episcopalis*.
Mp 245°. λ_{max} 202 (log ϵ 3.96); 242 (log ϵ 3.72); 383 (log ϵ 3.6); 452 (log ϵ 3.86) (MeOH).

2,3-Didehydro: ***Euthyroideone B***
[219566-38-8]
$C_{12}H_{11}BrN_2O_3S$ 343.201
Alkaloid from *Euthyroides episcopalis*.
Mp 244°. λ_{max} 208 (log ϵ 4.5); 310 (log ϵ 4.38); 436 (log ϵ 4.6) (MeOH).

7,8-Didehydro: ***Euthyroideone C***
[219566-40-2]
$C_{12}H_{11}BrN_2O_3S$ 343.201
Alkaloid from *Euthyroides episcopalis*. λ_{max} 203 (log ϵ 3.6); 280 (log ϵ 3.63); 391 (log ϵ 3.32) (MeOH).

Morris, B.D. *et al., J.O.C.*, 1998, **63**, 9545-9547

Exiguolide E-902



Relative Configuration

$C_{34}H_{48}O_8$ 584.748
Constit. of *Geodia exigua*. Viscous oil. $[\alpha]_D^{25}$ -92.5 (c, 0.07 in $CHCl_3$). λ_{max} 276 (ϵ 42200) (no solvent reported).

Ohta, S. *et al., Tet. Lett.*, 2006, **47**, 1957-1960 (*isol, pmr, cmr*)

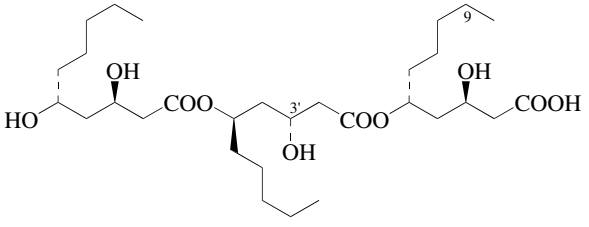
Exogastrula-inducing peptide D E-903

Peptide. Struct. constits of a chain of 53 amino-acid residues with 3 intramolecular disulfide bridges. Isol. from embryos of the Sea urchin *Anthocidaris crassispina*.

Suyemitsu, T. *et al., Cell Differ. Dev.*, 1989, **26**, 53 (*isol*)
Suyemitsu, T. *et al., Zool. Sci.*, 1991, **8**, 505 (*struct*)

Exophilin A E-904

[172703-87-6]



Absolute Configuration

$C_{30}H_{56}O_{10}$ 576.766
Prod. by *Exophiala pisciphila* and from the sponge *Mycale adhaerens*. Antibacterial agent. Viscous oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{27}$ -22.3 (c, 1 in $CHCl_3$).

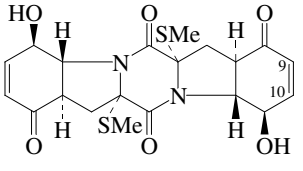
3′-Ac: ***Halymecin C***
[167173-82-2]
$C_{32}H_{58}O_{11}$ 618.804
Prod. by *Fusarium* sp. FE-71-1 from the marine alga *Halymenia dilatata*. Oil. $[\alpha]_D^{26}$ -9.2 (c, 3.2 in CH_2Cl_2).

9-Hydroxy: ***Halymecin E***
[167173-84-4]
$C_{30}H_{56}O_{11}$ 592.766
Prod. by *Fusarium* sp. FE-71-1 from the marine alga *Halymenia dilatata*. Stereochem. not confirmed.

Chen, C. *et al., J. Antibiot.*, 1996, **49**, 998 (*Halymecins*)
Doshida, J. *et al., J. Antibiot.*, 1996, **49**, 1105 (*isol, pmr, cmr, props*)

Exserohilone E-905

[99572-22-2]



Relative Configuration

$C_{20}H_{22}N_2O_6S_2$ 450.536

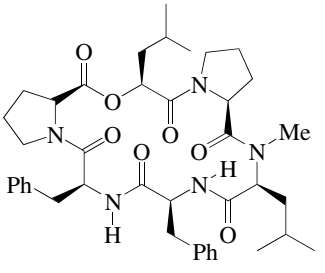
Diketopiperazine antibiotic. Prod. by *Exserohilum holmii* and a marine *Exserohilum rostrata*. Shows nonspecific phytotoxicity. Glass. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{21}$ -247 (c, 0.32 in $CHCl_3$).

9,10-Dihydro: ***Dihydroexserohilone***
$C_{20}H_{24}N_2O_6S_2$ 452.551
Prod. by *Exserohilum holmii*. Phytotoxin. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{21}$ -110 (c, 0.33 in $CHCl_3$).

Sugawara, K. *et al., J.O.C.*, 1985, **50**, 5631-5633 (*isol, pmr, cryst struct*)
Tan, R.X. *et al., J. Nat. Prod.*, 2004, **67**, 1374-1382 (*isol*)

Exumolide A E-906

[207227-48-3]



$C_{41}H_{55}N_5O_7$ 729.915

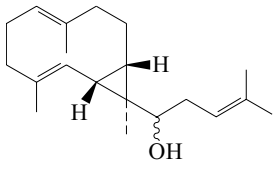
Depsipeptide antibiotic. Prod. by a marine fungus of the *Scytalidium* sp. Antimicroalgal agent. Solid. $[\alpha]_D$ -278 (c, 1.3 in $CHCl_3$). λ_{max} 203 (log ϵ 4.54) (MeOH).

N-*De-Me:* ***Exumolide B***
[207227-49-4]
$C_{40}H_{53}N_5O_7$ 715.888
Prod. by a *Scytalidium* sp. Antimicroalgal agent. Solid. $[\alpha]_D$ -288 (c, 2.1 in $CHCl_3$). λ_{max} 203 (log ϵ 4.52) (MeOH).

Jenkins, K.M. *et al., Tet. Lett.*, 1998, **39**, 2463-2466 (*isol, uv, ir, pmr, cmr*)

Faraunatin F-1

[161162-31-8]

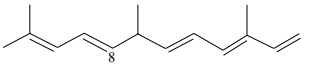


$C_{20}H_{32}O$ 288.472
Constit. of *Xenia faraunensis*.

Kashman, Y. *et al., Tet. Lett.*, 1994, **35**, 8855 (*isol, pmr, cmr*)

1,3,5,8,10-Farnesapentaene F-2

3,7,11-Trimethyl-1,3,5,8,10-dodecapentaene



$C_{15}H_{22}$ 202.339

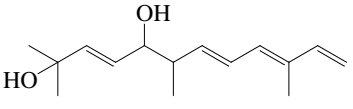
(3*E*,5*E*,8*E*)-*form* [73368-17-9]
Constit. of *Plexaurella grisea*.
Oil. $[\alpha]_D^{25}$ +55.1 (c, 0.45 in $CHCl_3$). λ_{max} 237 (ϵ 24960); 264 (ϵ 39640); 271 (ϵ 51380); 279 (ϵ 46240) (EtOH) (Derep).

(3*E*,5*E*,8*Z*)-*form* [73368-16-8]
Constit. of *Plexaurella grisea*.
Oil. $[\alpha]_D^{25}$ +50.2 (c, 0.33 in $CHCl_3$). λ_{max} 237 (ϵ 24960); 264 (ϵ 39640); 271 (ϵ 51380); 279 (ϵ 46240) (EtOH) (Derep).

Gopichand, Y. *et al., J.O.C.*, 1980, **45**, 2523

1,3,5,9-Farnesatetraene-8,11-diol F-3

2,6,10-Trimethyl-3,7,9,11-dodecatetraene-2,5-diol



$C_{15}H_{24}O_2$ 236.353

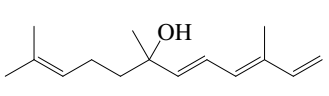
(3*E*,5*E*,9*E*)-*form*

Di-Ac: [340013-38-9]
$C_{19}H_{28}O_4$ 320.428
Constit. of *Plexaurella grisea*. Oil. $[\alpha]_D^{25}$ -2.1 (c, 0.28 in $CHCl_3$).

Rueda, A. *et al., J. Nat. Prod.*, 2001, **64**, 401-405 (*isol, pmr, cmr*)

1,3,5,10-Farnesatetraen-7-ol F-4

2,6,10-Trimethyl-2,7,9,11-dodecatetraen-6-ol, 9CI
[65580-18-9]



(3*E*,5*E*,7ξ)-*form*

$C_{15}H_{24}O$ 220.354

(3*E*,5*E*,7ξ)-*form* [67832-25-1]
[340013-36-7]
Constit. of *Ageratina aschenbornia*, *Ageratum fastigiatum*, *Brickellia* spp., *Plexaurella grisea* and *Critoniella acuminata*.
Oil. $[\alpha]_D^{25}$ -1.1 (c, 0.18 in $CHCl_3$).

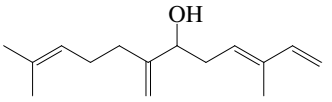
(3*Z*,5*E*,7ξ)-*form* [67832-24-0]
Constit. of *Ageratina aschenbornia*, *Brickellia californica*, *Critoniella acuminata* and *Eupatorium* spp.
Oil. $Bp_{0.1}$ 140°. $[\alpha]_D^{24}$ +15 (c, 1 in $CHCl_3$). λ_{max} 268; 278 (Et_2O).

[63147-23-9]

Bohlmann, F. *et al., Chem. Ber.*, 1977, **110**, 1321-1329 (*isol, pmr*)
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 566-567; 763-765; 1981, **20**, 1434-1435 (*isol, pmr*)
Rueda, A. *et al., J. Nat. Prod.*, 2001, **64**, 401-405 (*isol, pmr, cmr*)

1,3,7(14),10-Farnesatetraen-6-ol F-5

3,11-Dimethyl-7-methylene-1,3,10-dodecatrien-6-ol



$C_{15}H_{24}O$ 220.354

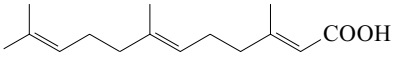
(3*E*,6ξ)-*form*

Ac: [340013-35-6]
$C_{17}H_{26}O_2$ 262.391
Oil. Constit. of *Plexaurella grisea*.
$[\alpha]_D^{25}$ +8.8 (c, 0.4 in $CHCl_3$). λ_{max} 228 (ϵ 14800) (MeOH).

Rueda, A. *et al., J. Nat. Prod.*, 2001, **64**, 401-405 (*isol, pmr, cmr*)

2,6,10-Farnesatrien-1-oic acid F-6

3,7,11-Trimethyl-2,6,10-dodecatrienoic acid. Farnesenic acid. Farnesylic acid. Farnesolic acid. ***Farnesic acid***
[7548-13-2]



$C_{15}H_{24}O_2$ 236.353
All isomers (*E,E; E,Z; Z,E;* and *Z,Z*) are known. Oil. Bp_{16} 202-206°.

Me ester: [10485-70-8]
$C_{16}H_{26}O_2$ 250.38
Produced by the mandibular glands of crustaceans. Moulting-inhibitory hormone. Also controls ovarian maturation and osmoregulation in different crustaceans studied. Oil. Bp_{10} 177-185°.

2,3-Dihydroxypropyl ester: [75957-03-8]
$C_{18}H_{30}O_4$ 310.433
Constit. of *Archidoris odhneri* and *Archidoris montereyensis*. Shows antibacterial props. Oil.

2-Acetoxy-3-hydroxypropyl ester:
$C_{20}H_{32}O_5$ 352.47
Constit. of *Archidoris odhneri*. Oil.

3-Acetoxy-2-hydroxypropyl ester:
$C_{20}H_{32}O_5$ 352.47
Constit. of *Archidoris odhneri*. Oil.

Me ester, 10,11-epoxide: Juvenile hormone III
[22963-93-5]
$C_{16}H_{26}O_3$ 266.38
Oil. $Bp_{0.08}$ 125-126°.

6S,7S:10R,11-Diepoxide, Me ester: ***Juvenile hormone B3****. Methyl 6,7:10,11-diepoxyfarnesate. Juvenile hormone III bisepoxide*
[120293-93-8]
$C_{16}H_{26}O_4$ 282.379
Constit. of the ring glands of *Drosophila melanogaster*.

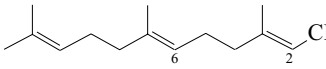
[68000-79-3, 137822-42-5, 146276-68-8]

Ohki, M. *et al., Agric. Biol. Chem.*, 1974, **38**, 175 (*synth*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1975, 913 (*cmr*)
Katzenellenbogen, J.A. *et al., J.A.C.S.*, 1976, **98**, 4925 (*synth*)
Pitzele, B.S. *et al., Tetrahedron*, 1976, **32**, 1347 (*synth*)
Kuhnz, W. *et al., Org. Magn. Reson.*, 1981, **16**, 138 (*cmr*)
Gustafson, K. *et al., Tetrahedron*, 1985, **41**, 1101-1108 (*2,3-dihydroxypropyl ester*)
Mori, K. *et al., Tetrahedron*, 1987, **43**, 4097 (*synth*)
Tobe, S.S. *et al., J. Exp. Zool.*, 1989, **249**, 165-171 (*occur, crustaceans*)
Richard, D.S. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1989, **86**, 1421 (*Juvenile hormone B3*)
Messeguer, A. *et al., Tetrahedron*, 1991, **47**, 1291 (*Juvenile hormone B3*)
Herlt, A.J. *et al., Chem. Comm.*, 1993, 1497 (*Juvenile hormone B_3*)
Rickards, R.W. *et al., Tet. Lett.*, 1993, **34**, 8369 (*Juvenile hormone B_3*)

Krug, P.J. *et al., Tetrahedron*, 1996, **52**, 6869 (*biosynth*)
Sen, S.E. *et al., J.O.C.*, 1997, **62**, 3529-3536 (*biosynth*)
Ungur, N. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 1263-1273 (*abs config*)

2,6,10-Farnesatrien-1-ol F-7

3,7,11-Trimethyl-2,6,10-dodecatrien-1-ol. ***Farnesol.*** *FEMA 2478*
[4602-84-0]



(2*E*,6*E*)*-form*

$C_{15}H_{26}O$ 222.37
Obt. synthetically as mixt. of geom. isomers by isom. of 1,6,10-Farnesatrien-3-ol. Component of many flower absolutes. Used in flower perfumes and as fixative in perfumery.
▶ LD_{50} (rat, orl) 6000 mg/kg. JR4979000

(2*E*,6*E*)*-form* [106-28-5]
Widespread. The main farnesol isomer, e.g. >90% of the farnesol component of the oil of *Hibiscus abelmoschus*. Nasonov pheromone of the honey bee *Apis mellifera*; constit. of temporal gland secretions of the African elephant (*Loxodonta africana*).
Liq. with a characteristic flowery odour. Bp_3 137°.

O-*Phosphate:* See 3,7,11-Trimethyl-2,6,10-dodecatrien-1-yl dihydrogen phosphate in *The Combined Chemical Dictionary.*

O-*[2-O-Acetyl-β-D-arabinopyranosyl-(1→4)-2,3-di-O-acetyl-β-D-arabinopyranoside]:*
$C_{31}H_{48}O_{12}$ 612.713
Constit. of a *Sinularia* sp.

O-*[α-L-Arabinopyranosyl-(1→3)-[α-L-rhamnopyranosyl-(1→2)][α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]:* ***Rubiginoside***
$C_{38}H_{64}O_{18}$ 808.913
Constit. of *Lepisanthes rubiginosa*. Glass. $[\alpha]_D$ -59 (c, 1 in MeOH).

Ac: [4128-17-0]
[29548-30-9] d_4^{20} 0.91. Mp 110°. $Bp_{0.3}$ 115-125°. n_D^{25} 1.4471.

Angeloyl: ***Farnesyl angelate***
[85527-05-5]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Lordhowea insularis*. Gum.

Hexanoyl: ***Farnesyl hexanoate***
[51532-28-6]
$C_{21}H_{36}O_2$ 320.514
Constit. of Dufour's gland secretion of *Andrena* spp.

Hexadecanoyl: ***Farnesyl palmitate***
[64144-82-7]
$C_{31}H_{56}O_2$ 460.782
Constit. of *Botryococcus braunii*.

9-Hexadecenoyl: ***Farnesyl palmitoleate***
[157501-13-8]
$C_{31}H_{54}O_2$ 458.766
Constit. of *Botryococcus braunii*.

9-Octadecenoyl: ***Farnesyl oleate***
[64144-81-6]
$C_{33}H_{58}O_2$ 486.82
Constit. of *Botryococcus braunii*.

9,12,15-Octadecatrienoyl: ***Farnesyl linolenate***
[157501-14-9]
$C_{33}H_{54}O_2$ 482.788
Constit. of *Botryococcus braunii*.

Aldehyde: 2,6,10-Farnesatrien-1-al. 3,7,11-Trimethyl-2,6,10-dodecatrienal. ***Farnesal***
[502-67-0]
[19317-11-4]
$C_{15}H_{24}O$ 220.354
Isol. from thoracic glands of male carpenter bees (*Xylocopa* spp.). Shows juvenile hormone activity. Oil. Bp_{14} 172-174°.

Aldehyde, semicarbazone: Mp 133-135°.

(2*E*,6*Z*)*-form* [3879-60-5] Bp_3 132°.

(2*Z*,6*E*)*-form* [3790-71-4]
Minor constit. of various essential oils including petitgrain oil.
Bp_3 135°.

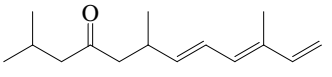
(2*Z*,6*Z*)*-form* [16106-95-9] Bp_3 127°.

[24163-97-1, 40266-29-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 149B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 226B; 226C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 219D; 220A (*ir*)
Bates, R.B. *et al., J.O.C.*, 1963, **28**, 1086 (*isol, struct*)
Burrell, J.W.K. *et al., J.C.S.(C)*, 1966, 2144 (*synth*)
Corey, E.J. *et al., J.A.C.S.*, 1967, **89**, 4245 (*synth*)
Hill, H.C. *et al., J.C.S.(C)*, 1968, 93 (*ms*)
Richards, J.B. *et al., Biochem. J.*, 1972, **128**, 1345 (*biosynth*)
Jacob, G. *et al., Phytochemistry*, 1972, **11**, 1683 (*biosynth*)
Evans, R.H. *et al., Chem. Comm.*, 1973, 465 (*biosynth*)
Nilles, G. *et al., J. Agric. Food Chem.*, 1973, **21**, 342 (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Tengo, J. *et al., J. Chem. Ecol.*, 1975, **1**, 253 (*hexanoyl, isol*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1975, 913 (*cmr*)
Cardillo, C.R. *et al., Chem. Comm.*, 1976, 190 (*synth*)
Pauling, H. *et al., Helv. Chim. Acta*, 1976, **59**, 1233 (*synth*)
Org. Synth., 1977, **56**, 112-117 (*synth, ir*)
Pickett, J.A. *et al., J. Chem. Ecol.*, 1980, **6**, 425 (*isol*)
Van Tamelen, E.E. *et al., Bioorg. Chem.*, 1982, **11**, 133-170 (*synth*)
Wheller, J.W. *et al., J. Chem. Ecol.*, 1982, **8**, 821 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 2537-2539 (*angelate*)
Amin, C *et al., Helv. Chim. Acta*, 1984, **67**, 1540-1546 (*synth, ir, pmr, ms*)
Yamagisawa, A. *et al., Chem. Lett.*, 1988, 1899-1902 (*synth*)
Andersen, J.F. *et al., J. Chem. Ecol.*, 1988, **14**, 1153 (*isol*)
Yoshioka, T. *et al., Phytochemistry*, 1990, **29**, 3469 (*biosynth*)
Shindo, T. *et al., Experientia*, 1992, **48**, 688-690 (*Sinularia glycoside*)
Christensen, D.J. *et al., Bioorg. Med. Chem.*, 1994, **2**, 631 (*synth*)
Inoue, H. *et al., Phytochemistry*, 1994, **36**, 1203 (*isol, iosynth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 277
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1059-1060
Leyes, A.E. *et al., Org. Lett.*, 1999, **1**, 1071-1074 (*biosynth*)
Adesanya, S.A. *et al., Phytochemistry*, 1999, **51**, 1039-1041 (*Rubiginoside*)
Yu, J.S. *et al., Org. Lett.*, 2005, **7**, 4803-4806 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAB800

1,3,5-Farnesatrien-9-one F-8

2,6,10-Trimethyl-7,9,11-dodecatrien-4-one



(3*E*,5*E*)*-form*

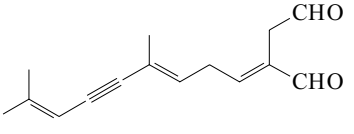
$C_{15}H_{24}O$ 220.354

(3*E*,5*E*)*-form* [340013-30-1]
Constit. of *Plexaurella grisea*.
Oil. $[\alpha]_D^{25}$ +38.4 (c, 0.87 in $CHCl_3$). λ_{max} 259 (ε 18000); 269 (ε 24600); 280 (ε 19500) (hexane).

(3*Z*,5*E*)*-form* [340013-33-4]
Constit. of *Plexaurella grisea*.
Oil. $[\alpha]_D^{25}$ +18.1 (c, 0.27 in $CHCl_3$). λ_{max} 260 (ε 16400); 280 (ε 16300) (hexane).

Rueda, A. *et al., J. Nat. Prod.*, 2001, **64**, 401-405 (*isol, pmr, cmr*)

3,6,10-Farnesatrien-8-yne-1,15-dial F-9

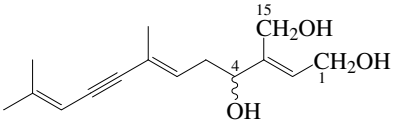


$C_{15}H_{18}O_2$ 230.306

(3*E*,6*E*)*-form*
Oxytoxin 2
[129932-68-9]

Constit. of *Oxynoe olivacea*; also from *Ascobulla fragilis* and *Lobiger serradifalci*.
Oil.
Cimino, G. *et al., Experientia*, 1990, **46**, 767-770 (*isol, pmr, cmr*)
Gavagnin, M. *et al., J. Exp. Mar. Biol. Ecol.*, 1994, **175**, 197-210

2,6,10-Farnesatrien-8-yne-1,4,15-triol F-10

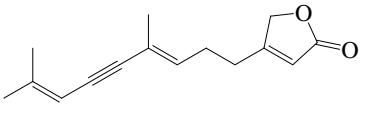


$C_{15}H_{22}O_3$ 250.337

(2Z,4ξ,6E)-form
1-O-*Tetradecanoyl, 4,15-di-Ac:* [488730-16-1]
$C_{33}H_{52}O_6$ 544.77
Constit. of *Caulerpa prolifera*.
1-O-*Hexadecanoyl, 4,15-di-Ac:* [488730-20-7]
$C_{35}H_{56}O_6$ 572.824
Constit. of *Caulerpa prolifera*.
1-O-*(9Z-Hexadecenoyl), 4,15-di-Ac:* [488730-17-2]
$C_{35}H_{54}O_6$ 570.808
Constit. of *Caulerpa prolifera*.
1-O-*(7Z,10Z,13Z-Hexadecatrienoyl), 4,15-di-Ac:* [488730-21-8]
$C_{35}H_{50}O_6$ 566.776
Constit. of *Caulerpa prolifera*.
1-O-*(9Z-Octadecenoyl), 4,15-di-Ac:* [488730-18-3]
$C_{37}H_{58}O_6$ 598.862
Constit. of *Caulerpa prolifera*.
1-O-*(9Z,12Z-Octadecadienoyl), 4,15-di-Ac:* [488730-19-4]
$C_{37}H_{56}O_6$ 596.846
Constit. of *Caulerpa prolifera*.
Smyrniotopoulos, V. *et al., J. Nat. Prod.*, 2003, **66**, 21-24 (*isol, pmr, cmr*)

2,6,10-Farnesatrien-8-yn-1,15-olide F-11

*4-(4,8-Dimethyl-3,7-nonadien-5-ynyl)-2(5*H*)-furanone*

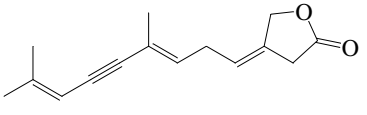


$C_{15}H_{18}O_2$ 230.306

(E)-form
Ascobullin A
[294199-62-5]
Constit. of *Ascobulla ulla*.
Cimino, G. *et al., Curr. Org. Chem.*, 1999, **3**, 327-372
Gavagnin, M. *et al., J. Chem. Ecol.*, 2000, **26**, 1563-1578 (*isol, pmr, cmr*)

3,6,10-Farnesatrien-8-yn-1,15-olide F-12

*4-(4,8-Dimethyl-3,7-nonadien-5-ynylidene)dihydro-2(3*H*)-furanone*

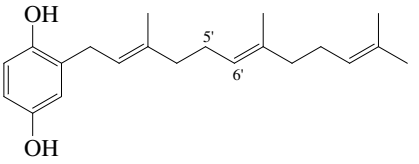


$C_{15}H_{18}O_2$ 230.306

(3Z,6E)-form
Ascobullin B
[294199-64-7]
Constit. of *Ascobulla ulla*.
Cimino, G. *et al., Curr. Org. Chem.*, 1999, **3**, 327-372
Gavagnin, M. *et al., J. Chem. Ecol.*, 2000, **26**, 1563-1578 (*isol, pmr, cmr*)

Farnesylhydroquinone F-13

2-(3,7,11-Trimethyl-2,6,10-dodecatrienyl)-1,4-benzenediol, 9CI

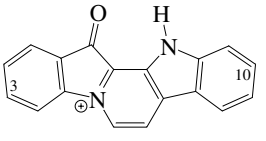


$C_{21}H_{30}O_2$ 314.467
For higher homologues see 2-Polyprenyl-1,4-benzenediol, P-547.

(E,E)-form
Constit. of *Wigandia kunthii* and from brown seaweed *Dictyopteris undulata*. Shows moderate antifungal activity. Viscous oil.
5′-Oxo: 1-(2,5-Dihydroxyphenyl)-3,7,11-trimethyl-2,6,10-dodecatrien-5-one. 2-(3,7,11-Trimethyl-5-oxo-2,6,10-dodecatrienyl)-1,4-benzenediol
[592533-85-2]
$C_{22}H_{30}O_3$ 342.477
Constit. of *Cystoseira crinita*. Oil. λ_{max} 244 (ϵ 9600); 289 (ϵ 2400) (EtOH).
*6′*Z*-Isomer, 5′-oxo:* [592533-86-3]
$C_{22}H_{30}O_3$ 342.477
Constit. of *Cystoseira crinita*. Oil. λ_{max} 244 (ϵ 25100); 286 (ϵ 8600) (EtOH).
Ochi, M. *et al., Chem. Lett.*, 1979, 831-832 (*isol*)
Gómez, F. *et al., Phytochemistry*, 1980, **19**, 2202-2203 (*isol, pmr, ms*)
Fisch, K.M. *et al., J. Nat. Prod.*, 2003, **66**, 968-975 (*5′-oxo derivs*)

Fascaplysin F-14

*12,13-Dihydro-13-oxopyrido[1,2-*a*:3,4-*b*′]diindol-5-ium(1+), 9CI. NSC 622398*
[114719-57-2]



$C_{18}H_{11}N_2O^{\oplus}$ 271.298
Pigment from the marine sponge *Fascaplysinopsis* sp. and from *Hyrtios erecta*, *Smenospongia* sp. and tunicate *Didemnum* sp. Exhibits antimicrobial and cytotoxic props. Inhibits HIV-1-rt and $p56^{LCK}$ tyrosine kinase. Shows antiplasmodial and antiviral activity. Red cryst. (MeOH or $CHCl_3$)(as chloride). Sol. MeOH, $CHCl_3$. Mp 232-235° (chloride). CAS no. refers to chloride. λ_{max} 210 (ϵ 30400); 237 (ϵ 6480); 274 (ϵ 5800); 332 (ϵ 5470); 398 (ϵ 2300); 427 (ϵ 2980); 453 (ϵ 2700) (MeOH/KOH) (Derep). λ_{max} 214 (ϵ 7000); 262 (ϵ 6400); 274 (ϵ 5450); 300 (ϵ 6800); 333 (ϵ 3560); 413 (ϵ 3100) (MeOH) (Derep).

Salt with Dehydroluffariellolide diacid, D-60: ***Fascaplysin A****. NSC 660649*
[132911-49-0]
$C_{43}H_{48}N_2O_5$ 672.863
Alkaloid-sesterterpene salt from the sponge *Fascaplysinopsis reticulata*. Red oil.

Salt with, 16-Oxo: ***Fascaplysin B***
[135091-13-3]
$C_{43}H_{46}N_2O_6$ 686.846
Alkaloid-sesterterpene salt from *Fascaplysinopsis reticulata*. No phys. props. reported.

3-Bromo: ***3-Bromofascaplysin****. NSC 700409*
$C_{18}H_{10}BrN_2O^{\oplus}$ 350.194
Isol. from a *Didemnum* sp. and from *Fascaplysinopsis reticulata*. Red solid (as chloride).

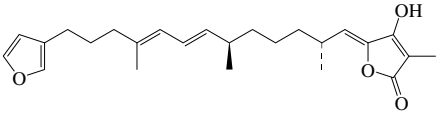
10-Bromo: ***10-Bromofascaplysin***
$C_{18}H_{10}BrN_2O^{\oplus}$ 350.194
Isol. from *Fascaplysinopsis reticulata*. Red solid (as chloride).

3,10-Dibromo: ***3,10-Dibromofascaplysin***
$C_{18}H_9Br_2N_2O^{\oplus}$ 429.09
Isol. from *Fascaplysinopsis reticulata*. Red solid (as chloride).

Roll, D.M. *et al., J.O.C.*, 1988, **53**, 3276 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Jimènez, C. *et al., J.O.C.*, 1991, **56**, 3403 (*Fascaplysin A*)
Jimènez, C. *et al., Tet. Lett.*, 1991, **32**, 1843 (*Fascaplysin B*)
Gribble, G.W. *et al., J.O.C.*, 1992, **57**, 3636 (*synth*)
Rocca, P. *et al., Tet. Lett.*, 1993, **34**, 7917 (*synth*)
Molina, P. *et al., Tet. Lett.*, 1994, **35**, 8851 (*synth*)
Radchenko, O.S. *et al., Tet. Lett.*, 1997, **38**, 5339 (*synth*)
Kirsch, G. *et al., J. Nat. Prod.*, 2000, **63**, 825-829 (*isol, pmr, cmr, activity*)
Segraves, N.L. *et al., Tet. Lett.*, 2003, **44**, 3471-3475 (*3-Bromofascaplysin*)
Segraves, N.L. *et al., J. Nat. Prod.*, 2004, **67**, 783-792 (*occur, 10-Bromofascaplysin, 3,10-Dibromofascaplysin*)

Fasciculatin† F-15

[37905-12-7]



Absolute Configuration

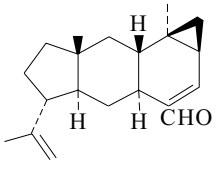
$C_{25}H_{34}O_4$ 398.541
Constit. of the sponge, *Ircinia fasciculata* and of *Ianthella basta*. Inosine monophosphate dehydrogenase inhibitor. Oil. $[\alpha]_D$ -15.6 (c, 0.5 in $CHCl_3$). λ_{max} 232 (sh) (ϵ 24700); 241 (ϵ 29200); 250 (sh) (ϵ 24500); 268 (ϵ 14500) (hexane) (Derep).

O-*Sulfate:*
$C_{25}H_{34}O_7S$ 478.605
Constit. of *Ircinia fasciculata*. Inosine monophosphate dehydrogenase inhibitor. Amorph. solid. $[\alpha]_D$ -4.5 (c, 2.7 in $CHCl_3$). λ_{max} 272 (ϵ 18000) (MeOH).

Cafieri, F. *et al., Tetrahedron*, 1972, **28**, 1579 (*struct, pmr, uv*)
Alfano, G. *et al., Experientia*, 1979, **35**, 1136 (*stereochem*)
Cimino, G. *et al., Tetrahedron*, 1985, **41**, 1093 (*isol*)
De Rosa, S. *et al., Nat. Prod. Lett.*, 1997, **10**, 7-12 (*sulfate*)

7,18-Fascioladien-17-al F-16

[102915-72-0]

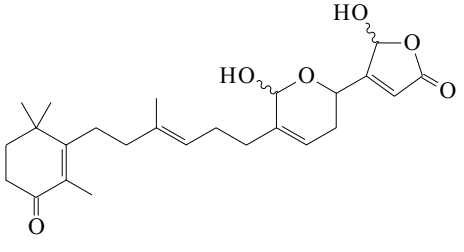


$C_{20}H_{28}O$ 284.441
Constit. of *Dilophus fasciola*. Cryst. (EtOH).
Mp 103-104°. $[\alpha]_D^{25}$ -150.9 (c, 1 in EtOH).

Tringali, C. *et al., J. Nat. Prod.*, 1986, **49**, 236

Fasciospongide A F-17

[153660-23-2]

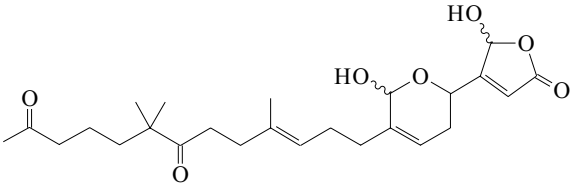


$C_{25}H_{34}O_6$ 430.54
Constit. of a *Fasciospongia* sp. Phospholipase A_2 inhibitor. Antiinflammatory agent. Oil. $[\alpha]_D$ +46 (c, 1 in $CHCl_3$). λ_{max} 244 (ϵ 7800) (MeOH) (Berdy).

Montagnac, A. *et al., J. Nat. Prod.*, 1994, **57**, 186 (*isol, pmr, cmr*)

Fasciospongide B F-18

[153660-24-3]

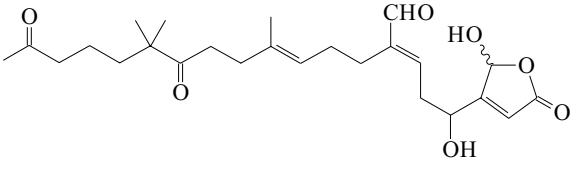


$C_{25}H_{36}O_7$ 448.555
Constit. of a *Fasciospongia* sp. Phospholipase A_2 inhibitor. Antiinflammatory agent. Oil. $[\alpha]_D$ +54 (c, 1 in $CHCl_3$).

Montagnac, A. *et al., J. Nat. Prod.*, 1994, **57**, 186 (*isol, pmr, cmr*)

Fasciospongide C F-19

[153660-25-4]

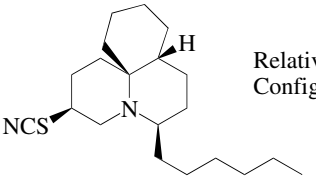


$C_{25}H_{36}O_7$ 448.555
Constit. of a *Fasciospongia* sp. Phospholipase A_2 inhibitor. Antiinflammatory agent. Oil. $[\alpha]_D$ +54 (c, 1 in $CHCl_3$).

Montagnac, A. *et al., J. Nat. Prod.*, 1994, **57**, 186 (*isol, pmr, cmr*)

Fasicularine F-20

[187618-62-8]



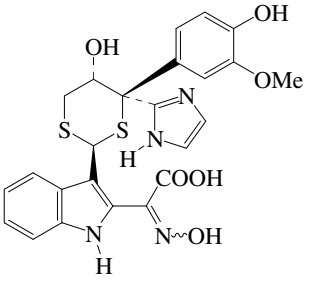
Relative Configuration

$C_{20}H_{34}N_2S$ 334.568
Alkaloid from the Micronesian ascidian *Nephteis fasicularis*. Shows selective activity against a DNA repair-deficient organism. Cytotoxic to Vero cells. Gum. Closely related to Cylindricine B, C-1094.

Patil, A.D. *et al., Tet. Lett.*, 1997, **38**, 363 (*isol, ir, pmr, cmr, ms, struct*)
Maeng, J.-H. *et al., Org. Lett.*, 2002, **4**, 331-333 (*synth*)
Fenster, M.D.B. *et al., Chem. Eur. J.*, 2005, **11**, 639-649 (*synth*)
Abe, H. *et al., J.A.C.S.*, 2005, **127**, 1473-1480 (*synth*)

Fasmerianamine B F-21

[383191-03-5]



Relative Configuration

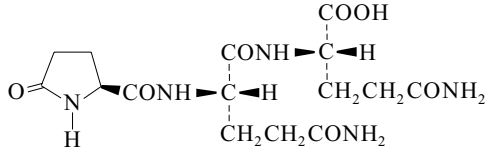
$C_{24}H_{22}N_4O_6S_2$ 526.593

Isol. from the ascidian *Hypsistozoa fasmeriana*. Brown gum. Related to 5-Hydroxy-4-(4-hydroxy-3-methoxyphenyl)-4-(2-imidazolyl)-1,2,3-trithiane, H-688.

Me ester: ***Fasmerianamine A***
[383191-02-4]
$C_{25}H_{24}N_4O_6S_2$ 540.62
Isol. from *Hypsistozoa fasmeriana*. Brown gum. $[\alpha]_D^{20}$ -17.5 (c, 0.4 in MeOH). Incorrect MF stated in ref. λ_{max} 206 (log ϵ 4.13); 283 (log ϵ 3.35); 311 (log ϵ 3.18) (MeOH).
Pearce, A.N. *et al., J.O.C.*, 2001, **66**, 8257-8259

Fastigiatine† F-22

L-5-Oxoprolinyl-L-α-glutaminyl-L-α-glutamine

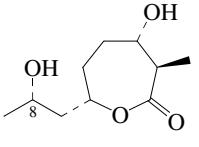


$C_{15}H_{23}N_5O_7$ 385.376
Isol. from the marine alga *Pelvetia fastigiata*. Mp 190-195° (natural) Mp 218-222° (synthetic). $[\alpha]_D^{20}$ -35.3 (synthetic). CAS no. not found 8-14Cl.

Dekker, C.A. *et al., J. Biol. Chem.*, 1949, **181**, 719-729 (*isol*)
Rudinger, J. *et al., Chem. Listy*, 1958, **52**, 120-129 (*synth, struct*)

Feigrisolide A F-23

4-Hydroxy-7-(2-hydroxypropyl)-3-methyl-2-oxepanone



$C_{10}H_{18}O_4$ 202.25
Struct. revised in 2006. Prob. identical with Nonactic acid, N-147 of which it is an alternative lactone form. Prod. by *Streptomyces griseus* GT 051022 and marine-derived *Streptomyces* spp. Antibacterial agent. Oil. $[\alpha]_D^{20}$ +3.4 (c, 0.3 in MeOH). λ_{max} 199 (log ϵ 3.47); 220 (log ϵ 3.27) (EtOH).

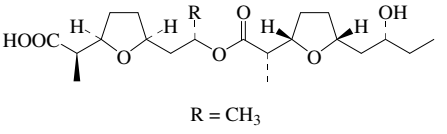
8-Epimer: ***Feigrisolide B***
$C_{10}H_{18}O_4$ 202.25
Prod. by *Streptomyces griseus* GT 051022 and marine-derived *Streptomyces* spp. Antibacterial agent. Oil. Racemic. λ_{max} 199 (log ϵ 3.36); 221 (log ϵ 3.27) (EtOH).

8-Epimer, 3-deoxy, 2,3-didehydro: 6,7-Dihydro-7-(2-hydroxypropyl)-3-methyl-2(5H)-oxepinone, 9CI. ***Feigrisolide E***
$C_{10}H_{16}O_3$ 184.235
Prod. by the marine-derived *Streptomyces* sp. B5375. Struct. prob. requires revision (2006).

Tang, Y.-Q. *et al., J. Antibiot.*, 2000, **53**, 934-943 (*isol*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)
Alvarez-Bercado, H. *et al., J.O.C.*, 2006, **71**, 5766-5769 (*synth, struct*)

Feigrisolide C F-24

Nonactyl homononactoate



Absolute Configuration

R = CH_3

$C_{21}H_{36}O_7$ 400.511

Struct. revised in 2005. Prod. by *Streptomyces griseus* GT 051022 and a marine-deived *Streptomyces* sp. Antibacterial agent. Powder. $[\alpha]_D^{20}$ +17.2 (c, 0.4 in MeOH). λ_{max} 201 (log ϵ 3.98) (EtOH).

Stereoisomer (?): ***Bonactin***
$C_{21}H_{36}O_7$ 400.511
Isol. from a marine *Streptomyces* sp. BD-21-2. Active against gram-positive and -negative bacteria and fungi. Viscous oil. Claimed to be a mixt. of racemic stereoisomers, but the stereochem. requires further investigation.

Tang, Y.-Q. *et al., J. Antibiot.*, 2000, **53**, 934-943 (*isol*)
Schumacher, R.W. *et al., J. Nat. Prod.*, 2003, **66**, 1291-1293 (*Bonactin*)
Shaaban, M. *et al., Dissertation*, Univ. of Göttingen, 2005, (*isol, marine*)
Kim, W.H. *et al., J.O.C.*, 2005, **70**, 8190-8192 (*synth, struct*)

Feigrisolide D F-25

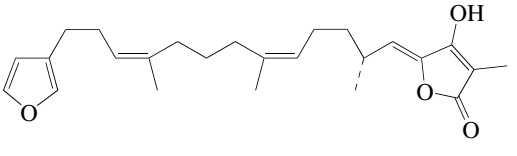
As Feigrisolide C, F-24 with
R = CH_2CH_3

$C_{22}H_{38}O_7$ 414.538

Struct. revision given here by analogy with Feigrisolide C, F-24, although this is not yet given in the lit. Prod. by *Streptomyces griseus* GT 051022 and a marine-derived *Streptomyces* sp. Antibacterial agent. Oil. $[\alpha]_D^{20}$ +15.7 (c, 0.2 in MeOH). λ_{max} 201 (log ϵ 3.97) (EtOH).

Tang, Y.Q. *et al., J. Antibiot.*, 2000, **53**, 934-943

Felixinin F-26

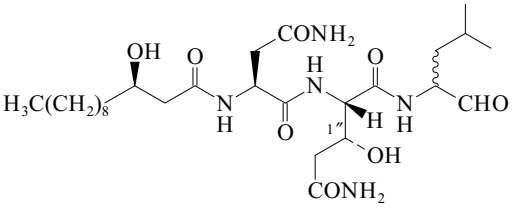


$C_{25}H_{34}O_4$ 398.541

(6Z,11Z,15R,16Z)-form [187038-73-9]
Constit. of *Ircinia felix*.
Martinez, A. *et al., Chem. Pharm. Bull.*, 1997, **45**, 181-184 (*isol, pmr, cmr*)

Fellutamide A F-27

[138682-08-3]



$C_{27}H_{49}N_5O_8$ 571.713

Lipopeptide antibiotic. Prod. by the marine fungus *Penicillium fellutanum*. Cytotoxic. Shows NGF inducing activity. Amorph. powder. $[\alpha]_D^{22}$ -12.7 (c, 1 in MeOH).

1″-Deoxy: ***Fellutamide B****. Antibiotic 1656B. 1656B. F 1652. Antibiotic F 1652*
[138752-26-8]
$C_{27}H_{49}N_5O_7$ 555.713
From *Penicillium fellutanum* and *Aspergillus* sp. F1656. Cytotoxic agent. Shows NGF inducing activity. Amorph. powder. Sol. DMSO. Mp 185-186°. $[\alpha]_D^{21}$ -24.7 (c, 0.5 in MeOH).

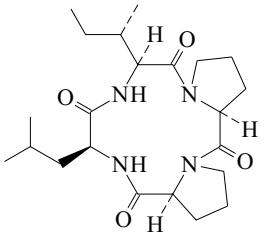
1″-Deoxy, di-Me acetal: ***Antibiotic 1656C****. 1656C*
[125850-33-1]
Prod. by *Aspergillus* sp. F1656. Cathepsin B inhibitor. Cytotoxic. Powder. Sol. MeOH, DMSO, AcOH; fairly sol. EtOAc, Me_2CO, $CHCl_3$; poorly sol. hexane, Et_2O, H_2O. $[\alpha]_D$ -25.3 (MeOH). λ_{max} 200 (MeOH).

[125882-62-4]

Eur. Pat., 1989, 318 254; *CA*, **112**, 137502 (*Antibiotic 1656B*)
Shigemori, H. *et al., Tetrahedron*, 1991, **47**, 8529-8534 (*isol, pmr, cmr*)
Yamaguchi, K. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 195-198 (*activity, Fellutamides A and B*)

Fenestin A F-28

Cyclo(isoleucylprolylprolylleucyl)
[118984-46-6]

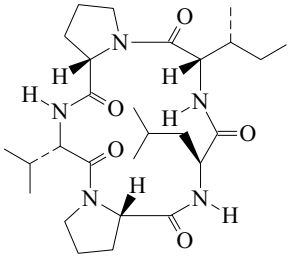


$C_{22}H_{36}N_4O_4$ 420.551
The proposed struct. illus. is doubtful. Isol. from the sponge *Leucophloeus fenestrata*.

Omar, S. *et al., Tet. Lett.*, 1988, **29**, 5489 (*isol, pmr, cmr*)
Schmidt, U. *et al., Angew. Chem., Int. Ed.*, 1990, **29**, 514 (*struct, synth*)

Fenestin B F-29

Cyclo(isoleucylprolylvalylprolylleucyl)
[118984-47-7]

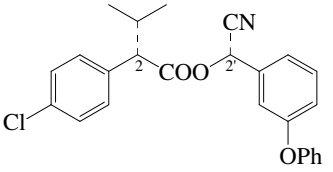


$C_{27}H_{45}N_5O_5$ 519.683
The proposed struct. illus. is almost certainly wrong. Cyclic peptide. Isol. from the sponge *Leucophloeus fenestrata*.

Omar, S. *et al., Tet. Lett.*, 1988, **29**, 5489 (*isol, pmr, cmr*)
Schmidt, U. *et al., Angew. Chem., Int. Ed.*, 1990, **29**, 514 (*struct, synth*)

Fenvalerate, BAN, BSI, ISO F-30

Cyano(3-phenoxyphenyl)methyl 4-chloro-α-(1-methylethyl)benzeneacetate, 9CI. α-Cyano-3-phenoxybenzyl 2-(4-chlorophenyl)-3-methylbutyrate. Belmark. Ectrin. Fenkill. Fenval. Pydrin. Sumicidin
[51630-58-1]



(2*S*,2′*S*)-*form*

$C_{25}H_{22}ClNO_3$ 419.906
Agricultural, public health and animal husbandry insecticide. Viscous yellow liq. d_{25}^{25} 1.18. Bp_{37} 300°.
▶ LD_{50} (rat, orl) 451 mg/kg. CY1576350

(2S,2′S)-form
Esfenvalerate, BSI, ISO*. Asana. Fenvalerate α. Sumi-alpha*
[66230-04-4]
Claimed isol. from the sponge *Haliclona cribricutis*. Insecticide. Has greater insecticidal activity than racemate. Cryst. d_4^{26} 1.26. Mp 59-60°. $[\alpha]_D^{25}$ -15 (c, 2.0 in MeOH). Presence in sponge certain to be as environmental contaminant.
▶ CY1576367

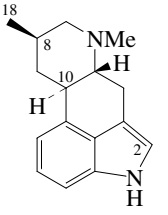
(2S,2′R)-form
Fenvalerate B
[66267-77-4]
Isol. from *Haliclona cribricutis*. Isol. certain to be as environmental contaminant.

[67614-32-8, 67614-33-9, 67890-39-5, 67890-40-8, 73367-17-6, 73367-18-7]

U.K. Pat., 1972, 1 439 615; *CA*, **80**, 120746w
Hattori, J. *et al., Jpn. Pestic. Inf.*, 1977, **33**, 13 (*rev, props*)
Aketa, K. *et al., Agric. Biol. Chem.*, 1978, **42**, 895 (*synth, pmr, activity*)
Ger. Pat., 1978, 2 737 297; *CA*, **88**, 152268y (*esfenvalerate*)
Yoshioka, H. *et al., Rev. Plant. Prot. Res.*, 1978, **11**, 39 (*rev, synth, tox*)
Horiba, M. *et al., Agric. Biol. Chem.*, 1982, **46**, 3041 (*abs config, bibl*)
Papadopoulou-Mourkidou, E. *et al., Residue Rev.*, 1983, **89**, 179 (*rev, detn*)
Wheeler, T.N. *et al., J. Agric. Food Chem.*, 1984, **32**, 1125 (*synth, activity*)
U.S. Pat., 1984, 4 432 908; *CA*, **100**, 209428y (*cryst struct*)
Oo'uchi, H. *et al., Jpn. Pestic. Inf.*, 1985, **46**, 21 (*esfenvalerate*)
Mikami, N. *et al., Pestic. Sci.*, 1985, **16**, 46 (*metab*)
Miyamoto, J. *et al., ACS Symp. Ser.*, 1986, **299**, 268 (*rev, tox*)
Lidgard, R.O. *et al., Biomed. Environ. Mass Spectrom.*, 1986, **13**, 677 (*ms*)
Papadopoulou-Mourkidou, E. *et al., Anal. Methods Pestic. Plant Growth Regul.*, 1988, **16**, 31 (*hplc*)
IARC Monog., 1991, **53**, 309 (*rev, tox*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A990; A207
Pesticide Manual, 11th edn., 1997, No. 319; *Pesticide Manual, 9th edn.*, 1991, No. 6340
Luzzio, F.A. *et al., J. Prakt. Chem.*, 2000, **342**, 498-501 (*synth*)
Goud, T.V. *et al., Indian J. Chem., Sect. B*, 2005, **44**, 607-610 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAR100

Festuclavine F-31

Dihydroagroclavine
[569-26-6]



Absolute Configuration

$C_{16}H_{20}N_2$ 240.347
Alkaloid from *Claviceps purpurea*, *Claviceps gigantea*, *Aspergillus fumigatus*, *Penicillium roquefortii*, *Penicillium crustosum*, *Argyreia*

nervosa and several other *Argyreia* spp., *Ipomoea hildebrandtii*, *Ipomoea violacea* and *Stictocardia tiliaefolia*. Mycotoxin, 5-HT receptor antagonist; active against gram-positive bacteria. Needles (MeOH). Sol. MeOH, $CHCl_3$.
Mp 249-252° (242-243°). $[\alpha]_D^{20}$ -113 (c, 0.25 in Py). $[\alpha]_D^{14}$ -67.4 (c, 0.12 in $CHCl_3$). λ_{max} 224 (log ϵ 4.53); 276 (log ϵ 3.82); 281 (log ϵ 3.84) (EtOH).

▶ LD_{50} (mus, ipr) 45 mg/kg. KE6334000

2-Bromo: ***Pibocine A***. *2-Bromofestuclavin*
[102394-16-1]
$C_{16}H_{19}BrN_2$ 319.244
Alkaloid from the ascidian *Eudistoma* sp. Moderate cytotoxic agent.
Mp 226-228°. $[\alpha]_D$ -36 (c, 0.14 in EtOH). λ_{max} 225 (ϵ 27400); 281 (ϵ 7000) (EtOH).

2-Bromo, N^1*-methoxy:* ***Pibocine B***
[388112-41-2]
$C_{17}H_{21}BrN_2O$ 349.27
Alkaloid from a *Eudistoma* sp. Cytotoxic. Thin cryst. (MeOH).
Mp > 358°. $[\alpha]_D$ -51 (c, 0.19 in EtOH). λ_{max} 231 (ϵ 4410); 283 (ϵ 2450) (MeOH).

18-Hydroxy: ***α-Dihydrolysergol***. *Dihydrolysergol. Dihydroelymoclavine*
[18051-16-6]
$C_{16}H_{20}N_2O$ 256.347
Alkaloid from *Claviceps gigantea*. Also present in the seeds of *Stictocardia campanulata* and *Ipomoea muelleri* (Convolvulaceae). 5-HT receptor antagonist, mycotoxin. Prisms (MeOH).
Mp 283°. $[\alpha]_D^{20}$ -60 (c, 0.13 in EtOH). $[\alpha]_D$ -92 (c, 0.5 in Py). λ_{max} 224 (log ϵ 4.6); 282 (log ϵ 3.92); 292 (log ϵ 3.88) (EtOH).

8-Epimer: ***Pyroclavine***
[478-89-7]
$C_{16}H_{20}N_2$ 240.347
Prod. by *Claviceps purpurea* and *Claviceps gigantea*, also *Penicillium* sp. 5-HT receptor antagonist, mycotoxin.
Mp 204°. $[\alpha]_D^{20}$ -90 (c, 0.2 in Py).

10-Epimer: ***Costaclavine***
[436-41-9]
$C_{16}H_{20}N_2$ 240.347
Alkaloid from *Claviceps purpurea* and *Penicillium chermesinum*.
Mp 182-184°. $[\alpha]_D$ +44 (Py). λ_{max} 275; 283; 293 (no solvent reported).

8,10-Diepimer: Epicostaclavine
Mp 132-135°.

Abe, M. *et al., Bull. Agric. Chem. Soc. Jpn.*, 1956, **20**, 59-60; 1959, **33**, 1031-1036; *CA*, **51**, 11365c; **59**, 2878c (*Costaclavine, Pyroclavine, isol, struct*)
Spilsbury, J.F. *et al., J.C.S.*, 1961, 2085-2089 (*isol, uv*)
Agurell, S.L. *et al., Experientia*, 1964, **20**, 25-26 (*Costaclavine, isol, uv, ir*)
Agurell, S. *et al., Acta Pharm. Suec.*, 1965, **2**, 231-238 (*Pyroclavine, Festuclavine, α-Dihydrolysergol, isol*)
Semononsky, M. *et al., Coll. Czech. Chem. Comm.*, 1966, **31**, 577-582 (*α-Dihydrolysergol, synth*)
Chao, J.M. *et al., Phytochemistry*, 1973, **12**, 2435-2440 (*Festuclavine, occur*)
Bach, N.J. *et al., J.O.C.*, 1974, **39**, 1272-1276 (*pmr, cmr*)
Voigt, D. *et al., Pharmazie*, 1974, **29**, 697 (*ms*)
Ohmomo, S. *et al., Agric. Biol. Chem.*, 1975, **39**, 1333-1336 (*isol, uv, ir*)
Ninomiya, I. *et al., Chem. Comm.*, 1976, 624-626 (*Costaclavine, Pyroclavine, pmr*)
Křepelka, J. *et al., Coll. Czech. Chem. Comm.*, 1976, **41**, 1416-1418 (*synth*)
Lee, T.M. *et al., Planta Med.*, 1979, **35**, 247-252 (*α-Dihydrolysergol, isol*)
Cole, R.J. *et al., J. Agric. Food Chem.*, 1983, **31**, 655-657 (*isol*)
Oppolzer, W. *et al., Tetrahedron*, 1983, **39**, 3695 (*Costaclavine, synth, ir, pmr, ms*)
Eich, E. *et al., Arzneim.-Forsch.*, 1985, **35**, 1760-1762 (*Festuclavine, activity*)
Osanai, K. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1587-1590 (*Costaclavine, synth*)
Makarieva, T.N. *et al., Tet. Lett.*, 1999, **40**, 1591-1594 (*Pibocine A*)
Makarieva, T.N. *et al., J. Nat. Prod.*, 2001, **64**, 1559-1561 (*Pibocine B, Festuclavine*)

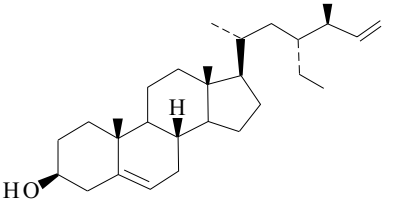
Mytilus edulis FFRF amide F-32

[143840-34-0]
Ala-D-Leu-Ala-Gly-Asp-His-Phe-Phe-Arg-Phe-NH_2
$C_{57}H_{78}N_{16}O_{12}$ 1179.343
Peptide containing a D-leucine residue. Isol. from the mussel *Mytilus edulis*. Neuropeptide.

Fujisawa, Y. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1992, **102**, 91-95 (*isol*)

Ficisterol F-33

23-Ethyl-24-methyl-27-norcholesta-5,25-dien-3-ol. 23-Ethyl-27-norergosta-5,25-dien-3-ol
[74137-07-8]



$C_{29}H_{48}O$ 412.698
Constit. of *Petrosia ficiformis*. Cryst. (MeOH).
Mp 143-145°. $[\alpha]_D^{20}$ -10.6 (c, 0.85 in $CHCl_3$).

Ac:
Cryst. Mp 102-103°.

Khalil, M.W. *et al., J.A.C.S.*, 1980, **102**, 2133 (*isol*)
Shu, A.Y.L. *et al., J.C.S. Perkin 1*, 1987, 1291 (*synth, struct*)

Ficulinic acid A F-34

2-Heptyl-10-oxo-11-nonadecenoic acid, 9CI
$H_3C(CH_2)_6CH{=}CHCO(CH_2)_7CH(COOH)(CH_2)_6CH_3$
$C_{26}H_{48}O_3$ 408.663

(E)-form [102791-30-0]
Isol. from the sponge *Ficulina ficus*. Shows weak cytotoxic props.
Sol. hexane, MeOH; poorly sol. H_2O.
Mp 33-35°. λ_{max} 230 (EtOH) (Berdy).
▶ LK3760000

Guyot, M. *et al., J. Nat. Prod.*, 1986, **49**, 307 (*isol*)

Ficulinic acid B F-35

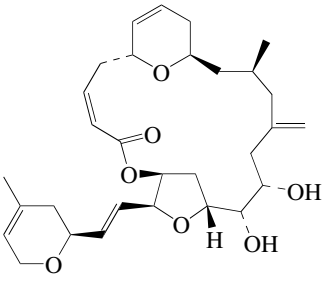
2-Heptyl-12-oxo-13-heneicosenoic acid, 9CI
$H_3C(CH_2)_6CH{=}CHCO(CH_2)_9CH(COOH)(CH_2)_6CH_3$
$C_{28}H_{52}O_3$ 436.717

(E)-form [102791-31-1]
Isol. from the sponge *Ficulina ficus*. Shows weak cytotoxic props.
Sol. hexane, MeOH; poorly sol. H_2O.
Mp 31-32°.
▶ LK3765000

Guyot, M. *et al., J. Nat. Prod.*, 1986, **49**, 307 (*isol*)

Fijianolide A F-36

Isolaulimalide. Isolaulamide
[115267-16-8]



$C_{30}H_{42}O_7$ 514.658
Macrolide antibiotic. Fijianolide A and Isolaulimalide have the same gross struct. but stereochem. varies. Constit. of *Spongia mycofijiensis*, *Hyatella* sp. and *Chromodoris lochi*. Shows

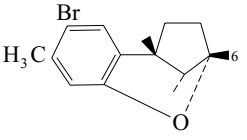
moderate *in vitro* cytotoxicity. $[\alpha]_D^{20}$ -8 (c, 0.04 in $CHCl_3$). λ_{max} 208 (ϵ 10500) (MeOH) (Derep).

[114995-72-1]

Quiñoà, E. *et al., J.O.C.*, 1988, **53**, 3642 (*isol, pmr, cmr*)
Corley, D.G. *et al., J.O.C.*, 1988, **53**, 3644-3646 (*isol, pmr, cmr*)
Tanaka, J. *et al., Chem. Lett.*, 1996, 255 (*isol, config*)

Filiformin F-37

7-Bromo-2,3,4,5-tetrahydro-2,5,8,10-tetramethyl-2,5-methano-1-benzoxepin, 9CI
[62311-75-5]



$C_{15}H_{19}BrO$ 295.218
Constit. of *Laurencia filiformis* and *Aplysia* sp. Cryst. (petrol). Mp 86.4-87.3°. $[\alpha]_D$ -20 (c, 1 in $CHCl_3$). Prob. artifact of cyclisation of, 7-Hydroxy, 10-bromo. λ_{max} 237 (ϵ 9150); 287 (ϵ 2700); 290 (ϵ 2680); 296 (ϵ 2840) (hexane).

6-Hydroxy: ***Filiforminol***
[62311-76-6]
$C_{15}H_{19}BrO_2$ 311.218
Constit. of *Laurencia filiformis.* Oil. $[\alpha]_D$ -13.7 (c, 1.1 in $CHCl_3$). λ_{max} 235 (ϵ 8240); 286 (ϵ 2820); 289 (ϵ 2780); 295 (ϵ 2870) (hexane).

6-Bromo: ***Bromoether A***
[63001-93-4]
$C_{15}H_{18}Br_2O$ 374.115
Isol. from *Laurencia glandulifera*. Cryst. (MeOH). Mp 86-87°. $[\alpha]_D^{23}$ +22 (c, 1.16 in $CHCl_3$).

6-Iodo: ***Iodoether A***
[72030-67-2]
$C_{15}H_{18}BrIO$ 421.115
Constit. of *Laurencia nana*. Cryst. Mp 99-102° dec. $[\alpha]_D$ +29 (c, 0.94 in $CHCl_3$).

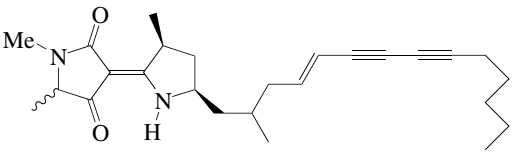
Debromo, 6-bromo: ***2-(Bromomethyl)-2,3,4,5-tetrahydro-5,8,10-trimethyl-2,5-methano-1-benzoxepin, 9CI***
[23526-41-2]
$C_{15}H_{19}BrO$ 295.218
Isol. from *Laurencia glandulifera*. λ_{max} 240 (ϵ 30000) (EtOH) (Derep).

Debromo, 6,6-dibromo: 2-(Dibromomethyl)-2,3,4,5-tetrahydro-5,8,10-trimethyl-2,5-methano-1-benzoxepin, 9CI. ***Bromoether B***
[63001-94-5]
$C_{15}H_{18}Br_2O$ 374.115
Isol. from *Laurencia glandulifera*. Cryst. (MeOH). Mp 125-126°. $[\alpha]_D^{21}$ +79 (c, 0.38 in $CHCl_3$).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1976, **29**, 2533-2539 (*isol, Filiforminol, uv, pmr, cmr, ir*)
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 3349-3351 (*Laurencia glandulifera constits*)
Izae, R.R. *et al., J.A.C.S.*, 1979, **101**, 6136-6139 (*Iodoether A*)
Goldsmith, D.J. *et al., J.O.C.*, 1980, **45**, 3989-3993 (*synth*)
Laronze, J.Y. *et al., Tetrahedron*, 1991, **47**, 10003-10014 (*synth*)
Nemoto, H. *et al., Heterocycles*, 1994, **39**, 467-470 (*synth*)
Yoo, S. *et al., Synthesis*, 1998, 771-774 (*Filiforminol, Bromoether A, synth, pmr, cmr, ir, ms*)
Gochfeld, D.J. *et al., J. Nat. Prod.*, 2001, **64**, 1477-1479 (*Filiformin, pmr*)

Fischerellin A F-38

[182227-56-1]



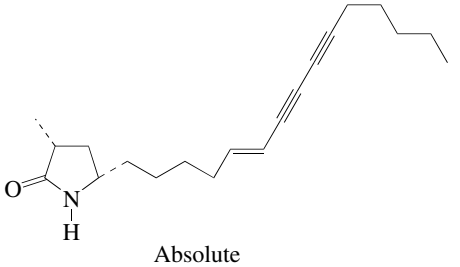
Relative Configuration

$C_{26}H_{36}N_2O_2$ 408.583
Isol. from the cyanobacterium *Fischerella muscicola*. Potent photosystem-II inhibitor. Exhibits antifungal and herbicidal activity. Powder. Unique struct.; unrelated to all other known cyanobacterial metabolites. λ_{max} 214 (log ϵ 53000); 229 (log ϵ 12000); 241 (log ϵ 16000); 253 (log ϵ 18000); 268 (log ϵ 20600); 284 (log ϵ 24000); 301 (log ϵ 22000) (no solvent reported).

Hagmann, L. *et al., Tet. Lett.*, 1996, **37**, 6539-6542 (*isol, uv, pmr, cmr, struct*)

Fischerellin B F-39

[186901-41-7]



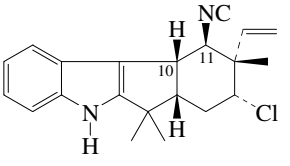
Absolute Configuration

$C_{20}H_{29}NO$ 299.455
Isol. from the cyanobacteria *Fischerella muscicola* and *Fischerella ambigua*. Yellowish solid. λ_{max} 240; 252; 267; 283 (MeOH).

Papke, U. *et al., Tet. Lett.*, 1997, **38**, 379 (*isol, uv, pmr, cmr, struct, abs config*)

Fischerindole L F-40

[144398-55-0]



$C_{21}H_{23}ClN_2$ 338.879
The suffix letters for the Fischerindoles are allocated on the basis of analogy with structurally similar Hapalindoles, therefore not all suffix letters are known. Alkaloid from the terrestrial blue-green alga *Fischerella muscicola*. λ_{max} 220 (ϵ 38000); 278 (ϵ 6800); 290 (sh) (ϵ 5000) (MeOH) (Derep).

10,11-Didehydro: ***12-Epifischerindole I isonitrile***
[159189-08-9]
$C_{21}H_{21}ClN_2$ 336.863
Isol. from *Hapalosiphon welwitschii*.

10-Epimer: ***12-Epifischerindole G isonitrile***
[159249-50-0]
$C_{21}H_{23}ClN_2$ 338.879
Isol. from *Hapalosiphon welwitschii*.
$[\alpha]_D$ +67 (c, 0.09 in CH_2Cl_2). λ_{max} 222 (ϵ 18600); 278 (ϵ 5880) (MeOH).

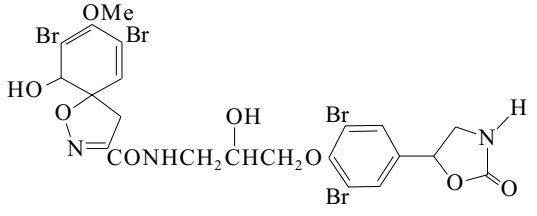
10-Epimer, dechloro: ***12-Epifischerindole U isonitrile***
[159189-06-7]
$C_{21}H_{24}N_2$ 304.434
Isol. from *Hapalosiphon welwitschii*. λ_{max} 226 (ϵ 17500); 278 (ϵ 5680) (MeOH).

10-Epimer, dechloro, isothiocyanate: ***12-Epifischerindole U isothiocyanate***
$C_{21}H_{24}N_2S$ 336.5
Isol. from *Hapalosiphon welwitschii*.
$[\alpha]_D$ +231 (c, 0.03 in CH_2Cl_2). Has -NCS replacing -NC. λ_{max} 206 (sh) (ϵ 16300); 228 (ϵ 23000); 278 (ϵ 5240) (MeOH).

Park, A. *et al., Tet. Lett.*, 1992, **33**, 3257-3260 (*isol, uv, pmr, cmr, ms*)
Stratmann, K. *et al., J.A.C.S.*, 1994, **116**, 9935-9942 (*derivs*)
Baran, P.S. *et al., J.A.C.S.*, 2005, **127**, 15394-15396 (*synth*)

Fistularin 1 F-41

[73622-20-5]

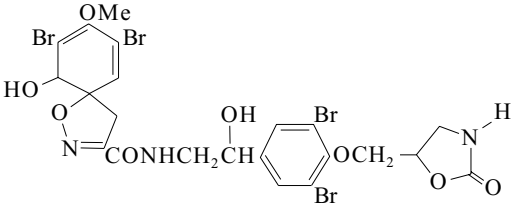


$C_{22}H_{21}Br_4N_3O_8$ 775.039
Metab. of the sponge *Aplysina fistularis* forma *fulva*. Amorph. solid. $[\alpha]_D$ +93.5 (c, 1.2 in MeOH). λ_{max} 230 (sh) (ϵ 15200); 284 (sh) (ϵ 5680) (MeOH) (Derep).

Di-O-*Ac:* Mp 168-171° dec. $[\alpha]_D$ +122.7 (c, 0.44 in $CHCl_3$).
Gopichand, Y. *et al., Tet. Lett.*, 1979, 3921 (*isol, uv, ir, pmr, struct*)

Fistularin 2 F-42

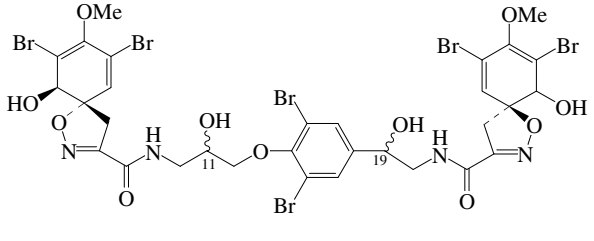
[73622-21-6]



$C_{22}H_{21}Br_4N_3O_8$ 775.039
Metab. of the sponge *Aplysina fistularis* forma *fulva*.
Gopichand, Y. *et al., Tet. Lett.*, 1979, 3921 (*isol, pmr, struct*)

Fistularin 3 F-43

[73622-22-7]



$C_{31}H_{30}Br_6N_4O_{11}$ 1114.022Metab. of the sponge *Aplysina fistularis* forma *fulva*, *Aplysina archeri*, *Agelas oroides*, *Pseudoceratina durissima*, *Verongula* sp., *Verongia aerophorba* and *Verongia cavernicola*. Inhibits the growth of feline leukaemia virus. Amorph. solid. $[\alpha]_D$ +104.2 (c, 1.67 in MeOH). λ_{max} 223 (sh) (ϵ 26545); 283 (sh) (ϵ 10387) (MeOH) (Derep).

Tetra-O-*Ac:* Mp 202-204° dec. $[\alpha]_D$ +149.4 (c, 1.32 in $CHCl_3$).

11-Ketone: ***11-Oxofistularin 3***. *11-Ketofistularin 3*
[142755-09-7]
$C_{31}H_{28}Br_6N_4O_{11}$ 1112.006
Metab. of the sponge *Aplysina archeri*. Inhibits the growth of feline leukaemia virus. Pale yellow gum. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{26}$ +130 (c, 0.1 in MeOH). λ_{max} 225 (ϵ 27000); 242 (ϵ 14000); 283 (ϵ 9900) (MeOH) (Berdy).

11-Deoxy: ***11-Deoxyfistularin 3***
[191112-19-3]
$C_{31}H_{30}Br_6N_4O_{10}$ 1098.023
Isol. from *Aplysina cavernicola* and *Aplysina fistularis insularis*. Cytotoxic agent. Powder.
Mp 128-130°. $[\alpha]_D^{25}$ +194.2 (c, 4.12 in MeOH). λ_{max} 232 (ϵ 19000); 284 (ϵ 11000) (MeOH). λ_{max} 209 (ϵ 42000); 235 (ϵ 21600); 283 (ϵ 11200) (MeOH).

19-Deoxy: ***19-Deoxyfistularin 3***
[153209-11-1]
$C_{31}H_{30}Br_6N_4O_{10}$ 1098.023
Metab. from a new sp. of sponge of the family Aplysinellidae, order Verongida, from the Coral Sea. Powder. $[\alpha]_D^{20}$ +155 (c, 0.17 in Me_2CO). λ_{max} 206 (ϵ 60400); 235 (ϵ 22000); 283 (ϵ 10400) (MeOH) (Berdy).

19-Deoxy, 11-ketone: ***19-Deoxy-11-oxofistularin 3***
[153209-12-2]
$C_{31}H_{28}Br_6N_4O_{10}$ 1096.007
Metab. from a new sp. of sponge of the family Aplysinellidae, order Verongida, from the Coral Sea. Powder. $[\alpha]_D^{20}$ +136 (c, 0.2 in Me_2CO). λ_{max} 205 (ϵ 18500); 280 (ϵ 3400) (MeOH) (Berdy).

11,19-Dideoxy: ***11,19-Dideoxyfistularin 3***
[179523-38-7]
$C_{31}H_{30}Br_6N_4O_9$ 1082.023
Metab. of the verongid sponge *Pseudoceratina durissima* and from *Aplysina lacunosa* and *Verongia cavernicola*. Unstable yellow powder. $[\alpha]_D$ +98.5 (c, 0.1 in MeOH). λ_{max} 224 (ϵ 26000); 257 (ϵ 16000); 284 (ϵ 10400) (MeOH) (Berdy).

11-Epimer: ***11-Epifistularin 3***
$C_{31}H_{30}Br_6N_4O_{11}$ 1114.022
Metab. from the marine sponge *Agelas oroides*. Exhibits antibacterial activity and moderate cytotoxicity towards cultured breast cancer cells. Amorph. solid. $[\alpha]_D^{25}$ +65.2 (c, 1.04 in Me_2CO). λ_{max} 233 (ϵ 13500); 283 (ϵ 2650) (EtOH) (Berdy).

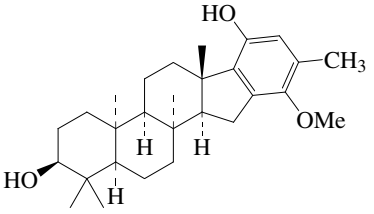
Stereoisomer: ***Isofistularin 3***
[87099-50-1]
$C_{31}H_{30}Br_6N_4O_{11}$ 1114.022
Isol. from *Verongia aerophoba* and *Aiolochroia crassa*. Cytotoxic agent. Shows antibiotic activity. Sol. Me_2CO, Et_2O. $[\alpha]_D$ +108 (c, 2.75 in MeOH). Isomeric at one or more chiral centres. Genus name often misspelt Ailochroia. λ_{max} 223 (sh) (ϵ 26545); 283 (sh) (ϵ 10387) (MeOH) (Derep).

Stereoisomer (2):
$C_{31}H_{30}Br_6N_4O_{11}$ 1114.022
Isol. from *Verongia aerophoba*. Pale yellow powder.
Mp 128°. $[\alpha]_D^{25}$ +51.6 (c, 0.6 in MeOH).

Gopichand, Y. *et al., Tet. Lett.*, 1979, **20**, 3921-3924 (*isol, uv, ir, pmr, struct*)
Cimino, G. *et al., Tet. Lett.*, 1983, **24**, 3029-3032 (*isol, pmr, struct, Isofistularin*)
Kernan, M.R. *et al., J. Nat. Prod.*, 1990, **53**, 615-622 (*11,19-Dideoxyfistularin 3*)
Gunasekera, S.P. *et al., J. Nat. Prod.*, 1992, **55**, 509-512 (*11-Oxofistularin 3*)
König, G.M. *et al., Heterocycles*, 1993, **36**, 1351-1358 (*11-Epifistularin 3*)
Mancini, I. *et al., J.C.S. Perkin 1*, 1993, 3121-3125 (*19-Deoxyfistularin 3, 19-Deoxy-11-oxofistularin 3*)
Ciminiello, P. *et al., Tetrahedron*, 1997, **53**, 6565-6572 (*11-Deoxyfistularin 3*)
Compagnone, R.S. *et al., J. Nat. Prod.*, 1999, **62**, 1443-1444 (*11-Deoxyfistularin 3*)
Gao, H. *et al., Tetrahedron*, 1999, **55**, 9717-9726 (*isol, cd, pmr, cmr*)
Aydoğmuş, Z. *et al., Turk. J. Chem.*, 1999, **23**, 339-344 (*Isofistularin 3, isol, activity, stereoisomer 2*)

Flabellinol F-44

[863548-85-0]



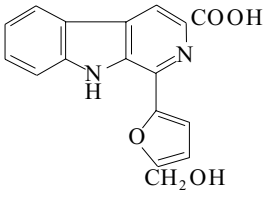
$C_{28}H_{42}O_3$ 426.638
Constit. of the tropical marine alga *Stypopodium flabelliforme*. Oil. $[\alpha]_D^{25}$ +18 (c, 0.12 in $CHCl_3$). λ_{max} 244 (ϵ 745); 284 (ϵ 960) (MeOH).

O-*De-Me, quinone:* ***Flabellinone***
[863548-86-1]
$C_{27}H_{38}O_3$ 410.595
Constit. of the tropical alga *Stypopodium flabelliforme*. Oil. $[\alpha]_D^{25}$ +25 (c, 0.12 in $CHCl_3$). λ_{max} 254 (ϵ 1240); 276 (ϵ 1039) (MeOH).

Sabry, O.M.M. *et al., J. Nat. Prod.*, 2005, **68**, 1022-1030 (*Flabellinol, Flabellinone*)

Flazine F-45

*1-[5-(Hydroxymethyl)-2-furanyl]-9*H*-pyrido[3,4-*b*]indole-3-carboxylic acid, 9CI*
[100041-05-2]



$C_{17}H_{12}N_2O_4$ 308.293
Constit. of the seeds of *Brucea javanica*. Prod. by the marine bacterium strain Bio215. Cryst. (MeOH).
Mp 231-233°. Fluorescent. λ_{max} 217 (log ϵ 4.87); 275 (log ϵ 4.85); 365 (log ϵ 3.02); 379 (log ϵ 3.11) (MeOH).

Me ester: ***Flazine methyl ester***
[104537-94-2]
$C_{18}H_{14}N_2O_4$ 322.32
Prod. by *Streptomyces* sp. K01-0031.
Mp 199-200°.

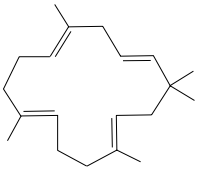
Me ether: ***Flazine methyl ether***. O-*Methylflazine*
[159898-11-0]
$C_{18}H_{14}N_2O_4$ 322.32
Alkaloid from freshly pressed juice of blackcurrant (*Ribes nigrum*).
Mp 199-200°.

*De(hydroxymethyl): 1-(2-Furanyl)-9*H*-pyrido[3,4-*b*]indole-3-carboxylic acid.* ***Dehydroxymethylflazine***
[76135-36-9]
$C_{16}H_{10}N_2O_3$ 278.267
From blackcurrant (*Ribes nigrum*).

Nakatsuka, S. *et al., Tet. Lett.*, 1986, **27**, 3399-3402 (*isol, uv, ir, pmr, struct*)
Gessner, W.P. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1988, **321**, 95-98 (*synth, uv, pmr*)
Blech, S. *et al., Z. Naturforsch., C*, 1994, **49**, 540-544 (*Flazine methyl ether, Dihydroxymethylflazine*)
Su, B.-N. *et al., Planta Med.*, 2002, **68**, 730-733 (*isol, pmr, cmr, ms*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)
Shiomi, K. *et al., J. Antibiot.*, 2005, **58**, 74-78 (*Me ester, isol*)

Flexibilene F-46

2,6,6,9,13-Pentamethyl-1,4,8,12-cyclopentadecatetraene
[62498-93-5]

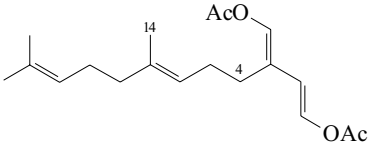


$C_{20}H_{32}$ 272.473
Constit. of *Sinularia flexibilis*.

Hérin, M. *et al., Bull. Soc. Chim. Belg.*, 1976, **85**, 801
McMurry, J. *et al., Tet. Lett.*, 1982, **23**, 1777 (*synth*)
McMurry, J.E. *et al., Tetrahedron*, 1987, **43**, 5489 (*synth*)

Flexilin F-47

[69625-33-8]



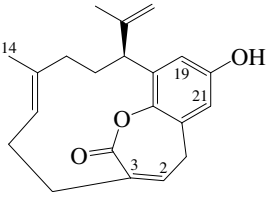
$C_{19}H_{28}O_4$ 320.428
Constit. of *Caulerpa flexilis*. Ichthyotoxin. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $Bp_{0.1}$ 100°.

14-Oxo: ***Preuplotin***
[154512-16-0]
$C_{19}H_{26}O_5$ 334.411
Isol. from *Euplotes crassus*. Cytotoxic to ciliates. λ_{max} 246 (ϵ 21400) (MeOH) (Berdy).

Blackman, A.J. *et al., Tet. Lett.*, 1978, 3063 (*isol*)
Guella, G. *et al., J.C.S. Perkin 1*, 1994, 161-166 (*Preuplotin*)

Floresolide B F-48

[588729-61-7]



$C_{21}H_{24}O_3$ 324.419
Constit. of an *Aplidium* sp. Cryst.
Mp 170°. $[\alpha]_D^{30}$ +164 (c, 0.2 in $CHCl_3$).

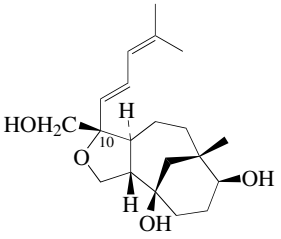
2α,3α-Epoxide: ***Floresolide A***
[588729-60-6]
$C_{21}H_{24}O_4$ 340.418
Constit. of an *Aplidium* sp. Cryst.
Mp 160-163°. $[\alpha]_D^{30}$ +26 (c, 0.6 in $CHCl_3$).

14-Hydroxy, 19,21-dibromo, 2α,3α-epoxide: ***Floresolide C***
[588729-62-8]
$C_{21}H_{22}Br_2O_5$ 514.21
Constit. of an *Aplidium* sp. Cryst.
Mp 178-180°. $[\alpha]_D^{30}$ +20 (c, 0.4 in $CHCl_3$).

Issa, H.H. *et al., Tet. Lett.*, 2003, **44**, 1243-1245 (*isol, pmr, cmr, cryst struct*)
Nicolaou, K.C. *et al., Chem. Comm.*, 2006, 600-602 (*synth*)

Florether A F-49

[217309-55-2]



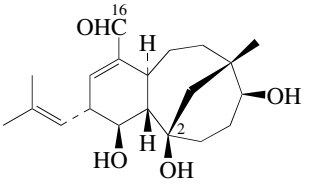
$C_{20}H_{32}O_4$ 336.47
Constit. of *Xenia florida*. Amorph. solid. $[\alpha]_D$ +52.3 (c, 0.11 in MeOH). λ_{max} 244 (log ϵ 4.12) (MeOH).

10-Epimer: ***Florether B***
[217309-56-3]
$C_{20}H_{32}O_4$ 336.47
Constit. of *Xenia florida*. Amorph. solid. $[\alpha]_D$ +79.4 (c, 0.08 in MeOH). λ_{max} 241 (log ϵ 4.24) (MeOH).

Iwagawa, T. *et al., J. Nat. Prod.*, 1998, **61**, 1513-1515 (*isol, pmr, cmr*)

Floridicin F-50

[158931-46-5]



$C_{20}H_{30}O_4$ 334.455
Constit. of *Xenia florida*. Needles.
Mp 182-183°. $[\alpha]_D$ -94.5 (c, 0.63 in MeOH). λ_{max} 235 (ϵ 8880) (MeOH) (Derep).

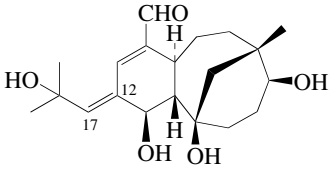
2-Me ether: ***2-O-Methylfloridicin***
$C_{21}H_{32}O_4$ 348.481
Constit. of *Xenia florida*. Oil. $[\alpha]_D$ -89.2 (c, 0.25 in MeOH). λ_{max} 230 (ϵ 9800) (MeOH).

16-Alcohol: ***Floridicin A***
$C_{20}H_{32}O_4$ 336.47
Constit. of *Xenia florida*. Oil. $[\alpha]_D$ -101.4 (c, 0.12 in MeOH). λ_{max} 209 (ϵ 9800) (MeOH).

Iwagawa, T. *et al., Chem. Comm.*, 1994, 2073 (*isol, pmr, cmr, cryst struct*)
Iwagawa, T. *et al., Tetrahedron*, 1997, **53**, 6809 (*isol, pmr, cmr, derivs*)

Floridicin B F-51

[191419-52-0]



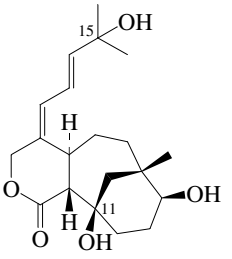
$C_{20}H_{30}O_5$ 350.454
Constit. of *Xenia florida*. Oil. $[\alpha]_D$ +382.5 (c, 0.12 in MeOH). λ_{max} 282 (ϵ 14500) (MeOH).

(12(17)-Z)-Isomer: ***Floridicin C***
[191419-53-1]
$C_{20}H_{30}O_5$ 350.454
Constit of *Xenia florida*. Oil. $[\alpha]_D$ +121.2 (c, 0.01 in MeOH). λ_{max} 280 (ϵ 18000) (MeOH).

Iwagawa, T. *et al., Tetrahedron*, 1997, **53**, 6809-6816 (*isol, pmr, cmr*)

Florlide A F-52

[132943-57-8]



$C_{20}H_{30}O_5$ 350.454
Constit. of *Xenia florida*. Amorph. solid. $[\alpha]_D$ +95.5 (c, 0.33 in MeOH). λ_{max} 246 (log ϵ 4.19) (MeOH). λ_{max} 246 (ϵ 15490) (MeOH) (Berdy).

15-Deoxy: ***Florlide B***
[132922-87-3]
$C_{20}H_{30}O_4$ 334.455
Constit. of *Xenia florida*. Amorph. solid. $[\alpha]_D$ +150 (c, 0.08 in MeOH). λ_{max} 245 (log ϵ 4.25) (MeOH). λ_{max} 244 (ϵ 17780) (MeOH) (Berdy).

11-Me ether: ***11-Methylflorlide A***
[267407-24-9]
$C_{21}H_{32}O_5$ 364.481
Constit. of *Xenia florida*. Oil. $[\alpha]_D$ +29 (c, 0.08 in MeOH). λ_{max} 239 (log ϵ 4.13) (MeOH).

Iwagawa, T. *et al., J. Nat. Prod.*, 1998, **61**, 1513-1515 (*isol, pmr, cmr*)
Iwagawa, T. *et al., J. Nat. Prod.*, 2000, **63**, 468-472 (*11-Methylflorlide A*)

FLRF amide F-53

[80690-77-3]

H-Phe-Leu-Arg-Phe-NH_2

$C_{30}H_{44}N_8O_4$ 580.729
Prob. present throughout molluscan phylum. Isol. from various molluscs incl. *Helisoma trivolvis* and *Lymnaea stagnalis*. Cardioregulatory neuropeptide.

Hydrochloride (1:2): [115993-58-3]
Cryst. + $2H_2O$. Mp 102° dec. $[\alpha]_D^{20}$ -6 (c, 0.5 in MeOH).

[104180-32-7]

Price, D.A. *et al., Am. Zool.*, 1986, **26**, 1007 (*rev*)
Kouge, K. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 4343 (*synth*)
Madrid, K.P. *et al., Peptides (Pergamon)*, 1994, **15**, 31 (*isol*)

Caenorhabditis elegans FLRF-amide peptides F-54

Ser-Ala-Asp-Pro-Asn-Phe-Leu-Arg-Phe-NH_2

Struct. of Peptide PF2 shown. Isol. from the nematode *Caenorhabditis elegans*. Neuropeptides.

SADPNFLRF amide
Peptide PF2
[143435-58-9]
$C_{49}H_{72}N_{14}O_{13}$ 1065.194
Also isol. from the nematode *Panagrellus redivivus*.

SQPNFLRF amide [149182-59-2]
$C_{47}H_{70}N_{14}O_{11}$ 1007.157
Indexed as the non-amide in CA.

ASGDPNFLRF amide [149203-83-8]
$C_{51}H_{75}N_{15}O_{14}$ 1122.246
Indexed as the non-amide in CA.

SDPNFLRF amide
Peptide PF1
[143435-57-8]
$C_{49}H_{72}N_{14}O_{13}$ 1065.194

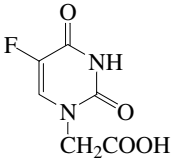
Also isol. from the nematode *Panagrellus redivivus*.

AAADPNFLRF amide [149182-61-6]
$C_{52}H_{77}N_{15}O_{13}$ 1120.273

PNFLRF amide [149182-62-7]
$C_{39}H_{57}N_{11}O_7$ 791.949
Indexed as the non-amide in CA.

Geary, T.G. *et al., Peptides (N.Y.)*, 1992, **13**, 209-214 (*isol, Panagrellus redivivus*)
Rosoff, M.L. *et al., Peptides (N.Y.)*, 1993, **14**, 331-338 (*isol, Caenorhabditis elegans*)

5-Fluoro-3,4-dihydro-2,4-dioxo-1(2*H*)-pyrimidineacetic acid F-55



$C_6H_5FN_2O_4$ 188.115

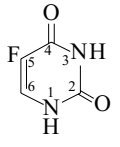
Me ester: 5-Fluoro-1-(methoxycarbonylmethyl)uracil
[56059-28-0]
$C_7H_7FN_2O_4$ 202.142
Isol. from the sponge *Phakellia fusca*. Needles (MeOH). Mp 178-179° (natural) Mp 185-186° (synthetic). λ_{max} 219 (ϵ 5725); 268 (ϵ 12813) (MeOH).

Hydrazide: [488713-02-6]
$C_6H_7FN_4O_3$ 202.145
Isol. from the sponge *Phakellia fusca*. Brown solid. Mp > 300°. λ_{max} 219 (ϵ 5763); 274 (ϵ 10909) (MeOH).

Tada, M. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 3427-3428 (*synth*)
Xu, X.-H. *et al., J. Nat. Prod.*, 2003, **66**, 285-288 (*isol*)

5-Fluoro-2,4(1*H*,3*H*)-pyrimidinedione, 9CI F-56

5-Fluoro-2,4-dihydroxypyrimidine. 5-Fluoro-2,4-pyrimidinediol. 5-Fluorouracil. ***Fluorouracil, BAN, INN, JAN, USAN****. Adrucil. Efudex. Fluoroplex. Fluracil. NSC 19893. Ro 2-9757. 5-FU*
[51-21-8]



$C_4H_3FN_2O_2$ 130.078
Isol. from the sponge *Phakellia fusca*. Reported from Chinese drug Mao Guo Yan Ming (roots of *Rabdosia lasiocarpus*). Antineoplastic agent. Used in combination with Adrenaline in the treatment of genital warts (AccuSite). Cryst. (H_2O). Mp 282-283° dec. Log P -0.97 (calc).

▶ Skin and respiratory tract irritant. Gastrointestinal, bone marrow depression and other adverse systemic effects when used therapeutically. Exp. reprod. and teratogenic effects. LD_{50} (rat, orl) 230 mg/kg. YR0350000

1-(2-Deoxy-β-D-ribofuranosyl): See 2′-Deoxy-5-fluorouridine in *The Combined Chemical Dictionary.*

1-β-D-Galactopyranosyl: OGT 719
[185843-61-2]
$C_{10}H_{13}FN_2O_7$ 292.22
Antineoplastic agent.

1-Me: 5-Fluoro-1-methyluracil
[155-16-8]
$C_5H_5FN_2O_2$ 144.105
Pale yellow needles (Me_2CO/EtOH). Mp 257-260° (255-257°).

3-Me: 5-Fluoro-3-methyluracil
[4840-69-1]
$C_5H_5FN_2O_2$ 144.105
Needles (Me_2CO/EtOH). Mp 170-171°.

1,3-Di-Me: [3013-92-1]
$C_6H_7FN_2O_2$ 158.132
Cryst. Mp 128-130°.

1-Et: 1-Ethyl-5-fluorouracil
[120889-35-2]
$C_6H_7FN_2O_2$ 158.132
Mp 183-185°.

1,3-Di-Et: 1,3-Diethyl-5-fluorouracil
[80115-67-9]
$C_8H_{11}FN_2O_2$ 186.185
Mp 66-68°.

1-Benzyl: 1-Benzyl-5-fluorouracil
[4871-13-0]
$C_{11}H_9FN_2O_2$ 220.203
Needles. Mp 173-174° (170-171°).

1,3-Dibenzyl: 1,3-Dibenzyl-5-fluorouracil
[75500-02-6]
$C_{18}H_{15}FN_2O_2$ 310.327
Needles. Mp 148-149°.

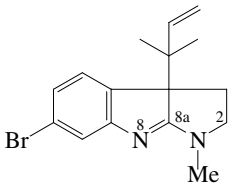
1-(2-Hydroxyethyl): 5-Fluoro-1-(2-hydroxyethyl)uracil
[53540-73-1]
$C_6H_7FN_2O_3$ 174.131
Isol. from the sponge *Phakellia fusca*. Needles. Mp 153-154°. λ_{max} 219 (ϵ 4823); 272 (ϵ 9159) (MeOH).

1-(2-Hydroxy-2-methoxyethyl): 5-Fluoro-1-(2-hydroxy-2-methoxyethyl)uracil
$C_7H_9FN_2O_4$ 204.158
Isol. from the sponge *Phakellia fusca*. Yellow amorph. powder. Mp 160-162°. λ_{max} 219 (ϵ 4479); 271 (ϵ 8895) (MeOH).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 809D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 362C (*nmr*)
Duschinsky, R. *et al., J.A.C.S.*, 1957, **79**, 4559 (*synth*)
Hoffer, M. *et al., J.A.C.S.*, 1959, **87**, 4112 (*synth*)
Robins, M.J. *et al., J.A.C.S.*, 1971, **93**, 5277 (*synth, uv, nmr, ms*)
Fallon, L. *et al., Acta Cryst. B*, 1973, **29**, 2549 (*cryst struct*)
Rudy, B.C. *et al., Anal. Profiles Drug Subst.*, 1973, **2**, 221 (*rev*)
Cech, D. *et al., J. Prakt. Chem.*, 1973, **315**, 149 (*synth*)
IARC Monog., 1981, **26**, 217; *Suppl.* 7, 210; *Suppl.* 6, 316 (*rev, tox*)
Chung, W.K. *et al., J. Het. Chem.*, 1983, **20**, 457 (*synth*)
Fuchikami, T. *et al., Chem. Lett.*, 1984, 1573 (*synth*)
Valeriote, F. *et al., Pharmacol. Ther.*, 1984, **24**, 107 (*rev, pharmacol*)
Chandrasekaran, S. *et al., J.O.C.*, 1985, **50**, 829 (*O-17 nmr*)
Morikawa, S. *et al., Nippon Kagaku Zasshi*, 1985, 2185; *CA*, **105**, 172147 (*synth*)
Leyland-Jones, B. *et al., Dev. Oncol.*, 1986, **47**, 131 (*rev, metab, pharmacol*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 154 (*synonyms*)
Wasternack, C. *et al., Pharmazie*, 1987, **42**, 73 (*rev*)
Ishikawa, I. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1922 (*derivs*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 480
Pat. Coop. Treaty (WIPO), 1997, (*Oxford GlycoSciences*)97 00 882; *CA*, **126**, 171853e (*OGT 719*)
Rohlff, C. *et al., Cancer Res.*, 1999, **59**, 1268-1272 (*OGT 719*)
Merck Index, 13th edn., 2001, No. 4208 (*bibl*)
Li, T.S.C. *et al., Chinese and Related North American Herbs*, CRC Press, 2002, 124 (*occur*)
Xu, X.-H. *et al., J. Nat. Prod.*, 2003, **66**, 285-288 (*Phakellia fusca uracils*)
Kheifets, G.M. *et al., Zh. Org. Khim.*, 2004, **40**, 106-112; *Russ. J. Org. Chem. (Engl. Transl.)2004,* **40**, 97-103 (*1-Me*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FMM000

Flustramine C F-57

[78127-86-3]



$C_{16}H_{19}BrN_2$ 319.243

Alkaloid from the marine bryozoan *Flustra foliacea*. Oil. λ_{max} 210 (sh) (ϵ 13000); 230 (ϵ 23000); 280 (ϵ 4600) (EtOH/HCl) (Derep). λ_{max} 210 (sh) (ϵ 10000); 232 (ϵ 27000); 290 (ϵ 9400); 307 (ϵ 4300) (EtOH) (Derep).

*8,8*a-*Dihydro:* ***Dihydroflustramine C***
[93930-02-0]
$C_{16}H_{21}BrN_2$ 321.259
Alkaloid from *Flustra foliacea*. Cryst. (Et_2O/petrol). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 82-84°. $[\alpha]_D^{25}$ -110 (c, 1.5 in CH_2Cl_2). λ_{max} 213 (ϵ 20000); 230 (ϵ 5600); 309 (ϵ 3400) (MeOH) (Berdy).

*8,8*a-*Dihydro,* N^1*-Oxide:* ***Dihydroflustramine C* N-*oxide***
[104387-11-3]
$C_{16}H_{21}BrN_2O$ 337.259
Minor metab. from *Flustra foliacea*. Oil. $[\alpha]_D^{25}$ -67.1 (c, 0.38 in CH_2Cl_2). Somewhat unstable. λ_{max} 226 (ϵ 2800); 283 (ϵ 2000) (MeOH) (Berdy).

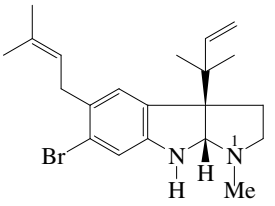
*8,8*a-*Dihydro, 8-(3-methyl-2-butenyl):* ***Flustramine A***
[71239-64-0]
$C_{21}H_{29}BrN_2$ 389.377
Alkaloid from the marine bryozoan *Flustra foliacea*. Muscle relaxant. Liq. Sol. MeOH, C_6H_6, $CHCl_3$; fairly sol. hexane. $[\alpha]_D^{20}$ -76.9 (c, 6.6 in EtOH). *cis*-3*a*,8*a*-Ring junction. λ_{max} 219 (ϵ 21000); 253 (ϵ 7700); 305 (ϵ 3500) (EtOH/HCl) (Derep). λ_{max} 218 (ϵ 20000); 262 (ϵ 9200); 317 (ϵ 3500) (EtOH) (Derep).

*8,8*a-*Dihydro, 2-oxo, 8-(3-methyl-2-butenyl):* ***Flustramide A***
[82534-44-9]
$C_{21}H_{27}BrN_2O$ 403.361
Alkaloid from the marine bryozoan *Flustra foliacea*. Oil. λ_{max} 216 (ϵ 18200); 260 (ϵ 7760); 310 (ϵ 3550) (EtOH) (Derep).

Carlé, J.S. *et al., J.A.C.S.*, 1979, **101**, 4012-4013 (*isol*)
Carlé, J.S. *et al., J.O.C.*, 1980, **45**, 1586-1589; 1981, **46**, 3440-3443 (*Flustramine A, Flustramine C, isol, uv, ir, pmr, ms, struct*)
Wulff, P. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **71**, 523-524 (*Flustramide A*)
Wright, J.L.C. *et al., J. Nat. Prod.*, 1984, **47**, 893-895 (*Dihydroflustramine C*)
Laycock, M.V. *et al., Can. J. Chem.*, 1986, **64**, 1312-1316 (*Dihydroflustramine* N^1*-oxide*)
Kawasaki, T. *et al., Tet. Lett.*, 1996, **37**, 7525-7528 (*synth, cmr*)
Morales-Rios, M.S. *et al., J.O.C.*, 1999, **64**, 1086-1087; 2001, **66**, 1186-1192 (*Flustramine A, Debromoflustramine A, Flustramide A, synth*)
Morales-Rios, M.S. *et al., Magn. Reson. Chem.*, 2002, **40**, 677-682 (*Flustramine A, pmr, cmr, conformn*)
Morales-Rios, M.S. *et al., Tetrahedron*, 2002, **58**, 1479-1484 (*Dihydroflustramine C, synth*)
Lysek, N. *et al., Z. Naturforsch., C*, 2002, **57**, 1056-1061 (*Flustramine A, isol, pmr, cmr*)
Fuchs, J.R. *et al., Org. Lett.*, 2005, **7**, 677-680 (*synth*)
Kawasaki, T. *et al., Chem. Comm.*, 2006, 420-422 (*Flustramine A, Flustramide A, synth*)

Flustramine D F-58

[104387-12-4]



Relative Configuration

$C_{21}H_{29}BrN_2$ 389.377

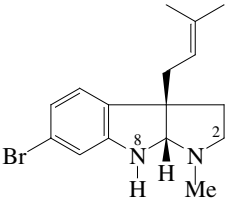
Metab. from the marine bryozoan *Flustra foliacea*. Oil. $[\alpha]_D^{25}$ -86.5 (c, 1.03 in CH_2Cl_2). λ_{max} 231 (ϵ 7100); 292 (ϵ 3100) (MeOH) (Berdy).

N^1*-Oxide:* ***Flustramine D* N-*oxide***
[104387-13-5]
$C_{21}H_{29}BrN_2O$ 405.377
Trace metab. from *Flustra foliacea*. Oil. Unstable. λ_{max} 224 (ϵ 7100); 285 (ϵ 3100) (MeOH) (Berdy).

Laycock, M.V. *et al., Can. J. Chem.*, 1986, **64**, 1312-1316 (*isol, uv, ir, pmr, cmr, ms, struct, oxide*)

Flustramine E F-59

[158642-05-8]



Absolute Configuration

$C_{16}H_{21}BrN_2$ 321.259

Rel. stereochem. only detd. Alkaloid from the marine bryozoan *Flustra foliacea*.
$[\alpha]_D^{20}$ -1136 (c, 0.0088 in EtOH). λ_{max} 210; 250; 308 (MeOH) (Berdy).

N^8*-(3-Methyl-2-butenyl):* ***Flustramine B***
[71239-65-1]
$C_{21}H_{29}BrN_2$ 389.377
Alkaloid from the marine bryozoan *Flustra foliacea*. Muscle relaxant. Sol. MeOH, C_6H_6, $CHCl_3$; fairly sol. hexane. λ_{max} 219 (ϵ 21000); 253 (ϵ 7700); 305 (ϵ 3500) (EtOH/HCl) (Derep). λ_{max} 218 (ϵ 20000); 262 (ϵ 9200); 317 (ϵ 3500) (EtOH) (Derep).

2-Oxo, N^8*-(3-methyl-2-butenyl):* ***Flustramide B***
[105708-75-6]
$C_{21}H_{27}BrN_2O$ 403.361
Minor alkaloid from *Flustra foliacea*. Oil. $[\alpha]_D^{20}$ -53.79 (EtOH). No stereochem. given. λ_{max} 216 (ϵ 18200); 260 (ϵ 7760); 310 (ϵ 3550) (EtOH) (Derep).

Debromo, N^8*-(3-methyl-2-butenyl):* ***Debromoflustramine B***
[158060-73-2]
$C_{21}H_{30}N_2$ 310.481
Trace alkaloid from *Flustra foliacea*.
$[\alpha]_D^{20}$ -98.2 (c, 0.0153 in $CHCl_3$). (+)-form has been synthesised.
λ_{max} 257; 308 (MeOH) (Berdy).

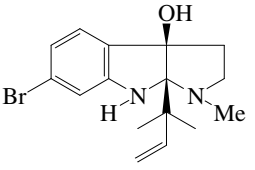
4′-Hydroxy, debromo: See Pseudophrynamine 258A in *The Combined Chemical Dictionary.*

Carlé, J.S. *et al., J.A.C.S.*, 1979, **101**, 4012-4013 (*isol, Flustramine B*)
Carlé, J.S. *et al., J.O.C.*, 1980, **45**, 1586-1589 (*isol, uv, ir, pmr, ms, struct, Flustramine B*)
Hino, T. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1806-1808 (*synth*)
Keil, P. *et al., Acta Chem. Scand., Ser. B*, 1986, **40**, 555-558 (*Flustramide B*)
Holst, P.B. *et al., J. Nat. Prod.*, 1994, **57**, 997-1000 (*Flustramine E, Debromoflustramine B*)
Bruncko, M. *et al., J.O.C.*, 1994, **59**, 5543-5549 (*Debromoflustramine B, synth*)

Somei, M. *et al., Heterocycles*, 1997, **45**, 2327-2330 (*synth, Debromoflustramine B*)
Morales-Rios, M.S. *et al., J.O.C.*, 1999, **64**, 1086-1087; 2001, **66**, 1186-1192 (*Flustramide B, Flustramine B, Debromoflustramine B, synth*)
Cardoso, A.S. *et al., Tet. Lett.*, 2001, **42**, 6663-6666 (*Debromoflustramine B, synth*)
Morales-Rios, M.S. *et al., Magn. Reson. Chem.*, 2002, **40**, 677-682 (*pmr, cmr, conformn*)
Morales-Rios, M.S. *et al., Tetrahedron*, 2002, **58**, 1479-1484 (*synth*)
Tan, G.H. *et al., Org. Lett.*, 2003, **5**, 1801-1803 (*synth*)
Kawasaki, T. *et al., Chem. Comm.*, 2006, 420-422 (*Flustramine B, Flustramide B, synth*)

Flustraminol A F-60

[78127-88-5]



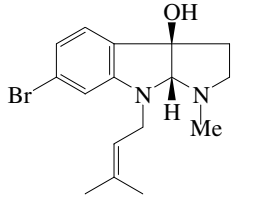
Relative Configuration

$C_{16}H_{21}BrN_2O$ 337.259
Alkaloid from the marine bryozoan *Flustra foliacea*. Brown oil. λ_{max} 215 (ϵ 18000); 234 (sh) (ϵ 8600); 246 (ϵ 5400); 306 (ϵ 2300) (EtOH/HCl) (Derep). λ_{max} 215 (ϵ 17000); 256 (ϵ 6500); 318 (ϵ 2300) (EtOH) (Derep).

Carlé, J.S. *et al., J.O.C.*, 1981, **46**, 3440-3443 (*isol, uv, ir, pmr, ms, struct*)

Flustraminol B F-61

[78127-89-6]



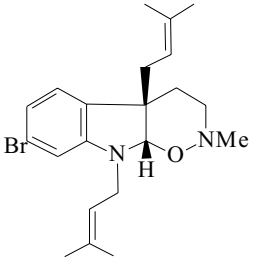
Relative Configuration

$C_{16}H_{21}BrN_2O$ 337.259
Alkaloid from the marine bryozoan *Flustra foliacea*. Brown oil. λ_{max} 220 (ϵ 17000); 240 (sh) (ϵ 6300); 298 (ϵ 2300) (EtOH/HCl) (Derep). λ_{max} 220 (ϵ 17000); 256 (ϵ 6300); 310 (ϵ 2300) (EtOH) (Derep).

Carlé, J.S. *et al., J.O.C.*, 1981, **46**, 3440-3443 (*isol, uv, ir, pmr, ms, struct*)

Flustrarine B F-62

[105708-76-7]



Relative configuration

$C_{21}H_{29}BrN_2O$ 405.377
Alkaloid from the marine bryozoan *Flustra foliacea*. Also obt. by H_2O_2 oxidn. of Flustramine E, F-59.
$[\alpha]_D^{20}$ -180 (EtOH). Prob. struct. Nat. prod may be Flustramine B *N*-oxide. λ_{max} 216 (ϵ 18200); 260 (ϵ 7760); 310 (ϵ 3550) (EtOH) (Derep).

Keil, P. *et al., Acta Chem. Scand., Ser. B*, 1986, **40**, 555-558 (*isol, uv, ir, pmr, cmr, ms, struct, synth*)

Fusinus ferrugineus FMRF amide-related peptides F-63

Ala-Leu-Thr-Asn-Asp-His-Phe-Leu-Arg-Phe-NH_2
Isol. from ganglia of the prosobranch mollusc *Fusinus ferrugineus*. Neuropeptides.

ALTNDHFLRF amide
$C_{57}H_{85}N_{17}O_{14}$ 1232.404
CAS no. not found 8-14CI.

LSSFVRI amide [148054-14-2]
$C_{38}H_{65}N_{11}O_9$ 820

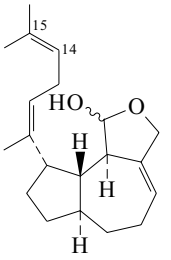
GSLFRF amide [135132-69-3]
$C_{35}H_{52}N_{10}O_7$ 724.859

SSLFRF amide [135132-70-6]
$C_{36}H_{54}N_{10}O_8$ 754.885

Kuroki, Y. *et al., Acta Biol. Hung.*, 1993, **44**, 41-44 (*isol*)

Focardin F-64

[177196-39-3]



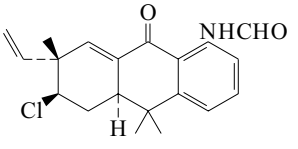
$C_{20}H_{30}O_2$ 302.456
Constit. of *Euplotes focardii*. Defensive agent.

14,15-Epoxide: ***Epoxyfocardin***
[177196-38-2]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Euplotes focardii*. Defensive agent. $[\alpha]_D^{20}$ +29 (c, 0.2 in EtOH).

Guella, G. *et al., Helv. Chim. Acta*, 1996, **79**, 439 (*isol, pmr, cmr*)

Fontonamide F-65

[109217-15-4]



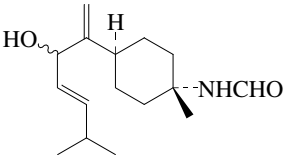
$C_{20}H_{22}ClNO_2$ 343.852
Apparently a seco-indole alkaloid which is a singlet oxygen oxidn. prod. of Hapalindole A, H-80. See also Hapalonamide G, H-86. Isol. from blue-green alga *Hapalosiphon fontinalis*.
Mp 156-157°. $[\alpha]_D$ -141 (c, 0.21 in $CHCl_3$). λ_{max} 240 (ϵ 5680); 289 (ϵ 4770); 345 (ϵ 1630) (MeOH) (Derep).

Decloro: ***Dechlorofontonamide***
[123498-02-2]
$C_{20}H_{23}NO_2$ 309.407
Minor alkaloid from *Hapalosiphon fontinalis*.
$[\alpha]_D$ -100 (c, 0.2 in $CHCl_3$).

Moore, R.E. *et al., J.O.C.*, 1987, **52**, 3773 (*isol, struct*)
Moore, R.E. *et al., Phytochemistry*, 1989, **28**, 1565 (*Dechlorofontonomide*)

3-Formamido-7(14),9-bisaboladien-8-ol F-66

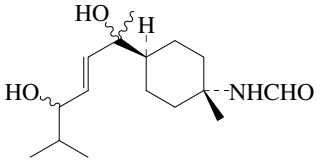
[245362-20-3]



$C_{16}H_{27}NO_2$ 265.395
Constit. of an *Axinyssa* sp. Oil.

8-Ketone: ***3-Formamido-7(14),9-bisaboladien-8-one***
[245360-32-1]
$C_{16}H_{25}NO_2$ 263.379
Constit. of an *Axinyssa* sp. Oil. $[\alpha]_D$ +28 (c, 0.25 in MeOH). λ_{max} 234 (MeOH).
Li, C.-J. *et al., J. Nat. Prod.*, 1999, **62**, 1330-1332 (*isol, pmr, cmr*)

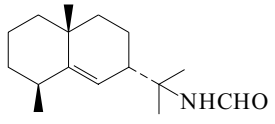
3-Formamido-8-bisabolene-7,10-diol F-67



$C_{16}H_{29}NO_3$ 283.41

7-Me ether: ***3-Formamido-7-methoxy-8-bisabolen-10-ol***
[245362-21-4]
$C_{17}H_{31}NO_3$ 297.437
Constit. of an *Axinyssa* sp. Oil.
Li, C.-J. *et al., J. Nat. Prod.*, 1999, **62**, 1330-1332 (*isol, pmr, cmr*)

11-Formamido-5-eudesmene F-68



$C_{16}H_{27}NO$ 249.395

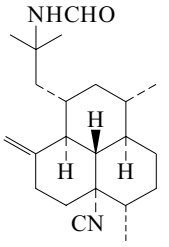
(4β,7α,10β)-*form*
Constit. of *Axinella cannabina*.
Oil.

Isocyanide: ***11-Isocyanato-5-eudesmene***
$C_{16}H_{25}N$ 231.38
Constit. of *Axinella cannabina* and *Phakellia* sp. Oil. $[\alpha]_D$ -85.7 (c, 0.8 in $CHCl_3$). Has –NC replacing –NHCHO.

Isothiocyanate: ***11-Isothiocyanato-5-eudesmene***
[108639-31-2]
$C_{16}H_{25}NS$ 263.446
Constit. of *Axinella cannabina*, *Acanthella klethra* and *Cadlina luteomarginata*. Oil. $[\alpha]_D$ -89.7 (c, 0.8 in $CHCl_3$). Has –NCS replacing –NHCHO.
Ciminiello, P. *et al., Can. J. Chem.*, 1987, **65**, 518
Angerhofer, C.K. *et al., J. Nat. Prod.*, 1992, **55**, 1787 (*isothiocyanate, isol*)
Burgoyne, D.L. *et al., Tetrahedron*, 1993, **49**, 4503

15-Formylamino-8-isocyano-11(20)-amphilectene F-69

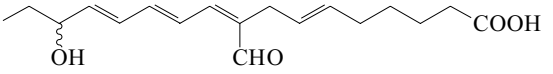
[70206-87-0]



$C_{22}H_{34}N_2O$ 342.523
Isol. from marine sponge *Hymeniacidon amphilecta*. Active against gram-positive bacteria and yeasts. Oil. $[\alpha]_D$ -24 (c, 1 in $CHCl_3$).
Wratten, S.J. *et al., Tet. Lett.*, 1978, 4345 (*isol, ir, pmr, cmr, struct*)

9-Formyl-15-hydroxy-6,9,11,13-heptadecatetraenoic acid F-70

9-(6-Hydroxy-2,4-octadienylidene)-10-oxodecanoic acid



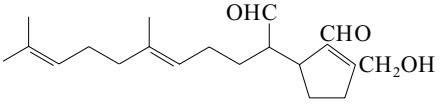
$C_{18}H_{26}O_4$ 306.401

(6*E*,9*Z*,11*E*,13*E*)-*form*
Me ester: [147292-96-4]
$C_{19}H_{28}O_4$ 320.428
Isol. from the green alga *Acrosiphonia coalita*. Light oil. C-15 config. not determined.

15-Ketone, Me ester: [147293-00-3]
$C_{19}H_{26}O_4$ 318.412
Isol. from *Acrosiphonia coalita*. Oil.
Bernart, M.W. *et al., J. Nat. Prod.*, 1993, **56**, 245 (*isol, struct*)

2-(2-Formyl-3-hydroxymethyl-2-cyclopentenyl)-6,10-dimethyl-5,9-undecadienal F-71

α-(4,8-Dimethyl-3,7-nonadienyl)-2-formyl-3-(hydroxymethyl)-2-cyclopentene-1-acetaldehyde, 9CI
[93888-62-1]

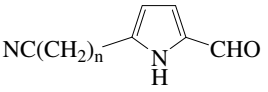


$C_{20}H_{30}O_3$ 318.455
Metab. of *Udotea flabellum*. Antifungal and antibacterial agent. Ichthyotoxin. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{25}$ -26.4 (c, 0.9 in $CHCl_3$). λ_{max} 251 (ε 5440) (MeOH) (Berdy).

Ac:
$C_{22}H_{32}O_4$ 360.492
Metab. of *Udotea flabellum*. Antifungal and antibacterial agent. Ichthyotoxin. Oil. $[\alpha]_D^{25}$ -28 (c, 1.5 in $CHCl_3$).
Paul, V.J. *et al., Tetrahedron*, 1984, **40**, 2913

5-Formyl-1*H*-pyrrole-2-alkanenitriles F-72

5-(ω-Cyanoalkyl)-2-pyrrolecarboxaldehydes



5-Formyl-1*H*-pyrrole-2-octadecanenitrile

*5-(17-Cyanoheptadecyl)-1*H*-pyrrole-2-carboxaldehyde.* ***Mycalenitrile 1***

[705973-45-1]

$C_{23}H_{38}N_2O$ 358.566

Alkaloid from the sponge *Mycale cecilia*. Oil. n = 17. λ_{max} 204 (ϵ 6025); 248 (ϵ 2540); 300 (ϵ 10125) (MeOH).

5-Formyl-1*H*-pyrrole-2-eicosanenitrile, 9CI

*5-(19-Cyanononadecyl)-1*H*-pyrrole-2-carboxaldehyde*

[233744-62-2]

$C_{25}H_{42}N_2O$ 386.62

Alkaloid from the sponges *Desmapsamma anchorata* and *Mycale microsigmatosa*. Antileishmanial agent. n = 19.

5-Formyl-1*H*-pyrrole-2-heneicosanenitrile

*5-(20-Cyanoeicosyl)-1*H*-pyrrole-2-carboxaldehyde.* ***Mycalenitrile 2***

[705973-46-2]

$C_{26}H_{44}N_2O$ 400.646

Alkaloid from the sponge *Mycale cecilia*. Oil. n = 20. λ_{max} 204 (ϵ 6030); 248 (ϵ 2710); 300 (ϵ 11790) (MeOH).

5-Formyl-1*H*-pyrrole-2-docosanenitrile

*5-(21-Cyanoheneicosyl)-1*H*-pyrrole-2-carboxaldehyde.* ***Mycalenitrile 3***

[705973-47-3]

$C_{27}H_{46}N_2O$ 414.673

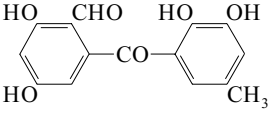
Alkaloid from the sponge *Mycale cecilia*. Oil. n = 21. λ_{max} 203 (ϵ 5950); 248 (ϵ 2510); 300 (ϵ 10000) (MeOH).

Compagnone, R.S. *et al., Nat. Prod. Lett.*, 1999, **13**, 203-211 (*5-Formyl-1H-pyrrole-2-eicosanenitrile*)

Ortega, M.J. *et al., Tetrahedron*, 2004, **60**, 2517-2524 (*Mycalenitriles*)

2-Formyl-2′,3,3′,5-tetrahydroxy-5′-methylbenzophenone F-73

2′,3,3′,5-Tetrahydroxy-5′-methylbenzophenone-2-carboxaldehyde



$C_{15}H_{12}O_6$ 288.256

3,3′-Di-Me ether: 2-Formyl-2′,5-dihydroxy-3,3′-dimethoxy-5′-methylbenzophenone. 2′,5-Dihydroxy-3,3′-dimethoxy-5′-methylbenzophenone-2-carboxaldehyde. ***Daldinal B***

[160889-33-8]

$C_{17}H_{16}O_6$ 316.31

Metab. of the fungus *Daldinia concentrica*. λ_{max} 214 (ϵ 26910); 272 (ϵ 16220); 323 (ϵ 11220) (EtOH).

2′,3,3′-Tri-Me ether: 2-Formyl-5-hydroxy-2′,3,3′-trimethoxy-5′-methylbenzophenone. 5-Hydroxy-2′,3,3′-trimethoxy-5′-methylbenzophenone-2-carboxaldehyde. ***Daldinal A***

[160889-21-4]

$C_{18}H_{18}O_6$ 330.337

Metab. of *Daldinia concentrica* and *Hypoxylon macrocarpum*. λ_{max} 213 (ϵ 24550); 262 (ϵ 10470); 321 (ϵ 9120) (EtOH).

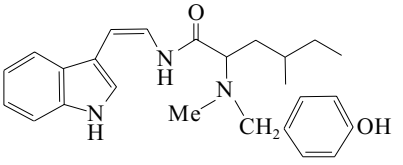
Hashimoto, T. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1528 (*isol, uv, ir, pmr, cmr*)

Muhlbauer, A. *et al., Mycol. Prog.*, 2002, **1**, 235-248 (*Daldinal A, occur*)

Fragilamide F-74

*2-[[(4-Hydroxyphenyl)methyl]methylamino]-*N*-[2-(1*H*-indol-3-yl)ethenyl]-4-methylhexanamide, 9CI*

[87168-33-0]



$C_{25}H_{31}N_3O_2$ 405.539

Alkaloid from the marine red alga *Martensia fragilis*. $[\alpha]_D$ -32 (c, 0.62 in MeOH). λ_{max} 229 (ϵ 15500); 280 (ϵ 10200) (EtOH) (Derep).

Kirkup, M.P. *et al., Tet. Lett.*, 1983, **24**, 2087 (*isol, uv, ir, pmr, cmr, ms, struct*)

Penaeus monodon FRMF amide-like neuropeptides F-75

Pem-FLP

Gly-Asp-Arg-Asn-Phe-Leu-Arg-Phe-NH_2

Struct. of Pem-FLP-1 shown. Isol. from the eyestalk of the giant tiger prawn *Penaeus monodon*.

Pem-FLP 1 [431944-93-3]

$C_{46}H_{70}N_{16}O_{11}$ 1023.16

Pem-FLP 2 [431944-94-4]

$C_{59}H_{86}N_{16}O_{15}$ 1259.427

Pem-FLP 3 [431944-95-5]

$C_{48}H_{81}N_{17}O_{11}S$ 1104.341

Pem-FLP 4 [431944-96-6]

$C_{48}H_{81}N_{17}O_{12}S$ 1120.341

Pem-FLP 5 [431944-97-7]

$C_{49}H_{84}N_{16}O_{11}S$ 1105.369

Pem-FLP 6 [431944-98-8]

$C_{57}H_{97}N_{21}O_{14}$ 1300.526

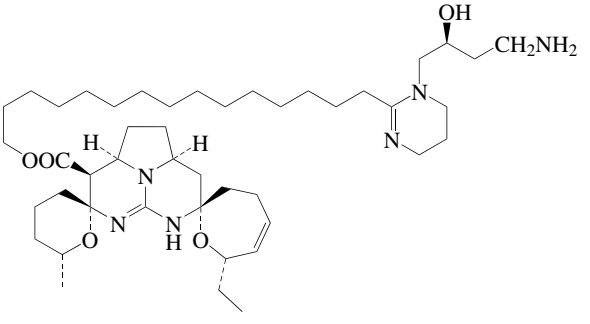
Pem-FLP 7 [431944-99-9]

$C_{66}H_{96}N_{18}O_{15}$ 1381.596

Sithigorngul, P. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2002, **131**, 325-327 (*isol*)

Fromiamycalin F-76

[163597-73-7]



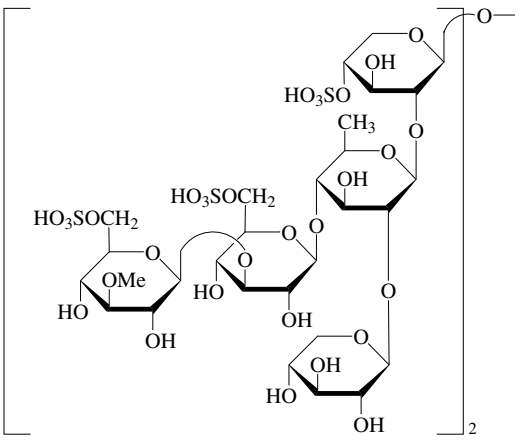
$C_{45}H_{78}N_6O_5$ 783.148

Alkaloid from the New Caledonian starfish *Fromia monilis*. Cytotoxic. $[\alpha]_D$ -12 (as hydrochloride).

Palagiano, E. *et al., Tetrahedron*, 1995, **51**, 3675-3682 (*isol, pmr, cmr, struct*)

Frondecaside F-77

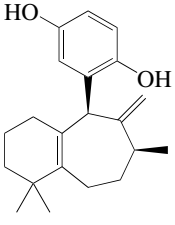
[139030-91-4, 139069-41-3]



$C_{58}H_{98}O_{63}S_6$ 1995.77
Isol. from the sea cucumber *Cucumaria frondosa*. Amorph. solid (as hexa-K or hexa-Na salt).
Mp 251-252° (hexa-K or hexa-Na salt). $[\alpha]_D^{23}$ -19.2 (c, 0.001 in Py aq.) (hexa-K or hexa-Na salt).

Findlay, J.A. *et al., J. Nat. Prod.*, 1992, **55**, 93-101 (*isol, pmr, cmr*)

Frondosin A F-78



(+)-*form*

$C_{21}H_{28}O_2$ 312.451
λ_{max} 232; 296 (MeOH) (Berdy).

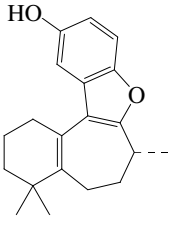
(+)-*form* [189514-05-4]
Constit. of *Dysidea frondosa*.
Powder.
Mp 111-113°. $[\alpha]_D$ +31.5 (c, 0.25 in MeOH). λ_{max} 232; 296 (MeOH).

(-)-*form* [203933-73-7]
Constit. of *Euryspongia* sp.
Solid. $[\alpha]_D$ -210 (c, 0.93 in MeOH). λ_{max} 210 (log ϵ 5.04); 296 (log ϵ 4.51) (MeOH).

Patil, A.D. *et al., Tetrahedron*, 1997, **53**, 5047-5060 (*isol, pmr, cmr*)
Hallock, Y.F. *et al., Nat. Prod. Lett.*, 1998, **11**, 153-160 (*isol*)

Frondosin B F-79

[189514-47-4]



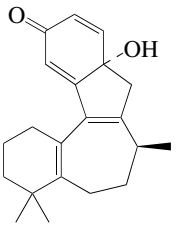
$C_{20}H_{24}O_2$ 296.408

(*R*)-*form*
Constit. of *Dysidea frondosa*.
Gum. $[\alpha]_D$ +18.6 (c, 0.17 in MeOH). λ_{max} 228; 245; 258 (MeOH).

Patil, A.D. *et al., Tetrahedron*, 1997, **53**, 5047-5060 (*isol, pmr, cmr*)
Inoue, M. *et al., J.A.C.S.*, 2001, **123**, 1878-1889 (*synth, abs config*)
Kerr, D.J. *et al., Org. Lett.*, 2004, **6**, 457-460 (*synth*)
Hughes, C.C. *et al., Tetrahedron*, 2004, **60**, 9675-9686 (*synth*)

Frondosin C F-80

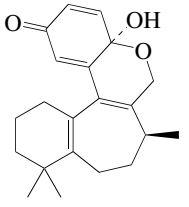
[189514-48-5]



$C_{21}H_{26}O_2$ 310.435
Constit. of *Dysidea frondosa*. Interleukin-8 receptor inhibitor. Protein kinase C inhibitor. Oil. $[\alpha]_D$ +9.4 (c, 0.12 in MeOH). λ_{max} 230; 245; 295 (MeOH).

Patil, A.D. *et al., Tetrahedron*, 1997, **53**, 5047-5060 (*isol, pmr, cmr*)

Frondosin D F-81



(+)-*form*

$C_{21}H_{26}O_3$ 326.435
λ_{max} 220; 245; 321 (MeOH) (Berdy).

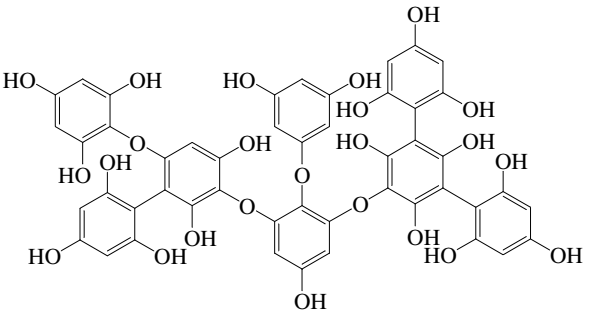
(+)-*form* [189514-84-9]
Constit. of *Dysidea frondosa*.
Solid. $[\alpha]_D$ +29.6 (c, 0.2 in MeOH). Error in struct. diag. in ref.
λ_{max} 220; 247; 321 (MeOH).

Me ether: ***Frondosin E***
[189515-22-8]
$C_{22}H_{28}O_3$ 340.461
Constit. of *Dysidea frondosa*. Interleukin-8 receptor inhibitor. Protein kinase C inhibitor. Oil. $[\alpha]_D$ +26.1 (c, 0.09 in MeOH). λ_{max} 228; 247; 299 (MeOH).

(-)-*form* [203933-76-0]
Constit. of *Euryspongia* sp.
Yellow solid. $[\alpha]_D$ -211 (c, 0.43 in MeOH). λ_{max} 221 (log ϵ 4.98); 337 (log ϵ 4.73) (MeOH).

Patil, A.D. *et al., Tetrahedron*, 1997, **53**, 5047-5060 (*isol, pmr, cmr*)
Hallock, Y.F. *et al., Nat. Prod. Lett.*, 1998, **11**, 153-160 (*isol*)

Fucodifucotetraphlorethol A F-82

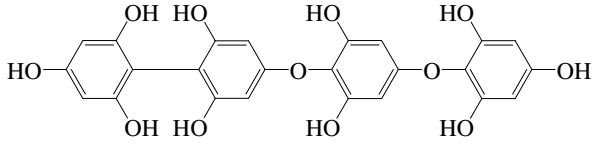


$C_{48}H_{34}O_{24}$ 994.782
Isol. from brown algae *Cystophora torulosa*, *Sargassum spinuligerum* and *Carpophyllum angustifolium*.

Glombitza, K.W. *et al., Phytochemistry*, 1997, **46**, 735-740; 1417-1422 (*isol, struct*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

Fucodiphlorethol A F-83

[64461-86-5]

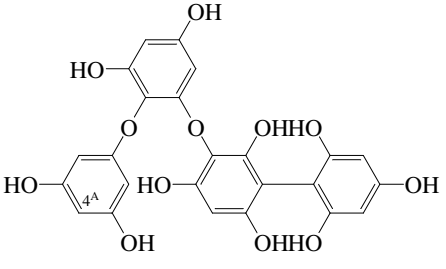


$C_{24}H_{18}O_{12}$ 498.399
Isol. from *Cystoseira baccata* and *Fucus vesiculosus*. Isol. as deca-Ac to which CAS no. refers.

Glombitza, K.W. *et al., Planta Med.*, 1977, **32**, 33-45 (*isol, struct*)
Glombitza, K.-W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1978, **311**, 393-399 (*isol*)

Fucodiphlorethol B F-84

3-[2-(3,5-Dihydroxyphenoxy)-3,5-dihydroxyphenoxy]-[1,1′-biphenyl]-2,2′,4,4′,6,6′-hexol, 9CI
[72380-14-4]



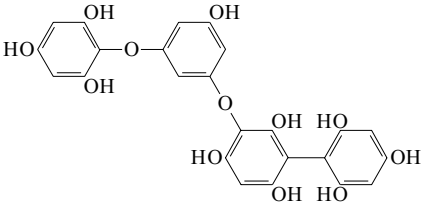
$C_{24}H_{18}O_{12}$ 498.399
Isol. from *Cystoseira baccata*, *Cystophora torulosa* and *Carpophyllum angustifolium*.

4^A-Hydroxy: ***Hydroxyfucodiphlorethol B***
$C_{24}H_{18}O_{13}$ 514.398
Isol. from *Cystophora torulosa*.

Glombitza, K.W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1978, **311**, 393-399 (*isol, struct*)
Glombitza, K.W. *et al., Phytochemistry*, 1997, **46**, 735-740 (*Hydroxyfucodiphlorethol B*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

Fucodiphlorethol C F-85

3-[3-Hydroxy-5-(2,4,6-trihydroxyphenoxy)phenoxy]-[1,1′-biphenyl]-2,2′,4,4′,6,6′-hexol, 9CI
[72380-13-3]

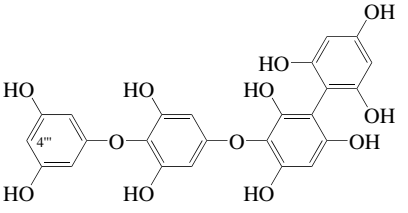


$C_{24}H_{18}O_{12}$ 498.399
Isol. from *Laminaria ochroleuca*.

Glombitza, K.W. *et al., CA*, 1980, **92**, 55043 (*isol*)

Fucodiphlorethol D F-86

3-[4-(3,5-Dihydroxyphenoxy)-3,5-dihydroxyphenoxy]-[1,1′-biphenyl]-2,2′,4,4′,6,6′-hexol, 9CI
[79005-82-6]



$C_{24}H_{18}O_{12}$ 498.399
Isol. from brown algae *Cystoseira baccata*, *Cystophora congesta*, *Carpophyllum angustifolium*, *Sargassum spinuligerum* and *Cystophora retroflexa*.

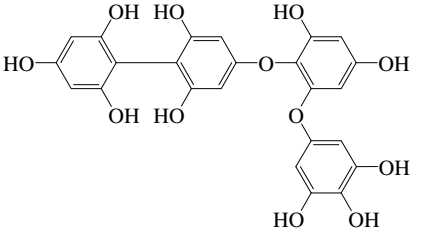
4‴-Hydroxy: ***Hydroxyfucodiphlorethol A***
$C_{24}H_{18}O_{13}$ 514.398
Isol. from brown algae *Sargassum spinuligerum*, *Carpophyllum maschalocarpum* and *Cystophora torulosa*. These phlorotannins are named in series according to their order of discovery. Hydroxyfucodiphlorethol A is a hydroxy deriv. of Fucodiphlorethol D, not A.

[79003-51-3]

Glombitza, K.W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1981, **314**, 602-608 (*isol, struct*)
Koch, M. *et al., Phytochemistry*, 1984, **23**, 2633-2637 (*isol*)
Glombitza, K.W. *et al., Phytochemistry*, 1991, **30**, 3423-3427; 1997, **46**, 1417-1422; 1999, **50**, 869-881 (*isol*)
Glombitza, K.W. *et al., Phytochemistry*, 1991, **30**, 3423-3427 (*Hydroxyfucodiphlorethol A*)
Glombitza, K.W. *et al., Nat. Toxins*, 1997, **5**, 58-63 (*Hydroxyfucodiphlorethol A, isol*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

Fucodiphlorethol F F-87

4′-[2,4-Dihydroxy-6-(2,4,6-trihydroxyphenoxy)phenoxy]-[1,1′-biphenyl]-2,2′,4,6,6′-pentol, 9CI
[64108-85-6]



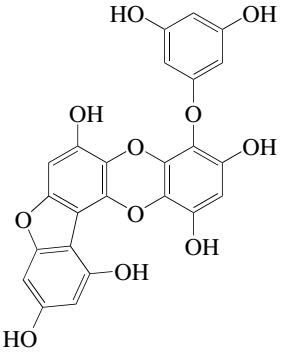
$C_{24}H_{18}O_{12}$ 498.399

Isol. from brown algae *Durvillaea antarctica*, *Sargassum spinuligerum*, *Cystophora torulosa* and *Fucus vesiculosus*. Isol. as per-Ac. Genus name often spelt as Durvillea.

Craigie, J.S. *et al., Can. J. Chem.*, 1977, **55**, 1575-1582 (*isol, pmr, cmr*)
Glombitza, K.-W. *et al., Nat. Toxins*, 1997, **5**, 58-63 (*isol*)

Fucofuroeckol A F-88

[96820-15-4]

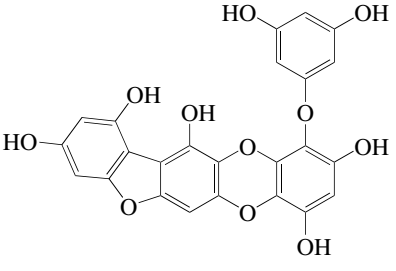


$C_{24}H_{14}O_{11}$ 478.368
Constit. of the brown alga *Eisenia arborea*. Isol. as hepta-Ac.

Glombitza, K.-W. *et al., Phytochemistry*, 1985, **24**, 543-551 (*isol, pmr*)

Fucofuroeckol B F-89

[96820-16-5]

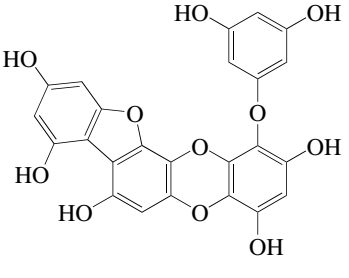


$C_{24}H_{14}O_{11}$ 478.368
Constit. of the brown alga *Eisenia arborea*. Isol. as hepta-Ac.

Glombitza, K.-W. *et al., Phytochemistry*, 1985, **24**, 543-551 (*isol, pmr*)

Fucofuroeckol C F-90

[96820-17-6]

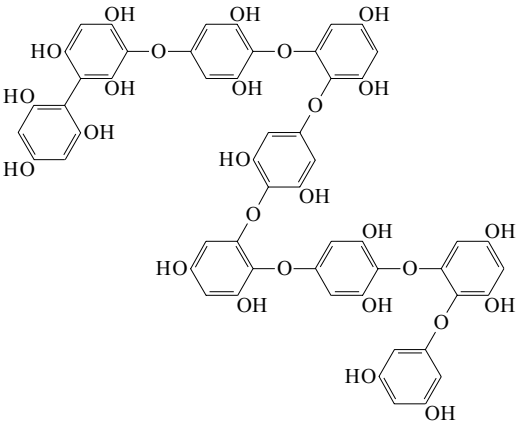


$C_{24}H_{14}O_{11}$ 478.368
Constit. of the brown alga *Eisenia arborea*.

Glombitza, K.-W. *et al., Phytochemistry*, 1985, **24**, 543-551 (*isol, pmr*)

Fucoheptaphlorethol A F-91

[97915-32-7]

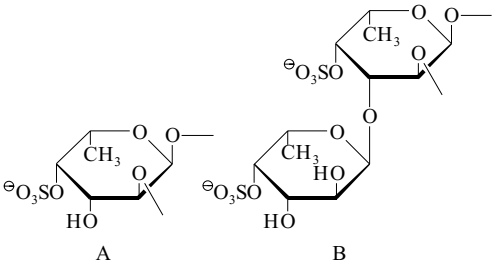


$C_{54}H_{38}O_{27}$ 1118.878
Isol. from *Cystoseira granulata* (as per-Ac).

Glombitza, K.W. *et al., Planta Med.*, 1985, **51**, 116 (*isol, pmr, cmr, ms*)

Fucoidin F-92

Fucoidan, 9CI, 8CI. Fucosidan
[9072-19-9]



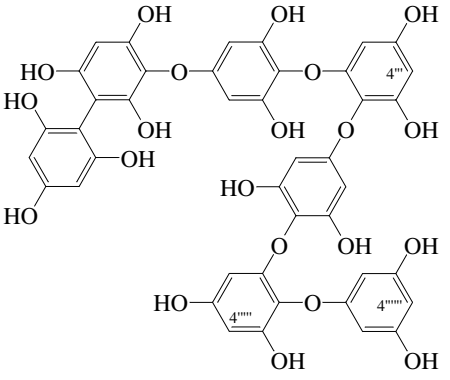
A B

A polysaccharide containing L-fucose and half sulfate ester. Small amounts of galactose, xylose and uronic acid are present. Two possible components are illustrated. The precise struct. of fucoidin in variants remains unclear (2000). Present in the intercellular tissues and surface exudates of Phaeophyceae, although the amount in some spp. is exceedingly small. The polysaccharide content varies with the depth at which the plant is located. *Pelvetia canaliculata* contains about 23% of the dry weight while in permanently submerged *Laminaria* it is V. hygroscopic, may prevent dehyd. of the plant upon long exp. Shows a range of biol. activities incl. antitumour and antiviral. $[\alpha]_D$ -118. Fucoins showing some structural differences isol. from *Sargassum linifolium* and from *Ascophyllum nodosum* have been termed Sargassan and Ascophylan respectively.

Conchie, J. *et al., J.C.S.*, 1950, 827
Black, W.A.P. *et al., J. Sci. Food Agric.*, 1954, **5**, 445 (*isol, occur*)
Larsen, B. *et al., Acta Chem. Scand.*, 1966, **20**, 219-230 (*Ascophylan*)
Percival, E. *et al., The Carbohydrates*, 2nd Ed., Academic Press, 1970, **2B**, 551 (*rev*)
Doner, L.W. *et al., Ind. Gums*, (Whistler, R.L., Ed.), 2nd Ed., Academic Press, New York, 1973, 115; *CA*, **81**, 27482t (*rev*)
Japan. Pat., 1975, 75 05 199; *CA*, **83**, 25277x (*manuf*)
Abdel-Fattah, A.F. *et al., Phytochemistry*, 1975, **12**, 1995-1998 (*Sargassan*)
Zvyagintseva, T.N. *et al., Carbohydr. Res.*, 1999, **322**, 32-39 (***isol, bibl***)
Marais, M.F. *et al., Carbohydr. Res.*, 2001, **336**, 155-159 (*isol, purifn*)
Lee, J.-B. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1091-1094 (*isol, ms*)

Fucopentaphlorethol A F-93

[97915-31-6]
[96738-78-2 (per-Ac)]



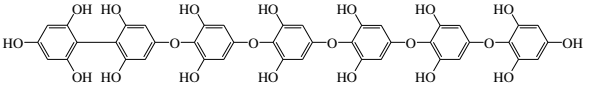
$C_{42}H_{30}O_{21}$ 870.686
Isol. from *Cystoseira granulata* (as per-Ac).

4‴‴‴-Hydroxy: ***Hydroxyfucopentaphlorethol A***
$C_{42}H_{30}O_{22}$ 886.686
Isol. from *Cystophora torulosa*.

4‴,4⁗,4⁗‴-Trihydroxy: ***Trihydroxyfucopentaphlorethol A***
[189171-34-4]
$C_{42}H_{30}O_{24}$ 918.685
Isol. from *Cystophora torulosa*. Isol. as per-Ac, to which CAS no. refers.

Glombitza, K.W. *et al., Planta Med.*, 1985, **51**, 116 (*isol, pmr, cmr, ms*)
Glombitza, K.W. *et al., Nat. Toxins*, 1997, **5**, 58-63 (*Hydroxyfucopentaphlorethol A*)

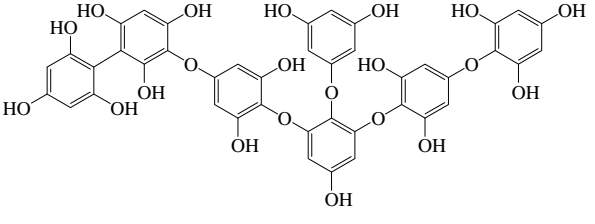
Fucopentaphlorethol B F-94



$C_{42}H_{30}O_{21}$ 870.686
Isol. from *Fucus vesiculosus*. Not indexed by CAS.

Preuss, B. *et al., Thesis, Bonn*, 1983,

Fucopentaphlorethol E F-95

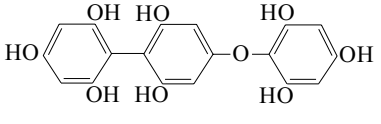


$C_{42}H_{30}O_{21}$ 870.686
Isol. from brown alga *Cystophora retroflexa*.

Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol, pmr, cmr, ms*)

Fucophlorethol A F-96

2,2′,4,6,6′-Pentahydroxy-4′-(2,4,6-trihydroxyphenoxy)biphenyl



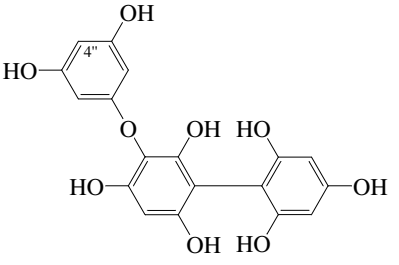
$C_{18}H_{14}O_9$ 374.303
Constit. of *Fucus vesiculosus* and other brown algae.

Octa-Me ether: [97049-74-6]
Cryst. Mp 205-207.5°.

Glombitza, K.-W. *et al., Planta Med.*, 1977, **32**, 33 (*isol*)
Ragan, M.A. *et al., Can. J. Chem.*, 1985, **63**, 291 (*synth*)

Fucophlorethol B F-97

3-(3,5-Dihydroxyphenoxy)-[1,1′-biphenyl]-2,2′,4,4′,6,6′-hexol, 9CI. 3-(3,5-Dihydroxyphenoxy)-2,2′,4,4′,6,6′-hexahydroxybiphenyl
[72380-15-5]



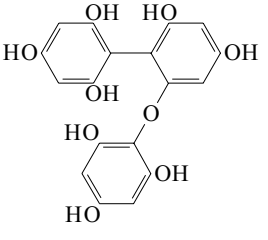
$C_{18}H_{14}O_9$ 374.303
Isol. from *Cystoseira baccata*, *Sargassum spinuligerum*, *Cystophora retroflexa* and *Carpophyllum angustifolium*.

4″-Hydroxy: ***Hydroxyfucophlorethol A***
[189171-30-0]
$C_{18}H_{14}O_{10}$ 390.303
Isol. from *Cystophora torulosa* and *Sargassum spinuligerum*. Isol. as per-Ac, to which CAS no. refers. Phlorotannins are named in order of discovery, so hydroxyfucophlorethol A is not an OH deriv. of Fucophlorethol A.

Glombitza, K.W. *et al., CA*, 1980, **92**, 55043 (*isol*)
Glombitza, K.W. *et al., Phytochemistry*, 1997, **46**, 1417-1422; 1999, **50**, 869-881 (*isol*)

Fucophlorethol C F-98

6′-(2,4,6-Trihydroxyphenoxy)-[1,1′-biphenyl]-2,2′,4,4′,6-pentol, 9CI. 2,2′,4,4′,6-Pentahydroxy-6′-(2,4,6-trihydroxyphenoxy)biphenyl
[123154-62-1]

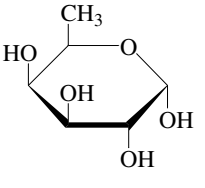


$C_{18}H_{14}O_9$ 374.303
Isol. from *Himanthalia elongata* and *Analipus japonicus* (as per-Ac).

Glombitza, K.W. *et al., Planta Med.*, 1985, **51**, 42-46; 1989, **55**, 171 (*isol*)

Fucose F-99

6-Deoxygalactose. Rhodeose. Galactomethylose



α-D-Pyranose-*form*

$C_6H_{12}O_5$ 164.158

An aq. soln. at 31°C contains 28% α-pyr, 67% β-pyr, =5% fur and 0.01% aldehyde.

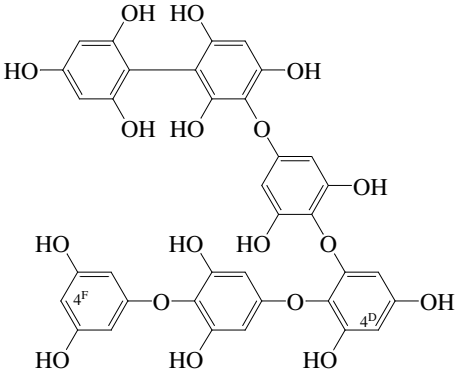
L-*form* [2438-80-4]
A constit. of the polysaccharides obt. from eggs of sea urchin, frog spawn, gum tragacanth and marine algae. Also found in glycoproteins obt. from mucins, blood group substances and milk. Prisms (EtOH).
Mp 145° (140-141°). $[\alpha]_D^{17}$ -124 → -76 (c, 2.0 in H_2O).

[3713-31-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 188A; 190A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 291A (*nmr*)
Percival, E. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 195 (*L-form, synth*)
Izumi, K. *et al., Agric. Biol. Chem.*, 1971, **35**, 1816-1818 (*pmr*)
Dejter-Juszynski, M. *et al., Carbohydr. Res.*, 1971, **18**, 219-226; 1972, **23**, 41-45; 1973, **28**, 61-74; 144-146 (*L-form, α-L-pyr benzyl derivs*)
Gorin, P.J. *et al., Can. J. Chem.*, 1975, **53**, 1212-1223 (*pmr*)
Flowers, H.M. *et al., Adv. Carbohydr. Chem. Biochem.*, 1981, **39**, 279-345 (***rev***)
Defaye, J. *et al., Carbohydr. Res.*, 1981, **95**, 131-141; 1984, **126**, 165-169 (*L-form, synth*)
Sarbajna, S. *et al., Carbohydr. Res.*, 1995, **270**, 93-96 (*L-form, !synth*)
Takanashi, S. *et al., J.C.S. Perkin 1*, 1997, 607-612 (*L-form, synth, pmr, cmr*)

Fucotetraphlorethol A F-100

[96738-77-1]



$C_{36}H_{26}O_{18}$ 746.591
Isol. from *Cystoseira granulata* and *Himanthalia elongata*. Isol. as per-Ac, to which CAS no. refers.

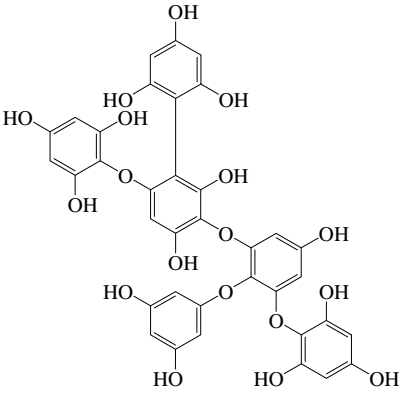
4^D-Hydroxy: ***Hydroxyfucotetraphlorethol A***
[189171-31-1]
$C_{36}H_{26}O_{19}$ 762.59
Isol. from *Cystophora torulosa*. Isol. as per-Ac, to which CAS no. refers.

4^D,4^F-Dihydroxy: ***Dihydroxyfucotetraphlorethol A***
[189171-33-3]
$C_{36}H_{26}O_{20}$ 778.589
Isol. from *Cystoseira torulosa*. Isol. as per-Ac, to which CAS no. refers.

Glombitza, K.W. *et al., Planta Med.*, 1985, **51**, 42-46; **15**, 116-120 (*Fucotetraphlorethol A*)
Glombitza, K.W. *et al., Nat. Toxins*, 1997, **5**, 58-68 (*Hydroxyfucotetraphlorethols*)

Fucotetraphlorethol B F-101

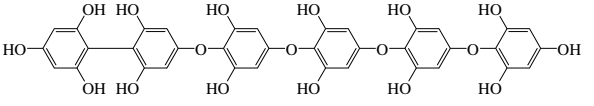
[96738-79-3]



$C_{36}H_{26}O_{18}$ 746.591
Isol. from *Cystophora retroflexa* and *Himanthalia elongata*. Isol. as per-Ac, to which CAS no. refers.

Glombitza, G.W. *et al., Planta Med.*, 1985, **50**, 42-46 (*isol, struct*)
Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol*)

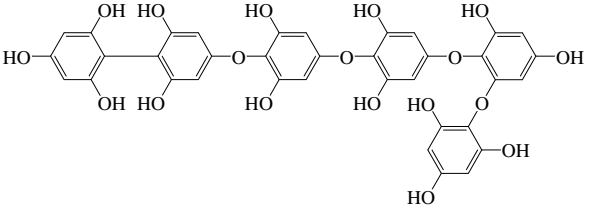
Fucotetraphlorethol C F-102



$C_{36}H_{26}O_{18}$ 746.591
Isol. from *Fucus vesiculosus*. Not indexed by CAS.

Preuss, B. *et al., Thesis*, Bonn, 1983,

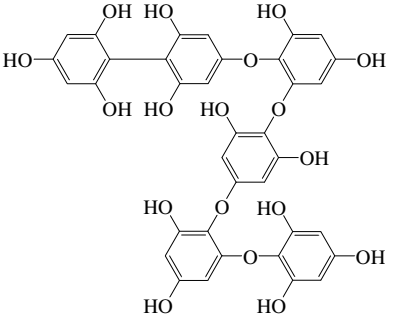
Fucotetraphlorethol D F-103



$C_{36}H_{26}O_{18}$ 746.591
Isol. from *Fucus vesiculosus*. Not indexed by CAS.

Preuss, B. *et al., Thesis*, Bonn, 1983,

Fucotetraphlorethol E F-104

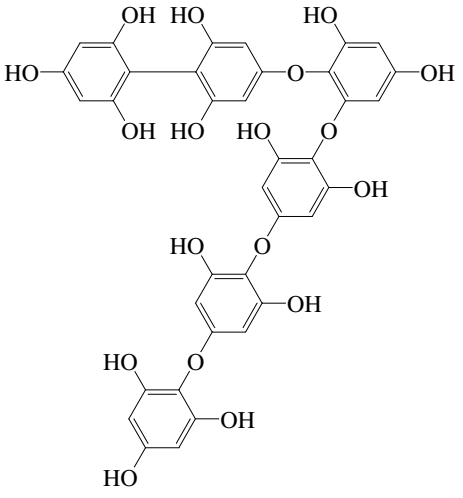


$C_{36}H_{26}O_{18}$ 746.591

Isol. from *Fucus vesiculosus*. Not indexed by CAS.

Preuss, B. *et al., Thesis*, Bonn, 1983,

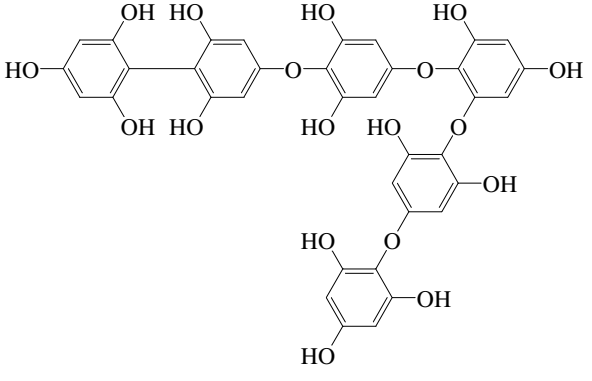
Fucotetraphlorethol F F-105



$C_{36}H_{26}O_{18}$ 746.591
Isol. from *Fucus vesiculosus*. Not indexed by CAS.

Preuss, B. *et al., Thesis*, Bonn, 1983,

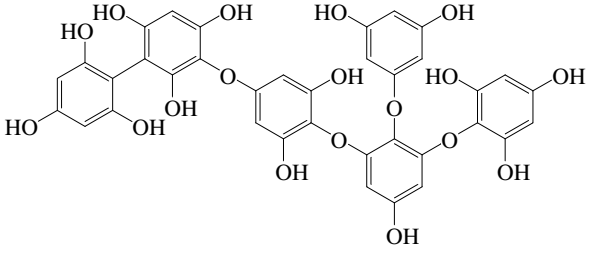
Fucotetraphlorethol G F-106



$C_{36}H_{26}O_{18}$ 746.591
Isol. from *Fucus vesiculosus*. Not indexed by CAS.

Preuss, B. *et al., Thesis*, Bonn, 1983,

Fucotetraphlorethol K F-107

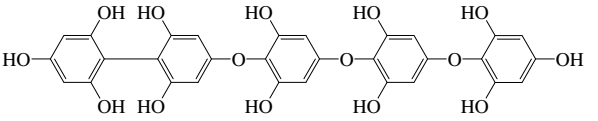


$C_{36}H_{26}O_{18}$ 746.591
Isol. from *Cystophora retroflexa*.

Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol, pmr, cmr, ms*)

Fucotriphlorethol A F-108

[64461-87-6]

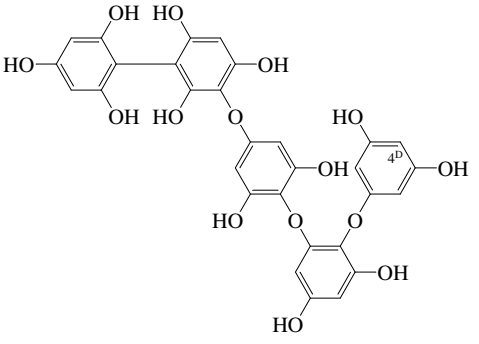


$C_{30}H_{22}O_{15}$ 622.495
Isol. from *Fucus vesiculosus*. Isol. as dodeca-Ac to which CAS no. refers.

Glombitza, K.W. *et al., Planta Med.*, 1977, **32**, 33-45 (*isol, struct, ms*)

Fucotriphlorethol B F-109

[96738-76-0]



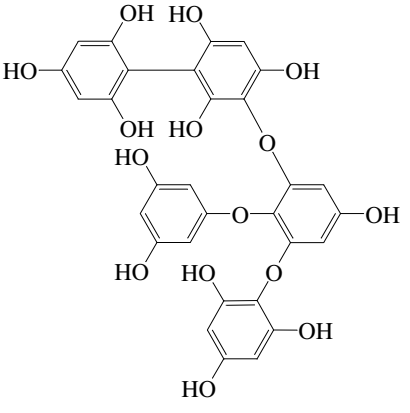
$C_{30}H_{22}O_{15}$ 622.495
Isol. from *Cystoseira granulata*, *Cystophora retroflexa* and *Carpophyllum angustifolium*. Isol. as per-Ac, to which CAS no. refers.

4^D-Hydroxy: ***Hydroxyfucotriphlorethol B***
[199857-66-4]
$C_{30}H_{22}O_{16}$ 638.494
Isol. from *Cystophora torulosa*. Isol. as trideca-Ac to which CAS no. refers.

Glombitza, K.W. *et al., Planta Med.*, 1985, **51**, 116-120 (*isol, pmr, ms*)
Glombitza, K.W. *et al., Phytochemistry*, 1997, **46**, 735-740; 1999, **50**, 869-881 (*isol, Hydroxyfucotriphlorethol B*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

Fucotriphlorethol C F-110

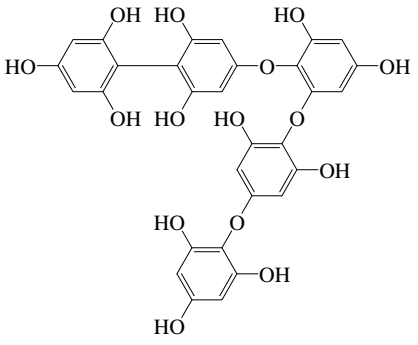
[96751-32-5]



$C_{30}H_{22}O_{15}$ 622.495
Isol. from *Himanthalia elongata*. Isol. as dodeca-Ac, to which CAS no. refers.

Glombitza, K.W. *et al., Planta Med.*, 1985, **51**, 42-46 (*isol, pmr, ms*)

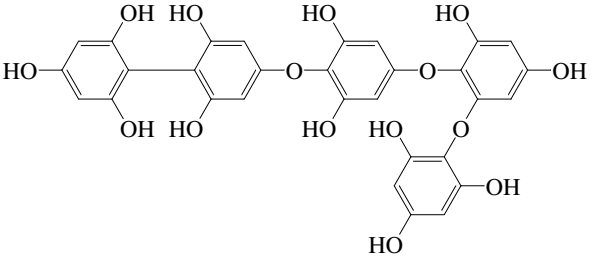
Fucotriphlorethol D F-111



$C_{30}H_{22}O_{15}^{\oplus}$ 622.495
Isol. from *Fucus vesiculosus*. Not indexed by CAS.

Preuss, B. *et al., Thesis*, Bonn, 1983,

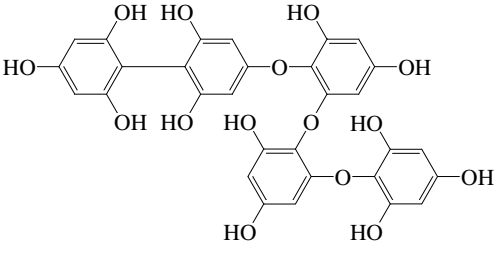
Fucotriphlorethol E F-112



$C_{30}H_{22}O_{15}$ 622.495
Isol. from *Fucus vesiculosus*. Not indexed by CAS.

Preuss, B. *et al., Thesis*, Bonn, 1983,

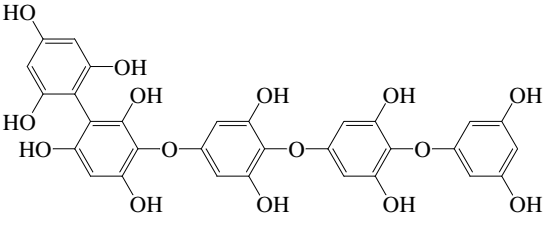
Fucotriphlorethol F F-113



$C_{30}H_{22}O_{15}$ 622.495
Isol. from *Fucus vesiculosus* and *Durvillaea antarctica*. Not indexed by CAS. Genus name often spelt as Durvillea.

Preuss, B. *et al., Thesis*, Bonn, 1983,

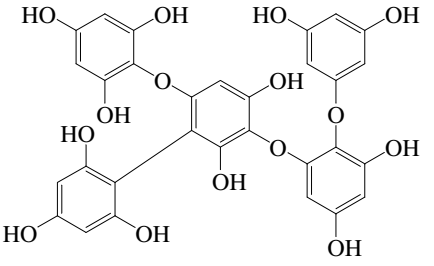
Fucotriphlorethol G F-114



$C_{30}H_{22}O_{15}$ 622.495
Isol. from *Cystophora retroflexa*.

Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol, pmr, cmr, ms*)

Fucotriphlorethol H F-115

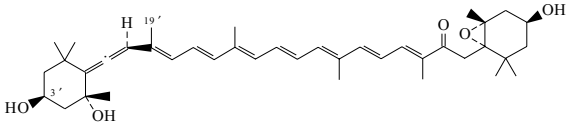


$C_{30}H_{22}O_{15}$ 622.495
Isol. from brown alga *Cystophora retroflexa*.

Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol, pmr, cmr, ms*)

Fucoxanthinol F-116

6′,7′-Didehydro-5,6-epoxy-5,5′,6,6′,7,8-hexahydro-3,3′,5′-trihydroxy-β,β-caroten-8-one
[7176-02-5]



$C_{40}H_{56}O_5$ 616.879
Constit. of *Paracentrotus lividus* and *Fucus vesiculosus*. Cryst. (C_6H_6/pentane).
Mp 134-138°. λ_{max} 445 (Me_2CO).

3′-Ac: ***Fucoxanthin***. *Fucoxanthol*
[3351-86-8]
$C_{42}H_{58}O_6$ 658.917
Constit. of brown algae, freshwater algae, and diatoms, for example *Fucus virsoides* , *Polysiphonia nigrescens*, *Colpomenia peregrina*, *Phaeodactylum tricornutum*, *Ceramium rubrum*. Major antioxidant in Japanese edible seaweed *Hijikia fusiformis*. Antioxidant. Antifouling agent. Red-brown prisms (MeOH). Sol. MeOH, Et_2O; poorly sol. hexane.
Mp 158-159° (168°). $[\alpha]_D^{18}$ +73.5 ($CHCl_3$) (cd). λ_{max} 436; 445; 452 (MeOH) (Berdy). λ_{max} 450 (E1%/1cm 1140) (EtOH) (Berdy). λ_{max} 444; 466 (Me_2CO).

▶ FI0329800

19′-Butanoyloxy, 3′-Ac: ***19′-Butanoyloxyfucoxanthin***. *3′-Acetoxy-6′,7′-didehydro-5,6-epoxy-5,5′,6,6′,7,8-hexahydro-3,5′-dihydroxy-8-oxo-19′-(1-oxobutoxy)-β,β-carotene*
[111234-30-1]
$C_{46}H_{64}O_8$ 745.007
Isol. from the marine crysophyte *Pelagococcus subviridis*. Cryst. (4-methyl-2-pentanone/hexane). λ_{max} 446; 473 (hexane). λ_{max} 454; 481 ($CHCl_3$).

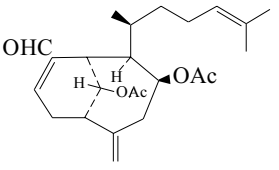
19′-Hexanoyloxy, 4-oxo, 3′-Ac: [279673-18-6]
$C_{48}H_{66}O_9$ 787.044
Constit. of *Emiliania huxleyi*. λ_{max} 443; 467 (Me_2CO). λ_{max} 455; 481 (C_6H_6). λ_{max} 443; 465 (MeOH).

Jensen, A. *et al., Acta Chem. Scand.*, 1964, **18**, 840-841 (*isol*)
Bonnett, R. *et al., Proc. Chem. Soc., London*, 1964, 419 (*struct*)
Galasko, G. *et al., J.C.S.(C)*, 1969, 1264-1265 (*isol*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97-102 (*cmr*)
Bernhard, K. *et al., Tet. Lett.*, 1976, 115-118 (*struct*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 368; 369 (*bibl*)
Haugan, J.A. *et al., Phytochemistry*, 1989, **28**, 2797-2798 (*isol*)
Bjornland, T. *et al., Phytochemistry*, 1989, **28**, 3347-3353 (*isol, pmr, uv, ms, 19′-butanoyloxy*)
Palermo, J.A. *et al., Phytochemistry*, 1991, **30**, 2983-2986 (*pmr, cmr*)

Haugan, J.A. *et al., Acta Chem. Scand.*, 1992, **46**, 389-395; 614-624 (*stereochem*)
Haugan, J.A. *et al., Phytochemistry*, 1992, **31**, 1359-1361 (*isol, stereochem*)
Haugan, J.A. *et al., Tet. Lett.*, 1994, **35**, 2245-2248 (*abs config*)
Yamano, Y. *et al., J.C.S. Perkin 1*, 1995, 1895-1904 (*synth*)
Yan, X.J. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 605-607 (*Fucoxanthin, isol, Hijikia*)
Egeland, E.S. *et al., J.C.S. Perkin 1*, 2000, 1223-1230 (*hexanoyloxy deriv*)
Mori, K. *et al., Mar. Drugs*, 2004, **2**, 63-72 (*Fucoxanthin, rev*)

Fukurinal F-117

[84667-04-9]

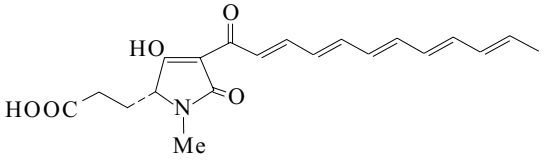


$C_{24}H_{34}O_5$ 402.53
Constit. of brown seaweed *Dilophus okamurai*. Cryst. Mp 132-134°.

Ochi, M. *et al., Chem. Lett.*, 1982, 1927

Fuligorubin A F-118

[108343-55-1]

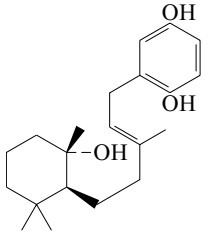


$C_{20}H_{23}NO_5$ 357.405
Tetramic acid deriv. Isol. from the slime mold *Fuligo septica* (Myxomycetes). Isol. from the sponge *Topsentia roquensis*. Prob. plays a role in slime mold phototaxis. Red cryst. + $2H_2O$. Mp 150° dec. λ_{max} 243 (ϵ 14454); 425 (ϵ 26900) (MeOH) (Berdy). λ_{max} 243; 377 (MeOH-NaOH) (Berdy).

Casser, I. *et al., Angew. Chem., Int. Ed.*, 1987, **26**, 586 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)
Ley, S.V. *et al., Tetrahedron*, 1992, **48**, 1145 (*synth*)

Fulvanin 2 F-119

[149298-03-3]



$C_{21}H_{32}O_3$ 332.482
Constit. of *Reniera fulva*.

Casapullo, A. *et al., J. Nat. Prod.*, 1993, **56**, 527 (*isol, pmr, cmr*)

Fulvellic acid F-120

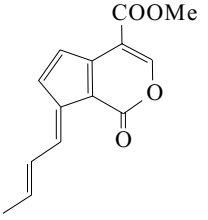
2-[(2,3-Dihydroxypropoxy)methyl]-2-propenoic acid. 1-Glyceryl α-(hydroxymethylacrylyl) ether
$H_2C{=}C(COOH)CH_2OCH_2CH(OH)CH_2OH$
$C_7H_{12}O_5$ 176.169
Present as acyl glycerides in lipids of the brown alga *Sargassum fulvellum* and present in other *Sargassum* spp. Could not be isol. as free acid by hydrol. of the lipids owing to instability.

[79894-99-8, 79895-00-4]

Kusumi, T. *et al., Chem. Lett.*, 1981, 1393-1396

Fulvoplumierin F-121

Methyl 7-(2-butenylidene)-1,7-dihydro-1-oxocyclopenta[c]pyran-4-carboxylate, 9CI, 8CI. Methyl 7-crotonylidenecyclopenta[c]pyran-1(7H)-one-4-carboxylate
[20867-01-0]

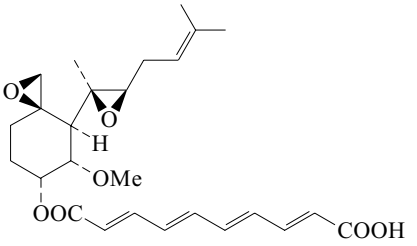


$C_{14}H_{12}O_4$ 244.246
Isol. from the rind of *Plumeria acutifolia* and *Plumeria rubra* var. *alba*. Also isol. from the marine mollusc *Nerita albicilla*. Shows antibiotic and anti-HIV props. Antimicrobial agent. Orange needles ($CHCl_3$/EtOH). Sol. Me_2CO, Py, $CHCl_3$; fairly sol. MeOH, C_6H_6, Et_2O, EtOAc, EtOH, butanol; poorly sol. H_2O, hexane.
Mp 151-152° dec. Log P 2.05 (calc). λ_{max} 272 (ϵ 7000); 365 (ϵ 33700) (MeOH) (Berdy). λ_{max} 278 (ϵ 5130); 366 (ϵ 36300) (EtOH) (Berdy).

Albers-Schönberg, G. *et al., Helv. Chim. Acta*, 1962, **45**, 1406 (*struct, nmr*)
Büchi, G. *et al., J.A.C.S.*, 1968, **90**, 5336; 1969, **91**, 6470 (*synth, ir, uv, ms, nmr, struct*)
Sanduja, R. *et al., J. Nat. Prod.*, 1985, **48**, 335-336 (*isol, Nerita*)
Tan, G.T. *et al., J. Nat. Prod.*, 1991, **54**, 143 (*anti-HIV activity*)

Fumagillin, BAN, INN F-122

Phagopedin sigma. Amebacilin. Fumidil. Fugillin. Amebex. Fumadil B. NSC 9168. U 5762
[23110-15-8]



$C_{26}H_{34}O_7$ 458.55
Isol. from *Aspergillus fumigatus* H3 and *Penicillium nigricans*. Antibiotic with antiphage and amoebicidal props. Inhibits RNA synthesis of *Octosporea muscae-domesticae*. Of limited use for the treatment of drug-resistant intestinal amoebiasis. Angiogenesis inhibitor. Yellow needles (MeOH aq.). Sol. dil. alkalis, MeOH, bases, $CHCl_3$; fairly sol. H_2O; poorly sol. Et_2O, acids, hexane. Mp 189-194°. $[\alpha]_D^{25}$ -26.6 (MeOH). Log P 2.63 (calc). Best stored in dark, evac. ampoules at low temp. λ_{max} 239 (ϵ 6870); 320 (sh) (ϵ 48000); 336 (ϵ 68700); 352 (ϵ 61800) (EtOH) (Derep). λ_{max} 239 (E1%/1cm 75); 336 (E1%/1cm 1464); 351 (E1%/1cm 1335) (MeOH) (Berdy).
▶ LD_{50} (mus, orl) 2000 mg/kg, LD_{50} (mus, scu) 800 mg/kg. Exp. reprod. and teratogenic effects. HE1750000

Dicyclohexylamine salt: Mp 147-148° dec.

Bis-2,4-dinitrophenylhydrazone: Mp 123-126°.

Me ester: [6035-64-9]
Needles (MeOH aq.). Mp 151-152°.

Deacyl: ***Fumagillol***
[108102-51-8]
$C_{16}H_{26}O_4$ 282.379

Isol. from *Penicillium jensenii*. Degradn. prod. of Fumagillin. Carcinolytic agent. Immunosuppressant. Cryst. (Et_2O/petrol). Mp 55.5-56°. $[\alpha]_D^{23}$ -68 (c, 1.73 in EtOH). Similar to FR 65814.

Deacyl, chloroacetylcarbamate: See 5-Methoxy-4-[2-methyl-3-(3-methyl-2-butenyl)oxiranyl]-1-oxaspiro[2.5]oct-6-yl chloroacetylcarbamate in *The Combined Chemical Dictionary.*

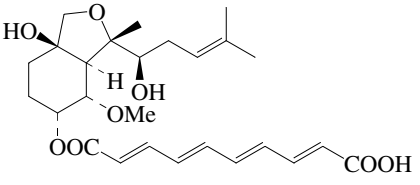
1,2-Deepoxy, 1,2-didehydro: ***Antibiotic Sch 528647***. *Sch 528647*
$C_{26}H_{34}O_6$ 442.551
Prod. by *Aspergillus fumigatus*. Antitumour agent. Yellow solid. Mp 144-146°. $[\alpha]_D^{25}$ -12.2 (c, 0.1 in MeOH). λ_{max} 240 (ϵ 72); 320 (sh) (ϵ 1012); 335 (ϵ 1478); 358 (ϵ 1338) (no solvent reported).

Demethoxy, O*-deacyl:* ***5-Demethoxyfumagillol***
[701277-78-3]
$C_{15}H_{24}O_3$ 252.353
Prod. by *Aspergillus fumigatus*. Angiogenesis inhibitor. Oil.

2′Z-Isomer: **cis-*Fumagillin***
[301823-84-7]
$C_{26}H_{34}O_7$ 458.55
Prod. by *Penicillium janczewski*. Methionine aminopeptidase inhibitor. Amorph. yellow solid (as Me ester). $[\alpha]_D$ +0.3 (MeOH) (Me ester). CAS no. refers to Me ester.

Eble, T.E. *et al., Antibiot. Chemother. (Washington, D.C.)*, 1951, **1**, 54-58 (*isol, props*)
Ross, J.M. *et al., J.A.C.S.*, 1956, **78**, 4675-4679 (*Fumagillol*)
Tarbell, D.S. *et al., J.A.C.S.*, 1960, **82**, 1005-1007 (*struct*)
Birch, A.J. *et al., J.C.S.(C)*, 1969, 1473-1474 (*biosynth*)
Corey, E.J. *et al., J.A.C.S.*, 1972, **94**, 2549-2550 (*synth*)
Hatanaka, H. *et al., J. Antibiot.*, 1988, **41**, 999-1008 (*Fumagillol*)
Kusaka, M. *et al., Biochem. Biophys. Res. Commun.*, 1991, **174**, 1070-1076 (*activity*)
Otsuka, T. *et al., J. Microb. Biotechnol.*, 1991, **1**, 163-168 (*FR 118487*)
Oikawa, T. *et al., Curr. Med. Chem.*, 1995, **1**, 406-417 (*activity*)
Oikawa, T. *et al., Curr. Med. Res. Opin.*, 1995, **174**, 1070-1076 (*activity*)
Terano, H. *et al., CA*, 1996, **125**, 131483g (*FR 118487, rev*)
Kim, D. *et al., Tet. Lett.*, 1997, **38**, 4437-4440 (*synth*)
Vosburg, D.A. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 971-974 (*Fumagillol, synth*)
Taber, D.F. *et al., J.A.C.S.*, 1999, **121**, 5589-5590 (*synth*)
Kwon, J.-Y. *et al., J. Antibiot.*, 2000, **53**, 799-806 (*cis-Fumagillin*)
Halasz, J. *et al., Tetrahedron*, 2000, **56**, 10081-10085 (*pmr, cmr, cryst struct*)
Chu, M. *et al., J. Antibiot.*, 2001, **54**, 1096-1099 (*Sch 528647*)
Boiteau, J.-G. *et al., Org. Lett.*, 2001, **3**, 2737-2740 (*Fumagillol, synth*)
Kim, D. *et al., Chem. Pharm. Bull.*, 2004, **52**, 447-450 (*Demethoxyfumagillol*)
Bedel, O. *et al., Eur. J. Org. Chem.*, 2004, 3813-3819 (*Fumagillol, synth*)
Yamaguchi, J. *et al., Angew. Chem., Int. Ed.*, 2006, **45**, 789-793 (*Fumagillol, synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 810
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FOZ000

Fumagiringillin F-123

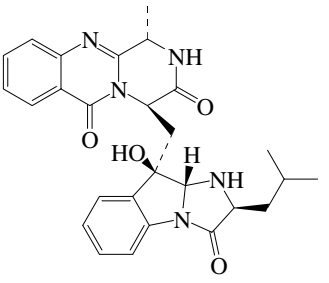


Relative Configuration

$C_{26}H_{36}O_8$ 476.566
Prod. by *Aspergillus fumigatus* (strain CANU A151) isol. from a saline lake. Pale yellow solid. $[\alpha]_D^{20}$ -12.5 (c, 1 in MeOH). λ_{max} 317 (sh) (log ϵ 2.18); 332 (log ϵ 2.29); 348 (log ϵ 2.23) (MeOH).

Jiao, W. *et al., J. Nat. Prod.*, 2004, **67**, 1434-1437 (*isol, pmr, cmr*)

Fumiquinazoline I F-124

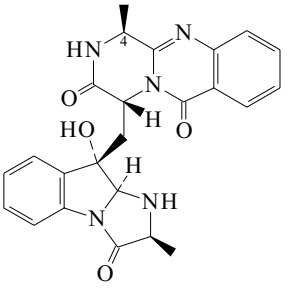


$C_{27}H_{29}N_5O_4$ 487.557
Isol. from an *Acremonium* sp. obt. from the tunicate *Ecteinascidia turbinata*. Solid.
Mp 116-120°. $[\alpha]_D$ -138 (c, 0.001 in $CHCl_3$). λ_{max} 224 (ϵ 63300); 230 (sh) (ϵ 57200); 255 (ϵ 26000); 266 (sh) (ϵ 21700); 277 (ϵ 17000); 304 (ϵ 5100) (MeOH).

Belofsky, G.N. *et al., Chem. Eur. J.*, 2000, **6**, 1355-1360
Snider, B.B. *et al., J.O.C.*, 2003, **68**, 545-563 (*synth*)

Fumiquinazoline A F-125

[140715-85-1]



$C_{24}H_{23}N_5O_4$ 445.477
Prod. by *Aspergillus fumigatus* isol. from the gastrointestinal tract of the fish *Pseudolabrus japonicus*. Cytotoxic agent. Cryst. (CH_2Cl_2).
Mp 178-182°. $[\alpha]_D^{33}$ -214.5 (c, 0.47 in $CHCl_3$). λ_{max} 226 (ϵ); 233 (sh) (ϵ); 256 (ϵ); 265 (sh) (ϵ); 277 (ϵ); 305 (ϵ); 327 (ϵ) (EtOH) (Derep). λ_{max} 208 (ϵ 37900); 226 (ϵ 30900); 233 (ϵ 27400); 256 (ϵ 14800); 265 (ϵ 13500); 277 (ϵ 10230); 305 (ϵ 3450); 327 (ϵ 2770) (MeOH) (Berdy).

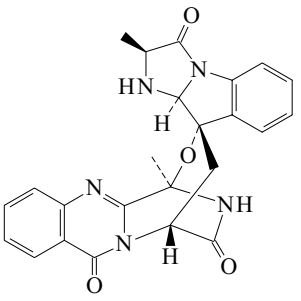
4-Epimer: ***Fumiquinazoline B***
[140852-71-7]
$C_{24}H_{23}N_5O_4$ 445.477
From *Aspergillus fumigatus* in *Pseudolabrus japonicus*. Cytotoxic agent. Cryst. (Me_2CO).
Mp 174-176°. $[\alpha]_D^{21}$ -196.7 (c, 0.38 in $CHCl_3$). λ_{max} 226 (ϵ); 233 (sh) (ϵ); 256 (ϵ); 265 (sh) (ϵ); 277 (ϵ); 305 (ϵ); 327 (ϵ) (EtOH) (Derep). λ_{max} 206 (ϵ 58500); 225 (ϵ 49200); 232 (ϵ 44700); 256 (ϵ 24000); 266 (ϵ 20900); 277 (ϵ 17300); 305 (ϵ 6150); 317 (ϵ 4800) (MeOH) (Berdy).

4-Methoxy: ***Fumiquinazoline E***
[140715-87-3]
$C_{25}H_{25}N_5O_5$ 475.503
Prod. by *Aspergillus fumigatus*. Cytotoxic agent. Pale yellow powder.
Mp 168-172°. $[\alpha]_D$ -143.3 (c, 0.2 in $CHCl_3$). λ_{max} 210 (log ϵ 4.54); 226 (log ϵ 4.48); 233 (log ϵ 4.44); 256 (log ϵ 4.16); 278 (log ϵ 4.06); 304 (log ϵ 3.62); 317 (log ϵ 3.52) (EtOH). λ_{max} 210; 216; 233; 256; 278; 304; 317 (MeOH) (Berdy).

Numata, A. *et al., Tet. Lett.*, 1992, **33**, 1621 (*isol, pmr, cmr, struct*)
Takahashi, C. *et al., J.C.S. Perkin 1*, 1995, 2345-2353 (*isol, uv, ir, pmr, cmr*)
Snider, B.B. *et al., J.O.C.*, 2003, **68**, 545-563 (*synth*)

Fumiquinazoline C F-126

[140924-01-2]



$C_{24}H_{21}N_5O_4$ 443.461

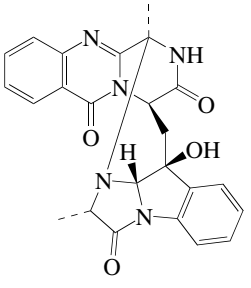
Prod. by *Aspergillus fumigatus* isol. from the gastrointestinal tract of the fish *Pseudolabrus japonicus*. Cytotoxic agent. Cryst. + $1Me_2CO$ (Me_2CO).

Mp 244-246°. $[\alpha]_D^{21}$ -193.7 (c, 0.31 in $CHCl_3$). λ_{max} 226 (ϵ); 233 (sh) (ϵ); 256 (ϵ); 265 (sh) (ϵ); 277 (ϵ); 305 (ϵ); 327 (ϵ) (EtOH) (Derep). λ_{max} 207 (ϵ 36300); 225 (ϵ 30100); 260 (ϵ 11450); 271 (ϵ 10500); 282 (ϵ 9850); 304 (ϵ 4050); 317 (ϵ 3120) (MeOH) (Berdy).

Numata, A. *et al., Tet. Lett.*, 1992, **33**, 1621 (*isol, pmr, cryst struct*)
Snider, B.B. *et al., J.O.C.*, 2003, **68**, 545-563 (*synth*)
Afiyatullov, S.S. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 236-238 (*isol, cmr*)

Fumiquinazoline D F-127

[140715-86-2]



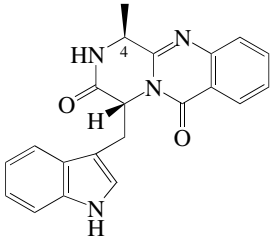
$C_{24}H_{21}N_5O_4$ 443.461

Prod. by *Aspergillus fumigatus*. Cytotoxic agent. Prisms (Me_2CO). Mp 214-216°. $[\alpha]_D^{22}$ +86.2 (c, 0.15 in $CHCl_3$). λ_{max} 205 (log ϵ 4.3); 225 (log ϵ 4.26); 232 (log ϵ 4.24); 254 (log ϵ 3.91); 265 (log ϵ 3.84); 276 (log ϵ 3.77); 304 (log ϵ 3.43); 316 (log ϵ 3.54) (EtOH).

Takahashi, C. *et al., J.C.S. Perkin 1*, 1995, 2345-2353 (*isol, uv, ir, cd, pmr, cmr, cryst struct*)
Afiyatullov, S.S. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 236-238 (*isol, cmr*)

Fumiquinazoline F F-128

[169626-35-1]



$C_{21}H_{18}N_4O_2$ 358.399

Prod. by a marine-derived *Aspergillus fumigatus*. Cytotoxic agent. Pale yellow powder.

Mp 88-90°. $[\alpha]_D$ -411.2 (c, 1.4 in $CHCl_3$). λ_{max} 207 (log ϵ 4.71); 219 (log ϵ 4.73); 270 (log ϵ 4.13); 277 (log ϵ 4.13); 289 (log ϵ 3.99); 306 (log ϵ 3.78); 320 (log ϵ 3.66) (EtOH).

4-Epimer: ***Fumiquinazoline G***

[169869-87-8]

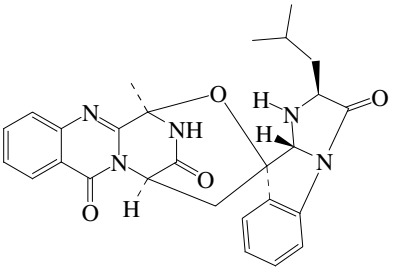
$C_{21}H_{18}N_4O_2$ 358.399

Prod. by a marine-derived *Aspergillus fumigatus*. Cytotoxic agent. Pale yellow powder.

Mp 119-121°. $[\alpha]_D$ -462.8 (c, 0.6 in $CHCl_3$). λ_{max} 208 (log ϵ 4.61); 220 (log ϵ 4.67); 273 (log ϵ 4.14); 278 (log ϵ 4.13); 288 (log ϵ 4.01); 307 (log ϵ 3.66); 323 (log ϵ 3.49) (EtOH).

Takahashi, C. *et al., J.C.S. Perkin 1*, 1995, 2345-2353 (*isol, uv, ir, pmr, cmr*)
He, F. *et al., Synlett*, 1997, 483-484 (*synth*)
Wang, H. *et al., J.O.C.*, 2000, **65**, 1022-1030 (*synth*)
Snider, B.B. *et al., Tetrahedron*, 2001, **57**, 3301-3307 (*synth*)
Liu, J.-F. *et al., J.O.C.*, 2005, **70**, 6339-5345 (*synth*)

Fumiquinazoline H F-129



$C_{27}H_{27}N_5O_4$ 485.541

Isol. from an *Acremonium* sp. obt. from the tunicate *Ecteinascidia turbinata*. Pale yellow solid.

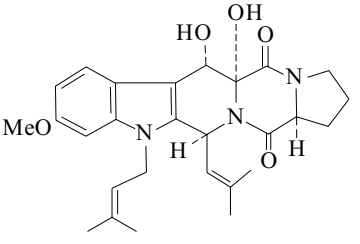
Mp 144-147°. $[\alpha]_D$ -59 (c. 0.001 in $CHCl_3$). λ_{max} 224 (ϵ 27700); 230 (sh) (ϵ 25800); 255 (ϵ 11500); 265 (ϵ 9700); 276 (ϵ 7600); 303 (ϵ 3000) (MeOH).

Belofsky, G.N. *et al., Chem. Eur. J.*, 2000, **6**, 1355-1360
Snider, B.B. *et al., J.O.C.*, 2003, **68**, 545-563 (*synth*)

Fumitremorgin B F-130

Lanosulin

[12626-17-4]



Absolute configuration

$C_{27}H_{33}N_3O_5$ 479.575

Prod. by *Aspergillus fumigatus, Aspergillus caespitosus, Penicillium lanosum* and *Penicillium piscarium*. Mycotoxin, tremorgen. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.

Mp 211-212° (204-206°). $[\alpha]_D^{25}$ +24 (c, 0.91 in $CHCl_3$). λ_{max} 228 (ϵ 39960); 278 (ϵ 11000); 295 (ϵ 12290) (MeOH) (Berdy). λ_{max} 226 (ϵ 31700); 278 (ϵ 7300); 295 (ϵ 7900) (EtOH) (Berdy).

▶ UY8709400

Tetrahydro: Mp 97-100°.

13-Epimer: Synthetic.

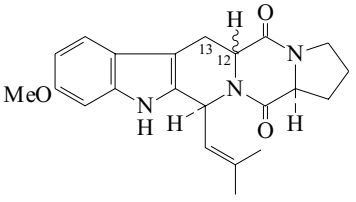
Cotton-like needles (EtOAc). Mp 231.5-232° (226-227°).

Dix, D.T. *et al., Chem. Comm.*, 1972, 1168 (*uv, ir, pmr, ms*)
Yamazaki, M. *et al., Tet. Lett.*, 1975, 27 (*cryst struct*)
Yamazaki, M. *et al., Chem. Pharm. Bull.*, 1980, **28**, 245 (*isol, uv, ir, pmr, cd, ms*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2220 (*uv, ir, pmr, ms, cd*)
Nakatsuka, S. *et al., Tet. Lett.*, 1986, **27**, 6361 (*synth, uv, ir, pmr*)
Kodato, S. *et al., Tetrahedron*, 1988, **44**, 359 (*synth, uv, ir, pmr, ms, cd*)

Hino, T. *et al., Heterocycles*, 1997, **46**, 673-704 (*rev, synth*)
Afiyatullov, S.S. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 236-238 (*isol, cmr*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 360

Fumitremorgin C F-131

SM-Q



$C_{22}H_{25}N_3O_3$ 379.458

Struct. revised in 1988. Config. at C-12 not specified. Of the two synthetic epimers the one with 12α-*H* config. possessed spectroscopic characteristics identical with those reported for natural Fumitremorgin C. (Hino *et al*).However, complete identification was not possible and the Mp's were widely different. A cryst. struct. determination mentioned in 1985 has not been publ. λ_{max} 224; 272; 294 (MeOH) (Berdy). λ_{max} 225; 273; 299 (EtOH) (Berdy).

Natural-*form* [118974-02-0]
Prod. by *Aspergillus fumigatus* and *Neosartorya fischeri*. Tremorgenic mycotoxin. Tremorgenic agent. Cryst. (EtOAc).
Mp 125-130°.

12,13-Epoxy: ***Epoxyfumitremorgin C***
$C_{22}H_{25}N_3O_4$ 395.457
From *Aspergillus fumigatus*. Tremorgenic mycotoxin.

12,13-Dihydroxy: ***12,13-Dihydroxyfumitremorgin C***
[111427-99-7]
$C_{22}H_{25}N_3O_5$ 411.457
From *Aspergillus fumigatus*. Tremorgenic mycotoxin. Yellow cryst.
Mp 197-198°. $[\alpha]_D$ +18.4.

Demethoxy: ***Demethoxyfumitremorgin C***
$C_{21}H_{23}N_3O_2$ 349.432
Prod. by *Aspergillus fumigatus*. Cell cycle progression Inhibitor, mycotoxin. Pale yellow needles. Sol. MeOH.
Mp 210-212°. $[\alpha]_D^{30}$ +8 (c, 0.2 in $CHCl_3$). λ_{max} 226 (ε 24950); 282 (ε 9000); 291 (sh) (ε 7450) (MeOH).

12α-*form*
Synthetic.
Powder (EtOAc). Mp 259.5-260.5° dec. $[\alpha]_D^{28}$ -13 (c, 0.53 in MeOH).

Demethoxy: [111768-16-2] Synthetic.
Cryst. (EtOH). Mp not reported.

12β-*form* [119066-64-7]
Synthetic. Pale yellow prisms (EtOH). Mp 240-247.5° dec. $[\alpha]_D^{28}$ + 239 (c, 0.11 in MeOH).

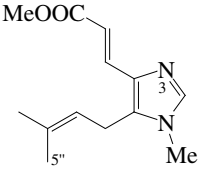
Demethoxy: [106211-91-0] Synthetic.
Cryst. + ⅓EtOAc (EtOAc). Mp 208-212°. $[\alpha]_D^{22}$ +281 (c, 0.1 in MeOH).

[118974-03-1, 119066-67-0, 119066-68-1, 119066-69-2]

Cole, R.J. *et al., J. Agric. Food Chem.*, 1977, **25**, 826-830 (*isol*)
Steyn, P.S. *et al., Prog. Chem. Org. Nat. Prod.*, 1985, **48**, 60 (*uv, pmr, cmr*)
Plate, R. *et al., J.O.C.*, 1987, **52**, 560-564 (*synth, uv, pmr, ms*)
O'Malley, G.J. *et al., Tet. Lett.*, 1987, **28**, 1131 (*synth, deriv*)
Hermkens, P.H.H. *et al., Tetrahedron*, 1988, **44**, 1991-2000 (*synth, uv, pmr, ms*)
Hino, T. *et al., Tetrahedron*, 1989, **45**, 1941-1944 (*synth, uv, ir, pmr, cmr, ms*)
Abraham, W.R. *et al., Phytochemistry*, 1990, **29**, 1025-1026 (*12,13-Dihydroxyfumitremorgin C*)
Cui, C.-B. *et al., J. Antibiot.*, 1996, **49**, 527-534; 534-540 (*pmr, cmr, demethoxy*)
Hino, T. *et al., Heterocycles*, 1997, **46**, 673-704 (*rev, synth*)
Bailey, P.D. *et al., Tet. Lett.*, 2001, **42**, 113-115 (*demethoxy, synth*)
Afiyatullov, S.S. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2004, **40**, 615-617 (*12,13-Dihydroxyfumitremorgin C*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 364

Fungerin F-132

Visoltricin
[185681-81-6]
[139874-44-5]



$C_{13}H_{18}N_2O_2$ 234.297
Alkaloid from *Fusarium tricinctum*, another *Fusarium* sp., *Metarhizium* sp. FKI-1079 and the marine *Microascus* sp. K14. Cytotoxic agent. Shows anticholinesterase and antifungal activities. Needles (hexane/EtOAc).
Mp 93-95°. λ_{max} 300 (ε 28000) (MeOH).

N^1-*Me:* **N-*Methylvisoltricin***
[156524-19-5]
[142750-50-3]
$C_{14}H_{21}N_2O_2^{\oplus}$ 249.332
Quaternary alkaloid prod. by *Fusarium* sp. Acetylcholinesterase inhibitor. Powder (as iodide).

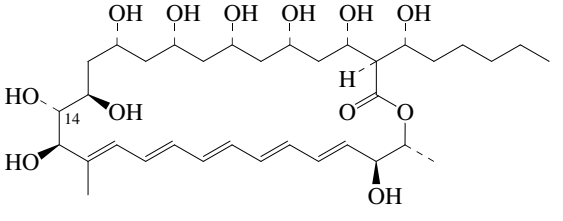
5″-Hydroxy: ***Hydroxyfungerin A***
$C_{13}H_{18}N_2O_3$ 250.297
Prod. by *Metarhizium* sp. FKI-1079. Pale yellow powder. λ_{max} 305 (ε 27000) (MeOH).

5″-Hydroxy, N-*de-Me, 3-Me (3*H-*form):* ***Hydroxyfungerin B***
$C_{13}H_{18}N_2O_3$ 250.297
Prod. by *Metarhizium* sp. FKI-1079. Pale yellow powder. λ_{max} 305 (ε 27200) (MeOH).

Marta, M. *et al., Acta Med. Rom.*, 1990, **28**, 343-346 (*N-Me*)
Visconti, A. *et al., J. Agric. Food Chem.*, 1994, **42**, 195-199 (*Visoltricin*)
Kato, Y. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 2081-2083 (*isol, uv, pmr, cmr, N-15 nmr*)
Benhida, R. *et al., Tet. Lett.*, 1998, **39**, 5963-5964 (*synth*)
Martin, G.E. *et al., J. Nat. Prod.*, 2000, **63**, 543-585 (*N-15 nmr*)
Rieder, J.M. *et al., Tet. Lett.*, 2002, **43**, 2375-2376 (*synth, struct*)
Koizumi, Y. *et al., J. Antibiot.*, 2004, **57**, 415-420 (*activity*)
Uchida, R. *et al., J. Antibiot.*, 2005, **58**, 804-809 (*Hydroxyfungerins*)

Fungichromin F-133

14-Hydroxyfilipin III. Cantricin. Cogomycin. Lagosin†. Moldcidin B. Moldocidin B. Pentamycin. A 246. FCRC 21. NSC 105388. Antibiotic A 246. Antibiotic FCRC 21
[6834-98-6]
[11006-45-4]



$C_{35}H_{58}O_{12}$ 670.836
Polyene antibiotic. Related to Filipin. Prod. by *Streptomyces cellulosae*, *Streptomyces griseofuscus*, *Streptomyces pentaticus* and other *Streptomyces* spp. incl marine *Streptomyces* sp. B7936. Antifungal agent. Needles (MeOH), hydrate pale-yellow cryst.
Mp 235° dec. (hydrate 205-210°). $[\alpha]_D$ -160 (c, 0.2 in MeOH). $[\alpha]_D$ -246 (c, 1 in Py). Contains 1 major and several minor

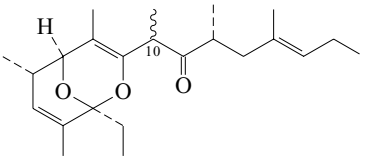
components; one is Filipin III. Fungichromin is a minor component of the Filipin complex. λ_{max} 310 (sh) (ϵ); 323 (ϵ 64300); 339 (ϵ 104000); 357 (ϵ 97800) (MeOH) (Derep).

▶ LD_{50} (mus, orl) 1624 mg/kg. LT3850000

Tytell, A.A. *et al., Antibiot. Annu.*, 1954, 716; 719 (*struct*)
Cope, A.C. *et al., J.A.C.S.*, 1962, **84**, 2170 (*abs config*)
Ceder, O. *et al., Acta Chem. Scand.*, 1964, **18**, 558 (*deriv*)
Dhar, M.L. *et al., J.C.S.*, 1964, 842; 862 (*struct*)
Golding, B.T. *et al., Tet. Lett.*, 1964, 2615 (*ms*)
Lematre, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1976, **282**, 763 (*cd, conformn*)
Holz, R.W. *et al., Antibiotics (N.Y.)*, 1979, **5**, 313 (*rev*)
Pandey, R.C. *et al., Biomed. Mass Spectrom.*, 1980, **7**, 93 (*isol, ms*)
Pandey, R.C. *et al., J. Antibiot.*, 1982, **35**, 988 (*pmr, cmr, cd*)
Noguchi, H. *et al., J.A.C.S.*, 1988, **110**, 2938 (*isol, biosynth, pmr, cmr*)
Matsumoto, K. *et al., Tet. Lett.*, 1993, **34**, 4935-4938 (*synth*)
Shih, H.-D. *et al., J. Agric. Food Chem.*, 2003, **51**, 95-99 (*isol, pmr, ms, activity*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FPC000

Funiculatin A F-134

[160632-41-7]

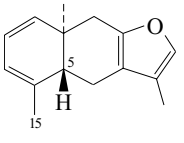


$C_{23}H_{36}O_3$ 360.536
Constit. of the mollusc *Siphonaria funiculata*.
$[\alpha]_D$ -41 ($CHCl_3$). λ_{max} 291 (ϵ 905) (no solvent reported).

10-Epimer: ***Funiculatin B***
[160709-09-1]
$C_{23}H_{36}O_3$ 360.536
Constit. of *Siphonaria funiculata*. λ_{max} 291 (ϵ 905) (no solvent reported).

Blanchfield, J.T. *et al., Aust. J. Chem.*, 1994, **47**, 2255-2269 (*isol, uv, ir, pmr, cmr*)

Furanoeudesma-1,3-diene F-135



(5β,10α)–*form*

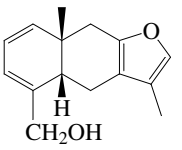
$C_{15}H_{18}O$ 214.307

(5β,10α)-*form*
Constit. of oil of myrrh.
Liq. $[\alpha]_D^{20}$ +59 (c, 0.82 in $CHCl_3$).

(5β,10β)-*form*
Tubipofuran
Isol. from *Tubipora musica*. Cytotoxic and ichthyotoxic.
Oil. $[\alpha]_D$ +5.7 (c, 0.6 in $CHCl_3$).

Brieskorn, C.H. *et al., Phytochemistry*, 1983, **22**, 187 (*isol, pmr, cmr*)
Iguchi, R. *et al., Chem. Lett.*, 1986, 1789 (*Tubipofuran*)
Ojida, A. *et al., J.O.C.*, 1994, **59**, 5970 (*synth*)
Blay, G. *et al., J.O.C.*, 1996, **61**, 3815 (*synth, abs config*)

Furanoeudesma-1,3-dien-15-ol F-136



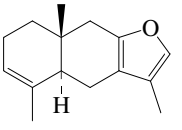
$C_{15}H_{18}O_2$ 230.306

Ac: ***15-Acetoxytubipofuran***
[106001-40-5]
$C_{17}H_{20}O_3$ 272.343
Isol. from *Tubipora musica*. Shows cytotoxic and ichthyotoxic props. Oil. $[\alpha]_D$ +10.7 (c, 0.5 in $CHCl_3$). λ_{max} 215 (ϵ 5500); 262 (ϵ 4300) (EtOH) (Derep).

Iguchi, R. *et al., Chem. Lett.*, 1986, 1789 (*isol, pmr, cmr, uv, ir*)
Ojida, A. *et al., J.O.C.*, 1994, **59**, 5970 (*synth*)
Kündig, E.P. *et al., J.A.C.S.*, 2003, **125**, 5642-5643 (*synth, abs config*)

Furanoeudesm-3-ene F-137

8,12-Epoxy-3,7,11-eudesmatriene
[632346-35-1]

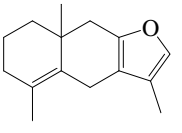


$C_{15}H_{20}O$ 216.322
Constit. of *Dasystenella acanthina*. Amorph. powder. $[\alpha]_D$ +70.2 (c, 0.5 in hexane).

Gavagnin, M. *et al., J. Nat. Prod.*, 2003, **66**, 1517-1519 (*isol, pmr, cmr*)

Furanoeudesm-4-ene F-138

[139742-33-9]

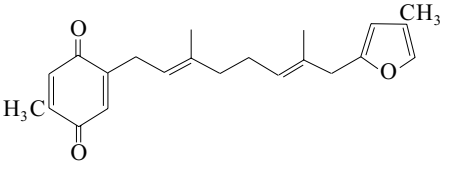


$C_{15}H_{20}O$ 216.322
Isol. from the gorgonian *Leptogorgia piccola*. Oil. $[\alpha]_D$ -22 (c, 0.002 in $CHCl_3$). λ_{max} 206 (ϵ 8000); 220 (ϵ 1500) (MeOH).

Roussis, V. *et al., New J. Chem.*, 1991, **15**, 959-961 (*isol, pmr, cmr, struct*)

Furanoquinone F-139

2-[3,7-Dimethyl-8-(4-methyl-2-furanyl)-2,6-octadienyl]-5-methyl-2,5-cyclohexadiene-1,4-dione, 9CI. Capillaquinone
[89014-06-2]

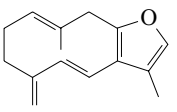


$C_{22}H_{26}O_3$ 338.446
Found in the soft coral *Sinularia capillosa*. Yellow cryst.
Mp 52-53°.

Hydroquinone: 2-[3,7-Dimethyl-8-(4-methyl-2-furanyl)-2,6-octadienyl]-5-methyl-1,4-benzenediol, 9CI. ***Furanoquinol***
[65557-84-8]
$C_{22}H_{28}O_3$ 340.461
Isol. from *Sinularia capillosa* and *Sinularia lochmodes*. Cryst. (hexane).

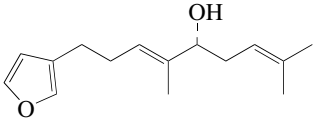
Mp 88-89°.
Coll, J.C. *et al., Aust. J. Chem.*, 1978, **31**, 157 (*Furanoquinol*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1983, **36**, 371 (*Furanoquinone*)

Furanotriene **F-140**
*8,12-Epoxy-1(10)*E*,4(15),5*E*,7,11-germacrapentaene*



$C_{15}H_{18}O$ 214.307
Struct. revised in 1990. Constit. of the sea plume *Pseudopterogorgia americana*. Oil.
Izac, R.R. *et al., Tetrahedron*, 1982, **38**, 301 (*isol*)
Chan, W.R. *et al., Tetrahedron*, 1990, **46**, 1499 (*isol, struct*)

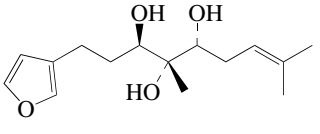
9-(3-Furanyl)-2,6-dimethyl-2,6-nonadien-5-ol **F-141**
8-Hydroxydendrolasin



$C_{15}H_{22}O_2$ 234.338

(5*R*,6*E*)-*form* [208926-17-4]
Constit. of *Ritterella rete.*
Oil. $[\alpha]_D$ +15.5 (c, 0.4 in MeOH). λ_{max} 210 (log ϵ 2.53); 274 (log ϵ 1.03) (MeOH).
6α,7α-Epoxide: ***6,7-Epoxy-8-hydroxydendrolasin***
[208926-20-9]
$C_{15}H_{22}O_3$ 250.337
Constit. of *Ritterella rete.* Yellow oil. $[\alpha]_D$ +52.8 (c, 0.5 in $CHCl_3$). λ_{max} 244 (log ϵ 3.58); 272 (log ϵ 1) ($CHCl_3$). λ_{max} 244 (ϵ 390); 272 (MeOH) (Berdy).
Lenis, L.A. *et al., Tetrahedron*, 1998, **54**, 5385-5406 (*isol, pmr, cmr, abs config*)

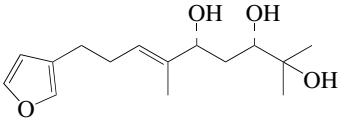
1-(3-Furanyl)-4,8-dimethyl-7-nonene-3,4,5-triol **F-142**
6,7-Dihydro-6,7,8-trihydroxydendrolasin. 6,7,8-Trihydroxydendrolasin (incorr.)



$C_{15}H_{24}O_4$ 268.352

(3*R*,4*R*,5*R*)-*form* [208926-18-5]
Constit. of *Ritterella rete.*
Pale yellow oil. $[\alpha]_D$ -14 (c, 0.12 in MeOH). λ_{max} 228 (log ϵ 2.77); 274 (log ϵ 2.18) (MeOH). λ_{max} 228 (ϵ 590); 274 (ϵ 151) (MeOH) (Berdy).
Lenis, L.A. *et al., Tetrahedron*, 1998, **54**, 5385-5406 (*isol, pmr, cmr*)

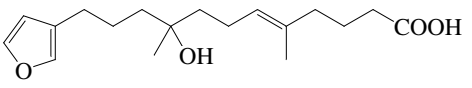
9-(3-Furanyl)-2,6-dimethyl-6-nonene-2,3,5-triol **F-143**
10,11-Dihydro-8,10,11-trihydroxydendrolasin. 8,10,11-Trihydroxydendrolasin (incorr.)



$C_{15}H_{24}O_4$ 268.352

(3*S*,5*R*,6*E*)-*form* [208926-19-6]
Constit. of *Ritterella rete.*
Pale yellow oil. $[\alpha]_D$ +14 (c, 0.35 in MeOH). λ_{max} 228; 274 (MeOH) (Berdy).
Lenis, L.A. *et al., Tetrahedron*, 1998, **54**, 5385-5406 (*isol, pmr, cmr*)

12-(3-Furanyl)-9-hydroxy-5,9-dimethyl-5-dodecenoic acid **F-144**
[87734-74-5]

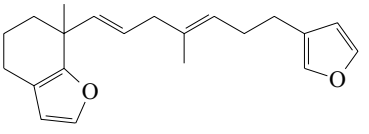


$C_{18}H_{28}O_4$ 308.417
Constit. of *Ircinia muscarum*.
$[\alpha]_D$ +4.7 (c, 0.3 in $CHCl_3$) (Me ester).

[87734-75-6 Me ester]

Gonzalez, A.G. *et al., An. Quim.*, 1983, **79**, 69-71

7-[7-(3-Furanyl)-4-methyl-1,4-heptadienyl]-4,5,6,7-tetrahydro-7-methylbenzofuran **F-145**

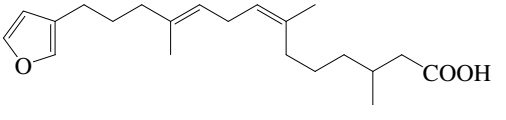


$C_{21}H_{26}O_2$ 310.435
Compd. not named in the paper. Constit. of *Fasciospongia cavernosa*. Oil. $[\alpha]_D^{28}$ +5 (c, 0.88 in $CHCl_3$).

[141631-71-2, 141634-59-5]

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 599 (*isol, pmr, cmr*)
Bando, T. *et al., Chem. Comm.*, 1996, 1357 (*synth*)

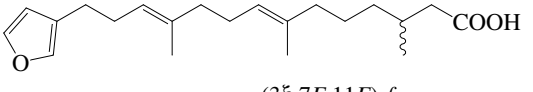
14-(3-Furanyl)-3,7,11-trimethyl-7,10-tetradecadienoic acid **F-146**



$C_{21}H_{32}O_3$ 332.482

(3ξ,7*Z*,10*E*)-*form* [82124-09-2]
Constit. of *Ircinia dendroides.*
González, A. *et al., J. Nat. Prod.*, 1983, **46**, 256-261 (*isol, pmr, cmr*)

14-(3-Furanyl)-3,7,11-trimethyl-7,11-tetradecadienoic acid, 9CI **F-147**



(3ξ,7*E*,11*E*)-*form*

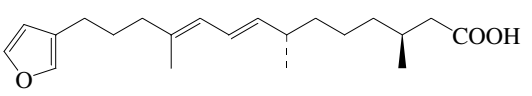
$C_{21}H_{32}O_3$ 332.482

(3ξ,7*E*,11*E*)-*form*
Variabilic acid
[82124-06-9]
The application of the name Variabilic acid to this compd. is tentative. Constit. of a *Sarcotragus* sp. Oil.

(3ξ,7*Z*,11*Z*)-*form* [82124-04-7]
Constit. of *Ircinia dendroides.*

González, A. *et al., J. Nat. Prod.*, 1983, **46**, 256-261 (*Ircinia dendroides constit*)
Barrow, C.J. *et al., J. Nat. Prod.*, 1988, **51**, 275-281 (*Variabilic acid*)

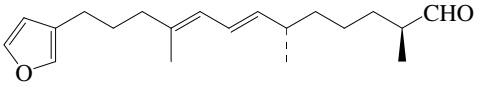
14-(3-Furanyl)-3,7,11-trimethyl-8,10-tetradecadienoic acid F-148



$C_{21}H_{32}O_3$ 332.482

(3*S*,7*S*,8*E*,10*E*)-*form* [138913-65-2]
Constit. of an unidentified marine sponge.
Oil. $[\alpha]_D^{20}$ +10 (c, 0.1 in $CHCl_3$). λ_{max} 238 (ϵ 21000) (MeOH).
Guella, G. *et al., Tet. Lett.*, 1991, **32**, 6415-6416 (*isol, pmr, cmr*)

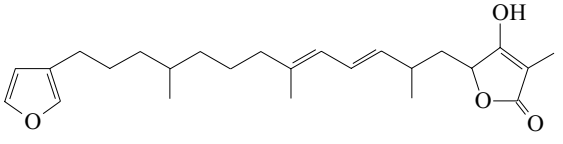
13-(3-Furanyl)-2,6,10-trimethyl-7,9-tridecadienal F-149



$C_{20}H_{30}O_2$ 302.456

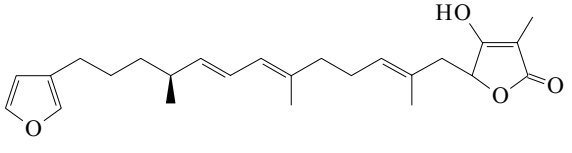
(2*S*,6*S*,7*E*,9*E*)-*form* [138913-66-3]
Constit. of an unidentified marine sponge.
Oil. $[\alpha]_D^{20}$ +9 (c, 0.08 in $CHCl_3$). λ_{max} 238 (ϵ 20200) (MeOH).
Guella, G. *et al., Tet. Lett.*, 1991, **32**, 6415-6416 (*isol, pmr, cmr*)

5-[13-(3-Furanyl)-2,6,10-trimethyl-3,5-tridecadienyl]-4-hydroxy-3-methyl-2(5*H*)-furanone F-150
[171438-67-8]



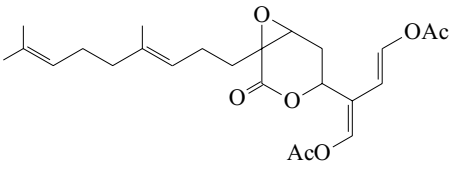
$C_{25}H_{36}O_4$ 400.557
Constit. of a *Psammocinia* sp. Oil. $[\alpha]_D$ -0.5 (c, 7.4 in $CHCl_3$). λ_{max} 201 (ϵ 17200); 238 (ϵ 16100) (MeOH) (Berdy).
Murray, L. *et al., Aust. J. Chem.*, 1995, **48**, 1899 (*isol, pmr, cmr*)

5-[13-(3-Furanyl)-2,6,10-trimethyl-2,6,8-tridecatrienyl]-4-hydroxy-3-methyl-2(5*H*)-furanone F-151
[125010-02-8]



$C_{25}H_{34}O_4$ 398.541
Constit. of *Psammocinia rugosa*. Oil. $[\alpha]_D$ +10.33 (c, 0.87 in $CHCl_3$).
Livkas, V. *et al., Aust. J. Chem.*, 1989, **42**, 1805 (*isol, pmr, cmr*)

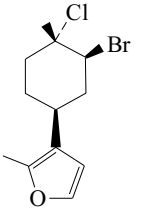
Furcellataepoxylactone F-152
1,20-Diacetoxy-6,7-epoxy-1,3(20),10,14-phytatetraen-19,4-olide



$C_{24}H_{32}O_7$ 432.513
Constit. of *Pseudochlorodesmis furcellata* and *Derbesia tenuissima*. Oil. $[\alpha]_D^{25}$ +1.6 (c, 0.7 in $CHCl_3$). λ_{max} 248 (ϵ 14000) (MeOH) (Berdy).
Paul, V.J. *et al., Phytochemistry*, 1988, **27**, 1011
Gavagnin, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1994, **108**, 107-115 (*isol*)

Furcelleran F-153
Furcelleran gum. Danish agar. Burtonitte 44
[9000-21-9]
A sulfated polysaccharide, the dominant hexose units of which are galactose, anhydrogalactose and their half-ester sulfates. Obt. by extraction of the red seaweed *Furcellaria fastigata* (Rhodophyceae).
Bjerre-Peterson, E *et al., Ind. Gums*, (ed. Whistler, R. L.), 2nd edn., Academic Press, 1973, 123-136 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1135-1139 (*use, props, salts*)

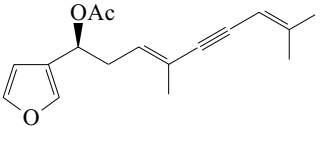
Furocaespitane F-154
3-(3-Bromo-4-chloro-4-methylcyclohexyl)-2-methylfuran
[51847-78-0]



Absolute configuration

$C_{12}H_{16}BrClO$ 291.614
Constit. of *Laurencia caespitosa*. Cryst. (C_6H_6).
Mp 83-85°. $[\alpha]_D$ 0 (c, 0.19 in $CHCl_3$).
González, A.G. *et al., Tet. Lett.*, 1973, 3625-3626; 1979, 2719-2722 (*isol, struct, cmr*)
Estrada, D.M. *et al., Tet. Lett.*, 1987, **28**, 687 (*abs config*)

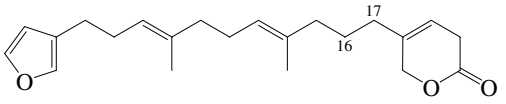
Furocaulerpin F-155
[80155-00-6]



$C_{17}H_{20}O_3$ 272.343
Constit. of *Caulerpa prolifera*. Oil. $[\alpha]_D^{20}$ -15 (c, 1 in $CHCl_3$).
De Napoli, L. *et al., Experientia*, 1981, **37**, 1132

Furodendin F-156

[74920-57-3]

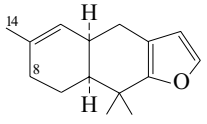


$C_{22}H_{30}O_3$ 342.477
Constit. of *Phyllospongia dendyi*. Oil.

*16,17-Didehydro(*E-*):* ***Dehydrofurodendin***
[808196-96-5]
$C_{22}H_{28}O_3$ 340.461
Constit. of *Lendenfeldia* spp. Oil.

Kazlauskas, R. *et al., Experientia*, 1980, **36**, 814 (*Furodendin*)
Chill, L. *et al., Tetrahedron*, 2004, **60**, 10619-10626 (*Dehydrofurodendin*)

Furodysin F-157



(+)–*form*

$C_{15}H_{20}O$ 216.322

(+)-*form* [70546-62-2]
[115889-38-8]
Constit. of *Dysidea* spp., and *Cadlina luteomarginata*, *Pleraplysilla* sp. and *Aplysilla* sp.
Cryst. (hexane). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 75°. $[\alpha]_D$ +36 (c, 0.5 in $CHCl_3$). λ_{max} 222 (ϵ 7000) (EtOH) (Derep).

8β-Acetoxy: ***8β-Acetoxyfurodysin***
[81619-63-8]
$C_{17}H_{22}O_3$ 274.359
Constit. of *Dysidea herbacea*. Oil. $[\alpha]_D$ +40 (c, 0.59 in $CHCl_3$).

14-(Acetylthio): ***Thiofurodysin acetate***
[70546-65-5]
$C_{17}H_{22}O_2S$ 290.426
Constit. of a *Dysidea* sp. Oil.

(-)-*form*
ent-*Furodysin*
[129783-56-8]
Isol. from *Dysidea fragilis*.
Mp 77-78° Mp 71-73° (synthetic). $[\alpha]_D^{25}$ -37.1 (c, 0.062 in $CHCl_3$). $[\alpha]_D$ -38 (c, 0.096 in $CHCl_3$) (synthetic).

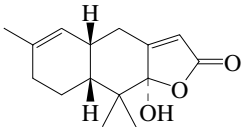
8α-Acetoxy: **ent-*8β-Acetoxyfurodysin***
[155322-16-0]
$C_{17}H_{22}O_3$ 274.359
Constit. of *Dysidea herbacea*. Oil. $[\alpha]_D^{25}$ -32 (c, 0.2 in CCl_4).

[70913-81-4]

Kaslauskas, R. *et al., Tet. Lett.*, 1978, 4951-4954 (*Furodysin, Thiofurodysin acetate*)
Dunlop, R.W. *et al., Aust. J. Chem.*, 1982, **35**, 95-103 (*Acetoxyfurodysin*)
Hellou, J. *et al., Tetrahedron*, 1982, **38**, 1875-1879 (*Furodysin*)
Hirota, H. *et al., Chem. Lett.*, 1987, 2079-2080 (*synth*)
Villaincourt, V. *et al., J.O.C.*, 1991, **56**, 378-387 (*synth, abs config*)
Su, J.-Y. *et al., Chin. J. Chem.*, 1993, **13**, 460-463 (*ent-Furodysin*)
Searle, P.A. *et al., Tetrahedron*, 1994, **50**, 3879-3888 (*8β-Acetoxyfurodysin, abs config*)
Ho, T.-L. *et al., Tet. Lett.*, 1995, **36**, 947-948 (*ent-Furodysin, synth*)
Moiseekov, A.M. *et al., Mendeleev Commun.*, 1996, 89-90 (*synth*)
Dumdei, E.J. *et al., Can. J. Chem.*, 1997, **75**, 773-789 (*Furodysin*)

Furodysin lactone F-158

[385801-56-9]

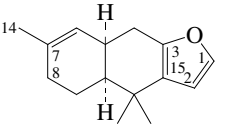


Relative Configuration

$C_{15}H_{20}O_3$ 248.321
Isol. from a *Dysidea* sp. Pale yellow oil. $[\alpha]_D^{23}$ +100 (c, 0.01 in MeOH). λ_{max} 216 (log ϵ 3.79) (MeOH).

Goetz, G.H. *et al., J. Nat. Prod.*, 2001, **64**, 1486-1488 (*isol, pmr, cmr*)

Furodysinin F-159



(+)-*form*

$C_{15}H_{20}O$ 216.322

(+)-*form* [70546-63-3]
Constit. of *Dysidea etheria*, *Hypselodoris zebra* and *Aplysilla* spp.
Cryst. (hexane).
Mp 55°. $[\alpha]_D$ +64 (c, 0.5 in $CHCl_3$). The abs. config. is (5*R*,10*S*) but some refs. misassign this. λ_{max} 222 (ϵ 7000) (EtOH).

8,9-Didehydro: ***9,10-Dehydrofurodysinin***
[157426-24-9]
$C_{15}H_{18}O$ 214.307
Constit. of *Hypselodoris webbi*. Toxic to brine shrimp, antifeedant, ichthyotoxin. Oil. Sol. MeOH, Me_2CO, Et_2O; poorly sol. H_2O.
$[\alpha]_D^{25}$ +259 (c, 0.22 in $CHCl_3$).

8α-Hydroxy: [72236-79-4]
$C_{15}H_{20}O_2$ 232.322
Isol. from *Dysidea herbacea*. Oil. $[\alpha]_D^{28}$ -10 (c, 0.3 in CCl_4).

8β-Hydroxy: [81702-30-9]
$C_{15}H_{20}O_2$ 232.322
Constit. of *Dysidea herbacea*. Oil. $[\alpha]_D^{26}$ -54.6 (c, 0.8 in CCl_4).

8β-Acetoxy: ***8β-Acetoxyfurodysinin***
[155322-13-7]
$C_{17}H_{22}O_3$ 274.359
Constit. of *Dysidea herbacea*. Cryst. (hexane).
Mp 107-108°. $[\alpha]_D$ +61.3 (c, 0.57 in $CHCl_3$).

14-Hydroxy: [81619-62-7]
$C_{15}H_{20}O_2$ 232.322
From *Dysidea herbacea*. Oil. $[\alpha]_D^{26}$ +2 (c, 0.25 in CCl_4).

14-Mercapto: ***Thiofurodysinin***
[70913-80-3]
$C_{15}H_{20}OS$ 248.388
From *Dysidea avara*. Oil. $[\alpha]_D$ +49.

14-(Acetylthio): ***Thiofurodysinin acetate***
[70546-64-4]
$C_{17}H_{22}O_2S$ 290.426
Isol. from a *Dysidea* sp. and from mollusc *Ceratosoma brevicaudatum*. Oil. $[\alpha]_D$ +49.3 (c, 12 in $CHCl_3$).

$\Delta^{7,14}$-Isomer: ***Isofurodysinin***
[81619-64-9]
$C_{15}H_{20}O$ 216.322
Isol. from *Dysidea herbacea*. Oil. $[\alpha]_D^{28}$ +36.5 (c, 0.2 in $CHCl_3$).

(-)-*form*
ent-*Furodysinin*
[98672-90-3]
Constit. of *Dysidea tupha*, *Dysidea fragilis* and *Dysidea herbacea*.
Needles.
Mp 56-57°. $[\alpha]_D^{25}$ -63.7 (c, 0.088 in $CHCl_3$). λ_{max} 252 (ϵ 19950); 270 (ϵ 30900) (hexane) (Derep).

*8-Acetoxy (*ent-*8α-):* **ent-*8α*-*Acetoxyfurodysinin**
[155322-17-1]
$C_{17}H_{22}O_3$ 274.359
Constit. of *Dysidea herbacea*. Oil. $[\alpha]_D$ -60.6 (c, 2.45 in $CHCl_3$).

*8-Acetoxy (*ent-*8β-):* **ent-*8β*-*Acetoxyfurodysinin**
[155322-15-9]
$C_{17}H_{22}O_3$ 274.359
Constit. of *Dysidea herbacea*. Oil. $[\alpha]_D^{25}$ -41 (c, 1 in $CHCl_3$).

1α,2α:3α,15α-Diepoxide: ***Furodysinin bis-α-epoxide***
[103302-75-6]
$C_{15}H_{20}O_3$ 248.321
Isol. from mollusc *Chromodoris funerea*. Unstable, dec. during chromatog.

1β,2β:3β,15β-Diepoxide: ***Furodysinin bis-β-epoxide***
[103202-16-0]
$C_{15}H_{20}O_3$ 248.321
Isol. from *Chromodoris funerea*. Unstable, dec. during chromatog.

14-(Methylthio): ***Methylthiofurodysinin***
[117569-46-7]
$C_{16}H_{22}OS$ 262.415
Constit. of *Ceratosoma brevicaudatum*.

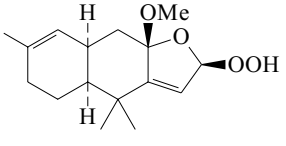
14-Mercapto, disulfide dimer: ***Dithiofurodysinin disulfide***. *Thiofurodysinin disulfide*
[128201-21-8]
$C_{30}H_{38}O_2S_2$ 494.761
Constit. of *Ceratosoma brevicaudatum* and *Dysidea herbacea*. Oil. $[\alpha]_D$ -27.8 (c, 0.009 in C_6H_6).

14-(Acetylthio): ***Thiofurodysinin acetate***
[128298-61-3]
$C_{17}H_{22}O_2S$ 290.426
Constit. of *Dysidea herbacea*. Oil. $[\alpha]_D$ -34.6 (c, 0.028 in C_6H_6).

Kaslauskas, R. *et al., Tet. Lett.*, 1978, 4951-4954 (*Methylthiofurodysinin*)
Dunlop, R.W. *et al., Aust. J. Chem.*, 1982, **35**, 95-103 (*8β-Hydroxyfurodysinin, 8β-Acetoxyfurodysinin, Isofurodysinin*)
Hellou, J. *et al., Tetrahedron*, 1982, **38**, 1875-1879 (*Furodysinin*)
Grode, S.H. *et al., J. Nat. Prod.*, 1984, **47**, 76-83 (*isol*)
Guella, G. *et al., Helv. Chim. Acta*, 1985, **68**, 1276-1282 (*isol*)
Carté, B. *et al., J.O.C.*, 1986, **51**, 3528 (*Furodysinin bis-epoxides*)
Hirota, H. *et al., Chem. Lett.*, 1987, 2079-2080 (*synth*)
Capon, R.J. *et al., J. Nat. Prod.*, 1987, **50**, 1136-1137 (*Thiofurodysinin, 14-Acetylthiofurodysinin, bibl*)
Ksebati, M.B. *et al., J. Nat. Prod.*, 1988, **51**, 857-861 (*Methylthiofurodysinin, Dithiofurodysinin disulfide*)
Horton, P. *et al., J. Nat. Prod.*, 1990, **53**, 143-151 (*ent-Furodysinin, isol*)
Vaillancourt, V. *et al., J.O.C.*, 1991, **56**, 378-387 (*synth, abs config*)
Su, J.-Y. *et al., Chin. J. Chem.*, 1993, **13**, 460-463 (*ent-Furodysinin*)
Fontana, A. *et al., J. Nat. Prod.*, 1994, **57**, 510-513 (*9,10-Dehydrofurodysinin*)
Searle, P.A. *et al., Tetrahedron*, 1994, **50**, 3879-3888 (*isol, abs config, derivs*)
Ho, T.-L. *et al., Chem. Comm.*, 1996, 1147 (*synth*)
Moiseekov, A.M. *et al., Mendeleev Commun.*, 1996, 89-90 (*synth*)
Dumdei, E.J. *et al., Can. J. Chem.*, 1997, **75**, 773-779 (*Furodysinin*)

Furodysinin hydroperoxide F-160

[103202-15-9]

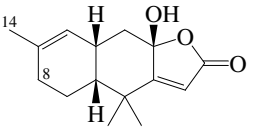


$C_{16}H_{24}O_4$ 280.363
Metab. of the nudibranch *Chromodoris funerea*. Also from *Dysidea herbacea*. Cryst. (Et_2O/hexane).
Mp 142-143°. $[\alpha]_D$ -63.4 (c, 0.5 in $CHCl_3$).

Carté, B. *et al., J.O.C.*, 1986, **51**, 3528-3532 (*isol, ir, pmr, cmr, cryst struct*)

Furodysinin lactone F-161

[89837-72-9]
[313510-10-0]



$C_{15}H_{20}O_3$ 248.321
Numbering systems vary. Constit. of *Dysidea etheria*, *Dysidea fragilis* and *Hypselodoris zebra*. Cryst.
Mp 168-170°. $[\alpha]_D^{25}$ +147 (c, 1 in $CHCl_3$). λ_{max} 222 (ε 10000) (MeOH).

Me ether: ***Furodysinin lactone methyl ether***. O-*Methylfurodysinin lactone*
[103202-14-8]
[313510-12-2]
$C_{16}H_{22}O_3$ 262.348
Constit. of *Chromodoris funerea*, *Dysidea herbacea* and *Dysidea* sp. 1519. Oil. $[\alpha]_D$ -84.8 (c, 0.5 in $CHCl_3$). λ_{max} 210 (ε 6000) (EtOH).

8α-Hydroxy: ***8-Hydroxyfurodysinin lactone***. *6-Hydroxyfurodysinin lactone*
[383896-81-9]
$C_{15}H_{20}O_4$ 264.321
Constit. of *Dysidea herbacea*.

8α-Hydroxy, Me ether: ***8-Hydroxyfurodysinin lactone methyl ether***
$C_{16}H_{22}O_4$ 278.347
Constit. of a *Dysidea* sp. 1524.
$[\alpha]_D$ +146 (c, 0.0035 in CH_2Cl_2).

8α-Hydroxy, Et ether: 8-Hydroxyfurodysinin lactone ethyl ether
[874359-41-8]
$C_{17}H_{24}O_4$ 292.374
Constit. of *Dysidea arenaria*.

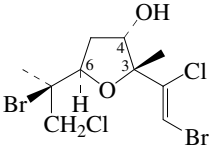
8-Oxo, Me ether: 8-Oxofurodysinin lactone methyl ether
[194020-47-8]
$C_{16}H_{20}O_4$ 276.332
Constit. of *Cadlina luteomarginata*. Oil. λ_{max} 220 (log ε 3.43) (hexane).

14-(Acetylthio): ***14-Acetylthioxyfurodysinin lactone***. *15-Acetylthioxyfurodysinin lactone*
[122771-73-7]
$C_{17}H_{22}O_4S$ 322.424
Metab. of sponge *Dysidea herbacea* and from an unspecified *Dysidea* sp. Potent LTB_4 receptor partial agonist. Cryst.
Mp 144-145°. $[\alpha]_D$ -178 ($CHCl_3$).

Grode, S.H. *et al., J. Nat. Prod.*, 1984, **47**, 76-83 (*Furodysinin lactone*)
Carté, B. *et al., J.O.C.*, 1986, **51**, 3528-3532 (*Me ether*)
Carté, B. *et al., Tet. Lett.*, 1989, **30**, 2725-2726 (*14-Acetylthioxyfurodysinin lactone*)
Dumdei, E.J. *et al., Can. J. Chem.*, 1997, **75**, 773-789 (*deriv*)
Reddy, N.S. *et al., Indian J. Chem., Sect. B*, 2000, **39**, 393-395 (*Furodysinin lactone, Me ether*)
Cameron, G.N. *et al., Tetrahedron*, 2000, **56**, 5247-5252 (*Dysidea constits*)
Dumrongchai, N. *et al., ACGC Chem. Res. Commun.*, 2001, **13**, 17-22; *CA*, **136**, 67123n (*8-Hydroxyfurodysinin lactone*)
Zhang, G.-W. *et al., Acta Cryst. E*, 2005, **61**, o172-o173 (*Furodysinin lactone, cryst struct*)
Piggott, A.M. *et al., Molecules*, 2005, **10**, 1292-1297 (*8-Hydroxyfurodysinin lactone ethyl ether*)

Furoplocamioid A F-162

[380847-41-6]



Relative Configuration

$C_{10}H_{14}Br_2Cl_2O_2$ 396.933
Constit. of *Plocamium cartilagineum*. Oil. $[\alpha]_D^{25}$ -47 (c, 0.3 in $CHCl_3$).

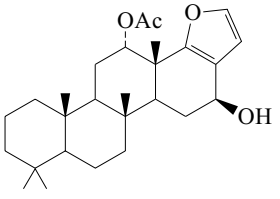
3-Epimer: ***Furoplocamioid B***
[380847-44-9]
$C_{10}H_{14}Br_2Cl_2O_2$ 396.933
Constit. of *Plocamium cartilagineum*. Oil. $[\alpha]_D^{25}$ -110 (c, 0.36 in $CHCl_3$).

6-Epimer: ***Furoplocamioid C***
[380847-46-1]
$C_{10}H_{14}Br_2Cl_2O_2$ 396.933
Constit. of *Plocamium cartilagineum*. Oil. $[\alpha]_D^{25}$ -81 (c, 0.2 in $CHCl_3$).

Darias, J. *et al., J. Nat. Prod.*, 2001, **64**, 1383-1387 (*isol, pmr, cmr*)
Díaz-Marrero, A.R. *et al., Tetrahedron*, 2002, **58**, 8539-8542 (*struct*)

Furoscalarol F-163

[64285-85-4]



$C_{27}H_{40}O_4$ 428.611
Isol. from the sponge *Cacospongia mollior* and mollusc *Hypselodoris tricolor*. Feeding inhibitor; platelet aggregation inhibitor. Cryst. (petrol).
Mp 181-183°. $[\alpha]_D$ +14.7 (c, 1 in $CHCl_3$). λ_{max} 215 (ϵ 8980); 272 (ϵ 2565) (MeOH).

Ac: ***16-Acetylfuroscalarol***
[186382-51-4]
$C_{29}H_{42}O_5$ 470.648
Constit. of *Cacospongia scalaris*. Oil. $[\alpha]_D$ +15 (c, 0.2 in $CHCl_3$). λ_{max} 224 (ϵ 3901); 270 (ϵ 672) (MeOH).

O-*De-Ac:* ***12-Deacetylfuroscalarol***. *Desacetylfuroscalarol*
$C_{25}H_{38}O_3$ 386.573
Constit. of *Hyrtios* sp. Stimulates nerve growth factor synth. Cryst. (MeOH).
Mp 238-242°. $[\alpha]_D^{20}$ +62 (c, 0.4 in $CHCl_3$). λ_{max} 217 (ϵ 6600) (MeOH) (Berdy).

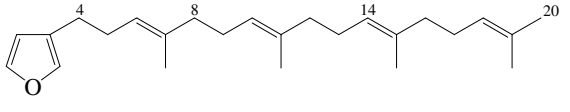
16-Ketone, O-*de-Ac:* ***12-Deacetylfuroscalar-16-one***. *12-Desacetylfuroscalar-16-one*
[215854-06-1]
$C_{25}H_{36}O_3$ 384.558
Constit. of a *Cacospongia* sp. Needles.
Mp 287-288°. $[\alpha]_D^{20}$ +44.8 (c, 0.13 in CH_2Cl_2). λ_{max} 260 (log ϵ 3.95) (CH_2Cl_2).

12,16-Diepimer, O-*de-Ac, 16-Ac:* [201213-04-9]
$C_{27}H_{40}O_4$ 428.611
Constit. of *Spongia agaricina*. Oil. $[\alpha]_D^{25}$ -44.2 (c, 0.33 in $CHCl_3$). λ_{max} 209 (ϵ 18840) (MeOH).

Cafieri, F. *et al., Gazz. Chim. Ital.*, 1977, **107**, 71-74 (*isol, pmr, ir, uv*)
Cimino, G. *et al., Tet. Lett.*, 1978, 2041-2044 (*cmr, abs config*)
Doi, Y. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2190-2191 (*Desacetylfuroscalarol, isol, pmr, cmr*)
Cimino, G. *et al., Experientia*, 1993, **49**, 582 (*isol*)
Rueda, A. *et al., J.O.C.*, 1997, **62**, 1481-1485 (*16-Acetylfuroscalarol*)
Rueda, A. *et al., J. Nat. Prod.*, 1998, **61**, 258-261 (*Spongia agaricina constit*)
Cambie, R.C. *et al., J. Nat. Prod.*, 1998, **61**, 1416-1417 (*12-Deacetylfuroscalar-16-one*)

Furospinulosin 1 F-164

3-(4,8,12,16-Tetramethyl-3,7,11,15-heptadecatetraenyl)furan, 9CI
[35890-95-0]



$C_{25}H_{38}O$ 354.575
Constit. of the sponges *Ircinia spinosula*, *Carteriospongia* sp., *Spongia idia*, *Thorecta* sp. and *Fasciospongia* sp. Ichthyotoxin. Oil. Sol. $CHCl_3$, hexane; poorly sol. H_2O. λ_{max} 218 (ϵ 4800) (cyclohexane) (Derep).

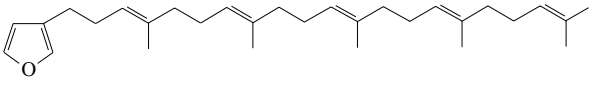
20-Carboxylic acid, 14,15-epoxide: 6,7-Epoxy-17-(3-furanyl)-2,6,10,14-tetramethyl-2,10,14-heptadecatrienoic acid
$C_{25}H_{36}O_4$ 400.557
Constit. of *Spongia* sp. Oil. $[\alpha]_D$ +8.7 (c, 6 in $CHCl_3$).

4,8-Dihydroxy: ***5,10-Dihydroxyfurospinulosin 1***
[705282-90-2]
$C_{25}H_{38}O_3$ 386.573
Isol. from the marine sponge *Hyrtios erectus*. Different numbering systems in use.

Cimino, G. *et al., Tetrahedron*, 1972, **28**, 1315
Searle, P.A. *et al., Tetrahedron*, 1994, **50**, 9893 (*isol, pmr, cmr*)
Qiu, Y. *et al., J. Nat. Prod.*, 2004, **67**, 921-924 (*5,10-Dihydroxyfurospinulosin 1*)

Furospinulosin 2 F-165

3-(4,8,12,16,20-Pentamethyl-3,7,11,15,19-heneicosapentaenyl)furan, 9CI
[35890-96-1]

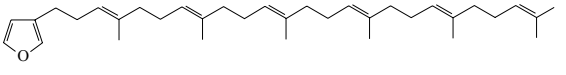


$C_{30}H_{46}O$ 422.693
Constit. of the sponge *Ircinia spinosula*. Oil. λ_{max} 218 (ϵ 4800) (cyclohexane) (Derep).

Cimino, G. *et al., Tetrahedron*, 1972, **28**, 1315 (*isol*)

Furospinulosin 3 F-166

3-(4,8,12,16,20,24-Hexamethyl-3,7,11,15,19,23-pentacosahexaenyl)furan, 9CI
[35890-97-2]

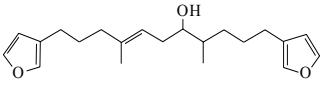


$C_{35}H_{54}O$ 490.811
Rare C_{35} linear terpenoid. Constit. of the sponge *Ircinia spinosula*. Oil. λ_{max} 218 (ϵ 4800) (cyclohexane) (Derep).

Cimino, G. *et al., Tetrahedron*, 1972, **28**, 1315

Furospongenol F-167

[60463-88-9]



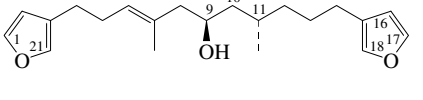
$C_{21}H_{30}O_3$ 330.466
Constit. of *Spongia* spp. Oil.

Ketone: ***Furospongenone***
[60463-89-0]
$C_{21}H_{28}O_3$ 328.45
From *Spongia* spp. Oil.

Kazlauskas, R. *et al., Tet. Lett.*, 1976, 1333

Furospongin 1 F-168

[35075-74-2]



Absolute Configuration

$C_{21}H_{30}O_3$ 330.466

Sesterterpene numbering shown. Absolute config. revised in 1992.
Constit. of *Spongia officinalis*, *Phyllospongia foliascens* and *Hippospongia communis*. Cryst. (petrol). Sol. MeOH.
Mp 35°. $[\alpha]_D$ +8.8 (c, 1 in $CHCl_3$). λ_{max} 220 (ϵ 9100) (cyclohexane) (Derep).

Ac: [34973-16-5]
$C_{23}H_{32}O_4$ 372.503
Constit. of *Dendrodoris grandiflora*.

*10,11*E*-Didehydro, 9-ketone:* ***Furospongin 2***
[35671-05-7]
$C_{21}H_{26}O_3$ 326.435
Isol. from *Spongia officinalis* and *Hippospongia communis*. Toxic to brine shrimp. Oil. Sol. MeOH, hexane; poorly sol. H_2O. λ_{max} 220 (ϵ 11400); 242 (ϵ 9000) (cyclohexane) (Derep). λ_{max} 242 (ϵ 23000) (MeOH) (Berdy).

*10,11*Z*-Didehydro, 9-ketone:* ***Isofurospongin 2***
[35671-04-6]
$C_{21}H_{26}O_3$ 326.435
Isol. from *Spongia officinalis* and *Hippospongia communis*. Oil.

*11,12*E*-Didehydro:* ***11,12-Didehydrofurospongin 1***. *12,13-Didehydrofurospongin 1*
[116331-45-4]
$C_{21}H_{28}O_3$ 328.45
Constit. of *Carteriospongia flabellifera* and *Fasciospongia cavernosa*.
$[\alpha]_D^{28}$ -8 (c, 0.92 in $CHCl_3$).

*11,12*E*-Didehydro, Me ether:*
$C_{22}H_{30}O_3$ 342.477
Constit. of *Fasciospongia cavernosa*. Oil. $[\alpha]_D^{28}$ +13 (c, 0.22 in $CHCl_3$).

1,2-Dihydro, 1-oxo, 3ξ,21-epoxide: [51943-35-2]
$C_{21}H_{30}O_5$ 362.465
Constit. of *Spongia officinalis*.

1,21-Dihydro, 1-oxo, 21ξ-hydroxy: [51943-39-6]
$C_{21}H_{30}O_5$ 362.465
Constit. of *Spongia officinalis*.

1,21-Dihydro, 21-oxo, 1ξ-hydroxy: [51943-37-4]
$C_{21}H_{30}O_5$ 362.465
Constit. of *Spongia officinalis*.

3ξ,21-Dihydro, 21-oxo, 1ξ,2ξ-epoxide: [51943-41-0]
$C_{21}H_{30}O_5$ 362.465
Constit. of *Spongia officinalis*.

15ξ,18-Dihydro, 18-oxo, 16ξ,17ξ-epoxide: [51943-40-9]
$C_{21}H_{30}O_5$ 362.465
Constit. of *Spongia officinalis*.

16,17-Dihydro, 17-oxo, 15,18-epoxide: [51943-42-1]
$C_{21}H_{30}O_5$ 362.465
Constit. of *Spongia officinalis*.

17,18-Dihydro, 17-oxo, 18ξ-hydroxy: [51943-38-5]
$C_{21}H_{30}O_5$ 362.465
Constit. of *Spongia officinalis*.

17,18-Dihydro, 18-oxo, 17ξ-hydroxy: [51943-36-3]
$C_{21}H_{30}O_5$ 362.465
Constit. of *Spongia officinalis*.

*Δ^7-Isomer(*E*-), 10,11*E*-didehydro, 9-ketone:* [126149-88-0]
$C_{21}H_{26}O_3$ 326.435
Constit. of *Spongia officinalis*. Oil. Sol. MeOH, hexane; poorly sol. H_2O. λ_{max} 267 (ϵ 26000) (MeOH).

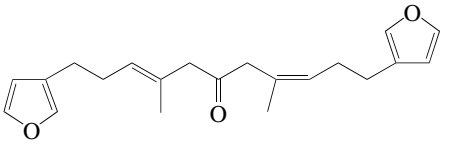
*Δ^7-Isomer(*Z*-), 10,11*E*-didehydro, 9-ketone:* [126149-87-9]
$C_{21}H_{26}O_3$ 326.435
Constit. of *Spongia officinalis*. Oil. λ_{max} 253 (ϵ 25000) (MeOH).

*Δ^7-Isomer (*Z*-), 10,11*Z*-didehydro, 9-ketone:* [126149-86-8]
$C_{21}H_{26}O_3$ 326.435
Constit. of *Spongia officinalis*. Oil. Sol. MeOH, hexane; poorly sol. H_2O. λ_{max} 265 (ϵ 24000) (MeOH).

Cimino, G. *et al., Tetrahedron*, 1971, **27**, 4673-4679; 1972, **28**, 267-273; 1985, **41**, 1093 (*Furospongin, Furospongin acetate, 11,12E-didehydro ketones, isol, struct*)
Cimino, G. *et al., Experientia*, 1974, **30**, 18-20 (*butenolide derivs*)
Schmitz, F.J. *et al., J. Nat. Prod.*, 1988, **51**, 745-748 (*isol, 11, 12-Didehydrofurospongin 1*)
De Giulio, A. *et al., J. Nat. Prod.*, 1989, **52**, 1258-1262 (*Isofurospongin 2 isomers*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 599-601 (*11,12-Didehydrofurospongin 1*)
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1992, 366-367 (*abs config*)
Garrido, L. *et al., J. Nat. Prod.*, 1997, **60**, 794-797 (*cmr*)

Furospongin 5 F-169

[192223-13-5]

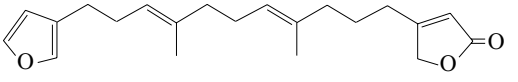


$C_{21}H_{26}O_3$ 326.435
Constit. of *Spongia officinalis*. Cytotoxic on P-388 cells. Oil. λ_{max} 204 (ϵ 11543) (MeOH).

Garrido, L. *et al., J. Nat. Prod.*, 1997, **60**, 794-797 (*isol, pmr, cmr, activity*)

Furospongolide F-170

[76343-80-1]

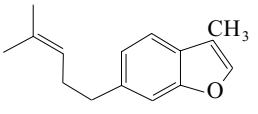


$C_{21}H_{28}O_3$ 328.45
Constit. of *Dysidea herbacea*. Antifouling agent. Oil.

Kashman, Y. *et al., Experientia*, 1980, **36**, 1279

Furoventalene F-171

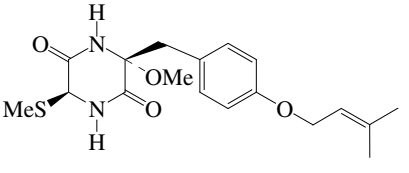
*3-Methyl-6-(4-methyl-3-pentenyl)benzo[*b*]furan*
[25074-12-8]



$C_{15}H_{18}O$ 214.307
Constit. of *Gorgonia ventalina*. Oil. Of unknown biosynth.; poss. an artifact of the isolation procedure.

Weinheimer, A.J. *et al., Tet. Lett.*, 1969, 3315 (*isol, struct*)
Kido, F. *et al., J.O.C.*, 1981, **46**, 4389 (*synth*)
Bergstrom, D.E. *et al., J. Het. Chem.*, 1983, **20**, 469 (*synth*)
Hagiwara, H. *et al., J.C.S. Perkin 1*, 1984, 91 (*synth*)

Fusaperazine B F-172



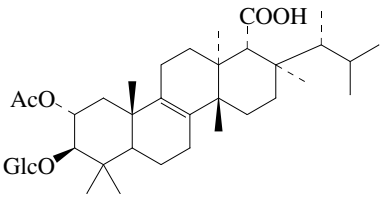
Relative Configuration

$C_{18}H_{24}N_2O_4S$ 364.465
Prod. by *Fusarium chlamydosporum* OUPS-N124. Needles. $[\alpha]_D$ -75.2 (c, 0.08 in dioxan). λ_{max} 227 (log ϵ 3.62); 277 (log ϵ 3.16); 283 (log ϵ 3.14) (EtOH).

Usami, Y. *et al., J. Antibiot.*, 2002, **55**, 655-659 (*isol, cd, uv, pmr, cmr*)

Fuscoatroside F-173

Antibiotic FR 207944. Antibiotic WF 217. FR 207944. WF 217
[476683-11-1]

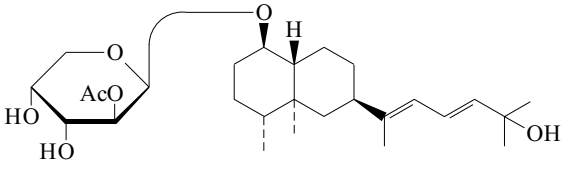


$C_{38}H_{62}O_{10}$ 678.902
Metab. of *Chaetomium* sp. No. 217, *Humicola fuscoatra* and the marine-derived *Humicola grisea* Gö 101/26. Antifungal agent.
Amorph. solid.
Mp 93-95°. $[\alpha]_D$ -26 (c, 0.3 in MeOH). λ_{max} 213 (ϵ 1400) (MeOH).

Joshi, B.K. *et al., J. Nat. Prod.*, 2002, **65**, 1734-1737 (*isol, pmr, cmr*)
Kobayashi, M. *et al., Biosci., Biotechnol., Biochem.*, 2005, **69**, 515-521; 1029-1032 (*isol, pmr, cmr, cryst struct, activity*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

Fuscoside A F-174

[133470-54-9]

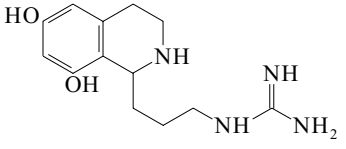


$C_{27}H_{44}O_7$ 480.64
Constit. of *Eunicea fusca*. Antiinflammatory agent. Oil. $[\alpha]_D$ -64 (c, 0.6 in $CHCl_3$). λ_{max} 239 (ϵ 28000) (MeOH) (Derep).

Shin, J. *et al., J.O.C.*, 1991, **56**, 3153 (*isol, pmr, cmr*)

Fuscusine F-175

[3-(1,2,3,4-Tetrahydro-6,8-dihydroxy-1-isoquinolinyl)propyl]guanidine, 9CI
[155210-58-5]

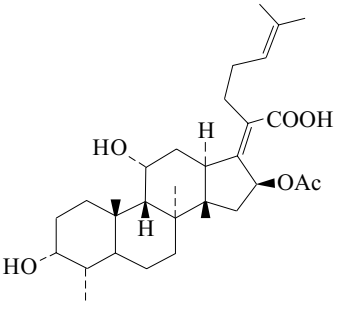


$C_{13}H_{20}N_4O_2$ 264.327
Alkaloid from the body wall of the seastar *Perknaster fuscus antarcticus*. Ichthyotoxin. Oil. CAS no. refers to monohydrochloride. λ_{max} 278 (ϵ 2510) (MeOH) (Derep).

Harper, M.K. *et al., Nat. Prod. Lett.*, 1992, **1**, 71-74 (*isol, pmr, cmr, uv, ir*)

Fusidic acid, BAN, INN, USAN F-176

Fusidin. Ramycin. NSC 56192. SQ 16603. Antibiotic SQ 16603
[6990-06-3]



$C_{31}H_{48}O_6$ 516.717
Steroid antibiotic. Constit. of *Fusidium* spp. Also prod. by dermatophytes. Isol. from a marine-derived *Stilbella aciculosa*. Mainly active against gram-positive bacteria; shows anti-HIV activity. Cryst. (Et_2O).
Mp 192-193°. $[\alpha]_D^{20}$ -9 (c, 1 in $CHCl_3$). Log P 5.31 (uncertain value) (calc). λ_{max} 204 (ϵ 9900) (95% EtOH) (Derep). λ_{max} 220 (ϵ 8300) (MeOH) (Derep).
▶ Skin irritant. Hepatic effects when used therapeutically. LD_{50} (mus,orl) 1500 mg/kg. RC1350000

Na salt: Fusidate sodium, USAN. Sodium fusidate, BAN, INN, JAN. Fucidin. Fusin. Stafusid. Stenicid. Verutex. Fucibet. SQ 16360
[751-94-0]
Hygroscopic powder.
▶ Skin irritant. Can cause hepatic effects when used therapeutically. LD_{50} (mus, scu) 313 mg/kg. LV5775000

16-O-*De-Ac:* ***16-Deacetylfusidic acid***
[13090-91-0]
$C_{29}H_{46}O_5$ 474.679
Prod. by *Fusidium coccineum*.

3-Ketone: [4680-37-9]
$C_{31}H_{46}O_6$ 514.701
Constit. of *Fusidium coccineum*. Cryst. (Et_2O).
Mp 177-178° Mp 191-192°. $[\alpha]_D^{20}$ +23 (c, 1.0 in $CHCl_3$). λ_{max} 204 (ϵ 10500); 225 (ϵ 7500) (EtOH) (Berdy).

11-Ketone: [16711-91-4]
$C_{31}H_{46}O_6$ 514.701
Constit. of *Fusidium coccineum*. Cryst. (Et_2O).
Mp 196-197°. $[\alpha]_D^{20}$ +55 (c, 1.0 in $CHCl_3$). λ_{max} 204 (ϵ 10900); 225 (ϵ 6950) (EtOH) (Berdy).

3-Epimer: [19030-42-3]
Constit. of *Fusidium coccineum*.
Cryst. ($CHCl_3$).
Mp 211°. $[\alpha]_D$ +10 (c, 1.0 in Py). λ_{max} 204 (ϵ 9800); 225 (ϵ 7350) (EtOH) (Berdy).

11-Epimer: [4680-36-8]
Constit. of *Fusidium coccineum*.
Cryst. (Et_2O).
Mp 202-203°. $[\alpha]_D^{20}$ +80 (c, 1.0 in Py). λ_{max} 204 (ϵ 9750); 225 (ϵ 7050) (EtOH) (Berdy).

16-Epimer, 16-O-*de-Ac:* [5951-83-7]
$C_{29}H_{46}O_5$ 474.679
Prod. by *Fusidium coccineum*.

Godtfredsen, W.O. *et al., Tetrahedron*, 1965, **21**, 3505 (*isol*)
Cooper, A. *et al., Tetrahedron*, 1968, **24**, 909 (*cryst struct*)
Tanaka, N. *et al., Antibiotics*, 1973, **3**, 436 (*rev*)
Ebersole, R.-C. *et al., J.A.C.S.*, 1974, **96**, 6499 (*biosynth*)
Ireland, R.E. *et al., J.O.C.*, 1977, **42**, 1276 (*synth*)
Tanabe, M. *et al., Tet. Lett.*, 1977, 1481 (*synth*)
Godtfredsen, W.O. *et al., Tetrahedron*, 1979, **35**, 2419
Suchova, G.S. *et al., Antibiotiki (Moscow)*, 1981, **26**, 16-19; *CA*, **94**, 172818e (*deacetyl derivs*)
Hikal, A.H. *et al., J. Pharm. Sci.*, 1982, **71**, 1297 (*hplc*)
Dauben, W.G. *et al., J.A.C.S.*, 1982, **104**, 303 (*synth*)
Perry, W.J. *et al., J. Antibiot.*, 1983, **36**, 1659 (*isol*)

Von Daehne, W. *et al., Drugs Pharm. Sci.*, 1984, **22**, 427 (*rev*)
Reeves, D.S. *et al., J. Antimicrob. Chemother.*, 1987, **20**, 467 (*rev, pharmacol*)
Czajkowski, J. *et al., J. Antimicrob. Chemother.*, 1989, **23**, 155 (*anti-HIV activity*)
Verbist, L. *et al., J. Antimicrob. Chemother.*, (Suppl. B), 1990, **25**, 1 (*rev, props*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 168
Kuznetsova, T.A. *et al., Biochem. Syst. Ecol.*, 2001, **29**, 873-874 (*Stilbella isol*)
Rastrup-Andersen, N. *et al., Magn. Reson. Chem.*, 2002, **40**, 471-473 (*pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FQU000; SHK000

FVNSRY amide F-177

[638174-66-0]

Phe-Val-Asn-Ser-Arg-Tyr-NH_2

$C_{36}H_{53}N_{11}O_9$ 783.883

Isol. from the pericardial organs of the crab *Cancer borealis.*

Li, L. *et al., J. Neurochem.*, 2003, **87**, 642-656 (*isol*)

FYANRY amide F-178

[638174-69-3]

Phe-Tyr-Ala-Asn-Arg-Tyr-NH_2

$C_{40}H_{53}N_{11}O_9$ 831.927

Isol. from the pericardial organs of the crab *Cancer borealis.*

Li, L. *et al., J. Neurochem.*, 2003, **87**, 642-656 (*isol*)

FYSQRY amide F-179

[638174-71-7]

Phe-Tyr-Ser-Gln-Arg-Tyr-NH_2

$C_{41}H_{55}N_{11}O_{10}$ 861.953

Isol. from the pericardial organs of the crab *Cancer borealis.*

Li, L. *et al., J. Neurochem.*, 2003, **87**, 642-656 (*isol*)

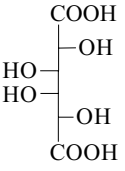
GAF G-1

Glycoprotein. Isol. from the coelemic fluid of *Glycera dibranchiata*. Shows antimicrobial activity. λ_{max} 280 (H_2O) (Berdy).

Chain, B.M. *et al., Biol. Bull. (Woods Hole, Mass.)*, 1983, **164**, 41-49 (*isol*)

Galactaric acid, 9CI, 8CI G-2

1,2,3,4-Tetrahydroxy-1,4-butanedicarboxylic acid. Mucic acid. Tetrahydroxyadipic acid. Galactosaccharic acid
[526-99-8]



$C_6H_{10}O_8$ 210.14

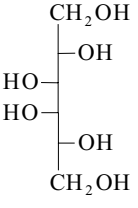
A *meso*-compd., certain derivs. induce asymmetry. For stereoisomers see Glucaric acid, Allaric acid, Mannaric acid, Galactaric acid, G-2 and Idaric acid. Isol. from sporophylls of brown algae, various fruits and fungi. Used as 2% aq. soln. to form colour complexes with Fe, Co, Cr(*III*), Mn, U(*VI*). (pH 3-10). Cryst. Sol. alkalis; spar. sol. H_2O.
Mp 213° Mp 225° Mp 230° dec.

▶ LD_{50} (mus, orl) 8000 mg/kg. LW5180000

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 458B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 524A (*ir*)
Anet, E.F.L.J. *et al., Nature (London)*, 1954, **174**, 930 (*isol*)
Togasawa, Y. *et al., CA*, 1955, **49**, 7064 (*isol*)
Burden, I.J. *et al., J.C.S. Perkin 1*, 1974, 863 (*pmr*)
Jeffrey, G.A. *et al., Carbohydr. Res.*, 1982, **108**, 205 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GAR000

Galactitol G-3

galacto-*Hexitol. Dulcose. Dulcite. Melampyrin. Dulcitol. Euonymit. Melampyrum*
[608-66-2]



$C_6H_{14}O_6$ 182.173
Occurs in various mannas such as *Melampyrum nemorosum*, *Gymnosporia diflexa* and *Maytenus ebenifolia*. Also present in *Evonymus atropurpureus*, in seaweeds and in the pentose fermenting yeast *Torula utilis*. Shows some antitumour effect. Mp 188.5°. Bp_1 275-280°. Log P -4.67 (calc). Opt. inactive, a *meso*-compd.

1,6-Di-Ac: 1,6-Di-O-acetylgalactitol
[20847-03-4]
$C_{10}H_{18}O_8$ 266.247
Mp 168°.

Hexa-Ac: Hexa-O-acetylgalactitol
$C_{18}H_{26}O_{12}$ 434.396
Mp 168-171°.

1,6-Dibenzoyl: 1,6-Di-O-benzoylgalactitol
[58917-44-5]
$C_{20}H_{22}O_8$ 390.389
Mp 206°.

Hexabenzoyl: Hexa-O-benzoylgalactitol
$C_{48}H_{38}O_{12}$ 806.821
Mp 189-191°.

Hexanitrate:
$C_6H_8N_6O_{18}$ 452.159
Mp 94-95°.

1,3:4,6-Dimethylene: 1,3:4,6-Di-O-methylenegalactitol
$C_8H_{14}O_6$ 206.195
Mp 249-250°.

1,3:4,6-Dibenzylidene: 1,3:4,6-Di-O-benzylidenegalactitol
$C_{20}H_{22}O_6$ 358.39
Mp 215-220°.

1,2:4,5-Di-O-isopropylidene: 1,2:4,5-Di-O-isopropylidenegalactitol
[20581-94-6]
$C_{12}H_{22}O_6$ 262.302
Prisms (95% EtOH). Mp 144-145°.

2,3,4,5-Tetra-Me: 2,3,4,5-Tetra-O-methylgalactitol
$C_{10}H_{22}O_6$ 238.28
Solid. Mp 60-62°.

1,6-Ditrityl: 1,6-Di-O-tritylgalactitol
$C_{44}H_{42}O_6$ 666.812
Solid. Mp 183-184°.

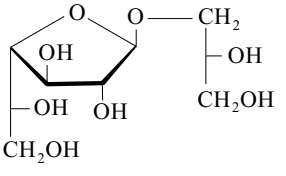
1,6-Ditrityl, 2,3,4,5-tetra-O-Me: 2,3,4,5-Tetra-O-methyl-1,6-di-O-tritylgalactitol
$C_{48}H_{50}O_6$ 722.919
Solid. Mp 180-182°.

[45007-61-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 186D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 290B (*nmr*)
Lespieau, M.R. *et al., Bull. Soc. Chim. Fr.*, 1934, 1374 (*synth*)
Lohmar, R. *et al., Adv. Carbohydr. Chem.*, 1949, **4**, 211 (*rev, derivs*)
Berman, H.M. *et al., Acta Cryst. B*, 1968, **24**, 435 (*cryst struct*)
Petersson, G. *et al., Tetrahedron*, 1969, **25**, 4437 (*ms*)
Bliss, C.A. *et al., Phytochemistry*, 1972, **11**, 1705 (*biosynth*)
Brimacombe, J.S. *et al., The Carbohydrates*, Academic Press, 1972, **1A**, 479 (*rev*)
Voelter, W. *et al., Tetrahedron*, 1973, **29**, 3845 (*conformn, cmr*)
Angyal, S.J. *et al., Carbohydr. Res.*, 1980, **84**, 201 (*cmr*)
Kopf, J. *et al., Carbohydr. Res.*, 1992, **229**, 17 (*cryst struct, hexa-Ac*)
König, B. *et al., Acta Cryst. C*, 1998, **54**, 1471-1473 (*1,2:4,5-disopropylidene, cryst struct*)
Shirota, O. *et al., Nat. Med. (Tokyo)*, 1998, **52**, 184-186; *CA*, **129**, 193564a (*isol, activity*)
Mancera, M. *et al., Carbohydr. Res.*, 2003, **338**, 1115-1119 (*2,3,4,5-tetra-Me, 1,6-ditrityl, 1,6-dirityl tetra-Me*)

1-*O*-β-D-Galactofuranosyl-D-glycerol G-4

(R)-2,3-Dihydroxypropyl β-D-galactofuranoside, 9CI. 1-Glyceryl β-D-galactofuranoside
[20196-73-0]



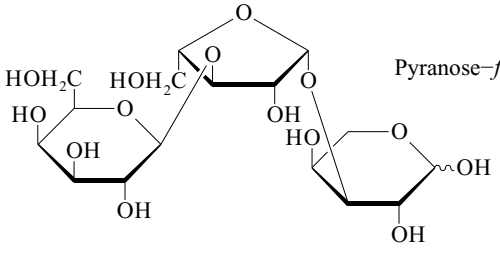
$C_9H_{18}O_8$ 254.236
Constit. of the lipids of *Bacteroides symbiosus*, *Mycoplasma mycoides* and a *Microbacterium* sp. associated with the sponge *Halichondria panicea*. Syrup. $[\alpha]_D$ -78 (c, 1.0 in H_2O).

Hexabenzoyl:
$C_{51}H_{42}O_{14}$ 878.884
Mp 135-136.5°. $[\alpha]_D$ -6.8 (c, 1.0 in $CHCl_3$).

Beving, H.F.G. *et al., Acta Chem. Scand.*, 1967, **21**, 2083-2086 (*synth*)
Plackett, P. *et al., Biochemistry*, 1967, **6**, 2746-2754 (*isol*)
Boren, H. *et al., CA*, 1972, **77**, 102045a (*rev*)
Wicke, C. *et al., J. Nat. Prod.*, 2000, **63**, 621-626 (*diacyl derivs*)

β-D-Galactopyranosyl-(1→3)-β-L-arabinofuranosyl-(1→3)-L-arabinose, 9CI G-5

[52287-02-2]



Pyranose–*form*

$C_{16}H_{28}O_{14}$ 444.389

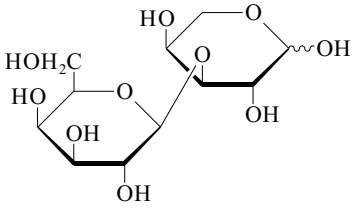
Isol. from the hydrolysate of *Rhizophora mangle* gum.

$[\alpha]_D^{30}$ -60 (c, 0.5 in H_2O).

Sarkar, M. *et al., Indian J. Chem., Sect. B*, 1974, **11**, 1129; 1978, **16**, 369 (*isol*)

3-*O*-β-D-Galactopyranosyl-L-arabinose, 9CI, 8CI G-6

[6055-00-1]



Pyranose–*form*

$C_{11}H_{20}O_{10}$ 312.273

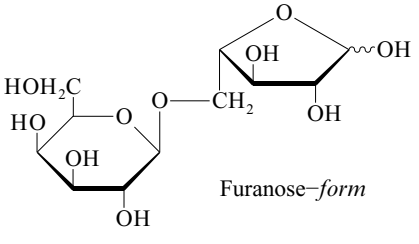
Isol. from partial acid hydrolysates of gum ghatti, *Rhizophora mangle* gum, *Aegle marmelos* gum (bael fruit), *Terminalia tomentosa* gum, *Anogeissus schimperi* gum, *Albizzia zygia* gum, and from the mucilage of *Opuntia ficus-indica* (Indian fig). Cryst. (MeOH/EtOH).

Mp 202-204° (192-194°). $[\alpha]_D$ +62 (in H_2O). $[\alpha]_D$ +57 (c, 0.2 in H_2O).

Aspinall, G.O. *et al., J.C.S.*, 1958, 4408; 1961, 3461 (*isol*)
Drummond, D.W. *et al., J.C.S.*, 1961, 3908
Gorin, P.A.J. *et al., Can. J. Chem.*, 1966, **44**, 2083 (*synth*)
Roy, A. *et al., Carbohydr. Res.*, 1975, **41**, 219
Audichya, T.D. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 601
McGarvie, D. *et al., Carbohydr. Res.*, 1981, **94**, 57 (*isol, struct*)

5-*O*-β-D-Galactopyranosyl-L-arabinose, 9CI G-7

[52287-01-1]



Furanose–*form*

$C_{11}H_{20}O_{10}$ 312.273

Isolated from partial acid hydrolysate of corn-hull hemicellulose and *Rhizophora mangle* gum.

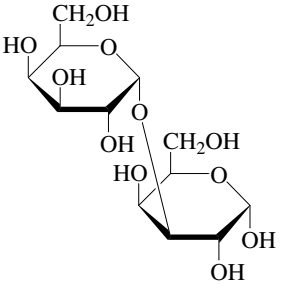
$[\alpha]_D$ -13 (H_2O). $[\alpha]_D^{30}$ -20 (c, 0.5 in H_2O). α- and β- anomers have been characterised as 6-octyl derivs.

[129229-17-0, 131285-16-0, 131285-17-1, 131285-18-2, 131285-19-3]

Srivastava, H.C. *et al., J.A.C.S.*, 1957, **79**, 982 (*isol*)
Goldstein, I.J. *et al., J.A.C.S.*, 1957, **79**, 3558 (*synth*)
Sarkar, M. *et al., Indian J. Chem., Sect. B*, 1973, **11**, 1129 (*isol*)
Cabaret, D. *et al., Can. J. Chem.*, 1990, **68**, 2253 (*synth, pmr*)

3-*O*-α-D-Galactopyranosyl-D-galactose, 9CI, 8CI G-8

[13168-24-6]



α-Pyranose-*form*

$C_{12}H_{22}O_{11}$ 342.299

Isol. from partial acetolysate of λ-carrageenan. Constit. of the products obt. by partial acetolysis of the algae galactans from *Aeodes ulvoidea* and *Pachymenia carnosa*. Constit. of the repeating unit of *Klebsiella* antigens.

$[\alpha]_D$ +184 (c, 1.25 in H_2O). $[\alpha]_D^{26}$ +149 (c, 1.0 in H_2O).

α-Pyranose-*form* [7313-98-6]

Octa-Ac: [56994-14-0]
$C_{28}H_{38}O_{19}$ 678.597
Mp 97-100°. $[\alpha]_D^{23}$ +137 (c, 2.0 in $CHCl_3$).

Me glycoside: Methyl 3-O-α-D-*galactopyranosyl-α-D-galactopyranoside, 9CI*
[104420-77-1]
$C_{13}H_{24}O_{11}$ 356.326
Mp 227-228°. $[\alpha]_D^{21}$ +252 (c, 1.0 in H_2O).

4-Nitrophenyl glycoside: [110891-71-9]
Cryst + $^1/_2H_2O$. Mp 217°. $[\alpha]_D^{21}$ +298 (c, 0.3 in MeOH aq.).

β-Pyranose-*form* [72597-57-0]

Octa-Ac: Mp 155-156°. $[\alpha]_D^{25}$ +110.8 (c, 0.71 in $CHCl_3$).

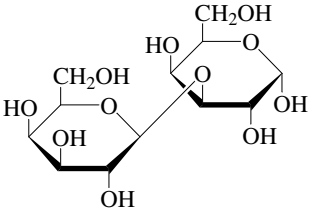
Me glycoside: Methyl 3-O-α-D-*galactopyranosyl-β-D-galactopyranoside, 9CI*
[18449-79-1]
$C_{13}H_{24}O_{11}$ 356.326
Mp 199°. $[\alpha]_D^{21}$ +142 (c, 0.5 in H_2O).

Me glycoside, heptabenzoyl:
$C_{62}H_{52}O_{18}$ 1085.082
$[\alpha]_D$ +131.9 (c, 0.9 in $CHCl_3$).

Morgan, K. *et al., Can. J. Chem.*, 1959, **37**, 1201
Farrant, A.J. *et al., Carbohydr. Res.*, 1972, **25**, 283; 1971, **19**, 161 (*occur*)
Alsobrook, A.J.R. *et al., Carbohydr. Res.*, 1975, **40**, 337 (*acetolysis*)
Chacon-Fuertes, M. *et al., Carbohydr. Res.*, 1975, **43**, 51 (*synth*)
Kenne, L. *et al., The Polysaccharides*, Acad. Press, London and New York (Ed. Aspinall, G.O.), 1983, **2**, 307; 323 (*occur*)
Nilsson, K.G.I. *et al., Carbohydr. Res.*, 1987, **167**, 95 (*Me gly*)
Takeo, K. *et al., J. Carbohydr. Chem.*, 1988, **7**, 309-316 (*synth*)
Stortz, C.A. *et al., J. Carbohydr. Chem.*, 1994, **13**, 235-247 (*conformn*)
Sakamoto, I. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1974-1977 (*synth*)

3-*O*-β-D-Galactopyranosyl-D-galactose, 9CI, 8CI G-9

[5188-48-7]



α-Pyranose-*form*

$C_{12}H_{22}O_{11}$ 342.299

Constit. of the hydrolysate of cashew nut shells and gums of an *Acacia* spp. (gum arabic) and *Rhizophora mangle*. Isol. from chondromucoprotein of bovine nasal septum.

Mp 225° (198-200°, 159-170°). $[\alpha]_D^{18}$ +50 (c, 0.2 in H_2O). $[\alpha]_D^{26}$ +71 → +62 (c, 1.0 in H_2O).

α-Pyranose-*form*

Octa-Ac:

$C_{28}H_{38}O_{19}$ 678.597

Cryst. (EtOAc). Mp 189-190°. $[\alpha]_D^{22}$ +53.8 (c, 0.4 in $CHCl_3$). β-Anomer also obt., probably noncryst.

β-Pyranose-*form*

Me glycoside: [81131-46-6]

$C_{13}H_{24}O_{11}$ 356.326

Mp 203-204°. $[\alpha]_D^{21}$ +25 (c, 0.9 in H_2O).

Me glycoside, hepta-Ac: [102854-37-5]

$C_{27}H_{38}O_{18}$ 650.586

Mp 189.5-190°. $[\alpha]_D$ -7.7 (c, 0.8 in $CHCl_3$).

Me glycoside, heptabenzoyl: [98056-61-2]

$C_{62}H_{52}O_{18}$ 1085.082

$[\alpha]_D$ +91 (c, 1.5 in $CHCl_3$).

2-Propenyl glycoside: [120094-96-4]

$C_{15}H_{26}O_{11}$ 382.364

Mp 213-215°. $[\alpha]_D^{21}$ +11 (c, 1.2 in H_2O).

Benzyl glycoside: [84553-71-9]

$C_{19}H_{28}O_{11}$ 432.424

Cryst. (MeOH). Mp 162-163°. $[\alpha]_D^{25}$ -4.2 (c, 1.8 in H_2O).

*Benzyl glycoside, 4,6-*O*-benzylidene:* [84553-70-8]

$C_{26}H_{32}O_{11}$ 520.532

Mp 263-264°. $[\alpha]_D^{25}$ +57 (c, 1.4 in DMF).

*Benzyl glycoside, 4,6-*O*-benzylidene, penta-Ac:* [84558-11-2]

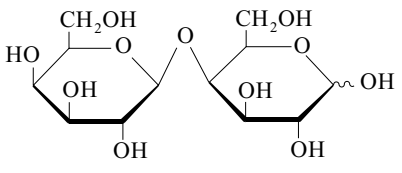
$C_{36}H_{42}O_{16}$ 730.718

Cryst. (Et_2O/petrol). Mp 114-116°. $[\alpha]_D^{26}$ -13.4 (c, 1.5 in $CHCl_3$).

Hirst, E.L. *et al., J.C.S.*, 1954, 2622 (*isol*)
Rodén, L. *et al., J. Biol. Chem.*, 1966, **241**, 5949 (*isol*)
Aspinall, G.O. *et al., Carbohydr. Res.*, 1968, **7**, 421 (*isol*)
Sarkar, M. *et al., Indian J. Chem.*, 1974, **11**, 1129 (*isol*)
Chacón-Fuertes, M.E. *et al., Carbohydr. Res.*, 1975, **43**, 51 (*synth*)
Takeo, K. *et al., Carbohydr. Res.*, 1983, **112**, 158 (*benzyl gly*)
Nilsson, K.G.I. *et al., Carbohydr. Res.*, 1987, **167**, 95; 1988, **180**, 53 (*glycosides*)
Ziegler, T. *et al., J. Carbohydr. Chem.*, 1990, **9**, 135 (*Me gly*)
Wang, L.X. *et al., J. Carbohydr. Chem.*, 1991, **10**, 349-361 (*octa-Ac*)

4-*O*-β-D-Galactopyranosyl-D-galactose, 9CI, 8CI G-10

[6206-28-6]



$C_{12}H_{22}O_{11}$ 342.299

Obt. by hydrol. of galactan from white birch wood (*Betula papyrifera*), white lupin seeds (*Lupinus albus*), aeodan (*Aeodes orbitosa*), flowers of *Bombax malabaricum* and of soya beans (*Glycine max*).

Mp 204°. $[\alpha]_D^{20}$ +68 (c, 1.0 in H_2O).

α-Pyranose-*form*

Octa-Ac:

$C_{28}H_{38}O_{19}$ 678.597

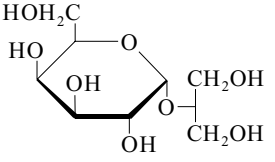
Mp 189-190°. $[\alpha]_D^{25}$ +54 (c, 1.8 in $CHCl_3$).

Curtis, E.J.C. *et al., Can. J. Chem.*, 1965, **43**, 2508 (*synth*)
Agrawal, G.D. *et al., Planta Med.*, 1972, **21**, 293; *CA*, **77**, 48734j (*isol*)
Chacon-Fuertes, M.E. *et al., Carbohydr. Res.*, 1975, **43**, 51 (*synth*)

2-*O*-α-D-Galactopyranosylglycerol G-11

2-Hydroxy-1-(hydroxymethyl)ethyl α-D-galactopyranoside, 9CI. 2-Glyceryl α-D-galactopyranoside. ***Floridoside***

[534-68-9]



$C_9H_{18}O_8$ 254.236

Constit. of many red algae such as *Plocamium cartilagineum*, *Laurencia pinnatifida*, *Iridaea laminaroides*; and the hydrolysate from *Bacillus coagulans* cell walls. The main reserve carbohydrate in most red algae. Prob. intracellular osmotic regulator.

Mp 128.5° Mp 86-87° (monohydrate). $[\alpha]_D$ +165 (c, 3.35 in H_2O).

Hexa-Ac: [3879-82-1]

$C_{21}H_{30}O_{14}$ 506.46

Constit. of *Ruellia brittoniana*.

Mp 101°. $[\alpha]_D$ +114 (c, 3.0 in Me_2CO).

Hexa-Me:

$C_{15}H_{30}O_8$ 338.397

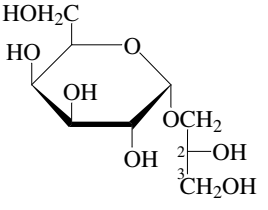
Syrup. $[\alpha]_D$ +156 (c, 2.86 in H_2O).

Putman, E.W. *et al., J.A.C.S.*, 1954, **76**, 2221-2223 (*isol, struct*)
Lindberg, B. *et al., Acta Chem. Scand.*, 1955, **9**, 1097; 1323 (*isol*)
Aplin, R.T. *et al., J.C.S.(C)*, 1967, 1346-1347 (*isol, pmr, ms*)
London, R.E. *et al., J.A.C.S.*, 1975, **97**, 3565-3573 (*cmr*)
Impellizzeri, G. *et al., Phytochemistry*, 1975, **14**, 1549-1557 (*isol*)
Meng, J. *et al., Carbohydr. Res.*, 1987, **161**, 171 (*pmr, cmr, ms, glc*)
Ahmad, V.U. *et al., J. Nat. Prod.*, 1990, **53**, 960-963 (*isol, hexa-Ac, pmr, cmr, cryst struct*)
Abreu, P.M. *et al., Phytochemistry*, 1997, **45**, 1601-1603 (*isol, pmr, cmr*)
Simon-Colin, C. *et al., Carbohydr. Res.*, 2002, **337**, 279-280; 2003, **338**, 2413-2416 (*purifn, pmr, cmr, cryst struct*)

1-*O*-Galactopyranosylglycerol G-12

2,3-Dihydroxypropyl galactopyranoside, 9CI. Glyceryl galactopyranoside

[7420-23-7]



α-D-(2*R*)-*form*

$C_9H_{18}O_8$ 254.236

α-D-(2*R*)-*form*

Isofloridoside

[23202-76-8]

Constit. of various marine red algae.

Cryst. (EtOH/MeOH).

Mp 150-152°. $[\alpha]_D^{20}$ +158 (c, 1.8 in H_2O).

β-D-(2*R*)-*form* [16232-91-0]
Isol. from wheat flour lipids and the brown alga *Sargassum thunbergii*. Cryst. (MeOH). Mp 140.5-141.5°. $[\alpha]_D^{15}$ -9 (c, 0.6 in H_2O).

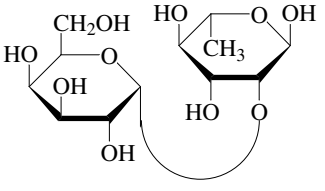
α-D-(2*S*)-*form* [38841-15-5]
Constit. of a red alga *Porphyra* sp. Cryst. Mp 104-107°. $[\alpha]_D^{20}$ + 2 (c, 2 in H_2O).

[42869-31-8]

Carter, H.E. *et al., J.A.C.S.*, 1956, **78**, 3735-3738 (*β-D-2R-form, isol*)
Wickberg, B. *et al., Acta Chem. Scand.*, 1958, **12**, 1187-1201 (*β-D-2R-form, β-D-2S-form, synth, ir*)
Silhavy, T.J. *et al., J. Biol. Chem.*, 1973, **248**, 6571-6574 (*synth*)
Gent, P.A. *et al., J.C.S. Perkin 1*, 1975, 364-370 (*synth*)
Impellizzeri, G. *et al., Phytochemistry*, 1975, **14**, 1549-1557 (*isol*)
Beier, R.C. *et al., Can. J. Chem.*, 1980, **58**, 2800-2804 (*cmr*)
Beier, R.C. *et al., Carbohydr. Res.*, 1981, **93**, 141-143 (*synth*)
Boos, W. *et al., Methods Enzymol.*, 1982, **89D**, 59-64 (*synth*)
Michelsen, P. *et al., Chem. Scr.*, 1985, **25**, 217-218 (*ord, cd*)
Meng, J. *et al., Carbohydr. Res.*, 1987, **161**, 171-180 (*isol, pmr, cmr, abs config, bibl*)
Son, B.W. *et al., Bull. Korean Chem. Soc.*, 1992, **13**, 584-586 (*β-D-2R-form, isol*)

2-*O*-α-D-Galactopyranosyl-L-rhamnose G-13

[67508-21-8]

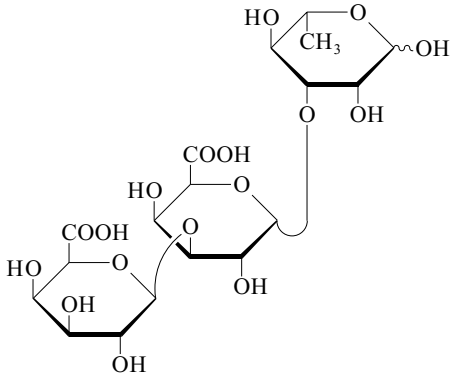


α-Pyranose-*form*

$C_{12}H_{22}O_{10}$ 326.3
Reducing disaccharide. Isol. from the gum of *Rhizophora* sp. Constit. of the repeating unit of the O-antigen from *Pseudomonas cepacia* (strain IMV 598/2). $[\alpha]_D^{30}$ +105 (+94) (H_2O).

α-Pyranose-*form* [94061-76-4]
Benzyl glycoside, 3,4-dibenzoyl, tetrabenzyl: [105285-87-8]
$C_{61}H_{60}O_{12}$ 985.138
$[\alpha]_D$ +54 (c, 0.5 in $CHCl_3$).
Sarkar, M. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 369 (*isol*)
Lipkind, G.M. *et al., Bioorg. Khim.*, 1984, **10**, 1670; *Sov. J. Bioorg. Chem. (Engl. Transl.)*, 1984, **10**, 912 (*conformn, pmr*)
Norberg, T. *et al., Carbohydr. Res.*, 1986, **152**, 301 (*synth*)

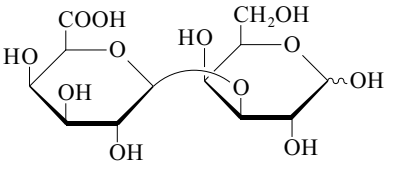
β-D-Galactopyranuronosyl-(1→3)-β-D-galactopyranuronosyl-(1→3)-L-rhamnose G-14



$C_{18}H_{28}O_{17}$ 516.409
Isol. from the hydrolysate of the gum of *Rhizophora mangle*. $[\alpha]_D^{30}$ +120 (c, 0.1 in H_2O).
Sarkar, M. *et al., Indian J. Chem.*, 1973, **11**, 1129 (*isol*)

3-*O*-β-D-Galactopyranuronosyl-D-galactose, 9CI G-15

[7268-75-9]

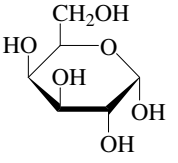


Pyranose–*form*

$C_{12}H_{20}O_{12}$ 356.283
Isol. from the partial acid hydrolysate of *Rhizophora mangle* gum and from *Spondias dulcis* (ambarella) gum (Anacardiaceae). $[\alpha]_D$ +56.2 (H_2O).
Parikh, V.M. *et al., Can. J. Chem.*, 1966, **44**, 327
Sarkar, M. *et al., Indian J. Chem.*, 1974, **11**, 1129 (*isol*)
Roy, A. *et al., Carbohydr. Res.*, 1975, **41**, 219
Basu, S. *et al., Carbohydr. Res.*, 1981, **94**, 215 (*isol*)

Galactose, 9CI, 8CI, USAN G-16

Cerebrose
[26566-61-0]



α-D-Pyranose-*form*

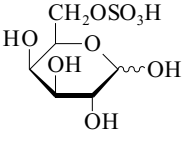
$C_6H_{12}O_6$ 180.157
An aq. soln. at 31° contains 30% α-pyr, 64% β-pyr, 2.5% α-fur, 3.5% β-fur and 0.02% aldehyde. Active ingredient of Levovist™, used in echo-enhancement in sonographic Doppler-B-mode imaging. Ultrasound contrast medium.

L-*form* [15572-79-9]
Occurs in agar-agar, chagual gum, red algae, flaxseed mucilage and a snail galactan. The L-galactose obt. from the hydrolysates of these polysaccharides can be freed from the enantiomer present by fermentation of the D-form. Mp 163-165°. $[\alpha]_D^{22}$ -78 (H_2O).

[4198-47-4, 41846-88-2, 41846-89-3, 42789-83-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 192A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 298B; 298C (*nmr*)
Methods Carbohydr. Chem., 1962, **1**, 120; 122; 127 (*D-form, L-form*)
Araki, C. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 122 (*synth, L-form*)
Frush, H.L. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 127 (*synth, L-form*)
Stothers, J.B. *et al., Carbon-13 NMR Spectroscopy*, Academic Press, 1972,
Schaffer, R. *et al., The Carbohydrates*, 1972, **1A**, 69 (*occur*)
Dmietriev, B.A. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1975, 142
Ko, S.Y. *et al., Science (Washington, D.C.)*, 1983, **220**, 949 (*total synth, L-form*)
Sturgeon, R.J. *et al., Carbohydr. Res.*, 1990, **200**, 499 (*occur, enantiomers*)
Vogt, D.C. *et al., Carbohydr. Res.*, 1990, **206**, 333 (*pmr, cmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 774
Binch, H. *et al., Carbohydr. Res.*, 1998, **306**, 409-419 (*synth, L-form*)
Kroger, K. *et al., Eur. J. Ultrasound*, 1998, **8**, 17-24 (*use*)
Takeuchi, M. *et al., Synthesis*, 1999, 341-354 (*L-form, synth*)

Galactose 6-sulfate G-17



$C_6H_{12}O_9S$ 260.221
The L-enantiomer is a component of the polysaccharides of *Porphyra umbilicalis*.

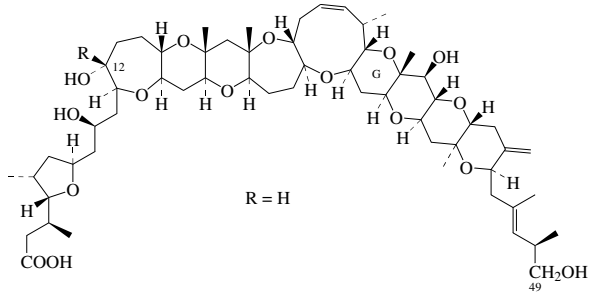
Peat, S. *et al., J.C.S.*, 1960, 4761 (*synth*)
Turvey, J.R. *et al., Nature (London)*, 1961, **189**, 831 (*isol*)
Archbald, P.J. *et al., Carbohydr. Res.*, 1981, **93**, 177 (*cmr*)

Galactose-6-sulfurylase G-18

E.C. 2.5.1.5. D-*Galactose-6-sulfate:alkyltransferase (cyclising)*. *Porphyran sulfatase*
[9030-36-8]
Enzyme. Isol. from *Porphyra umbilicalis*. Catalyses the elimination of sulfate from the D-galactose 6-sulfate residues of porphyran to prod. 3,6-anhydrogalactose residues.
Rees, D.A. *et al., Biochem. J.*, 1961, **80**, 449-453; **81**, 347-352

Gambieric acid A G-19

[138434-64-7]



Absolute Configuration

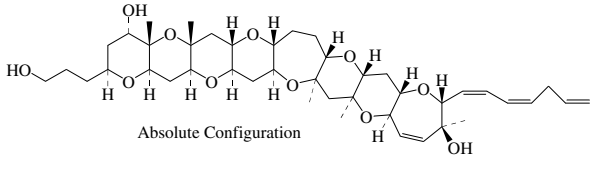
$C_{59}H_{92}O_{16}$ 1057.366
Polyether antibiotic. Isol. from dinoflagellate *Gambierdiscus toxicus*. Antifungal agent, allelopathic, growth enhancer. Amorph. $[\alpha]_D^{20}$ +33 (c, 0.49 in MeOH).
▶ LU5247400
O^{49}-*(4-Carboxy-3*S*-methylbutanoyl)*: ***Gambieric acid C***
[138458-89-6]
$C_{65}H_{100}O_{19}$ 1185.494
From *Gambierdiscus toxicus*. Antifungal agent. Obt. as a mixt. with Gambieric acid D.
Nagai, H. *et al., J.O.C.*, 1992, **57**, 5448 (*isol, pmr, cmr, struct*)
Morohashi, A. *et al., Tetrahedron*, 2000, **56**, 8995-9001 (*abs config*)

Gambieric acid B G-20

[141363-65-7]
As Gambieric acid A, G-19 with
R = CH_3
$C_{60}H_{94}O_{16}$ 1071.393
Polyether antibiotic. Isol. from *Gambierdiscus toxicus*. Antifungal agent. Phycotoxin. Growth enhancer. Amorph.
▶ LU5247000
O^{50}-*(4-Carboxy-3*S*-methylbutanoyl)*: ***Gambieric acid D***
[141363-66-8]
$C_{66}H_{102}O_{19}$ 1199.52
From *Gambierdiscus toxicus*. Antifungal agent. Growth enhancer. Obt. as a mixt. with Gambieric acid C.
Nagai, H. *et al., J.O.C.*, 1992, **57**, 5448 (*isol, pmr, cmr, struct*)
Morohashi, A. *et al., Tetrahedron*, 2000, **56**, 8995-9001 (*abs config*)

Gambierol G-21

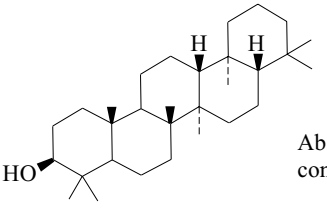
[146763-62-4]



Absolute Configuration

$C_{43}H_{64}O_{11}$ 756.972
Isol. from the marine dinoflagellate *Gambierdiscus toxicus*. Phycotoxin. Amorph. solid. Sol. MeOH, Py, CH_2Cl_2; poorly sol. H_2O. λ_{max} 237 (ϵ 15800) (MeOH) (Derep).
▶ LD_{50} (mus, ipr) .05 mg/kg.
Satake, M. *et al., J.A.C.S.*, 1993, **115**, 361 (*isol, pmr, cmr, struct*)
Morohashi, A. *et al., Tet. Lett.*, 1999, **40**, 97-100 (*abs config*)
Fuwa, H. *et al., Org. Lett.*, 2002, **4**, 2981-2984 (*synth*)
Kadota, I. *et al., J.A.C.S.*, 2003, **125**, 11893-11899 (*synth*)
Johnson, H.W.B. *et al., Chem. Eur. J.*, 2006, **12**, 1736-1746; 1747-1753 (*synth*)

3-Gammaceranol G-22



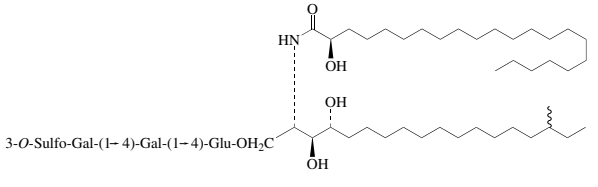
Absolute configuration

$C_{30}H_{52}O$ 428.74

3β-*form*
Tetrahymanol. *Wallichiniol*
[2130-17-8]
Constit. of *Tetrahymena pyriformis*, *Adiantum* spp. and other ferns. Also isol. from marine sediments.
Cryst. (MeOH).
Mp 312.5-314.5° (291-292°). $[\alpha]_D$ +12 ($CHCl_3$).
Ac:
$C_{32}H_{54}O_2$ 470.777
Isol. from *Oleandra wallichii*. Cryst.
Mp 315-320° (298-301°). $[\alpha]_D$ +43.
Mallory, F.B. *et al., J.A.C.S.*, 1963, **85**, 1362 (*isol*)
Tsuda, Y. *et al., Tet. Lett.*, 1965, 1427 (*struct, synth*)
Pandey, G.N. *et al., Phytochemistry*, 1969, **8**, 327 (*isol, acetate*)
v. Tamelen, E.E. *et al., J.A.C.S.*, 1972, **94**, 8228 (*synth*)
Aberhart, D.J. *et al., J.A.C.S.*, 1979, **101**, 1013 (*biosynth*)
Benson, M. *et al., J. Nat. Prod.*, 1983, **46**, 274 (*pmr*)
Ten Haven, H.L. *et al., Geochim. Cosmochim. Acta*, 1989, **53**, 3073-3079 (*marine sedinet constit*)
Shiojima, K. *et al., Tet. Lett.*, 1989, **30**, 4977 (*pmr, cmr*)

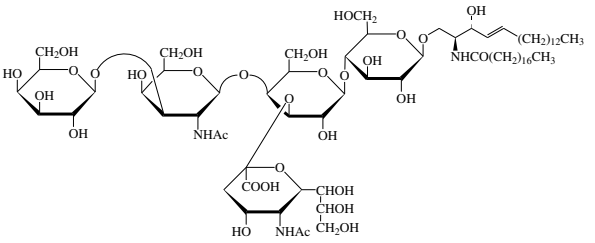
Luidia maculata Ganglioside 1 G-23

LMG 1
[195434-92-5]



$C_{59}H_{113}NO_{23}S$ 1236.601
Isol. from the starfish *Luidia maculata*. Exhibits neuritogenic activity. Amorph. powder.
Kawatake, S. *et al., Liebigs Ann./Recl.*, 1997, 1797-1800 (*isol, pmr, cmr*)

Gangliosides G-24



A large class of glycosphingolipids composed of hexoses, Sphingosine, fatty acids and sialic acids. The differences between the gangliosides are mainly in the carbohydrate moieties. Four major gangliosides referred to as GM_1 (illus.), DD_{1a}, GD_{1b}, GT_{1b}. Found in the CNS and widely distributed in other tissues. Gangliosides are the main cause of cell surface negative charge. They are also thought to be involved in many different cell functions e.g. metabolism, growth and malignant transformation. A monoganglioside prepn. has been used in the treatment of cerebrovascular disorders.

Ganglioside GM_1

Ganglioside G_1. Siagoside. Sygen

[37758-47-7]

$C_{73}H_{131}N_3O_{31}$ 1546.839

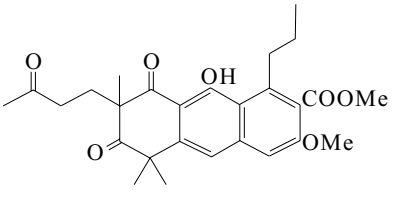
Isol. from bovine brain. Constit. of mammalian vertebrate cell membranes. Particularly abundant in the central and peripheral nervous systems. Used in the treatment of peripheral neuropathies, cerebrovascular disorders and spinal cord injury. Positive effects still need to be confirmed. Now used in the treatment of Parkinson's disease.

[19553-76-5, 19600-01-2, 54827-14-4, 59247-13-1, 62010-37-1, 69345-49-9, 71012-19-6, 85305-87-9, 85305-88-0, 89678-50-2]

Kuhn, R. *et al., Chem. Ber.*, 1963, **96**, 866-880 (*isol, struct*)
Klenk, E. *et al., Prog. Chem. Fats Other Lipids*, 1970, **10**, 411
Gigg, R.H. *et al., Rodd's Chem. Carbon Compd. (3rd edn.)*, 1976, **1E**, 394
Sillerud, L.O. *et al., Carbohydr. Res.*, 1983, **113**, 173-188 (*cmr*)
Fishman, P.H. *et al., Chem. Phys. Lipids*, 1986, **42**, 137-151 (*rev, props*)
Sonnino, S. *et al., Adv. Exp. Med. Biol.*, 1988, **228**, 437 (*rev*)
Jack, D.B. *et al., J. Clin. Pharm. Ther.*, 1990, **15**, 233 (*rev*)
Skaper, S.D. *et al., Adv. Exp. Med. Biol.*, 1991, **296**, 257-266 (*rev*)
Rost, K.L. *et al., Clin. Pharmacol. Ther. (St. Louis)*, 1991, **50**, 141-149 (*pharmacokinet*)
Rodden, F.A. *et al., J. Neurosurg.*, 1991, **74**, 606 (*rev*)
Sandhoff, K. *et al., Adv. Lipid Res.*, 1993, **26**, 119 (*rev, metab, biosynth*)
Hasegawa, A. *et al., J. Carbohydr. Chem.*, 1993, **12**, 703-718 (*synth, GM1*)
Walker, J.B. *et al., Neurosci. Lett.*, 1993, **161**, 174-178 (*bibl*)
Nobile-Orazio, E. *et al., Drugs*, 1994, **47**, 576-585 (*rev, struct, pharmacol, tox*)
Schneider, J.S. *et al., Neurology*, 1995, **45**, 1149-1154 (*anti-Parkinsonian pilot study*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1708
Ishida, H. *et al., J. Carbohydr. Chem.*, 1997, **16**, 413-428 (*synth*)
Duclos, R.I. *et al., Carbohydr. Res.*, 2000, **328**, 489-507 (*synth, GM3*)
Bhattacharya, S.K. *et al., J.O.C.*, 2000, **65**, 144-151 (*synth, GM1*)
Ito, H. *et al., J. Carbohydr. Chem.*, 2001, **20**, 207-225 (*synth*)

Garvalone A G-25

[109872-45-9]



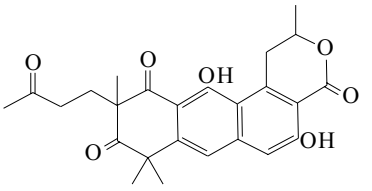
$C_{27}H_{32}O_7$ 468.546

Constit. of *Garveia annulata*. Pale-yellow oil.

Fahy, E. *et al., Can. J. Chem.*, 1987, **65**, 376

Garvalone B G-26

[109894-26-0]



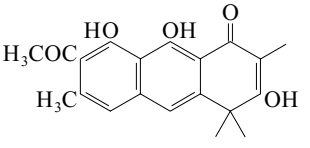
$C_{25}H_{26}O_7$ 438.476

Mol. formula given in the paper as $C_{26}H_{28}O_6$, apparently incorrectly. Constit. of *Garveia annulata*. Light-yellow oil. $[\alpha]_D$ +136.9 (c, 0.39 in $CHCl_3$).

Fahy, E. *et al., Can. J. Chem.*, 1987, **65**, 376

Garveatin A G-27

[95388-04-8]



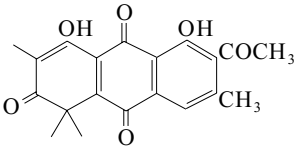
$C_{20}H_{20}O_5$ 340.375

Constit. of *Garveia annulata*. Orange needles (Me_2CO). Sol. MeOH, EtOAc; poorly sol. H_2O, hexane.

Mp 236-240°. λ_{max} 232 (ϵ 16000); 282 (ϵ 8500); 323 (sh) (ϵ 3900); 432 (ϵ 3800) (MeOH) (Derep).

Fahy, E. *et al., J.O.C.*, 1985, **50**, 1149

Garveatin A quinone G-28



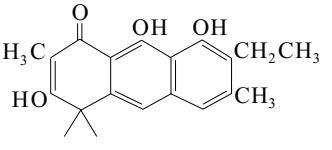
$C_{20}H_{18}O_6$ 354.359

Constit. of *Garveia annulata*. Red oil. Some confusion over *CA* number. λ_{max} 216; 276; 384 (MeOH) (Berdy).

Fahy, E. *et al., Can. J. Chem.*, 1987, **65**, 376

Garveatin B G-29

[99457-96-2]



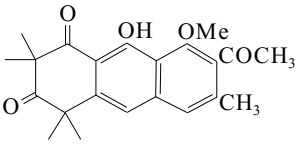
$C_{20}H_{22}O_4$ 326.391

Metab. of *Garveia annulata*. Yellow oil. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 240 (ϵ 16000); 260 (ϵ 9000); 317 (ϵ 3900); 417 (ϵ 3800) (MeOH) (Derep).

Fahy, E. *et al., J.O.C.*, 1986, **51**, 57

Garveatin C G-30

[99475-52-2]

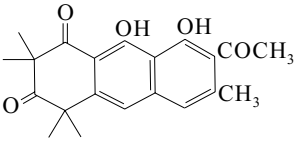


$C_{22}H_{24}O_5$ 368.429
Metab. of *Garveia annulata*. Orange cryst. (hexane). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 125°. λ_{max} 228 (ϵ 13700); 274 (ϵ 19700); 305 (sh) (ϵ 3300); 389 (ϵ 4400) (MeOH) (Derep).

Fahy, E. *et al., J.O.C.*, 1986, **51**, 57

Garveatin D G-31

[109872-42-6]

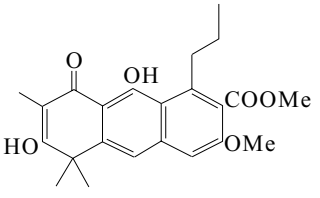


$C_{21}H_{22}O_5$ 354.402
Mol. formula given in the paper as $C_{21}H_{20}O_5$, apparently incorrectly. Constit. of *Garveia annulata*. Yellow oil.

Fahy, E. *et al., Can. J. Chem.*, 1987, **65**, 376

Garvin A G-32

[109872-44-8]

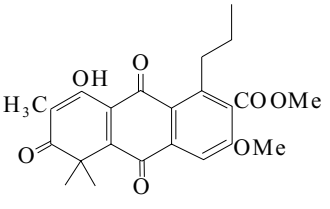


$C_{23}H_{26}O_6$ 398.455
Constit. of *Garveia annulata*. Yellow solid.

Fahy, E. *et al., Can. J. Chem.*, 1987, **65**, 376

Garvin A quinone G-33

[99457-98-4]

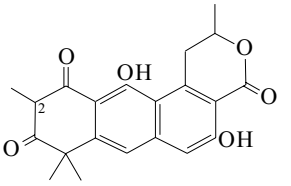


$C_{23}H_{24}O_7$ 412.438
Metab. of *Garveia annulata*. Orange-red amorph. solid. Called Garveatin A quinone in index guide but *CA* gives this struct. λ_{max} 216 (ϵ); 276 (ϵ); 384 (ϵ) (MeOH) (Derep).

Fahy, E. *et al., J.O.C.*, 1986, **51**, 57

Garvin B G-34

[109872-43-7]



$C_{21}H_{20}O_6$ 368.385
Enolised β-diketone. Constit. of *Garveia annulata*. Yellow solid.
2-Hydroxy: ***2-Hydroxygarvin B***
$C_{21}H_{20}O_7$ 384.385
Constit. of *Garveia annulata*. Yellow solid.

Fahy, E. *et al., Can. J. Chem.*, 1987, **65**, 376

Nephrops Gastric peptide G-35

SEGGQDFWL
[138538-52-0]
Ser-Glu-Gly-Gly-Gln-Asp-Phe-Trp-Leu
$C_{47}H_{63}N_{11}O_{16}$ 1038.079
Isol. from the stomach of the marine crustacean *Nephrops norvegicus*. Gastin/cholecystokinin-like peptide.

Favrel, P. *et al., Biochimie*, 1991, **73**, 1233-1239 (*isol*)

Oncorhynchus mykiss Gastrin-releasing peptide G-36

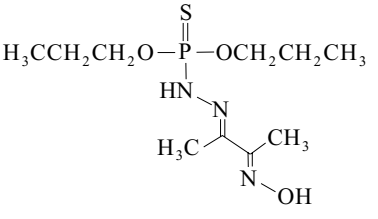
[145523-58-6]

$C_{110}H_{169}N_{35}O_{29}S$ 2477.828
Isol. from the stomach of the rainbow trout *Oncorhynchus mykiss*.

Jensen, J. *et al., Peptides (N.Y.)*, 1992, **13**, 995-999 (*isol*)

GB4 Toxin G-37

2-(1-Methyl-2-oxopropylidene)phosphorohydrazidothioate oxime
[82638-81-1]

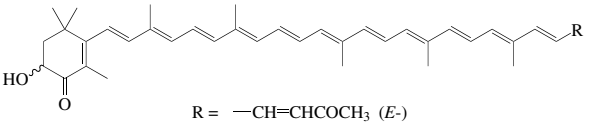


$C_{10}H_{22}N_3O_3PS$ 295.342
Isol. from the Florida red tide dinoflagellate *Gymnodinium breve (Ptychodiscus brevis)*. Ichthyotoxin. Needles (C_6H_6).
Mp 82-83°. λ_{max} 230 (solvent not reported) (Derep).

Alam, M. *et al., J.A.C.S.*, 1982, **104**, 5232 (*isol, cryst struct, ms, ir, pmr*)

Gelliodenone G-38

[111536-18-6]



$C_{40}H_{50}O_3$ 578.833
Isol. from the sponge *Gelliodes callista*. Poss. artifact derived from Gelliodesxanthin, G-39.

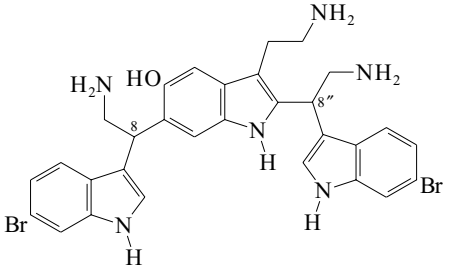
Tanaka, Y. *et al., CA*, 1987, **107**, 233403b (*isol, struct*)

Gelliodesxanthin G-39

3′,4′-Didehydro-3-hydroxy-4-oxo-2′-apo-β,ψ-carotenal, 9CI
[111536-19-7]
As Gelliodenone, G-38 with
R = –CHO
$C_{37}H_{46}O_3$ 538.769
Isol. from the sponge *Gelliodes callista*. Dark red cryst.
Mp 193-194° (161-165°). λ_{max} 467; 495; 527 (no solvent reported).

Tanaka, Y. *et al., CA*, 1987, **107**, 233403b (*isol, struct*)
Bernhard, K. *et al., Pure Appl. Chem.*, 1991, **63**, 35-44 (*synth*)

Gelliusine A G-40



$C_{30}H_{30}Br_2N_6O$ 650.415

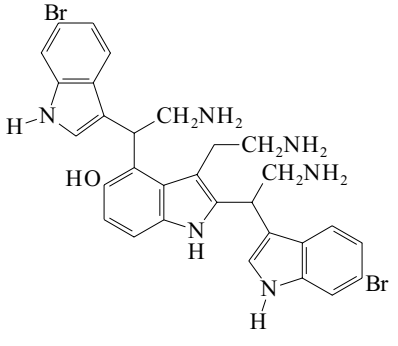
(±)-*form* [159903-67-0]
Alkaloid from a deep water New Caledonian marine sponge (*Gellius* or *Orina* sp.). Serotonin receptor agonist. λ_{max} 226 (ϵ 52000); 285 (ϵ 15000) (MeOH) (Berdy).

Diastereoisomer: ***Gelliusine B***
[159992-42-4]
$C_{30}H_{30}Br_2N_6O$ 650.415
From a deep water New Caledonian marine sponge (*Gellius* or *Orina* sp.). Serotonin receptor agonist. Racemate with different rel. configs. at C-8 and C-8″ from (±)-Gelliusine A. λ_{max} 226 (ϵ 52000); 285 (ϵ 15000) (MeOH) (Berdy).

Bifulco, G. *et al., J. Nat. Prod.*, 1994, **57**, 1294 (*isol, uv, pmr, cmr, struct*)

Gelliusine C G-41

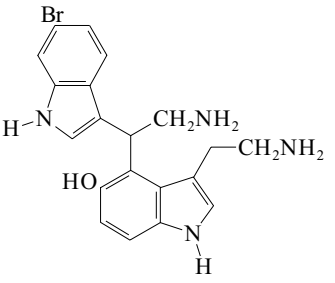
[171090-79-2]



$C_{30}H_{30}Br_2N_6O$ 650.415
Alkaloid from the deep-water New Caledonian marine sponge *Orina* sp. and from *Gellius* sp. Shows antiserotonin activity. Racemic. λ_{max} 230 (ϵ 35234); 284 (ϵ 13272) (MeOH) (Berdy).

Bifulco, G. *et al., J. Nat. Prod.*, 1995, **58**, 1254 (*isol, uv, pmr, cmr, struct*)

Gelliusine D G-42

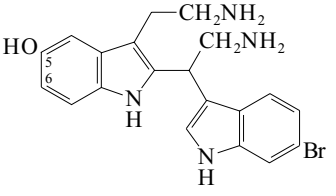


$C_{20}H_{21}BrN_4O$ 413.316

(±)-*form* [171090-80-5]
Alkaloid from the deep-water New Caledonian marine sponge *Orina* sp. and from *Gellius* sp. Shows antiserotonin activity. λ_{max} 230 (E1%/1cm 284) (MeOH) (Berdy).

Bifulco, G. *et al., J. Nat. Prod.*, 1995, **58**, 1254-1260 (*isol, pmr, cmr, struct*)

Gelliusine E G-43



$C_{20}H_{21}BrN_4O$ 413.316

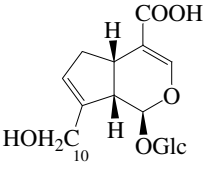
(±)-*form* [171090-81-6]
Alkaloid from the deep-water New Caledonian marine sponge *Orina* sp. and *Gellius* sp. Shows antiserotonin activity. Neuropeptide Y receptor binding agent. λ_{max} 230; 284 (MeOH) (Berdy).

5-Deoxy, 6-bromo: ***Gelliusine F***
[171090-82-7]
$C_{20}H_{20}Br_2N_4$ 476.213
From *Orina* sp. and *Gellius* sp. Antiserotonin agent, neuropeptide Y binding agent. λ_{max} 230; 284 (MeOH) (Berdy).

Bifulco, G. *et al., J. Nat. Prod.*, 1995, **58**, 1254-1260 (*isol, pmr, cmr, struct*)

Geniposidic acid G-44

Premnosidic acid
[27741-01-1]



$C_{16}H_{22}O_{10}$ 374.344
Constit. of *Genipa americana* (genipap) and *Premna barbata*.
$[\alpha]_D^{24}$ +19.3 (c, 1 in MeOH). Struct. of Premnosidic acid incorr. in ref.

*10-(5-Phenyl-2*E*,4*E*-pentadienoyl), Me ester:* ***10-(5-Phenyl-2,4-pentadienoyl)geniposide***
[97868-32-1]
$C_{28}H_{32}O_{11}$ 544.554
Constit. of *Avicennia marina*. λ_{max} 308 (log ϵ 4.47) (MeOH) (Me ester).

10-O-E-*Cinnamoyl:* [405283-36-5]
$C_{25}H_{28}O_{11}$ 504.49
Constit. of *Avicennia marina*.

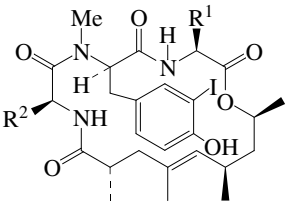
10-O-(4-Hydroxy-E-cinnamoyl): [405283-37-6]
$C_{25}H_{28}O_{12}$ 520.489
Constit. of *Avicennia marina*.

10-O-(3,4-Dihydroxy-E-cinnamoyl): [367513-00-6]
$C_{25}H_{28}O_{13}$ 536.488
Constit. of *Leonotis nepetaefolia* and *Avicennia marina*.

Koenig, G. *et al., Phytochemistry*, 1985, **24**, 1245-1248 (*Phenylpentadienoylgeniposide*)
Shaker, K.H. *et al., Z. Naturforsch., C*, 2001, **56**, 965-968 (*Avicennia marina constits*)

Geodiamolide A G-45

[108675-63-4]



$R^1 = R^2 = CH_3$

$C_{28}H_{40}IN_3O_6$ 641.545

Depsipeptide antibiotic. Isol. from the marine sponge *Geodia* sp. and from *Cymbastela* sp. Exhibits some antifungal props. Cytotoxic. Prisms ($MeCN/CH_2Cl_2$). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 217-218°. $[\alpha]_D^{25}$ +53 (c, 0.04 in $CHCl_3$). λ_{max} 219 (ϵ 13800); 284 (ϵ 3200); 292 (ϵ 3000) (MeOH).

Bromo analogue: ***Geodiamolide B***
[108675-64-5]
$C_{28}H_{40}BrN_3O_6$ 594.544
From *Geodia* sp. and *Cymbastela* sp. Exhibits some antifungal props. Cryst. ($MeCN/CH_2Cl_2$). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 203-204°. $[\alpha]_D^{22}$ +101 (c, 0.04 in $CHCl_3$). λ_{max} 214 (ϵ 15400); 281 (ϵ 2700); 290 (ϵ 2500) (MeOH).

Chloro analogue: ***Geodiamolide C***
[126596-02-9]
$C_{28}H_{40}ClN_3O_6$ 550.093
From the sponge *Pseudaxinyssa* sp. and *Cymbastela* sp. No phys. props. reported. λ_{max} 214 (ϵ 15400); 281 (ϵ 2700); 290 (ϵ 2500) (MeOH).

Chan, W.R. *et al., J.O.C.*, 1987, **52**, 3091-3093 (*Geodiamolides A,B, isol, struct*)
Hirai, Y. *et al., Heterocycles*, 1989, **29**, 1865 (*synth*)
Dilip de Silva, E. *et al., Tet. Lett.*, 1990, **31**, 489-492 (*Geodiamolide C*)
Imaeda, T. *et al., Tet. Lett.*, 1994, **35**, 591 (*synth*)
Shioiri, T. *et al., Heterocycles*, 1997, **46**, 421-442 (*synth*)
Tinto, W.F. *et al., Tetrahedron*, 1998, **54**, 4451-4458 (*cmr*)

Geodiamolide D G-46

[126596-03-0]
As Geodiamolide A, G-45 with
$R^1 = CH_3$, $R^2 = H$
$C_{27}H_{38}IN_3O_6$ 627.518

Depsipeptide antibiotic. Isol. from the sponge *Pseudaxinyssa* sp. and *Cymbastela* sp. Cytotoxic. λ_{max} 219 (ϵ 13800); 284 (ϵ 3200); 292 (ϵ 3000) (MeOH).

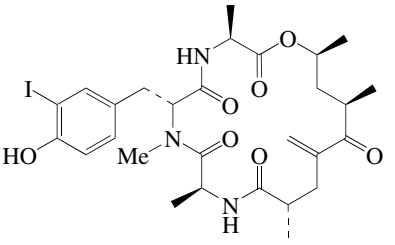
Bromo analogue: ***Geodiamolide E***
[126596-04-1]
$C_{27}H_{38}BrN_3O_6$ 580.518
From a *Pseudaxinyssa* sp. and *Cymbastela* sp. Cytotoxic. λ_{max} 214 (ϵ 15400); 281 (ϵ 2700); 290 (ϵ 2500) (MeOH) (Derep). λ_{max} 219; 284; 292 (MeOH) (Berdy).

Chloro analogue: ***Geodiamolide F***
[126596-05-2]
$C_{27}H_{38}ClN_3O_6$ 536.066
From a *Pseudaxinyssa* sp. and *Cymbastela* sp. Cytotoxic. λ_{max} 214 (ϵ 15400); 281 (ϵ 2700); 290 (ϵ 2500) (MeOH) (Derep). λ_{max} 219; 284; 292 (MeOH) (Berdy).

Dilip de Silva, E. *et al., Tet. Lett.*, 1990, **31**, 489-492 (*isol, pmr, cmr, struct*)

Geodiamolide G G-47

[169181-23-1]



$C_{28}H_{38}IN_3O_7$ 655.529

Depsipeptide antibiotic. Isol. from the sponge *Cymbastela* sp. and *Pseudaxinyssa* sp. Cytotoxic. Glass.

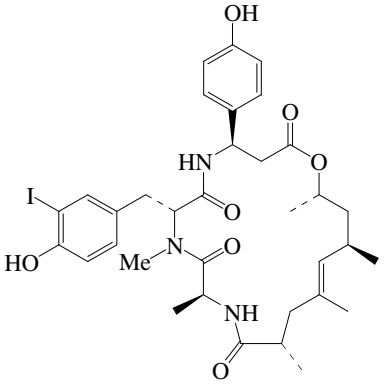
Bromo analogue: ***Geodiamolide J***
$C_{28}H_{38}BrN_3O_7$ 608.528
Isol. from a *Cymbastela* sp. Glass.

Chloro analogue: ***Geodiamolide K***
$C_{28}H_{38}ClN_3O_7$ 564.077
Isol. from a *Cymbastela* sp. Glass.

Coleman, J.E. *et al., Tetrahedron*, 1995, **51**, 10653-10662 (*isol, ir, pmr, cmr*)
Coleman, J.E. *et al., J. Nat. Prod.*, 1999, **62**, 1137-1141 (*isol, pmr, cmr*)

Geodiamolide H G-48

[207385-07-7]



Absolute Configuration

$C_{34}H_{44}IN_3O_7$ 733.642
Isol. from the sponge *Geodia* sp. Cytotoxic.
Mp 186-189°. $[\alpha]_D$ +19.1 (c, 0.17 in $CHCl_3$). λ_{max} 215 (ϵ 12500); 280 (ϵ 2800) (EtOH).

Bromo analogue: ***Geodiamolide I***
[207385-08-8]
$C_{34}H_{44}BrN_3O_7$ 686.642
Isol. from a *Geodia* sp. and *Suberites japonicus*.
Mp 168-170°. $[\alpha]_D$ +39.3 (c, 0.14 in $CHCl_3$). λ_{max} 214 (ϵ 14000); 280 (ϵ 3000) (EtOH).

Chloro analogue: ***Seragamide F***
$C_{34}H_{44}ClN_3O_7$ 642.19
Isol. from *Suberites japonicus*. Glass. $[\alpha]_D^{24}$ +10 (c, 0.02 in $CHCl_3$). λ_{max} 229 (ϵ 4700); 279 (ϵ 1400) (MeOH).

Tinto, W.F. *et al., Tetrahedron*, 1998, **54**, 4451-4458 (*isol, pmr, cmr, cryst struct*)
Tanaka, C. *et al., Tetrahedron*, 2006, **62**, 3536-3542 (*Seragamide F*)

Geodiamolide L G-49

[244157-94-6]
As Geodiamolide A, G-45 with
$R^1 = CH_2OH$, $R^2 = CH_3$
$C_{28}H_{40}IN_3O_7$ 657.544
Depsipeptide. Isol. from the marine sponge *Cymbastela* sp. Glass.
Bromo analogue: ***Geodiamolide M***
[244157-95-7]
$C_{28}H_{40}BrN_3O_7$ 610.544
Isol. from *Cymbastela* sp. Glass.
Chloro analogue: ***Geodiamolide N***
[244157-96-8]
$C_{28}H_{40}ClN_3O_7$ 566.093
Isol. from *Cymbastela* sp. Glass.
Coleman, J.E. *et al., J. Nat. Prod.*, 1999, **62**, 1137-1141 (*Geodiamolides L-N*)

Geodiamolide O G-50

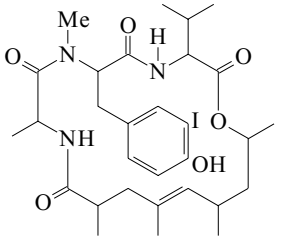
[244157-97-9]
As Geodiamolide A, G-45 with
$R^1 = CH_3$, $R^2 = CH_2OH$
$C_{28}H_{40}IN_3O_7$ 657.544
Depsipeptide. Isol. from the marine sponge *Cymbastela* sp. Glass.
Bromo analogue: ***Geodiamolide P***
[244157-98-0]
$C_{28}H_{40}BrN_3O_7$ 610.544
Isol. from *Cymbastela* sp. Glass.
Chloro analogue: Geodiamolide Q
$C_{28}H_{40}ClN_3O_7$ 566.093
Not found as a nat. prod., but the name has been reserved in anticipation of its future discovery.
Coleman, J.E. *et al., J. Nat. Prod.*, 1999, **62**, 1137-1141 (*Geodiamolides O-Q*)

Geodiamolide R G-51

[244157-99-1]
As Geodiamolide A, G-45 with
$R^1 = CH_2OH$, $R^2 = H$
$C_{27}H_{38}IN_3O_7$ 643.518
Cyclic depsipeptide. Isol. from the marine sponge *Cymbastela* sp. Glass.
Coleman, J.E. *et al., J. Nat. Prod.*, 1999, **62**, 1137-1141 (*isol, pmr, cmr*)

Geodiamolide TA G-52

[157207-91-5]



$C_{30}H_{44}IN_3O_6$ 669.599
Depsipeptide antibiotic. Isol. from the marine sponge *Hemiasterella minor*. Cytotoxic agent. Glass. $[\alpha]_D$ +30 (c, 0.03 in $CHCl_3$). Related to Neosiphoniamolide A, N-81.
Talpir, R. *et al., Tet. Lett.*, 1994, **35**, 4453-4456 (*isol, pmr, cmr, ms*)

Geodiastatin G-53

Chromoproteins. Isol. from the marine sponge *Geodia mesotriaena*. Shows antitumour activity.

Geodiastatin 1
Shiny brownish-black solid. Sol. H_2O; poorly sol. hexane. Contains 34% protein.

Geodiastatin 2
Shiny brownish-black solid. Sol. H_2O; poorly sol. hexane. Contains 28% protein.
Pettit, G.R. *et al., J. Nat. Prod.*, 1981, **44**, 588-592 (*isol*)

Geodiatoxins G-54

Struct. unknown. Isol. from the marine sponge *Geodia mesotriaena*. Toxins.
▶ LD_{50} (mus, ipr) 8 mg/kg.

Geodiatoxin 1 [80450-67-5]
Contains 24% protein.

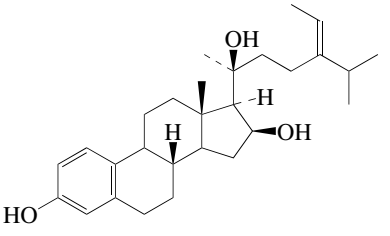
Geodiatoxin 2 [131594-48-4]
Dark brown solid.

Geodiatoxin 3 [131594-49-5]
Dark brown solid.

Geodiatoxin 4 [131594-50-8]
Brownish-black solid.
Pettit, G.R. *et al., J. Nat. Prod.*, 1981, **44**, 588-592 (*Geodiatoxin 1, isol*)
Pettit, G.R. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1990, **96**, 305-306 (*Geodiatoxins 2-4, isol*)

Geodisterol G-55

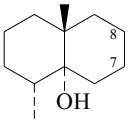
[185146-75-2]



$C_{28}H_{42}O_3$ 426.638
Constit. of a *Geodia* sp.
$[\alpha]_D$ +67 (c, 0.31 in CH_2Cl_2/MeOH).
Wang, G.-Y.-S. *et al., Tet. Lett.*, 1996, **37**, 8145-8146 (*isol, pmr, cmr*)

Geosmin G-56

*Octahydro-4,8*a*-dimethyl-4*a*(2*H*)-naphthalenol, 9CI. 1,10-Dimethyl-9-decalol. 11,12,13-Trinor-5-eudesmanol*
[19700-21-1]



Absolute configuration

$C_{12}H_{22}O$ 182.305
Noreudesmane numbering shown. Odorous substance produced by *Streptomyces* spp. and blue-green algae. Implicated in off-flavour of shellfish, freshwater fish, drinking water and some vegetables. Oil with characteristic penetrating earthy odour. $[\alpha]_D^{25}$ -140 (MeOH). $[\alpha]_D$ -16.5 ($CHCl_3$). Stereoisomers known synthetically.
▶ QK4249000
*7,8-Didehydro: 1,2,3,4,4*a*,5,8,8*a*-Octahydro-4,8*a*-dimethylnaphthalen-4*a*-ol. 11,12,13-Trinor-7-eudesmen-5-ol.* ***Dehydrogeosmin***
$C_{12}H_{20}O$ 180.289
Constit. of various cactus spp. flower scents. Oil.

(±)-form [16423-19-1]
Oil, cryst. on standing. Mp 78-82°.

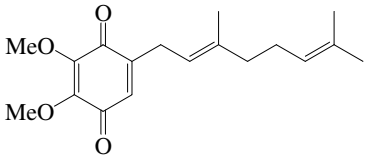
[5173-69-3, 5173-70-6, 16452-32-7, 23333-91-7, 62823-65-8, 73428-92-9]

Marshall, J.A. *et al., J.O.C.*, 1966, **31**, 1020; 1968, **33**, 2593 (*synth*)
Gerber, N.N. *et al., Tet. Lett.*, 1968, 2971 (*isol, struct*)

Ayer, W.A. *et al., Can. J. Chem.*, 1976, **54**, 3276 (*isol, struct, synth, abs config*)
Gerber, N.N. *et al., J. Chem. Ecol.*, 1977, **3**, 475 (*isol*)
Gerber, N.N. *et al., Phytochemistry*, 1977, **16**, 2025 (*cmr*)
Gerber, N.N. *et al., Dev. Ind. Microbiol.*, 1978, **20**, 225 (*rev*)
Maga, J.A. *et al., Food Res. Int.*, 1987, **3**, 269-284 (*occur, rev*)
Kaiser, R. *et al., Helv. Chim. Acta*, 1990, **73**, 133 (*isol, synth, ms, pmr, cmr*)
Hansson, L. *et al., Acta Chem. Scand.*, 1992, **46**, 103 (*synth*)
Swarts, H.J. *et al., Tetrahedron*, 1992, **48**, 5497 (*synth*)
Huber, U. *et al., Helv. Chim. Acta*, 1993, **76**, 1949 (*synth, abs config*)
Feng, Z. *et al., Helv. Chim. Acta*, 1993, **76**, 2547 (*biosynth*)
Conte, E.D. *et al., J. Agric. Food Chem.*, 1996, **44**, 829-835 (*anal, occur*)
Saito, A. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 2923 (*synth*)
Fuhshuku, K. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 2267-2272 (*synth*)
Dickschat, J.S. *et al., J.O.C.*, 2005, **70**, 5174-5182 (*biosynth*)
Cane, D.E. *et al., J. Antibiot.*, 2006, **59**, 471-479 (*biosynth*)
Jiang, J. *et al., J.A.C.S.*, 2006, **128**, 8128-8129 (*biosynth*)

5-Geranyl-2,3-dimethoxy-1,4-benzoquinone G-57

5-(3,7-Dimethyl-2,6-octadienyl)-2,3-dimethoxy-2,5-cyclohexadien-1,4-dione, 9CI. ***Glabruquinone A***. *Desmethylubiquinone Q_2*
[124373-52-0]



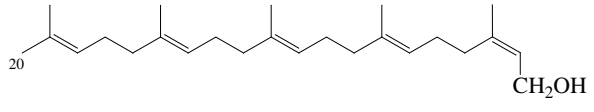
$C_{18}H_{24}O_4$ 304.385
Isol. from the ascidian *Aplidium glabrum*. Constit. of *Wigandia caracasana*. Yellow oil.
▶ Contact allergen, cytotoxic.

Z-Isomer: 2,3-Dimethoxy-5-neryl-1,4-benzoquinone. ***Glabruquinone B***
$C_{18}H_{24}O_4$ 304.385
Isol. from *Aplidium glabrum*. Yellow oil.

Reynolds, G.W. *et al., Contact Dermatitis*, 1989, **21**, 65-68 (*isol, props*)
Shubina, L.K. *et al., Tet. Lett.*, 2005, **46**, 559-562 (*isol, synth, pmr, cmr*)

Geranylfarnesol G-58

3,7,11,15,19-Pentamethyl-2,6,10,14,18-eicosapentaen-1-ol, 9CI



$C_{25}H_{42}O$ 358.606
Major component of archaebacterial lipids, together with its hydrogenated analogues (pentamethyleicosanoids or PMEs). Considered as a taxonomic marker for archaea.

(2Z,6E,10E,14E)-form [22488-05-7]
Constit. of the wax of *Ceroplastes albolineatus*.
Wax.

10,11,14,15,18,19-Hexahydro: ***3,7,11,15,19-Pentamethyl-2,6-eicosadien-1-ol***
[26549-03-1]
$C_{25}H_{48}O$ 364.654
Constit. of the leaves of *Solanum tuberosum* and in archaebacterial lipids. Pale yellow oil.

6,7,10,11,14,15,18,19-Octahydro: ***3,7,11,15,19-Pentamethyl-2-eicosen-1-ol***
[625416-21-9]
$C_{25}H_{50}O$ 366.669
Constit. of *Croton hieronymi*. Gum.

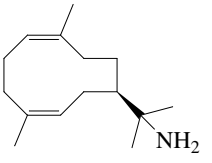
20-Hydroxy: ***ω-Hydroxygeranylfarnesol***
$C_{25}H_{42}O_2$ 374.606
Constit. of *Ceroplastes albolineatus*. Oil.

(2Z,6Z,10E,14E)-form [80373-83-7]
Constit. of seed oils of Theaceae and Gramineae.

Rós, T. *et al., Chem. Comm.*, 1969, 214 (*isol*)
Toyoda, M. *et al., Tet. Lett.*, 1969, 4879 (*hexahydro*)
Quijano, L. *et al., Chem. Lett.*, 1979, 1387 (*isol*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 31 (*synth*)
Akihisa, T. *et al., Lipids*, 1999, **34**, 1151-1157 (*6Z-isomer*)
Catalán, C.A.N. *et al., Phytochemistry*, 2003, **64**, 625-629 (*octahydro*)

1(10),4-Germacradien-11-amine G-59

11-Amino-1(10),4-germacradiene

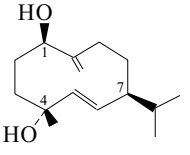


$C_{15}H_{27}N$ 221.385

(1(10)Z,4Z)-form [674817-51-7]
Constit. of *Axinyssa* n. sp.
Oil. $[\alpha]_D^{25}$ +28 (c, 0.2 in $CHCl_3$).

Satitpatipan, V. *et al., J. Nat. Prod.*, 2004, **67**, 503-505 (*isol, pmr, cmr*)

5,10(14)-Germacradiene-1,4-diol G-60



(1β,4α*OH*,5*E*)*–form*

$C_{15}H_{26}O_2$ 238.369

(1β,4αOH,5E)-form [109362-70-1]
Isol. from *Laurencia subopposita*, *Parthenium lozanianum* and *Achillea pannonica*.
Cryst.
Mp 118-120°. $[\alpha]_D^{20}$ +55 (c, 2.5 in $CHCl_3$). $[\alpha]_D^{24}$ -13 (c, 1.3 in $CHCl_3$). $[\alpha]_D^{20}$ -89 (c, 0.48 in CH_2Cl_2). Discrepancy in opt. rotns. unexplained.

1-Ac: [63181-40-8]
$C_{17}H_{28}O_3$ 280.406
Constit. of soft coral *Lemnalia africana*. Oil. $[\alpha]_D$ +23 (c, 1.39 in $CHCl_3$).

(1β,4βOH,5E)-form [63181-39-5]
Isol. from *Senecio adenophyllus* and *Juniperus communis* subsp. *hemisphaerica*.
Cryst. (hexane).
Mp 84-86°. $[\alpha]_D^{24}$ -13 (c, 1.3 in $CHCl_3$). $[\alpha]_D^{25}$ -147.9 (c, 0.3 in $CHCl_3$).

(ent-1β,4βOH,5E)-form
Nephthediol
Isol. from the soft coral *Nephthea* sp.
Amorph. $[\alpha]_D^{21}$ +82 (c, 1.2 in $CHCl_3$).

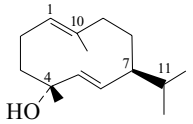
1-Hydroperoxide: 1-Hydroperoxy-5,10(14)-germacradien-4-ol. ***Nephtheoxydiol***
$C_{15}H_{26}O_3$ 254.369
Amorph. solid. $[\alpha]_D^{21}$ +14 (c, 1.2 in $CHCl_3$).

(1α,4βOH,5E)-form
Constit. of *Juniperus communis* subsp. *hemisphaerica*.

Wratten, S.J. *et al., J.O.C.*, 1977, **42**, 3343 (*isol*)
Izac, R.R. *et al., Tetrahedron*, 1982, **38**, 301 (*isol, acetate*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1987, **35**, 124 (*Nephthediol, Nephtheoxydiol*)
Jakupovic, J. *et al., Phytochemistry*, 1987, **26**, 761 (*isol*)
Dupré, S. *et al., Phytochemistry*, 1991, **30**, 1211 (*isol, pmr*)

San Feliciano, A. *et al., J. Nat. Prod.*, 1995, **58**, 1059 (*isol, pmr, cmr, synth*)
Sosa, S. *et al., Planta Med.*, 2001, **67**, 654-658 (*Achillea pannonica constit*)

1(10),5-Germacradien-4-ol G-61



(1(10)*E*,4α,5*E*)–*form*

$C_{15}H_{26}O$ 222.37

(1(10)*E*,4α,5*E*)-*form* [64197-30-4]
Constit. of the soft coral *Lemnalia africana* and *Peucedanum palustre*.
Oil. $[\alpha]_D^{26}$ +122 (c, 1.22 in $CHCl_3$).

O-*β*-D-*Glucopyranoside:* [403985-49-9]
$C_{21}H_{36}O_6$ 384.512
Constit. of *Pittosporum viridiflorum viridiflorum*. Amorph. solid. $[\alpha]_D$ +49.7 (c, 0.61 in $CHCl_3$).

O-*(2*-O-*Acetyl-β*-D-*glucopyranoside):* [403985-51-3]
$C_{23}H_{38}O_7$ 426.549
Constit. of *Pittosporum viridiflorum viridiflorum*. Amorph. solid.

O-*(6*-O-*Acetyl-β*-D-*glucopyranoside):* [403985-50-2]
$C_{23}H_{38}O_7$ 426.549
Constit. of *Pittosporum viridiflorum viridiflorum*. Amorph. solid.

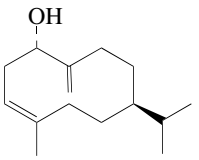
11-Hydroxy: ***1(10),5-Germacradiene-4,11-diol***
[82443-68-3]
$C_{15}H_{26}O_2$ 238.369
Isol. from the gorgonian *Pacifigorgia media*. Cryst.
Mp 172-173°. $[\alpha]_D$ -1.3 (c, 0.99 in $CHCl_3$).

(1(10)*E*,4β,5*E*)-*form*
***β*-Germacrenol**
[74841-87-5]
Constit. of *Pseudobrickellia brasiliensis* and *Juniperus communis* ssp. *hemisphaerica*.
Oil. $[\alpha]_D^{24}$ -109 (c, 0.02 in $CHCl_3$).

(1(10)*E*,4α,5*E*,7β*H*)-*form*
***Nephthenol*†**
Constit. of a *Nephthea* coral.
Oil. $[\alpha]_D^{20}$ +184 (c, 3.1 in $CHCl_3$).

(1(10)*E*,4ξ,5*E*)-*form*
Constit. of *Neodiprion sertifer*.
Izac, R.R. *et al., Tetrahedron*, 1982, **38**, 301 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1984, **23**, 1798 (*isol*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1987, **35**, 124
Schmaus, G. *et al., Planta Med.*, 1989, **55**, 482 (*isol, pmr, cmr*)
Bergström, G. *et al., Acta Chem. Scand.*, 1995, **48**, 187 (*isol*)
San Feliciano, A. *et al., J. Nat. Prod.*, 1995, **58**, 1059 (*isol, pmr, cmr*)
Cornwell, C.P. *et al., Flavour Fragrance J.*, 2001, **16**, 263-273 (*β-Germacrenol*)
Ramanandraibe, V. *et al., Magn. Reson. Chem.*, 2001, **39**, 762-764 (*glucosides*)

3,10(14)-Germacradien-3-ol G-62



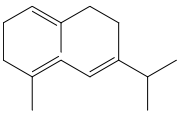
$C_{15}H_{26}O$ 222.37

(1α,3*Z*)-*form*
Oil. $[\alpha]_D$ +96.4 (c, 0.75 in $CHCl_3$).

Ac: [160543-30-6]
$C_{17}H_{28}O_2$ 264.407
Constit. of *Nephthea chabroli*. Oil. $[\alpha]_D$ +73.1 (c, 1 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 32-39 (*isol, pmr, cmr*)

1(10),4,6-Germacratriene G-63

4-Isopropyl-1,7-dimethyl-1,3,7-cyclodecatriene



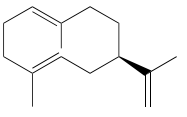
(1(10)*E*,4*E*,6*E*)-*form*

$C_{15}H_{24}$ 204.355

(1(10)*E*,4*E*,6*E*)-*form*
Germacrene C
[34323-15-4]
Constit. of the dried fruits of *Kadsura japonica*.
Oil. $[\alpha]_D^{24}$ 0 (c, 5.55 in $CHCl_3$).

(1(10)*E*,4*Z*,6*E*)-*form*
Constit. of *Nephthea* sp.
Morikawa, K. *et al., Tet. Lett.*, 1969, 1799; 1971, 1131 (*isol, struct, biosynth*)
Koenig, G.M. *et al., Planta Med.*, 1989, **55**, 583-584 (*isol*)

1(10),4,11-Germacratriene G-64



(1(10)*E*,4*E*)-*form*

$C_{15}H_{24}$ 204.355

(1(10)*E*,4*E*)-*form*
Germacrene A
[28387-44-2]
[28028-64-0]
Constit. of *Eunicea mammosa*. Alarm pheromone of the spotted alfalfa aphid *Therioaphis maculata*.
Oil. $[\alpha]_D^{25}$ -3.2 (c, 4.4 in $CHCl_3$).

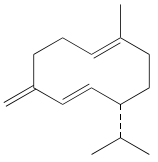
(1(10)*E*,4*Z*)-*form*
(+)-Helminthogermacrene
[675105-92-7]
Constit. of *Scapania undulata*.
Oil.

(*ent*-1(10)*E*,4*E*)-*form*
Isogermacrene A
[783322-20-3]
Constit. of *Saccogyna viticulosa*.
Oil.

(*ent*-1(10)*E*,4*Z*)-*form*
Helminthogermacrene
[75023-40-4]
Constit. of *Helminthosporium sativum*.
Oil. $[\alpha]_D^{25}$ -28 (c, 0.5 in CCl_4).
Weinheimer, W.J. *et al., Tet. Lett.*, 1970, 497 (*Germacrene A*)
Itoh, A. *et al., Tet. Lett.*, 1978, 2903 (*Germacrene A, synth*)
Winter, R.E.K. *et al., J.O.C.*, 1980, **45**, 4786 (*Helminthogermacrene*)
McMurry, J.E. *et al., Tet. Lett.*, 1985, **26**, 2171 (*Helminthogermacrene, synth*)
De Kraker, J.-W. *et al., Phytochemistry*, 2001, **58**, 481-487 (*Germacrene A, isol, ms*)
Calvert, M.J. *et al., J.A.C.S.*, 2002, **124**, 11636-11641 (*biosynth*)
Prosser, I. *et al., Phytochemistry*, 2002, **60**, 691-702 (*biosynth*)
Adio, A.M. *et al., Phytochemistry*, 2004, **65**, 199-206 (*(+)-Helminthogermacrene*)
Hackl, T. *et al., Phytochemistry*, 2004, **65**, 2261-2275 (*Isogermacrene A*)

1(10),4(15),5-Germacratriene G-65

3-Isopropyl-6-methyl-10-methylene-1,6-cyclodecadiene



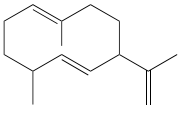
(1(10)*E*,5*E*,7*R*)-*form*

$C_{15}H_{24}$ 204.355

(1(10)*E*,5*E*,7*R*)-*form*
(+)-Germacrene D
[68005-97-0]
Constit. of *Sinularia mayi*, *Pseudopterogorgia americana*, *Solidago canadensis*, *Solidago altissima* and the liverworts *Preissia quadrata* and *Jackiella javanica*.
Oil. $[\alpha]_D^{22}$ +190 (c, 1 in $CHCl_3$).

(1(10)*E*,5*E*,7*S*)-*form*
Germacrene D
[23986-74-5]
Constit. of *Pseudotsuga japonica*, *Tanacetum vulgare*, *Xylopia aethiopica* and many other essential oils. Isol from *Sinularia erecta*. Biosynth. precursor of many sesquiterpenoids. Oil. $[\alpha]_D^{23}$ -240.
Yoshihara, K. *et al., Tet. Lett.*, 1969, 2263 (*isol*)
Beechan, C.M. *et al., Tetrahedron*, 1978, **34**, 2503-2508 (*Sinularia mayi constit*)
Niwa, M. *et al., Chem. Pharm. Bull.*, 1980, **28**, 997-999 (*Solidago altissima constits*)
Kitahara, T. *et al., J.O.C.*, 1984, **49**, 3281 (*synth*)
Mori, M. *et al., J.C.S. Perkin 1*, 1990, 1769-1777 (*pmr*)
Chan, W.R. *et al., Tetrahedron*, 1990, **46**, 1499-1502 (*Pseudopterogorgia americana constit*)
König, W.A. *et al., Phytochemistry*, 1996, **43**, 629-633 (*Preissia quadrata constit*)
Nabeta, K. *et al., J.C.S. Perkin 1*, 1997, 2065-2070 (*biosynth*)
Nagashima, F. *et al., Phytochemistry*, 1997, **46**, 1203-1208 (*Jackiella javanica constit*)
Schmidt, C.O. *et al., Angew. Chem., Int. Ed.*, 1998, **37**, 1400-1402 (*biosynth*)
Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*cmr*)
Steliopoulos, P. *et al., Phytochemistry*, 2002, **60**, 13-20 (*biosynth*)
Umlauf, D. *et al., Phytochemistry*, 2004, **65**, 2463-2470 (*biosynth*)

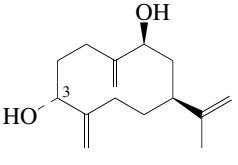
1(10),5,11-Germacratriene G-66



$C_{15}H_{24}$ 204.355

(1(10)*E*,5*E*)-*form*
Germacrene E
[208391-97-3]
Constit. of *Sinularia erecta*.
Oil. $[\alpha]_D$ +2.1 (c, 0.23 in MeOH).
Rudi, A. *et al., J. Nat. Prod.*, 1998, **61**, 872-875 (*isol, pmr, cmr*)

4(15),10(14),11-Germacratriene-3,9-diol G-67



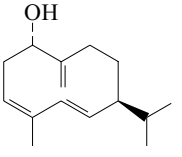
(3α,9β)-*form*

$C_{15}H_{24}O_2$ 236.353

(3α,9β)-*form*
Di-Ac: ***Chrysanthediacetate C***
[189156-54-5]
$C_{19}H_{28}O_4$ 320.428
Constit. of *Chrysanthemum morifolium*. Oil. $[\alpha]_D^{17}$ -46.6 (c, 0.7 in MeOH).

(3β,9β)-*form*
Sinugibberodiol
[864530-17-6]
Constit. of *Sinularia gibberosa*.
Oil. $[\alpha]_D^{25}$ -5 (c, 0.2 in $CHCl_3$).
Di-Ac: ***Chrysanthediacetate B***
[189156-56-7]
[864530-18-7]
$C_{19}H_{28}O_4$ 320.428
Constit. of *Chrysanthemum morifolium*. Oil. $[\alpha]_D^{17}$ +45.5 (c, 0.8 in MeOH).
Hu, L. *et al., Phytochemistry*, 1997, **44**, 1287-1290 (*Chrysanthediacetates A and B*)
Ahmed, A.F. *et al., J. Nat. Prod.*, 2005, **68**, 1208-1212 (*Sinugibberodiol*)

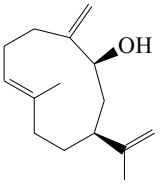
3,5,10(14)-Germacratrien-1-ol G-68



$C_{15}H_{24}O$ 220.354

(1α,3*Z*,5*E*)-*form*
Oil. $[\alpha]_D$ +96.8 (c, 0.85 in $CHCl_3$).
Ac: [160543-31-7]
$C_{17}H_{26}O_2$ 262.391
Constit. of *Nephthea chabroli*. Oil. $[\alpha]_D$ +80.2 (c, 1,1 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 32-39 (*isol, pmr, cmr*)

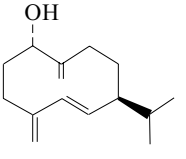
3,10(14),11-Germacratrien-9-ol G-69



$C_{15}H_{24}O$ 220.354

(3*E*,9β)-*form* [132679-81-3]
Constit. of *Dictyopteris divaricata*.
$[\alpha]_D$ -23.6 (c, 0.97 in $CHCl_3$).
Suzaki, M. *et al., Chem. Lett.*, 1990, 2187 (*isol, pmr, cryst struct*)

4(15),5,10(14)-Germacratrien-1-ol G-70



(1α,5*E*)–*form*

$C_{15}H_{24}O$ 220.354

(1α,5*E*)-*form* [65882-79-3]
Constit. of *Inula cuspidata*.
Oil. $[\alpha]_D$ -180.3 ($CHCl_3$).

Ac:
$C_{17}H_{26}O_2$ 262.391
Constit. of *Dilophus fasciola*. Oil. $[\alpha]_D$ -106.5 (c, 1 in $CHCl_3$).

1-Ketone: ***4(15),5,10(14)-Germacratrien-1-one***
[84002-60-8]
$C_{15}H_{22}O$ 218.338
Constit. of *Calea reticulata*. Oil. $[\alpha]_D$ +30 (c, 0.1 in $CHCl_3$).

(1β,5*E*)-*form* [81968-62-9]
Constit. of seeds of *Artemisia annua*.
Oil. $[\alpha]_D$ -106 (c, 0.2 in $CHCl_3$).

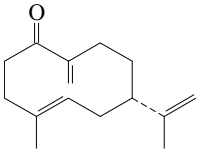
(*ent*-1α,5*E*)-*form*
Constit. of *Jackiella javanica*.
Oil. $[\alpha]_D$ +88.4 (c, 2.41 in $CHCl_3$).

(*ent*-1β,5*E*)-*form*
Constit. of *Jackiella javanica*.
Oil. $[\alpha]_D$ +146 (c, 2.89 in $CHCl_3$).

Fattorusso, E. *et al., Tet. Lett.*, 1978, 4149 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 157; 1793 (*isol*)
Nagashima, F. *et al., Phytochemistry*, 1990, **29**, 2169 (*isol, pmr, cmr*)
Brown, G.D. *et al., Phytochemistry*, 2003, **64**, 303-323 (*Artemisia annua constit*)

4,10(14),11-Germacratrien-1-one G-71

[128718-17-2]

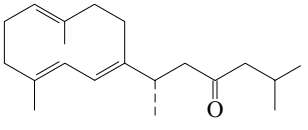


$C_{15}H_{22}O$ 218.338
Constit. of *Dictyopteris divaricata*. Oil. $[\alpha]_D^{24}$ +33.5 (c, 0.76 in $CHCl_3$).

Segawa, M. *et al., Phytochemistry*, 1990, **29**, 973 (*isol, pmr, cmr*)

Germacrexeniolone G-72

2-(4,8-Dimethyl-1,3,7-cyclodecatrien-1-yl)-6-methyl-4-heptanone, 9CI
[107168-63-8]

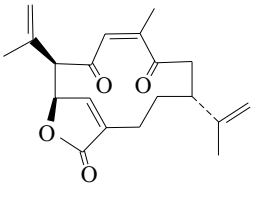


$C_{20}H_{32}O$ 288.472
Isol. from an Okinawan soft coral *Xenia* sp. Oil. $[\alpha]_D^{20}$ +33 (c, 1.4 in $CHCl_3$).

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4641 (*isol, struct, uv, ir, ms, pmr, cmr*)

Gersemolide G-73

[106293-82-7]

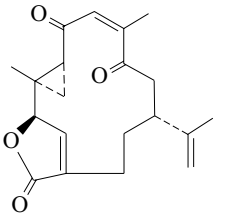


$C_{20}H_{24}O_4$ 328.407
Constit. of *Gersemia rubiformis*. Needles. λ_{max} 233 (ϵ 9000) (MeOH) (Derep).

Williams, D. *et al., J.O.C.*, 1987, **52**, 332-335 (*Gersemolide, cryst struct*)
Marrero, J. *et al., Tetrahedron*, 2006, **62**, 6998-7008 (*Gersemolide, pmr, cmr*)

Gersolide G-74

[116214-76-7]



$C_{20}H_{24}O_4$ 328.407
Constit. of soft coral *Gersemia rubiformis*. Needles (MeOH).
Mp 176-178°. $[\alpha]_D$ -51.9 (c, 0.31 in CH_2Cl_2). λ_{max} 209 (ϵ 4200); 237 (sh) (ϵ) (MeOH) (Derep).

Williams, D.E. *et al., Tet. Lett.*, 1987, **28**, 5079-5080 (*Gersolide, cryst struct*)
Marrero, J. *et al., Tetrahedron*, 2006, **62**, 6998-7008 (*Gersolide, pmr: cmr*)

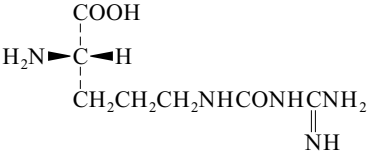
Gigantoxins G-75

Three peptides, Gigantoxins I (48 residues), II (44 residues) and III (48 residues). Isol. from the sea anemone *Stichodactyla gigantea*. Toxic to crabs; Gigantoxin I is an epidermal growth factor-like toxin, Gigantoxins II and III are sodium-channel toxins.

Shiomi, K. *et al., Toxicon*, 2003, **41**, 229-236 (*isol*)
Hermann, P.M. *et al., Curr. Pharm. Des.*, 2004, **10**, 3885-3892 (*Gigantoxin I, rev*)

Gigartinine G-76

N^5-*[[(Aminoiminomethyl)amino]carbonyl]ornithine, 9CI. 5-(3-Amidinoureido)-2-aminovaleric acid*



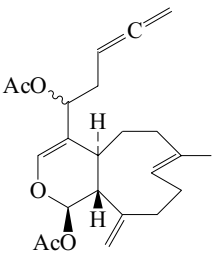
$C_7H_{15}N_5O_3$ 217.227

(*S*)-*form* [7536-90-5]
[7536-92-7 (nitrate)]
Constit. of many spp. of red algae, e.g. *Gymnogongrus flabelliformis, Gelidium amansii, Grateloupia livida, Grateloupia filicina, Polyopes polyideoides, Carpopeltis flabellata, Hypnea japonica* and *Gracilaria textorii*.
Plates (EtOH)(as nitrate).
Mp 197°. $[\alpha]_D^{22}$ +7.5 (c, 2.0 in H_2O).

Ito, K. *et al., Nature (London)*, 1966, **211**, 417 (*isol, uv, ir*)
Ito, K. *et al., CA*, 1968, **68**, 87527c; **69**, 93635y (*isol*)
Laycock, M.V. *et al., Can. J. Biochem.*, 1977, **55**, 27 (*isol, pmr, cmr*)
Wakamiya, T. *et al., Tetrahedron*, 1984, **40**, 235 (*isol*)

Ginamallene G-77

[116242-03-6]

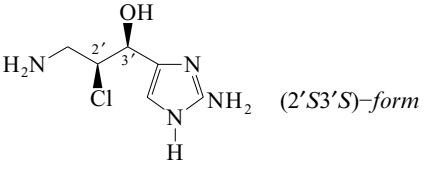


$C_{23}H_{30}O_5$ 386.487
Constit. of *Acalycigorgia* spp. Oil. $[\alpha]_D$ +53 (c, 1.05 in $CHCl_3$).

Fusetani, N. *et al., Tetrahedron*, 1989, **45**, 1647-1652

Giracodazole, INN G-78

*2-Amino-α-(2-amino-1-chloroethyl)-1*H*-imidazole-4-methanol, 9CI. 4-Amino-1-(2-amino-4-imidazolyl)-2-chloro-1-butanol.* ***Girolline****. NSC 627434. RP 49532*



$C_6H_{11}ClN_4O$ 190.632
Protein synthesis inhibitor, antineoplastic agent. Sol. MeOH, EtOH.

(2′S,3′S)-form [135824-74-7]
Isol. from the sponge *Pseudaxinyssa cantharella*.
Powder (as hydrochloride). $[\alpha]_D^{20}$ +7.9 (c, 0.84 in MeOH). Log P -2.03 (calc). CAS no. refers to hydrochloride.

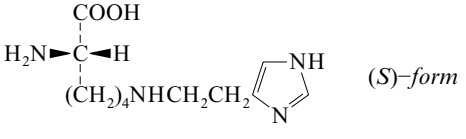
(2′RS,3′SR)-form [127909-96-0]
Mp 191-193° (hydrochloride).

[110883-46-0, 117678-06-5, 117678-08-7, 132618-95-2]

Ahond, A. *et al., C. R. Hebd. Seances Acad. Sci. Ser. 2*, 1988, **307**, 145 (*isol*)
Bedoya Zurita, M. *et al., Tetrahedron*, 1989, **45**, 6713 (*synth, pmr*)
Chiaroni, A. *et al., C. R. Hebd. Seances Acad. Sci. Ser. 2*, 1991, **312**, 49 (*cryst struct, abs config*)
Commercon, A. *et al., Tet. Lett.*, 1991, **32**, 1419; 4905 (*synth, config*)
Colson, G. *et al., Biochem. Pharmacol.*, 1992, **43**, 1717 (*pharmacol*)
Ahond, A. *et al., Tetrahedron*, 1992, **48**, 4327 (*synth*)
Marchais, S. *et al., Tet. Lett.*, 1998, **39**, 8085-8088 (*synth*)

Gizzerosine G-79

N^6*-[2-(1*H*-Imidazol-4-yl)ethyl]lysine, 9CI. 2-Amino-9-(4-imidazolyl)-7-azanonanoic acid. Black vomit toxin*



$C_{11}H_{20}N_4O_2$ 240.305

(R)-form
D-form
[103548-50-1 (hydrochloride salt)]
Cryst. (MeOH) (as dihydrochloride). Mp 252-254° dec. (dihydrochloride). $[\alpha]_D^{22}$ -9.1 (c, 1.26 in H_2O).

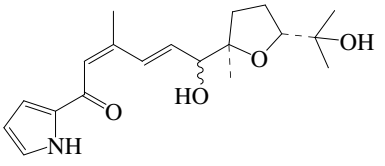
(S)-form
L-form
[89238-78-8]
Isol. from mackerel meal. Prod. as a contaminant during fish meal manufacturing by reaction between histidine and protein in the fish meat. Causes gizzard erosion ("black vomit") in chicks. Cryst. (MeOH aq.) (as dihydrochloride). Mp 251-252° dec. (dihydrochloride). $[\alpha]_D^{22}$ +10.3 (c, 1.28 in H_2O).

(±)-form [88252-77-1]
[88238-60-2]
Fine prisms (MeOH aq.)(as dihydrochloride). Mp 253-256° dec. (as dihydrochloride).

Okazaki, T. *et al., Agric. Biol. Chem.*, 1983, **47**, 2949 (*isol*)
Mori, K. *et al., Tetrahedron*, 1985, **41**, 5307 (*synth*)
Murakita, H. *et al., J. Chromatogr.*, 1990, **515**, 527-530 (*hplc*)
Rosselot, G. *et al., Poultry Sci.*, 1996, **75**, 873-880
Shimasaki, Y. *et al., Synthesis*, 2005, 3191-3192 (*synth*)

Glaciapyrrole A G-80

[853885-46-8]

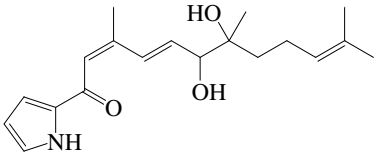


$C_{19}H_{27}NO_4$ 333.427
Metab. of a marine-sediment derived *Streptomyces* sp. Glass. $[\alpha]_D^{22}$ +16.8 (c, 0.02 in MeOH). λ_{max} 285 (sh) (ε 6700); 333 (ε 14400) (MeOH).

Macherla, V.R. *et al., J. Nat. Prod.*, 2005, **68**, 780-783 (*Glaciapyrrole A*)

Glaciapyrrole B G-81

[853885-48-0]

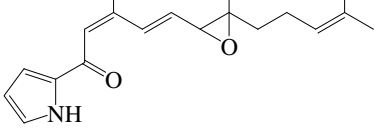


$C_{19}H_{27}NO_3$ 317.427
Metab. of a marine-sediment derived *Streptomyces* sp. Glass. λ_{max} 285 (sh); 335 (MeCN aq.).

Macherla, V.R. *et al., J. Nat. Prod.*, 2005, **68**, 780-783 (*Glaciapyrrole B*)

Glaciapyrrole C G-82

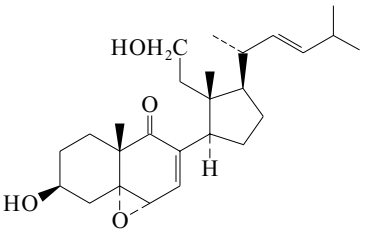
[853885-50-4]



$C_{19}H_{25}NO_2$ 299.412
Constit. of a marine-sediment derived *Streptomyces* sp. Glass. λ_{max} 285 (sh); 335 (MeCN aq.).

Macherla, V.R. *et al., J. Nat. Prod.*, 2005, **68**, 780-783 (*Glaciapyrrole C*)

Glaciasterol A G-83



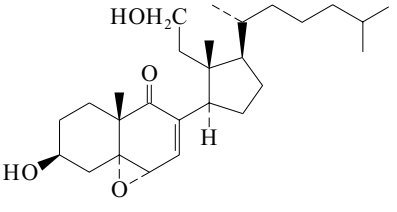
$C_{26}H_{40}O_4$ 416.6
Constit. of *Aplysilla glacialis*. Cytotoxic agent. MDR inhibitor. Amorph. solid.

[144369-45-9]

Pika, J. *et al., Can. J. Chem.*, 1992, **70**, 1506 (*isol, pmr, cmr, activity*)

Glaciasterol B G-84

5,6-Epoxy-3,11-dihydroxy-11,12-secocholest-7-ene-9-one
[144676-37-9]



$C_{27}H_{44}O_4$ 432.642
Constit. of *Aplysilla glacialis*. Cytotoxic agent. Needles (MeOH aq.) (as di-Ac).
Mp 55-57° (di-Ac).

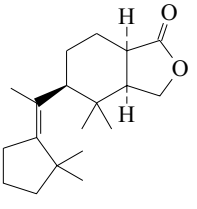
3-Ac: [223682-38-0]
$C_{29}H_{46}O_5$ 474.679
Constit. of *Fasciospongia cavernosa*. Cryst. (hexane/MeOH). Mp 97-99°. $[\alpha]_D$ +4.2 (c, 0.15 in $CHCl_3$). λ_{max} 241 (ϵ 4100) (MeOH).

[144369-46-0]

Pika, J. *et al., Can. J. Chem.*, 1992, **70**, 1506 (*isol, pmr, cmr, activity*)
De Rosa, S. *et al., Nat. Prod. Lett.*, 1999, **13**, 15-20 (*3-Ac*)

Glaciolide G-85

[125482-27-1]



$C_{19}H_{30}O_2$ 290.445
Constit. of nudibranch *Cadlina luteomarginata* and the sponge *Aplysilla glacialis*. Needles (hexane).
Mp 102-103°. $[\alpha]_D$ +18.9 (c, 0.14 in EtOH).

Tischler, M. *et al., Tet. Lett.*, 1989, **30**, 5717-5720 (*isol*)

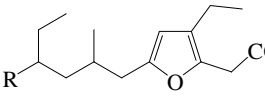
Glacontryphan M G-86

Asn-Gla-Ser-Gla-Cys-Pro-D-Trp-His-Pro-Trp-Cys-NH_2
$C_{61}H_{77}N_{17}O_{17}S_2$ 1384.515
Peptide containing 4-carboxyglutamate residues at positions 2 and 4 and a D-tryptophan residue at position 7. Isol. from venom of *Conus marmoreus*.

Hansson, K. *et al., J. Biol. Chem.*, 2004, **279**, 32453-32463 (*isol*)
Grant, M.A. *et al., J. Biol. Chem.*, 2004, **279**, 32464-32473 (*pmr, struct*)

Glanvillic acid A G-87

3-Ethyl-5-(4-ethyl-2-methyl-5-octenyl)-2-furanacetic acid



R = -CH=CHCH$_2$CH$_3$(*E*-)

$C_{19}H_{30}O_3$ 306.444
Isol. from *Plakortis halichondrioides*. Oil (as Me ester). $[\alpha]_D^{25}$ -23.8 (c, 0.21 in CH_2Cl_2) (Me ester). λ_{max} 233 (ϵ 5300) (CH_2Cl_2) (Me ester).

Williams, D.E. *et al., J. Nat. Prod.*, 2001, **64**, 281-285

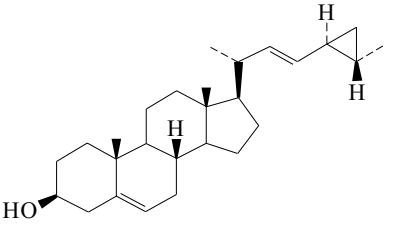
Glanvillic acid B G-88

3-Ethyl-5-(4-ethyl-2-methylheptyl)-2-furanacetic acid
As Glanvillic acid A, G-87 with
R = $CH_2CH_2CH_3$
$C_{18}H_{30}O_3$ 294.433
Isol. from *Plakortis halichondrioides*. Oil (as Me ester). $[\alpha]_D^{25}$ -23.1 (c, 0.13 in CH_2Cl_2) (Me ester). λ_{max} 230 (ϵ 5810) (CH_2Cl_2) (Me ester).

Williams, D.E. *et al., J. Nat. Prod.*, 2001, **64**, 281-285

Glaucasterol G-89

23-(2-Methylcyclopropyl)-24-norchola-5,22-dien-3-ol, 9CI. 22-Dehydro-24,26-cyclocholesterol. 24,26-Cyclocholesta-5,22-dien-3-ol. Papakusterol
[84871-06-7]
[85761-48-4 (*R,R*)-isomer]



$C_{27}H_{42}O$ 382.628
Papakusterol isol. as a mixt. of . of (24*S*,25*S*)- (illus.) and (24*R*,25*R*)-forms in ratio 3:1. Glaucasterol was characterised as the stereoisomer illus. Isol. fom *Sarcophyton glaucum* and unidentified gorgonians. Cryst.
Mp 112-113°.

3-O-(4,8,12-Trimethyltridecanoyl): [137042-62-7]
$C_{43}H_{72}O_2$ 621.041
Constit. of a *Xestospongia* sp. Gum. $[\alpha]_D^{25}$ +6 (c, 0.02 in $CHCl_3$). Stereochem. of side chain not certain.

5α,6-Dihydro: 24,26-Cyclocholest-22-en-3-ol. ***5,6-Dihydroglaucasterol***
[87084-97-7]
$C_{27}H_{44}O$ 384.644
Constit. of soft coral *Sarcophyton glaucum*. Cryst.
Mp 120-124°.

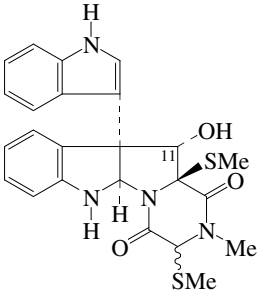
22,23-Dihydro: 24,26-Cyclocholesterol. 24,26-Cyclo-5-cholesten-3-ol
[87984-70-1]
$C_{27}H_{44}O$ 384.644
Constit. of sponge *Spheciospongia vagabunda*. Cryst.
Mp 130-133°.

7,8-Didehydro: ***Dehydropapakusterol***
[85727-98-6]
$C_{27}H_{40}O$ 380.612
Constit. of a gorgonian *Acanthagorgia* sp. Isol. as a mixt. of stereoisomers.

Catalan, C.A.N. *et al., Steroids*, 1982, **40**, 455-463 (*24,26-Cyclocholesterol, isol, struct*)
Kobayashi, M. *et al., Steroids*, 1982, **40**, 665-672 (*Glaucasterol*)
Kobayashi, M. *et al., Ann. Chim. Farm.*, 1983, **31**, 1803 (*5,6-dihydro*)
Bonini, C. *et al., Tet. Lett.*, 1983, **24**, 277-280 (*Papukasterol, Dehydropapukasterol*)
Catalan, C.A.N. *et al., Tet. Lett.*, 1983, **24**, 3461-3464 (*24,26-Cyclocholesterol, abs config*)
Fujimoto, Y. *et al., Tet. Lett.*, 1984, **25**, 1805-1808 (*synth, abs config*)
Gunasekera, S.P. *et al., J. Nat. Prod.*, 1991, **54**, 1119-1122 (*ester*)

Gliocladin A G-90

[749216-45-3]



Relative Configuration

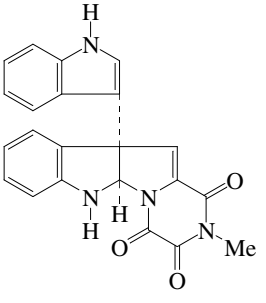
$C_{24}H_{24}N_4O_3S_2$ 480.611
Prod. by *Gliocladium roseum* OUPS-N132 isol. from *Aplysia kurodai*. Cryst. (CH_2Cl_2/MeOH).
Mp 174-176°. $[\alpha]_D^{16}$ +263 (c, 0.14 in $CHCl_3$). λ_{max} 242 (log ϵ 4.36); 283 (log ϵ 4.12); 291 (log ϵ 4.11) (EtOH).

11-Deoxy: ***Gliocladin B***
[749216-46-4]
$C_{24}H_{24}N_4O_2S_2$ 464.611
Prod. by *Gliocladium roseum* OUPS-N132 from *Aplysia kurodai*. Cryst. (CH_2Cl_2/MeOH).
Mp 145-148°. $[\alpha]_D^{16}$ +200 (c, 0.06 in $CHCl_3$). λ_{max} 283 (log ϵ 3.78); 292 (log ϵ 3.77) (EtOH).

Usami, Y. *et al., Heterocycles*, 2004, **63**, 1123-1129 (*isol, cd, pmr, cmr*)

Gliocladin C G-91

[749216-47-5]

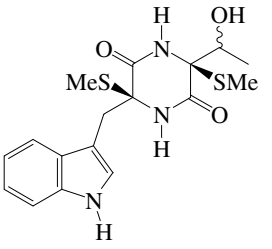


$C_{22}H_{16}N_4O_3$ 384.393
Prod. by *Gliocladium roseum* OUPS-N132 isol. from *Aplysia kurodai*. Cytotoxic. Pale yellow powder (CH_2Cl_2/MeOH).
Mp 180-183°. $[\alpha]_D^{16}$ +131.4 (c, 0.07 in $CHCl_3$). λ_{max} 242 (log ϵ 5.11); 283 (log ϵ 4.88); 292 (log ϵ 4.89) (EtOH).

Usami, Y. *et al., Heterocycles*, 2004, **63**, 1123-1129 (*isol, cd, pmr, cmr*)

Glioperazine G-92

[749216-48-6]

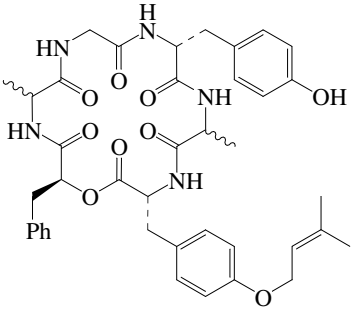


Relative Configuration

$C_{17}H_{21}N_3O_3S_2$ 379.503
Prod. by *Gliocladium roseum* OUPS-N132 isol. from *Aplysia kurodai*. Cryst. (CH_2Cl_2/MeOH).
Mp 170-173°. $[\alpha]_D^{16}$ +52.6 (c, 0.11 in $CHCl_3$). λ_{max} 274 (log ϵ 3.61); 283 (log ϵ 3.62); 292 (log ϵ 3.56) (EtOH).

Usami, Y. *et al., Heterocycles*, 2004, **63**, 1123-1129 (*isol, cd, pmr, cmr*)

Gliotide G-93

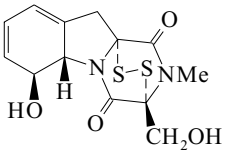


$C_{40}H_{47}N_5O_9$ 741.839
Prod. by a marine-derived *Gliocladium* sp. Amorph. solid. $[\alpha]_D^{20}$ +6.6 (c, 0.33 in MeOH).

Lang, G. *et al., J. Nat. Prod.*, 2006, **69**, 621-624 (*isol, pmr, cmr*)

Gliotoxin G-94

*2,3,5*a*,6-Tetrahydro-6-hydroxy-3-(hydroxymethyl)-2-methyl-10*H*-3,10*a*-epidithiopyrazino[1,2-*a*]indole-1,4-dione, 9CI, 8CI. Aspergillin*†*. SN 12870. Antibiotic SN 12870*
[67-99-2]



$C_{13}H_{14}N_2O_4S_2$ 326.397
Epithiodioxopiperazine antibiotic. Isol. from *Gliocladium fimbriatum*, *Aspergillus fumigatus*, *Penicillium* spp. and *Pseudallescheria* sp. (MFB165). Present in both terrestrial and marine fungi. Shows antiviral activity, of limited use as agricultural fungicide. Now superseded. Also shows immunomodulating activity. Monoclinic cryst. (MeOH).
Mp 221° dec. $[\alpha]_D^{25}$ -290 (c, 0.078 in EtOH). Log P 1.13 (uncertain value) (calc). λ_{max} 269 (ϵ 4500); 310 (ϵ); 340 (ϵ) (MeOH) (Derep).
▶ LD_{50} (mus, orl) 67 mg/kg, hepatotoxic. KB4725000

Ac: ***Acetylgliotoxin***
$C_{15}H_{16}N_2O_5S_2$ 368.434
Isol. from *Penicillium terlikowskii*. Antibiotic. Pale yellow rhombic cryst. (C_6H_6). Sol. MeOH, Et_2O; poorly sol. H_2O.

Mp 162-163°. $[\alpha]_D^{19}$ -197 (c, 0.6 in $CHCl_3$). λ_{max} 268 (ϵ 6300) (EtOH) (Berdy).

▶ LD_{50} (mus, ipr) 50 mg/kg.

Dibenzoyl:
Plates ($CHCl_3$/MeOH). Mp 192-193° dec. $[\alpha]_D^{22}$ -20 (c, 1 in $CHCl_3$).

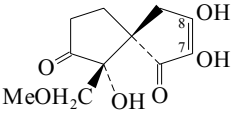
Bis(4-bromobenzoyl):
Needles (dioxan aq.). Mp 193° dec. $[\alpha]_D$ -20 (c, 1 in $CHCl_3$).

Bis(4-nitrobenzoyl):
Prismatic rods ($CHCl_3$/MeOH). Mp 189° dec. $[\alpha]_D^{22}$ -13 (c, 1 in $CHCl_3$).

Johnson, D. *et al., J.A.C.S.*, 1943, **65**, 2005 (*isol, uv, props*)
Bell, M.R. *et al., J.A.C.S.*, 1958, **80**, 1001 (*struct, uv, ir*)
Beecham, A.F. *et al., Tet. Lett.*, 1966, 3131 (*cryst struct, abs config*)
Bose, A.K. *et al., J.A.C.S.*, 1968, **90**, 1038 (*biosynth, ms*)
Johns, N. *et al., J.C.S. Perkin 1*, 1975, 383 (*biosynth*)
Fukuyama, T. *et al., J.A.C.S.*, 1976, **98**, 6723 (*synth*)
Kirby, G.W. *et al., J.C.S. Perkin 1*, 1980, 119; 1988, 301 (*isol, synth, pmr*)
Fukuyama, T. *et al., Tetrahedron*, 1981, **37**, 2045 (*synth*)
Nagarajan, R. *et al., Dev. Food Sci.*, 1984, **8**, 351 (*rev*)
Wróbel, J.T. *et al., Alkaloids (N.Y.)*, 1985, **26**, 67 (*rev*)
Waring, P. *et al., Tet. Lett.*, 1986, **27**, 735 (*isol, struct, ms*)
Kirby, G.W. *et al., Tet. Lett.*, 1986, **27**, 5539 (*synth*)
Yoshida, K. *et al., Prog. Biochem. Pharmacol.*, 1988, **22**, 66 (*rev, pharmacol, synth*)
Kaouadji, M. *et al., J. Nat. Prod.*, 1990, **53**, 717 (*pmr, cmr*)
Pesticide Manual, 9th edn., 1991, No. 6920
Grovel, O. *et al., Toxicon*, 2003, **42**, 297-300 (*isol*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 571; 575
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ARO250

Gloiosiphone A G-95

2,3,6-Trihydroxy-6-(methoxymethyl)spiro[4.4]non-2-ene-1,7-dione, 9CI
[152406-60-5]

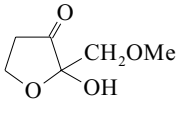


$C_{11}H_{14}O_6$ 242.228
Constit. of the red alga *Gloiosiphonia verticillaris*. Oil (as 7,8-di-Me ether). Racemic.

Chen, J.L. *et al., J. Nat. Prod.*, 1993, **56**, 1205
Sturino, C.F. *et al., Tetrahedron*, 1997, **53**, 8913 (*synth, ir, pmr, cmr*)
Sha, C.-K. *et al., J. Chin. Chem. Soc. (Taipei)*, 1999, **46**, 469-475 (*synth*)

Gloiosiphone B G-96

4,5-Dihydro-2-hydroxy-2-(methoxymethyl)-3(2H)-furanone
[152406-61-6]

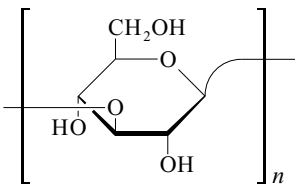


$C_6H_{10}O_4$ 146.143
Constit. of the red alga *Gloiosiphonia verticillaris*. Oil. Racemic.

Chen, J.L. *et al., J. Nat. Prod.*, 1993, **56**, 1205-1210

β-D-(1→3)-Glucan G-97

Pachyman. Callose. Paramylon
[51052-65-4]



Isol. from many fungi, bacteria, plants and algae. A practical laboratory source is the fungus *Poria cocos* (94% of dry weight). Synthetic source of 3-*O*-β-D-Glucopyranosyl-D-glucose, G-100, Laminaritriose and higher homologues. Sol. H_2O. Curdlan below is a well-studied variant having n = 540. Also closely related is Laminarin, L-21 which has a limited amount of chain branching.

Curdlan

Cerdlan. Kerdlan. TAK-N
[54724-00-4]
Extracellular polysaccharide prod. by *Alcaligenes faecalis* var. *myxogenes*, structural or reserve polysaccharide of yeasts, fungi and higher plants. Gelling agent for foods. Claimed to show anti-HIV activity by inhibiting attachment of the virus to T-cells. Insol. H_2O but absorbs H_2O. Suspensions heated >54° form a firm gel. Phase 1 clinical trials (1995)

Sulfate: ***Curdlan sulfate***
[115743-28-7] Semisynthetic polysaccharide. Used in the treatment of AIDS myelopathy, dementia.

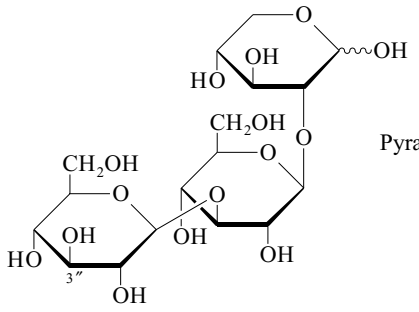
Wheelan, W.J. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 330 (*isol, bibl*)
Harada, T. *et al., ACS Symp. Ser.*, 1977, **45**, 265 (*rev, synth, props, use*)
Marchenault, R.H. *et al., Carbohydr. Res.*, 1979, **75**, 231-242 (*struct*)
Deslandes, Y. *et al., Macromolecules*, 1980, **13**, 1466 (*cryst struct, bibl*)
Saito, H. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 2093; 1987, **60**, 4259; 1989, **62**, 392 (*conformn, cmr*)
Okuyama, K. *et al., J. Carbohydr. Chem.*, 1991, **10**, 645-656 (*Curdlan, struct*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **16**, 595
Demleitner, S. *et al., Carbohydr. Res.*, 1992, **226**, 239; 247 (*synth, pharmacol*)
Kai, A. *et al., Carbohydr. Res.*, 1993, **240**, 153 (*bibl, biosynth*)
Gordon, M. *et al., J. Med. (Westbury, N.Y.)*, 1994, **25**, 163-180; 1995, **26**, 97-131; 1997, **28**, 108-128 (*pharmacol, curdlan sulfate*)
Yoshida, T. *et al., Carbohydr. Res.*, 1995, **276**, 425 (*curdlan sulfate*)
Alban, S. *et al., Thromb. Res.*, 1995, **78**, 201 (*curdlan sulfate*)
Kulicke, W.M. *et al., Carbohydr. Res.*, 1997, **297**, 135-143 (*struct, props*)
Müller, A. *et al., Carbohydr. Res.*, 1997, **299**, 203-208 (*isol, purifn*)
Masihi, K.N. *et al., Int. J. Immunopharmacol.*, 1997, **19**, 463-468 (*curdlan sulfate*)
Tylianakis, M. *et al., Carbohydr. Res.*, 1999, **315**, 16-34 (*cmr*)
Shimizu, J. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 466-469 (*curdlan*)
Naito, T. *et al., J. Acquir. Immune Defic. Syndr.*, 2001, **26**, 512-513 (*curdlan sulfate*)

1,3-Glucan phosphorylase G-98

E.C. 2.4.1.97. 1,3-β-D-Glucan:phosphate α-D-glucosyltransferase. Laminarin phosphoryltransferase. Laminarin phosphorylase
[37340-31-1]
Hexosyltransferase enzyme. Isol. from *Ochromonas malhamensis*. Catalyses the reaction of $(1,3\text{-}\beta\text{-D-glucosyl})_n$ with phosphate to give $(1,3\text{-}\beta\text{-D-glucosyl})_{n-1}$ and α-D-glucose 1-phosphate. Acts on β-1,3-oligoglucans and on glucans of the laminarin type.

Albrecht, G.J. *et al., Phytochemistry*, 1971, **10**, 1293-1298

β-D-Glucopyranosyl-(1 →3)-β-D-glucopyranosyl-(1 →2)-D-xylose, 9CI G-99



Pyranose–*form*

$C_{17}H_{30}O_{15}$ 474.415
Constit. of Holotoxin A and B, isol. from sea cucumber *Stichopus japonicus*.

Pyranose-*form*

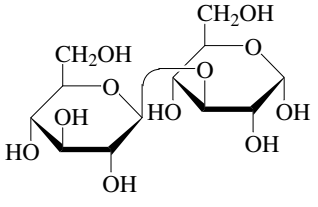
Me glycoside, nona-Me: [55727-75-8]
$C_{27}H_{50}O_{15}$ 614.683
Amorph. $[\alpha]_D^{28}$ +2 (c, 0.3 in $CHCl_3$).

3′′-Me, nona-Ac: [55762-44-2]
$C_{36}H_{50}O_{24}$ 866.777
Amorph.

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1976, **24**, 275 (*constit, Me pyr deriv, nona-Ac deriv, ir, pmr*)

3-*O*-β-D-Glucopyranosyl-D-glucose, 9CI G-100

Laminaribiose, 8CI. *Laminarabiose*
[34980-39-7]



α-Pyranose-*form*

$C_{12}H_{22}O_{11}$ 342.299
Constit. of pine needles, seeds of *Cycas revoluta*, laminaran, pachyman, yeast glucans and seaweed lichenans.
Mp 205° (90°). $[\alpha]_D$ +18 (c, 2.0 in H_2O).

Phenylosazone: Mp 195°. $[\alpha]_D^{10}$ -79.6 (EtOH).

α-Pyranose-*form*

Octa-Ac: 3-O-*Tetra*-O-*acetyl-β-D-glucopyranosyl tetra*-O-*acetyl-α-D-glucopyranoside*
$C_{28}H_{38}O_{19}$ 678.597
Mp 77-78°. $[\alpha]_D$ +20 ($CHCl_3$).

Benzyl glycoside: Benzyl 3-O-*β-D-glucopyranosyl-α-D-glucopyranoside*
$C_{19}H_{28}O_{11}$ 432.424
$[\alpha]_D$ +77.2 (c, 1.8 in H_2O).

1-Bromo, 1-deoxy, hepta-Ac: Acetobromolaminaribiose
$C_{26}H_{35}BrO_{17}$ 699.456
Mp 180.5-182°. $[\alpha]_D^{18}$ +85 ($CHCl_3$).

β-Pyranose-*form*

Octa-Ac: 3-O-*Tetra*-O-*acetyl-β-D-glucopyranosyl tetra*-O-*acetyl-β-D-glucopyranoside*
$C_{28}H_{38}O_{19}$ 678.597
Mp 161°. $[\alpha]_D^{18}$ -29 (c, 2.5 in $CHCl_3$).

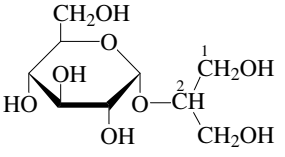
Me glycoside: Methyl 3-O-*β-D-glucopyranosyl-β-D-glucopyranoside*
$C_{13}H_{24}O_{11}$ 356.326
Mp 165-166°. $[\alpha]_D$ -28 (H_2O).

Ph glycoside: Phenyl 3-O-*β-D-glucopyranosyl-β-D-glucopyranoside*
[72656-07-6]
$C_{18}H_{26}O_{11}$ 418.397
Solid. Mp 77° Mp 129-131°. $[\alpha]_D^{20}$ -39.1 (c, 1.07 in H_2O).

Bächli, P. *et al., J.C.S.*, 1952, 1243 (*synth, β-pyr octa-Ac*)
Barry, V.C. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 328 (*isol*)
Pazur, J.H. *et al., The Carbohydrates*, Academic Press, 2nd Ed., 1970, 69 (*rev*)
Matsui, M. *et al., Chem. Pharm. Bull.*, 1971, **19**, 395 (*pmr*)
Colson, P. *et al., J.A.C.S.*, 1974, **96**, 8081 (*cmr*)
Villa, T.G. *et al., Carbohydr. Res.*, 1979, **74**, 369-370 (*enzymic synth*)
Takeo, K. *et al., Carbohydr. Res.*, 1979, **77**, 131; 245; 1980, **86**, 151; 1981, **93**, 157 (*synth, derivs*)
Lambda, D. *et al., Carbohydr. Res.*, 1986, **153**, 205 (*cryst struct, octa-Ac*)
Wang, L.X. *et al., Carbohydr. Res.*, 1991, **219**, 133 (*enzymic synth, octa-Ac*)
Noguchi, K. *et al., Carbohydr. Res.*, 1992, **237**, 33 (*cryst struct, β-Me gly*)
Ikegami, M. *et al., Carbohydr. Res.*, 1994, **253**, 29 (*cryst struct, α-Me gly hepta-Ac*)
Drone, J. *et al., Eur. J. Org. Chem.*, 2005, 1977-1983 (*β-Ph gly*)

2-*O*-Glucopyranosylglycerol G-101

2-Hydroxy-1-(hydroxymethyl)ethyl glucopyranoside, 9CI, 8CI



$C_9H_{18}O_8$ 254.236

α-D-*form*

Isol. from a marine blue-green alga *Oscillatoria* sp.
Viscous oil. $[\alpha]_D$ -37 (c, 0.6 in H_2O).

β-D-*form*

Lilioside B
[10588-30-4]
Constit. of *Lilium longiflorum*.
Mp 166-167°. $[\alpha]_D^{26}$ -30.2 (H_2O).

1-Ac: ***Lilioside A***. *2-(Acetyloxy)-1-(hydroxymethyl)ethyl β-D-glucopyranoside, 9CI*
[55729-18-5]
$C_{11}H_{20}O_9$ 296.274
Constit. of *Lilium longiflorum*.
Mp 146-148°. $[\alpha]_D^{23}$ -21.8 (H_2O). 2-Config. not determined.

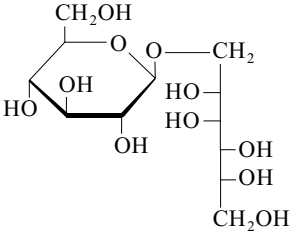
Hexa-Ac: Mp 128°. $[\alpha]_D^{18}$ -15.5 ($CHCl_3$).

[131831-28-2]

Dutton, G.G.S. *et al., J. Chromatogr.*, 1968, **36**, 283 (*Liliosides, glc*)
Kaneda, M. *et al., Tet. Lett.*, 1974, 3937 (*Liliosides, isol, pmr*)
Kaneda, M. *et al., Phytochemistry*, 1990, **29**, 3559 (*Liliosides, synth, abs config*)
Choi, J.S. *et al., Bull. Korean Chem. Soc.*, 1999, **20**, 1121-1122 (*α-D-form*)

1-*O*-D-Glucopyranosyl-D-mannitol, 8CI G-102

[28971-30-4]



$C_{12}H_{24}O_{11}$ 344.315

α-*form*

E953

[20942-99-8]

Prepd. on large scale from sucrose. Low nutritive sweetener with half sweetness of sucrose. Mp 122-125°. $[\alpha]_D^{20}$ +87.3 (c, 0.2 in H_2O).

β-*form*

Constit. of *Fucus vesiculosus* and other brown algae.
Mp 140-141°. $[\alpha]_D^{20}$ -18 (c, 2.0 in H_2O).

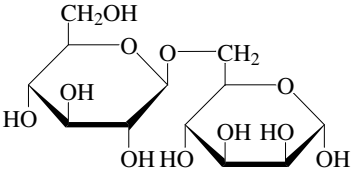
[64519-82-0]

Lindberg, B. *et al., Acta Chem. Scand.*, 1953, **7**, 1119; 1218; 1954, **8**, 817; 1547; 1955, **9**, 168 (*isol, synth, β-form*)
Manners, D.J. *et al., Carbohydr. Res.*, 1968, **7**, 291-298 (*α-form, synth*)
Helferich, B. *et al., Chem. Ber.*, 1973, **106**, 2508-2512 (*α-form, synth*)
Lindner, H.J. *et al., Carbohydr. Res.*, 1981, **93**, 1315 (*cryst struct*)

6-*O*-β-D-Glucopyranosyl-D-mannose G-103

Epigentiobiose

[25538-26-5]



α-Pyranose-*form*

$C_{12}H_{22}O_{11}$ 342.299

Occurs in the free state in various seaweeds, e.g. *Pelvetia canaliculata, Laminaria cloustoni* and *Fucus spiralis*. Also isol. from the partial acid hydrolysate of "insoluble laminarin". Cryst. + H_2O.
Mp 137-138°. $[\alpha]_D$ -11 (H_2O).

Phenylosazone: Mp 166-170°.

α-Pyranose-*form*

Octa-Ac:
$C_{28}H_{38}O_{19}$ 678.597
Mp 110-112°. $[\alpha]_D$ +26 ($CHCl_3$).

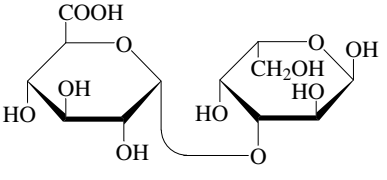
β-Pyranose-*form*

Octa-Ac: Mp 132-140°. $[\alpha]_D$ -20.6 ($CHCl_3$).

2-(Trichloroacetyl), hepta-Ac:
$C_{28}H_{35}Cl_3O_{18}$ 765.932
Mp 185°. $[\alpha]_D^{21}$ -7.2 (c, 1.2 in $CHCl_3$).

Lindberg, B. *et al., Acta Chem. Scand.*, 1953, **7**, 1218; 1218; 1954, **8**, 817; 1547 (*occur, synth*)
Bouveng, H.O. *et al., Acta Chem. Scand.*, 1955, **9**, 168 (*occur*)
Peat, S. *et al., J.C.S.*, 1958, 729; 1960, 175 (*isol, synth*)
Bredereck, H. *et al., Chem. Ber.*, 1960, **93**, 1201; 1962, **95**, 3064 (*synth, Ac*)

3-*O*-α-D-Glucopyranuronosyl-L-galactose G-104



α-Pyranose-*from*

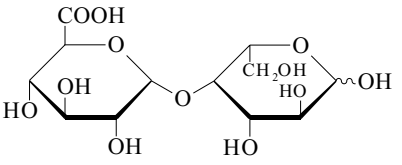
$C_{12}H_{20}O_{12}$ 356.283

α-Pyranose-*form* [62069-78-7]

Isol. from unicellular red alga *Rhodella reticulata* and of the polysaccharide of hornwort *Anthoceros caucasicus*.
No phys. props. reported.

Jaseja, M. *et al., Carbohydr. Res.*, 1989, **186**, 313 (*pmr, cmr*)
Geresh, S. *et al., Carbohydr. Res.*, 1990, **208**, 301 (*Rhodella rediculata constit, isol, struct*)
Popper, Z.A. *et al., Phytochemistry*, 2003, **64**, 325-335 (*Anthoceros caucasicus constit, isol, pmr, cmr*)

4-*O*-α-D-Glucopyranuronosyl-L-galactose, 9CI G-105



Pyranose–*form*

$C_{12}H_{20}O_{12}$ 356.283

Pyranose-*form* [50692-51-8]

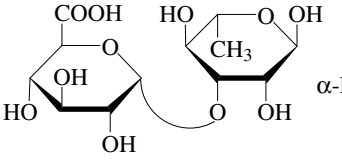
Isol. from the partial acid hydrolysate of the polysaccharide from the red alga *Anatheca dentata*.
$[\alpha]_D$ +24 (c, 0.5 in H_2O).

Nunn, J.R. *et al., Carbohydr. Res.*, 1973, **29**, 281

3-*O*-α-D-Glucopyranuronosyl-L-rhamnose G-106

[218780-33-7]

[76819-10-8]



α-Pyranose-*form*

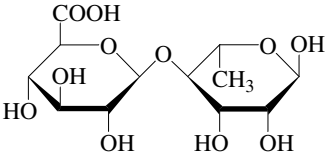
$C_{12}H_{20}O_{11}$ 340.283

Isol. from the acid hydrolysate of an acidic polysaccharide from *Chlorella vulgaris* cells. Powder. $[\alpha]_D^{28}$ +74 (c, 1 in H_2O).

Ogawa, K. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 2030-2031 (*isol, pmr, cmr*)

4-*O*-β-D-Glucopyranuronosyl-L-rhamnose G-107

[67109-66-4]



α-Pyranose-*form*

$C_{12}H_{20}O_{11}$ 340.283

Reducing disaccharide. Isol. from partial acid hydrolysate from the seaweeds *Acrosiphonia centralis* and *Ulva lactuca*. Constit. of the repeating unit of the capsular antigen of *Klebsiella* K70 and capsular antigen of *Escherichia coli* 06:K54:H10.
$[\alpha]_D$ -41 (-30) (H_2O).

α-Pyranose-*form*

Me glycoside, 2,3-O-*isopropylidene, tri-Ac, Me ester:* [79291-99-9]
$C_{23}H_{34}O_{14}$ 534.513
Powder. $[\alpha]_D^{23}$ -33.5 (c, 2.1 in $CHCl_3$).

[84366-53-0]

O'Donnell, J.J. *et al., J.C.S.*, 1959, 2168 (*isol*)
McKinnell, P.J. *et al., J.C.S.*, 1962, 2082
Dutton, G.G.S. *et al., Carbohydr. Res.*, 1978, **62**, 321 (*isol, pmr*)
Betaneli, V.I. *et al., Carbohydr. Res.*, 1981, **94**, C1 (*deriv, cmr*)
Hofmann, P. *et al., Carbohydr. Res.*, 1985, **139**, 261 (*isol, cmr, pmr*)

Glucosylglycerol phosphate synthase G-108

*E.C. 2.4.1.213. ADP-glucose:*sn-*glycerol-3-phosphate 2-β-D-glucosyltransferase*

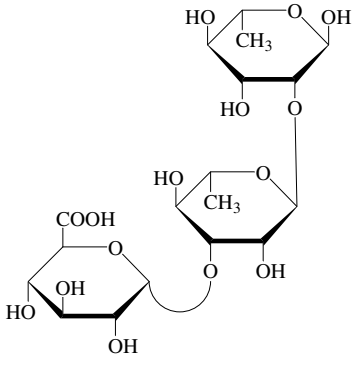
A hexosyltransferase enzyme. Isol. from salt-stressed cells of the marine cyanobacterium *Synechocystis*. Catalyses the reaction of

ADP-D-glucose with *sn*-glycerol 3-phosphate to give ADP and 2-(β-D-glucosyl)-*sn*-glycerol 3-phosphate.

Hagemann, M. *et al., Curr. Microbiol.*, 2001, **43**, 278-283

α-D-Glucuronopyranosyl-(1 →3)-α-L-rhamnopyranosyl-(1 →2)-α-L-rhamnopyranose G-109

[256374-54-6]



α-Pyranose-*form*

$C_{18}H_{30}O_{15}$ 486.426

Constit. of the cells of *Chlorella vulgaris* K-22. Solid.
Mp 166-176° dec. $[\alpha]_D^{24}$ +46 (c, 0.3 in H_2O) (nat.). $[\alpha]_D$ +12.1 (c, 0.32 in H_2O) (equilib.) (synthetic).

Ogawa, K. *et al., Carbohydr. Res.*, 1999, **321**, 128-131 (*isol, struct*)
Sajtos, F. *et al., Carbohydr. Res.*, 2001, **334**, 253-259 (*synth*)

Glumitocin G-110

[Ser⁴,Gln⁸]oxytocin

[10052-67-2]

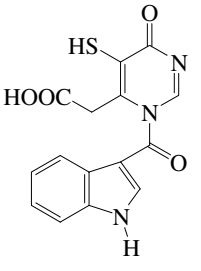
Cys-Tyr-Ile-Ser-Asn-Cys-Pro-Gln-Gly-NH_2

$C_{40}H_{60}N_{12}O_{13}S_2$ 981.119

Peptide; struct. of reduced form shown. Isol. from the ray *Raja clavata*.

Acher, R. *et al., Biochim. Biophys. Acta*, 1965, **107**, 393-396 (*isol*)
Klieger, E. *et al., Experientia*, 1968, **24**, 13-14 (*synth*)
Manning, M. *et al., Experientia*, 1968, **24**, 659-660 (*synth*)

Glusun I G-111

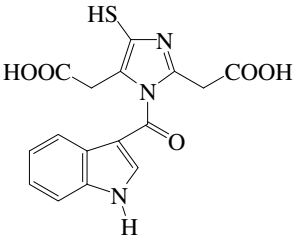


$C_{15}H_{11}N_3O_4S$ 329.336

Prod. by the marine-derived *Halomonas* sp. RK377. Yellow solid.
Mp 150° dec. λ_{max} 271 (log ϵ 3.31); 278 (log ϵ 3.32); 356 (log ϵ 3.35) (MeOH).

Liang, L. *et al., Dissertation*, Univ. of Göttingen, 2003, (*isol, uv, pmr, cmr, ms*)

Glusun II G-112



$C_{16}H_{13}N_3O_5S$ 359.362

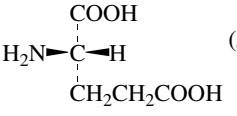
Prod. by the marine-derived *Halomonas* sp. RK377. Orange solid.
λ_{max} 272 (log ϵ 3.72); 365 (log ϵ 3.56) (MeOH).

Liang, L. *et al., Dissertation*, Univ. of Göttingen, 2003, (*isol, uv, pmr, cmr, ms*)

Glutamic acid G-113

2-Aminopentanedioic acid, 9CI. 2-Aminoglutaric acid. Glutaminic acid. Glu. E620. FEMA 3285

[6899-05-4]



(*S*)-*form*

$C_5H_9NO_4$ 147.13

(*R*)-*form*

D-*form*

[6893-26-1]

Component of bacterial cell proteins and peptidolipids.
Leaflets (H_2O).
Mp 213° dec. (rapid heating). $[\alpha]_D^{26}$ -12.9 (H_2O). $[\alpha]_D$ +31 (aq. HCl). Tasteless.

Hydrochloride: [617-61-8]
Prisms (HCl aq.). Mp 209° dec. $[\alpha]_D^{20}$ -24.5 (H_2O).

N-*Me:* N-*Methyl-D-glutamic acid*
[77481-28-8]
$C_6H_{11}NO_4$ 161.157
Isol. from the mollusc *Scapharca broughtonii*.

(*S*)-*form*

L-*form*

[56-86-0]

Obt. from acid hydrol. of proteins. Seasoning additive in food manuf. (as Na, K and NH_4 salts). Intermed. in 2,5-Diaminopentanoic acid, D-122 biosynth. Excitatory CNS transmitter. Dietary supplement, nutrient. Rhombic cryst. (EtOH aq.). Spar. sol. EtOH, H_2O (0.84 g/100g at 25°).
Mp 224-225° (211-213°, 247-249°) dec. $[\alpha]_D^{25}$ +17 (c, 2 in H_2O). $[\alpha]_D^{25}$ +46.8 (c, 2 in 5*M* HCl). pK_{a1} 2.2; pK_{a2} 4.2; pK_{a3} 9.6 (25°,NH_2). Isoelectric point 3.24. Appetising taste.
▶ Human systemic effects by ingestion and intravenous routes.
LZ9700000

Hydrochloride: [138-15-8] Dietary supplement, nutrient, flavouring agent and enhancer. Used in treatment of achlorhydria or hypochlorhydria. Mp 202° dec Mp 213° (rapid heating).

N-*Me:* N-*Methyl-L-glutamic acid*
[6753-62-4]
$C_6H_{11}NO_4$ 161.157
Isol. from the mollusc *Scapharca broughtonii*. Hygroscopic solid (as hydrochloride).
Mp 139-142° (hydrochloride). $[\alpha]_D^{25}$ +2.7 (c, 7.0 in H_2O).

[997-42-2, 5996-22-5, 7558-63-6, 11070-68-1, 19285-83-7, 21752-29-4, 24938-00-9, 25513-46-6, 25683-11-8, 63663-21-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 589D; 590A; 590C; 678B; 781D (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1077C; 1120A; 1277B (*nmr*)
Org. Synth., Coll. Vol., 1, 1932, 286 (*synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, (Chapter 25), Wiley, N.Y., 1961, 1929 (*isol, synth, rev*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Sequieira, A. *et al., Acta Cryst. B*, 1972, **28**, 2514 (*cryst struct*)
Voelter, W. *et al., Monatsh. Chem.*, 1974, **105**, 1110-1135 (*cmr*)
Traldi, P. *et al., Org. Mass Spectrom.*, 1982, **17**, 245 (*ms*)
Dunitz, J.D. *et al., Acta Cryst. C*, 1995, **51**, 1377 (*cryst struct*)
Burger, K. *et al., Eur. J. Org. Chem.*, 2000, 199-204 (*N-Me*)
Tarui, A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2003, **134**, 79-84 (*N-Me Scapharca constits*)

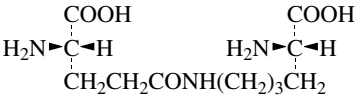
Glutamylglycyl-4-hydroxystyrylamine G-114

α-Glutamyl-N-*[2-(4-hydroxyphenyl)ethenyl]glycinamide, 9CI*

$C_{15}H_{19}N_3O_5$ 321.332

(*S*)-(*E*)-*form* [154887-09-9]
Isol. from the sponge *Anchinoe tenacior*.
$[\alpha]_D$ -4.6 (c, 1 in MeOH). λ_{max} 220 (ε 7320); 283 (ε 9650); 290 (sh); 320 (sh) (MeOH).
Casapullo, A. *et al., Tet. Lett.*, 1994, **35**, 2421 (*isol, pmr, cmr, uv, ir*)
Gurjar, M.K. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 1244 (*synth, pmr*)

N^6-γ-Glutamyllysine G-115



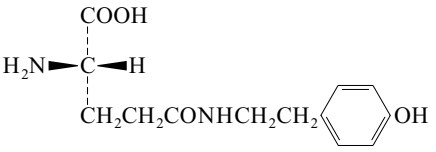
$C_{11}H_{21}N_3O_5$ 275.304

L-L-*form* [17105-15-6]
Cross-linking agent in the protein of the hair of mammals. Also found in fish eggs.
Cryst. (EtOH aq.). $[\alpha]_D^{30}$ +34.3 (c, 1 in 0.1 *M* HCl). Dec. at 250°.
N^{Glu}-*Benzyloxycarbonyl:*
Cryst. (H_2O). Mp 204°.

[75684-67-2, 153882-32-7]

Zahn, H. *et al., Chem. Ber.*, 1963, **96**, 2566 (*synth*)
Caldwell, J.B. *et al., Aust. J. Chem.*, 1971, **24**, 435 (*synth*)
Harding, H.W.J. *et al., Biochim. Biophys. Acta*, 1972, **257**, 37 (*isol*)
Finot, P.A. *et al., Adv. Exp. Med. Biol.*, 1978, **105**, 549 (*synth*)
Griffin, M. *et al., Mol. Cell. Biochem.*, 1984, **58**, 37 (*rev*)
Kubilus, J. *et al., Mol. Cell. Biochem.*, 1984, **58**, 129 (*rev*)
Lloyd, J.R. *et al., Biomed. Environ. Mass Spectrom.*, 1988, **15**, 399 (*ms*)
Kumazawa, Y. *et al., Fish. Sci.*, 1996, **62**, 331 (*isol*)

γ-Glutamyltyramine G-116



$C_{13}H_{18}N_2O_4$ 266.296

(*S*)-*form*
L-*form*
[65520-56-1]
Isol. from aerial parts of *Tephrosia noctiflora*. Also prod. by the mollusc *Aplysia californica*.
Cryst.
Mp 218-219°. $[\alpha]_D^{20}$ +18 (c, 1 in 1*M* HCl).
Forgacs, P. *et al., Phytochemistry*, 1980, **19**, 1225
McCaman, M.W. *et al., J. Neurochem.*, 1985, **45**, 1828

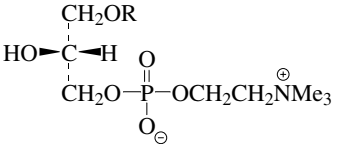
Glycerol, INN G-117

1,2,3-Propanetriol, 9CI. Glycerin, JAN, USAN. Glyceritol. Amylac. Babylax. Bulboid. Cristal. Dagralax. Glyrol. Luxoral. Meprolax. Osmoglyn. E422. FEMA 2525. Many other names
[56-81-5]
$HOCH_2CH(OH)CH_2OH$
$C_3H_8O_3$ 92.094
Many acyl derivs. (glycerides) have separate entries. Obt. on large scale by alkaline hydrol. of fats during soap manuf. and by other routes. Found extensively in esterified form in animal and plant glycerides. Humectant, emollient and solvent, used in cosmetics and pharmaceutical products, foods, tobacco processing and extensively in numerous industrial and domestic prods. Component of alkyd resins and polyurethanes. Used for detn. of B; photometric detn. of Co. Mild laxative and diuretic. Syrup with sweet taste. Misc. H_2O, EtOH; insol. C_6H_6, $CHCl_3$, CCl_4. d_{15}^{15} 1.27.
Mp 17.8°. Bp 290° part. dec. Bp_{20} 182°. n_D^{20} 1.4720. pK_{a1} 14.4. V. hygroscopic. Steam-volatile.
▶ Fl. p. 160°, autoignition temp. 370/393°. Reacts violently or explosively with many oxid. agents. OES: long-term 10 mg m^{-3} (mist). Skin and eye irritant. Ingestion can cause headache and vomiting. Exp. reprod. effects. MA8050000

[6990-26-7, 18673-08-0, 28959-04-8, 36887-04-4, 51432-61-2, 69790-27-8, 117591-83-0, 117591-84-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 183A; 224D; 225D; 1157C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 283C; 341A; **2**, 397C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 262A; 295A; 296C (*ir*)
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, New York, 1947, **1**, 91 (*use*)
Gidez, L.I. *et al., J.A.C.S.*, 1952, **74**, 2413 (*synth*)
Miner, C.S. *et al., Glycerol, Am. Chem. Soc. Monograph No. 117*, N.Y., 1953, (*rev*)
Nessonova, G.D. *et al., Zavod. Lab.*, 1959, **25**, 786 (*detn, Co*)
Newman, A.A. *et al., Glycerol, Am. Chem. Soc. Monograph No. 117*, Morgan-Grampian, London, 1968, (*rev*)
Voelter, W. *et al., Angew. Chem., Int. Ed.*, 1970, **9**, 803 (*cmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 139
Van de Sande, C.C. *et al., J.A.C.S.*, 1975, **97**, 4613 (*ms*)
Budden, R. *et al., Arzneim.-Forsch.*, 1978, **28**, 1579 (*pharmacol*)
Carmaniu, S. *et al., Arch. Int. Physiol. Biochim.*, 1980, **88**, 255 (*metab*)
Frank, M.S. *et al., Pharmacotherapy (Carlisle, Mass.)*, 1981, **1**, 147 (*rev, pharmacol*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **12**, 681 (*rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 204-206
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 7th edn., Akademie-Ve lag*, 1994, 169 (*synonyms*)

Glycerol 1-alkanoate 3-phosphocholines G-118



The *R*-enantiomers (illus.), to which props. given refer, are the biol. important species. Intermeds. in lipid biosynth.

Glycerol 1-dodecanoate 3-phosphocholine [3476-42-4]
[20559-18-6]
$C_{20}H_{42}NO_7P$ 439.528
No phys. props. reported.

Glycerol 1-(2,12-dimethyltridecanoate) 3-phosphocholine
Stellettacholine B

$C_{23}H_{48}NO_7P$ 481.609
Constit. of a *Stelletta* sp. Amorph. solid. $[\alpha]_D^{21}$ -3.2 (c, 0.09 in MeOH).

Glycerol 1-tetradecanoate 3-phosphocholine
4,7-Dihydroxy-N,N,N-*trimethyl-10-oxo-3,5,9-trioxa-4-phosphatricosan-1-aminium inner salt 4-oxide, 9CI*
[13699-45-1]
[20559-16-4]

$C_{22}H_{46}NO_7P$ 467.582
No phys. props. reported.

Glycerol 1-hexadecanoate 3-phosphocholine
4,7-Dihydroxy-N,N,N-*trimethyl-10-oxo-3,5,9-trioxa-4-phosphapentacosan-1-aminium hydroxide inner salt 4-oxide, 9CI. Choline hydroxide dihydrogen phosphate inner salt 3-ester with 1-monopalmitin. 1-Palmitoylglycero-3-phosphocholine. Choline phosphate 3-ester with 1-monopalmitin.* ***α-Lysolecithin***
[17364-16-8]

$C_{24}H_{50}NO_7P$ 495.635
Constit. of biomembranes.
$[\alpha]_{Hg}^{22}$ -4.3 (c, 3.5 in $CHCl_3$/MeOH).

Glycerol 1-octadecanoate 3-phosphocholine
4,7-Dihydroxy-N,N,N-*trimethyl-10-oxo-3,5,9-trioxa-4-phosphaheptacosan-1-aminium hydroxide inner salt 4-oxide, 9CI*
[19420-57-6]

$C_{26}H_{54}NO_7P$ 523.689
Cryst. Mp 235-237°. $[\alpha]_D^{20}$ -3 (c, 5.0 in 1:1 $CHCl_3$/MeOH).

Glycerol 1-(3,17-dimethyloctadecanoate) 3-phosphocholine
Homaxicholine A

$C_{28}H_{58}NO_7P$ 551.743
Constit. of *Homaxinella* sp. Amorph. solid.

Glycerol 1-(*cis*-11,12-methyleneoctadecanoate) 3-phosphocholine
1-O-*[10-(2-Hexylcyclopropyl)decanoyl]glycero-3-phosphocholine*
[251092-30-5]

$C_{27}H_{54}NO_7P$ 535.7
Constit. of *Spirastrella abata*. Amorph. solid.

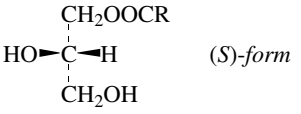
Glycerol 1-(13*Z*-eicosenoate) 3-phosphocholine
1-O-*(13-Eicosenoyl)glycero-3-phosphocholine*
[251092-31-6]

$C_{28}H_{56}NO_7P$ 549.727
Constit. of *Spirastrella abata*. Amorph. solid.

Arnold, D. *et al., Annalen*, 1967, **709**, 234-239 (*hexadecanoate, octadecanoate, synth*)
Brandt, A.E. *et al., Biochim. Biophys. Acta*, 1967, **144**, 605-612 (*dodecanoate, synth*)
Eibl, H. *et al., Annalen*, 1970, **738**, 161-169 (*hexadecanoate, synth*)
Dorset, D.L. *et al., Biochim. Biophys. Acta*, 1975, **380**, 257-263 (*hexadecanoate, cryst struct*)
Spiker, R.C. *et al., Biochim. Biophys. Acta*, 1975, **388**, 361-373 (*hexadecanoate, Raman*)
Yabusaki, K.K. *et al., Chem. Phys. Lipids*, 1976, **17**, 120-127 (*hexadecanoate, synth*)
Ger. Pat., 1976, 2 604 283; *CA*, **85**, 176860z (*octadecanoate, synth, R-form*)
Smith, N.B. *et al., Can. J. Biochem.*, 1978, **56**, 1149-1153 (*hexadecanoate, synth, pmr*)
Lammers, J.G. *et al., Chem. Phys. Lipids*, 1978, **22**, 293-305 (*octadecanoate, synth, ir, pmr*)
Radhakrishnan, R. *et al., Methods Enzymol.*, 1981, **72**, 408-433 (*tetradecanoate, synth*)
Tokumura, A. *et al., Chem. Pharm. Bull.*, 1983, **31**, 4425-4435 (*hexadecanoate, ms*)
Eibl, H. *et al., Angew. Chem., Int. Ed.*, 1984, **23**, 257-271 (*rev*)
Eibl, H. *et al., Chem. Phys. Lipids*, 1988, **47**, 63-68 (*octadecanoate, !synth*)
Ali, S. *et al., Chem. Phys. Lipids*, 1989, **50**, 11-21 (*octadecanoate, synth*)
Baba, N. *et al., Chem. Comm.*, 1990, 1281-1282 (*octadecanoate, synth, S-form*)
Tamura, Y. *et al., Synth. Commun.*, 1994, **24**, 2907-2914 (*octadecanoate, tetradecanoate, synth*)
The Lipid Handbook, (eds. Gunstone, F.D. *et al*), Chapman & Hall, 1994, 634-645 (*rev, biochem*)
Shin, B.A. *et al., J. Nat. Prod.*, 1999, **62**, 1554-1557 (*Spirastrella abata constits*)
Zhao, Q. *et al., J. Nat. Prod.*, 2003, **66**, 725-728 (*Stellettacholine B*)
Hong, C.-O.L. *et al., Lipids*, 2005, **40**, 981-985 (*Homaxicholine A*)

Glycerol 1-alkanoates G-119

1-O-*Acylglycerols. 1-Monoacylglycerols*



(*S*)-*form*

Chiral compds. The *S*-enantiomers correspond to 1-*O*-acyl-*sn*-glycerol. Synth. by protection of 1,2-positions in glycerol or glycerol synthons, esterification of 3-position and deprotection. Enzymatic (lipase-catalysed) routes from glycerol or triacylglycerols have been developed. Stepwise mammalian metabolism of triacylglycerols at the *sn*-1,3-positions by, successively, lingual, gastric, and pancreatic lipases produces 2-monoacylglycerols. Small amounts of *sn*-1,2 and *sn*-2,3-diacylglycerols are intermediates. Further metabolism of 2-monoacylglycerols to glycerol may proceed via isomerisations to 1(3)-monoacylglycerols, but the relevance of this acyl migration has been questioned. In a wider study of the action of lipases of animal and microbial origin, stereoselective preference was mainly for the *sn*-1 position. The *Candida antarctica* A lipase is one of a small number of lipases that will hydrolyse the *sn*-2 position in triacylglycerols. Regioisomerically pure derivatives used for the synthesis of defined triacylglycerols, phospholipids and glycolipids. Long-chain commercial mixtures are non-ionic surfactants used as emulsifiers in food, cosmetics and pharmaceutical manufacturing.
Acyl migrations, particularly under the influence of heat, acidic or alkaline conditions, can result in the interconversion of 1(3)-acyl- and 2-acylglycerols.

Glycerol 1-(2ξ,12-dimethyltridecanoate)
1-O-*(2,12-Dimethyltridecanoyl)glycerol*

$C_{18}H_{36}O_4$ 316.48
Isol. from the sponge *Stelletta* sp. Amorph. solid. $[\alpha]_D^{21}$ -3.5 (c, 0.14 in MeOH) (*S*-form).

Glycerol 1-(13-methyltetradecanoate)
1-O-*(13-Methyltetradecanoyl)glycerol*

$C_{18}H_{36}O_4$ 316.48
Isol. from the sponge *Stelletta* sp. Amorph. solid. $[\alpha]_D^{21}$ +3.4 (c, 0.1 in MeOH) (*S*-form).

Glycerol 1-pentadecanoate
1-O-*Pentadecanoylglycerol*

$C_{18}H_{36}O_4$ 316.48
Isol. from the sponge *Stelletta* sp. Amorph. solid. $[\alpha]_D^{21}$ +2.6 (c, 0.11 in MeOH) (*S*-form).

Glycerol 1-hexadecanoate
1-O-*Hexadecanoylglycerol. α-Monopalmitin. Glycerol 1-palmitate. 1-Palmitoylglycerol. Hexadexanoic acid 2,3-dihydroxypropyl ester*
[542-44-9]
[5309-46-6, 19670-51-0, 26657-96-5, 32899-41-5]

$C_{19}H_{38}O_4$ 330.507
Minor component of olive oil and other vegetable oils.
Mp 71-72° (*R*-form) Mp 77° (± -form). $[\alpha]_D$ -4.3 (c, 10 in Py) (±-form).

3-O-*β-D-Galactopyranoside: 1*-O-*β-D-Galactopyranosyl-3*-O-*hexadecanoylglycerol*
[35949-84-9]
$C_{25}H_{48}O_9$ 492.649
Constit. of the marine alga *Oscillatoria rosea* and *Spongia* cf. *hispida*. Platelet aggregation inhibitor. Amorph. powder.
Mp 119-121°. $[\alpha]_D^{31}$ +9.2 (c, 0.8 in MeOH). C-2 shows (*S*)-config.

3-O-*β*-*D*-*Glucopyranoside:* ***Codioside A***
[358368-42-0]
$C_{25}H_{48}O_9$ 492.649
Isol. from the green alga *Codium iyengarii*.
$[\alpha]_D$ +16.3 (c, 0.7 in MeOH).

Glycerol 1-(9-hexadecenoate)
$C_{19}H_{36}O_4$ 328.491
3-O-*β*-*D*-*Galactopyranoside:* [157807-76-6]
$C_{25}H_{46}O_9$ 490.633
Isol. from the marine alga *Oscillatoria rosea* NIES-208. Platelet aggregation inhibitor. Amorph. powder. $[\alpha]_D^{31}$ +8.6 (c, 0.7 in MeOH).

Glycerol 1-(4,7,10,13-hexadecatetraenoate)
$C_{19}H_{30}O_4$ 322.444
3-O-*β*-*D*-*Galactopyranoside:* [189373-34-0]
$C_{25}H_{40}O_9$ 484.586
Constit. of the marine alga *Oltmannsiellopsis unicellularis* NIES-359. Amorph. powder. $[\alpha]_D^{23}$ -18.7 (c, 1.6 in MeOH).

Glycerol 1-(9*Z*-octadecenoate)
1-O-*(9Z-Octadecenoyl)glycerol*. *α-Monoolein*. *1-Oleoylglycerol*
[30836-40-9]
[111-03-5, 25496-72-4, 34487-30-4, 37220-82-9]
Cryst. Mp 35° (± -form). $[\alpha]_D$ -3.6 (c, 10 in Py) (*R*-form). Exhibits polymorphism.

3-O-*β*-*D*-*Glucopyranoside:* ***Codioside B***
[358368-50-0]
$C_{27}H_{50}O_9$ 518.687
Isol. form the green alga *Codium iyengarii*.
$[\alpha]_D$ +79.9 (c, 0.1 in MeOH).

Glycerol 1-(6*Z*,9*Z*,12*Z*,15*Z*-octadecatetraenoate)
$C_{21}H_{34}O_4$ 350.497
3-O-*β*-*D*-*Galactopyranoside:* ***Hemolysin 1***
[119105-25-8]
$C_{27}H_{44}O_9$ 512.639
Isol. from *Amphidinium carteri* and *Hymenomonas* sp.

Glycerol 1-(10-methyl-9*Z*-octadecenoate)
1-O-*(10-Methyl-9-octadecenoyl)glycerol*
[177602-94-7]
$C_{22}H_{42}O_4$ 370.571
Isol. from the marine fungus *Microsphaeropsis olivacea*. Oil. λ_{max} 210 (MeOH).

Glycerol 1-(2*S*-methoxy-12ξ-methyl-7*Z*,17-octadecadien-5-ynoate)
1-O-*(2-Methoxy-12-methyl-7,17-octadecadien-5-ynoyl)glycerol*
$C_{23}H_{38}O_5$ 394.55
Isol. from the sponge *Stelletta* sp. Pale yellow oil. $[\alpha]_D^{21}$ -1 (c, 0.18 in MeOH) (*S*-form).

Glycerol 1-(7*Z*,9*Z*,12*Z*-octadecatrien-5-ynoate)
1-O-*(7,9,11-Octadecatrien-5-ynoyl)glycerol*
[76152-36-8]
$C_{21}H_{32}O_4$ 348.481
Isol. from red alga *Liagora farinosa*.
$[\alpha]_D$ -1.5 (c, 0.5 in $CHCl_3$).

Glycerol 1-(20-methyl-5*Z*-heneicosenoate)
1-O-*(20-Methyl-5-heneicosenoyl)glycerol*
$C_{25}H_{48}O_4$ 412.652
Isol. from the sponge *Stelletta* sp. Pale yellow oil. $[\alpha]_D^{21}$ +3.4 (c, 0.1 in MeOH) (*S*-form).

Glycerol 1-(4,7,10,13,16,19-docosahexaenoate) (*all-Z*)
Present in annelid worm *Hydroides ezoensis*. Larval metamorphosis hormone.

Glycerol 1-(23-methyl-5*Z*,9*Z*-tetracosadienoate)
1-O-*(23-Methyl-5,9-tetracosadienoyl)glycerol*
$C_{28}H_{52}O_4$ 452.716
Isol. from the sponge *Stelletta* sp. Pale yellow oil. $[\alpha]_D^{21}$ +2.9 (c, 0.05 in MeOH).

Glycerol 1-(8,9-methylenehexadecanoate)
1-O-*[7-(2-Hexylcyclopropyl)heptanoyl]glycerol*. ***Homaxinolin B***
[873304-48-4]
$C_{20}H_{38}O_4$ 342.518
Constit. of a *Homaxinella* sp. Amorph. powder. (*S*)-form.

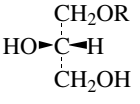
Glycerol 1-(6-bromo-21-methyl-5*E*,9*Z*-docosadienoate)
1-O-*(6-Bromo-21-methyl-5,9-docosadienoyl)glycerol*. ***Homaxinolin A***
[873304-47-3]
$C_{26}H_{47}BrO_4$ 503.559
Constit. of *Homaxinella* sp. Oil. (*S*)-form.

[28060-90-4]

Crossley, A. *et al., J.C.S.*, 1959, 760-764 (*acyl migration*)
Serdavich, B. *et al., J. Am. Oil Chem. Soc.*, 1967, **44**, 381-393 (*acyl migration*)
Jensen, R.G. *et al., Adv. Lipid Res.*, 1976, **14**, 213-247 (*rev, synth*)
Paul, V.J. *et al., Tet. Lett.*, 1980, **21**, 3327-3330 (*Liagora farinosa constit*)
Kobayashi, J. *et al., J.C.S. Perkin 1*, 1989, 101-103 (*Hymenomonas constit*)
Aliya, R. *et al., Pak. J. Pharm. Sci.*, 1991, **4**, 103-111 (*Codium iyengarii constits*)
Yu, C.-M. *et al., Can. J. Chem.*, 1996, **74**, 730-735 (*Microsphaeropsis olivacea constit*)
Rho, M.C. *et al., J. Nat. Prod.*, 1996, **59**, 308-309 (*hexadecanoyl galactoside*)
Rho, M.C. *et al., Planta Med.*, 1996, **62**, 473-474 (*9-hexadecenoyl galactoside*)
Pettit, G.R. *et al., Can. J. Chem.*, 1997, **75**, 920-925 (*1-hexadecanoyl galactoside*)
Rho, M.C. *et al., Phytochemistry*, 1997, **44**, 1507-1509 (*hexadecatetraenoyl galactoside*)
Watanabe, N. *et al., J. Mar. Biotechnol.*, 1998, **6**, 11-15 (*1-docosahexaenoate*)
Lyubachevskaya, G. *et al., Lipids*, 2000, **35**, 1353-1358 (*acyl migration, metab*)
Ali, M.S. *et al., Z. Naturforsch., B*, 2001, **56**, 837-841 (*Codiosides*)
Zhao, Q. *et al., J. Nat. Prod.*, 2003, **66**, 725-728 (*Stelletta alkanoates*)
Qi, S.-H. *et al., Chem. Pharm. Bull.*, 2004, **52**, 986-988 (*1-heptacosanoate*)
Mansoor, T.A. *et al., Lipids*, 2005, **40**, 981-985 (*Homaxinolins*)

Glycerol 1-alkyl ethers G-120

3-O-*Alkyl-1,2-propanediol*



For shorter-chain alkyl ethers see under Glycerol, G-117. Where the abs. configs. are known, the naturally occurring compds. are the *S*-enantiomers illus. (1-*O*-alkyl *sn*-glycerol). Found as lipid components of a variety of species, esp. marine organisms.

Glycerol 1-tridecyl ether
1-O-*Tridecylglycerol*. *3-Tridecyloxy-1,2-propanediol*
[10431-00-2]
[86803-75-0, 126923-58-8 (racemate)]
$C_{16}H_{34}O_3$ 274.443
Constit. of the sponge *Desmapsamma anchorata*. Also detected in the scent gland secretions of the rattlesnake *Crotalus atrox*.
Mp 50.2-51.9° (racemate).

Glycerol 1-tetradecyl ether
3-Tetradecyloxy-1,2-propanediol
[1561-06-4]
[82873-41-4]
Constit. of *Desmapsamma anchorata* and fish oils.

Glycerol 1-(8*Z*-tetradecenyl) ether
3-(8-Tetradecenyloxy)-1,2-propanediol
[488862-82-4]
$C_{17}H_{34}O_3$ 286.454
Constit. of the brown alga *Ishige okamurae*.

Glycerol 1-pentadecyl ether
3-Pentadecyloxy-1,2-propanediol
[10431-02-4]

[124770-96-3]
$C_{18}H_{38}O_3$ 302.496
Constit. of *Desmapsamma anchorata* and *Tethya aurantiaca*.

Glycerol 1-hexadecyl ether
3-Hexadecyloxy-1,2-propanediol. 1-O-*Hexadecyl*-sn-*glycerol. Chimyl alcohol*
[25378-11-4]
[506-03-6, 6145-69-3]
$C_{19}H_{40}O_3$ 316.523
Constit. of squid liver, shark liver and other elasmobranch fish oils. Isol. from mollusc *Archidoris montereyensis*. Constit. of the sponges *Desmapsamma anchorata* and *Tethya aurantia*.
Mp 64.5-65.5° Mp 60° (racemate). Opt. rotn. concn. dependent.

3-O-α-L-*Fucopyranoside:*
$C_{25}H_{50}O_7$ 462.666
Constit. of *Sinularia grandilobata*.
$[\alpha]_D^{25}$ -76.5 (c, 0.92 in H_2O). Config. of glycerol group undefined.

2-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 3*-O-*β-D-xylopyranoside:* ***Myrmekioside A***
[256446-78-3]
$C_{36}H_{68}O_{17}$ 772.923
Constit. of the marine sponge *Myrmekioderma* sp. Amorph. solid. $[\alpha]_D^{22}$ -19.8 (c, 0.5 in MeOH).

2-Ac: 2-O-*Acetyl-1*-O-*hexadecyl*-sn-*glycerol*
[77133-35-8]
$C_{21}H_{42}O_4$ 358.56
Biosynth. precursor to Platelet activating factor. Stimulates cell differentiation and possesses hypotensive activity.

Di-Ac: [10152-42-8]
$C_{23}H_{44}O_5$ 400.598
Isol. from *Aplysia kurodai*. Laxative. $[\alpha]_D^{20}$ -12.8 (c, 0.2 in hexane).

Ditetradecanoyl:
$C_{47}H_{92}O_5$ 737.241
Mp 49-49.5°.

3-O-*Hexadecanoyl: 1*-O-*Hexadecyl-3*-O-*hexadecanoylglycerol*
$C_{35}H_{70}O_4$ 554.936
Isol. from *Lobophytum* sp. (*R*)-config.

Dihexadecanoyl: [1116-45-6]
$C_{51}H_{100}O_5$ 793.348
Isol. from the soft coral *Lobophytum* sp. Solid.
Mp 56-57°. $[\alpha]_D^{20}$ +7.4 (c, 1.0 in $CHCl_3$).

2-Me ether: 1-O-*Hexadecyl-2*-O-*methyl*-sn-*glycerol. 3-(Hexadecyloxy)-2-methoxy-1-propanol*
[96960-92-8]
$C_{20}H_{42}O_3$ 330.55
Inhibitor of protein kinase. Mp 29-30° (35-36°). $[\alpha]_D^{20}$ -9.92 (c, 1.64 in $CHCl_3$).

Glycerol 1-(10-methylhexadecyl) ether
3-[(10-Methylhexadecyl)oxy]-1,2-propanediol. 1-O-*(10-Methylhexadecyl)glycerol*
$C_{20}H_{42}O_3$ 330.55
Constit. of a *Stelletta* sp.

2-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 3*-O-*β-D-xylopyranoside:* ***Myrmekioside B***
$C_{37}H_{70}O_{17}$ 786.95
Constit. of the marine sponge *Myrmekioderma* sp. Amorph. solid. $[\alpha]_D^{22}$ -19.5 (c, 0.5 in MeOH). Possesses 2*R*-config.

Glycerol 1-(13-methylhexadecyl) ether
3-(13-Methylhexadecyloxy)-1,2-propanediol, 9CI
[88948-43-0]
$C_{20}H_{42}O_3$ 330.55
Isol. from a marine sponge *Aaptos* sp.

Glycerol 1-(2*R*-methoxyhexadecyl) ether
1-O-*(2-Methoxyhexadecyl)glycerol. 3-[(2-Methoxyhexadecyl)oxy]-1,2-propanediol*
[130052-37-8]
[16725-32-9 (undefined config), 130052-34-5 (stereoisomer), 130052-41-4, 130052-44-7]
$C_{20}H_{42}O_4$ 346.549
Isol. from shark liver oil. Exhibits antitumour activity.
Mp 39.5° Mp 44.2-44.7° (dimorph.). $[\alpha]_D^{20}$ -3.3 (c, 5 in THF). All 4 stereoisomers have been synthesised.

Glycerol 1-(1*Z*-hexadecenyl) ether
3-(1-Hexadecenyloxy)-1,2-propanediol
[56194-19-5]
[1559-76-8, 34677-26-4]
$C_{19}H_{38}O_3$ 314.507
Isol. from pig's heart plasmalogen; also from *Tethya aurantia*.
Mp 37-39°. $[\alpha]_D^{20}$ -2.1 (c, 1 in $CHCl_3$).

Glycerol 1-(15-methyl-1*Z*-hexadecenyl) ether [180048-12-8]
$C_{20}H_{40}O_3$ 328.534
Constit. of *Gryphus vitreus*.

Glycerol 1-(2*R*-methoxy-3*Z*-hexadecenyl) ether [167171-41-7]
$C_{20}H_{40}O_4$ 344.534
Isol. from shark liver oil.

Glycerol 1-(2*R*-methoxy-4*Z*-hexadecenyl) ether [16725-33-0]
$C_{20}H_{40}O_4$ 344.534
Isol. from shark liver oil and *Gryphus vitreus*.

Glycerol 1-(9*Z*-hexadecenyl) ether
3-(9-Hexadecenoyloxy)-1,2-propanediol
[10431-06-8]
$C_{19}H_{38}O_3$ 314.507
Constit. of the shark *Centrophorus squamosus*.

Glycerol 1-heptadecyl ether
3-Heptadecyloxy-1,2-propanediol
[1607-33-6]
$C_{20}H_{42}O_3$ 330.55
Constit. of *Desmapsamma anchorata* and *Centrophorus squamosus*.

3-O-*Hexadecanoyl: 1*-O-*Heptadecyl-3*-O-*hexadecanoylglycerol*
[843651-44-5]
$C_{36}H_{72}O_4$ 568.962
Isol. from *Lobophytum* sp. (*R*)-config.

Glycerol 1-(15-methylheptadecyl) ether
1-O-*(15-Methylheptadecyl)glycerol. 3-(15-Methylheptadecyloxy)-1,2-propanediol*
[109113-52-2]
$C_{21}H_{44}O_3$ 344.577
Constit. of the lipids of the sponge *Tethya aurantia*. 15′-Config. undetermined.

Glycerol 1-(16-methylheptadecyl) ether
1-O-*(16-Methylheptadecyl)glycerol. 3-(16-Methylheptadecyloxy)-1,2-propanediol*
[109113-51-1]
$C_{21}H_{44}O_3$ 344.577
Constit. of the lipids of the sponge *Tethya aurantia*.

Glycerol 1-(16-methyl-1*Z*-heptadecenyl) ether [180048-11-7]
$C_{21}H_{42}O_3$ 342.561
Constit. of *Gryphus vitreus*.

Glycerol 1-octadecyl ether
3-(Octadecyloxy)-1,2-propanediol. Glyceryl α-steryl ether. 1-O-*Octadecylglycerol. Batyl alcohol.* ***Batilol***
[6129-13-1]
[544-62-7 (undefined config), 10438-95-6 (racemate), 10567-22-3]
$C_{21}H_{44}O_3$ 344.577
Constit. of shark liver and other elasmobranch fish oils and other marine organisms incl. *Desmapsamma anchorata*, *Palythoa liscia*, *Sinularia* sp., *Mycale mytilorum*. Radioprotective agent. Sol. Me_2CO, C_6H_6; fairly sol. MeOH; poorly sol. H_2O, hexane.
Mp 70.5-71.5°. Opt. rotn. concn. dependent. Racemate cryst. Mp.71-73°.
▶ LD_{50} (mus, ipr) 750 mg/kg.

3-O-α-D-*Arabinopyranoside:* [189560-10-9]
$C_{26}H_{52}O_7$ 476.693
Constit. of *Lobophytum microlobulatum*. Abs. config of this and the other glycosides not definitely establ.

3-O-*β*-D-*Arabinopyranoside:* [351443-77-1]
$C_{26}H_{52}O_7$ 476.693
Constit. of a *Cladiella* sp. Cryst. ($CHCl_3$/MeOH).
Mp 98-100°. $[\alpha]_D^{25}$ +80 (c, 0.3 in MeOH).

3-O-*β*-D-*Lyxofuranoside: Batyl lyxofuranoside.* ***Sarsoliside***
[169181-42-4]
$C_{26}H_{52}O_7$ 476.693
Constit. of *Sarcophyton solidum.*

3-O-*(6-Deoxy-β-D-allopyranoside):* ***Lochmodoside***
[120996-02-3]
$C_{27}H_{54}O_7$ 490.719
Isol. from the coral *Sinularia lochmodes.*
Mp 131-132°. $[\alpha]_D^{25}$ -78.6 (c, 0.1 in EtOH).

3-O-*α*-D-*Fucopyranoside:* [283169-79-9]
$C_{27}H_{54}O_7$ 490.719
Constit. of *Sinularia gravis.* Flakes ($CHCl_3$/MeOH).
Mp 138-140°. $[\alpha]_D^{25}$ -10 (c, 0.3 in MeOH).

3-O-*α*-L-*Fucopyranoside:* [263016-44-0]
$C_{27}H_{54}O_7$ 490.719
Isol. from *Sinularia* sp. Prisms (MeOH).
Mp 135-138°. $[\alpha]_D^{30}$ -73 (c, 0.1 in MeOH).

Di-Ac: [18330-40-0]
Mp 39-40°. $[\alpha]_D^{22}$ -11.8 (c, 0.27 in hexane).

3-O-*Hexadecanoyl: 1*-O-*Hexadecanoyl-3*-O-*octadecylglycerol*
[843651-45-6]
$C_{37}H_{74}O_4$ 582.989
Isol. from *Lobophytum* sp. (*R*)-config.

Isopropylidene: $[\alpha]_D^{22}$ -16.2 (c, 0.46 in hexane).

Glycerol 1-(15-methyloctadecyl) ether
3-[(15-Methyloctadecyl)oxy]-1,2-propanediol. 1-O-*(15-Methyloctadecyl)glycerol*
[88948-44-1]
$C_{22}H_{46}O_3$ 358.604
Isol. from a marine sponge *Aaptos* sp.

Glycerol 1-(9-octadecenyl) ether
1-O-*(9Z-Octadecenyl)glycerol. 3-(9-Octadecenyloxy)-1,2-propanediol. Selachyl alcohol. Glyceryl α-oleyl ether. α-Oleyl glyceryl ether*
[34043-91-9]
[15863-83-9, 21994-81-0, 34783-94-3]
$C_{21}H_{42}O_3$ 342.561
Constit. of shark liver and other elasmobranch fish oils. Oil. $[\alpha]_D^{22}$ -15.2 (c, 0.34 in hexane) (as isopropylidene deriv.). Opt. rotn. concn.-dependent. Racemate, low-melting cryst., Mp. 17.6-18.5°.

Glycerol 1-(11-octadecenyl) ether
3-(11-Octadecenyloxy)-1,2-propanediol, 9CI. 1-O-*(11-Octadecenyl)glycerol.* ***Paramecyl alcohol***
[76971-20-5]
$C_{21}H_{42}O_3$ 342.561
Constit. of phospholipids of *Paramecium tetraurelia* and *Paramecium caudatum.*

Glycerol 1-nonadecyl ether
3-Nonadecyloxy-1,2-propanediol
[158789-23-2]
$C_{22}H_{46}O_3$ 358.604

3-O-*Hexadecanoyl: 1*-O-*Hexadecanoyl-3*-O-*nonadecylglycerol*
[843651-46-7]
$C_{38}H_{76}O_4$ 597.016
Isol. from *Lobophytum* sp. (*R*)-Config.

Glycerol 1-eicosyl ether
3-Eicosyloxy-1,2-propanediol. 3-Icosyloxy-1,2-propanediol
[158850-88-5]
$C_{23}H_{48}O_3$ 372.63
Constit. of *Desmapsamma anchorata.*

Glycerol 1-heneicosyl ether
3-Heneicosyloxy-1,2-propanediol
[158789-24-3]
$C_{24}H_{50}O_3$ 386.657
Constit. of *Desmapsamma anchorata.*

Glycerol 1-(17*Z*-tetracosenyl) ether
3-(17-Tetracosenyloxy)-1,2-propanediol
[85210-26-0]
[85210-25-9]
$C_{27}H_{54}O_3$ 426.722
Isol. from sponges *Cinachyra alloclada* and *Ulosa ruetzieri.*

Di-O-*β*-D-*xylopyranoside:* [149151-07-5]
$C_{37}H_{70}O_{11}$ 690.953
Isol. from the sponge *Trikentrion loeve.*
Mp 98-100°. $[\alpha]_D^{25}$ -26.9 (MeOH). The glycoside has *R*-abs. config.

Glycerol 1-(1*Z*,16*Z*-tetracosadienyl) ether
3-(1,6-Tetracosadienyloxy)-1,2-propanediol. ***Hanishenol A***
[188479-74-5]
$C_{27}H_{52}O_3$ 424.706
Isol. from the sponge *Acanthella carteri*. Oil. $[\alpha]_D^{25}$ +4 (c, 0.1 in MeOH).

Glycerol 1-(2-methyl-1*E*,6*Z*-tetracosadienyl) ether
3-O-*(2-methyl-1,6-tetracosadienyloxy)-1,2-propanediol.* ***Hanishenol B***
[188479-75-6]
$C_{28}H_{54}O_3$ 438.733
Isol. from the sponge *Acanthella carteri* (*Acanthella aurentiaca*). Oil. $[\alpha]_D^{25}$ +5 (c, 0.1 in MeOH).

Glycerol 1-pentacosyl ether
3-O-*(Pentacosyloxy)-1,2-propanediol. 1*-O-*Pentacosylglycerol*
[140160-20-9]
$C_{28}H_{58}O_3$ 442.764
Isol. from an unidentified sponge from the South China sea.
Mp 51-52°. MF incorrectly given as C_{26} in the CAS abstract.

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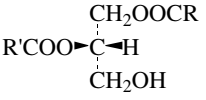
Glycerol 1,2-dialkanoates G-121

1,2-Di-O-*acylglycerols*



(*S*)-*form*

Chiral molecules, whether R and R′ are the same or different. The biol. important S-enantiomer corresponds to 1,2-diacyl-*sn*-glycerol. 3-Phosphates have the *R*-config. Props. of individual compds. refer to this enantiomer unless otherwise stated. See also 1,2-Diacylglycerol 6-sulfoquinovosides, D-111. Synth. by protection of 1,2 and 3-positions in glycerol, deprotection and esterification of 1,2-positions and deprotection of 3-position. Glycerol synthons (oxiranemethanol; 2-propen-1-ol; (chloromethyl)oxirane; 2,3-dihydroxypropanoic acid; and glyceraldehyde) are also utilised, esp. for stereospecific synth. Stepwise mammalian metab. of triacylglycerols at the *sn*-1,3-positions by, successively, lingual, gastric, and pancreatic lipases produces 2-monoacylglycerols. Small amounts of *sn*-1,2 and *sn*-2,3-diacylglycerols are intermediates. Further metab. of 2-monoacylglycerols to glycerol may proceed via isomerisation to 1(3)-monoacylglycerols, but the relevance of this acyl migration has been questioned. In a wider study of the action of lipases of animal and microbial origin, stereoselective preference was mainly for the *sn*-1 position. The *Candida antarctica* A lipase is one of a small number of lipases that will hydrol. the *sn*-2 position in triacylglycerols. Regioisomerically pure derivs. used for the synth. of defined triacylglycerols, phospholipids and glycolipids. Surfactants, used as food emulsifiers. Other food-processing uses for mixts. of mono- and diglycerides include dough strengthener, formulation aid, flavouring agent, lubricant, stabiliser, surface active agent, and texturiser.
Acyl migration, particularly under the influence of heat, acidic or alkaline conditions, can result in the interconversion of 1,2-di-*O*-acyl- and 1,3-di-*O*-acylglycerols. Commercial preps., prepared by chemical glycerolysis of triacylglycerols, contain mixts. of mono- and diacylglycerols. The diacylglycerol component forms an equilib. mixt. with a mole ratio of approx. 1.5:1 of the 1,3- and 1,2(2,3)-regioisomers.

Glycerol 1,2-dioctanoate
Octanoic acid 1-(hydroxymethyl)-1,2-ethanediyl ester. 1,2-Di-O-*octanoylglycerol. α,β-Dicaprylin. Glycerol 1,2-dicaprylate. 1,2-Dioctanoin*
[1069-87-0]
[60514-48-9, 104195-35-9, 113973-38-9]
$C_{19}H_{36}O_5$ 344.49
Protein kinase C activator. Liq. d 0.98. $[\alpha]_D^{22}$ +3.5 (neat). $[\alpha]_D^{22}$ -3.4 (c, 10 in $CHCl_3$). n_D^{23} 1.4745.

Glycerol 1-dodecanoate 2-(3*Z*-hexenoate)
$C_{21}H_{38}O_5$ 370.528
3-O-*[α-D-Galactopyranosyl-(1→6)-α-D-galactopyranoside]:* ***Capsoside A***
[340682-67-9]
$C_{33}H_{58}O_{15}$ 694.812
Constit. of the fruit of *Capsicum annuum* var. *acuminatum*. $[\alpha]_D^{25}$ +30 (c, 0.2 in H_2O).

Glycerol 1,2-didodecanoate
Dodecanoic acid 1-(hydroxymethyl)-1,2-ethanediyl ester. 1,2-Di-O-*dodecanoylglycerol. 1,2-Dilauroylglycerol. α,β-Dilaurin*
[17598-94-6]
[59540-17-9, 60562-15-4]
$C_{27}H_{52}O_5$ 456.705
Cryst. Mp 45-47° (*S*-form) Mp 20° (racemate) Mp 39° (racemate). $[\alpha]_D^{23}$ +6.9 (c, 7.33 in $CHCl_3$). Exhibits polymorphism.

Glycerol 1,2-ditetradecanoate
Tetradecanoic acid 1-(hydroxymethyl)-1,2-ethanediyl ester. 1,2-Di-O-*tetradecanoylglycerol. 1,2-Dimyristoylglycerol. α,β-Dimyristin*
[20255-94-1]
[1069-82-5, 56270-93-0, 60562-16-5]
$C_{31}H_{60}O_5$ 512.812
Cryst. Mp 58.5-60° (*S*-form) Mp 37.5° (racemate) Mp 54° (racemate) Mp 59° (racemate). Shows polymorphism.
3-O-*(6-Deoxy-6-sulfo-α-D-glucopyranoside): 1,2-Di*-O-*myristoyl-3*-O-*(6-sulfoquinovopyranosyl)glycerol*
$C_{37}H_{70}O_{12}S$ 739.019
Constit. of the leaves of craboo (*Byrsonima crassifolia*) (nance). $[\alpha]_D^{25}$ +43 (c, 1 in MeOH) (as Na salt).
Phosphate: See Glycerol 1,2-ditetradecanoate 3-phosphate in *The Combined Chemical Dictionary.*

Glycerol 1-hexadecanoate 2-tetradecanoate
$C_{33}H_{64}O_5$ 540.866
3-O-*β-D-Galactopyranoside:*
$C_{39}H_{74}O_{10}$ 703.008
From *Phormidium tenue*. Oil. $[\alpha]_D^{24}$ -2.8 (c, 0.5 in $CHCl_3$).

Glycerol 2-hexadecanoate 1-tetradecanoate
$C_{33}H_{64}O_5$ 540.866
1-O-*(6-Deoxy-6-sulfo-β-D-glucopyranoside):* ***Crassicaulisin***
$C_{39}H_{74}O_{12}S$ 767.072
Constit. of the red alga *Chondria crassicaulis*. Amorph. powder (as Na salt). $[\alpha]_D$ +43 (c, 0.13 in MeOH) (Na salt).

Glycerol 1,2-dihexadecanoate
1,2-Di-O-*hexadecanoylglycerol. Glycerol 1,2-palmitate. 1,2-Dipalmitin. α,β-Dipalmitin. 1,2-Dipalmitoylglycerol*
[761-35-3]
[6076-30-8, 26657-95-4, 30334-71-5, 109430-50-4, 128308-90-7]
$C_{35}H_{68}O_5$ 568.919
Cryst. ($CHCl_3$/petrol). Mp 68-69°. $[\alpha]_D^{23}$ -2.75 (c, 7.62 in $CHCl_3$).
3-Phosphate: See Glycerol 1,2-dihexadecanoate 3-phosphate in *The Combined Chemical Dictionary.*
3-O-*β-D-Glucopyranoside: 1*-O-*β-D-Glucopyranosyl-2,3-di*-O-*palmitoylglycerol.* ***Codioside D***
[358368-55-5]
$C_{41}H_{78}O_{10}$ 731.061
Isol. from the green alga *Codium iyengarii*.
$[\alpha]_D$ +23 (c, 0.3 in MeOH).
3-O-*(6-Deoxy-6-sulfo-α-D-glucopyranoside): 1,2-Di*-O-*palmitoyl-3*-O-*(6-sulfoquinovopyranosyl)glycerol*
[122991-48-4]
$C_{41}H_{78}O_{12}S$ 795.126
Constit. of the leaves of *Byrsonima crassifolia* (nance) and the algae *Gracilaria verrucosa* and *Sargassum parvivesiculosum*. Amorph. powder. $[\alpha]_D^{25}$ +42.5 (c, 1 in MeOH).

Glycerol 1-(9*Z*-hexadecenoate) 2-tetradecanoate
$C_{33}H_{62}O_5$ 538.85
3-O-*β-D-Galactopyranoside:* [133174-19-3]
$C_{39}H_{72}O_{10}$ 700.992
From cyanobacterium *Phormidium tenue*. Algicide, autolytic agent. Oil. $[\alpha]_D^{24}$ -2.8 (c, 0.5 in $CHCl_3$).

Glycerol 1,2-di-(8*E*-hexadecenoate)
1,2-Di-O-*(8*E*-hexadecenoyl)glycerol*
$C_{35}H_{64}O_5$ 564.888

3-O-*β*-D-*Glucopyranoside: 1*-O-*β*-D-*Glucopyranosyl-2,3-di*-O-*(8-hexadecenoyl)glycerol*
$C_{41}H_{74}O_{10}$ 727.03
Constit. of the leaves of *Byrsonima crassifolia* (nance).
$[\alpha]_D^{25}$ -8 (c, 1 in MeOH).

3-O-*(6-Deoxy-6-sulfo-α-D-glucopyranoside): 1,2-Di*-O-*(8-hexadecenoyl)-3*-O-*(6-sulfoquinovopyranosyl)glycerol*
$C_{41}H_{74}O_{12}S$ 791.094
Constit. of the leaves of *Byrsonima crassifolia* (nance).
$[\alpha]_D^{25}$ +50 (c, 1 in MeOH).

Glycerol 1,2-di-(9*Z*-hexadecenoate)
$C_{35}H_{64}O_5$ 564.888

3-O-*β*-D-*Galactopyranoside:* [404582-92-9]
$C_{41}H_{74}O_{10}$ 727.03
Isol. from the marine bacillariophycean microalga *Nitzschia* sp.
Viscous liq. $[\alpha]_D$ -5 (c, 0.2 in $CHCl_3$).

Glycerol 1,2-di(7*Z*,10*Z*-hexadecadienoate)
1,2-Di-(7,10-hexadecadienoyl)glycerol
$C_{35}H_{60}O_5$ 560.856

3-O-*β*-D-*Galactopyranoside:* [171743-40-1]
$C_{41}H_{70}O_{10}$ 722.998
Isol. from the green alga *Chlorella vulgaris*. Antitumour promotor.
Oil. $[\alpha]_D^{26}$ -2.1 (c, 0.2 in $CHCl_3$).

Glycerol 1-octadecanoate 2-hexadecanoate
2-O-*Hexadecanoyl-1*-O-*octadecanoylglycerol. α-Stearo-β-palmitin*
$C_{37}H_{72}O_5$ 596.973
Cryst. (hexane) (racemate). Mp 69-71° (racemate).

Glycerol 2-octadecanoate 1-hexadecanoate
Octadecanoic acid 1-(hydroxymethyl)-2-[(1-oxohexadecyl)oxy]ethyl ester, 9CI. 1-O-*Hexadecanoyl-2*-O-*octadecanoylglycerol. α-Palmito-β-stearin*
[20296-26-8]
$C_{37}H_{72}O_5$ 596.973
Cryst. (hexane) (racemate). Mp 59-61° (racemate).

Glycerol 1,2-dioctadecanoate
Octadecanoic acid 1-(hydroxymethyl)-1,2-ethanediyl ester. 1,2-Di-O-octadecanoylglycerol. Glycerol 1,2-distearate. α,β-Distearin. Cithrol EDS. E471
[1188-58-5]
[1323-83-7, 1429-59-0, 10567-21-2, 51063-97-9]
$C_{39}H_{76}O_5$ 625.026
Cryst. Mp 74-76° (*S*-form) Mp 59.5° (racemate) Mp 71-72° (racemate). Shows polymorphism.

3-Phosphate: See Glycerol 1,2-dioctadecanoate 3-phosphate in *The Combined Chemical Dictionary.*

3-O-*(6-Deoxy-6-sulfo-α-D-glucopyranoside):* [267900-52-7]
[184914-82-7 (Na salt)]
$C_{45}H_{86}O_{12}S$ 851.233
Isol. from the marine dinoflagellate *Amphidinium carterae.*

3-O-*(6-Amino-6-deoxy-α-D-glucopyranoside):* ***Avrainvilloside***
$C_{45}H_{87}NO_9$ 786.184
Isol. from the green alga *Avrainvillea nigricans*. Amorph. solid.
$[\alpha]_D^{25}$ +25 (c, 0.3 in MeOH).

Glycerol 1-(9*Z*-octadecenoate) 2-tetradecanoate
1-O-*(9Z-Octadecenoyl)-2*-O-*tetradecanoylglycerol. 2*-O-*Myristoyl-1*-O-*oleoylglycerol*
$C_{35}H_{66}O_5$ 566.903

3-Phosphate:
$C_{35}H_{67}O_8P$ 646.883
No phys. props. reported.

3-O-*β*-D-*Galactopyranoside:* [133174-21-7]
$C_{41}H_{76}O_{10}$ 729.045
From *Phormidium tenue*. Oil. $[\alpha]_D^{24}$ -2.5 (c, 0.5 in $CHCl_3$).

Glycerol 1-(9*E*-octadecenoate) 2-hexadecanoate
$C_{37}H_{70}O_5$ 594.957

3-O-*(6-Deoxy-6-sulfo-α-D-glucopyranoside): 1-Oleoyl-2-palmitoyl-3-(6-sulfoquinovopyranosyl)glycerol*
[222991-63-1]
$C_{43}H_{80}O_{12}S$ 821.164
Constit. of the brown alga *Dictyota ciliolata*. Amorph. solid.
Incorrect struct. assigned in CA.

Glycerol 1-(9*Z*-octadecenoate) 2-hexadecanoate
9-Octadecenoic acid 3-hydroxy-2-[(1-oxohexadecyl)oxy]propyl ester. 2-O-*Hexadecanoyl-1-(9Z-octadecenoyl)glycerol*
[38991-91-2]
$C_{37}H_{70}O_5$ 594.957
Oil. *R*-enantiomer prepd.

3-Phosphate: 9-Octadecenoic acid 1-[[(1-oxohexadecyl)oxy]-methyl]-2-(phosphonoxy)ethyl ester
[10015-87-9]
$C_{37}H_{71}O_8P$ 674.937
Racemate prepd.

3-O-*[β-D-Galactopyranosyl-(1→4)-β-D-glucopyranoside]:* ***Codioside C***
[358368-88-4]
$C_{49}H_{90}O_{15}$ 919.241
Isol. from the green alga *Codium iyengarii*.
$[\alpha]_D$ +6.9 (c, 1 in MeOH). Position of fatty acids may be reversed.

Glycerol 2-(9*Z*-octadecenoate) 1-hexadecanoate
9-Octadecenoic acid 1-(hydroxymethyl)-2-[(1-oxohexadecyl)oxy]ethyl ester. 1-O-*Hexadecanoyl-2*-O-*(9Z-octadecenoyl)glycerol. 2-Oleoyl-1-palmitoylglycerol. α-Palmito-β-olein*
[29541-66-0]
[3123-73-7]
$C_{37}H_{70}O_5$ 594.957

3-Phosphate:
$C_{37}H_{71}O_8P$ 674.937
Mp 192-194° (as NH_4 salt). $[\alpha]_D$ +4.5 (c, 3 in $CHCl_3$) (NH_4 salt).

3-O-*β*-D-*Galactopyranoside: 1*-O-*β*-D-*Galactopyranosylglycerol 3-hexadecanoate 2-(9-octadecenoate)*
$C_{43}H_{80}O_{10}$ 757.099
Constit. of *Arisaema amurense*. Stereochem. not confirmed.

3-O-*[α-D-Galactopyranosyl-(1→6)-β-D-galactopyranoside]:*
$C_{49}H_{90}O_{15}$ 919.241
Constit. of *Arisaema amurense*. Stereochem. not confirmed.

Glycerol 1-(9*Z*-octadecenoate) 2-octadecanoate
9-Octadecenoic acid 3-hydroxy-2-[(1-oxooctadecyl)oxy]propyl ester, 9CI. 2-O-*Octadecanoyl-1*-O-*(9Z-octadecenoyl)glycerol. 1*-O-*Oleoyl-2*-O-*stearoylglycerol. α-Oleo-β-stearin*
[38635-46-0]
[73788-95-1]
$C_{39}H_{74}O_5$ 623.011
Mp 19-20° (racemate).

Glycerol 2-(9*Z*-octadecenoate) 1-octadecanoate
9-Octadecenoic acid 1-(hydroxymethyl)-2-[(1-oxooctadecyl)oxy]ethyl ester, 9CI. 1-O-*Octadecanoyl-2*-O-*(9Z-octadecenoyl)glycerol. 2*-O-*Oleoyl-1*-O-*stearoylglycerol. α-Stearo-β-olein*
[53702-48-0]
[21059-30-3]
$C_{39}H_{74}O_5$ 623.011
Mp 39.5-40° (racemate). $[\alpha]_D$ -2.8 (c, 9.2 in $CHCl_3$) (*S*-form).

Glycerol 1,2-di-(9*E*-octadecenoate)
1,2-Di-O-9E-*octadecenoylglycerol. 1,2-Dielaidoylglycerol*
$C_{39}H_{72}O_5$ 620.995
Mp 25°. $[\alpha]_D^{25}$ -1.85 (c, 1.0 in $CHCl_3$).

Glycerol 1,2-di-(9*Z*-octadecenoate)
1,2-Di-O-9Z-*octadecenoylglycerol. 1,2-Dioleoylglycerol. α,β-Diolein*
[24529-88-2]
[2442-61-7, 3738-74-7, 25637-84-7, 33735-55-6]
$C_{39}H_{72}O_5$ 620.995
Oil. $[\alpha]_D^{25}$ -1.91 (c, 6.2 in $CHCl_3$).
► RK1250000

3-Phosphate: 9-Octadecenoic acid 1-[(phosphonoxy)methyl]-1,2-ethanediyl ester, 9CI. Dioleoylphosphatidic acid
[61617-08-1]

[5487-64-9, 14268-17-8]
$C_{39}H_{73}O_8P$ 700.975
$[\alpha]_D^{22}$ +3.8 (c, 5 in $CHCl_3$) (*R*-form).

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-tetradecanoate
$C_{35}H_{64}O_5$ 564.888
3-O-*β*-D-*Galactopyranoside:* [133174-20-6]
$C_{41}H_{74}O_{10}$ 727.03
From *Phormidium tenue*. Oil. $[\alpha]_D^{24}$ -2.3 (c, 0.8 in $CHCl_3$).

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-hexadecanoate
$C_{37}H_{68}O_5$ 592.941
3-O-*β*-D-*Galactopyranoside:*
$C_{43}H_{78}O_{10}$ 755.083
From *Phormidium tenue*. Oil. $[\alpha]_D^{24}$ -3.4 (c, 0.6 in $CHCl_3$).

Glycerol 2-(9*Z*,12*Z*-octadecadienoate) 1-hexadecanoate
9,12-Octadecadienoic acid 1-(hydroxymethyl)-2-[(1-oxohexadecyl)oxy]ethyl ester. 1-O-*Hexadecanoyl-2*-O-*(9Z,12Z-octadecadienoyl)glycerol. 1*-O-*Palmitoyl-2*-O-*linoleoylglycerol*
[51621-26-2]
[73649-99-7, 96613-82-0]
$C_{37}H_{68}O_5$ 592.941
Oil. $[\alpha]_D^{25}$ +2.5 (neat).
3-O-*[α-D-Galactopyranosyl-(1→6)-β-D-galactopyranoside]:*
[145033-48-3]
$C_{49}H_{88}O_{15}$ 917.225
Constit. of *Arisaema amurense* and wheat flour.
3-O-*β*-D-*Galactopyranoside: 1*-O-*β*-D-*Galactopyranosylglycerol 3-hexadecanoate 2-(9,12-octadecadienoate)*
[28069-27-4]
$C_{43}H_{78}O_{10}$ 755.083
Constit. of *Arisaema amurense* (Araceae).

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-(4*Z*-hexadecenoate)
3-O-*β*-D-*Galactopyranoside:*
$C_{43}H_{76}O_{10}$ 753.067
Isol. from a marine *Oscillatoria* sp. Viscous solid. $[\alpha]_D$ -6 (c, 0.2 in $CHCl_3$).

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-octadecanoate
2-O-*Octadecanoyl-1*-O-*(9Z,12Z-octadecadienoyl)glycerol. 1*-O-*Linoleoyl-2*-O-*stearoylglycerol. α-Linoleo-β-stearin*
$C_{39}H_{72}O_5$ 620.995
Oil. Mp 18.5° (*S*-form) Mp 9-10° (racemate).

Glycerol 2-(9*Z*,12*Z*-octadecadienoate) 1-octadecanoate
9,12-Octadecadienoic acid 1-(hydroxymethyl)-2-[(1-oxooctadecyl)oxy]ethyl ester. 2-O-*(9Z,12Z-Octadecadienoyl)-1*-O-*octadecanoylglycerol. 2*-O-*Linoleoyl-1*-O-*stearoylglycerol. α-Stearo-β-linolein*
[34487-26-8]
$C_{39}H_{72}O_5$ 620.995
Mp 17.5° (*S*-form) Mp 13.5° (racemate).
3-O-*[α-D-Galactopyranosyl-(1→6)-β-D-galactopyranoside]:*
$C_{51}H_{92}O_{15}$ 945.279
Constit. of *Arisaema amurense* (Araceae).

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-(9*Z*-octadecenoate)
9,12-Octadecadienoic acid 3-hydroxy-2-[(1-oxo-9-octadecenyl)oxy]propyl ester. 1-O-*(9Z,12Z-Octadecadienoyl)-2*-O-*(9Z-octadecenoyl)glycerol. 1*-O-*Linoleoyl-2*-O-*oleoylglycerol*
$C_{39}H_{70}O_5$ 618.979
$[\alpha]_D^{20}$ -4.47 (*R*-form).
3-O-*β*-D-*Galactopyranoside: 1*-O-*β*-D-*Galactopyranosylglycerol 2-(9,12-octadecadienoate) 3-(9-octadecenoate)*
$C_{45}H_{80}O_{10}$ 781.121
Constit. of *Arisaema amurense* (Araceae). Has 2*S*-config.

Glycerol 2-(9*Z*,12*Z*-octadecadienoate) 1-(9*Z*-octadecenoate)
2-O-*(9Z,12Z-Octadecadienoyl)-1*-O-*(9Z-octadecenoyl)glycerol. 2-Linoleoyl-1-oleoylglycerol. α-Oleo-β-linolein*
$C_{39}H_{70}O_5$ 618.979
Oil. $[\alpha]_D^{20}$ -2.6 (c, 2.0 in $CHCl_3$) (*R*-form).

Glycerol 1,2-di-(9*Z*,12*Z*-octadecadienoate)
*9,12-Octadecadienoic acid 1-(hydroxymethyl)-1,2-ethanediyl ester. Glycerol 1,2-di-*O-*linoleoate. 1,2-Dilinoleoylglycerol*
[24529-89-3]
[2442-62-8, 68069-29-4, 125356-49-2]
$C_{39}H_{68}O_5$ 616.963
Oil. $[\alpha]_D^{25}$ -2 (c, 1.1 in $CHCl_3$).
3-Phosphate: [13397-95-0]
[17966-17-5]
$C_{39}H_{69}O_8P$ 696.943
No phys. props. reported.
3-O-*β*-D-*Galactopyranoside: 1*-O-*β*-D-*Galactopyranosylglycerol 2,3-di-(9,12-octadecadienoate)*
[88195-88-4]
$C_{45}H_{78}O_{10}$ 779.105
Constit. of *Arisaema amurense* and *Sonchus arvensis*.
$[\alpha]_D$ +26 (MeOH).

Glycerol 2-(9,12,15-octadecatrienoate) 1-hexadecanoate
1-O-*Hexadecanoyl-2*-O-*(9Z,12Z,15Z-octadecatrienoyl)glycerol*
$C_{37}H_{66}O_5$ 590.925
3-O-*[α-D-Galactopyranosyl-(1→6)-β-D-galactopyranoside]:* ***Inulagalactolipid A***
[178174-88-4]
$C_{49}H_{86}O_{15}$ 915.209
Constit. of *Arisaema amurense* and *Inula viscosa*.

Glycerol 1-(9*Z*,12*Z*,15*Z*-octadecatrienoate) 2-tetradecanoate
$C_{35}H_{62}O_5$ 562.872
3-O-*β*-D-*Galactopyranoside:* [133174-17-1]
$C_{41}H_{72}O_{10}$ 725.014
Isol. from the cyanobacterium *Phormidium tenue*. Algicide, tumour inhibitor. Oil. $[\alpha]_D^{24}$ -2.7 (c, 0.7 in $CHCl_3$).

Glycerol 1-(9*Z*,12*Z*,15*Z*-octadecatrienoate) 2-hexadecanoate
$C_{37}H_{66}O_5$ 590.925
3-O-*β*-D-*Galactopyranoside:*
$C_{43}H_{76}O_{10}$ 753.067
From *Phormidium tenue*. Obt. as a mixt. with 1-*O*-(9,12,15-octadecatrienoyl), 2-*O*-(9*E*-hexadecenoyl) ester.

Glycerol 1-(9*Z*,12*Z*,15*Z*-octadecatrienoate) 2-(9*E*-hexadecenoate)
$C_{37}H_{64}O_5$ 588.91
3-O-*β*-D-*Galactopyranoside:* [133174-18-2]
$C_{43}H_{74}O_{10}$ 751.052
From *Phormidium tenue*. Algicide, antitumour agent. Oil. $[\alpha]_D^{24}$ -3.4 (c, 0.8 in $CHCl_3$).

Glycerol 1-(9*Z*,12*Z*,15*Z*-octadecatrienoate) 2-(4*Z*,7*Z*,10*Z*,13*Z*-hexadecatetraenoate)
3-O-*β*-D-*Galactopyranoside:*
$C_{43}H_{68}O_{10}$ 745.004
Isol. from *Dunaliella acidophila*.

Glycerol 1-(9*Z*,12*Z*,15*Z*-octadecatrienoate) 2-(7*Z*,10*Z*,13*Z*-hexadecatrienoate)
$C_{37}H_{60}O_5$ 584.878
3-O-*β*-D-*Galactopyranoside:*
$C_{43}H_{70}O_{10}$ 747.02
Isol. from *Caulerpa taxifolia* and *Chlorella vulgaris*. Oil. $[\alpha]_D^{25}$ -2.8 (c, 0.1 in $CHCl_3$).

Glycerol 2-(9*Z*,12*Z*,15*Z*-octadecatrienoate) 1-(7*Z*,10*Z*,13*Z*-hexadecatrienoate)
$C_{37}H_{60}O_5$ 584.878
3-O-*β*-D-*Galactopyranoside:*
$C_{43}H_{70}O_{10}$ 747.02
Isol. from *Caulerpa taxifolia* and *Chlorella vulgaris*. Oil. $[\alpha]_D^{25}$ -2.8 (c, 0.2 in $CHCl_3$).

Glycerol 2-(9*Z*,12*Z*,15*Z*-octadecatrienoate) 1-octadecanoate
1-O-*Octadecanoyl-2*-O-*(9Z,12Z,15Z-octadecatrienoyl)glycerol*
$C_{39}H_{70}O_5$ 618.979

3-O-*β*-D-*Galactopyranoside:* [178174-86-2]
$C_{45}H_{80}O_{10}$ 781.121
Constit. of *Arisaema amurense*.

Glycerol 1,2-di-(9*Z*,12*Z*,15*Z*-octadecatrienoate)
1,2-Di-O-*(9Z,12Z,15Z-octadecatrienoyl)glycerol. 1,2-Di*-O-*linolenoylglycerol. Glycerol 1,2-dilinolenoate*
[87584-95-0, 111187-16-7]
$C_{39}H_{64}O_5$ 612.932

3-Phosphate: 9,12,15-Octadecatrienoic acid 1-[(phosphonoxy)methyl]-1,2-ethanediyl ester
[94086-57-4]
[34961-23-4]
$C_{39}H_{65}O_8P$ 692.911
$[\alpha]_D^{20}$ +31 (c, 3.5 in $CHCl_3$).

3-O-*β*-D-*Galactopyranoside:*
$C_{45}H_{74}O_{10}$ 775.074
Isol. from the cyanobacterium *Phormidium tenue* and the fruit of *Rosa canina*. Also from *Caulerpa taxifolia*, *Chlorella vulgaris* and *Euphorbia nicaensis*. Oil. $[\alpha]_D^{25}$ -3.8 (c, 0.3 in $CHCl_3$).

3-O-*[9Z,12Z,15Z-Octadecatrienoyl-(→6)-β-D-galactopyranoside]:*
$C_{63}H_{102}O_{11}$ 1035.492
Constit. of the leaves of *Feijoa sellowiana* (feijoa). Oil. $[\alpha]_D$ +6.9 (c, 1.1 in EtOH).

3-O-*(6-Amino-6-deoxy-α-D-glucopyranoside):* ***Strangulatoside A***
[339524-99-1]
$C_{45}H_{75}NO_9$ 774.089
Constit. of *Serratula strangulata* rhizomes. Gum. $[\alpha]_D^{24}$ +25.5 (c, 3 in MeOH). C2-config. unknown.

3-O-*[[3-(4-Hydroxyphenyl)propanoyl]-(→6)-6-amino-6-deoxy-α-D-glucopyranoside]:* ***Strangulatoside B***
[339525-07-4]
$C_{54}H_{83}NO_{11}$ 922.25
Constit. of *Serratula strangulata*. Gum. $[\alpha]_D^{24}$ +25.8 (c, 2.7 in MeOH). C2-config. unknown.

3-O-*[β-D-Allopyranosyl-(1→6)-α-D-glucopyranoside]:* ***Strangulatoside C***
[339525-08-5]
$C_{51}H_{84}O_{15}$ 937.216
Constit. of *Serratula strangulata*. Gum. $[\alpha]_D^{24}$ +25.3 (c, 6 in MeOH). C2-Config. not known.

Glycerol 1,2-di-(6*Z*,9*Z*,12*Z*,15*Z*-octadecatetraenoate)
$C_{39}H_{60}O_5$ 608.9

3-O-*β*-D-*Galactopyranoside (2*R-*):* ***Heterosigma glycolipid I***
[121312-93-4]
$C_{45}H_{70}O_{10}$ 771.042
Isol. from the dinoflagellate *Heterosigma akashiwo*. Oil. $[\alpha]_D^{25}$ -4.5 (c, 1.3 in $CHCl_3$).

3-O-*[α-D-Galactopyranosyl-(1→6)-β-D-galactopyranoside] (2*S-*):*
$C_{51}H_{80}O_{15}$ 933.184
Isol. from *Amphidinium carterae*. Pale yellow powder. $[\alpha]_D^{25}$ +52 (c, 0.8 in MeOH).

Glycerol 1-(3*Z*,6*Z*,9*Z*,12*Z*,15*Z*-octadecapentaenoate) 2-(6*Z*,9*Z*,12*Z*,15*Z*-octadecatetraenoate)
$C_{39}H_{58}O_5$ 606.884

3-O-*β*-D-*Galactopyranoside:* ***Heterosigma glycolipid III***
[144118-09-2]
$C_{45}H_{68}O_{10}$ 769.026
Isol. from the dinoflagellate *Heterosigma akashiwo*. Oil. $[\alpha]_D^{25}$ -4.5 (c, 1.3 in $CHCl_3$).

3-O-*(6*-O-*Octadecanoyl-β-D-glucopyranoside):*
$C_{63}H_{102}O_{11}$ 1035.492
Isol. from *Amphidinium* sp. Oil. $[\alpha]_D^{25}$ -3.9 (c, 0.4 in $CHCl_3$).

3-O-*[β-D-Galactopyranosyl-(1→6)-β-D-galactopyranoside]:*
$C_{51}H_{78}O_{15}$ 931.168
Isol. from the dinoflagellate *Heterocapsa circularisquama*. $[\alpha]_D^{25}$ +54 (c, 0.85 in MeOH).

Glycerol 1,2-di(3*Z*,6*Z*,9*Z*,12*Z*,15*Z*-octadecapentaenoate)
$C_{39}H_{56}O_5$ 604.868

3-O-*β*-D-*Galactopyranoside:* [156458-56-9]
$C_{45}H_{66}O_{10}$ 767.01
Isol. from the marine dinoflagellate *Scrippsiella trochoidea*. Amorph. powder. $[\alpha]_D^{25}$ -6 (c, 0.4 in $CHCl_3$).

Glycerol 1-(5*Z*,8*Z*,11*Z*,14*Z*,17*Z*-eicosapentaenoate) 2-(9*Z*-hexadecenoate)
$C_{39}H_{64}O_5$ 612.932

3-O-*β*-D-*Galactopyranoside:* [404581-88-0]
$C_{45}H_{74}O_{10}$ 775.074
Isol. from a *Nitzschia* sp. Amorph. solid. $[\alpha]_D$ -8 (c, 0.2 in $CHCl_3$).

Glycerol 1-(5*Z*,8*Z*,11*Z*,14*Z*,17*Z*-eicosapentaenoate) 2-(6*Z*,9*Z*,12*Z*,15*Z*-octadecatetraenoate)
$C_{41}H_{62}O_5$ 634.938

3-O-*β*-D-*Galactopyranoside (2*R-*):* ***Heterosigma glycolipid II***
[121245-05-4]
$C_{47}H_{72}O_{10}$ 797.08
Isol. from the dinoflagellate *Heterosigma akashiwo*. Oil. $[\alpha]_D$ -4.1 (c, 1.3 in $CHCl_3$).

Glycerol 2-(5,8,11,14,17-eicosapentaenoate) 1-(6,9,12,15-octadecatetraenoate)
$C_{41}H_{62}O_5$ 634.938

3-O-*[α-D-Galactopyranosyl-(1→6)-α-D-galactopyranoside]:* ***Heterosigma glycolipid IV***
[144118-10-5]
$C_{53}H_{82}O_{15}$ 959.222
Isol. from the dinoflagellate *Heterosigma akashiwo*.

Glycerol 1,2-dioctacosanoate
Octacosanoic acid 1-(hydroxymethyl)-1,2-ethanediyl ester. 1,2-Di-O-*octacosanoylglycerol. α,β-Dimontanylglycerol*
[52363-45-8]
[127039-57-0]
$C_{59}H_{116}O_5$ 905.562
Constit. of *Morus alba* root (white mulberry) bark. Cryst. (EtOAc).
Mp 82-82.5°. Abs. config. of nat. prod. not known.

Ac:
Cryst. (MeOH/$CHCl_3$). Mp 68-69.5°.

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Dai, J.Q. *et al., Phytochemistry*, 2001, **58**, 1305-1309 (*Strangulatosides*)
Ali, M.S. *et al., Z. Naturforsch., B*, 2001, **56**, 837-841 (*Codiosides*)
Shao, Z.Y. *et al., J. Asian Nat. Prod. Res.*, 2002, **4**, 205-209 (*Crassicaulisin*)
Hiraga, Y. *et al., J. Nat. Prod.*, 2002, **65**, 1494-1496 (*Heterocapsa digalactoside*)
Qi, S.-H. *et al., Chem. Pharm. Bull.*, 004, **52**, 986-988 (*Sargassum parvivesiculosum constit*)
Ruberto, G. *et al., Phytochemistry*, 2004, **65**, 2947-2951 (*Feijoa sellowiana galactoside*)
Wu, J. *et al., Chem. Pharm. Bull.*, 2005, **53**, 330-332 (*Amphidinium carterae digalactoside*)
Andersen, R.J. *et al., J. Nat. Prod.*, 2005, **68**, 1428-1430 (*Avrainvilloside*)
Kamal, A. *et al., Tetrahedron: Asymmetry*, 2005, **16**, 1855-1859 (*dihexadecanoate, synth*)

Glycerol 1,3-dialkanoates G-122

*1,3-Di-*O*-acylglycerols*

$RCOOCH_2CH(OH)CH_2OOCR'$

Meso-compds. if the R groups are identical. Potentially opt. active if they are different. Data given here refers to racemates unless stated otherwise. Synth. by protection of 1,2-positions in glycerol or glycerol synthons, esterification of 3-position, deprotection and selective esterification of 1-position. Enzymatic (lipase-catalysed) routes from glycerol or triacylglycerols have been developed. Stepwise mammalian metabolism of triacylglycerols at the *sn*-1,3-positions by, successively, lingual, gastric, and pancreatic lipases produces 2-monoacylglycerols. Small amounts of *sn*-1,2- and *sn*-2,3-diacylglycerols are intermediates. Further metabolism of 2-monoacylglycerols to glycerol may proceed via isomerisation to 1(3)-monoacylglycerols, but the relevance of this acyl migration has been questioned. In a wider study of the action of lipases of animal and microbial origin, stereoselective preference was mainly for the *sn*-1 position. The *Candida antarctica* A lipase is one of a small number of lipases that will hydrolyse the *sn*-2 position in triacylglycerols. Surfactants, used as food emulsifiers. Other food-processing uses for mixtures of mono- and diglycerides include dough strengtheners, formulation aids, flavouring agents, lubricants, stabilisers, surface active agents, and texturisers.

Acyl migration, particularly under the influence of heat, acidic or alkaline conditions, can result in the interconversion of 1,2-di-*O*-acyl- and 1,3-di-*O*-acylglycerols. Commercial preparations, prepared by chemical glycerolysis of triacylglycerols, contain mixtures or mono- and diacylglycerols. The diacylglycerol component forms an equilibrium mixture with a mole ratio of approximately 1.5:1 of the 1,3- and 1,2(2,3)-regioisomers.

Glycerol 1,3-dihexadecanoate

*Hexadecanoic acid 2-hydroxy-1,3-propanediyl ester. 1,3-Di-*O*-hexadecanoylglycerol. Glycerol 1,3-dipalmitate. 1,3-Dipalmitin. α,α′-Dipalmitin*

[502-52-3]
[26657-95-4]

$C_{35}H_{68}O_5$ 568.919

Constit. of *Panax ginseng* (ginseng) and the sea urchin *Temnopleurus toreumaticus*. Cryst. (Me_2CO/hexane at 0°).
Mp 73-74°.

Crossley, A. *et al., J.C.S.*, 1959, 760-764 (*acyl migration*)
Mattson, F.H. *et al., J. Lipid Res.*, 1962, **3**, 281-296 (*rev, acyl migration*)
Serdavich, B. *et al., J. Am. Oil Chem. Soc.*, 1967, **44**, 381-393 (*acyl migration*)
Jensen, R.G. *et al., Adv. Lipid Res.*, 1976, **14**, 213-247 (*rev, synth*)
Rogalska, E. *et al., Chirality*, 1993, **5**, 24-30 (*metab*)
Babu, U.V. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 995-997 (*isol, sea urchin*)

sn-Glycerol 3-phosphate 1-galactosyltransferase G-123

*E.C. 2.4.1.96. UDP-galactose:*sn*-glycerol-3-phosphate 1-α-*D*-galactosyltransferase. Isofloridoside phosphate synthase*

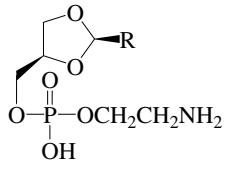
[9076-70-4]

Hexosyltransferase enzyme. Isol. from *Ochromonas* spp. Catalyses the reaction of UDP-D-galactose with *sn*-glycerol 3-phosphate to give UDP and isofloridoside phosphate. Involved in osmoregulation.

Kauss, H. *et al., FEBS Lett.*, 1971, **19**, 131-135
Kauss, H. *et al., Plant Physiol.*, 1976, **58**, 295-298

Glycerophosphoethanolamine acetals G-124

Fuelgen's acetalphosphatides



Absolute Configuration

Related to Phosphatidylethanolamine, P-363. Originally regarded as artifacts, now shown to be genuine natural prods.

Glycerophosphoethanolamine hexadecanal acetal

$C_{21}H_{44}NO_6P$ 437.556

Isol. from the sea anemone *Actinogeton* sp. R = $-(CH_2)_{14}CH_3$.

Glycerophosphoethanolamine heptadecanal acetal

Isol. from *Actinogeton* sp. R = $-(CH_2)_{15}CH_3$.

Glycerophosphoethanolamine 15-methylhexadecanal acetal

Isol. from *Actinogeton* sp. R = $-(CH_2)_{12}CH(CH_3)_2$.

Glycerophosphoethanolamine octadecanal acetal

$C_{23}H_{48}NO_6P$ 465.609

Isol. from *Actinogeton* sp.
$[\alpha]_D$ +15.1. R = $-(CH_2)_{16}CH_3$.

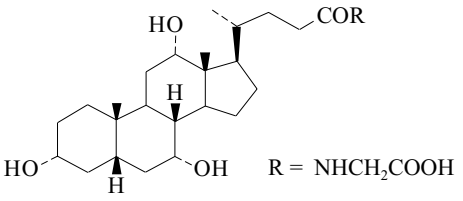
Glycerophosphoethanolamine 9*Z*-octadecenal acetal

Isol. from *Actinogeton* sp. R = $-(CH_2)_7CH{=}CH(CH_2)_7CH_3$.

Tanaka, R. *et al., Lipids*, 2000, **35**, 665-671 (*isol, pmr, ms, struct, abs config, bibl*)

Glycocholic acid G-125

Cholylglycine
[475-31-0]



$C_{26}H_{43}NO_6$ 465.629
Constit. of serum bile acids. Small needles (EtOH aq.). Mp 140-142° Mp 154-155° dec. $[\alpha]_D^{13}$ +27.8 (EtOH). pK_a 4.4.

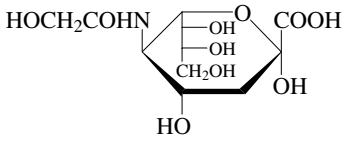
Na salt: [863-57-0]
Cryst. (EtOH/Et_2O). Mp 230-240°. $[\alpha]_D^{23}$ +29.2 (H_2O).

▶ MB9265100

Cortese, F. *et al., J.A.C.S.*, 1935, **57**, 1393 (*synth*)
Cortese, F. *et al., J.A.C.S.*, 1937, **59**, 2532 (*synth*)
Begemann, F. *et al., Z. Klin. Chem. Klin. Biochem.*, 1972, **10**, 29-32 (*isol*)
Games, D.E. *et al., Tet. Lett.*, 1974, **27**, 2377 (*ms*)
Tserng, K.-Y. *et al., J. Lipid Res.*, 1977, **18**, 404 (*synth*)
Shaw, R. *et al., Biomed. Mass Spectrom.*, 1978, **5**, 433 (*ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1234-1235

N-Glycolylneuraminic acid G-126

3,5-Dideoxy-5-[(hydroxyacetyl)amino]-D-glycero-*D*-galacto-*2-nonulosonic acid, 9CI. Porcine sialic acid. NGNA*
[1113-83-3]



α-D-Pyranose-*form*

$C_{11}H_{19}NO_{10}$ 325.272
Isol. from hog submaxillary mucin and starfish *Asterias rubens*. Also found in certain gangliosides and sialoproteins of other animal spp., e.g. horse erythrocytes, horse kidney and beef serum. Mp 185-187°. $[\alpha]_D$ -32 (H_2O). $[\alpha]_D^{22}$ -26.9 (c, 1.34 in H_2O) (1h, equilib.).

8-Me ether: [106073-67-0]
$C_{12}H_{21}NO_{10}$ 339.299
Occurs in gangliosides from the starfish *Asterias forbesi*, *Asterias amurensis* and *Asterias rubens*.

8-Me ether, 9-Ac: [128885-12-1]
$C_{14}H_{23}NO_{11}$ 381.336
Occurs in sialic acids of starfish *Asterias rubens*.

Blix, G. *et al., Nature (London)*, 1955, **175**, 340 (*isol*)
Zilliken, F. *et al., Adv. Carbohydr. Chem.*, 1958, **13**, 237 (*rev*)
Gottschalk, A. *et al., The Chemistry and Biology of Sialic Acids and Related Substances*, Cambridge Univ. Press, 1960, (*rev*)
Warren, L. *et al., Biochim. Biophys. Acta*, 1964, **83**, 129-131 (*8-Me ether, isol*)
Schoop, H.J. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1969, **350**, 155
Schauer, R. *et al., Angew. Chem., Int. Ed.*, 1973, **12**, 127
Corfield, A.P. *et al., Eur. J. Biochem.*, 1976, **68**, 597 (*biosynth*)
Codington, J.F. *et al., Methods Carbohydr. Chem.*, 1976, **7**, 226 (*occur, purifn*)
Kochetkov, N.K. *et al., Biochim. Biophys. Acta*, 1982, **712**, 650-658 (*isol, struct*)
Bergwerff, A.A. *et al., Biochimie*, 1992, **74**, 25-37 (*occur, 8-Me ether, 8-Me ether 9-Ac*)
Kuboki, A. *et al., Tetrahedron*, 1997, **53**, 2387-2400 (*synth, pmr, cmr*)

Sargassum kjellmanianum Glycoprotein G-127

Sulfated glycoprotein antibiotic. Isol. from the alga *Sargassum kjellmanianum*. Antitumour agent. Sol. H_2O, Py; poorly sol. MeOH, $CHCl_3$. $[\alpha]_D$ -82 (H_2O).

Japan. Pat., 1983, 83 174 329; *CA*, **100**, 12641f (*isol*)

Glycoprotein 1 G-128

Glycoprotein. Isol. from *Chlorella vulgaris*. Shows antitumour activity. Sol. H_2O; poorly sol. hexane.

Matsueda, S. *et al., Yakugaku Zasshi*, 1982, **102**, 447-451; 1987, **107**, 694-697 (*isol*)

Glycylalanylprolylmethionylphenylalanylvalinamide G-129

MIP-2
[115525-99-0]
H-Gly-^{2}Ala-Pro-^{4}Met-Phe-Val-NH_2
$C_{29}H_{45}N_7O_6S$ 619.784
Isol. from the pedal ganglion and the anterior byssus retractor muscle of *Mytilus edulis* (blue mussel). Muscle contraction inhibitor.

2-L-Proline analogue: Glycylprolylprolylmethionylphenylalanylvalinamide. MIP-A6
[142629-94-5]
$C_{31}H_{47}N_7O_6S$ 645.822
Isol. from *Achatina fulica*.

2-L-Serine analogue: Glycylserylprolylmethionylphenylalanylvalinamide. MIP-1
[115525-98-9]
$C_{29}H_{45}N_7O_7S$ 635.783
Isol. from the pedal ganglion and the anterior byssus retractor muscle of *Mytilus edulis* (blue mussel). Muscle contraction inhibitor.

4-L-Alanine analogue: Glycylalanylprolylalanylphenylalanylvalinamide
[152247-83-1]
$C_{27}H_{41}N_7O_6$ 559.664
Isol. from the nervous system of the snail *Helix pomatia*.

4-L-Arginine analogue: Glycylalanylprolylarginylphenylalanylvalinamide
[152247-84-2]
$C_{30}H_{48}N_{10}O_6$ 644.773
Isol. from *Helix pomatia* and from *Aplysia kurodai*.

4-L-Leucine analogue: Glycylalanylprolylleucylphenylalanylvalinamide
[152247-94-4]
$C_{30}H_{47}N_7O_6$ 601.745
Isol. from *Helix pomatia*.

4-L-Lysine analogue: Glycylalanylprolyllysylphenylalanylvalinamide. MIP-A2
[142629-90-1]
$C_{30}H_{48}N_8O_6$ 616.759
Isol. from the snails *Achatina fulica* and *Helix pomatia*.

4-L-Phenylalanine analogue: Glycylalanylprolylphenylalanylphenylalanylvalinamide. MIP-A7
[142629-95-6]
$C_{33}H_{45}N_7O_6$ 635.762
Isol. from *Achatina fulica*.

4-L-Tyrosine analogue: Glycylalanylprolyltyrosylphenylalanylvalinamide. MIP-A4
[142629-92-3]
$C_{33}H_{45}N_7O_7$ 651.761
Isol. from *Achatina fulica* and *Helix pomatia*.

4-L-Valine analogue: Glycylalanylprolylvalylphenylalanylvalinamide. MIP-A3
[142629-91-2]
$C_{29}H_{45}N_7O_6$ 587.718
Isol. from *Achatina fulica*.

2-L-Serine, 4-L-tyrosine analogue: Glycylserylprolyltyrosylphenylalanylvalinamide. Helix aspersa *Peptide Ha3*
[152247-89-7]
$C_{33}H_{45}N_7O_8$ 667.761
Isol. from *Helix pomatia* and *Helix aspersa*.

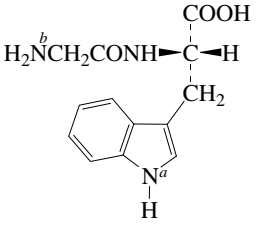
2-L-Valine, 4-L-tyrosine analogue: Glycylvalylprolyltyrosylphenylalanylvalinamide
[152247-92-2]
$C_{35}H_{49}N_7O_7$ 679.815
Isol. from *Helix pomatia*.

2-L-Proline, 4-L-arginine analogue: Glycylprolylprolylargininylphenylalanylvalinamide
[152247-86-4]
$C_{32}H_{50}N_{10}O_6$ 670.81
Isol. from *Helix pomatia*.

Hirata, T. *et al., Biochem. Biophys. Res. Commun.*, 1988, **152**, 1376-1382 (*isol, Mytilus edulis*)
Fujisawa, Y. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1991, **100**, 525-531 (*isol, Mytilus edulis*)
Ikeda, T. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1992, **101**, 245-249 (*isol, Achatina fulica*)
Ikeda, T. *et al., CA*, 1994, **120**, 50479e (*isol*)
Ohtani, M. *et al., Gen. Pharmacol.*, 1997, **29**, 103-111 (*isol, Helix aspersa*)
Fujisawa, Y. *et al., J. Neurosci.*, 1999, **19**, 9618-9634 (*isol, Aplysia constit*)

N-Glycyltryptophan, 9CI G-130

[2189-26-6]



(*S*)-*form*

$C_{13}H_{15}N_3O_3$ 261.28

D-*form* [50632-89-8]
$[\alpha]_D^{26}$ -34.2 (c, 2 in 5*M* HCl).

L-*form* [2390-74-1]
$[\alpha]_D^{25}$ +34.3 (c, 2 in 5M HCl).

Amide: Glycyltryptophanamide. GW amide
[1510-05-0]
[58761-04-9]
$C_{13}H_{16}N_4O_2$ 260.295
Isol. from optic lobes of mature female cuttlefish *Sepia officinalis*.
Myotropic neuropeptide.

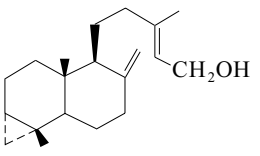
N^b-tert-*Butyloxycarbonyl, Me ester:* [57769-48-9]
$C_{19}H_{25}N_3O_5$ 375.424
Mp 55°. $[\alpha]_D^{25}$ +40.8 (c, 0.5 in $CHCl_3$) (98% ee).

N^b-*Benzyloxycarbonyl:*
$C_{21}H_{21}N_3O_5$ 395.414
Cryst. (AcOH/petrol). Mp 141-142°. $[\alpha]_D^{24}$ +33.3 (c, 2.34 in EtOH).

Rao, K.R. *et al., J. Biol. Chem.*, 1952, **198**, 507 (*synth*)
Robinson, D.S. *et al., J. Biol. Chem.*, 1953, **202**, 1 (*synth*)
Weygand, F. *et al., Chem. Ber.*, 1960, **93**, 2983
Theodoropoulos, D.M. *et al., Biochemistry*, 1962, 933
Katakai, R. *et al., J.O.C.*, 1972, **37**, 327 (*synth*)
Christensen, M. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1978, **359**, 813-818 (*amide, synth*)
Henry, J. *et al., Peptides (N.Y.)*, 1997, **18**, 1469-1474 (*amide, isol*)
Caballero, E. *et al., Tetrahedron: Asymmetry*, 1998, **9**, 3025-3028 (*N-tert-butyloxycarbonyl, Me ester, synth, nmr*)

8(17),13-Gnaphaladien-15-ol G-131

3,18-Cyclo-8(17),13-labdadien-15-ol



(3α,4α,13*E*)–*form*

$C_{20}H_{32}O$ 288.472

(3α,4α,13*E*)-*form*

Carboxylic acid: 8(17),13-Gnaphaladien-15-oic acid. ***Cycloanticopalic acid****. Metasequoic acid B*
[109291-60-3]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Pinus strobus* and *Metasequoia glyptostroboides*. Cryst. Sol. MeOH, hexane, $CHCl_3$; poorly sol. H_2O.
Mp 124-125°. $[\alpha]_D$ +94.

Carboxylic acid, Me ester: [109291-62-5]
$[\alpha]_D^{20}$ +87.5 (c, 1.4 in $CHCl_3$).

(3β,4β,13*E*)-*form*

Carboxylic acid: ***Metasequoic acid A***
[113626-22-5]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Metasequoia glyptostroboides*. Cryst. Sol. MeOH, $CHCl_3$, hexane; poorly sol. H_2O.
Mp 112-113°. $[\alpha]_D$ +36.3.

(*ent*-3α,4α,9β*H*,13*E*)-*form*

Preparguerene
Constit. of *Laurencia filiformis*.
Oil. $[\alpha]_D$ -62.9 (c, 0.6 in $CHCl_3$). Misleading name as it it an alcohol.

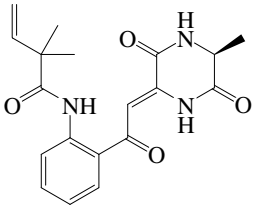
Zinkel, D.F. *et al., Phytochemistry*, 1987, **26**, 769 (*Cycloanticopalic acid*)
Sakan, F. *et al., Chem. Lett.*, 1988, 123 (*Metasequoic acids*)
Rochfort, S.J. *et al., Aust. J. Chem.*, 1996, **49**, 19 (*Preparguerene*)
Abad, A. *et al., J.C.S. Perkin 1*, 1997, 1837-1843 (*synth*)

Octopus GnRH-like peptide G-132

5-OxoPro-Asn-Tyr-His-Phe-Ser-Asn-Gly-Trp-His-Pro-Gly-NH_2
$C_{66}H_{80}N_{20}O_{17}$ 1425.482
Isol. from *Octopus vulgaris*.

Iwakoshi, E. *et al., Biochem. Biophys. Res. Commun.*, 2002, **291**, 1187-1193 (*isol*)

Golmaenone G-133



Absolute Configuration

$C_{19}H_{21}N_3O_4$ 355.393
Alkaloid from the marine fungus *Aspergillus* (culture MFA 212). Radical scavenger and uv protectant. Yellow cryst. ($CHCl_3$).
Mp 160-161°. $[\alpha]_D$ +7.1 (c, 0.4 in $CHCl_3$). CAS no. not found CA 141. λ_{max} 222 (log ϵ 1.8); 247 (log ϵ 2); 327 (log ϵ 1.9); 368 (log ϵ 1.7) ($CHCl_3$).

Li, Y. *et al., Chem. Pharm. Bull.*, 2004, **52**, 375-376 (*isol, cd, pmr, cmr*)

Odontesthes bonariensis Gonadotropin-releasing hormone G-134

[308098-61-5]
5-OxoPro-His-Trp-Ser-Phe-Gly-Leu-Ser-Pro-Gly-NH_2
$C_{52}H_{68}N_{14}O_{13}$ 1097.195
Isol. from brain of the teleost fish *Odontesthes bonariensis* (pejerrey). Chicken GnRH-II and salmon GnRH also isol.

Montaner, A.D. *et al., Endocrinology (Baltimore)*, 2001, **142**, 1453-1460 (*isol*)

Petromyzon marinus Gonadotropin-releasing hormone G-135

*Lamprey GnRH III. **Peforelin, INN**. Luteinizing hormone-releasing factor III (Petromyzon marinus), 9CI*
[147859-97-0]
5-OxoPro-His-Trp-Ser-His-Asp-Trp-Lys-Pro-Gly-NH_2
$C_{59}H_{74}N_{18}O_{14}$ 1259.346
Isol. from brain of the sea lamprey *Petromyzon marinus*.
Gonadotrophin releasing hormone analogue with preferential follicle stimulating hormone (FSH) action.

Sower, S.A. *et al., Endocrinology (Baltimore)*, 1993, **132**, 1125-1131 (*isol*)
Yu, W.H. *et al., Exp. Biol. Med.*, 2002, **227**, 786-793 (*pharmacol*)
Amstalden, M. *et al., Reproduction*, 2004, **127**, 35-43 (*pharmacol, bibl*)

Squalus acanthus Gonadotropin-releasing hormone G-136

Dogfish GnRH. dfGnRH
[101509-61-9]
5-OxoPro-His-Trp-Ser-His-Gly-Trp-Leu-Pro-Gly-NH_2
$C_{57}H_{71}N_{17}O_{12}$ 1186.295
Isol. from the dogfish *Squalus acanthus*.

Lovejoy, D.A. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1992, **89**, 6373-6377 (*isol*)

Gongrine G-137

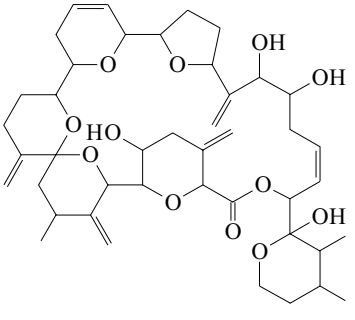
4-[[[(Aminoiminomethyl)amino]carbonyl]amino]butanoic acid, 9CI. γ-(Guanylureido)butanoic acid. 1-Amidino-3-(3-carboxypropyl)urea. γ-(Amidinoureido)butyric acid
[5998-99-2]
$HN{=}C(NH_2)NHCONH(CH_2)_3COOH$
$C_6H_{12}N_4O_3$ 188.186
Isol. from red algae *Gymnogongrus flabelliformis* and *Grateloupia filicina*. Prisms (H_2O).
Mp 208-209° dec.

Picrate: [21808-08-2]
Yellow needles. Mp 208-210° dec. Sinters at ca. 196°.

Ito, K. *et al., Agric. Biol. Chem.*, 1965, **29**, 832; 1969, **33**, 237 (*isol, synth*)
Frankel, M. *et al., J.C.S.(C)*, 1967, 2698 (*synth*)
Wakamiya, T. *et al., Tetrahedron*, 1984, **40**, 235 (*isol, bibl*)

Goniodomin A G-138

[112923-40-7]



$C_{43}H_{60}O_{12}$ 768.94
Polyether macrolide antibiotic. Isol. from the dinoflagellate *Alexandrium hiranoi* (formerly *Goniodoma pseudogoniaulax*). Antifungal agent. $[\alpha]_D^{20}$ +28 (c, 0.13 in MeOH).
▶ MP4780230

Murakami, M. *et al., Tet. Lett.*, 1988, **29**, 1149 (*isol, struct*)
Murakami, M. *et al., Phytochemistry*, 1998, **48**, 85-88 (*biosynth*)

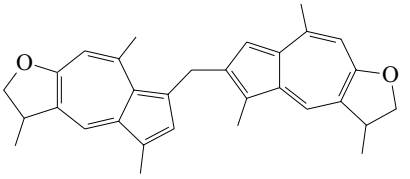
Goniopora toxin G-139

GPT
Polypeptide. Isol. from the coral *Goniopora* sp. Toxin.

Fujiwara, M. *et al., J. Pharmacol. Exp. Ther.*, 1979, **210**, 153-157 (*isol*)

Gorgiabisazulene G-140

[152845-74-4]

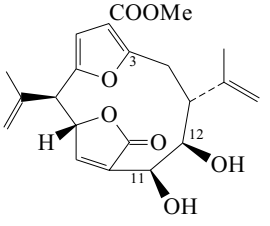


$C_{31}H_{32}O_2$ 436.593
Constit. of an *Acalycigorgia* sp. Purple amorph. solid. $[\alpha]_D^{20}$ -92 (c, 0.05 in $CHCl_3$).

Ochi, M. *et al., Chem. Lett.*, 1993, 2003 (*isol, pmr, cmr*)

Gorgiacerodiol G-141

[138828-00-9]



$C_{21}H_{24}O_7$ 388.416
Constit. of *Pseudopterogorgia acerosa*. Gum. $[\alpha]_D$ +98 (c, 0.29 in $CHCl_3$).

11-Me ether: ***Methoxygorgiacerol***
[138828-02-1]
$C_{22}H_{26}O_7$ 402.443
Constit. of *Pseudopterogorgia acerosa*. Gum. $[\alpha]_D$ +124.4 (c, 0.75 in $CHCl_3$).

3α,4α:5α,6α-Diepoxide: ***Diepoxygorgiacerodiol***
$C_{21}H_{24}O_9$ 420.415
Constit. of *Pseudopterogorgia acerosa*. Semi-solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -0.34 (c, 7.8 in $CHCl_3$). λ_{max} 246 (ε 1200) (MeOH) (Berdy).

12-Deoxy: ***11-Gorgiacerol***
$C_{21}H_{24}O_6$ 372.417
Constit. of *Pseudopterogorgia acerosa*. Gum. $[\alpha]_D$ +22 (c, 0.1 in $CHCl_3$).

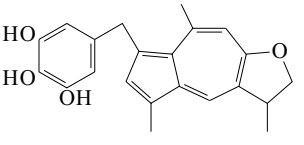
11-Deoxy, 12-ketone: ***Gorgiacerone***
[138827-99-3]
$C_{21}H_{22}O_6$ 370.401
Isol. from *Pseudopterogorgia acerosa*. Gum. $[\alpha]_D$ -184 (c, 0.36 in $CHCl_3$).

11-Deoxy, 12-ketone, 3α,4α:5α,6α-diepoxide: ***Diepoxygorgiacerone***
$C_{21}H_{22}O_8$ 402.4
Constit. of *Pseudopterogorgia acerosa*. Cryst.
Mp 180-181°. $[\alpha]_D$ -319 (c, 0.27 in $CHCl_3$).

Tinto, W.F. *et al., Tetrahedron*, 1991, **47**, 8679 (*isol, pmr, cmr*)
Paquette, L.A. *et al., J.A.C.S.*, 1992, **114**, 3910; 3926 (*synth*)
Tinto, W.F. *et al., J. Nat. Prod.*, 1995, **58**, 1975 (*11-Gorgiacerol*)
Rodriguéz, A.D. *et al., Chem. Pharm. Bull.*, 1996, **44**, 91 (*Diepoxygorgiacerodiol*)

Gorgiagallylazulene G-142

[152845-75-5]



$C_{22}H_{22}O_4$ 350.413

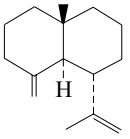
Constit. of an *Acalycigorgia* sp. Purple amorph. solid. $[\alpha]_D^{21}$ -30 (c, 0.11 in $CHCl_3$).

Ochi, M. *et al., Chem. Lett.*, 1993, 2003 (*isol, pmr, cmr*)

4(15),11-Gorgonadiene G-143

β-Gorgonene

[20071-48-1]



Absolute configuration

$C_{15}H_{24}$ 204.355

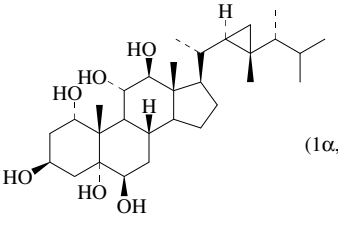
Constit. of *Pseudopterogorgia americana*. Oil. $[\alpha]_D^{25}$ +13.9 (neat).

$AgNO_3$ complex:

Cryst. (Me_2CO/hexane). Mp 132.5-133.5°.

Bilayet Hossain, M. *et al., J.A.C.S.*, 1968, **90**, 6607 (*struct*)
Boeckman, R.K. *et al., J.O.C.*, 1975, **40**, 1755 (*synth*)
Hčkl, T. *et al., Phytochemistry*, 2004, **65**, 2261-2275 (*pmr, cmr*)

Gorgostane-1,3,5,6,11,12-hexol G-144



(1α,3β,5α,6β,11α,12β,24*R*)-*form*

$C_{30}H_{52}O_6$ 508.737

(1α,3β,5α,6β,11α,12β,24*R*)-*form*

12-Ac: [467227-49-2]

$C_{32}H_{54}O_7$ 550.774

Constit. of *Isis hippuris*. Glass. $[\alpha]_D^{25}$ +5 (c, 0.49 in $CHCl_3$).

(1α,3β,5α,6β,11α,12β,24*S*)-*form*

12-Ac: ***Isihippurol A***

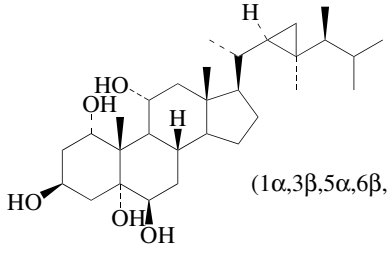
[364599-47-3]

$C_{32}H_{54}O_7$ 550.774

Constit. of *Isis hippuris*. Amorph. powder. $[\alpha]_D^{25}$ +30.2 (c, 0.05 in MeOH).

Shen, Y.-C. *et al., Steroids*, 2001, **66**, 721-725 (*isol, pmr, cmr*)
Tanaka, J. *et al., Tetrahedron*, 2002, **58**, 6259-6266 (*isol, pmr, cmr*)

Gorgostane-1,3,5,6,11-pentol G-145



(1α,3β,5α,6β,11α)-*form*

$C_{30}H_{52}O_5$ 492.738

(1α,3β,5α,6β,11α)-*form* [117569-43-4]

Constit. of *Isis hippuris*. Cryst. Mp 295-297°.

(1α,3β,5β,6β,11α)-*form*

6-Ketone: ***1,3,5,11-Tetrahydroxygorgostan-6-one***

[868279-60-1]

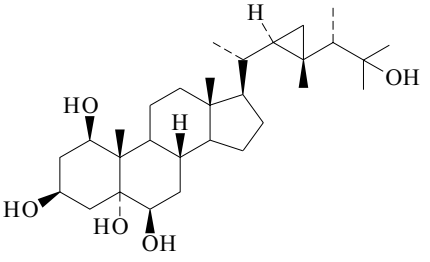
$C_{30}H_{50}O_5$ 490.722

Constit. of *Isis hippuris*. Powder.

Mp 218-220°. $[\alpha]_D$ -5 (c, 0.44 in $CHCl_3$).

Rao, C.B. *et al., J. Nat. Prod.*, 1988, **51**, 954
Chao, C.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1366-1370 (*6-ketone*)

Gorgostane-1,3,5,6,25-pentol G-146



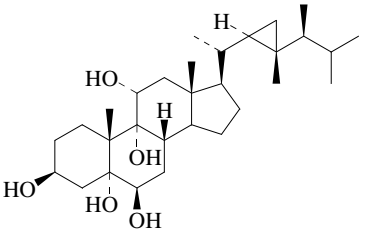
$C_{30}H_{52}O_5$ 492.738

(1β,3β,5α,6β)-*form* [142780-43-6]

Constit. of *Sarcophyton subviride*.

Raja, B.L. *et al., J. Nat. Prod.*, 1992, **55**, 904 (*isol, pmr, cmr*)

Gorgostane-3,5,6,9,11-pentol G-147



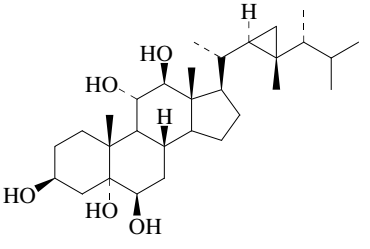
$C_{30}H_{52}O_5$ 492.738

(3β,5α,6β,9α,11α)-*form* [313511-68-1]

Constit. of *Eunicea laciniata*. Powder. Mp 243-247°. $[\alpha]_D$ +15.5 (c, 0.51 in MeOH).

D'Armas, H.T. *et al., J. Nat. Prod.*, 2000, **63**, 1669-1671 (*isol, pmr, cmr*)

Gorgostane-3,5,6,11,12-pentol G-148



$C_{30}H_{52}O_5$ 492.738

(3β,5α,6β,11α,12β)-*form*

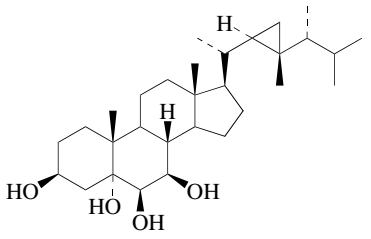
12-Ac: [467227-48-1]

$C_{32}H_{54}O_6$ 534.775

Constit. of *Isis hippuris*. Glass. $[\alpha]_D^{25}$ -14 (c, 0.49 in $CHCl_3$).

Tanaka, J. *et al., Tetrahedron*, 2002, **58**, 6259-6266 (*isol, pmr, cmr*)

Gorgostane-3,5,6,7-tetrol G-149

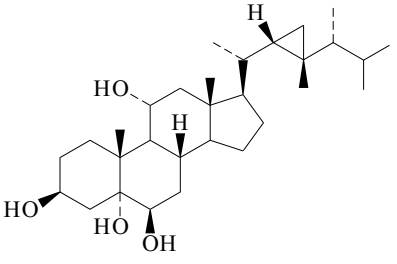


$C_{30}H_{52}O_4$ 476.738

(3β,5α,6β,7β)-*form*

7-Ac: ***Xeniasterol D***
[107168-60-5]
$C_{32}H_{54}O_5$ 518.776
Isol. from a soft coral of *Xenia* sp. Needles (EtOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 285-286°. $[\alpha]_D^{22}$ +32 (c, 1 in Py).
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4590-4596 (*isol, pmr, cmr*)

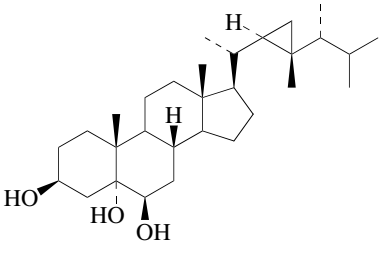
Gorgostane-3,5,6,11-tetrol G-150



$C_{30}H_{52}O_4$ 476.738

(3β,5α,6β,11α)-*form*
Sarcoaldesterol A
[180313-84-2]
Constit. of a *Sarcophyton* sp.
Amorph. powder.
Mp 285.5-287°. $[\alpha]_D^{25}$ -40.5 (c, 0.97 in Py).
Umeyama, A. *et al., J. Nat. Prod.*, 1996, **59**, 894-895 (*isol, pmr, cmr*)

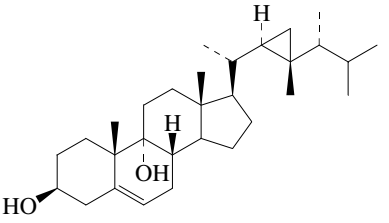
Gorgostane-3,5,6-triol G-151



$C_{30}H_{52}O_3$ 460.739

(3β,5α,6β)-*form*
Xeniasterol C
[107168-59-2]
Isol. from a soft coral of *Xenia* sp.
Needles ($CHCl_3$). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 255-256°. $[\alpha]_D^{22}$ -3 (c, 0.9 in $CHCl_3$/MeOH).
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4590-4596 (*isol, pmr, cmr*)

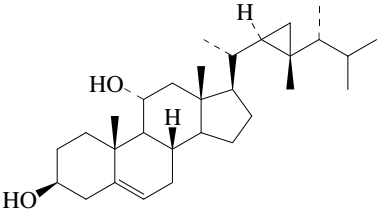
Gorgost-5-ene-3,9-diol G-152



$C_{30}H_{50}O_2$ 442.724

(3β,9α)-*form* [395070-86-7]
Constit. of *Plexaurella grisea*.
Amorph. solid. $[\alpha]_D$ -41.3 (c, 0.08 in $CHCl_3$).
Rueda, A. *et al., Steroids*, 2001, **66**, 897-904 (*isol, pmr, cmr*)

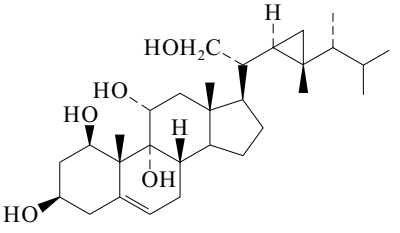
Gorgost-5-ene-3,11-diol G-153



$C_{30}H_{50}O_2$ 442.724

(3β,11α)-*form* [253195-22-1]
Constit. of a *Sarcophyton* sp.
Cryst. ($CHCl_3$/MeOH).
Mp 180-182°. $[\alpha]_D^{25}$ +36 (c, 0.08 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 2000, **63**, 112-118 (*isol, pmr, cmr*)

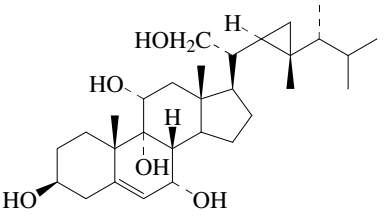
Gorgost-5-ene-1,3,9,11,21-pentol G-154



$C_{30}H_{50}O_5$ 490.722

(1β,3β,9α,11α)-*form* [147151-92-6]
Constit. of *Lobophytum strictum*.
Cryst.
Mp 301-303°. $[\alpha]_D$ -33 (c, 0.78 in Py).
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1993, 112 (*isol, pmr, cmr*)

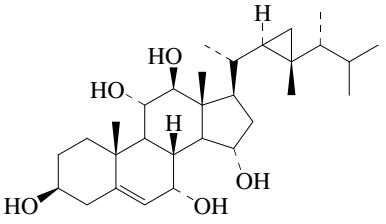
Gorgost-5-ene-3,7,9,11,21-pentol G-155



$C_{30}H_{50}O_5$ 490.722

(3β,7α,9α,11α)-*form* [281680-34-0]
Constit. of *Lobophytum strictum*.
Vanisree, M. *et al., J. Asian Nat. Prod. Res.*, 2000, **2**, 87-95; *CA*, **133**, 86889w (*isol, pmr, cmr*)

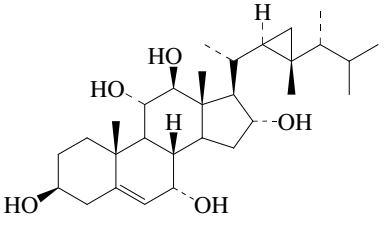
Gorgost-5-ene-3,7,11,12,15-pentol G-156



$C_{30}H_{50}O_5$ 490.722

(3β,7α,11α,12β,15α)-*form*
11,15-Di-Ac: [467227-45-8]
$C_{34}H_{54}O_7$ 574.796
Constit. of *Isis hippuris*. Glass. $[\alpha]_D^{25}$ -9.2 (c, 0.45 in $CHCl_3$).
5β,6β-Epoxide: 5,6-Epoxygorgostane-3,7,11,12,15-pentol
$C_{30}H_{50}O_6$ 506.721
5β,6β-Epoxide, 11,15-di-Ac: [467227-46-9]
$C_{34}H_{54}O_8$ 590.796
Constit. of *Isis hippuris*. Glass. $[\alpha]_D^{25}$ +24 (c, 0.62 in $CHCl_3$).
Tanaka, J. *et al., Tetrahedron*, 2002, **58**, 6259-6266 (*isol, pmr, cmr*)

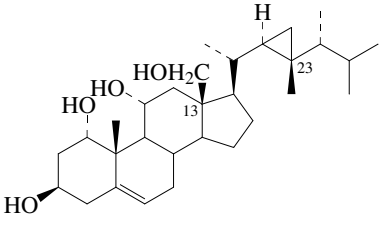
Gorgost-5-ene-3,7,11,12,16-pentol G-157



$C_{30}H_{50}O_5$ 490.722

(3β,7α,11α,12β,16α)-*form*
12,16-Di-Ac: [467227-44-7]
$C_{34}H_{54}O_7$ 574.796
Constit. of *Isis hippuris*. Glass. $[\alpha]_D^{25}$ -2.4 (c, 0.64 in $CHCl_3$).
5β,6β-Epoxide: 5,6-Epoxygorgostane-3,7,11,12,16-pentol
$C_{30}H_{50}O_6$ 506.721
5β,6β-Epoxide, 11,16-di-Ac: [467227-47-0]
$C_{34}H_{54}O_8$ 590.796
Constit. of *Isis hippuris*. Glass. $[\alpha]_D^{25}$ +23 (c, 0.26 in $CHCl_3$).
Tanaka, J. *et al., Tetrahedron*, 2002, **58**, 6259-6266 (*isol, pmr, cmr*)

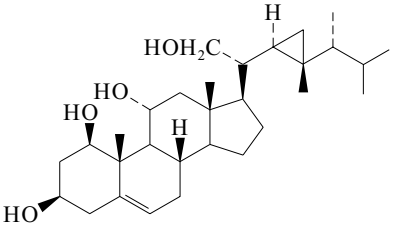
Gorgost-5-ene-1,3,11,18-tetrol G-158



$C_{30}H_{50}O_4$ 474.723

(1α,3β,11α)-*form* [862261-35-6]
Constit. of *Sinularia dissecta*.
Amorph. powder. $[\alpha]_D^{20}$ -19 (c, 0.08 in MeOH).
18-Ac: [862261-36-7]
$C_{32}H_{52}O_5$ 516.76
Constit. of *Sinularia dissecta*. Gum. $[\alpha]_D^{20}$ -27 (c, 0.07 in MeOH).
18-Aldehyde: ***1,3,11-Trihydroxygorgost-5-en-18-al***
[97190-45-9]
Constit. of *Sinularia dissecta*.
18-Carboxylic acid: ***1,3,11-Trihydroxygorgost-5-en-18-oic acid***
[97190-40-4]
$C_{30}H_{48}O_5$ 488.706
From *Sinularia dissecta*.
18-Carboxylic acid, 3-Ac: [862261-34-5]
$C_{32}H_{50}O_6$ 530.743
Constit. of *Sinularia dissecta*. Gum. $[\alpha]_D^{20}$ -25.2 (c, 0.12 in MeOH).
Jagodzinska, B.M. *et al., J.O.C.*, 1985, **50**, 2988-2992 (*18-aldehyde, 18-carboxylic acid*)
Jin, P. *et al., Steroids*, 2005, **70**, 487-493 (*Sinularia dissecta constits*)

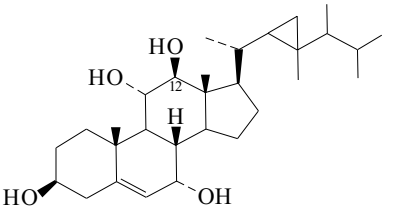
Gorgost-5-ene-1,3,11,21-tetrol G-159



$C_{30}H_{50}O_4$ 474.723

(1β,3β,11α)-*form* [147151-93-7]
Constit. of *Lobophytum strictum*. Cryst. Mp 270-272°.
$[\alpha]_D$ -23 (c, 1.2 in Py).
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1993, 112 (*isol, pmr, cmr*)

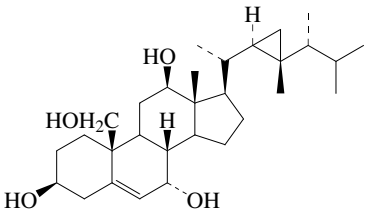
Gorgost-5-ene-3,7,11,12-tetrol, 9CI G-160



$C_{30}H_{50}O_4$ 474.723

(3β,7α,11α,12β)-*form*
12-Ac: [83173-20-0]
$C_{32}H_{52}O_5$ 516.76
Constit. of gorgonian *Isis hippuris*. Cryst. Mp 197-200°.
5β,6β-Epoxide: 5,6-Epoxygorgostane-3,7,11,12-tetrol
$C_{30}H_{50}O_5$ 490.722
5β,6β-Epoxide, 12-Ac: [467227-43-6]
$C_{32}H_{52}O_6$ 532.759
Constit. of *Isis hippuris*. Solid. $[\alpha]_D^{22}$ +2.6 (c, 0.1 in $CHCl_3$).
Tanaka, J. *et al., Chem. Lett.*, 1982, 1295
Tanaka, J. *et al., Tetrahedron*, 2002, **58**, 6259-6266 (*epoxide*)

Gorgost-5-ene-3,7,12,19-tetrol G-161

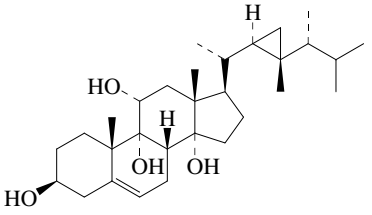


$C_{30}H_{50}O_4$ 474.723

(3β,7α,12β)-*form*

12-Ac: [494858-30-9]
$C_{32}H_{52}O_5$ 516.76
Constit. of *Capnella lacertiliensis*. Oil. $[\alpha]_D^{22}$ -98 (c, 0.01 in $CHCl_3$).
Wright, A.D. *et al., J. Nat. Prod.*, 2002, **66**, 157-160 (*isol, pmr, cmr*)

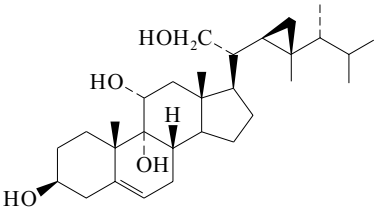
Gorgost-5-ene-3,9,11,14-tetrol G-162



$C_{30}H_{50}O_4$ 474.723

(3β,9α,11α,14α)-*form* [395070-87-8]
Constit. of *Plexaurella grisea*.
Amorph. solid. $[\alpha]_D$ -15 (c, 0.1 in MeOH).
Rueda, A. *et al., Steroids*, 2001, **66**, 897-904 (*isol, pmr, cmr*)

Gorgost-5-ene-3,9,11,21-tetrol G-163

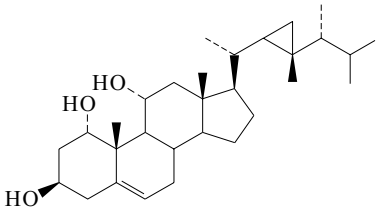


$C_{30}H_{50}O_4$ 474.723

(3β,9α,11α)-*form*
Andamansterol
[133883-21-3]
Constit. of a *Sclerophytum* sp. Cryst. Mp 265-266°. $[\alpha]_D^{22}$ -34 (c, 1 in Py).
Kobayashi, M. *et al., J.C.S. Perkin 1*, 1991, 493 (*isol, pmr, cmr, cryst struct*)

Gorgost-5-ene-1,3,11-triol G-164

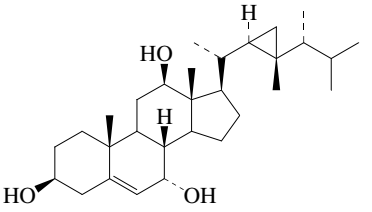
1,11-Dihydroxygorgosterol



$C_{30}H_{50}O_3$ 458.723

(1α,3β,11α)-*form* [95513-63-6]
Constit. of *Sinularia dissecta*. Cryst. Mp 212-214°.
Jagodzinska, B.M. *et al., J.O.C.*, 1985, **50**, 1435 (*isol, ms, pmr*)

Gorgost-5-ene-3,7,12-triol G-165

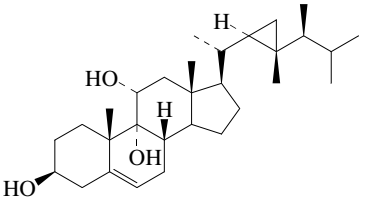


$C_{30}H_{50}O_3$ 458.723

(3β,7α,12β)-*form*

12-Ac: [494858-28-5]
$C_{32}H_{52}O_4$ 500.76
Constit. of *Capnella lacertiliensis*. Oil. $[\alpha]_D^{22}$ -64 (c, 0.01 in $CHCl_3$).
Wright, A.D. *et al., J. Nat. Prod.*, 2002, **66**, 157-160 (*isol, pmr, cmr*)

Gorgost-5-ene-3,9,11-triol G-166

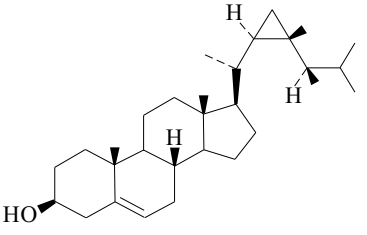


$C_{30}H_{50}O_3$ 458.723

(3β,9α,11α)-*form* [313511-62-5]
Constit. of *Eunicea laciniata*. Needles. Mp 188-190°.
D'Armas, H.T. *et al., J. Nat. Prod.*, 2000, **63**, 1669-1671 (*isol, pmr, cmr*)

Gorgosterol G-167

Gorgost-5-en-3-ol, 9CI. 23,24-Dimethyl-22,23-methylenecholest-5-en-3-ol
[29782-65-8]



$C_{30}H_{50}O$ 426.724
Isol. from cnidarians *Plexaura flexuosa*, *Palythoa tuberculosa*, *Palythoa mammilosa* and *Sarcophyton glaucum* and from molluscs *Tridacna gigas*, *Hippopus hippopus* and other marine animals. Shown to be produced by symbiotic dinoflagellates inhabiting cnidarian tissues. Cryst. (EtOH). Poorly sol. hexane.
Mp 186.5-188°. $[\alpha]_D$ -45. A compd., Mp 175-178°, isol. from a soft coral was assigned the same gross struct. It is not clear from the abstr. whether this was Gorgosterol or claimed as a new stereoisomer.

Djerassi, C. *et al., J.A.C.S.*, 1970, **92**, 2179; 5281 (*isol, struct*)
Finer, J. *et al., J.O.C.*, 1978, **43**, 1990 (*cryst struct*)
Li, R. *et al., CA*, 1982, **97**, 107457
Withers, N.W. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1982, **79**, 3764-3768; 6390 (*occur, dinoflagellates*)

Terasawa, T. *et al., Chem. Comm.*, 1983, 1180 (*synth*)
Giner, J.-L. *et al., J.O.C.*, 1991, **56**, 2357 (*biosynth*)

GPFGLNKHG amide G-168

GPFG-9
[151808-91-2]
Gly-Pro-Phe-Gly-Leu-Asn-Lys-His-Gly-NH_2
$C_{42}H_{64}N_{14}O_{10}$ 925.055
Isol. from the anterior byssus retractor muscle of the edible mussel *Mytilus edulis.*

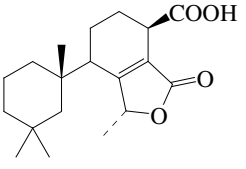
Fujisawa, Y. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1993, **106**, 261-267 (*isol*)

GPFGTHIK amide G-169

GPFG-8
[151808-90-1]
Gly-Pro-Phe-Gly-Thr-His-Ile-Lys-NH_2
$C_{40}H_{62}N_{12}O_9$ 855.005
Isol. from the anterior byssus retractor muscle of the edible mussel *Mytilus edulis.*

Fujisawa, Y. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1993, **106**, 261-267 (*isol*)

8(14)-Gracilen-15,7-olid-16-oic acid G-170



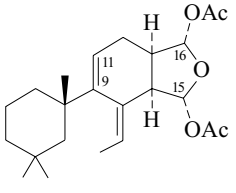
$C_{19}H_{28}O_4$ 320.428

Me ester: [676348-91-7]
$C_{20}H_{30}O_4$ 334.455
Constit. of *Dendrilla membranosa*. Oil. $[\alpha]_D^{25}$ +70 (c, 0.27 in $CHCl_3$).

Díiaz-Marrero, A.R. *et al., Tetrahedron*, 2004, **60**, 1073-1078 (*isol, pmr, cmr, cryst struct, abs config*)

Gracilin A G-171

[96313-94-9]



$C_{23}H_{34}O_5$ 390.519
Constit. of sponge *Spongionella gracilis* and *Aplysilla tango.* Phospholipase A2 inhibitor. Oil. $[\alpha]_D$ -60.5 (c, 1.3 in $CHCl_3$). λ_{max} 225 (ϵ 7700) (MeOH) (Derep).

9α,11-Dihydro: ***9,11-Dihydrogracilin A***
[106231-25-8]
$C_{23}H_{36}O_5$ 392.534
Constit. of *Dendrilla membranosa*. Oil. Sol. CH_2Cl_2, 1-propanol. $[\alpha]_D$ -11 (c, 1.3 in $CHCl_3$).

16-Deacetoxy: ***Gracilin E***
[106199-81-9]
$C_{21}H_{32}O_3$ 332.482
Isol. from *Spongionella gracilis.*
$[\alpha]_D$ -55.6 (c, 0.8 in $CHCl_3$). λ_{max} 224 (ϵ 6530) (MeOH) (Derep).

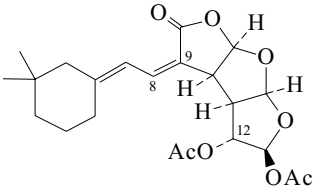
16-Deacetoxy, O^{15}-de-Ac: ***Gracilin F***
[106199-80-8]
$C_{19}H_{30}O_2$ 290.445
Constit. of *Spongionella gracilis.* Oil. $[\alpha]_D$ +0.5 (c, 1.2 in $CHCl_3$). λ_{max} 224 (ϵ 6530) (MeOH) (Derep).

O^{16}-De-Ac, 16-ketone: See 15-Hydroxy-17-nor-5,6-seco-7,9(11)-spongiadien-16,15-olide, H-824

Mayol, L. *et al., Tet. Lett.*, 1985, **26**, 1357 (*isol*)
Mayol, L. *et al., Tetrahedron*, 1986, **42**, 5369 (*isol, struct*)
Molinski, T.F. *et al., J.O.C.*, 1987, **52**, 296 (*isol*)
Poiner, A. *et al., Aust. J. Chem.*, 1990, **43**, 1713 (*isol, pmr, cmr*)
Puliti, R. *et al., Acta Cryst. C*, 1993, **49**, 1373 (*cryst struct*)

Gracilin B G-172

[96313-95-0]



$C_{22}H_{28}O_8$ 420.458
Constit. of sponge *Spongionella gracilis.* Cryst.
Mp 167-168°. $[\alpha]_D$ +191 (c, 1.0 in $CHCl_3$). λ_{max} 296 (ϵ 20150) (MeOH) (Derep).

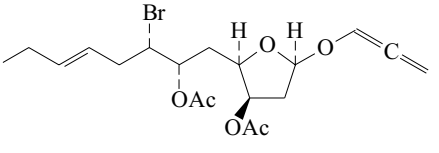
12-Deacetyl, 12-propanoyl: ***Gracilin D***
[106849-36-9]
$C_{23}H_{30}O_8$ 434.485
From *Spongionella gracilis.* Oil. $[\alpha]_D^{25}$ +130.1 (c, 1.1 in $CHCl_3$).

*8*E*-Isomer:* ***Gracilin C***
[106621-85-6]
$C_{22}H_{28}O_8$ 420.458
From *Spongionella gracilis.* Cryst. (MeOH).
Mp 240-241°. $[\alpha]_D^{25}$ +273.3 (c, 1.4 in $CHCl_3$).

Mayol, L. *et al., Tet. Lett.*, 1985, **26**, 1253
Mayol, L. *et al., J. Nat. Prod.*, 1986, **49**, 823 (*isol, struct*)
Mayol, L. *et al., Tetrahedron*, 1986, **42**, 5369 (*isol, struct*)
Corey, E.J. *et al., J.A.C.S.*, 1995, **37**, 9616 (*synth*)

Graciosallene G-173

[119285-22-2]

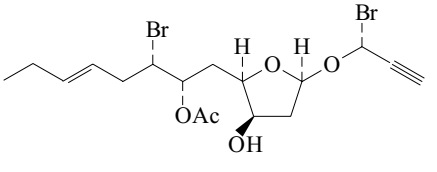


$C_{19}H_{27}BrO_6$ 431.323
Metab. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ -83.3 (c, 0.018 in $CHCl_3$).

Norté, M. *et al., Phytochemistry*, 1988, **27**, 3537

Graciosin G-174

[119285-19-7]



$C_{17}H_{24}Br_2O_5$ 468.182
Metab. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ -14.5 (c, 0.62 in $CHCl_3$).

González, A.G. *et al., Tetrahedron*, 1984, **40**, 3443 (*isol*)
Norte, M. *et al., Phytochemistry*, 1988, **27**, 3537 (*isol, cryst struct*)

Grammistins G-175

[53026-69-0]

A family of peptides containing 13-28 amino acid residues. Isol. from skin secretions of the soapfish *Pogonoperca punctata* (Grammistin Pp) and *Grammistes sexlineatus* (Grammistin Gs). Show haemolytic and ichthyotoxic activity.

Grammistin Gs A

$C_{148}H_{226}N_{40}O_{35}$ 3125.66

Grammistin Gs B

$C_{70}H_{108}N_{16}O_{14}$ 1397.722

Grammistin Gs C

$C_{127}H_{213}N_{35}O_{31}S$ 2758.362

Grammistin Gs D

Grammistin Pp 1

[349533-22-8]

$C_{79}H_{117}N_{17}O_{15}$ 1544.898

Grammistin Gs E

Grammistin Pp 2b

[349533-24-0]

$C_{76}H_{119}N_{15}O_{15}$ 1482.868

Grammistin Gs F

Grammistin Gs 1

[254732-65-5]

$C_{130}H_{210}N_{36}O_{32}$ 2789.311

Grammistin Gs G

Grammistin Gs 2. *Grammistin Pp 4a*

[254732-66-6]

$C_{127}H_{206}N_{30}O_{26}$ 2569.21

Grammistin Pp 2a [349533-23-9]

Grammistin Pp 3 [349533-25-1]

$C_{118}N_{192}N_{32}O_{33}$ 5082.779

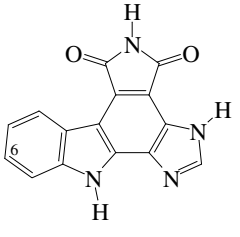
Grammistin Pp 4b [349533-26-2]

Shiomi, K. *et al., Toxicon*, 2000, **38**, 91-103 (*Grammistin Gs F-G*)
Shiomi, K. *et al., Fish. Sci.*, 2001, **67**, 163-169; 928-929 (*Grammistin Pp*)
Sugiyama, N. *et al., Toxicon*, 2005, **45**, 595-601 (*Grammistin Gs A-E*)

Granulatimide G-176

*1*H-*Imidazo[4,5*-a*]pyrrolo[3,4*-c*]carbazole-4,6-(5*H*,11*H*)-dione, 9CI*

[219828-99-6]



$C_{15}H_8N_4O_2$ 276.254

Alkaloid from the ascidian *Didemnum granulatum*. G2 specific cell cycle checkpoint inhibitor. Yellow solid.

6-Bromo: ***6-Bromogranulatimide***

[330846-92-9]

$C_{15}H_7BrN_4O_2$ 355.15

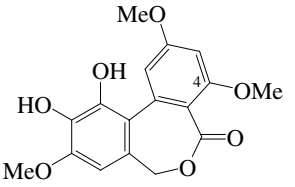
Alkaloid from *Didemnum granulatum*. Amorph. yellow solid. λ_{max} 236; 282; 308; 386 (MeOH).

Berlinck, R.G.S. *et al., J.O.C.*, 1998, **63**, 9850-9856 (*isol, synth, pmr, cmr, activity*)
Britton, R. *et al., J. Nat. Prod.*, 2001, **64**, 254-255 (*6-Bromogranulatimide, isol, pmr, cmr*)
Yoshida, T. *et al., Chem. Pharm. Bull.*, 2002, **50**, 872-876; 2003, **51**, 209-214 (*synth*)

Graphislactone D G-177

*10,11-Dihydroxy-2,4,9-trimethoxydibenz[*c,e*]oxepin-5(7*H*)-one, 9CI*

[194924-01-1]



$C_{17}H_{16}O_7$ 332.309

Metab. of the spore-derived mycobiont of *Graphis scripta* var. *pulverulenta*. Cryst.

Mp 110-112°. λ_{max} 209 (log ϵ 4.22); 236 (log ϵ 4.25); 254 (sh) (log ϵ 4.18); 278 (sh) (log ϵ 3.83); 303 (sh) (log ϵ 3.69) (MeOH).

O^4*-De-Me: 4,10,11-Trihydroxy-2,9-dimethoxydibenz[*c,e*]oxepin-5(7*H*)-one, 9CI.* ***Ulocladol***

$C_{16}H_{14}O_7$ 318.282

Metab. of the marine fungus *Ulocladium botrytis*. Also prod. by *Microsphaeropsis olivacea*. Tyrosine kinase inhibitor. Powder. Mp 110-111°. λ_{max} 251 (log ϵ 4.11); 299 (log ϵ 3.54) (EtOH).

Tanahashi, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1183-1185 (*isol*)
Höller, U. *et al., Eur. J. Org. Chem.*, 1999, 2949-2955 (*Ulocladol*)
Abe, H. *et al., Tet. Lett.*, 2005, **46**, 3197-3200 (*synth*)
Hormazabal, E. *et al., Z. Naturforsch., C*, 2005, **60**, 11-21 (*Ulocladol*)

Grateloupine G-178

4-[(Aminocarbonyl)amino]butanoic acid, 9CI. N-*Carbamoyl-γ-aminobutyric acid*. *γ-Ureidobutyric acid*

[2609-10-1]

$H_2NCONHCH_2CH_2CH_2COOH$

$C_5H_{10}N_2O_3$ 146.146

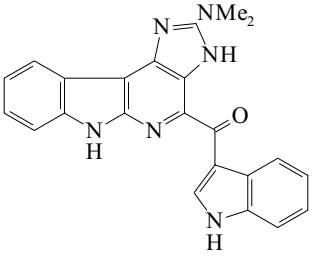
Isol. from the red alga *Grateloupia filicina*. Cryst. (H_2O).

Mp 178-179° dec.

Wakamiya, T. *et al., Tetrahedron*, 1984, **40**, 235-240 (*isol, pmr, cmr, struct, synth*)

Grossularine 1 G-179

[94935-97-4]



$C_{23}H_{18}N_6O$ 394.435

Struct. revised in 1989. First examples of a naturally occurring α-carboline (see also Grossularine 2, G-180). Cmr assignments revised in 1996. Isol. from the tunicate *Dendrodoa grossularia*. Exhibits marked cytotoxicity toward murine and human tumour cells. Amorph. yellow powder.

Mp 350°. λ_{max} 202; 235; 264 (sh); 340; 360 (EtOH) (Derep).

N,N-*Di-de-Me:* **N,N-*Didemethylgrossularine 1***

[175170-89-5]

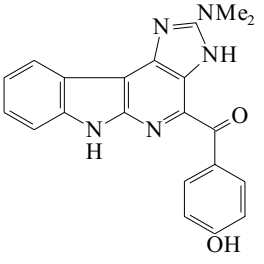
$C_{21}H_{14}N_6O$ 366.381

Alkaloid from the ascidian *Polycarpa aurata*. Yellow needles (MeOH/Me_2CO).
Mp 333-335°.

Moquin, C. *et al., Tet. Lett.*, 1984, **25**, 5047-5048 (*isol, ms*)
Moquin-Pattey, C. *et al., Tetrahedron*, 1989, **45**, 3445-3450 (*isol, uv, ms, struct*)
Abas, S.A. *et al., J.O.C.*, 1996, **61**, 2709-2712 (*N,N-Didemethylgrossularine 1*)
Loukaci, A. *et al., Magn. Reson. Chem.*, 1996, **34**, 143-145 (*pmr, cmr*)
Molina, P. *et al., Tetrahedron*, 1998, **54**, 9623-9638 (*synth*)
Miyake, F.Y. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 3280-3282 (*synth*)

Grossularine 2 G-180

[102488-58-4]

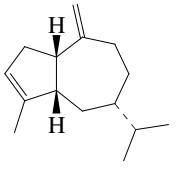


$C_{21}H_{17}N_5O_2$ 371.398

Cmr spectral assignments revised in 1996. Isol. from the tunicate *Dendrodoa grossularia*. Exhibits marked cytotoxicity toward murine and human tumour cells. Cryst. (THF/MeOH).
Mp 281-283°. λ_{max} 235 (ϵ); 255 (ϵ); 340 (ϵ); 360 (ϵ) (EtOH) (Derep).

Moquin-Pattey, C. *et al., Tetrahedron*, 1989, **45**, 3445 (*isol, pmr, cmr, ms, struct*)
Loukaci, A. *et al., Magn. Reson. Chem.*, 1996, **34**, 143 (*pmr, cmr*)
Molina, P. *et al., Tetrahedron*, 1998, **54**, 9623-9638 (*synth*)

3,10(14)-Guaiadiene G-181



(1β,5β,7β*H*)-*form*

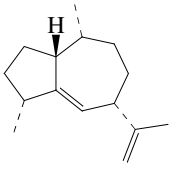
$C_{15}H_{24}$ 204.355

(1β,5β,7β*H*)-*form*
3α,4α-Epoxide: ***3,4-Epoxy-10(14)-guaiene***
[282101-69-3]
$C_{15}H_{24}O$ 220.354
Constit. of a *Nephthea* sp. Oil. $[\alpha]_D^{25}$ +69 (c, 0.011 in $CHCl_3$).

(1ξ,5ξ,7ξ)-*form*
Sclerosporene
[69394-03-2]
Metab. of *Sclerotinia fructicola*.

Katayama, M. *et al., Tet. Lett.*, 1979, 1773 (*Sclerosporene*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 2000, **39**, 42-56 (*epoxide*)

5,11-Guaiadiene G-182



(1β,4α,7α,10β)-*form*

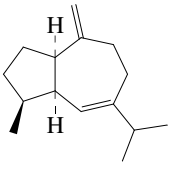
$C_{15}H_{24}$ 204.355

(1β,4α,7α,10β)-*form*
Epi-γ-gurjunene
Constit. of *Cymbastela hooperi*.
Oil. $[\alpha]_D$ +34.6 (c, 0.11 in $CHCl_3$).

(1β,4α,7β,10α)-*form*
γ-Gurjunene
[22567-17-5]
Constit. of *Dipterocarpus dyeri*.
$[\alpha]_D$ +147.

Ehret, C. *et al., Tetrahedron*, 1969, **25**, 1785
König, G.M. *et al., J.O.C.*, 1997, **62**, 3837-3840 (*isol, pmr, cmr*)

6,10(14)-Guaiadiene G-183



(1α,4β,5α)-*form*

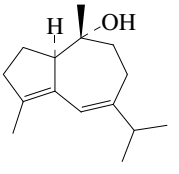
$C_{15}H_{24}$ 204.355

(1α,4β,5α)-*form* [847374-78-1]
Constit. of *Cupressus macrocarpa* foliage.

(1α,4ξ,5β)-*form* [290819-13-5]
Constit. of *Nephthea chabrolii*.

Rao, M.R. *et al., J. Chem. Res., Synop.*, 2000, 245-247 (*isol, pmr, cmr*)
Cool, L.G. *et al., Phytochemistry*, 2005, **66**, 249-260 (*Cupressus macrocarpa constit*)

4,6-Guaiadien-10-ol G-184

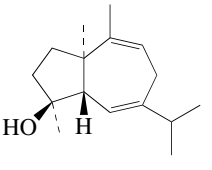


$C_{15}H_{24}O$ 220.354

(1α,10α)-*form* [290819-14-6]
Constit. of *Nephthea chabrolii*.

Rao, M.R. *et al., J. Chem. Res., Synop.*, 2000, 245-247 (*isol, pmr, cmr*)

6,9-Guaiadien-4-ol G-185

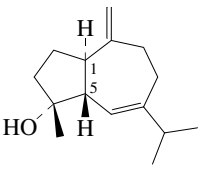


$C_{15}H_{24}O$ 220.354

(1α,4β,5β)-*form* [160543-32-8]
Constit. of *Nephthea chabroli*.
Oil. $[\alpha]_D$ +68.5 (c, 1.1 in $CHCl_3$).

Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 32-39 (*isol, pmr, cmr*)

6,10(14)-Guaiadien-4-ol G-186



(1α,4α,5β)-*form*

$C_{15}H_{24}O$ 220.354

(1α,4α,5β)-*form*
Constit. of *Nephthea chabrolii*.
Oil. $[\alpha]_D$ 0 (c, 0.1 in $CHCl_3$).

(1α,4β,5β)-*form*
Alismol. *Valerol*
[87827-55-2]
[75556-47-7, 140223-02-5]
Constit. of *Alisma plantago-aquatica*, *Alisma aquatica* and *Valeriana wolgensis.*
Oil. $[\alpha]_D$ +8.7 (c, 0.24 in $CHCl_3$). Struct. revised in 1992 and again in 1994. Only relative config. of Valerol is known.
Ac: [148371-07-7]
$C_{17}H_{26}O_2$ 262.391
Constit. of *Lemnalia africana*. Oil. $[\alpha]_D$ 0 (c, 0.1 in $CHCl_3$).

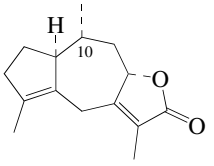
(1β,4α,5α)-*form*
Lactiflorenol
[85404-63-3]
Constit. of *Artemisia lactiflora* and *Chromolaena laevigata*.

(1ξ,4α,5α)-*form* [72646-96-9]
Constit. of *Athanasia dregeana*.
Oil. $[\alpha]_D^{24}$ -27.5 (c, 2 in $CHCl_3$).

[162238-69-9]

Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 995 (*isol*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1980, **33**, 1833 (*isol, pmr, cmr*)
Xu, C. *et al., Zhongcaoyao*, 1982, **13**, 529-533; *CA*, **98**, 157839b (*Lactiflorenol*)
Oshima, Y. *et al., Phytochemistry*, 1983, **22**, 183 (*isol*)
Konovalova, O.A. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1991, **27**, 125-126 (*Valerol*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2582; 1994, **42**, 1813 (*isol, pmr, cmr, struct*)
Jurek, Y. *et al., J. Nat. Prod.*, 1993, **56**, 508 (*isol, pmr, cmr*)
Lange, G.L. *et al., J.O.C.*, 1999, **64**, 6738-3744 (*synth*)

4,7(11)-Guaiadien-12,8-olide G-187



(1α,8α,10α)-*form*

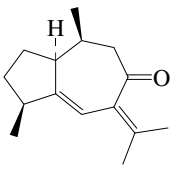
$C_{15}H_{20}O_2$ 232.322

(1α,8α,10α)-*form*
Americanolide D
[185614-61-3]
Constit. of *Pseudopterogorgia americana*.
Unstable yellow oil. $[\alpha]_D^{23}$ -15 (c, 1 in $CHCl_3$). λ_{max} 208 (ϵ 7467) (MeOH). λ_{max} 208 (ϵ 7467) (MeOH) (Berdy).

(1α,8α,10β)-*form*
Americanolide F
[185614-68-0]
Constit. of *Pseudopterogorgia americana*.
Unstable yellow oil. $[\alpha]_D^{23}$ -2 (c, 0.5 in $CHCl_3$). λ_{max} 208 (ϵ 6670) (MeOH).

Rodríguez, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 207-211 (*isol, pmr, cmr*)

5,7(11)-Guaiadien-8-one G-188



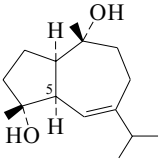
$C_{15}H_{22}O$ 218.338

(1α,4β,10β)-*form*
Guaiacophine
[757954-42-0]
Constit. of *Sarcophyton glaucum*.
Oil. $[\alpha]_D^{25}$ -20 (c, 0.01 in $CHCl_3$).

Feller, M. *et al., J. Nat. Prod.*, 2004, **67**, 1303-1308 (*isol, pmr, cmr*)

6-Guaiene-4,10-diol G-189

[74513-46-5]



(1α,4α,5α,10α)–*form*

$C_{15}H_{26}O_2$ 238.369

(1α,4α,5α,10α)-*form*
Constit. of *Silphium perfoliatum*.
Cryst. (Et_2O/petrol).
Mp 144°. $[\alpha]_D^{24}$ -1.1 (c, 0.9 in $CHCl_3$).

(1α,4α,5β,10α)-*form*
Constit. of *Silphium perfoliatum* and *Sparattanthelium botocudorum*.
Cryst. (Et_2O/petrol).
Mp 111.5°. $[\alpha]_D$ 0.
4-Me ether: 4-Methoxy-6-guaien-10-ol
[331736-11-9]
$C_{16}H_{28}O_2$ 252.396
Constit. of *Sarcophyton buitendijki*. Oil. $[\alpha]_D^{25}$ -0.34 (c, 1.5 in $CHCl_3$).
4-Et ether: 4-Ethoxy-6-guaien-10-ol
[331736-09-5]
$C_{17}H_{30}O_2$ 266.423
Constit. of *Sarcophyton buitendijki*. Oil. $[\alpha]_D^{25}$ -0.36 (c, 1.5 in $CHCl_3$).

(1α,4β,5α,10β)-*form*
10-Me ether: 10-Methoxy-6-guaien-4-ol
[377088-42-1]
$C_{16}H_{28}O_2$ 252.396
Constit. of a Red Sea sponge *Diacarnus erythraenus.* Oil. $[\alpha]_D$ +22 (c, 0.15 in CH_2Cl_2).

(1α,4β,5β,10α)-*form*
Alismoxide
[87701-68-6]
Constit. of *Alisma plantago-aquatica* and *Alisma orientale.*
Oil. $[\alpha]_D$ +31.1 (c, 0.63 in $CHCl_3$). The name Alismoxide is now misleading. Struct. revised in 1992 and again in 1994.
10-Me ether: [290819-11-3]
Constit. of *Alisma orientale* and *Nephthea chabrolii.*
Oil.

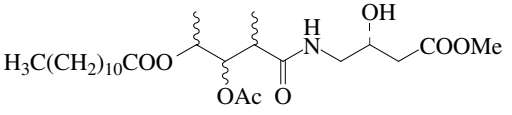
(1β,4α,5α,10β)-*form*
Nephalbidol
[593261-05-3]
Constit. of *Nephthea albida*.

Cryst.
Mp 132-133°. $[\alpha]_D^{20}$ -1.2 (c, 0.336 in EtOH).

Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1987
Oshima, Y. *et al., Phytochemistry*, 1983, **22**, 183
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2582; 1994, **42**, 1813 (*cmr, struct, isol, pmr*)
Nakajima, Y. *et al., Phytochemistry*, 1994, **36**, 119 (*isol, pmr, cmr*)
El Sayed, K.A. *et al., J. Nat. Prod.*, 1996, **59**, 687 (*isol, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 2000, **39**, 773-778 (*Sarcopyton buitendijki constits*)
Rao, M.R. *et al., J. Chem. Res., Synop.*, 2000, 245-247 (*Me ether*)
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2001, **64**, 1332-1335 (*Diacarnus erythraenus constit*)
Su, J.-Y. *et al., Huaxue Xuebao*, 2003, **61**, 1097-1100 (*Nephalbidol*)
Blay, G. *et al., J.O.C.*, 2006, **71**, 7866-7869 (*synth*)

Guamamide G-190

[657401-19-9]



$C_{25}H_{45}NO_8$ 487.632
Alkaloid from a *Symploca* sp. Cytotoxic. Amorph. powder. $[\alpha]_D^{21}$ +6 (c, 0.4 in MeOH). λ_{max} 201 (log ϵ 3.71) (MeOH).

Williams, P.G. *et al., J. Nat. Prod.*, 2004, **67**, 49-53 (*isol, pmr, cmr*)

Guamerin G-191

Polypeptide containing 57 amino acids. Isol. from the leech *Hirudo nipponia*. Human leukocyte elastase inhibitor.

Jung, H.I. *et al., J. Biol. Chem.*, 1995, **270**, 13879-13884 (*isol, struct*)

Guanidinoacetic acid G-192

N-*(Aminoiminomethyl)glycine, 9CI. Glycocyamine.* N-*Guanylglycine. [(Aminoiminomethyl)amino]acetic acid. Guanidineacetic acid. (Carboxymethyl)guanidine*
[352-97-6]
HN═C(NH$_2$)NHCH$_2$COOH
$C_3H_7N_3O_2$ 117.107
Occurs in the sea anemone *Anthopleura japonica* and other spp. Has cardiotonic props. Plates (H_2O).
Mp 280-284° dec. pK_a 2.82 (25°).

Hydrochloride: [14901-20-3]
Plates (conc. HCl). Mp 200° dec.

N-*Me:* See Creatine in *The Combined Chemical Dictionary.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 820D (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 680B (*nmr*)
Walter, W. *et al., Angew. Chem.*, 1955, **67**, 275 (*synth*)
Org. Synth., Coll. Vol., 3, 1955, 440 (*synth*)
Fasold, H. *et al., Biochem. Z.*, 1961, **335**, 86 (*synth*)
Cramer, F. *et al., Chem. Ber.*, 1962, **95**, 1670 (*synth*)
Pant, R. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1964, **335**, 272 (*synth*)

4-Guanidinobutanoic acid G-193

4-[(Aminoiminomethyl)amino]butanoic acid, 9CI. GGBA
[463-00-3]
HN═C(NH$_2$)NHCH$_2$CH$_2$CH$_2$COOH
$C_5H_{11}N_3O_2$ 145.161
Occurs in plants and animals, e.g. *Pinus* spp., *Lunaria annua*, sea anemone *Anthopleura japonica*, green alga *Enteromorpha intestinalis*. Found in soybean, tea and *Citrus* spp. Depressive neurotransmitter, displays similarities to 4-Aminobutanoic acid. Cryst. + 2H_2O (H_2O).
▶ Toxic to chick embryos.

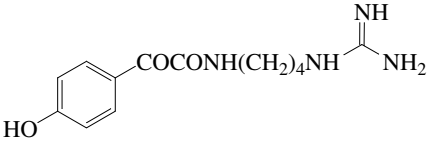
Hydrochloride: [13890-14-7]
Mp 184°.

Amide: 4-Guanidinobutyramide. ***Tiformin, INN****. Tyformin, BAN*
[4210-97-3]
$C_5H_{12}N_4O$ 144.176
Oral hypoglycaemic agent. Log P -2.9 (calc).

Amide; hydrochloride: HL 523. Augmentin†
[23256-39-5]
Cryst. (MeOH). Mp 108°.

Robin, Y. *et al., Bull. Soc. Chim. Biol.*, 1953, **35**, 285 (*biosynth*)
Irreverre, F. *et al., Nature (London)*, 1957, **80**, 704 (*occur*)
Makisumi, S. *et al., J. Biochem. (Tokyo)*, 1961, **49**, 284 (*isol*)
Pant, R. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1964, **335**, 272 (*synth*)
Reinbothe, H. *et al., Phytochemistry*, 1964, **3**, 327 (*biosynth*)
Tomita, K. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 3628 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 13387
Okabe, N. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1992 (*cryst struct*)

N-(4-Guanidinobutyl)-2-(4-hydroxyphenyl)-2-oxoacetamide G-194



$C_{13}H_{18}N_4O_3$ 278.31
Isol. from the hydroid *Campanularia* sp. Oil. λ_{max} 209 (log ϵ 3.84); 295 (log ϵ 3.89) (MeOH).

Houssen, W.E. *et al., J. Nat. Prod.*, 2005, **68**, 453-455

2-Guanidinoethanesulfinic acid, 8CI G-195

2-[(Aminoiminomethyl)amino]ethanesulfinic acid, 9CI. Hypotaurocyamine
[1119-54-6]
[35365-99-2]
HN═C(NH$_2$)NHCH$_2$CH$_2$SO$_2$H
$C_3H_9N_3O_2S$ 151.189
Isol. from *Arenicola marina* and *Phascolosoma* spp.
Mp 187-188°.

Phosphate: 2-[[Imino(phosphonoamino)methyl]amino]ethanesulfinic acid, 9CI. 2-(3-Phosphonoguanidino)ethanesulfinic acid, 8CI. Hypotaurocyanaminephosphoric acid
[4378-69-2]
$C_3H_{10}N_3O_5PS$ 231.169
Isol. from marine annelids.

Robin, Y. *et al., Biochim. Biophys. Acta*, 1962, **63**, 481 (*isol*)
Desvages, G. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1968, **267**, 1868 (*synth*)
Berthou, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1972, **274**, 157 (*cryst struct*)

4-Guanidino-3-hydroxybutanoic acid G-196

4-[(Aminoiminomethyl)amino]-3-hydroxybutanoic acid, 9CI
[7010-89-1]
HN═C(NH$_2$)NHCH$_2$CH(OH)CH$_2$COOH
$C_5H_{11}N_3O_3$ 161.16
Occurs in the sea anemone *Anthopleura japonica*. Cryst. (H_2O).
Mp 260° dec.

Robin, Y. *et al., Bull. Soc. Chim. Biol.*, 1953, **35**, 285 (*biosynth*)
Makisumi, S. *et al., J. Biochem. (Tokyo)*, 1961, **49**, 284 (*isol*)
Japan. Pat., 1963, 63 2 860; *CA*, **59**, 11263 (*synth*)

5-Guanidino-2-oxopentanoic acid G-197

5-[(Aminoiminomethyl)amino]-2-oxopentanoic acid, 9CI. α-Keto-δ-guanidinovaleric acid
[3715-10-4]
HN═C(NH$_2$)NHCH$_2$CH$_2$CH$_2$COCOOH
$C_6H_{11}N_3O_3$ 173.171
Occurs in insects and marine invertebrates. Also found in *Phlox decussata* and *Picea glauca*. Cryst. + 1H_2O (H_2O).
Mp 250°. Darkens at 221°.

2,4-Dinitrophenylhydrazone: Mp 250°. Darkens at 218°.

Robin, Y. *et al., Biochim. Biophys. Acta*, 1953, **11**, 403 (*isol*)
Brandner, G. *et al., Acta Chem. Scand.*, 1964, **18**, 574 (*isol*)
Biellmann, J.F. *et al., Bioorg. Chem.*, 1977, **6**, 89 (*synth*)
Cooper, A.J.L. *et al., J. Biol. Chem.*, 1978, **253**, 5407 (*synth*)

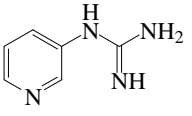
3-Guanidinopropanoic acid G-198

N-*(Aminoiminomethyl)-β-alanine, 9CI*. N-*Amidino-β-alanine, 8CI. Guanidinepropionic acid*
[353-09-3]
$HN{=}C(NH_2)NHCH_2CH_2COOH$
$C_4H_9N_3O_2$ 131.134
Occurs in the sea anemone *Anthopleura japonica*. Cryst. (EtOH aq.). Mp 209-211°.

Mourgue, M. *et al., Bull. Soc. Chim. Fr.*, 1948, 181 (*synth*)
Makisumi, S. *et al., J. Biochem. (Tokyo)*, 1961, **49**, 284 (*isol*)
Steward, E.G. *et al., Acta Cryst. B*, 1974, **30**, 813 (*cryst struct*)

3-Guanidinylpyridine G-199

3-Pyridinylguanidine, 9CI, 8CI. ***Pyraxinine***
[67087-03-0]

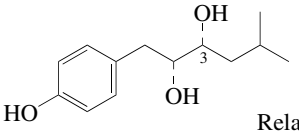


$C_6H_8N_4$ 136.156
Isol. from the New Caledonian marine sponge *Cymbastela cantharella*. Amorph. solid. λ_{max} 203 (ϵ 2300); 231 (ϵ 1900); 260 (sh) (ϵ 1100) (EtOH). λ_{max} 215 (ϵ 2800); 243 (ϵ 2000); 277 (ϵ 900) (EtOH/NaOH aq).

Al Mourabit, A. *et al., J. Nat. Prod.*, 1997, **60**, 290-291 (*isol, synth, uv, ir, pmr, cmr*)

Guaymasol G-200

1-(4-Hydroxyphenyl)-5-methyl-2,3-hexanediol
[208997-42-6]



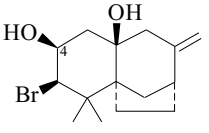
Relative Configuration

$C_{13}H_{20}O_3$ 224.299
Isol. from a marine *Bacillus* sp. (CNA-995). Viscous oil. $[\alpha]_D$ +30.4 (c, 1.13 in $CHCl_3$).

3-Epimer: ***Epiguaymasol***
[208997-43-7]
$C_{13}H_{20}O_3$ 224.299
Isol. from a marine *Bacillus* sp. (CNA-995). Viscous oil. $[\alpha]_D$ -7.2 (c, 0.17 in $CHCl_3$).
Trischman, J.A. *et al., Nat. Prod. Lett.*, 1998, **11**, 279-284 (*isol, pmr, cmr*)

Guimarediol G-201

[94835-99-1]

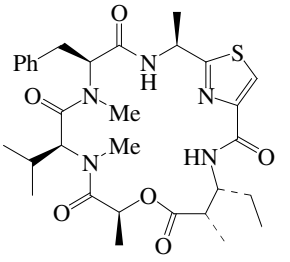


$C_{15}H_{23}BrO_2$ 315.249
Constit. of red alga *Laurencia* sp.

4-Ac:
Cryst. Mp 94-95°. $[\alpha]_D^{27}$ +30 (c, 1.2 in $CHCl_2$).
Gonzalez, A.G. *et al., Chem. Lett.*, 1984, 1865 (*cryst struct*)

Guineamide A G-202

[560082-02-2]

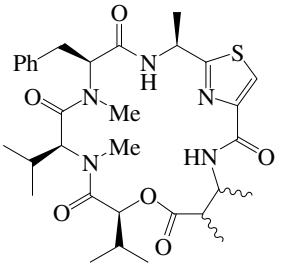


$C_{31}H_{43}N_5O_6S$ 613.777
Isol. from *Lyngbya majuscula*. Oil. $[\alpha]_D^{26}$ -8 (c, 0.1 in $CHCl_3$). λ_{max} 214 (ϵ 14400) (MeOH).

Tan, L.T. *et al., J. Nat. Prod.*, 2003, **66**, 764-771 (*isol, pmr, cmr*)

Guineamide B G-203

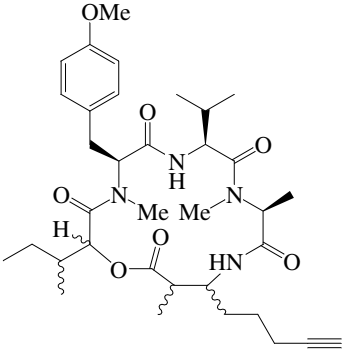
[560082-04-4]



$C_{32}H_{45}N_5O_6S$ 627.803
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D$ -5 (c, 0.17 in $CHCl_3$). λ_{max} 213 (ϵ 24900) (EtOH).

Tan, L.T. *et al., J. Nat. Prod.*, 2003, **66**, 764-771 (*isol, pmr, cmr*)

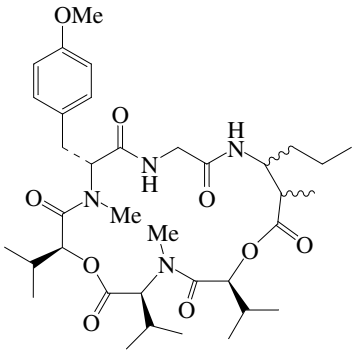
Guineamide C G-204



$C_{35}H_{52}N_4O_7$ 640.818
Isol. from *Lyngbya majuscula*. Oil. $[\alpha]_D^{26}$ -76 (c, 0.1 in MeOH). λ_{max} 222 (ϵ 16400) (MeOH).

Tan, L.T. *et al., J. Nat. Prod.*, 2003, **66**, 764-771 (*isol, pmr, cmr*)

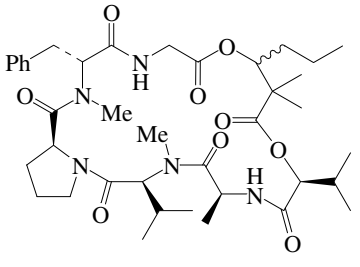
Guineamide D G-205



$C_{36}H_{56}N_4O_9$ 688.860
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{26}$ +55 (c, 0.95 in $CHCl_3$). λ_{max} 210 (ϵ 21200) (EtOH).

Tan, L.T. *et al., J. Nat. Prod.*, 2003, **66**, 764-771 (*isol, pmr, cmr*)

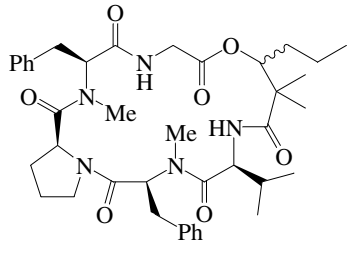
Guineamide E G-206



$C_{39}H_{59}N_5O_9$ 741.923
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{26}$ -2.7 (c, 0.18 in $CHCl_3$). λ_{max} 215 (ϵ 38300) (EtOH).

Tan, L.T. *et al., J. Nat. Prod.*, 2003, **66**, 764-771 (*isol, pmr, cmr*)

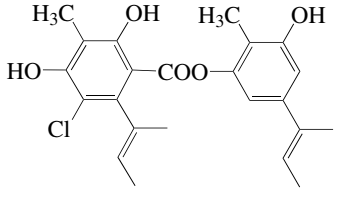
Guineamide F G-207



$C_{40}H_{55}N_5O_7$ 717.904
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{26}$ -49 (c, 0.37 in $CHCl_3$). λ_{max} 215 (ϵ 28700) (EtOH).

Tan, L.T. *et al., J. Nat. Prod.*, 2003, **66**, 764-771 (*isol, pmr, cmr*)

Guisinol G-208



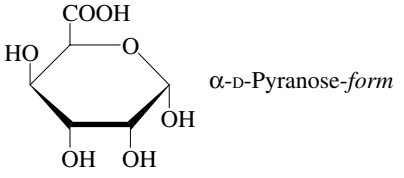
$C_{23}H_{25}ClO_5$ 416.9

Metab. of the marine derived fungus *Emericella unguis*. Antibacterial agent. Yellowish oil. λ_{max} 216 (sh) (log ϵ 4.53); 254 (log ϵ 4.09); 318 (log ϵ 3.81) (MeOH). λ_{max} 254 (ϵ 34670); 318 (ϵ 6456) (MeOH) (Berdy).

Nielsen, J. *et al., Phytochemistry*, 1999, **50**, 263-265 (*isol, uv, pmr, cmr, ms*)

Guluronic acid, 9CI, 8CI G-209

[1986-15-8]



$C_6H_{10}O_7$ 194.141

D-*form*
Cryst. + $1H_2O$ (as Na salt). $[\alpha]_D^{23}$ +31 (3 min.) → +48 (16 min., equilib.). Prepared and used as Na or brucine salt; Na salt shows no definite Mp.

L-*form* [56688-68-7]
Occurs in alginic acids from seaweed.
Syrup.

Na salt: [51433-33-1]
Needles. $[\alpha]_D^{23}$ +31 → +48 (c, 2 in H_2O). Mp indefinite (as hydrate).

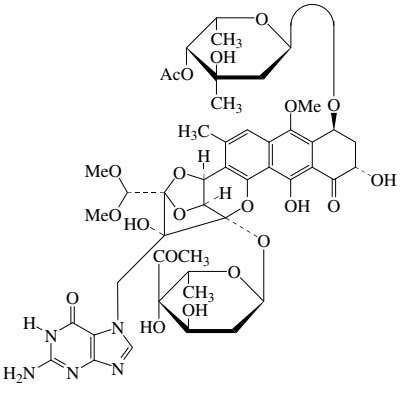
*2,3:4,5-Diisopropylidene, Me ester: Methyl 2,3:4,5-di-*O*-isopropylidene-L-guluronate*
$C_{13}H_{20}O_7$ 288.297
Syrup. $[\alpha]_D^{23}$ -82 (c, 0.64 in $CHCl_3$).

[15769-56-9, 21675-52-5]

Sutter, M. *et al., Helv. Chim. Acta*, 1938, **21**, 1210 (*synth*)
Whistler, R.L. *et al., J.A.C.S.*, 1958, **80**, 5701 (*isol*)
Drummond, D.W. *et al., J.C.S.*, 1962, 1208 (*isol*)
Anthonsen, T. *et al., Acta Chem. Scand.*, 1973, **27**, 2671 (*pmr*)
Atkins, E.D. *et al., Biopolymers*, 1973, **12**, 1879 (*cryst struct*)
Morris, E.R. *et al., J.C.S. Perkin 2*, 1975, 1418 (*cd, conformn*)
Siddiqui, I.R. *et al., Carbohydr. Res.*, 1978, **63**, 312; 1980, **80**, 343 (*isol, L-form, Na salt, synth*)
Mo, F. *et al., Carbohydr. Res.*, 1985, **145**, 13 (*cryst struct, L-form, Na salt*)
Grasdalen, H. *et al., Carbohydr. Res.*, 1990, **203**, 281 (*pmr, cmr*)
Chida, N. *et al., J. Carbohydr. Chem.*, 1992, **11**, 137-148 (*2,3:4,5-diisopropylidene, Me ester*)

Gutingimycin G-210

[690998-82-4]



$C_{47}H_{57}N_5O_{21}$ 1027.988

Closely related to Trioxacarcin A, T-752. Prod. by a marine streptomycete (isolate B8652). Yellow solid. $[\alpha]_D^{20}$ -56.5 (c, 0.5 in $CHCl_3$). λ_{max} 269 (log ϵ 5.53); 399 (log ϵ 4.96) (MeOH).

Maskey, R.P. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 1281-1283 (*isol, pmr, cmr*)

GYIRF amide G-211

[163359-58-8]

H-Gly-Tyr-Ile-Arg-Phe-NH_2

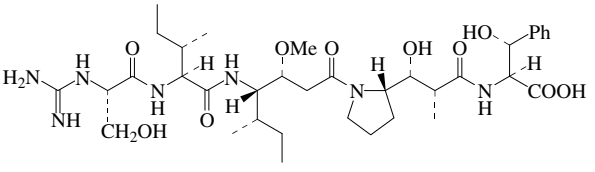
$C_{32}H_{47}N_9O_6$ 653.78

Isol. from the marine turbellarians *Bdelloura candida* and *Dugesia tigrina*. Neuropeptide.

Johnston, R.N. *et al., Biochem. Biophys. Res. Commun.*, 1995, **209**, 689 (*isol*)

Johnston, R.N. *et al., J. Neurochem.*, 1996, **67**, 814 (*isol, struct, props*)

Gymnangiamide G-212



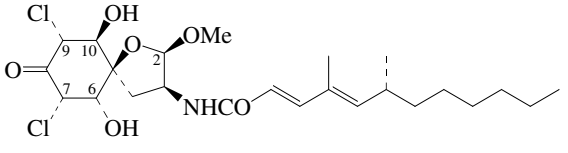
$C_{36}H_{59}N_7O_{10}$ 749.903

Isol. from the marine hydroid *Gymnangium regae*. Cytotoxic. Amorph. solid. $[\alpha]_D$ -32.5 (c, 0.24 in MeOH). λ_{max} 258 (log ϵ 2.99) (MeOH).

Milanowski, D.J. *et al., J.O.C.*, 2004, **69**, 3036-3042 (*isol, pmr, cmr, ms*)

Gymnastatin C G-213

[195729-59-0]



$C_{24}H_{37}Cl_2NO_6$ 506.465

Metab. of the fungus *Gymnascella dankaliensis* isol. from the sponge *Halichondria japonica*. Cytotoxic agent. Powder. Mp 104.7-107.5°. $[\alpha]_D$ -101.2 (c, 0.1 in $CHCl_3$). Related to Aranorosin. λ_{max} 265 (log ϵ 4.42) (EtOH).

6,10-Dideoxy, 6,7,9,10-tetradehydro, 2-O-de-Me: ***Gymnastatin A***
[195729-55-6]
Metab. of *Gymnascella dankaliensis* from *Halichondria japonica*. Cytotoxic agent. Powder.
Mp 74.2-76°. $[\alpha]_D$ -3.8 (c, 0.7 in $CHCl_3$). Mixt. of C-2 stereoisomers. λ_{max} 266 (log ϵ 4.63) (EtOH).

Dibromo analogue: ***Gymnastatin K***
[234757-10-9]
$C_{24}H_{37}Br_2NO_6$ 595.367
Metab. of *Gymnascella dankaliensis.*

Dibromo analogue, 6,7-didehydro: ***Gymnastatin J***
[234757-09-6]
$C_{24}H_{35}Br_2NO_6$ 593.352
Metab. of *Gymnascella dankaliensis.*

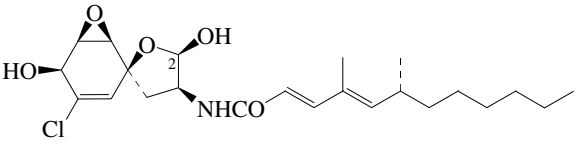
Dibromo analogue, 6,10-dideoxy, 6,7,9,10-tetradehydro, 2-O-de-Me: ***Gymnastatin I***
[234757-08-5]
$C_{23}H_{31}Br_2NO_4$ 545.31
Metab. of *Gymnascella dankaliensis.*

7-Epimer, 10-deoxy, 9,10-didehydro: ***Gymnastatin B***
[195729-57-8]
$C_{24}H_{35}Cl_2NO_5$ 488.45
Metab. of *Gymnascella dankaliensis* from *Halichondria japonica*. Cytotoxic agent. Powder.
Mp 73.5-77.5°. $[\alpha]_D$ -122.1 (c, 0.3 in $CHCl_3$). λ_{max} 265 (log ϵ 4.5) (EtOH).

Amagata, T. *et al., J.C.S. Perkin 1*, 1998, 3585-3599
Amagata, T. *et al., CA*, 1999, **131**, 129789s (*Gymnastatins I,J,K*)
Gurjar, M.K. *et al., Heterocycles*, 2000, **53**, 143-149 (*Gymnastatin A, synth*)

Gymnastatin D G-214

[220150-98-1]
[220151-09-7 (C-2 stereoisomer)]



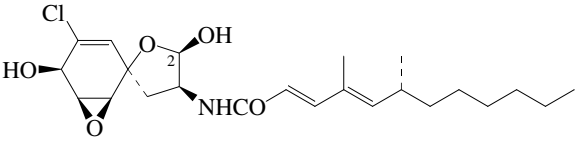
$C_{23}H_{34}ClNO_5$ 439.978

A mixt. of C-2 stereoisomers. Metab. of *Gymnascella dankaliensis* from *Halichondria japonica*. Cytotoxic. Amorph. powder.
Mp 86.4-88.2°. $[\alpha]_D$ -8.9 (c, 0.45 in $CHCl_3$). λ_{max} 265 (log ϵ 4.44) (EtOH).

Amagata, T. *et al., J.C.S. Perkin 1*, 1998, 3585-3599 (*isol, ir, pmr, cmr, uv, ms, cd*)

Gymnastatin E G-215

[220151-00-8]



$C_{23}H_{34}ClNO_5$ 439.978

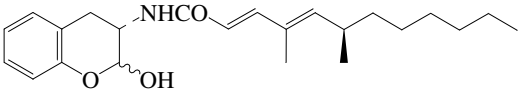
A mixt. of C-2 stereoisomers. Metab. of *Gymnascella dankaliensis* from *Halichondria japonica*. Cytotoxic agent. Amorph. powder.
Mp 87.3-88°. $[\alpha]_D$ -8.5 (c, 0.52 in $CHCl_3$). λ_{max} 266 (log ϵ 4.63) (EtOH).

[220151-14-4 (C-2 stereoisomer)]

Amagata, T. *et al., J.C.S. Perkin 1*, 1998, 3585-3599 (*isol, ir, pmr, cmr, uv, ms, cd*)

Gymnastatin L G-216

[234757-11-0]



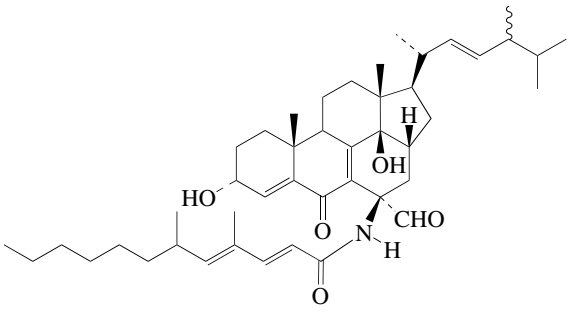
$C_{23}H_{33}NO_3$ 371.519

Metab. of *Gymnascella dankaliensis* isol. from the sponge *Halichondria japonica*.

Amagata, T. *et al., CA*, 1999, **131**, 129789s (*isol*)

Gymnasterone A G-217

[209169-57-3]

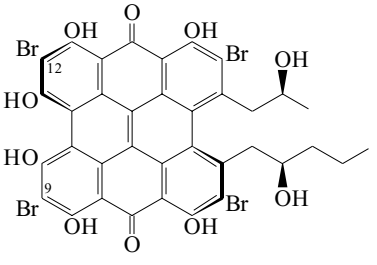


$C_{45}H_{67}NO_5$ 702.028
Constit. of *Gymnascella dankaliensis* isol from the sponge *Halichondria japonica*. Pale yellow oil. $[\alpha]_D$ -110.7 (c, 1.44 in $CHCl_3$). λ_{max} 270 (log ϵ 4.22) (EtOH). λ_{max} 270 (ϵ 16600) (MeOH) (Berdy).

Amagata, T. *et al., Tet. Lett.*, 1998, **39**, 3773-3774 (*isol, pmr, cmr*)

Gymnochrome A G-218

[137363-67-8]



$C_{36}H_{24}Br_4O_{10}$ 936.196
Constit. of the stalked crinoid *Gymnocrinus richeri*. Violet pigment. λ_{max} 216 (sh) (ϵ 41000); 235 (ϵ 44000); 256 (ϵ 42000); 298 (ϵ 31300); 332 (ϵ 24000); 500 (ϵ 12700); 553 (ϵ 17000); 597 (ϵ 33800) (MeOH).

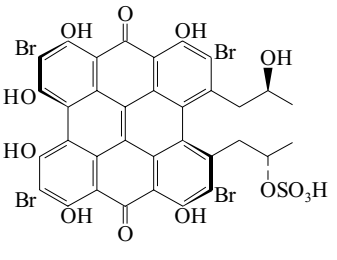
9 or 12-Debromo: ***Gymnochrome B***
[137363-72-5]
$C_{36}H_{25}Br_3O_{10}$ 857.299
Constit. of *Gymnocrinus richeri*. Violet pigment. λ_{max} 216 (ϵ 48000); 233 (ϵ 51500); 295 (sh) (ϵ 32000); 329 (ϵ 27200); 485 (ϵ 13800); 553 (ϵ 19800); 596 (ϵ 39300) (MeOH).

[137490-27-8 (Isogymnochrome B)]

De Riccardis, F. *et al., J.O.C.*, 1991, **56**, 6781-6787 (*isol, pmr, uv, ir, ms*)
Etzlstorfer, C. *et al., Monatsh. Chem.*, 1993, **124**, 1031-1039 (*tautom*)

Gymnochrome C G-219

[137363-68-9]

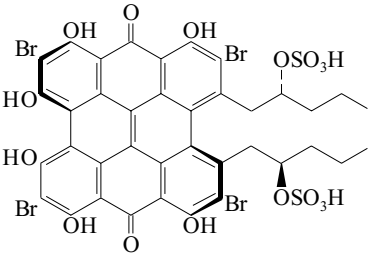


$C_{34}H_{20}Br_4O_{13}S$ 988.206
Isol. from *Gymnocrinus richeri*. Violet pigment. λ_{max} 215 (ϵ 36800); 234 (ϵ 34000); 297 (ϵ 21000); 338 (ϵ 15700); 500 (ϵ 8500); 553 (ϵ 8000); 597 (ϵ 19000) (MeOH).

De Riccardis, F. *et al., J.O.C.*, 1991, **56**, 6781-6787 (*isol, pmr, uv, ir, ms*)

Gymnochrome D G-220

[137363-69-0]

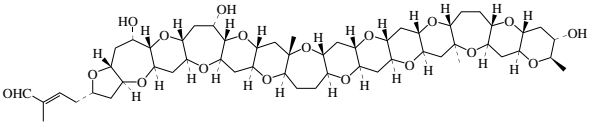


$C_{38}H_{28}Br_4O_{16}S_2$ 1124.378
Isol. from the stalked crinoid *Gymnocrinus richeri*. Violet pigment.

Diastereoisomer: ***Isogymnochrome D***
[137490-24-5]
$C_{38}H_{28}Br_4O_{16}S_2$ 1124.378
Isol. from *Gymnocrinus richeri*. Violet pigment.

De Riccardis, F. *et al., J.O.C.*, 1991, **56**, 6781-6787 (*isol, uv, ir, pmr*)
Etzlstorfer, C. *et al., Monatsh. Chem.*, 1993, **124**, 1031-1039 (*tautom*)

Gymnocin A G-221

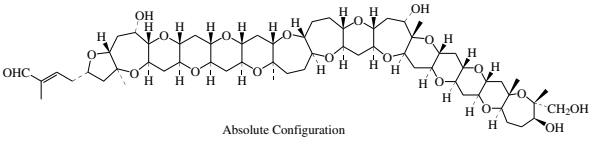


Absolute Configuration

$C_{55}H_{80}O_{18}$ 1029.226
Isol. from the red tide dinoflagellate *Karenia* (formerly *Gymnodinium*) *mikimotoi*. Cytotoxic. Amorph. solid. $[\alpha]_D^{20}$ +12.5 (c, 0.11 in $CHCl_3$). λ_{max} 236 (ϵ 16000) (no solvent reported).

Satake, M. *et al., Tet. Lett.*, 2002, **43**, 5829-5832 (*isol, pmr, cmr, ms*)
Tsukano, C. *et al., J.A.C.S.*, 2005, **127**, 4326-4335 (*synth*)
Tsukano, C. *et al., Tet. Lett.*, 2006, **47**, 6803-6807 (*sar*)

Gymnocin B G-222



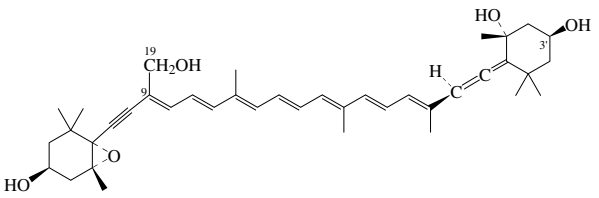
Absolute Configuration

$C_{62}H_{92}O_{20}$ 1157.397
Isol. from the red tide dinoflagellate *Karenia mikimotoi* (formerly *Gymnodinium mikimotoi*). Cytotoxic. Amorph. solid. λ_{max} 230 (ϵ 17300) (no solvent reported).

Tanaka, K. *et al., J.A.C.S.*, 2005, **127**, 9561-9570 (*abs config*)
Satake, M. *et al., Tet. Lett.*, 2005, **46**, 3537-3540 (*isol, pmr, cmr, ms*)

Gymnodimine G-223

[173792-58-0]



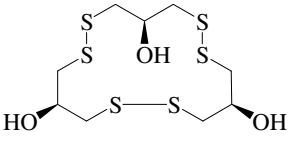
$C_{32}H_{45}NO_4$ 507.712
Isol. from New Zealand oysters (*Tiostrea chilensis*) and the dinoflagellate *Gymnodinium* cf. *mikimotoi*. Shows potent ichthyotoxicity. Amorph. solid. $[\alpha]_D^{25}$ -10.4 (c, 0.13 in MeOH).

*$\Delta^{17,29}$-Isomer, 18*R*-hydroxy:* ***Gymnodimine C***
$C_{32}H_{45}NO_5$ 523.711
Prod. by *Karenia selliformis* (formerly *Gymnodinium selliforme*).

*$\Delta^{17,29}$-Isomer, 18*S*-hydroxy:* ***Gymnodimine B***
$C_{32}H_{45}NO_5$ 523.711
Isol. from *Karenia selliformis* (formerly *Gymnodinium selliforme*).

Seki, T. *et al., Tet. Lett.*, 1995, **36**, 7093-7096 (*isol, pmr, cmr, struct*)
Stewart, M. *et al., Tet. Lett.*, 1997, **38**, 4889-4890 (*cryst struct, abs config*)
Miles, C.O. *et al., J. Agric. Food Chem.*, 2000, **48**, 1373-1376; 2003, **51**, 4838-4840 (*Gymnodimines B,C*)

Gymnorrhizol G-224



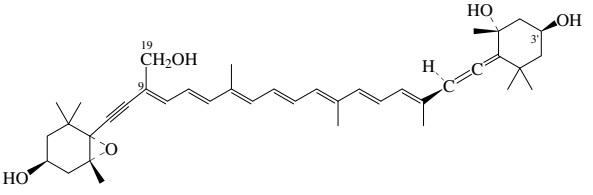
$C_9H_{18}O_3S_6$ 366.635
Isol. from the mangrove *Bruguiera gymnorrhiza*. Cryst. Mp 144-146°. λ_{max} 249 (ϵ 2520) (MeOH).
Sun, Y.-Q. *et al., Tet. Lett.*, 2004, **45**, 5533-5535 (*isol, pmr, cmr*)

GYNRSFLRF amide G-225

[138968-16-8]
Gly-Tyr-Asn-Arg-Ser-Phe-Leu-Arg-Phe-NH_2
$C_{54}H_{79}N_{17}O_{12}$ 1158.325
FMRF amide-related peptide. Isol. from the blue crab *Callinectes sapidus.*
Krajniak, K.G. *et al., Peptides (N.Y.)*, 1991, **12**, 1295-1302 (*isol*)

Gyroxanthin G-226

[201364-25-2]

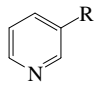


$C_{40}H_{54}O_5$ 614.864
Constit. of *Gymnodinium galatheanum*. λ_{max} 408; 434; 461 (Me_2CO).

19-Dodecanoyl, 3′-Ac: ***Gyroxanthin diester***
[326865-47-8]
$C_{54}H_{78}O_7$ 839.206
Constit. of *Gymnodinium galatheanum*. λ_{max} 418; 442; 470 (hexane).

*9*Z*-Isomer, 19-dodecanoyl, 3′-Ac: 9-*cis*-Gyroxanthin diester*
[326586-72-5]
$C_{54}H_{78}O_7$ 839.206
Constit. of *Gymnodinium galatheanum*. λ_{max} 325; 414; 438; 465 (hexane).
Bjornland, T. *et al., Tetrahedron*, 2000, **56**, 9047-9056 (*isol, pmr, cmr*)

Hachijodines H-1



Hachijodine A R = -$(CH_2)_{12}$NHOMe
B R = -$(CH_2)_9$CH(CH_3)CH_2CH_2NHOMe
C R = -$(CH_2)_{10}$CH(CH_3)CH_2NHOMe
D R = -CH_2CH(CH_3)$(CH_2)_{10}$NHOMe
E R = -$(CH_2)_{13}$NMeOH
F R = -$(CH_2)_4C{\equiv}C(CH_2)_8$NMeOH
G R = -$(CH_2)_4C{\equiv}CCH{=}CH(CH_2)_8$NMeOH
Cribochaline B R = -$(CH_2)_{11}$CH(CH_3)CH_2NHOMe

Alkaloids from either *Amphimedon* sp. or *Xestospongia* sp. Cytotoxic agents.

Hachijodine A [265114-90-7]
$C_{18}H_{32}N_2O$ 292.464
From a *Xestospongia* sp. λ_{max} 260 (ϵ 3300) (MeOH).

Hachijodine B [265114-91-8]
$C_{19}H_{34}N_2O$ 306.49
From a *Xestospongia* sp. λ_{max} 260 (ϵ 3300) (MeOH).

Hachijodine C
Cribochaline A
[265114-92-9]
$C_{19}H_{34}N_2O$ 306.49
Isol. from the sponges *Xestospongia* sp. and *Cribrochalina* sp. $[\alpha]_D^{24}$ -1 (c, 0.2 in MeOH). Related to Niphatesine C, N-117. λ_{max} 260 (ϵ 3200) (MeOH). λ_{max} 210 (ϵ 5630); 262 (ϵ 4530); 269 (ϵ 3330) (MeOH).

Hachijodine D [265114-93-0]
$C_{19}H_{34}N_2O$ 306.49
From a *Xestospongia* sp. λ_{max} 260 (ϵ 3200) (MeOH).

Hachijodine E [265114-94-1]
$C_{19}H_{34}N_2O$ 306.49
From an *Amphimedon* sp.

Hachijodine F [265114-95-2]
$C_{20}H_{32}N_2O$ 316.486
From an *Amphimedon* sp.

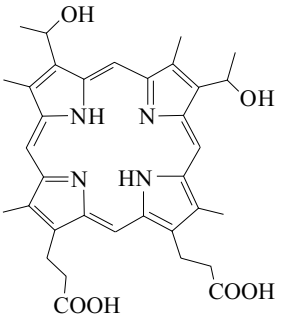
Hachijodine G [265114-96-3]
$C_{22}H_{34}N_2O$ 342.523
From an *Amphimedon* sp.

Cribochaline B
$C_{20}H_{36}N_2O$ 320.517
Isol. from the sponge *Cribrochalina* sp.

Tsukamoto, S. *et al., J. Nat. Prod.*, 2000, **63**, 682-684 (*isol, pmr, Hachijodines B-G*)
Nicholas, G.M. *et al., Tetrahedron*, 2000, **56**, 2921-2927 (*Cribochalines A,B*)
Goundry, W.R.F. *et al., Tetrahedron*, 2003, **59**, 1719-1729 (*Hachijodines F,G, synth*)
Romeril, S.P. *et al., Tet. Lett.*, 2004, **45**, 3273-3277 (*Hachijodine B, synth*)

Haematoporphyrin H-2

Haematoporphyrin IX. Hematoporphyrin
[14459-29-1]



$C_{34}H_{38}N_4O_6$ 598.697
Obt. from Haemin or Haematin by removal of Fe with conc. acids. Isol. from a *Chlorella vulgaris* mutant. Antidepressant. Treatment of haematoporphyrin with H_2SO_4/AcOH followed by NaOH yields a complex mixt. of ester, ether and C–C linked dimers and trimers known as HPD, which is used as a photosensitiser for photodynamic tumour therapy (PDT). Purple cryst. (Et_2O/AcOH). Log P 4.75 (calc). Use limited by chemical instability.

▶ LD_{50} (mus, ivn) 307 mg/kg. TS5500000

Di-Me ester: [32562-61-1]
$C_{36}H_{42}N_4O_6$ 626.751
Violet cryst. ($CHCl_3$/MeOH). Mp 212°.

[17696-69-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 575C (*ir*)
Fischer, H. *et al., Die Chemie des Pyrrols*, Akademische Verlag, Leipzig, Vol. II, (i), 1937, 421
Granick, S. *et al., J. Biol. Chem.*, 1953, **202**, 801 (*isol*)
Falk, J.E. *et al., Porphyrins and Metalloporphyrins*, (ed. Smith, K.M.), Elsevier, New York, 1964, 175 (*rev*)
Sano, S. *et al., Biochem. J.*, 1965, **97**, 250 (*pmr*)
Evans, N. *et al., J. Chromatogr.*, 1975, **115**, 325 (*hplc, ms*)
Luzgina, V.N. *et al., Khim.-Farm. Zh.*, 1977, **11**, 26 (*rev, synth, pharmacol*)
Kessel, D. *et al., Photochem. Photobiol.*, 1984, **39**, 851 (*rev, pharmacol*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 8024
Henderson, B.W. *et al., Photochem. Photobiol.*, 1992, **55**, 145 (*PDT review*)
Henderson, B.W. *et al., Photodynamic Therapy*, M. Dekker, New York, 1992, (*book*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1376
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PHV275

Haemerythrin H-3

Hemerythrin
[$Fe_2N_5O_5$]

Non-haem binuclear O_2-carrier protein. Consists of 8 subunits (each of 113 amino acid residues) with 2 Fe/subunit. Found among invertebrates; particularly annelids, molluscs and arthropods. MW *ca*. 108,000.

Stenkamp, R.E. *et al., Acta Cryst. B*, 1983, **39**, 697 (*cryst struct*)
Wilkins, R.G. *et al., Adv. Inorg. Biochem.*, 1983, **5**, 51 (*rev*)
Klotz, I.M. *et al., Acc. Chem. Res.*, 1984, **17**, 16 (*rev*)
Brunori, M. *et al., Top. Mol. Struct. Biol.*, 1985, **7**, 263 (*rev*)
Wilkins, P.C. *et al., Coord. Chem. Rev.*, 1987, **79**, 195 (*rev*)
Que, L. *et al., Met. Ions Biol. Syst.*, (Ed. Sigel, H.), Vol. 21, Marcel Dekker, N.Y., 1987, 87 (*rev, nmr*)
Janin, J. *et al., J. Mol. Biol.*, 1988, **204**, 155 (*struct*)
Reem, R.C. *et al., J.A.C.S.*, 1989, **111**, 4688

Haemocyanin H-4

Hemocyanin
Metalloprotein with a multisubunit struct incl. 2 Cu atoms. Present in the blood of most molluscs and some arthropods such as the horseshoe crab (*Limulus polyphemus*). Respiratory

protein. Cu atoms reversibly bind an O_2 molecule. Oxygenation causes a colour change between the colourless Cu(I) deoxygenated form and the blue Cu(II) oxygenated form.

Van Holde, K.E. *et al., Q. Rev. Biophys.*, 1982, **15**, 1-129 (*rev*)
Van Holde, K.E. *et al., Adv. Protein Chem.*, 1995, **47**, 1-81 (*rev*)
Van Holde, K.E. *et al., J. Biol. Chem.*, 2001, **276**, 15563-15566 (*rev*)

Hagfish intestinal antimicrobial peptides H-5

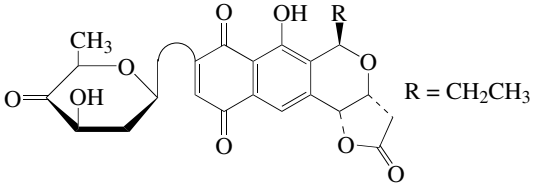
HFIAP

Three peptides containing 30-37 amino acid residues; members of the Cathelicidin family. Isol. from intestinal tissues of the Atlantic hagfish *Myxine glutinosa*. Antimicrobial agents.

Uzzell, T. *et al., Peptides (N.Y.)*, 2003, **24**, 1655-1667 (*isol*)

Halawanone A H-6

[213547-25-2]



$C_{23}H_{22}O_9$ 442.421

Prod. by a marine-derived *Streptomyces* sp. λ_{max} 217 (ϵ 20300); 255 (ϵ 6360); 325 (ϵ 2550); 428 (ϵ 2300) (MeOH).

Ford, P.W. *et al., J. Nat. Prod.*, 1998, **61**, 1232-1236 (*isol, cd, uv, ir, pmr, cmr, ms*)

Halawanone B H-7

[213547-26-3]

As Halawanone A, H-6 with

R = CH_3

$C_{22}H_{20}O_9$ 428.395

Prod. by a marine-derived *Streptomyces* sp.

Ford, P.W. *et al., J. Nat. Prod.*, 1998, **61**, 1232-1236 (*isol, cd, uv, ir, pmr, cmr, ms*)

Halcurin H-8

[189257-65-6]

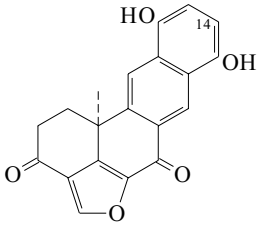
Peptide containing 47 amino acid residues. Isol. from the sea anemone *Halcurias* sp. Toxin, lethal to crabs.

Ishida, M. *et al., Toxicon*, 1997, **35**, 537-544 (*isol*)

Halenaquinol H-9

*8,11-Dihydroxy-12*b-*methyl-1*H-*benzo[6,7]phenanthro[10,1-*bc*]furan-3,6(2*H,*12*bH*)-dione, 9CI*

[96603-02-0]



Absolute configuration

$C_{20}H_{14}O_5$ 334.328

Constit. of sponge *Xestospongia sapra* and *Xestospongia carbonaria*. Potent irreversible inhibitor of Rous sarcoma virus. Inhibitor of protein tyrosine kinase. Yellow solid. Sol. Me_2CO. $[\alpha]_{577}$ +179 (Me_2CO). Unstable to heat and light. λ_{max} 228 (ϵ 36000); 284 (sh) (ϵ 20000); 302 (ϵ 23000); 431 (ϵ 4000) (MeOH) (Derep).

O^{16}-Sulfate: [99528-87-7]
$C_{20}H_{14}O_8S$ 414.392

Constit. of *Xestospongia sapra*. Yellow solid. Sol. Me_2CO. $[\alpha]_{577}$ +106 (MeOH). λ_{max} 225 (ϵ 41000); 275 (ϵ 20000); 296 (ϵ 22000); 318 (sh) (ϵ 12000); 398 (ϵ 6000) (MeOH) (Derep).

12,15-Quinone: ***Halenaquinone***
[86690-14-4]
$C_{20}H_{12}O_5$ 332.312

Constit. of *Xestospongia exigua*, *Xestospongia carbonaria*, *Adocia* sp. and *Spongia* sp. Inhibitor of protein tyrosine kinase and topoisomerase. Yellow solid. Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 250° dec. $[\alpha]_D^{25}$ +22.2 (c, 0.124 in CH_2Cl_2). λ_{max} 216 (ϵ 18100); 232 (sh) (ϵ 16500); 253 (ϵ 21600); 260 (sh) (ϵ 20400); 278 (ϵ 15900); 325 (sh) (ϵ 6000) (MeCN) (Derep). λ_{max} 222 (ϵ 31600); 245 (ϵ 18700); 265 (sh) (ϵ 13400); 293 (sh) (ϵ 7400); 305 (sh) (ϵ 7100); 317 (ϵ 6900) (MeOH) (Derep).

12,15-Quinone, 14-methoxy: ***14-Methoxyhalinaquinone***
[150931-83-2]
$C_{21}H_{14}O_6$ 362.338

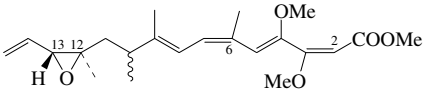
Constit. of *Xestospongia* cf. *carbonaria*. Inhibitor of protein tyrosine kinase. Reddish-yellow solid. λ_{max} 216; 237; 246; 351 (MeOH) (Berdy).

12,15-Quinone, 3-deoxo: See Xestoquinone, X-52

Roll, D.M. *et al., J.A.C.S.*, 1983, **105**, 6177-6178 (*Halenaquinone, cryst struct*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1305-1308 (*isol, sulfate*)
Harada, N. *et al., J.A.C.S.*, 1989, **111**, 5668-5674 (*abs config*)
Alvi, K.A. *et al., J.O.C.*, 1993, **58**, 4871-4880 (*isol, pmr, cmr, activity*)
Harada, N. *et al., J.O.C.*, 1994, **59**, 6606-6613 (*synth*)
Kojima, A. *et al., Synthesis*, 1998, 581-589 (*synth*)
Sutherland, H.S. *et al., J.O.C.*, 2001, **66**, 3639-3641 (*Halenaquinone, synth*)
Wipf, P. *et al., Org. Biomol. Chem.*, 2005, **3**, 2053-2061 (*rev*)

Haliangicin A H-10

Antibiotic SMP 2. SMP 2



Relative Configuration

$C_{22}H_{32}O_5$ 376.492

Polyene antibiotic. Prod. by the marine myxobacterium *Haliangium ochraceum* AJ13395. Antifungal agent. Light yellow oil. $[\alpha]_D^{22}$ +34.6 (c,0.3 in MeOH). λ_{max} 257 (ϵ 15900); 291 (ϵ 15100) (MeOH).

12,13-cis-*Isomer:* **cis-*Haliangicin A***
$C_{22}H_{32}O_5$ 376.492
Prod. by *Haliangium ochraceum* AJ13395. Antifungal agent. Light yellow oil. $[\alpha]_D^{22}$ +29.3 (c, 0.21 in MeOH). Not obt. free of the *trans*-isomer. λ_{max} 245 (sh) (ϵ 11000); 295 (sh) (ϵ 7600) (MeOH).

(2Z)-Isomer: ***Haliangicin B***
$C_{22}H_{32}O_5$ 376.492
Prod. by *Haliangium ochraceum* AJ13395. Antifungal agent. Light yellow oil. $[\alpha]_D^{22}$ +38 (c, 0.11 in MeOH). Obt. as a mixt. of 12,13-*trans*- and *cis*-isomers (2:1). λ_{max} 254 (ϵ 9500); 341 (ϵ 11000) (MeOH).

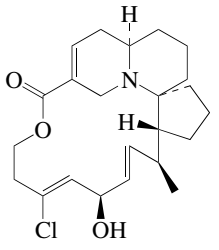
*(4*E*)-Isomer:* ***Haliangicin C***
$C_{22}H_{32}O_5$ 376.492
Prod. by *Haliangium ochraceum* AJ13395. Antifungal agent. Light yellow oil. $[\alpha]_D^{22}$ -40 (c, 0.04 in MeOH). Obt. as a mixt. of 12,13-*trans*- and *cis*-isomers (2:1). λ_{max} 247 (ϵ 9100); 277 (ϵ 9200) (MeOH).

*(4*E*,6*E*)-Isomer:* ***Haliangicin D***
$C_{22}H_{32}O_5$ 376.492
Prod. by *Haliangium ochraceum* AJ13395. Antifungal agent. Light yellow oil. $[\alpha]_D^{22}$ -20 (c, 0.05 in MeOH). λ_{max} 286 (ϵ 27000) (MeOH).

Fudou, R. *et al., J. Antibiot.*, 2001, **54**, 149-152; 153-156 (*isol, pmr, cmr*)
Kundim, B.A. *et al., J. Antibiot.*, 2003, **56**, 630-638 (*isol, pmr, cmr*)

Halichlorine H-11

[178176-75-5]



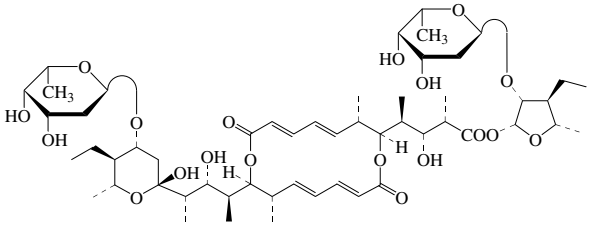
Absolute configuration

$C_{23}H_{32}ClNO_3$ 405.963

Alkaloid from the marine sponge *Halichondria okadai*. Shows antiinflammatory, antimetastatic and immunosuppressive props. Mp 183.5-185.5°. $[\alpha]_D$ +240.7 (c, 0.54 in MeOH).

Kuramoto, M. *et al., Tet. Lett.*, 1996, **37**, 3867-3870 (*isol, ir, pmr, cmr, struct*)
Arimoto, H. *et al., Tet. Lett.*, 1998, **39**, 861-862 (*abs config*)
Trauner, D. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 3542-3545 (*synth*)
Matsumura, Y. *et al., Org. Lett.*, 2004, **6**, 965-968 (*synth*)
Zhang, H.-L. *et al., J.O.C.*, 2005, **70**, 4954-4961 (*synth*)
Andrade, R.B. *et al., Org. Lett.*, 2005, **7**, 5733-5735 (*synth*)

Halichoblelide H-12



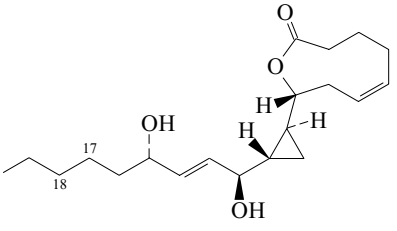
$C_{54}H_{86}O_{19}$ 1039.262

Macrolide antibiotic. Prod. by *Streptomyces hygroscopicus* from a marine fish (*Halichoeres bleekeri*). Cytotoxic. Powder. Mp 137-139°. $[\alpha]_D$ -16 (c, 0.16 in EtOH). λ_{max} 252 (log ϵ 4.56) (EtOH).

Yamada, T. *et al., Tet. Lett.*, 2002, **43**, 1721-1724 (*isol, pmr, cmr*)

Halicholactone H-13

[124190-20-1]



$C_{20}H_{32}O_4$ 336.47

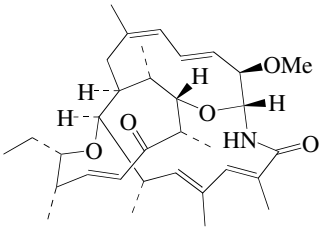
Metab. of sponge *Halichondria okadai*. Potent 5-lipoxygenase inhibitor. Oil. $[\alpha]_D^{23}$ -85.4 (c, 1.16 in $CHCl_3$).

17Z,18-Didehydro: ***Neohalicholactone***
[124190-21-2]
$C_{20}H_{30}O_4$ 334.455
Metab. of *Halichondria okadai*. 5-Lipoxygenase inhibitor. Cryst. (Et_2O/pentane).
Mp 69-70°. $[\alpha]_D^{16}$ -54.2 (c, 0.73 in $CHCl_3$).

Niwa, H. *et al., Tet. Lett.*, 1989, **30**, 4543
Kigoshi, H. *et al., Tet. Lett.*, 1991, **32**, 2427 (*cryst struct*)
Proteau, P.J. *et al., J. Nat. Prod.*, 1994, **57**, 1717 (*isol, abs config*)
Critcher, D.J. *et al., J.O.C.*, 1997, **62**, 6638-6657 (*synth*)
Takemoto, Y. *et al., Tet. Lett.*, 2000, **41**, 3653-3656 (*synth*)
Baba, Y. *et al., J.O.C.*, 2001, **66**, 81-88 (*synth*)
Takahashi, T. *et al., Heterocycles*, 2002, **58**, 99-104 (*synth*)

Halichomycin H-14

[157078-49-4]



Relative Configuration

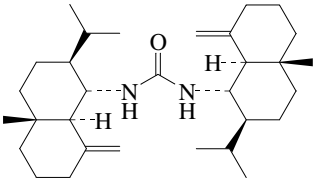
$C_{33}H_{49}NO_5$ 539.754

Prod. by a *Streptomyces hygroscopicus* from a marine fish (*Halichoeres bleekeri*). Cytotoxic agent. Oil. $[\alpha]_D^{20}$ +3.8 (c, 1.2 in $CHCl_3$). λ_{max} 242 (log ϵ 4.31); 275 (log ϵ 3.88) (EtOH).

Takahashi, C. *et al., Tet. Lett.*, 1994, **35**, 5013-5014 (*isol, uv, ir, pmr, cmr*)

Halichonadin A H-15

[847605-76-9]



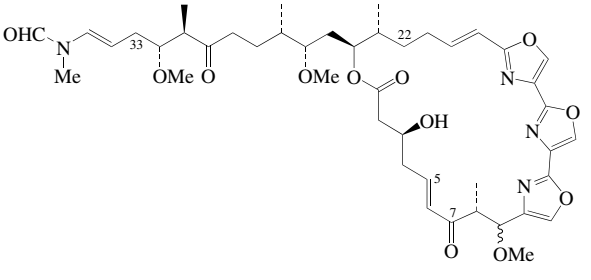
$C_{31}H_{52}N_2O$ 468.765

Constit. of a *Halichondria* sp. Cryst.
Mp 114-116°. $[\alpha]_D^{24}$ -30 (c, 1 in $CHCl_3$).

Ishiyama, H. *et al., Tetrahedron*, 2005, **61**, 1101-1105 (*isol, pmr, cmr*)

Halichondramide H-16

[113275-14-2]



$C_{44}H_{60}N_4O_{12}$ 836.978

Macrolide antibiotic. Related to Kabiramide C, K-1. Prod. by sponge *Halichondria* sp., *Haliclona* sp. and *Polycitorella* sp. Antifungal agent, insectide, toxic to sea urchins. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 66-68°. $[\alpha]_D$ -100.7 (c, 0.42 in MeOH). λ_{max} 232 (ϵ 23400) (MeOH) (Derep).

5,6-Dihydro: ***Dihydrohalichondramide***
[116302-29-5]
$C_{44}H_{62}N_4O_{12}$ 838.993
Isol. from *Halichondria* sp. and *Hexabranchus sanguineus*. Glass. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -69.7 (c, 1.68 in MeOH). λ_{max} 247 (ϵ 32000) (MeOH) (Berdy). λ_{max} 245 (ϵ 26800) (EtOH) (Berdy).

*5,6-Dihydro, 7*R*-alcohol:* ***Tetrahydrohalichondramide***
[116302-33-1]

$C_{44}H_{64}N_4O_{12}$ 841.009
Isol. from *Halichondria* sp. Glass. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -27 (c, 0.54 in MeOH). λ_{max} 247 (ϵ 34000) (MeOH) (Berdy).

*5*S-*Hydroxy, 5,6-dihydro:* ***Jaspisamide A***
[149420-76-8]
$C_{44}H_{62}N_4O_{13}$ 854.993
Isol. from the Okinawan marine sponge *Jaspis* sp. Cytotoxic. Solid. $[\alpha]_D^{17}$ -51 (c, 0.13 in MeOH). λ_{max} 244 (ϵ 24000) (MeOH) (Berdy).

*22*S-*Hydroxy:* ***Jaspisamide B***
[149420-77-9]
$C_{44}H_{60}N_4O_{13}$ 852.977
Isol. from *Jaspis* sp. Cytotoxic. Solid. $[\alpha]_D^{20}$ -112 (c, 0.19 in MeOH). λ_{max} 230 (ϵ 36000) (MeOH) (Berdy).

*5*S-*Amino, 5,6-dihydro:* ***Halishigamide A***
$C_{44}H_{63}N_5O_{12}$ 854.008
Metab. from the Okinawan marine sponge *Halichondria* sp. Cytotoxic. Antifungal agent. Amorph. solid. $[\alpha]_D^{25}$ +38 (c, 0.51 in MeOH). λ_{max} 263 (ϵ 15000) (MeOH).

5Z-Isomer: ***Isohalichondramide***
[116302-30-8]
$C_{44}H_{60}N_4O_{12}$ 836.978
Minor prod. from *Halichondria* sp. Ichthyotoxin, feeding deterrent and spongicide. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

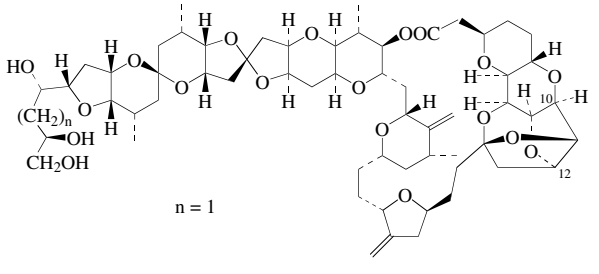
*33*R-*Methyl:* ***Jaspisamide C***
[149420-78-0]
$C_{45}H_{62}N_4O_{12}$ 851.004
Isol. from *Jaspis* sp. Cytotoxic. Solid. $[\alpha]_D^{19}$ -76 (c, 0.37 in MeOH). λ_{max} 230 (ϵ 32000) (MeOH) (Berdy).

*33*R-*Methyl, 5,6-dihydro:* ***33-Methyldihydrohalichondramide****. Dihydrojaspisamide*
[119147-13-6]
$C_{45}H_{64}N_4O_{12}$ 853.02
Isol. from the egg masses of *Hexabranchus* sp. Cytotoxic. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{23}$ -53 (c, 0.5 in $CHCl_3$). λ_{max} 242 (ϵ 24600) (MeOH).

Kernan, M.R. *et al., J.O.C.*, 1988, **53**, 5014-5020 (*isol, pmr, cmr*)
Matsunaga, S. *et al., J.O.C.*, 1989, **54**, 1360-1363 (*33-Methyldihydrohalichondramide*)
Kobayashi, J. *et al., J. Nat. Prod.*, 1993, **56**, 787-791 (*Jaspisamides A,B,C*)
Kobayashi, J. *et al., J. Nat. Prod.*, 1997, **60**, 150-154 (*Halishigamide*)

Halichondrin B H-17

[103614-76-2]



$C_{60}H_{86}O_{19}$ 1111.328
Polyether macrolide. Isol. from the marine sponges *Axinella* spp., *Halichondria okadai*, *Phakellia carteri* and *Lissodendoryx* sp. Cytotoxic agent. Shows antimitotic and microtubule assembly inhibiting activities. Undergoing preclinical trials at U.S. Natl. Cancer Inst. (1994). Cryst. Sol. MeOH, EtOH, Py; poorly sol. H_2O.
Mp 164-166°. $[\alpha]_D$ -58.9 (c, 0.94 in MeOH). Halichondrin A is not known. It is used by CA as a parent struct.

10-Hydroxy: Isohalichondrin C. ***Halistatin 1***
[147427-91-6]
$C_{60}H_{86}O_{20}$ 1127.327
Isol. from the sponges *Phakellia carteri* and *Axinella carteri*. Cytotoxic agent. Inhibits tubulin polym. Amorph. solid. $[\alpha]_D^{25}$ -58.4 (c, 0.57 in MeOH). λ_{max} 201 (ϵ 8000) (MeOH) (Derep).

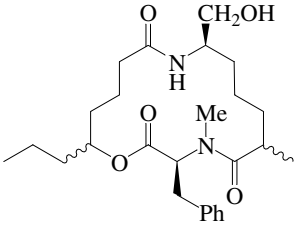
12-Hydroxy: ***Halichondrin C***
[101383-38-4]
$C_{60}H_{86}O_{20}$ 1127.327
Isol. from *Halichondria okadai*. Cytotoxic agent. Cryst. Sol. MeOH, butanol, Py; poorly sol. H_2O.
Mp 169-172°. $[\alpha]_D$ -41.6 (c, 0.49 in MeOH).

Homologue (n = 2): ***Halistatin 3****. Neohomohalichondrin B*
[156742-01-7]
$C_{61}H_{88}O_{19}$ 1125.355
Isol. from the sponges *Lissodendoryx* sp. and *Phakellia* sp. Cytotoxic agent.
Mp 185-187°. $[\alpha]_D^{25}$ -62 (c, 0.04 in MeOH). λ_{max} 201 (ϵ 8000) (MeOH).

[102721-98-2]

Hirata, Y. *et al., Pure Appl. Chem.*, 1986, **58**, 701 (*isol*)
Bai, R.L. *et al., J. Biol. Chem.*, 1991, **266**, 15882-15889 (*pharmacol*)
Aicher, T.D. *et al., J.A.C.S.*, 1992, **114**, 3162 (*synth, abs config*)
Canadian Pat., 1993, 2 092 108; *CA*, **121**, 130563p (*Halistatin 3, isol*)
Pettit, G.R. *et al., Gazz. Chim. Ital.*, 1993, **123**, 371 (*isol*)
Pettit, G.R. *et al., J.O.C.*, 1993, **58**, 2538 (*Halistatin 1*)
Eur. Pat., 1994, 608 108 (*Halistatin 1*)
Pettit, G.R. *et al., Chem. Comm.*, 1995, 383 (*Halistatin 3, uv, pmr, isol*)
Norcross, R.D. *et al., Chem. Rev.*, 1995, **95**, 2041 (*rev, synth*)
Litaudon, M. *et al., J.O.C.*, 1997, **62**, 1868-1871 (*Neohomohalichondrin B*)
Burke, S.D. *et al., Spec. Publ. - Chem. Soc.*, 1997, **198**, 73-85 (*rev, synth*)
Munro, M.H. *et al., J. Biotechnol.*, 1999, **70**, 15-25 (*rev*)
Towle, M.J. *et al., Cancer Res.*, 2001, **61**, 1013-1021 (*analogues*)

Haliclamide H-18

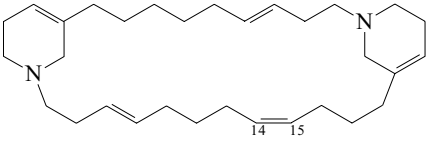


$C_{26}H_{40}N_2O_5$ 460.612
Isol. from the Vanuatu sponge *Haliclona* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D$ -4.8 (c, 0.006 in $CHCl_3$).

Randazzo, A. *et al., Tetrahedron*, 2001, **57**, 4443-4446

Haliclamine B H-19

[126622-63-7]

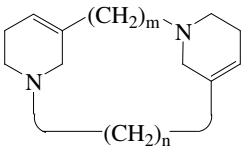


$C_{31}H_{50}N_2$ 450.749
Alkaloid from an unidentified marine sponge of the genus *Haliclona*. Cytotoxic agent. Oil.

14,15-Dihydro: ***Haliclamine A***
[126622-64-8]
$C_{31}H_{52}N_2$ 452.765
Alkaloid from *Haliclona* sp. Oil.

Fusetani, N. *et al., Tet. Lett.*, 1989, **30**, 6891-6894 (*isol, ir, pmr, cmr, ms, struct*)
Morimoto, Y. *et al., Tetrahedron*, 1998, **54**, 12197-12214 (*synth*)
Baldwin, J.E. *et al., Tet. Lett.*, 2000, **41**, 733-736 (*synth*)
Michelliza, S. *et al., J.O.C.*, 2002, **67**, 6474-6478 (*Haliclamine A, synth*)

Haliclamine C H-20



m = 9, n = 11

$C_{30}H_{54}N_2$ 442.77
Alkaloid from the Arctic sponge *Haliclona viscosa*. CAS no. not found in CA 142.

Volk, C.A. *et al., Eur. J. Org. Chem.*, 2004, 3154-3158 (*isol, pmr, cmr, ms*)

Haliclamine D H-21

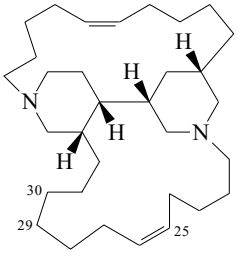
As Haliclamine C, H-20 with
m = 10, n = 11

$C_{31}H_{56}N_2$ 456.797
Alkaloid from the Arctic sponge *Haliclona viscosa*. CAS no. not found in CA 142.

Volk, C.A. *et al., Eur. J. Org. Chem.*, 2004, 3154-3158 (*isol, pmr, cmr, ms*)

Haliclonacyclamine A H-22

[179733-14-3]



Relative configuration

$C_{32}H_{56}N_2$ 468.808
Alkaloid from the tropical marine sponge *Haliclona* sp. Exhibits pronounced cytotoxic, antibacterial and antifungal activity. Needles.
Mp 149-150°. $[\alpha]_D$ -3.4 (c, 1.21 in CH_2Cl_2).

Methiodide (1:2):
Yellow needles (MeOH/EtOAc). Mp 196-197° dec.

15,16-Dihydro: ***Haliclonacyclamine C***
$C_{32}H_{58}N_2$ 470.824
From *Haliclona* sp. Gum. $[\alpha]_D$ +4.8 (c, 0.3 in CH_2Cl_2).

25,26-Dihydro, 27,28-didehydro: ***Haliclonacyclamine B***
[179733-15-4]
$C_{32}H_{56}N_2$ 468.808
From *Haliclona* sp. Exhibits pronounced cytotoxic, antibacterial and antifungal activity. Needles.
Mp 145-146°. $[\alpha]_D$ +3.4 (c, 0.55 in CH_2Cl_2). Struct. revised in 1998.

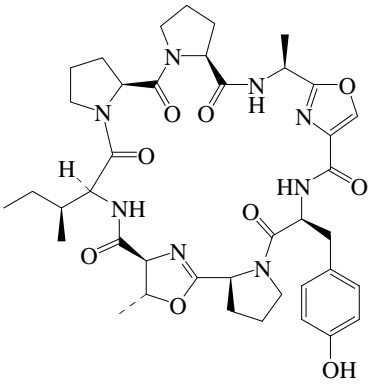
25,26-Dihydro, 29,30-didehydro, methiodide (1:2):
Yellow needles (MeOH/EtOAc). Mp 170-175° dec.

15,16,25,26-Tetrahydro, 27,28-didehydro: ***Haliclonacyclamine D***
$C_{32}H_{58}N_2$ 470.824
From *Haliclona* sp. Gum. $[\alpha]_D$ +16.1 (c, 0.3 in CH_2Cl_2).

Charan, R.D. *et al., Tetrahedron*, 1996, **52**, 9111 (*isol, pmr, cmr, cryst struct*)
Clark, R.J. *et al., Tetrahedron*, 1998, **54**, 8811-8826 (*isol, pmr, cmr, cryst struct*)

Haliclonamide B H-23

[248270-62-4]



$C_{40}H_{52}N_8O_9$ 788.899
Isol. from the marine sponge *Haliclona* sp.
$[\alpha]_D^{24}$ -1.01.

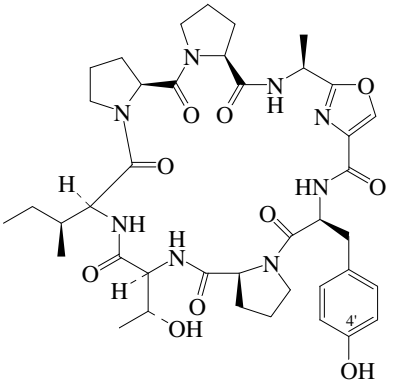
O-*(3-Methyl-2-butenyl):* ***Haliclonamide A***
[350593-22-5]
$C_{45}H_{60}N_8O_9$ 857.017
Isol. from a *Haliclona* sp.
$[\alpha]_D^{24}$ -0.23.

O-*(2-Hydroxy-3-methyl-3-butenyl):* ***Haliclonamide C***
[489446-55-1]
$C_{45}H_{60}N_8O_{10}$ 873.017
Isol. from a *Haliclona* sp.

Guan, L.L. *et al., Biochem. Biophys. Res. Commun.*, 2001, **283**, 976-981 (*isol, ir, pmr, cmr*)
Sera, Y. *et al., Mar. Biotechnol.*, 2002, **4**, 441-446 (*isol*)

Haliclonamide D H-24

[489446-56-2]



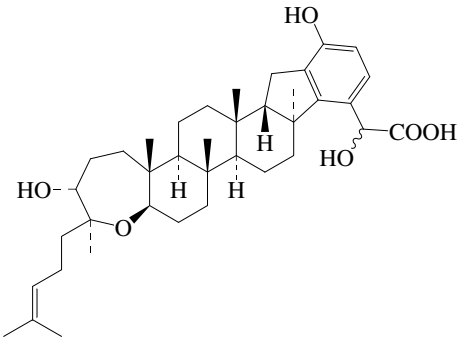
$C_{40}H_{54}N_8O_{10}$ 806.914
Isol. from a *Haliclona* sp.

4′-O-*(3-Methyl-2-butenyl):* ***Haliclonamide E***
[489446-57-3]
$C_{45}H_{62}N_8O_{10}$ 875.032
Isol. from a *Haliclona* sp.

Sera, Y. *et al., Mar. Biotechnol.*, 2002, **4**, 441-446 (*isol*)

Haliclotriol A H-25

[325690-71-9]

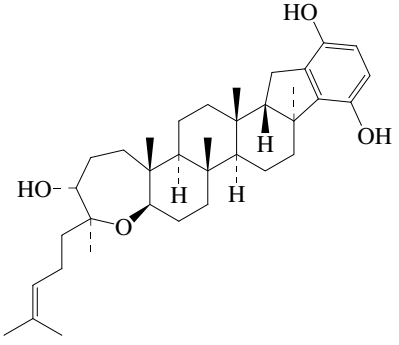


$C_{38}H_{56}O_6$ 608.857
Constit. of a *Haliclona* sp. Brown powder. $[\alpha]_D^{25}$ -39.4 (c, 7.63 in MeOH). λ_{max} 214; 226; 278 (MeOH).

Crews, P. *et al., Tetrahedron*, 2000, **56**, 9039-9046 (*isol, pmr, cmr*)

Haliclotriol B H-26

[325690-73-1]

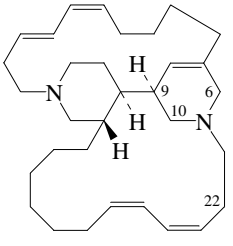


$C_{36}H_{54}O_4$ 550.82
Constit. of a *Haliclona* sp. Powder. $[\alpha]_D^{25}$ -9.5 (c, 1.86 in MeOH). λ_{max} 214; 226; 278 (MeOH).

Crews, P. *et al., Tetrahedron*, 2000, **56**, 9039-9046 (*isol, pmr, cmr*)

Halicyclamine A H-27

[156280-95-4]



$C_{32}H_{50}N_2$ 462.76
Alkaloid from the marine sponges *Amphimedon* sp. and *Haliclona* sp. Cytotoxic. Yellowish solid. $[\alpha]_D$ -7.3 (c, 0.72 in CH_2Cl_2). $[\alpha]_D^{25}$ -24 (c, 0.1 in MeOH). λ_{max} 236 (MeOH).

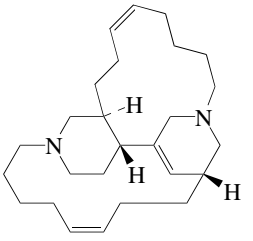
*6,9,10,*N-*Dehydro:* ***Tetradehydrohalicyclamine A***
$C_{32}H_{47}N_2^{\oplus}$ 459.737
Quaternary alkaloid from *Amphimedon* sp. Cytotoxic. Amorph. solid (as TFA salt). $[\alpha]_D^{25}$ -14.7 (c, 0.1 in MeOH) (TFA salt). λ_{max} 232; 273 (MeOH) (TFA salt).

22ξ-Hydroxy: ***22-Hydroxyhalicyclamine A***
$C_{32}H_{50}N_2O$ 478.76
Alkaloid from *Amphimedon* sp. Amorph. solid. $[\alpha]_D^{25}$ +21 (c, 0.1 in MeOH). λ_{max} 234; 273 (MeOH).

Jaspars, M. *et al., J.O.C.*, 1994, **59**, 3253-3255 (*isol, ir, pmr, cmr, ms*)
Matzanke, N. *et al., Org. Prep. Proced. Int.*, 1998, **30**, 3-51 (*rev*)
Matsunaga, S. *et al., J. Nat. Prod.*, 2004, **67**, 1758-1760 (*isol, pmr, cmr*)

Halicyclamine B H-28

[185559-26-6]



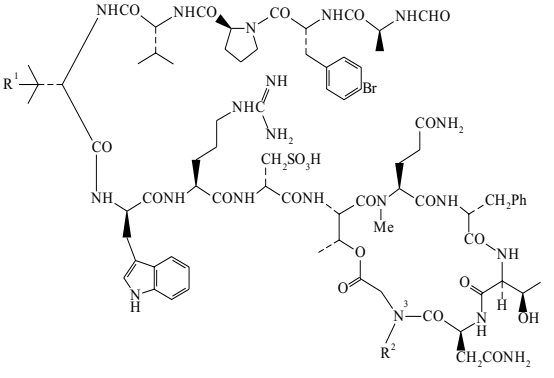
Relative Configuration

$C_{26}H_{42}N_2$ 382.631
Alkaloid from the marine sponge *Xestospongia* sp. $[\alpha]_D$ -143.5.

Harrison, B. *et al., Tet. Lett.*, 1996, **37**, 9151 (*isol, pmr, cmr, cryst struct*)

Halicylindramide A H-29

[160824-55-5]



R^1 = H, R^2 = CH_3

$C_{78}H_{109}BrN_{20}O_{22}S$ 1790.81
Depsipeptide antibiotic. Isol. from the sponge *Halichondria cylindrata*. Antifungal and cytotoxic agent. Solid. $[\alpha]_D^{23}$ -1.4 (c, 0.6 in MeOH).

Li, H.-Y. *et al., J. Med. Chem.*, 1995, **38**, 338 (*isol, uv, ir, pmr, cmr, ms*)

Halicylindramide B H-30

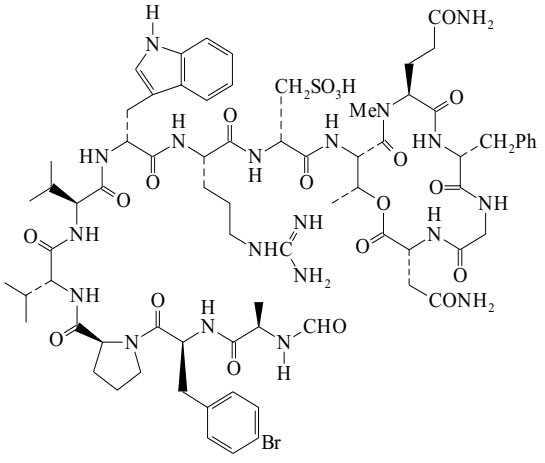
[160858-95-7]
As Halicylindramide A, H-29 with
R^1 = CH_3, R^2 = H
$C_{78}H_{109}BrN_{20}O_{22}S$ 1790.81
Depsipeptide antibiotic. Isol. from the sponge *Halichondria cylindrata*. Antifungal and cytotoxic agent. Solid. $[\alpha]_D^{23}$ -4.5 (c, 4 in MeOH).

N^3-*Me:* ***Halicylindramide C***
[160824-56-6]
$C_{79}H_{111}BrN_{20}O_{22}S$ 1804.837
Isol. from *Halichondria cylindrata*. Antifungal and cytotoxic agent. Solid. $[\alpha]_D^{23}$ -6.1 (c, 0.5 in MeOH).

Li, Y. *et al., J. Med. Chem.*, 1995, **38**, 338 (*isol, uv, ir, pmr, cmr, ms*)

Halicylindramide D H-31

[172548-80-0]



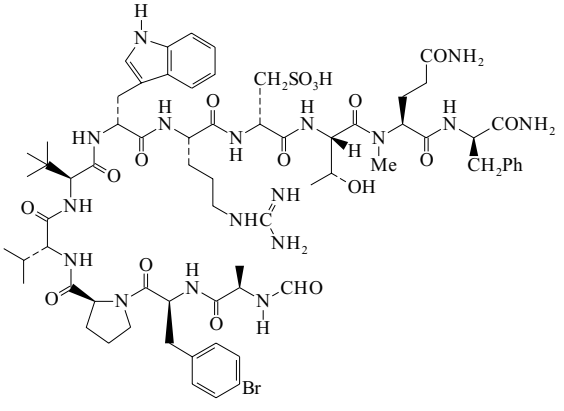
$C_{73}H_{100}BrN_{19}O_{20}S$ 1675.678

Depsipeptide antibiotic. Isol. from the sponge *Halichondria cylindrata*. Antifungal and cytotoxic agent. Powder (as Na salt). $[\alpha]_D$ +5.1 (c, 0.2 in Me_2CO aq.) (Na salt). λ_{max} 213 (ϵ 42000); 279 (ϵ 5600); 288 (ϵ 4500) (MeOH).

Li, H.-Y. *et al., J. Nat. Prod.*, 1996, **59**, 163-166 (*isol, uv, ir, pmr, cmr, ms*)

Halicylindramide E H-32

[172519-51-6]



$C_{68}H_{96}BrN_{17}O_{17}S$ 1535.58

Polypeptide antibiotic. Isol. from the sponge *Halichondria cylindrata*. Antifungal and cytotoxic agent. Powder (as Na salt). $[\alpha]_D$ +9 (c, 0.3 in MeOH) (Na salt). λ_{max} 214 (ϵ 43500); 280 (ϵ 5400 br.); 288 (ϵ 4300) (MeOH).

Li, H.-Y. *et al., J. Nat. Prod.*, 1996, **59**, 163-166 (*isol, uv, ir, pmr, cmr, ms*)

Halicynone B H-33

26,31-Dihydroxy-?-methyl-4-hentriacontene-1,27,29-triyn-3-one

$HOH_2CC{\equiv}CC{\equiv}CCH(OH)(CH_2)_mCH(CH_3)(CH_2)_nCH{=}CHCOC{\equiv}CH$

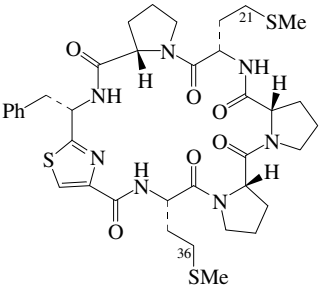
$C_{32}H_{50}O_3$ 482.745

m + n = 19. Isol. from the sponge *Haliclona* sp. Oil.

Zhou, G.-X. *et al., Mar. Drugs*, 2003, **1**, 46-53 (*isol, pmr*)

Haligramide A H-34

[282096-24-6]



$C_{37}H_{49}N_7O_6S_3$ 784.035

Isol. from the sponge *Haliclona nigra*. Amorph. powder. $[\alpha]_D$ -36.5 (c, 0.1 in MeOH). λ_{max} 206 (log ϵ 4.35); 242 (log ϵ 4.11); 254 (log ϵ 4.15); 260 (log ϵ 3.99) (EtOH).

36-S-*Oxide:* ***Haligramide B***

[282096-25-7]

$C_{37}H_{49}N_7O_7S_3$ 800.035

Isol. from *Haliclona nigra*. Amorph. powder. $[\alpha]_D$ -32.5 (c, 0.09 in MeOH). λ_{max} 206 (log ϵ 4.26); 240 (log ϵ 3.63) (EtOH).

21,36-S,S-*Dioxide:* ***Waiakeamide***

[179667-64-2]

$C_{37}H_{49}N_7O_8S_3$ 816.034

Cyclic hexapeptide. Isol. from the sponge *Ircinia dendroides* and a Palauan *Haliclona* sp. Amorph. solid. $[\alpha]_D$ -54 (c, 0.5 in MeOH). λ_{max} 206 (ϵ 13000); 239 (ϵ 4400) (MeOH).

21,21,36-S,S,S-*Trioxide:* ***Waiakeamide 21-sulfone***

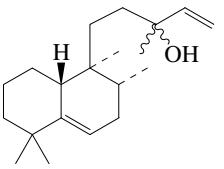
[518315-43-0]

$C_{37}H_{49}N_7O_9S_3$ 832.034

Isol. from a Palauan *Haliclona* sp. Amorph. solid. $[\alpha]_D^{26}$ -108 (c, 0.16 in $CHCl_3$).

Mau, C.M.S. *et al., J.O.C.*, 1996, **61**, 6302-6304 (*Waiakeamide*)
Rashid, M.A. *et al., J. Nat. Prod.*, 2000, **63**, 956-959 (*Haligramides A,B*)
Fujii, K. *et al., Tetrahedron*, 2002, **58**, 6873-6879 (*Waiakeamide, abs config*)
Sera, Y. *et al., J. Nat. Prod.*, 2003, **66**, 719-721 (*Waiakeamide, Waiakeamide 21-sulfone*)

5,14-Halimadien-13-ol H-35



$C_{20}H_{34}O$ 290.488

(ent-ξ)-form

Nosyberkol

[805228-56-2]

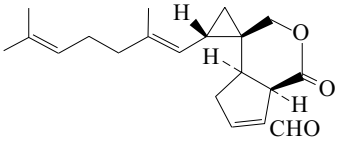
Constit. of a *Raspailia* sponge.

$[\alpha]_D^{25}$ +16.8 (c, 0.25 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 2004, **67**, 1932-1935 (*isol, pmr, cmr*)

Halimedalactone H-36

[93888-71-2]



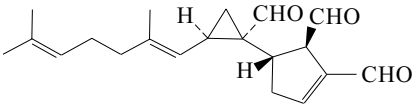
$C_{20}H_{26}O_3$ 314.424

Metabolite of green algae *Halimeda tuna* and *Halimeda scabra*. Ichthyotoxin. Yellow oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{25}$ 0 (c, 1.3 in $CHCl_3$). λ_{max} 236 (ϵ 11400) (MeOH) (Derep). λ_{max} 236 (ϵ 7300) (MeOH) (Berdy).

Paul, V.J. *et al., Tetrahedron*, 1984, **40**, 3053

Halimedatrial H-37

[87425-38-5]

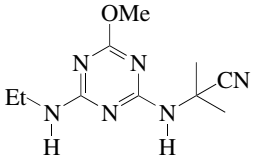


$C_{20}H_{26}O_3$ 314.424

Metab. of green alga *Halimeda* spp. Antifeedant. Ichthyotoxin. Feeding deterrent. Yellow oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{25}$ -59 (c, 0.9 in $CHCl_3$). λ_{max} 236 (ϵ 11400) (MeOH) (Derep). λ_{max} 244 (ϵ 11400) (MeOH) (Berdy). λ_{max} 236 (ϵ 11400) (EtOH) (Berdy).

Paul, V.J. *et al., Tetrahedron*, 1984, **40**, 3053 (*isol*)
Nagaoka, H. *et al., Tet. Lett.*, 1990, **31**, 1573 (*synth, abs config*)

Halimedin H-38

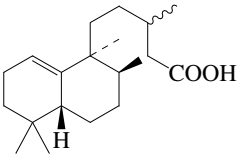


$C_{10}H_{16}N_6O$ 236.276

First example of a naturally occurring 1,3,5-triazine. Alkaloid from the alga *Halimeda xishaensis*. Cryst. Mp 164-165°.

Su, J.-Y. *et al., Phytochemistry*, 1998, **48**, 583-584 (*isol, ir, pmr, cmr, ms, cryst struct*)

1(10)-Halimen-15-oic acid H-39



$C_{20}H_{34}O_2$ 306.487

(9α,13ξ)-*form*

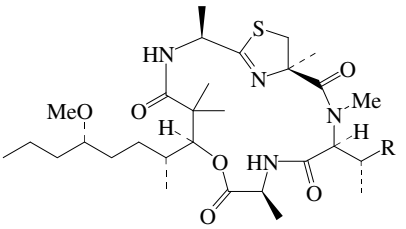
*2,3-Dihydroxypropyl ester (*S-*):* ***Austrodorin***
[169238-54-4]
$C_{23}H_{40}O_4$ 380.567
Constit. of *Austrodoris kerguelenensis*.

(1,3-Dihydroxy-2-propyl) ester: [588701-38-6]
$C_{23}H_{40}O_4$ 380.567
Constit. of *Austrodoris kerguelenensis*. Amorph. solid. $[\alpha]_D^{25}$ +24.2 (c, 0.2 in $CHCl_3$).

(2-Acetoxy-1-hydroxymethylethyl) ester (S-): [250163-08-7]
$C_{25}H_{42}O_5$ 422.604
Constit. of *Austrodoris kerguelenensis*. Amorph. solid. $[\alpha]_D^{25}$ +29.1 (c, 0.1 in $CHCl_3$).

Gavagnin, M. *et al., Tet. Lett.*, 1995, **36**, 7319-7322 (*isol, pmr, cmr*)
Gavagnin, M. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 2647-2650 (*abs config*)
Gavagnin, M. *et al., Tetrahedron*, 2003, **59**, 5579-5583 (*isol, pmr, cmr*)

Halipeptin A H-40



Absolute Configuration

R = -$CH_2^{5'}CH_2OH$

$C_{31}H_{54}N_4O_7S$ 626.856

Struct. revised in 2002. MF originally given as $C_{31}H_{54}N_4O_9$. Isol. from the sponge *Haliclona* sp. Potent antiinflammatory agent. Amorph. solid. $[\alpha]_D$ -16.6 (c, 0.03 in $CHCl_3$).

O-*De-Me:* ***Halipeptin B***
$C_{30}H_{52}N_4O_7S$ 612.829
Isol. from *Haliclona* sp. Amorph. solid. $[\alpha]_D$ -22.7 (c, 0.002 in $CHCl_3$).

5′-Deoxy: ***Halipeptin D***
[866555-47-7]
$C_{31}H_{54}N_4O_6S$ 610.857
Isol. from the sponge *Leiosella* cf. *arenifibrosa*. Viscous oil. $[\alpha]_D^{25}$ -26 (c, 0.2 in $CHCl_3$).

Randazzo, A. *et al., J.A.C.S.*, 2001, **123**, 10870-10876 (*isol, pmr, cmr, N-15 nmr*)
Monica, C.D. *et al., Tet. Lett.*, 2002, **43**, 5707-5710 (*struct*)
Nicolaou, K.C. *et al., Chem. Eur. J.*, 2005, **11**, 6197-6211 (*Halipeptin D*)
Yu, S. *et al., Chem. Eur. J.*, 2006, **12**, 6572-6584 (*synth*)
Nicolaou, K.C. *et al., J.A.C.S.*, 2006, **128**, 4460-4470 (*synth*)
Hara, S. *et al., Tet. Lett.*, 2006, **47**, 1081-1085 (*synth*)

Halipeptin C H-41

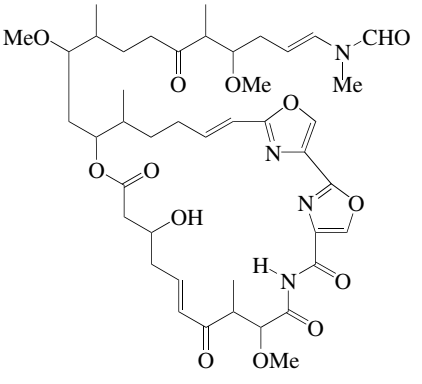
As Halipeptin A, H-40 with
R = CH_3

$C_{30}H_{52}N_4O_6S$ 596.83
Isol. from the sponge *Haliclona* sp. Amorph. solid. $[\alpha]_D$ -30 (c, 0.3 in $CHCl_3$).

Monica, C.D. *et al., Tet. Lett.*, 2002, **43**, 5707-5710 (*isol, pmr, cmr*)
Yu, S. *et al., Chem. Eur. J.*, 2006, **12**, 6572-6584 (*synth*)

Halishigamide B H-42

[185847-12-5]



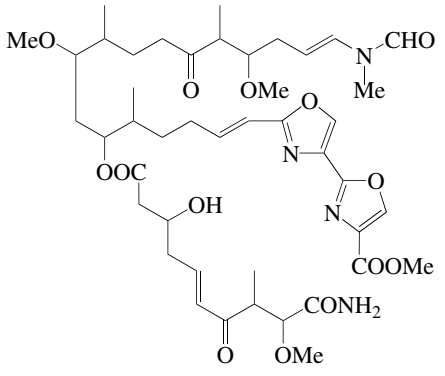
$C_{43}H_{60}N_4O_{13}$ 840.966

Metab. from the Okinawan marine sponge *Halichondria* sp. Exhibits weak cytotoxicity and modest antifungal activity. Amorph. solid. $[\alpha]_D^{25}$ -72 (c, 0.06 in MeOH). λ_{max} 231 (ϵ 66000); 260 (sh) (MeOH).

Kobayashi, J. *et al., J. Nat. Prod.*, 1997, **60**, 150-154 (*isol, uv, ir, pmr, cmr, struct*)

Halishigamide C H-43

[185847-13-6]



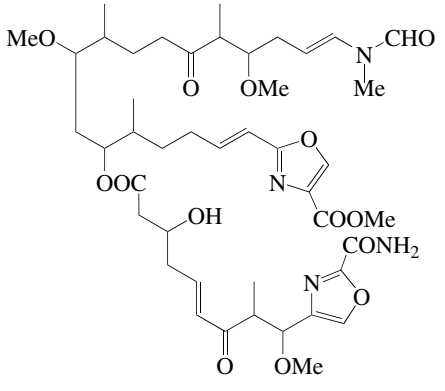
$C_{44}H_{64}N_4O_{14}$ 873.008

Metab. from the Okinawan marine sponge *Halichondria* sp. Exhibits weak cytotoxicity and modest antifungal activity. Amorph. solid. $[\alpha]_D^{27}$ -70 (c, 0.12 in $CHCl_3$). λ_{max} 231 (ϵ 56000) (MeOH).

Kobayashi, J. *et al., J. Nat. Prod.*, 1997, **60**, 150-154 (*isol, uv, ir, pmr, cmr, struct*)

Halishigamide D H-44

[185847-14-7]



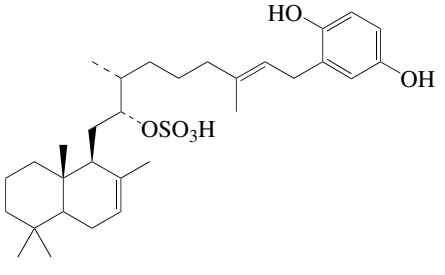
$C_{44}H_{64}N_4O_{14}$ 873.008

Metab. from the Okinawan marine sponge *Halichondria* sp. Exhibits weak cytotoxicity and modest antifungal activity. Amorph. solid. $[\alpha]_D^{25}$ -88 (c, 0.03 in MeOH). λ_{max} 235 (ϵ 15000) (MeOH).

Kobayashi, J. *et al., J. Nat. Prod.*, 1997, **60**, 150-154 (*isol, uv, ir, pmr, cmr, struct*)

Halisulfate 1 H-45

[116302-38-6]



$C_{31}H_{48}O_6S$ 548.783

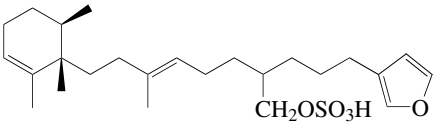
Constit. of a sponge (Halichondriidae). Active against gram-positive bacteria and *Candida albicans*. Phospholipase A2 and serine protease inhibitor. Needles. $[\alpha]_D$ -27.3 (c, 0.01 in MeOH).

1,7,9-Trimethylguaninium salt: [201667-10-9]
$C_{39}H_{59}N_5O_7S$ 741.99
Isol. from the sponge *Coscinoderma mathewsi*. Cryst. Mp 165-170°. λ_{max} 260 (log ϵ 4.04); 287 (log ϵ 3.96) (MeOH).

Kernan, M.R. *et al., J.O.C.*, 1988, **53**, 4574-4578 (*isol, pmr, cmr, activity*)
Kimura, J. *et al., J. Nat. Prod.*, 1998, **61**, 248-250; 862 (*trimethylguaninium salt*)
Singh, M. *et al., Planta Med.*, 1999, **65**, 2-8 (*rev*)

Halisulfate 2 H-46

[116302-39-7]



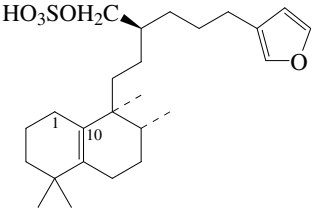
$C_{25}H_{40}O_5S$ 452.654

Constit. of a sponge (Halichondriidae). Solid.

Kernan, M.R. *et al., J.O.C.*, 1988, **53**, 4574-4578 (*isol, pmr, cmr*)

Halisulfate 3 H-47

[116302-40-0]



$C_{25}H_{40}O_5S$ 452.654

Constit. of a sponges incl. *Ircinia* and *Igernella* spp. Solid. Mp 162-166°.

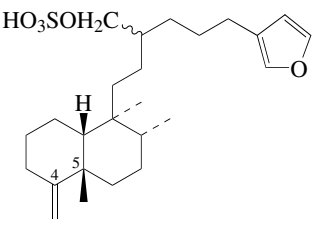
*$\Delta^{1(10)}$-Isomer (5α*H*), 9-epimer:* ***Halisulfate 7***
[246868-56-4]
$C_{25}H_{40}O_5S$ 452.654
Constit. of a *Coscinoderma* sponge. Struct. revised in 2004.

*8-Epimer, $\Delta^{1(10)}$-isomer (5β*H*), 2-oxo:* ***Halisulfate 8***
[577704-97-3]
$C_{25}H_{38}O_6S$ 466.638
Constit. of *Darwinella australensis*. Amorph. solid. Mp 55-57°. $[\alpha]_D^{25}$ -74.8 (c, 0.36 in MeOH). λ_{max} 245 (log ϵ 4.22) (MeOH).

Kernan, M.R. *et al., J.O.C.*, 1988, **53**, 4574-4578 (*isol, pmr, cmr*)
Müller, E.L. *et al., Tetrahedron*, 1997, **53**, 5373-5380 (*abs config, pmr, cmr*)
Fu, X. *et al., J. Nat. Prod.*, 1999, **62**, 1190-1191 (*Halisulfate 7*)
Makarieva, T.N. *et al., J. Nat. Prod.*, 2003, **66**, 1010-1012 (*Halisulfate 8*)
Phuwapraisirisan, P. *et al., Tet. Lett.*, 2004, **45**, 2125-2128 (*Halisulfate 7, struct*)

Halisulfate 5 H-48

[116302-42-2]



$C_{25}H_{40}O_5S$ 452.654

Constit. of a sponge (Halichondriidae).

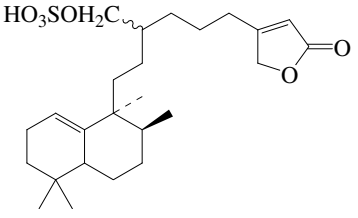
5-Epimer: ***Halisulfate 6***
[116348-54-0]
$C_{25}H_{40}O_5S$ 452.654
Constit. of a sponge (Halichondriidae).

Δ^4-Isomer: ***Halisulfate 4***
[116302-41-1]
$C_{25}H_{40}O_5S$ 452.654
Constit. of a Halichondriid sponge. The C-13 config. need not be identical.

Kernan, M.R. *et al., J.O.C.*, 1988, **53**, 4574-4578 (*isol, pmr, cmr*)

Halisulfate 9 H-49

[577704-98-4]

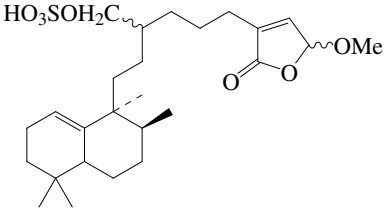


$C_{25}H_{40}O_6S$ 468.653
Constit. of *Darwinella australensis*. Amorph. solid.
Mp 53-54°. $[\alpha]_D^{25}$ -57.9 (c, 0.31 in MeOH). λ_{max} 206 (log ϵ 4.06) (MeOH).

Makarieva, T.N. *et al., J. Nat. Prod.*, 2003, **66**, 1010-1012 (*isol, pmr, cmr*)

Halisulfate 10 H-50

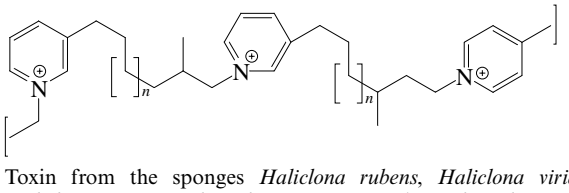
[577704-99-5]



$C_{26}H_{42}O_7S$ 498.68
Constit. of *Darwinella australensis*. Amorph. solid.
Mp 69-71°. $[\alpha]_D^{25}$ -42.2 (c, 0.21 in MeOH). λ_{max} 204 (log ϵ 3.96) (MeOH).

Makarieva, T.N. *et al., J. Nat. Prod.*, 2003, **66**, 1010-1012 (*isol, pmr, cmr*)

Halitoxin H-51

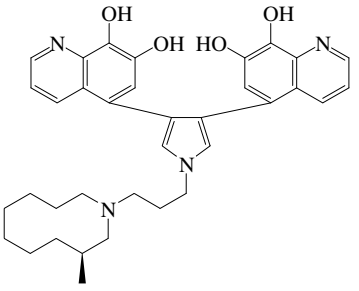


Toxin from the sponges *Haliclona rubens*, *Haliclona viridis*, *Haliclona erina*, *Amphimedon compressa* and *Amphimedon viridis*. Neurotoxin. Haemolytic, ichthyotoxic and antimitotic agent. Neuromuscular blocker. λ_{max} 267; 273 (EtOH).
▶ LD_{50} (mus, ipr) 2-5 mg/kg.

[54990-72-6]

Schmitz, F.J. *et al., J.O.C.*, 1978, **43**, 3916-3922 (*isol, uv, pmr, cmr*)

Halitulin H-52



Absolute Configuration

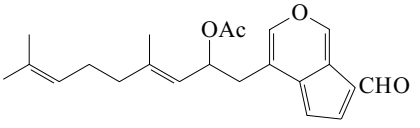
$C_{35}H_{40}N_4O_4$ 580.725

(S)-form [221367-90-4]
Alkaloid from the marine sponge *Haliclona tulearensis*. Cytotoxic agent. Orange foaming oil. $[\alpha]_D$ +7.5 (c, 2.8 in MeOH). λ_{max} 212 (ϵ 29200); 252 (ϵ 31600); 364 (ϵ 4400) (MeOH). λ_{max} 214 (ϵ 24700); 264 (ϵ 14800); 350 (ϵ 4650) (MeOH/NaOH) (Berdy).

Kashman, Y. *et al., Tet. Lett.*, 1999, **40**, 997-1000 (*isol, uv, ir, pmr, cmr, ms*)
Banwell, M.G. *et al., J.C.S. Perkin 1*, 2002, 1340-1343 (*synth, struct*)
Heinrich, M.R. *et al., Tetrahedron*, 2003, **59**, 9239-9247 (*synth, abs config*)

Halitunal H-53

[133076-08-1]

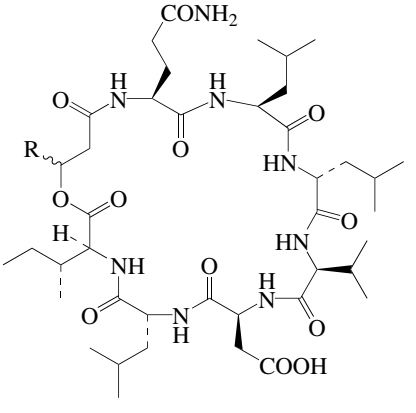


$C_{22}H_{26}O_4$ 354.445
Constit. of *Halimeda tuna*. Shows antiviral activity. λ_{max} 227 (ϵ 8500); 240 (ϵ 7860); 287 (ϵ 6180); 310 (ϵ 3920); 426 (ϵ 4640) (EtOH) (Derep). λ_{max} 227 (ϵ 8500); 240 (ϵ 7860); 287 (ϵ 6180); 310 (ϵ 3920); 426 (ϵ 5640) (EtOH) (Berdy).

Koehn, F.E. *et al., Tet. Lett.*, 1991, **32**, 169 (*isol, pmr, cmr*)
Shimano, K. *et al., Tet. Lett.*, 1996, **37**, 2253 (*synth*)

Halobacillin H-54

[158204-41-2]



R = $(CH_2)_{11}CH_3$

$C_{53}H_{94}N_8O_{12}$ 1035.372
Cyclic lipopeptide antibiotic. Prod. by the marine *Bacillus* sp. CND-914. Cytotoxic. Non-cryst. solid. Sol. MeOH, butanol. $[\alpha]_D$ -10.6 (c, 2.8 in MeOH).

Trischman, J.A. *et al., Tet. Lett.*, 1994, **35**, 5571-5574 (*isol, ir, pmr, cmr, ms*)

Halocidin H-55

[460079-92-9]

Thr—Leu—Asn—Ala—Leu—Leu—His—His—Gly—Leu—Asn—Cys—Ala—Lys—Gly—Val—Leu—Ala
Ala—Leu—Leu—His—His—Gly—Leu—Asn—Cys—Ala—Lys—Gly—Val—Leu—Ala

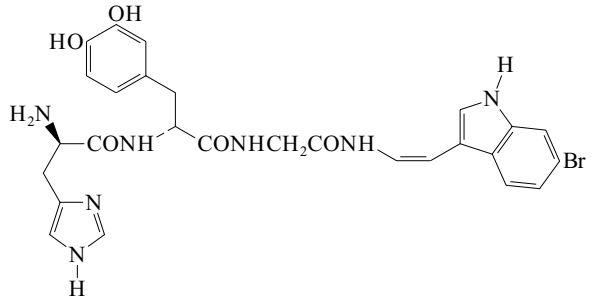
$C_{155}H_{251}N_{47}O_{38}S_2$ 3445.112

Peptide consisting of 2 subunits (18 and 15 amino acid residues) linked by a disulfide bond. Isol. from haemocytes of the solitary tunicate *Halocynthia aurantium*. Shows antimicrobial activity.

Jang, W.S. *et al., FEBS Lett.*, 2002, **521**, 81-86 (*isol, struct, synth*)

Halocyamine A H-56

[122548-03-2]



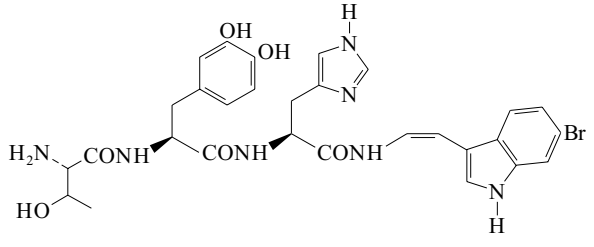
$C_{27}H_{28}BrN_7O_5$ 610.466

Oligopeptide antibiotic. Isol. from the haemocytes of the ascidian *Halocynthia roretzi*. Active against several bacteria and yeasts. Sol. MeOH, Me_2CO. $[\alpha]_D^{26}$ +5.2 (c, 0.5 in MeOH).

Azumi, K. *et al., Biochemistry*, 1990, **29**, 159-165 (*isol*)

Halocyamine B H-57

[122548-04-3]



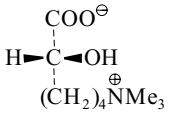
$C_{29}H_{32}BrN_7O_6$ 654.519

Oligopeptide antibiotic. Isol. from the haemocytes of the ascidian *Halocynthia roretzi*. Active against several bacteria and yeasts. Sol. MeOH, Me_2CO. $[\alpha]_D^{25}$ +63.1 (c, 0.5 in MeOH). λ_{max} 203 (E1%/1cm 785); 232 (E1%/1cm 428); 282 (E1%/1cm 276) (MeOH) (Berdy).

Azumi, K. *et al., Biochemistry*, 1990, **29**, 159-165 (*isol*)

Halocynine H-58

5-Carboxy-5-hydroxy-N,N,N-*trimethyl-1-pentanaminium hydroxide inner salt, 9CI. 2-Hydroxy-6-trimethylammoniohexanoate*



$C_9H_{19}NO_3$ 189.254

Analogue of 6-*N*-Trimethyllysine betaine, T-716.

(*R*)-*form*

D-form

[90934-32-0]

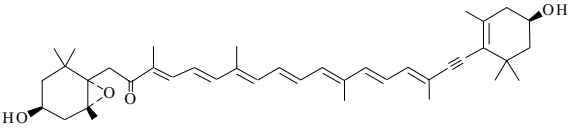
Isol. from muscle of ascidian *Halocynthia roretzi*. Hygroscopic gum.

Watanabe, K. *et al., Tet. Lett.*, 1984, **25**, 2003-2004 (*isol, ms, cd, pmr, cmr*)

Halocynthiaxanthin H-59

7′,8′-Didehydro-5,6-epoxy-3,3′-dihydroxy-5,6,7,8-tetrahydro-β,β-caroten-8-one

[81306-52-7]



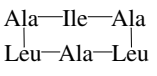
$C_{40}H_{54}O_4$ 598.864

Constit. of *Halocynthia roretzi*. HIV-1 and HIV-2 reverse transcriptase (HIV-rt) inhibitor. Antibarnacle agent. Reddish needles (petrol). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 158-160°. λ_{max} 430 (sh) (ϵ); 452 (ϵ); 470 (ϵ) (solvent not reported) (Derep). λ_{max} 430; 452; 470 (Et_2O) (Berdy).

Matsuno, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 4309
Loya, S. *et al., Arch. Biochem. Biophys.*, 1992, **293**, 208-212 (*activity*)
Yamano, Y. *et al., J.C.S. Perkin 1*, 1995, 1895 (*synth*)

Halolitoralin A H-60

Cyclo(alanylisoleucylalanylleucylalanylleucyl)



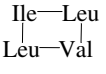
$C_{27}H_{48}N_6O_6$ 552.713

Isol. from the marine-derived *Halobacillus litoralis* YS3106. Antifungal agent. Amorph. solid.
Mp 170-171°. $[\alpha]_D^{20}$ -175.2 (c, 0.24 in MeOH). λ_{max} 204 (ϵ 36000) (MeOH).

Yang, L. *et al., Tet. Lett.*, 2002, **43**, 6545-6548 (*isol, struct*)

Halolitoralin B H-61

Cyclo(isoleucylleucylvalylleucyl)



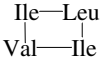
$C_{23}H_{42}N_4O_4$ 438.609

Isol. from a marine-derived *Halobacillus litoralis* YS3106. Antifungal agent. Amorph. solid.
Mp 198-199°. $[\alpha]_D^{20}$ -115 (c, 0.28 in MeOH). Incorrect struct. shown in ref. λ_{max} 204 (ϵ 32000) (MeOH).

Yang, L. *et al., Tet. Lett.*, 2002, **43**, 6545-6548 (*isol, struct*)

Halolitoralin C H-62

Cyclo(isoleucylleucylisoleucylvalyl)

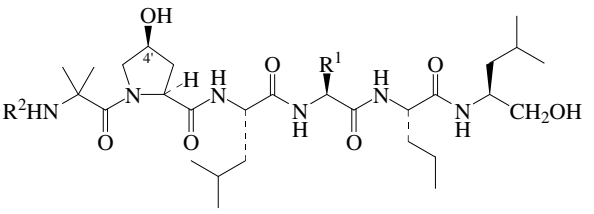


$C_{23}H_{42}N_4O_4$ 438.609

Isol. from the marine-derived *Halobacillus litoralis* YS3106. Antifungal agent. Amorph. solid.
Mp 201-202°. $[\alpha]_D^{20}$ -105 (c, 0.25 in MeOH). λ_{max} 204 (ϵ 37000) (MeOH).

Yang, L. *et al., Tet. Lett.*, 2002, **43**, 6545-6548 (*isol, struct*)

Halovir H-63



Halovir A $R^1 = -CH(CH_3)_2$, $R^2 = -CO(CH_2)_{12}CH_3$
B $R^1 = CH_3$, $R^2 = -CO(CH_2)_{12}CH_3$
D $R^1 = -CH(CH_3)_2$, $R^2 = -CO(CH_2)_{10}CH_3$

Peptide antibiotic complex. Prod. by a marine fungus *Scytalidium* sp. Antiviral agent.

Halovir A
$C_{45}H_{83}N_7O_9$ 866.192
Amorph. solid. $[\alpha]_D$ -13 (c, 0.73 in MeOH). λ_{max} 226 (log ϵ 2.58) (MeOH).

4′-Deoxy: ***Halovir C***
$C_{45}H_{83}N_7O_8$ 850.193
Amorph. solid. $[\alpha]_D$ -20 (c, 0.38 in MeOH). λ_{max} 227 (log ϵ 2.9) (MeOH).

Halovir B
$C_{43}H_{79}N_7O_9$ 838.139
Amorph. solid. $[\alpha]_D$ -8 (c, 0.25 in MeOH). λ_{max} 225 (log ϵ 3.01) (MeOH).

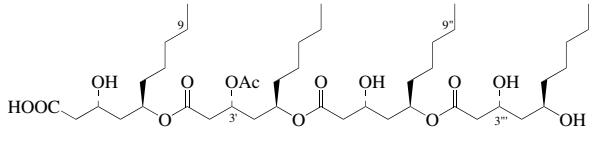
Halovir D
$C_{43}H_{79}N_7O_9$ 838.139
Amorph. solid. $[\alpha]_D$ -27 (c, 0.28 in MeOH).

4′-Deoxy: ***Halovir E***
$C_{43}H_{79}N_7O_8$ 822.139
Amorph. solid. $[\alpha]_D$ -14 (c, 0.42 in MeOH).

Rowley, D.C. *et al., Bioorg. Med. Chem.*, 2003, **11**, 4263-4274 (*isol, pmr, cmr, activity*)

Halymecin A H-64

[165561-10-4]



$C_{42}H_{76}O_{14}$ 805.054
Prod. by *Fusarium* sp. FE-71-1 from the marine alga *Halymenia dilatata*. Antimicroalgal agent. Oil. $[\alpha]_D^{26}$ -4.3 (c, 1.5 in CH_2Cl_2).

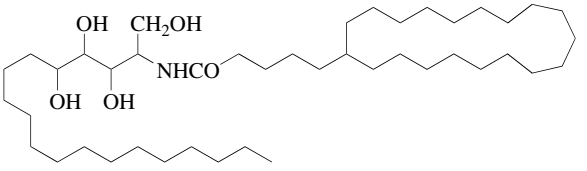
3‴-O-β-D-Mannopyranoside: ***Halymecin B***
[167173-81-1]
$C_{48}H_{86}O_{19}$ 967.196
Prod. by *Fusarium* spp. FE-71-1 from *Halymenia dilatata*. Antimicroalgal agent. Oil. $[\alpha]_D^{26}$ -24.4 (c, 6.6 in CH_2Cl_2).

9,9″-Dihydroxy, 3′-de-O-Ac: ***Halymecin D***
[167173-83-3]
$C_{40}H_{74}O_{15}$ 795.016
Prod. by *Acremonium* sp. FK-N30 from *Halymenia dilatata*. Config. not confirmed.

Japan. Pat., 1995, 95 118 206; *CA*, **123**, 81764k (*isol, struct*)
Chen, C. *et al., J. Antibiot.*, 1996, **49**, 998-1005 (*isol, ir, pmr, cmr, ms*)

Halyminine H-65

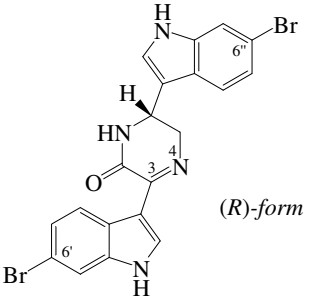
N-*[2,3,4-Trihydroxy-1-(hydroxymethyl)octadecyl]cyclononadecanepentanamide, 9CI*
[129780-95-6]



$C_{43}H_{85}NO_5$ 696.148
Isol. from the red alga *Halymenia porphyroides*. Amorph. solid.

Bano, S. *et al., Planta Med.*, 1990, **56**, 233 (*isol, struct*)

Hamacanthin A H-66



(*R*)-*form*

$C_{20}H_{14}Br_2N_4O$ 486.165
Abs. configs. not certain. Hamacanthin A itself has now been shown to have *S*-config. but the minor congeners appear to be *R*-.

(R)-form [354538-21-9]

*3*R*,4-Dihydro:* **cis-*3,4-Dihydrohamacanthin A***
[264624-42-2]
$C_{20}H_{16}Br_2N_4O$ 488.181
Alkaloid from the sponge *Rhaphisia lacazei*.
$[\alpha]_D^{25}$ +8.1 (c, 0.2 in MeOH). Abs. config. not confirmed.

*3*S*,4-Dihydro:* **trans-*3,4-Dihydrohamacanthin A***
[264624-43-3]
Alkaloid from *Rhaphisia lacazei* and *Spongosorites* sp.
$[\alpha]_D^{23}$ +16 (c, 1.1 in MeOH).

6′-Debromo: ***(R)-6′-Debromohamacanthin A***
$C_{12}H_{15}BrN_4O$ 311.181
Alkaloid from the sponge *Spongosorites* sp. Amorph. yellow powder. $[\alpha]_D^{23}$ -91 (c, 0.2 in MeOH).

*6′-Debromo, 3*S*,4-dihydro:* **trans-*6′-Debromo-3,4-dihydrohamacanthin A***
[264624-44-4]
$C_{20}H_{17}BrN_4O$ 409.285
Alkaloid from the sponge *Rhaphisia lacazei*.
$[\alpha]_D^{25}$ +4.8 (c, 0.07 in MeOH). Abs. config. not confirmed.

6″-Debromo: ***(R)-6″-Debromohamacanthin A***
$C_{12}H_{15}BrN_4O$ 311.181
Alkaloid from the sponge *Spongosorites* sp. Amorph. yellow powder. $[\alpha]_D^{23}$ -76 (c, 0.05 in MeOH).

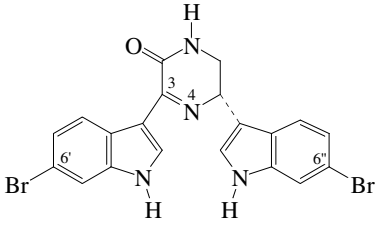
*6″-Debromo, 3*S*,4-dihydro:* **trans-*6″-Debromo-3,4-dihydrohamacanthin A***
[264624-45-5]
$C_{20}H_{17}BrN_4O$ 409.285
Alkaloid from *Rhaphisia lacazei*.
$[\alpha]_D^{25}$ +4.9 (c, 0.1 in MeOH). Abs. config. not confirmed.

(S)-form [160098-92-0]
Alkaloid from a deep-water marine sponge *Hamacantha* sp. Shows antimicrobial activity. Pale yellow powder. $[\alpha]_D^{24}$ +84 (c, 0.1 in MeOH). λ_{max} 219 (ϵ 76500); 280 (ϵ 20600); 325 (ϵ 13300) (MeOH).

Gunasekera, S.P. *et al., J. Nat. Prod.*, 1994, **57**, 1437-1441 (*isol, uv, ir, pmr, cmr, ms, struct*)
Casapullo, A. *et al., J. Nat. Prod.*, 2000, **63**, 447-451 (*3,4-Dihydrohamacanthins*)
Jiang, B. *et al., J.O.C.*, 2001, **66**, 4865-4869; 7560 (*synth, abs config*)
Miyake, F.Y. *et al., Org. Lett.*, 2002, **4**, 941-943 (*synth*)
Bao, B. *et al., J. Nat. Prod.*, 2005, **68**, 711-715 (*isol, pmr, cmr, abs config*)
Garg, N.K. *et al., Tet. Lett.*, 2005, **46**, 2423-2426 (*3,4-Dihydrohamacanthins, synth*)
Kouko, T. *et al., Tetrahedron*, 2005, **61**, 2309-2318 (*synth*)

Hamacanthin B H-67

[160098-93-1]



Absolute Configuration

$C_{20}H_{14}Br_2N_4O$ 486.165
Alkaloid from a deep-water marine sponge *Hamacantha* sp. Shows significant antimicrobial activity. Pale yellow powder. $[\alpha]_D^{24}$ +172 (c, 0.1 in MeOH). λ_{max} 219 (ϵ 76500); 280 (ϵ 20600); 325 (ϵ 13300) (MeOH) (Berdy).

*3,4-Dihydro(*cis-*):* **cis-*3,4-Dihydrohamacanthin B***
[264624-39-7]
$C_{20}H_{16}Br_2N_4O$ 488.181
Alkaloid from the sponges *Rhaphisia lacazei* and *Spongosorites* sp. Amorph. yellow powder. $[\alpha]_D^{21}$ +101 (c, 0.8 in MeOH).

6′-Debromo: ***6′-Debromohamacanthin B***
$C_{20}H_{15}BrN_4O$ 407.269
Alkaloid from the sponge *Spongosorites* sp. Amorph. yellow solid.
Mp 210-212°. $[\alpha]_D^{25}$ -100 (c, 0.2 in MeOH). λ_{max} 217 (log ϵ 4); 224 (log ϵ 3.94); 274 (log ϵ 3.46); 328 (log ϵ 3.7) (no solvent reported).

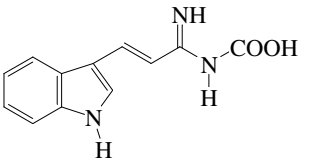
*6′-Debromo, 3,4-dihydro(*cis-*):* **cis-*6′-Debromo-3,4-dihydrohamacanthin B***
[264624-40-0]
$C_{20}H_{17}BrN_4O$ 409.285
Alkaloid from the sponge *Rhaphisia lacazei*.
$[\alpha]_D^{25}$ +23.2 (c, 0.1 in MeOH).

6′′-Debromo: ***6′′-Debromohamacanthin B***
$C_{20}H_{15}BrN_4O$ 407.269
Alkaloid from the sponge *Spongosorites* sp. Amorph. yellow powder. $[\alpha]_D^{23}$ +43 (c, 0.3 in MeOH).

*6′′-Debromo, 3,4-dihydro(*cis-*):* **cis-*6′′-Debromo-3,4-dihydrohamacanthin B***
[264624-41-1]
$C_{20}H_{17}BrN_4O$ 409.285
Alkaloid from the sponge *Rhaphisia lacazei*.
$[\alpha]_D^{25}$ +52.1 (c, 0.1 in MeOH).

Gunasekera, S.P. *et al., J. Nat. Prod.*, 1994, **57**, 1437-1441 (*isol, uv, ir, pmr, cmr, ms, struct*)
Casapullo, A. *et al., J. Nat. Prod.*, 2000, **63**, 447-451 (*3,4-Dihydrohamacanthins*)
Jiang, B. *et al., J.O.C.*, 2002, **67**, 1396-1398 (*synth*)
Miyake, F.Y. *et al., Org. Lett.*, 2002, **4**, 941-943 (*synth*)
Oh, K.-B. *et al., Bioorg. Med. Chem. Lett.*, 2005, **15**, 4927-4931 (*6′-Debromohamacanthin B*)
Bao, B. *et al., J. Nat. Prod.*, 2005, **68**, 711-715 (*6′′-Debromohamacanthin B*)
Kouko, T. *et al., Tetrahedron*, 2005, **61**, 2309-2318 (*synth*)

Hamigeramide H-68

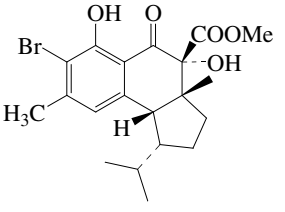


$C_{12}H_{11}N_3O_2$ 229.238
Alkaloid from the sponge *Hamigera hamigera*. Pale yellow powder. λ_{max} 228; 346 (MeOH).

Hassan, W. *et al., Mar. Drugs*, 2004, **2**, 88-100 (*isol, pmr, cmr, ms*)

Hamigeran A H-69

Hamigerin A (incorr.)
[255882-01-0]



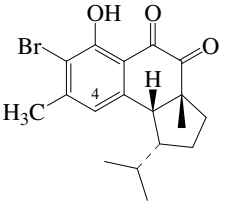
$C_{20}H_{25}BrO_5$ 425.319
Constit. of *Hamigera tarangaensis*. Yellow needles.
Mp 207-209°. $[\alpha]_D^{25}$ -22.5 (c, 0.5 in CH_2Cl_2).

Debromo: ***Debromohamigeran A***
[255830-26-3]
$C_{20}H_{26}O_5$ 346.422
Constit. of *Hamigera tarangaensis*. Cryst.
Mp 88.5-90°. $[\alpha]_D^{25}$ -38.5 (c, 0.11 in CH_2Cl_2).

Wellington, K.D. *et al., J. Nat. Prod.*, 2000, **63**, 79-85 (*isol, pmr, cmr*)
Cambie, R.C. *et al., Acta Cryst. C*, 2001, **57**, 958-960 (*cryst struct*)
Nicolaou, K.C. *et al., J.A.C.S.*, 2004, **126**, 613-627; *Angew. Chem., Int. Ed.*, 2001, **40**, 3679-3683 (*synth*)
Trost, B.M. *et al., J.A.C.S.*, 2004, **126**, 4480-4481 (*synth*)

Hamigeran B H-70

[255882-02-1]



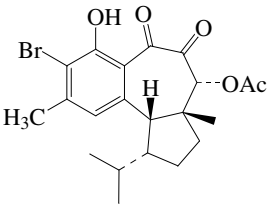
$C_{18}H_{21}BrO_3$ 365.266
Constit. of *Hamigera tarangaensis*. Yellow plates.
Mp 163-165°. $[\alpha]_D^{25}$ -151 (c, 0.15 in CH_2Cl_2).

4-Bromo: ***4-Bromohamigeran B***
[255830-27-4]
$C_{18}H_{20}Br_2O_3$ 444.162
Constit. of *Hamigera tarangaensis*. Yellow solid.
Mp 144-148°. $[\alpha]_D^{25}$ -81.2 (c, 0.37 in CH_2Cl_2).

Wellington, K.D. *et al., J. Nat. Prod.*, 2000, **63**, 79-85 (*isol, pmr, cmr*)
Mehta, G. *et al., Tet. Lett.*, 2003, **44**, 7049-7053 (*synth*)
Nicolaou, K.C. *et al., J.A.C.S.*, 2004, **126**, 607-612; *Angew. Chem., Int. Ed.*, 2001, **40**, 3679-3683 (*synth*)
Clive, D.L.J. *et al., J.O.C.*, 2004, **69**, 2773-2784 (*synth*)
Trost, B.M. *et al., Chem. Eur. J.*, 2005, **11**, 951-959 (*synth*)

Hamigeran C H-71

[255882-08-7]

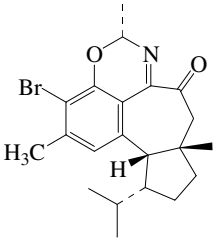


$C_{21}H_{25}BrO_5$ 437.33
Constit. of *Hamigera tarangaensis*. Yellow needles.
Mp 156-158°. $[\alpha]_D^{25}$ -136 (c, 0.29 in CH_2Cl_2).

Wellington, K.D. *et al., J. Nat. Prod.*, 2000, **63**, 79-85 (*isol, pmr, cmr*)

Hamigeran D H-72

[255882-09-8]

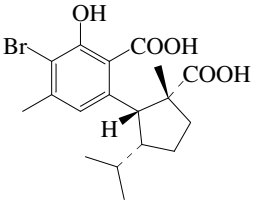


$C_{21}H_{26}BrNO_2$ 404.346
Isol. from the sponge *Hamigera tarangaensis*. Cytotoxic agent.
Pale yellow solid. $[\alpha]_D^{25}$ -47.1 (c, 0.21 in CH_2Cl_2).

Wellington, K.D. *et al., J. Nat. Prod.*, 2000, **63**, 79-85

Hamigeran E H-73

[166407-31-4]



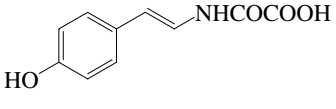
$C_{18}H_{23}BrO_5$ 399.281
Struct. revised in 2000. Previously assigned a bezobicyclic lactone struct. Isol. from the sponge *Hamigera tarangaensis*. Oil. $[\alpha]_D^{25}$ +30.5 ($CHCl_3$) (as tri-Et ether).

Debromo: ***Debromohamigeran E***
[255830-30-9]
$C_{18}H_{24}O_5$ 320.385
Constit. of *Hamigera tarangaensis*.
$[\alpha]_D^{25}$ +38.6 (c, 0.05 in $CHCl_3$) (as Et ether, di-Et ester).

Cambie, R.C. *et al., J. Nat. Prod.*, 1995, **58**, 940 (*isol, pmr, cmr*)
Wellington, K.D. *et al., J. Nat. Prod.*, 2000, **63**, 79-85 (*isol, pmr, cmr, struct*)
Nicolaou, K.C. *et al., J.A.C.S.*, 2004, **126**, 613-617 (*synth*)

Hamigeroxalamic acid H-74

[2-(4-Hydroxyphenyl)vinyl]oxamic acid



$C_{10}H_9NO_4$ 207.185

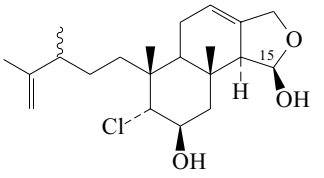
Alkaloid from the sponge *Hamigera hamigera*. Pale yellow powder. λ_{max} 248; 320 (MeOH).

Imine: [2-(4-Hydroxyphenyl)vinylamino]iminoacetic acid. ***Hamigeramine***
$C_{10}H_{10}N_2O_3$ 206.201
Alkaloid from the sponge *Hamigera hamigera*. Pale yellow powder. λ_{max} 227; 324 (MeOH).

Hassan, W. *et al., Mar. Drugs*, 2004, **2**, 88-100 (*isol, pmr, cmr, ms*)

Hamiltonin B H-75

[166774-51-2]



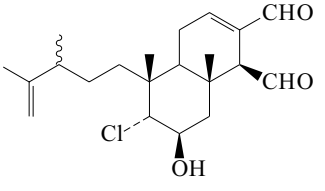
$C_{21}H_{33}ClO_3$ 368.943
Constit. of *Chromodoris hamiltoni*. Oil. $[\alpha]_D$ -8 (c, 0.29 in CH_2Cl_2).

15-Ketone (lactone): ***Hamiltonin A***
[166774-50-1]
$C_{21}H_{31}ClO_3$ 366.927
Constit. of *Chromodoris hamiltoni*. Oil. $[\alpha]_D$ -60 (c, 0.027 in CH_2Cl_2).

Pika, J. *et al., Tetrahedron*, 1995, **51**, 8189-8198 (*isol, pmr, cmr*)

Hamiltonin C H-76

[166774-52-3]

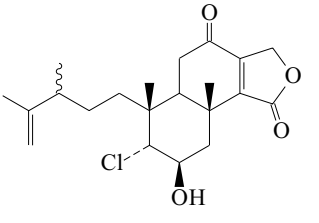


$C_{21}H_{31}ClO_3$ 366.927
Constit. of *Chromodoris hamiltoni*. Oil.

Pika, J. *et al., Tetrahedron*, 1995, **51**, 8189-8198 (*isol, pmr, cmr*)

Hamiltonin D H-77

[166774-53-4]

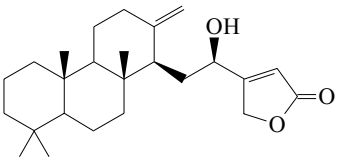


$C_{21}H_{29}ClO_4$ 380.91
Constit. of *Chromodoris hamiltoni*. Oil.

Pika, J. *et al., Tetrahedron*, 1995, **51**, 8189-8198 (*isol, pmr, cmr*)

Hamiltonin E H-78

[166797-74-6]



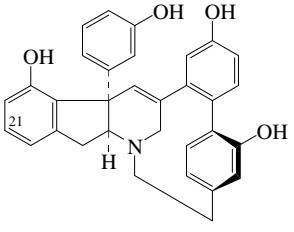
$C_{25}H_{38}O_3$ 386.573

Constit. of *Chromodoris hamiltoni*. Oil. Incorrect struct. given in CA.

Pika, J. *et al., Tetrahedron*, 1995, **51**, 8189-8198 (*isol, pmr, cmr*)

Haouamine A H-79

[496962-05-1]



$C_{32}H_{27}NO_4$ 489.57

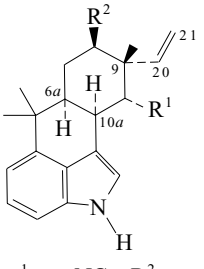
Alkaloid from the ascidian *Aplidium haouarianum*. Cytotoxic. Solid. $[\alpha]_D^{29}$ -52 (c, 0.4 in MeOH). Dec. at 170°. λ_{max} 205 (ϵ 62000); 275 (ϵ 11000) (MeOH).

21-Hydroxy: ***Haouamine B***
[496962-06-2]
$C_{32}H_{27}NO_5$ 505.569
Alkaloid from *Aplidium haouarianum*. Solid (as penta-Ac). $[\alpha]_D^{26}$ -27.1 (c, 0.14 in $CHCl_3$) (penta-Ac). λ_{max} 204 (ϵ 48100); 238 (ϵ 20300) (MeOH) (penta-Ac).

Garrido, L. *et al., J.O.C.*, 2003, **68**, 293-299 (*isol, pmr, cmr, cryst struct*)
Baran, P.S. *et al., J.A.C.S.*, 2006, **128**, 3908-3909 (*synth*)
Jeong, J.H. *et al., Org. Lett.*, 2006, **8**, 2309-2312 (*synth*)

Hapalindole A H-80

*8-Chloro-9-ethenyl-2,6,6*a*,7,8,9,10,10*a*-octahydro-10-isocyano-6,6,9-trimethylnaphth[1,2,3-*cd*]indole, 9CI*
[92219-95-9]



R^1 = —NC, R^2 = Cl

$C_{21}H_{23}ClN_2$ 338.879

Numbering systems vary. Isol. from the blue-green alga *Hapalosiphon fontinalis*. Algicide. Antibacterial and antimycotic agent. Yellow plates (CH_2Cl_2/heptane). Sol. MeOH, butanol, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 160-167° dec. $[\alpha]_D^{25}$ -78 (c, 1.2 in CH_2Cl_2). λ_{max} 222 (ϵ 38000); 280 (ϵ 7000); 291 (ϵ 5800) (MeOH) (Derep).

20,21-Epoxide: ***Hapalindole N***
[106865-65-0]
$C_{21}H_{23}ClN_2O$ 354.878
From *Hapalosiphon fontinalis* ATCC39964. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -31.5 (c, 1.7 in $CHCl_3$). Config. at C-20 not known. λ_{max} 220 (ϵ 34000); 273 (ϵ 5700); 280 (ϵ 5800); 290 (ϵ 4500) (MeOH) (Derep).

*6*a*,10*a*-Didehydro:* ***Hapalindole K***
[106865-63-8]
$C_{21}H_{21}ClN_2$ 336.863
From *Hapalosiphon fontinalis* ATCC39964. Thick yellow plates (CH_2Cl_2/heptane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 110-240° dec. $[\alpha]_D^{25}$ -12.5 (c, 1.8 in $CHCl_3$). λ_{max} 226 (ϵ 19300); 301 (ϵ 9600) (MeOH) (Derep).

*10,10*a*-Didehydro:* ***Hapalindole I***
[101968-76-7]
$C_{21}H_{21}ClN_2$ 336.863
From *Hapalosiphon fontinalis*.
Mp 180° dec. $[\alpha]_D^{25}$ -12 (c, 0.2 in CH_2Cl_2). λ_{max} 224 (ϵ 25800); 240 (sh) (ϵ 13000); 274 (ϵ 6700); 322 (ϵ 13400) (MeOH) (Derep). λ_{max} 222; 224 (ϵ 25800); 274 (ϵ 6700); 280; 291; 322 (ϵ 13900) (MeOH) (Berdy).

*10a*β*-Hydroxy:* ***Hapalindole V****. 10-Hydroxyhapalindole G*
[106865-68-3]
$C_{21}H_{23}ClN_2O$ 354.878
From *Hapalosiphon fontinalis* ATCC39964. No phys. props. reported. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 220 (ϵ 34000); 273 (ϵ 5700); 280 (ϵ 5800); 290 (ϵ 4500) (MeOH) (Derep).

Dechloro: ***Hapalindole J***
[106928-26-1]
$C_{21}H_{24}N_2$ 304.434
From *Hapalosiphon fontinalis* ATCC39964. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ +54.4 (c, 0.9 in $CHCl_3$). λ_{max} 222 (ϵ 38700); 280 (ϵ 7000); 291 (ϵ 5700) (MeOH) (Derep).

*6*a*-Epimer:* ***Hapalindole H***
[101968-75-6]
$C_{21}H_{23}ClN_2$ 338.879
From *Hapalosiphon fontinalis*.
Mp 190-193°. $[\alpha]_D^{25}$ +152 (c, 4.1 in CH_2Cl_2). λ_{max} 222 (ϵ 38700); 280 (ϵ 7000); 291 (ϵ 5700) (MeOH) (Derep).

9-Epimer: ***Hapalindole L***
[106928-27-2]
$C_{21}H_{23}ClN_2$ 338.879
From *Hapalosiphon fontinalis* ATCC39964. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -74 (c, 1.1 in $CHCl_3$). λ_{max} 222 (ϵ 38000); 280 (ϵ 7000); 291 (ϵ 5800) (MeOH) (Derep).

*10*a*-Epimer:* ***Hapalindole G***
[102045-13-6]
$C_{21}H_{23}ClN_2$ 338.879
From *Hapalosiphon fontinalis*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 185° dec. $[\alpha]_D^{25}$ -43.9 (c, 0.28 in CH_2Cl_2). λ_{max} 222 (ϵ 38000); 280 (ϵ 7000); 291 (ϵ 5800) (MeOH) (Derep).

*10*a*-Epimer, dechloro:* ***Hapalindole U***
[106928-30-7]
$C_{21}H_{24}N_2$ 304.434
From *Hapalosiphon fontinalis* ATCC39964. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ +12 (c, 0.6 in CH_2Cl_2). λ_{max} 222 (ϵ 38700); 280 (ϵ 7000); 291 (ϵ 5700) (MeOH) (Derep). λ_{max} 222; 282; 291 (MeOH) (Berdy).

?-Epimer, 20,21-epoxide: ***Hapalindole P***
[106928-28-3]
$C_{21}H_{23}ClN_2O$ 354.878
From *Hapalosiphon fontinalis* ATCC39964. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D$ -16.3 (c, 0.8 in $CHCl_3$). λ_{max} 220 (ϵ 34000); 273 (ϵ 5700); 280 (ϵ 5800); 290 (ϵ 4500) (MeOH) (Derep). λ_{max} 222; 280; 291 (MeOH) (Berdy).

*6*a*,9-Diepimer:* ***12-Epihapalindole H***
[174063-68-4]
$C_{21}H_{24}ClN_2$ 339.887
Alkaloid from *Hapalosiphon laingii*. Sol. MeOH.
Mp 187-189°. $[\alpha]_D$ +217.3 (c, 0.16 in CH_2Cl_2). λ_{max} 221 (ϵ 28140); 282 (ϵ 5150); 291 (sh) (ϵ 4130) (MeOH).

*9,10*a-*Diepimer:* ***12-Epihapalindole G.*** *12*-epi-*Hapalindole G*
[173241-59-3]
$C_{21}H_{23}ClN_2$ 338.879
Isol. from *Hapalosiphon laingii*. Sol. MeOH. λ_{max} 222 (ϵ 37220); 280 (ϵ 8200); 291 (sh) (ϵ 6640) (MeOH).
Moore, R.E. *et al., J.A.C.S.*, 1984, **106**, 6456 (*isol, uv, ir, pmr, cmr*)
Moore, R.E. *et al., J.O.C.*, 1987, **52**, 1036 (*isol, ir, pmr, cmr, cryst struct*)
Muratake, H. *et al., Tetrahedron*, 1990, **46**, 6331; 6351 (*synth, Hapalindoles H,J,U*)
Fukuyama, T. *et al., J.A.C.S.*, 1994, **116**, 3125 (*synth, Hapalindole G*)
Klein, D. *et al., J. Nat. Prod.*, 1995, **58**, 1781-1785 (*12-Epihapalindoles G,H*)

Hapalindole B H-81

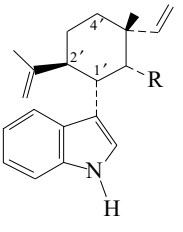
[92219-96-0]
As Hapalindole A, H-80 with
R^1 = –NCS, R^2 = Cl
$C_{21}H_{23}ClN_2S$ 370.945
Isol. from the blue-green alga *Hapalosiphon fontinalis*. Algicide. Antibacterial and antimycotic agent. Oil. Sol. MeOH, $CHCl_3$, butanol; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -194 (c, 5.1 in CH_2Cl_2). λ_{max} 222 (ϵ 38000); 280 (ϵ 7000); 291 (ϵ 5700) (MeOH) (Derep).

Dechloro: ***Hapalindole M***
[106865-64-9]
$C_{21}H_{24}N_2S$ 336.5
From *Hapalosiphon fontinalis* ATCC39964. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -83.1 (c, 1.8 in $CHCl_3$). λ_{max} 223 (ϵ 40000); 281 (ϵ 7300); 291 (ϵ 5900) (MeOH) (Derep).

Dechloro, 8β-hydroxy: ***Hapalindole O***
[106865-66-1]
$C_{21}H_{24}N_2OS$ 352.499
From *Hapalosiphon fontinalis* ATCC39964. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -106 (c, 2.4 in $CHCl_3$). λ_{max} 222 (ϵ 38000); 279 (ϵ 7000); 290 (ϵ 5700) (MeOH) (Derep). λ_{max} 223; 281; 291 (MeOH) (Berdy).
Moore, R.E. *et al., J.A.C.S.*, 1984, **106**, 6456 (*isol, pmr*)
Moore, R.E. *et al., J.O.C.*, 1987, **52**, 1036 (*isol, ir, pmr, cmr, struct*)
Muratake, H. *et al., Tetrahedron*, 1990, **46**, 6331 (*synth, Hapalinodole M*)
Sakagami, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1393 (*synth, Hapalindole O*)

Hapalindole C H-82

[101968-71-2]



R= NC

$C_{21}H_{24}N_2$ 304.434
Rel. config. illus. Isol. from the blue-green alga *Hapalosiphon fontinalis*. Sol. MeOH, butanol, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 138-143°. $[\alpha]_D^{25}$ +76.5 (c, 0.41 in CH_2Cl_2). λ_{max} 222 (ϵ 38700); 280 (ϵ 7000); 291 (ϵ 5700) (MeOH) (Derep).

4′β-Chloro: ***Hapalindole E***
[101968-73-4]
$C_{21}H_{23}ClN_2$ 338.879
From *Hapalosiphon fontinalis*. Sol. MeOH, butanol, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 88-90°. $[\alpha]_D^{25}$ +25.2 (c, 3.1 in CH_2Cl_2). λ_{max} 222 (ϵ 38000); 280 (ϵ 7000); 291 (ϵ 5800) (MeOH) (Derep).

5′-Epimer: ***12-Epihapalindole C isonitrile***
[159249-52-2]
$C_{21}H_{24}N_2$ 304.434
Alkaloid from the freshwater blue-green alga *Hapalosiphon welwitschii* and from *Westiella intricata* and *Hapalosiphon laingii*. Ichthyotoxic. $[\alpha]_D$ +10.4 (c, 0.54 in CH_2Cl_2). Authors' numbering and nomenclature. λ_{max} 219 (ϵ 18000); 282 (ϵ 4800) (MeOH) (Berdy). λ_{max} 222 (ϵ 26900); 283 (ϵ 4460); 290 (ϵ 4060) (EtOH) (Berdy).

5′-Epimer, 4′β-chloro: ***12-Epihapalindole E isonitrile***
[159249-51-1]
$C_{21}H_{23}ClN_2$ 338.879
Alkaloid from *Hapalosiphon welwitschii*, *Hapalosiphon laingii* and *Westiella intricata*. Ichthyotoxic. $[\alpha]_D$ +42.9 (c, 0.3 in CH_2Cl_2). Authors' numbering and nomenclature. λ_{max} 221 (ϵ 28400); 282 (ϵ 5000); 290 (ϵ 4480) (MeOH) (Berdy).

1′,2′,5′-Triepimer: ***12-Epihapalindole Q isonitrile***
[173241-60-6]
$C_{21}H_{24}N_2$ 304.434
Alkaloid from *Hapalosiphon laingii*. Ichthyotoxic. Sol. MeOH. Authors' numbering and nomenclature. λ_{max} 222 (ϵ 24160); 283 (ϵ 4850); 291 (sh) (ϵ 4300) (MeOH).
Moore, R.E. *et al., J.O.C.*, 1987, **52**, 1036 (*isol, pmr, cmr, struct*)
Stratmann, K. *et al., J.A.C.S.*, 1994, **116**, 9935 (*12-Epihapalindole C isonitrile, 12-Epihapalindole E isonitrile*)
Klein, D. *et al., J. Nat. Prod.*, 1995, **58**, 1781-1785 (*12-Epihapalindole Q isonitrile*)

Hapalindole D H-83

[101968-72-3]
As Hapalindole C, H-82 with
R = –NCS
$C_{21}H_{24}N_2S$ 336.5
Rel. config. illus. Isol. from the blue-green alga *Hapalosiphon fontinalis*. Yellow-orange prisms (CH_2Cl_2).
Mp 105-107°. $[\alpha]_D$ +239 (c, 3.1 in CH_2Cl_2). λ_{max} 223 (ϵ 40000); 281 (ϵ 7300); 291 (ϵ 5900) (MeOH) (Derep).

4′β-Chloro: ***Hapalindole F***
[101968-74-5]
$C_{21}H_{23}ClN_2S$ 370.945
From *Hapalosiphon fontinalis*.
Mp 176-179°. $[\alpha]_D^{25}$ +93.2 (c, 0.22 in CH_2Cl_2). λ_{max} 222 (ϵ 38000); 280 (ϵ 7000); 291 (ϵ 5700) (MeOH) (Derep).

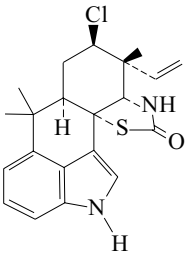
5′-Epimer: ***12-Epihapalindole D isothiocyanate***
[159249-54-4]
$C_{21}H_{24}N_2S$ 336.5
Alkaloid from the freshwater blue-green alga *Hapalosiphon welwitschii*. Authors' numbering and nomenclature.

5′-Epimer, 4′β-chloro: ***12-Epihapalindole F isothiocyanate***
[159249-53-3]
$C_{21}H_{23}ClN_2S$ 370.945
Alkaloid from *Hapalosiphon welwitschii*.
$[\alpha]_D$ +102 (c, 0.5 in CH_2Cl_2). Authors' numbering and nomenclature.

1′,2′-Diepimer: ***Hapalindole Q***
[106928-29-4]
$C_{21}H_{24}N_2S$ 336.5
From *Hapalosiphon fontinalis*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ +24.1 (c, 1.1 in CH_2Cl_2). λ_{max} 223 (ϵ 40000); 281 (ϵ 7300); 291 (ϵ 5900) (MeOH) (Derep).
Moore, R.E. *et al., J.O.C.*, 1987, **52**, 1036 (*isol, pmr, cryst struct*)
Stratmann, K. *et al., J.A.C.S.*, 1994, **116**, 9935 (*12-Epihapalindole D isothiocyanate, 12-Epihapalindole F isothiocyanate*)
Kinsman, A.C. *et al., J.A.C.S.*, 2003, **125**, 14120-14125 (*Hapalindole Q, synth*)

Hapalindole T H-84

[106865-67-2]



$C_{21}H_{23}ClN_2OS$ 386.944

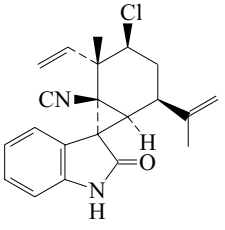
Isol. from the blue-green alga *Hapalosiphon fontinalis* ATCC39964. Antibacterial and antimycotic agent. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -137 (c, 1.5 in CH_2Cl_2). λ_{max} 222 (ϵ 35400); 283 (ϵ 7100) (MeOH) (Derep).

Moore, R.E. *et al., J.O.C.*, 1987, **52**, 1036 (*isol, uv, ir, pmr, cmr, struct*)

Hapalindolinone A H-85

*3-Chloro-2-ethenyl-1-isocyano-2-methyl-5-(1-methylethenyl)spiro[bicyclo[4.1.0]heptane-7,3′-[3*H*]indol]-2′(1′*H*)-one, 9CI*

[109151-56-6]



$C_{21}H_{21}ClN_2O$ 352.862

Isol. from a cultured cyanobacterium and from *Fischerella* sp. and *Hapalosiphon laingii*. Adenylate cyclase inhibitor, vasopressin antagonist and ichthyotoxin. Cryst.

Mp 92-96° dec. $[\alpha]_D^{25}$ -30. Related to Hapalindole A, H-80. λ_{max} 217 (ϵ 77000); 253 (ϵ 3200); 300 (sh) (ϵ 1500) (no solvent specified) (Derep). λ_{max} 223 (ϵ 24380); 261 (ϵ 4620) (MeOH) (Berdy).

Dechloro: ***Hapalindolinone B***

[109151-57-7]

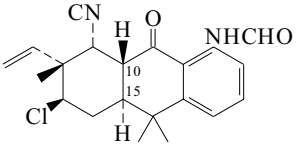
$C_{21}H_{22}N_2O$ 318.418

Isol. from a cultured cyanobacterium and from *Fischerella* sp. Adenylate cyclase inhibitor. Oil. λ_{max} 217 (ϵ 77000); 253 (ϵ 3200); 300 (sh) (ϵ 1500) (MeOH) (Derep). λ_{max} 223 (ϵ 24600); 261 (ϵ 4570) (MeOH) (Berdy).

Schwartz, R.E. *et al., J.O.C.*, 1987, **52**, 3704 (*isol, ir, pmr, cmr, cryst struct*)

Hapalonamide G H-86

[109281-38-1]



$C_{21}H_{23}ClN_2O_2$ 370.878

Author's numbering shown. See also Fontonamide, F-65. Minor alkaloid from the blue-green alga *Hapalosiphon fontinalis*. Also obt. by oxidn. of Hapalindole A, H-80.

10β-Hydroxy: ***Hapalonamide V***

[123498-01-1]

$C_{21}H_{23}ClN_2O_3$ 386.877

Minor alkaloid from *Hapalosiphon fontinalis*.

10,15-Diepimer, dechloro: ***Hapalonamide H***

[123498-00-0]

$C_{21}H_{24}N_2O_2$ 336.433

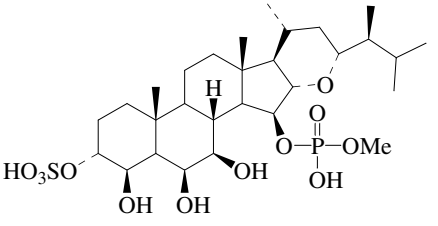
Minor alkaloid from *Hapalosiphon fontinalis*.

$[\alpha]_D$ +13.7 (c, 0.15 in $CHCl_3$).

Moore, R.E. *et al., J.O.C.*, 1987, **52**, 3773 (*synth, pmr*)
Moore, R.E. *et al., Phytochemistry*, 1989, **28**, 1565 (*isol*)

Haplosamate A H-87

[242150-93-2]



$C_{29}H_{51}O_{12}PS$ 654.755

Constit. of a *Xestospongia* sp. and a *Cribrochalina* sp. Solid (Na salt).

Mp 210° (dec.) (Na salt). $[\alpha]_D$ -32 (c, 0.4 in MeOH) (Na salt). $[\alpha]_D^{24}$ -6.9 (c, 2.5 in MeOH). Struct. revised in 2001. λ_{max} 269 (ϵ 9100) (MeOH) (Na salt).

7-O-Phosphate: ***Haplosamate B***

[242150-94-3]

$C_{29}H_{52}O_{15}P_2S$ 734.734

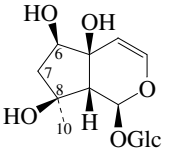
Constit. of a *Xestospongia* sp. Solid (di-Na salt).

Mp 213° (dec.) (di-Na salt). $[\alpha]_D$ -8 (c, 0.1 in MeOH) (di-Na salt). Struct. revised in 2001. λ_{max} 269 (ϵ 5200) (MeOH) (di-Na salt).

Qureshi, A. *et al., Tetrahedron*, 1999, **55**, 8323-8330 (*isol, pmr, cmr*)
Fujita, M. *et al., Tetrahedron*, 2001, **57**, 3885-3890 (*isol, pmr, cmr, struct*)

Harpagide H-88

[6926-08-5]



$C_{15}H_{24}O_{10}$ 364.349

Constit. of *Melittis melissophyllum*. Antiarthritic, antiinflammatory agent. Log P -6.4 (uncertain value) (calc).

7α-Chloro: ***Linarioside***. *Avicennioside*

[35927-36-7]

[79549-53-4]

$C_{15}H_{23}ClO_{10}$ 398.793

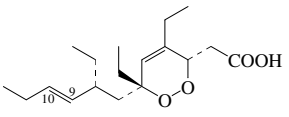
Constit. of *Linaria japonica* and *Avicennia officinalis*. Pale yellow hygroscopic amorph. solid. $[\alpha]_D^{24}$ -140 (dioxan aq.). Unstable. Avicennioside shown to be identical to Linarioside (1996).

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1973, **21**, 1978-1987 (*Linarioside*)
König, G. *et al., Phytochemistry*, 1987, **26**, 423-427 (*Avicennioside*)
Nass, R. *et al., Phytochemistry*, 1996, **41**, 489-498 (*Avicennioside, struct*)

HarveyicinProd. by the marine bacterium *Beneckea harveyi* SY. Bacteriocin. H-89

McCall, J.O. *et al., Appl. Environ. Microbiol.*, 1979, **38**, 974-979 (*isol*)

Haterumadioxin A H-90



Absolute Configuration

$C_{18}H_{30}O_4$ 310.433
Similar to Plakortic acid, P-472. Isol. from *Plakortis lita*. Cytotoxic. Oil. $[\alpha]_D^{29}$ -102 (c, 1.56 in MeOH).

9,10-Dihydro: ***Haterumadioxin B***
$C_{18}H_{32}O_4$ 312.448
Isol. from *Plakortis lita*. Cytotoxic. Oil. $[\alpha]_D^{29}$ -28 (c, 0.42 in MeOH). Stereochem. not determined.

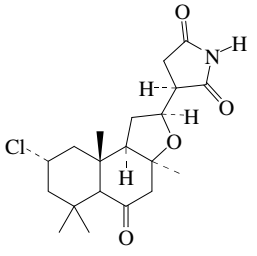
*7,8-Didehydro(*E-*), 4α,5-dihydro, 9,10-epoxide, Me ester(1):* ***Plakorstatin 1***
[761441-65-0]
$C_{19}H_{32}O_5$ 340.459
Isol. from *Plakortis nigra*. Antineoplastic agent. Oil. $[\alpha]_D^{25}$ -177 (c, 0.1 in MeOH). Rel. config. only determined. Has (9*R*,10*R*)- or (9*S*,10*R*)-config.

*7,8-Didehydro(*E-*), 4α,5-dihydro, 9,10-epoxide, Me ester(2):* ***Plakorstatin 2***
[761441-66-1]
$C_{19}H_{32}O_5$ 340.459
Isol. from *Plakortis nigra*. Antineoplastic agent. Oil. $[\alpha]_D^{25}$ -220 (c, 0.1 in MeOH). Rel. config. only determined. 9,10-Diepimer of Plakorstatin 1.

Takada, N. *et al., J. Nat. Prod.*, 2001, **64**, 356-359 (*Haterumadioxins*)
Pettit, G.R. *et al., J. Nat. Prod.*, 2004, **67**, 1611-1613 (*Plakorstatins*)

Haterumaimide I H-91

[368421-37-8]

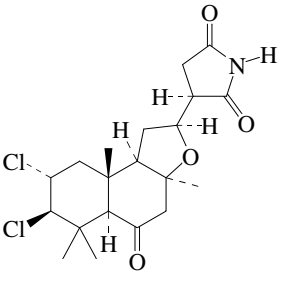


$C_{20}H_{28}ClNO_4$ 381.898
Constit. of a *Lissoclinum* sp. Oil. $[\alpha]_D^{32}$ +62 (c, 0.77 in MeOH). λ_{max} 210 (log ϵ 3.56) (MeOH).

Uddin, M.J. *et al., J. Nat. Prod.*, 2001, **64**, 1169-1173 (*isol, pmr, cmr*)

Haterumaimide C H-92

[338949-10-3]

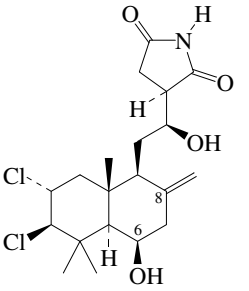


$C_{20}H_{27}Cl_2NO_4$ 416.343
Isol. from a *Lissoclinum* sp. Cytotoxic. $[\alpha]_D^{28}$ +66.6 (c, 0.06 in MeOH).

Uddin, M.J. *et al., Heterocycles*, 2001, **54**, 1039-1048 (*isol, pmr, cmr*)

Haterumaimide E H-93

[338949-12-5]



$C_{20}H_{29}Cl_2NO_4$ 418.359
Isol. from a *Lissoclinum* sp. Cytotoxic. $[\alpha]_D^{29}$ +29.6 (c, 0.16 in MeOH).

6-Ketone: ***Haterumaimide B***
[338949-09-0]
$C_{20}H_{27}Cl_2NO_4$ 416.343
Isol. from a *Lissoclinum* sp. Cytotoxic. $[\alpha]_D^{33}$ +32.6 (c, 0.48 in MeOH).

Δ^7-Isomer, 6-ketone: ***Haterumaimide D***
[338949-11-4]
$C_{20}H_{27}Cl_2NO_4$ 416.343
Isol. from a *Lissoclinum* sp. Cytotoxic. $[\alpha]_D^{29}$ -27.7 (c, 0.16 in MeOH).

2-Dechloro, 6-ketone: ***Haterumaimide M***
[735278-27-0]
$C_{20}H_{28}ClNO_4$ 381.898
Constit. of *Pleurobranchus albiguttatus*. Amorph. solid. $[\alpha]_D$ +14.4 (c, 0.36 in CH_2Cl_2).

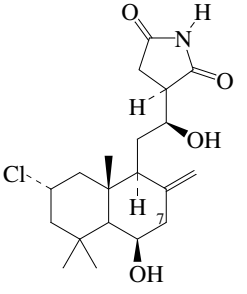
2-Dechloro, Δ^7-isomer, 6-ketone: ***Haterumaimide L***
[735278-28-1]
$C_{20}H_{28}ClNO_4$ 381.898
Constit. of *Pleurobranchus albiguttatus* and *Pleurobranchus forskalii*. Amorph. solid. $[\alpha]_D$ -7.2 (c, 0.43 in CH_2Cl_2).

3-Dechloro, 3β-hydroxy: ***3-Hydroxychlorolissoclimide***
[733753-15-6]
$C_{20}H_{30}ClNO_5$ 399.913
Constit. of *Pleurobranchus albiguttatus*. Amorph. solid.

Uddin, M.J. *et al., Heterocycles*, 2001, **54**, 1039-1048 (*isol, pmr, cmr*)
Fu, X. *et al., J. Nat. Prod.*, 2004, **67**, 1415-1418 (*Haterumaimides L-M, 3-Hydroxychlorolissoclimide*)

Haterumaimide F H-94

[368421-34-5]



$C_{20}H_{30}ClNO_4$ 383.914
Constit. of a *Lissoclinum* sp. Oil. $[\alpha]_D^{29}$ +53.7 (c, 0.35 in MeOH). λ_{max} 210 (log ϵ 3.57) (MeOH).

6-Ketone: ***Haterumaimide G***
[368421-35-6]
$C_{20}H_{28}ClNO_4$ 381.898
Constit. of a *Lissoclinum* sp. Oil. $[\alpha]_D^{29}$ +63.5 (c, 0.58 in MeOH). λ_{max} 207 (log ϵ 3.56) (MeOH).

6-Deoxy, 18-hydroxy: ***Haterumaimide J***
[479249-29-1]
$C_{20}H_{30}ClNO_4$ 383.914
Isol. from a *Lissoclinum* sp. Cytotoxic agent. Oil. $[\alpha]_D^{29}$ +68 (c, 0.92 in MeOH). λ_{max} 210 (ϵ 3800) (MeOH).

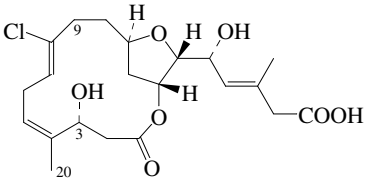
6-Deoxy, 18-acetoxy: ***Haterumaimide K***
[479249-30-4]
$C_{22}H_{32}ClNO_5$ 425.951
Isol. from a *Lissoclinum* sp. Cytotoxic. $[\alpha]_D^{29}$ +59.6 (c, 0.19 in MeOH). λ_{max} 210 (ϵ 3600) (MeOH).

Δ^7-Isomer, 6-ketone: ***Haterumaimide H***
[368421-36-7]
$C_{20}H_{28}ClNO_4$ 381.898
Constit. of a *Lissoclinum* sp. Oil. $[\alpha]_D^{32}$ +47.6 (c, 0.31 in MeOH). λ_{max} 205 (log ϵ 3.7); 238 (log ϵ 3.9) (MeOH).

Uddin, M.J. *et al., J. Nat. Prod.*, 2001, **64**, 1169-1173 (*isol, pmr, cmr*)
Uddin, M.J. *et al., Chem. Lett.*, 2002, 1028-1029 (*Haterumamides J,K*)

Haterumalide NE H-95

Haterumalide E
[245342-52-3]



Absolute Configuration

$C_{21}H_{29}ClO_7$ 428.909
Macrolide antibiotic. Isol. from an *Ircinia* sp. and prod. by *Serratia plymuthica* A153. Cytotoxic agent. Oil.

3-Ac: ***Haterumalide NA****. Haterumalide A. Oocydin A. FR 177391. Antibiotic FR 177391*
[245342-48-7]
[260362-86-5, 288581-04-4]
$C_{23}H_{31}ClO_8$ 470.946
Isol. from an *Ircinia* sp., prod. by *Serratia marcescens*, *Serratia liquefaciens* FR 177391 and *Serratia plymuthica* A153. Cytotoxic, antihyperlipidaemic and anti-oomycetic agent. Powder. Mp 106-108°. $[\alpha]_D^{26}$ -3 (c, 0.05 in MeOH). $[\alpha]_D$ +18.2 (MeOH). $[\alpha]_D$ +32 (c, 0.85 in MeOH). Stereochemical identity of the various isolates has not been demonstrated.

3-Ac, butyl ester: ***Haterumalide NB***
[245342-49-8]
$C_{27}H_{39}ClO_8$ 527.053
Isol. from an *Ircinia* sp. Cytotoxic agent. Oil.

3-Ac, (2-methylene-3-oxobutyl) ester: ***Haterumalide B***
[245122-93-4]
$C_{28}H_{37}ClO_9$ 553.048
Isol. from a *Lissoclinum* sp., prod. by *Serratia plymuthica* A153. Cytotoxic agent. Oil. $[\alpha]_D$ 0 ($CHCl_3$). λ_{max} 206 (ϵ 12000) (MeOH).

3-Ac, (2-sulfoethyl)amide: ***Biselide D****. Taurohaterumalide NA*
$C_{25}H_{36}ClNO_{10}S$ 578.079
Alkaloid from a *Didemnum* sp. Oil.

δ-Lactone, 3-Ac: ***Haterumalide X***
[343573-61-5]
$C_{23}H_{29}ClO_7$ 452.931
Prod. by *Serratia plymuthica* A153. Cytotoxic agent.

*9*R*-Hydroxy, 3-Ac:* ***Haterumalide ND***
[245342-51-2]
$C_{23}H_{31}ClO_9$ 486.945
Isol. from an *Ircinia* sp. Cytotoxic agent. Oil.

*9*R*-Hydroxy, 3-Ac, butyl ester:* ***Haterumalide NC***
[245342-50-1]
$C_{27}H_{39}ClO_9$ 543.052
Isol. from an *Ircinia* sp. Cytotoxic agent. Oil.

20-Hydroxy, 3-Ac: ***Biselide C***
$C_{23}H_{31}ClO_9$ 486.945
Constit. of a *Didemnum* sp. Cytotoxic. Oil.

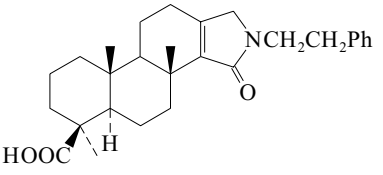
20-Acetoxy, 3-Ac: ***Biselide A***
$C_{25}H_{33}ClO_{10}$ 528.982
Constit. of a *Didemnum* sp. Oil.

20-Acetoxy, 3-Ac, (2-methylene-3-oxobutyl) ester: ***Biselide B***
$C_{30}H_{39}ClO_{11}$ 611.084
Constit. of a *Didemnum* sp. Oil.

Strobel, G. *et al., Microbiology (Reading, U.K.)*, 1999, **145**, 3557-3564 (*Oocydin A*)
Ueda, K. *et al., Tet. Lett.*, 1999, **40**, 6305-6308; 6309-6312 (*isol, pmr, cmr*)
Pat. Coop. Treaty (WIPO), 2001, 40442; *CA*, **135**, 32806q (*Haterumalide X*)
Kigoshi, H. *et al., Org. Lett.*, 2003, **5**, 957-960 (*synth, abs config*)
Gu, Y. *et al., Org. Lett.*, 2003, **5**, 4385-4388 (*synth*)
Sato, B. *et al., J. Antibiot.*, 2005, **58**, 634-639; 640-647; 648-653; 654-662 (*FR 177391*)
Hoye, T.R. *et al., J.A.C.S.*, 2005, **127**, 6950-6951 (*Haterumalide NA, synth*)
Teruya, T. *et al., Tetrahedron*, 2005, **61**, 6561-6567 (*Biselides*)

Haumanamide H-96

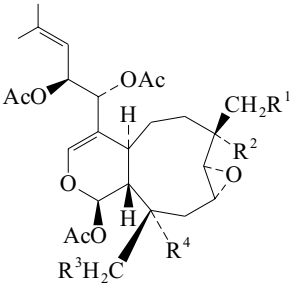
4,8-Dimethyl-15-oxo-16-(2-phenylethyl)-16-aza-18-norandrost-13-ene-4-carboxylic acid, 9CI
[141266-06-0]



$C_{28}H_{37}NO_3$ 435.605
Alkaloid from a *Spongia* sp. Cytotoxic agent. Powder. $[\alpha]_D$ -163.2 (c, 0.13 in $CHCl_3$). λ_{max} 250 (ϵ 340) (EtOH) (Derep).

Pham, A.T. *et al., Tet. Lett.*, 1992, **33**, 1147 (*isol, pmr, cmr*)

7(18)-Havannachlorohydrin H-97



R^1 = Cl, R^2 = OH, R^3,R^4 = —O—

$C_{26}H_{35}ClO_{10}$ 543.009
Constit. of *Xenia membranacea*. Amorph. $[\alpha]_D$ +22 (c, 1.4 in $CHCl_3$).

Almourabit, A. *et al., J. Nat. Prod.*, 1988, **51**, 282-292

11(19)-Havannachlorohydrin H-98

As 7(18)-Havannachlorohydrin, H-97 with R^1R^2 = –O-, R^3 = Cl, R^4 = OH
$C_{26}H_{35}ClO_{10}$ 543.009
Constit. of *Xenia membranacea*. Cryst. (EtOH).
Mp 145°. $[\alpha]_D$ -1 (c, 2.4 in $CHCl_3$).

O^{13}-De-Ac: ***13-Deacetyl-11(9)-havannachlorohydrin***
$C_{24}H_{33}ClO_9$ 500.972
Constit. of *Xenia membranacea*. Amorph.

Almourabit, A. *et al., J. Nat. Prod.*, 1988, **51**, 282-292

7(18),11(19)-Havannadichlorohydrin H-99

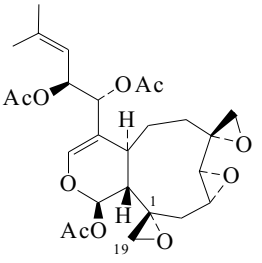
As 7(18)-Havannachlorohydrin, H-97 with
$R^1 = R^3 = Cl$, $R^2 = R^4 = OH$

$C_{26}H_{36}Cl_2O_{10}$ 579.47
Constit. of *Xenia membranacea*. Amorph. $[\alpha]_D$ -5 (c, 1.6 in $CHCl_3$).

Almourabit, A. *et al., J. Nat. Prod.*, 1988, **51**, 282-292

Havannahine H-100

[110201-59-7]



$C_{26}H_{34}O_{10}$ 506.549
Constit. of *Xenia membranacea*. Cryst.
Mp 181°. $[\alpha]_D$ +33 (c, 1.27 in $CHCl_3$). λ_{max} 205 (ϵ 20000) (MeOH) (Derep).

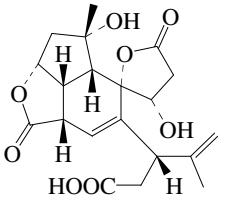
1,19-Deepoxy: ***Deoxyhavannahine***
[124580-88-7]
$C_{26}H_{34}O_9$ 490.549
Constit. of *Xenia membranacea*. Amorph. solid. $[\alpha]_D$ +48 (c, 0.6 in $CHCl_3$).

6-Epimer, 1,19-deepoxy: ***6-Epideoxyhavannahine****. 7-Epideoxyhavannahine*
[110201-60-0]
$C_{26}H_{34}O_9$ 490.549
From *Xenia membranacea* and *Xenia garciae*. Cryst.
Mp 138-139°. $[\alpha]_D$ +35 (c, 0.005 in $CHCl_3$). 6-Config. revised in 1989. λ_{max} 205 (ϵ 20000) (MeOH) (Derep).

6,7,8-Triepimer, 1,19-deepoxy: ***6,7,8-Triepideoxyhavannahine****. 7,8,9-Triepideoxyhavannahine*
[124580-89-8]
$C_{26}H_{34}O_9$ 490.549
Constit. of *Xenia membranacea*. Amorph. solid.

Lelong, H. *et al., J. Nat. Prod.*, 1987, **50**, 203-210 (*isol, cryst struct*)
Almourabit, A. *et al., J. Nat. Prod.*, 1988, **51**, 282-292 (*abs config*)
König, G.M. *et al., J. Nat. Prod.*, 1989, **52**, 294-299 (*isol, cryst struct, 6-Epideoxyhavannine*)
Almourabit, A. *et al., J. Nat. Prod.*, 1989, **52**, 1080-1087 (*Deoxyhavannahine, 6,7,8-Triepideoxyhavannahine*)

Havellockic acid H-101



$C_{20}H_{24}O_8$ 392.405

Me ester: Methyl havellockate. ***Havellockate***
[201859-57-6]
$C_{21}H_{26}O_8$ 406.432
Constit. of *Sinularia granosa*. Cryst.
Mp 212-213°. $[\alpha]_D$ +23.7 (c, 0.43 in Py).

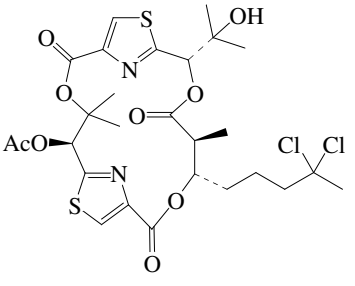
Anjaneyulu, A.S.R. *et al., Tet. Lett.*, 1998, **39**, 139-142 (*isol, pmr, cmr, cryst struct*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 2000, **39**, 530-535 (*isol, pmr, cmr*)

Head-activator peptide H-102

Peptide (hydra-head activator), 9CI
[79943-68-3]
H-5-OxoPro-Pro-Pro-Gly-Gly-Ser-Lys-Val-Ile-Leu-Phe-OHIsol. from *Anthopleura elegantissima* and *Hydra attenuata*. Also present in other animals such as frogs and mammals.

Birr, C. *et al., FEBS Lett.*, 1981, **131**, 317-321 (*synth*)
Schaller, H.C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1981, **78**, 7000 (*isol*)
Bodenmuller, H. *et al., Biochim. Biophys. Acta*, 1985, **825**, 261 (*rev*)
Schaller, H.C. *et al., Biol. Chem. Hoppe-Seyler*, 1985, **366**, 1003 (*rev*)
Saffrich, R. *et al., Biochim. Biophys. Acta*, 1989, **997**, 144 (*pmr*)

Hectochlorin H-103



Absolute Configuration

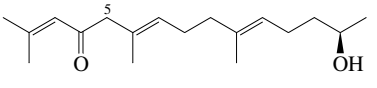
$C_{27}H_{34}Cl_2N_2O_9S_2$ 665.611
Isol. from *Bursatella leachii* and *Lyngbya majuscula*. Promoter of actin polym. Antifungal and cytotoxic agent. Pale yellow solid. $[\alpha]_D^{25}$ -8.7 (c, 1.04 in MeOH).

O-*De-Ac:* ***Deacetylhectochlorin***
$C_{25}H_{32}Cl_2N_2O_8S_2$ 623.574
Isol. from the sea hare *Bursatella leachii*. Potent stimulator of actin assembly. Cytotoxic. Amorph. solid. $[\alpha]_D^{20}$ -26 (c, 0.1 in MeOH).

Marquez, B.L. *et al., J. Nat. Prod.*, 2002, **65**, 866-871 (*isol, ir, pmr, cmr, cryst struct*)
Cetusic, J.R.P. *et al., Org. Lett.*, 2002, **4**, 1307-1310 (*synth*)
Suntornchashwej, S. *et al., J. Nat. Prod.*, 2005, **68**, 951-955 (*isol, pmr, cmr*)

Hedaol B H-104

14-Hydroxy-2,6,10-trimethyl-2,6,10-pentadecatrien-4-one
[346610-25-1]



$C_{18}H_{30}O_2$ 278.434
Constit. of a *Sargassum* sp. Oil. $[\alpha]_D^{29}$ -79 (c, 0.047 in $CHCl_3$).

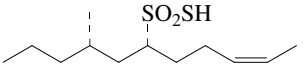
*Δ^5-Isomer(*E-*): 14-Hydroxy-2,6,10-trimethyl-2,5,10-pentadecatrien-4-one.* ***Hedaol C***
[346610-26-2]
$C_{18}H_{30}O_2$ 278.434
Constit. of a *Sargassum* sp. Oil. $[\alpha]_D^{28}$ -3 (c, 0.047 in $CHCl_3$).

*Δ^5-Isomer(*Z-*):* ***Hedaol A***
[346610-24-0]
$C_{18}H_{30}O_2$ 278.434
Constit. of a *Sargassum* sp. Oil. $[\alpha]_D^{29}$ -1.9 (c, 0.057 in $CHCl_3$).

Takada, N. *et al., J. Nat. Prod.*, 2001, **64**, 653-655 (*isol, pmr, cmr*)
Li, Y. *et al., Synth. Commun.*, 2003, **33**, 1417-1423 (*synth, ir, pmr, ms*)

Hedathiosulfonic acid A H-105

1-(2-Methylpentyl)-4-hexenesulfonothioic acid, 9CI. 8-Methyl-2-undecene-6-sulfonothioic acid



Absolute Configuration

$C_{12}H_{24}O_2S_2$ 264.452

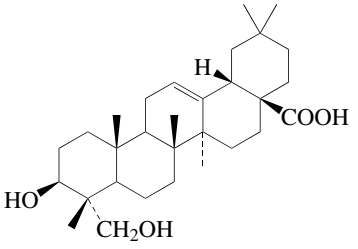
First known natural thiosulfonic acids. Isol. from the deep sea urchin *Echinocardium cordatum*. Oil. $[\alpha]_D^{26}$ +2.1 (c, 0.07 in MeOH).

▶ Highly toxic to mice.

1,2-Didehydro: 3-Methyl-1-(3-pentenyl)-5-hexenesulfonothioic acid. ***Hedathiosulfonic acid B***
$C_{12}H_{22}O_2S_2$ 262.437
Isol. from *Echinocardium cordatum*. Oil. $[\alpha]_D^{26}$ -2.2 (c, 0.28 in MeOH).

Kita, M. *et al., Tetrahedron*, 2002, **58**, 6405-6412 (*isol, pmr, cmr*)

Hederagenin 28-glycosyl esters H-106



Glycosyl esters of Hederagenin with glycoside residues at C-28 only.

28-O-[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranosyl] ester:
[170032-83-4]
$C_{41}H_{66}O_{13}$ 766.965
Constit. of *Pometia eximia*. Cryst.
Mp 222-224°. $[\alpha]_D^{25}$ -7.4 (c, 0.43 in MeOH).

28-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranosyl] ester: ***Calthasaponin F***
[108195-61-5]
$C_{42}H_{68}O_{13}$ 780.991
Constit. of *Caltha polypetala*. Powder. Mp 139-140°.

28-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester: ***Dipsacussaponin A***
[99624-66-5]
$C_{42}H_{68}O_{14}$ 796.991
Constit. of *Dipsacus asper* and *Dipsacus asperoides*.
Mp 186-188°. $[\alpha]_D^{30}$ +19.3 (c, 1.19 in MeOH).

28-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester, 23-O-sulfate: ***Sulfapatrinoside II***
[120204-05-9]
$C_{42}H_{68}O_{17}S$ 877.055
Constit. of *Patrinia scabiosaefolia*. Cryst. (EtOH).
Mp 242-244°. $[\alpha]_D^{20}$ +25.3 (c, 0.39 in Py).

28-O-[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester: ***Cussonoside A***. *HN Saponin H. Pulsatiloside C*
[57539-70-5]
$C_{48}H_{78}O_{18}$ 943.133
Isol. from *Cussonia barteri*, *Pulsatilla campanella* and *Hedera nepalensis*. Powder (MeOH/EtOAc).
Mp 198-202° dec. $[\alpha]_D$ -3.3 (c, 3 in MeOH).

28-O-[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranosyl] ester, 23-sulfate: [218457-82-0]
$C_{48}H_{78}O_{22}S$ 1039.197
Constit. of *Gypsophila bermejoi*. Amorph. powder.
Mp 234-236°. $[\alpha]_D$ +6.5 (c, 1.5 in MeOH). λ_{max} 270 (log ε 3.2); 300 (sh) (log ε 2.9) (MeOH).

28-O-[β-D-Glucuronopyranosyl-(1→4)-β-D-glucopyranosyl] ester:
[261955-56-0]
$C_{42}H_{66}O_{15}$ 810.974
Constit. of *Aralia dasyphylla*.

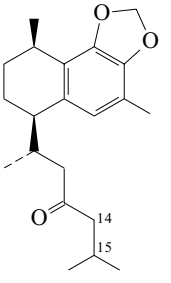
3-(Methylmalonoyl), 28-O-[α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: ***Begoniifolide C***
[333329-90-1]
$C_{52}H_{82}O_{21}$ 1043.207
Constit. of *Anemone begoniifolia*. Cryst. Mp 168-170°.

23-(Methylmalonoyl), 28-O-[α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: ***Begoniifolide B***
[333329-48-9]
$C_{52}H_{82}O_{21}$ 1043.207
Constit. of *Anemone begoniifolia*. Cryst. Mp 175-178°.

Woo, W.S. *et al., Phytochemistry*, 1983, **22**, 1045-1047 (*Patrinia scabiosaefolia saponin*)
Kizu, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 3324-3329 (*HN saponin H*)
Vulgal'ter, M.M. *et al., Khim. Prir. Soedin.*, 1986, **22**, 712-716; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 665-668 (*Calthasaponin F*)
Dubois, M.A. *et al., Planta Med.*, 1986, **52**, 80-83 (*Cussonoside A*)
Choi, J.S. *et al., Planta Med.*, 1987, **53**, 62-65 (*Patrinia scabiosaefolia saponin*)
Inada, A. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4269-4274 (*Sulfapatrinoside II*)
Li, X.-C. *et al., Phytochemistry*, 1990, **29**, 595-599 (*Pulsatiloside C*)
Zhang, Y.W. *et al., Yaoxue Xuebao*, 1991, **26**, 911; *CA*, **117**, 44545v (*Dipsacus asper saponin*)
Zhang, Y.W. *et al., Yaoxue Xuebao*, 1992, **27**, 912; 1993, **28**, 358; *CA*, **118**, 120975y; **119**, 177572q (*Dipsacus asper saponin*)
Jung, K.Y. *et al., Arch. Pharmacal Res.*, 1993, **16**, 32 (*Dipsacussaponin A*)
Yang, S. *et al., CA*, 1994, **120**, 73428b; 101953q (*Dipsacus asperoides saponin*)
Jayasinghe, L. *et al., Phytochemistry*, 1995, **40**, 891-897 (*Pometia eximia glycosides*)
Acebes, B. *et al., J. Nat. Prod.*, 1998, **61**, 1557-1559 (*Gypsophilia bermejoi saponin*)
Xiao, K. *et al., Tianran Chanwu Yanjiu Yu Kaifa*, 1999, **11**, 14-18; *CA*, **132**, 234268q (*Aralia dasyphylla constit*)
Liao, X. *et al., Yaoxue Xuebao*, 2000, **35**, 821-825 (*Begoniifolides*)

Helioporin B H-107

[138264-49-0]



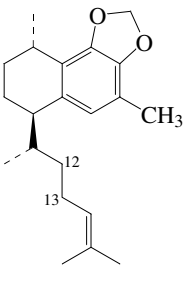
$C_{21}H_{30}O_3$ 330.466
Constit. of *Heliopora coerula*. Oil. $[\alpha]_D^{24}$ +18.8 (c, 2.55 in $CHCl_3$). λ_{max} 212 (ε 19500); 287 (ε 1660) (MeOH) (Derep).

14,15-Didehydro: ***Helioporin C***
[138264-50-3]
$C_{21}H_{28}O_3$ 328.45
Constit. of *Heliopora coerula*. Oil. $[\alpha]_D^{22}$ +8.3 (c, 0.58 in $CHCl_3$). λ_{max} 237 (ε 10000); 287 (ε 1700) (MeOH) (Derep). λ_{max} 212; 290 (MeOH) (Berdy).

Tanaka, J. *et al., Tetrahedron*, 1993, **49**, 811 (*isol, pmr, cmr*)
Dehmel, F. *et al., Org. Lett.*, 2001, **3**, 3579-3582 (*synth*)

Helioporin D H-108

[138264-51-4]



$C_{21}H_{30}O_2$ 314.467

Stereochem. revised in 1998. It is epimeric with closely related nat. prods. Constit. of *Heliopora coerula*. Oil. $[\alpha]_D^{23}$ +6.3 (c, 0.36 in $CHCl_3$). λ_{max} 212 (ϵ 19500); 287 (ϵ 1660) (MeOH) (Derep).

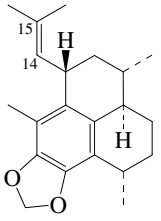
12,13-Didehydro (E-): ***Helioporin G***
[138264-54-7]
$C_{21}H_{28}O_2$ 312.451
Constit. of *Heliopora coerula*. Oil. $[\alpha]_D^{23}$ -50 (c, 0.69 in $CHCl_3$). λ_{max} 230 (ϵ 10000); 287 (ϵ 1700) (MeOH) (Derep).

12,13-Didehydro (Z-): ***Helioporin F***
[138264-53-6]
$C_{21}H_{28}O_2$ 312.451
Constit. of *Heliopora coerula*. Oil. $[\alpha]_D^{23}$ -17 (c, 0.23 in $CHCl_3$). λ_{max} 230 (ϵ 10000); 287 (ϵ 1700) (MeOH) (Derep).

Tanaka, J. *et al., Tetrahedron*, 1993, **49**, 811 (*isol, pmr, cmr*)
Geller, T. *et al., Tet. Lett.*, 1998, **39**, 1541-1544 (*config*)

Helioporin E H-109

[138264-52-5]



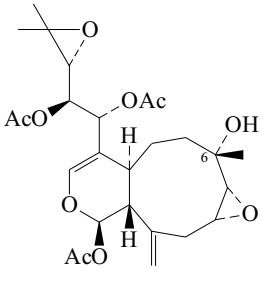
$C_{21}H_{28}O_2$ 312.451
Stereochem. revised in 2000. Constit. of *Heliopora coerulea*. Oil. $[\alpha]_D^{23}$ +111 (c, 0.55 in $CHCl_3$). λ_{max} 213 (ϵ 20000); 290 (ϵ 1900) (MeOH) (Derep).

14α,15-Epoxide: ***Helioporin A***
[138264-48-9]
$C_{21}H_{28}O_3$ 328.45
Constit. of *Heliopora coerulea*. Oil. $[\alpha]_D^{24}$ +65 (c, 4.4 in $CHCl_3$). λ_{max} 213 (ϵ 20000); 290 (ϵ 1900) (MeOH) (Derep).

Tanaka, J. *et al., Tetrahedron*, 1993, **49**, 811 (*isol, pmr, cmr*)
Lazerwith, S.E. *et al., Org. Lett.*, 2000, **2**, 2389-2392 (*struct*)

Helioxenicin A H-110

[157878-23-4]



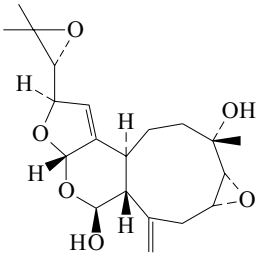
$C_{26}H_{36}O_{10}$ 508.564
Constit. of *Heliopora coerulea*. Gum. $[\alpha]_D^{24}$ -4.2 (c, 0.6 in $CHCl_3$).

6-Ac: ***Helioxenicin B***
[157878-24-5]
$C_{28}H_{38}O_{11}$ 550.602
Constit. of *Heliopora coerulea*. Cryst. (EtOH).
Mp 166-168°. $[\alpha]_D^{24}$ +34 (c, 0.22 in $CHCl_3$).

Tanaka, J.-I. *et al., Tetrahedron*, 1994, **50**, 9989 (*isol, pmr, cmr, cryst struct*)

Helioxenicin C H-111

[157878-25-6]

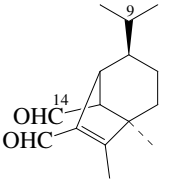


$C_{20}H_{28}O_6$ 364.438
Constit. of *Heliopora coerulea*. Cryst. (hexane/C_6H_6).
Mp 154-156°. $[\alpha]_D^{24}$ -92 (c, 0.1 in $CHCl_3$).

Tanaka, J.-I. *et al., Tetrahedron*, 1994, **50**, 9989 (*isol, pmr, cmr*)

Helminthosporal H-112

1,7-Dimethyl-4-(1-methylethyl)bicyclo[3.2.1]oct-6-ene-6,8-dicarboxaldehyde, 9CI. 4-Isopropyl-1,7-dimethylbicyclo[3.2.1]oct-6-ene-6,8-dicarboxaldehyde
[723-61-5]



$C_{15}H_{22}O_2$ 234.338
Prod. by *Helminthosporium sativum* and *Cochliobolus sativus*. Phytotoxin. Cryst. Sol. MeOH, Et_2O; poorly sol. H_2O, hexane. Mp 56-59°. $[\alpha]_D$ -49 (c, 1.2 in $CHCl_3$). λ_{max} 266 (ϵ 11000) (EtOH) (Derep). λ_{max} 266 (ϵ 9700) (EtOH) (Berdy).

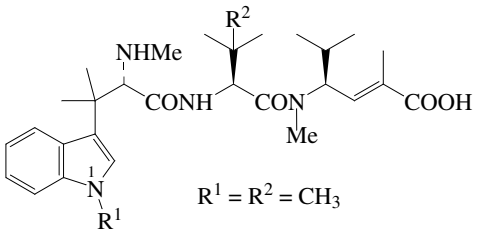
14-Alcohol: ***Helminthosporol***
[1619-29-0]
$C_{15}H_{24}O_2$ 236.353
Metab. of *Helminthosporium sativum* and *Drechslera dematioidea*. Cryst. (hexane). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 98°. $[\alpha]_D$ -28.7 (c, 1.9 in $CHCl_3$). λ_{max} 266 (ϵ 11000) (EtOH) (Derep). λ_{max} 267 (ϵ 9700) (MeOH) (Berdy).

9-Hydroxy, 14-alcohol: ***9-Hydroxyhelminthosporol***
[40517-86-0]
$C_{15}H_{24}O_3$ 252.353
Metab. of *Drechslera dematioidea* isol. from the marine alga *Liagora viscida*. Amorph. powder. $[\alpha]_D^{22}$ +50 (c, 0.4 in EtOH). λ_{max} 268 (log ϵ 3.66) (EtOH).

De Mayo, P. *et al., Can. J. Chem.*, 1965, **43**, 1357 (*isol*)
Corey, E.J. *et al., J.A.C.S.*, 1965, **87**, 5728 (*synth*)
Sommereyns, G. *et al., Arch. Int. Physiol. Biochim.*, 1977, **85**, 431 (*isol, props*)
Piers, E. *et al., Can. J. Chem.*, 1977, **55**, 1039 (*synth, bibl*)
Yanagiya, M. *et al., Tet. Lett.*, 1979, **20**, 1761 (*synth*)
Shizuri, Y. *et al., Chem. Comm.*, 1986, 63 (*synth*)
Gray, B.D. *et al., Chem. Comm.*, 1987, 1136 (*synth*)
Nagaoka, H. *et al., Tet. Lett.*, 1991, **32**, 6741 (*synth*)
Wenkert, E. *et al., J.A.C.S.*, 1992, **114**, 644 (*synth*)
Osterhage, C. *et al., J. Nat. Prod.*, 2002, **65**, 306-313 (*9-Hydroxyhelminthosporol*)

Hemiasterlin H-113

Milnamide B
[157207-90-4]



$C_{30}H_{46}N_4O_4$ 526.718

Peptide antibiotic. Isol. from the marine sponges *Auletta* sp., *Cymbastela* sp. and *Hemiasterella minor*. Cytotoxic. Microtubule formation inhibitor. Cryst. (MeOH/hexane). Mp 120-130°. $[\alpha]_D$ -95 (c, 0.06 in MeOH). λ_{max} 220 (ϵ 30000); 270 (ϵ 9000); 295 (ϵ 5000) (MeOH) (Derep).

N^1-De-Me: ***Hemiasterlin A***
[169181-24-2]
$C_{29}H_{44}N_4O_4$ 512.691
Isol. from sponges *Cymbastela* sp. and *Siphonochalina* sp. Cytotoxic. Amorph. solid. Sol. MeOH. $[\alpha]_D$ -45 (c, 0.25 in MeOH). λ_{max} 218 (ϵ 23400); 280 (ϵ 2800) (MeOH).

Talpir, R. *et al., Tet. Lett.*, 1994, **35**, 4453-4456 (*isol, pmr, cmr, ms*)
Coleman, J.E. *et al., Tetrahedron*, 1995, **51**, 10653-10662 (*Hemiasterlin A*)
Coleman, J.E. *et al., Acta Cryst. C*, 1996, **52**, 1525-1527 (*cryst struct*)
Gamble, W.R. *et al., Bioorg. Med. Chem.*, 1999, **7**, 1611-1615 (*isol, activity*)
Vedejs, E. *et al., J.O.C.*, 2001, **66**, 7355-7364 (*synth, pmr, cmr*)
Nieman, J.A. *et al., J. Nat. Prod.*, 2003, **66**, 183-199 (*synth, pmr, cmr, activity*)
Chevallier, C. *et al., Org. Lett.*, 2003, **5**, 3737-3739 (*isol, activity*)
Sonnenschein, R. *et al., Org. Lett.*, 2004, **6**, 779-782 (*isol, activity*)

Hemiasterlin B H-114

[169181-25-3]
As Hemiasterlin, H-113 with
$R^1 = R^2 = H$
$C_{28}H_{42}N_4O_4$ 498.664
Isol. from the sponge *Cymbastela* sp. Cytotoxic agent. Microtubule formation inhibitor. Amorph. solid. Sol. MeOH.

Coleman, J.E. *et al., Tetrahedron*, 1995, **51**, 10653-10662 (*isol, pmr, cmr*)

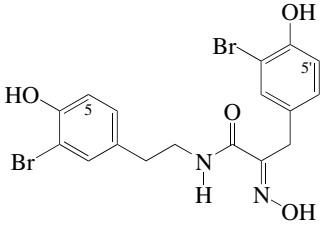
Hemiasterlin C H-115

[246847-61-0]
As Hemiasterlin, H-113 with
$R^1 = CH_3$, $R^2 = H$
$C_{29}H_{44}N_4O_4$ 512.691
Isol. from the sponge *Siphonochalina* sp. Cytotoxic agent. $[\alpha]_D$ -18.8 (c, 0.11 in MeOH).

Gamble, W.R. *et al., Bioorg. Med. Chem.*, 1999, **7**, 1611-1615

Hemibastadin 1 H-116

[134981-79-6]



$C_{17}H_{16}Br_2N_2O_4$ 472.132
Numbering systems vary. Minor constit. of the Australian marine sponge *Ianthella basta*. Solid.

4-Sulfate: ***4-O-Sulfohemibastadin 1***. *1*-O-*Sulfohemibastadin 1*
$C_{17}H_{16}Br_2N_2O_7S$ 552.197
Constit. of *Ianthella basta*. Amorph. solid (as Na salt).

4′-Me ether: ***4′-O-Methylhemibastadin 1***. *1′-Methoxyhemibastadin 1*
[182496-48-6]
$C_{18}H_{18}Br_2N_2O_4$ 486.159
Constit. of *Ianthella basta*. Oil. λ_{max} 213 (log ϵ 4.53); 280 (log ϵ 3.87) (MeOH).

5-Bromo: ***Hemibastadin 3***
[182806-14-0]
$C_{17}H_{15}Br_3N_2O_4$ 551.029
Constit. of *Ianthella basta*.

5′-Bromo: ***Hemibastadin 2***
[134981-80-9]
$C_{17}H_{15}Br_3N_2O_4$ 551.029
Constit. of *Ianthella basta*. Solid.

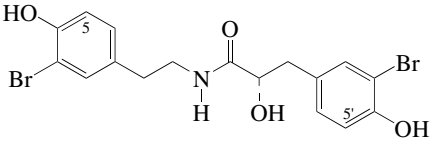
5′-Bromo, 4-sulfate: ***4-O-Sulfohemibastadin 2***. *1*-O-*Sulfohemibastadin 2*
$C_{17}H_{15}Br_3N_2O_7S$ 631.093
Constit. of *Ianthella basta*. Amorph. solid. λ_{max} 204; 282 (MeOH).

5′-Bromo, 4′-Me ether: ***4′-O-Methylhemibastadin 2***. *1′-Methoxyhemibastadin 2*
[182496-49-7]
$C_{18}H_{17}Br_3N_2O_4$ 565.055
Constit. of *Ianthella basta*. Solid. λ_{max} 213 (log ϵ 4.5); 281 (log ϵ 3.87) (MeOH).

Butler, M.S. *et al., Aust. J. Chem.*, 1991, **44**, 287-296 (*isol, pmr, ms, struct*)
Pettit, G.R. *et al., J. Nat. Prod.*, 1996, **59**, 927-934 (*4′-O-Methylhemibastadins, Hemibastadin 3*)
Wasserman, H.H. *et al., J.O.C.*, 1998, **63**, 5581-5586 (*Hemibastadin 2, synth*)
Masuno, M.N. *et al., Mar. Drugs*, 2004, **2**, 176-184 (*4-Sulfohemibastadins*)

Hemibastadinol 1 H-117

[182806-09-3]



$C_{17}H_{17}Br_2NO_4$ 459.134
Isol. from the Papua New Guinea marine sponge *Ianthella basta*. Solid. $[\alpha]_D^{23}$ -31 (c, 1.83 in MeOH). λ_{max} 208 (log ϵ 4.43); 281 (log ϵ 3.69) (MeOH).

5′-Bromo: ***Hemibastadinol 2***
[182806-11-7]
$C_{17}H_{16}Br_3NO_4$ 538.03
From *Ianthella basta*. Oil. $[\alpha]_D^{23}$ -24 (c, 0.10 in MeOH). Inseparable mixt. with Hemibastadinol 3, to which data refer.

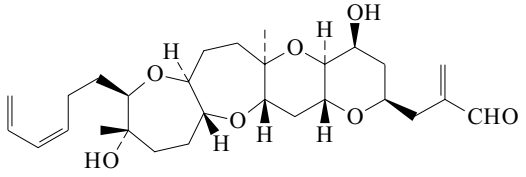
5-Bromo: ***Hemibastadinol 3***
[182806-12-8]
$C_{17}H_{16}Br_3NO_4$ 538.03
From *Ianthella basta*. Inseparable mixt. with Hemibastadinol 2.

Pettit, G.R. *et al., J. Nat. Prod.*, 1996, **59**, 927 (*isol, uv, ir, pmr, cmr, ms, struct*)

Hemibrevetoxin B H-118

GB-N

[122271-91-4]

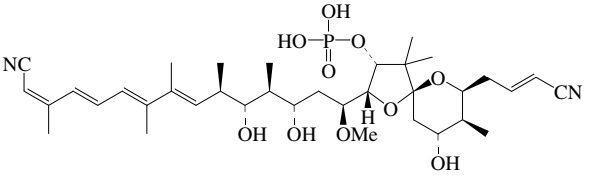


$C_{28}H_{42}O_7$ 490.636

Prod. by the dinoflagellate red-tide organism *Gymnodinium breve*. Cytotoxic agent. Non-cryst. solid. $[\alpha]_D^{22}$ +115 (c, 0.1 in $CHCl_3$). λ_{max} 222 (ϵ 15500) (MeOH) (Derep).

Prasad, A.V. *et al., J.A.C.S.*, 1989, **111**, 6476 (*pmr, cmr, struct*)
Nicolaou, K.C. *et al., J.A.C.S.*, 1993, **115**, 3558 (*synth, pmr, cmr*)
Morimoto, M. *et al., Tet. Lett.*, 1996, **37**, 6365 (*synth*)
Mori, Y. *et al., J.O.C.*, 1998, **63**, 6200-6209 (*synth*)
Kadota, I. *et al., J.O.C.*, 1998, **63**, 6597-6606 (*synth*)
Rainier, J.D. *et al., J.O.C.*, 2001, **66**, 1380-1386 (*synth*)
Zakarian, A. *et al., J.A.C.S.*, 2003, **125**, 7822-7824 (*synth*)
Holland, J.M. *et al., J.O.C.*, 2003, **68**, 747-753 (*synth*)
Fujiwara, K. *et al., Tet. Lett.*, 2004, **45**, 5243-5246 (*synth*)

Hemicalyculin A H-119



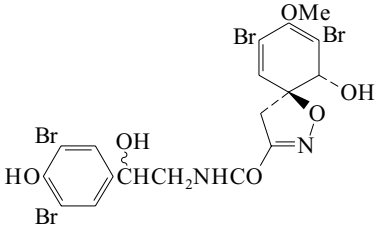
$C_{36}H_{55}N_2O_{10}P$ 706.812

Isol. from the sponge *Discodermia calyx*. Amorph. solid. $[\alpha]_D^{20}$ -107 (c, 0.5 in MeOH). λ_{max} 237 (ϵ 3700); 340 (ϵ 19000) (MeOH).

Wakimoto, T. *et al., Chem. Biol.*, 2002, **9**, 309-319 (*isol, pmr, cmr*)

Hemifistularin 3 H-120

[153415-35-1]



$C_{18}H_{16}Br_4N_2O_6$ 675.95

Metab. from a new sp. of sponge of the family Aplysinellidae, order Verongida, from the Coral Sea. Powder (hexane/Et_2O). Mp 73-75°. $[\alpha]_D^{20}$ +110 (c, 0.2 in Me_2CO). λ_{max} 207 (ϵ 39000); 281 (ϵ 6900) (MeOH) (Berdy).

Mancini, I. *et al., J.C.S. Perkin 1*, 1993, 3121 (*isol, uv, ir, pmr, cmr, struct*)

12,18-Heneicosadiene-1,3,8,10,20-pentayne H-121

Callypentayne. *Callyberyne A*

$HC{\equiv}CC{\equiv}C(CH_2)_3C{\equiv}CC{\equiv}CCH{=}CH(CH_2)_3CH{=}CH$
$C{\equiv}CH$

$C_{21}H_{20}$ 272.389

(*Z,Z*)-*form* [185548-30-5]

Isol. from the sponge *Callyspongia truncata* and *Callyspongia* sp. nov. Induces metamorphosis in ascidians. Oil. Uv data of two sets of workers not in agreement. λ_{max} 207 (ϵ 33200); 214 (ϵ 41800); 253 (ϵ 8100); 267 (ϵ 11900); 283 (ϵ 9500) (MeOH) (Berdy). λ_{max} 214 (ϵ 26000); 225 (ϵ 30000); 269 (ϵ 40000); 285 (ϵ 34000) ($CHCl_3$) (Berdy).

3,4-Dihydro (Z-): 3,12,18-Heneicosatriene-1,8,10,20-tetrayne.
Callyberyne B

[185614-74-8]

$C_{21}H_{22}$ 274.405

Isol. from *Callyspongia* sp. nov. Oil. λ_{max} 214 (ϵ 41000); 225 (ϵ 39000); 269 (ϵ 39000); 286 (ϵ 47000) ($CHCl_3$) (Berdy).

Tsukamoto, S. *et al., J. Nat. Prod.*, 1997, **60**, 126-130 (*isol, uv, ir, pmr, cmr*)
Umeyama, A. *et al., J. Nat. Prod.*, 1997, **60**, 131-133 (*isol, uv, pmr, cmr*)
López, S. *et al., J.O.C.*, 2006, **71**, 2802-2810 (*synth*)

3,18-Heneicosadiene-1,8,10,20-tetrayne H-122

Callytetrayne. *Callyberyne C*

$HC{\equiv}CCH{=}CH(CH_2)_6C{\equiv}CC{\equiv}C(CH_2)_3CH{=}CHC{\equiv}CH$

$C_{21}H_{24}$ 276.421

(*Z,Z*)-*form* [185548-29-2]

Isol. from the sponge *Callyspongia truncata* and *Callyspongia* sp. nov. Induces metamorphosis in ascidians. Oil. Uv data of two sets of workers not in agreement. λ_{max} 215 (ϵ 34900); 253 (ϵ 8500); 267 (ϵ 10800); 283 (ϵ 9800) (MeOH) (Berdy). λ_{max} 239 (ϵ 13000); 269 (ϵ 1000); 286 (ϵ 800) ($CHCl_3$) (Berdy).

Tsukamoto, S. *et al., J. Nat. Prod.*, 1997, **60**, 126-130 (*isol, uv, ir, pmr, cmr*)
Umeyama, A. *et al., J. Nat. Prod.*, 1997, **60**, 131-133 (*isol, uv, pmr, cmr*)
López, S. *et al., J.O.C.*, 2006, **71**, 2802-2810 (*synth*)

7,15-Heneicosadienoic acid H-123

$H_3C(CH_2)_4CH{=}CH(CH_2)_6CH{=}CH(CH_2)_5COOH$

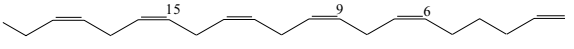
$C_{21}H_{38}O_2$ 322.53

Isol. from the marine bivalve *Megangulus zyonoensis*.

Kawashima, H. *et al., Lipids*, 2004, **39**, 265-271 (*isol*)

1,6,9,12,15,18-Heneicosahexaene, 9CI, 8CI H-124

[65341-44-8]



$C_{21}H_{32}$ 284.484

(all-*Z*)-*form* [33439-58-6]

Isol. from *Fucus vesiculosus* and the brown alga *Notheia anomala*. Also constit. of *Agarum cribrosum*, *Alaria esculenta* and *Bryocladia cuspidata*.

Highly unstable oil. $Bp_{0.05}$ 138°.

6,7:15,16-Diepoxide: 6,7:15,16-Diepoxy-1,9,12,18-heneicosatetraene. 6,7:15,16-Bisepoxy-3,9,12,20-heneicosatetraene (incorr.)

$C_{21}H_{32}O_2$ 316.483

Isol. from *Notheia anomala*. Yellow oil. $[\alpha]_D$ +9.1 (c, 0.3 in $CHCl_3$).

9,10:15,16-Diepoxide: 9,10:15,16-Diepoxy-1,6,12,18-heneicosatetraene. 6,7:12,13-Bisepoxy-3,9,15,20-heneicosatetraene (incorr.)

[138195-56-9]

$C_{21}H_{32}O_2$ 316.483

Isol. from *Notheia anomala*. Oil. $[\alpha]_D$ +15.6 (c, 0.3 in $CHCl_3$).

6,7:12,13:15,16-Triepoxide: 6,7:12,13:15,16-Triepoxy-1,9,18-heneicosatriene. 6,7:9,10:15,16-Trisepoxy-3,12,20-heneicosatriene (incorr.)

[138195-58-1]

$C_{21}H_{32}O_3$ 332.482

From *Notheia anomala*. Yellow oil. $[\alpha]_D$ +12.3 (c, 1.7 in $CHCl_3$).

18,19-Dihydro: 1,6,9,12,15-Heneicosapentaene, 9CI, 8CI

[33439-59-7]

$C_{21}H_{34}$ 286.5

Isol. from *Notheia anomala*, *Fucus vesiculosus* and *Bryocladia cuspidata*. Highly unstable oil.

18,19-Dihydro, 9,10:15,16-diepoxide: 9,10:15,16-Diepoxy-1,6,12-heneicosatriene. 6,7:12,13-Bisepoxy-9,15,20-heneicosatriene (incorr.)

[138213-66-8]

$C_{21}H_{34}O_2$ 318.498

From *Notheia anomala*. Unstable oil. $[\alpha]_D$ +8.6 (c, 0.5 in $CHCl_3$).

*18,19-Dihydro, 12*S*,13*R*:15*S*,16*R*-diepoxide: 12,13:15,16-Diepoxy-1,6,9-heneicosatriene*
[129436-93-7]
$C_{21}H_{34}O_2$ 318.498
Isol. from *Notheia anomala*. Unstable oil. $[\alpha]_D$ +25.6 (c, 0.7 in $CHCl_3$).

18,19-Dihydro, 6ξ,7ξ:9ξ,10ξ:12ξ,13ξ-triepoxide: 6,7:9,10:12,13-Triepoxy-1,15-heneicosadiene
$C_{21}H_{34}O_3$ 334.498
Isol. from brown alga *Notheia anomala*. Mod. stable oil. $[\alpha]_D^{20}$ +35.5 (c, 0.1 in $CHCl_3$). Wrongly numbered in the lit.

18,19-Dihydro, 6,7:12,13:15,16-triepoxide: 6,7:12,13:15,16-Triepoxy-1,9-heneicosadiene. 6,7:9,10:15,16-Trisepoxy-12,20-heneicosadiene (incorr.)
[138195-57-0]
$C_{21}H_{34}O_3$ 334.498
From *Notheia anomala*. Yellow oil. $[\alpha]_D$ +5.9 (c, 2.3 in $CHCl_3$).

18,19-Dihydro, 9ξ,10ξ:12ξ,13ξ:15ξ,16ξ-triepoxide: 9,10:12,13:15,16-Triepoxy-1,6-heneicosadiene
$C_{21}H_{34}O_3$ 334.498
Isol. from brown alga *Notheia anomala*. Mod. stable oil. $[\alpha]_D^{20}$ +33.3 (c, 0.8 in $CHCl_3$). Wrongly numbered in the lit.

[65341-43-7]

Halsall, T.G. *et al., Chem. Comm.*, 1971, 448 (*isol, pmr*)
Caccamese, S. *et al., Experientia*, 1978, **34**, 1129 (*ms*)
Wright, J.L. *et al., Phytochemistry*, 1980, **19**, 143 (*isol, cmr*)
Broekhof, N.L.J.M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1986, **105**, 436 (*synth, ir, pmr*)
Barrow, R.A. *et al., Aust. J. Chem.*, 1990, **43**, 895 (*isol, pmr, ms*)
Murray, L.M. *et al., Aust. J. Chem.*, 1991, **44**, 843
Rochfort, S. *et al., J. Nat. Prod.*, 1992, **55**, 1332-1335 (*6,7:9,10:12,13-triepoxide, 9,10:12,13:15,16-triepoxide*)
Holmeide, A.K. *et al., J.C.S. Perkin 1*, 2001, 1942-1946 (*synth*)

3,6,9,12,15,18-Heneicosahexaene H-125

[127702-72-1]
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH_3$
$C_{21}H_{32}$ 284.484

(all-*E*)-*form* [32779-95-6]
Isol. from *Emerita analoga* and *Macrocystis pyrifera*.

(all-*Z*)-*form* [29118-86-3]
Isol. from marine algae and plankton. Ir ν 3020, 715 (C=C) cm^{-1}.

[32779-95-6]

Lee, R.F. *et al., Biochim. Biophys. Acta*, 1970, **202**, 386 (*isol, struct, ms*)
Blumer, M. *et al., Mar. Biol. (Berlin)*, 1970, **6**, 226 (*isol, struct, uv, ir, ms*)
Wright, J.L.C. *et al., Phytochemistry*, 1980, **19**, 143 (*cmr*)

1,21-Heneicosanediol H-126

$HOH_2C(CH_2)_{19}CH_2OH$
$C_{21}H_{44}O_2$ 328.577
Constit. of apple and carnauba waxes. Also from *Pancratium* sp. Component of carnauba wax used in floor polishes etc. Cryst. (EtOH).
Mp 105-105.5°. $Bp_{1.5}$ 223-224°.

Di-O-*sulfate:* [189822-33-1]
$C_{21}H_{44}O_8S_2$ 488.706
Isol. from the tunicate *Ascidia mentula* (as di-Na salt). Antiproliferative agent.

Di-Ac:
$C_{25}H_{48}O_4$ 412.652
Cryst. (petrol). Mp 60°.

4-Hydroxy-E-*cinnamoyl: 21-Hydroxyheneicosyl* trans-p-*coumarate*
$C_{30}H_{50}O_4$ 474.723
Constit. of the roots of *Tanacetum longifolium*. Amorph. powder.

Chuit, P. *et al., Helv. Chim. Acta*, 1929, **12**, 850 (*synth*)
Lukes, R. *et al., Coll. Czech. Chem. Comm.*, 1961, **26**, 1719 (*synth*)
Mazliak, P. *et al., Phytochemistry*, 1962, **1**, 79 (*occur*)
Ahmed, Z.F. *et al., J. Nat. Prod.*, 1964, **27**, 115 (*occur*)
Aiello, A. *et al., Tetrahedron*, 1997, **53**, 5877 (*isol, sulfate*)
Mahmood, U. *et al., Phytochemistry*, 2003, **64**, 851-853 (*trans-p-coumarate*)

3,6,9,12,15-Heneicosapentaene H-127

[66887-59-0]
$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH_3$
$C_{21}H_{34}$ 286.5
Found in sand crabs (*Emerita analoga*) and the kelp (*Macrocystis pyrifera*).

(all-*Z*)-*form* [33426-22-1]
Constit. of *Polytrichum commune* and benthic green algae.

Youngblood, W.W. *et al., Mar. Biol. (Berlin)*, 1971, **8**, 190 (*isol*)
Karunen, P. *et al., Phytochemistry*, 1974, **13**, 2209 (*isol*)
Rossi, S.S. *et al., CA*, 1979, **91**, 2755c (*occur*)

3-Heneicosene-1,8,20-triyne H-128

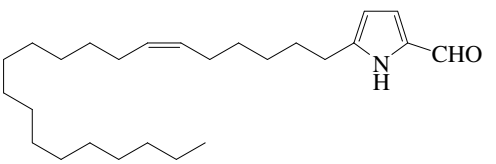
Aikupikanyne B
$HC{\equiv}C(CH_2)_{10}C{\equiv}C(CH_2)_3CH{=}CHC{\equiv}CH$
$C_{21}H_{30}$ 282.468

(*Z*)-*form*
Isol. from a *Callyspongia* sp.
Oil.

Youssef, D.T.A. *et al., J. Nat. Prod.*, 2000, **63**, 1406-1410,

5-(6-Heneicosenyl)-1*H*-pyrrole-2-carboxaldehyde, 9CI H-129

*2-Formyl-5-(6-heneicosenyl)-1*H*-pyrrole*



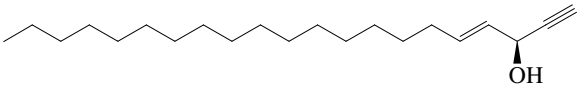
$C_{26}H_{45}NO$ 387.648

(*Z*)-*form* [262351-88-2]
Isol. from *Mycale mytilorum*.
Pale yellow flakes.
Mp 40-43°. λ_{max} 302 (ε 16000) (EtOH).

Reddy, G.B.S. *et al., Bioorg. Med. Chem.*, 2000, **8**, 27-36 (*Z-form, ir, ms, pmr, cmr*)

4-Heneicosen-1-yn-3-ol H-130

[146333-91-7]



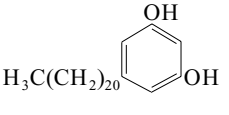
$C_{21}H_{38}O$ 306.531

(3*S*,4*E*)-*form* [173938-19-7]
Isol. from the sponge *Cribrochalina vasculum*.
Solid. $[\alpha]_D$ +11 (c, 0.21 in MeOH).

Hallock, Y.F. *et al., J. Nat. Prod.*, 1995, **58**, 1801-1807 (*isol, pmr, cmr, ms, config*)

5-Heneicosyl-1,3-benzenediol H-131

5-Heneicosylresorcinol
[70110-59-7]



$C_{27}H_{48}O_2$ 404.675

Constit. of wheat and other cereal grains. Also formed in encysting *Azotobacter vinelandii*. Cryst. (hexane).
Mp 99.5-100.5°.

Di-Ac:
Cryst. (EtOH). Mp 72.5-73°.

Di-Me ether: 1-Heneicosyl-3,5-dimethoxybenzene
Cryst. (EtOAc). Mp 63.5-64.5°.

*3,4,6,7,9,10,12,13,15,16,18,19-Dodecakisdehydro(*all-Z*):* ***5-(3,6,9,12,15,18-Heneicosahexaenyl)-1,3-benzenediol***
[138168-61-3]
Isol. from sponge *Haliclona* sp.
Oil. Darkens in air.

12′,13′-Didehydro(Z-): 5-(12-Heneicosenyl)-1,3-benzenediol. 5-(12-Heneicosenyl)resorcinol
[189562-00-3]
$C_{27}H_{46}O_2$ 402.659
Constit. of wheat and rye flour.

14′,15′-Didehydro(Z-): 5-(14-Heneicosenyl)-1,3-benzenediol. 5-(14-Heneicosenyl)resorcinol
$C_{27}H_{46}O_2$ 402.659
Constit. of wheat and rye flour.

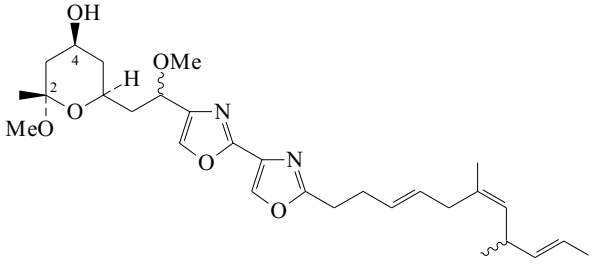
16′,17′-Didehydro(Z-): 5-(16-Heneicosenyl)-1,3-benzenediol. 5-(16-Heneicosenyl)resorcinol
[189562-08-1]
$C_{27}H_{46}O_2$ 402.659
Constit. of wheat and rye flour.

12′,13′,15′,16′-Tetradehydro(Z,Z-): 5-(12,15-Heneicosadienyl)-1,3-benzenediol. 5-(12,15-Heneicosadienyl)resorcinol
[189562-03-6]
$C_{27}H_{44}O_2$ 400.643
Constit. of wheat and rye flour.

Wenkert, E. *et al., J.O.C.*, 1964, **29**, 435 (*anal, synth*)
Reusch, R.N. *et al., J. Bacteriol.*, 1979, **139**, 448; 1981, **145**, 889 (*isol*)
Gohil, S. *et al., J. Sci. Food Agric.*, 1988, **45**, 43 (*isol*)
Barrow, R.A. *et al., Aust. J. Chem.*, 1991, **44**, 1393 (*deriv*)
Suzuki, Y. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 480-486 (*isol, ms*)
Ross, A.B. *et al., J. Agric. Food Chem.*, 2003, **51**, 4111-4118 (*occur*)

Hennoxazole A H-132

[132564-95-5]



$C_{29}H_{42}N_2O_6$ 514.661
Alkaloid from the marine sponge *Polyfibrospongia* sp. Possesses antiviral and peripheral analgesic activities. Light yellow oil. $[\alpha]_D^{25}$ -47 (c, 3.12 in $CHCl_3$) (-42.7). λ_{max} 254 (ϵ 12000) (MeOH) (Derep).

4-Ac: ***4-O-Acetylhennoxazole A***
$C_{31}H_{44}N_2O_7$ 556.698
Alkaloid from a *Polyfibrospongia* sp. CAS no. not found 13-14CI.

O^2*-De-Me:* ***Hennoxazole E***
$C_{28}H_{40}N_2O_6$ 500.634
Alkaloid from *Polyfibrospongia* sp. CAS no. not found 13-14CI.

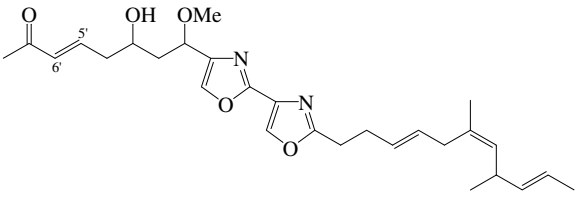
O^2*-De-Me,* O^2*-Et:* ***Hennoxazole B***
[132564-96-6]
$C_{30}H_{44}N_2O_6$ 528.687
Alkaloid from *Polyfibrospongia* sp. Analgesic. λ_{max} 254 (ϵ 12000) (MeOH) (Derep).

O^2*-De-Me,* O^2*-butyl:* ***Hennoxazole C***
[132564-97-7]
$C_{32}H_{48}N_2O_6$ 556.741
Alkaloid from *Polyfibrospongia* sp. λ_{max} 254 (ϵ 12000) (MeOH) (Derep).

4-Deoxy: ***Hennoxazole D***
[132564-98-8]
$C_{29}H_{42}N_2O_5$ 498.661
From *Polyfibrospongia* sp. Light yellow oil. λ_{max} 254 (ϵ 12000) (MeOH) (Derep).

Ichiba, T. *et al., J.A.C.S.*, 1991, **113**, 3173-3174 (*isol, struct*)
Higa, T. *et al., Pure Appl. Chem.*, 1994, **66**, 2227-2230 (*4-Acetylhennoxazole A, Hennoxazole E*)
Williams, D.R. *et al., J.A.C.S.*, 1999, **121**, 4924-4925 (*synth*)
Yokokawa, F. *et al., Tetrahedron*, 2001, **57**, 6311-6327 (*synth, ir, pmr, cmr, ms*)

Hennoxazole F H-133

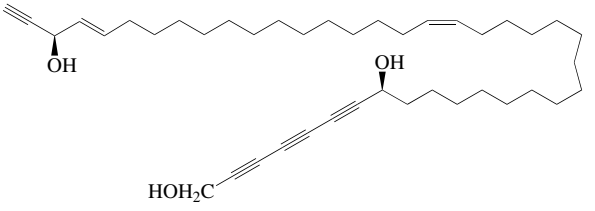


$C_{28}H_{38}N_2O_5$ 482.619
Alkaloid from the sponge *Polyfibrospongia* sp. Not in CA.

5′,6′-Dihydro, 5′-hydroxy: ***Hennoxazole G***
$C_{28}H_{40}N_2O_6$ 500.634
Alkaloid from *Polyfibrospongia* sp.

Higa, T. *et al., Pure Appl. Chem.*, 1994, **66**, 2227-2230

23,37-Hentetracontadiene-2,4,6,40-tetrayne-1,8,39-triol H-134



$C_{41}H_{64}O_3$ 604.955

(8R*,23Z,37E,39S*)-form
Triangulyne D
[182314-10-9]
Isol. from the sponge *Pellina triangulata*. Cytotoxic agent. Oil. $[\alpha]_D$ -10.7 (c, 0.01 in $CHCl_3$). Prob. has (8*S*,39*R*)-config. as shown. λ_{max} 203 (log ϵ 3.6); 230 (log ϵ 3.1); 256 (log ϵ 2.8) (MeOH). λ_{max} 203 (ϵ 3980); 230 (ϵ 1260); 256 (ϵ 630) (MeOH) (Berdy).

Dai, J.-R. *et al., J. Nat. Prod.*, 1996, **59**, 860-865 (*isol, uv, ir, pmr, cmr, ms*)

1,22-Hentriacontadiene H-135

[28914-20-7]
$H_3C(CH_2)_7CH{=}CH(CH_2)_{19}CH{=}CH_2$
$C_{31}H_{60}$ 432.815

(E)-form [188828-93-5]
Isol. from the green alga *Botryococcus braunii*.

(Z)-form [104899-42-5]
Isol. from *Botryococcus braunii*, *Emiliania huxleyi* and *Isochrysis galbana*.

Metzger, P. *et al., Phytochemistry*, 1986, **25**, 1869-1872; 1997, **44**, 1071-1075 (*isol*)
Rieley, G. *et al., Lipids*, 1998, **33**, 617-625 (*isol*)

1,24-Hentriacontadiene H-136

$H_3C(CH_2)_5CH{=}CH(CH_2)_{21}CH{=}CH_2$

$C_{31}H_{60}$ 432.815

(Z)-form [211238-14-1]

Isol. from the haplophyte *Isochrysis galbana*.

Rieley, G. *et al., Lipids*, 1998, **33**, 617-625 (*isol*)

2,22-Hentriacontadiene H-137

$H_3C(CH_2)_7CH{=}CH(CH_2)_{18}CH{=}CHCH_3$

$C_{31}H_{60}$ 432.815

(Z,Z)-form [211238-02-7]

Isol. from the haplophyte *Emiliania huxleyi*.

Rieley, G. *et al., Lipids*, 1998, **33**, 617-625 (*isol*)

2,24-Hentriacontadiene H-138

$H_3C(CH_2)_5CH{=}CH(CH_2)_{20}CH{=}CHCH_3$

$C_{31}H_{60}$ 432.815

(Z,Z)-form [211238-20-9]

Isol. from the haplophyte *Emiliania huxleyi*.

Rieley, G. *et al., Lipids*, 1998, **33**, 617-625 (*isol*)

3,22-Hentriacontadiene H-139

$H_3C(CH_2)_7CH{=}CH(CH_2)_{17}CH{=}CHCH_2CH_3$

$C_{31}H_{60}$ 432.815

(Z,Z)-form [211238-09-4]

Isol. from the haplophyte *Emiliania huxleyi*.

Rieley, G. *et al., Lipids*, 1998, **33**, 617-625 (*isol*)

4,28-Hentriacontadiene-2,30-diynoic acid H-140

Petroformynic acid

$HC{\equiv}CCH{=}CH(CH_2)_{22}CH{=}CHC{\equiv}CCOOH$

$C_{31}H_{50}O_2$ 454.735

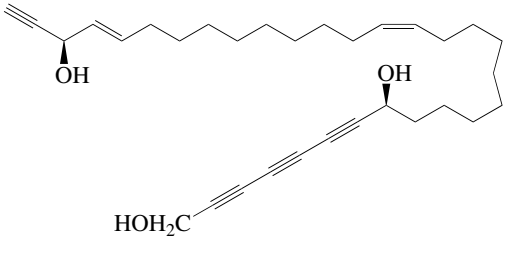
(Z,Z)-form

Isol. from the sponge *Petrosia ficiformis*.

Oil. λ_{max} 230 (ϵ 19200) (MeOH). λ_{max} 230 (ϵ 19200) (MeOH) (Berdy).

Guo, Y. *et al., J. Nat. Prod.*, 1998, **61**, 333-337 (*isol, uv, pmr, cmr*)

17,27-Hentriacontadiene-2,4,6,30-tetrayne-1,8,29-triol H-141



$C_{31}H_{44}O_3$ 464.687

Probable stereochem. shown.

(8S,17Z,27E,29R)-form

Triangulyne C

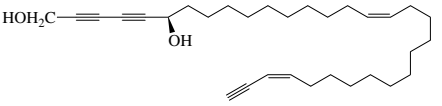
[182314-05-2]

Isol. from the sponge *Pellina triangulata*. Cytotoxic agent. Powder. $[\alpha]_D$ -19 (c, 0.7 in $CHCl_3$). λ_{max} 204 (log ϵ 3.4); 231 (log ϵ 2.8); 243 (log ϵ 2.7); 257 (log ϵ 2.5) (MeOH). λ_{max} 204 (ϵ 2510); 231 (ϵ 630); 243 (ϵ 500); 257 (ϵ 316) (MeOH) (Berdy).

Dai, J.-R. *et al., J. Nat. Prod.*, 1996, **59**, 860-865 (*isol, uv, ir, pmr, cmr, ms*)

16,28-Hentriacontadiene-2,4,30-triyne-1,6-diol H-142

Strongylodiol E



(6*R*,16*Z*,28*Z*)-*form*

$C_{31}H_{48}O_2$ 452.719

(6R,16Z,28Z)-form [334973-94-3]

Isol. from *Strongylophora* sp.

Amorph. solid. $[\alpha]_D^{25}$ -1.8 (c, 0.5 in $CHCl_3$). Obt. as a partial racemate (22% o.p.). λ_{max} 223 (log ϵ 3.95); 257 (log ϵ 2.63) (EtOH).

16,17-Didehydro: 28-Hentriacontene-2,4,16,30-tetrayne-1,6-diol.

Strongylodiol F

[334904-87-9 (6*S*-form), 334973-95-4 (6*R*-form)]

$C_{31}H_{46}O_2$ 450.703

Isol. from a *Strongylophora* sp. Amorph. solid. $[\alpha]_D^{25}$ -5.3 (c, 0.36 in $CHCl_3$). Partial racemate (60% o.p.). λ_{max} 221 (log ϵ 4); 256 (log ϵ 2.88) (EtOH).

[334904-86-8 (*S,Z,Z*-form)]

Watanabe, K. *et al., CA*, 2000, **134**, 308117e (*Strongylodiol F*)

Watanabe, K. *et al., J. Nat. Prod.*, 2005, **68**, 1001-1005 (*Strongylodiol E*)

Hentriacontanoic acid, 9CI H-143

Melissic acid B

[38232-01-8]

$H_3C(CH_2)_{29}COOH$

$C_{31}H_{62}O_2$ 466.83

Has been confused with Triacontanoic acid owing to analytical misidentification. Isol. from leaf wax of *Agave sisalana* and other plants. Cryst. (Me_2CO).

Mp 93-93.2°.

Pentyl ester: Pentyl hentriacontanoate

$C_{36}H_{72}O_2$ 536.964

Isol. from the red alga *Chondria armata*.

Mp 60-62°.

Nonacosyl ester: Nonacosyl hentriacontanoate

$C_{60}H_{120}O_2$ 873.607

Constit. of *Swertia chirata*. Cryst.

Mp 75-77°.

[77630-51-4]

Piper, S.H. *et al., Biochem. J.*, 1934, **28**, 2175 (*synth*)

Razafindrazaka, J. *et al., Bull. Soc. Chim. Fr.*, 1963, 1633 (*isol*)

Rao, S.J. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 208 (*synth*)

Govenkar, M.B. *et al., Phytochemistry*, 2000, **54**, 979-981 (*pentyl ester*)

Pant, N. *et al., Indian J. Chem., Sect. B*, 2002, **41**, 1980-1986 (*nonacosyl ester*)

1,22,24-Hentriacontatriene H-144

$H_3C(CH_2)_5CH{=}CHCH{=}CH(CH_2)_{19}CH{=}CH_2$

$C_{31}H_{58}$ 430.799

(22Z,24Z)-form

Isol. from the green alga *Botryococcus braunii*.

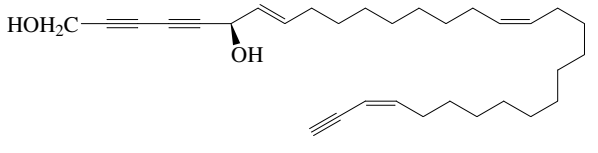
(22ξ,24ξ)-form

Isol. from *Botryococcus braunii*. An (*E,Z*)-isomer.

Metzger, P. *et al., Phytochemistry*, 1997, **44**, 1071-1075 (*isol, pmr, cmr*)

7,16,28-Hentriacontatriene-2,4,30-triyne-1,6-diol H-145

Strongylodiol J



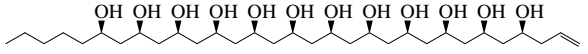
$C_{31}H_{46}O_2$ 450.703

(6*R*,7*E*,16*Z*,28*Z*)-*form*
Isol. from the sponge *Strongylophora* sp.
Oil. $[\alpha]_D^{22}$ -32.6 (c, 0.44 in $CHCl_3$). Obt. as a partial racemate (96% op). λ_{max} 208 (log ϵ 3.79) (MeOH).
Watanabe, K. *et al., J. Nat. Prod.*, 2005, **68**, 1001-1005 (*isol, pmr, cmr*)

5,9,24-Hentriacontatrienoic acid **H-146**
$H_3C(CH_2)_5CH{=}CH(CH_2)_{13}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{31}H_{56}O_2$ 460.782

(*all-Z*)-*form* [187657-40-5]
Isol. from the sponge *Haliclona cinerea*.
Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*isol, ms*)

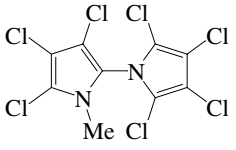
1-Hentriacontene-4,6,8,10,12,14,16,18,20,22,24,26-dodecol **H-147**



$C_{31}H_{62}O_{12}$ 626.824

(4*S*,6*S*,8*S*,10*S*,12*S*,14*S*,16*R*,18*R*,20*R*,22*R*,24*R*,26*R*)-*form*
Dodeca-Me ether: 4,6,8,10,12,14,16,18,20,22,24,26-Dodecamethoxy-1-hentriacontene
[265649-29-4]
$C_{43}H_{86}O_{12}$ 795.145
Isol. from the cyanobacterium *Aphanizomenon ovalisporum*.
Banker, R. *et al., J. Nat. Prod.*, 2000, **63**, 387-389

2,3,3′,4,4′,5,5′-Heptachloro-1′-methyl-1,2′-bi-1*H*-pyrrole **H-148**
Q1



$C_9H_3Cl_7N_2$ 387.305
Widespread in natural sources. Distribution pattern resembles that of environmental contaminants, e.g. PCBs, but appears to be a genuine nat. prod. Cryst.
Mp 154-155.5°. Readily oxidises and polymerises.
Wu, J. *et al., Angew. Chem., Int. Ed.*, 2002, **41**, 1740-1743 (*synth, cryst struct*)
Vetter, W. *et al., Chemosphere*, 2003, **52**, 415-422 (*isol, pmr, cmr*)
Vetter, W. *et al., Rapid Commun. Mass Spectrom.*, 2006, **20**, 3018-3022 (*cmr, occur*)
Vetter, W. *et al., Rev. Environ. Contam. Toxicol.*, 2006, **188**, 1-57 (*rev, occur*)

1,18-Heptacosadiene **H-149**
$H_3C(CH_2)_7CH{=}CH(CH_2)_{15}CH{=}CH_2$
$C_{27}H_{52}$ 376.708

(*E*)-*form* [104899-45-8]
Isol. from the green alga *Botryococcus braunii*.

(*Z*)-*form* [104899-40-3]
Isol. from *Botryococcus braunii*.
Metzger, P. *et al., Phytochemistry*, 1986, **25**, 1869; 1993, **33**, 1125 (*isol, pmr, cmr*)

5,9-Heptacosadienoic acid **H-150**
[155093-08-6]
$H_3C(CH_2)_{16}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{27}H_{50}O_2$ 406.691

(*Z,Z*)-*form* [129596-73-2]
Constit. of various sponges incl. *Dysidea fragilis*, *Hymeniacidon sanguinea* and *Trikentrion loeve*.
Zimmermann, M.P. *et al., Lipids*, 1989, **24**, 210-216 (*isol*)
Christie, W.W. *et al., Lipids*, 1992, **27**, 640-644 (*isol*)
Christie, W.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1994, **109**, 245-252 (*isol*)

1,3,5,18-Heptacosatetraene **H-151**
$H_3C(CH_2)_7CH{=}CH(CH_2)_{11}CH{=}CHCH{=}CHCH{=}CH_2$
$C_{27}H_{48}$ 372.676

(*all-E*)-*form* [151298-51-0]
Isol. from the green alga *Botryococcus braunii*.

(3*E*,5*E*,18*Z*)-*form* [151298-49-6]
Isol. from *Botryococcus braunii*.
[151298-48-5, 151298-50-9]
Metzger, P. *et al., Phytochemistry*, 1993, **33**, 1125 (*isol, pmr, cmr*)

1,3,18-Heptacosatriene **H-152**
$H_3C(CH_2)_7CH{=}CH(CH_2)_{13}CH{=}CHCH{=}CH_2$
$C_{27}H_{50}$ 374.692

(3*E*,18*E*)-*form* [151298-47-4]
Isol. from the green alga *Botryococcus braunii*.

(3*E*,18*Z*)-*form* [151298-45-2]
Isol. from *Botryococcus braunii*.

(3*Z*,18*E*)-*form* [151298-46-3]
Isol. from *Botryococcus braunii*.

(3*Z*,18*Z*)-*form* [151298-44-1]
Isol. from *Botryococcus braunii*.
Metzger, P. *et al., Phytochemistry*, 1993, **33**, 1125 (*isol, pmr, cmr*)

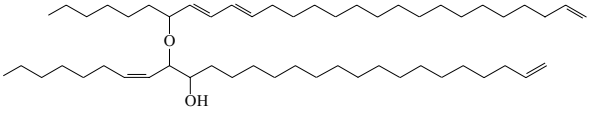
1,18,20-Heptacosatriene **H-153**
$H_3C(CH_2)_5CH{=}CHCH{=}CH(CH_2)_{15}CH{=}CH_2$
$C_{27}H_{50}$ 374.692

(*Z,Z*)-*form* [144223-42-7]
Prod. by *Botryococcus braunii*.
Villarreal-Rosales, E. *et al., Phytochemistry*, 1992, **31**, 3021 (*isol, pmr, cmr*)

5,9,20-Heptacosatrienoic acid **H-154**
[59708-92-8]
$H_3C(CH_2)_5CH{=}CH(CH_2)_9CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{27}H_{48}O_2$ 404.675
Isol. from the sponges *Microciona prolifera* and *Halichondria panicea*.

(*all-Z*)-*form* [152336-67-9]
Isol. from the sponges *Baicalospongia bacillifera*, *Baicalospongia intermedia* and *Lubomirskia baicalensis*.
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206-216 (*isol*)
Dembitsky, V.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1993, **106**, 825-831; 1994, **109**, 415-426 (*isol*)

9-[(8,10,26-Heptacosatrien-7-yl)oxy]-7,26-heptacosadien-10-ol **H-155**
9-[(1-Hexyl-2,4,20-heneicosatrienyl)oxy]-7,26-heptacosadien-10-ol, 9CI
[135631-43-5]



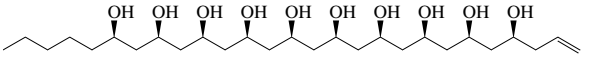
$C_{54}H_{100}O_2$ 781.383

(7Z,8′E,10′E)-form
Constit. of *Botryococcus braunii*.
Metzger, P. *et al., Phytochemistry*, 1991, **30**, 1439-1444 (*isol, pmr, cmr, ms*)
Villareal-Rosales, E. *et al., Phytochemistry*, 1992, **31**, 3021-3027 (*isol*)

1-Heptacosene H-156

[15306-27-1]
$H_3C(CH_2)_{24}CH{=}CH_2$
$C_{27}H_{54}$ 378.724
Isol. from the green alga *Botryococcus braunii*, the labial glands of the bee *Chalicodoma sicula*, *Hippophae rhamnosides* and *Quercus robor* oils. Low-melting solid.
Iyer, R. *et al., J. Indian Chem. Soc.*, 1985, **62**, 887-890 (*synth*)
Metzger, P. *et al., Phytochemistry*, 1997, **44**, 1071 (*isol*)

1-Heptacosene-4,6,8,10,12,14,16,18,20,22-decol H-157



$C_{27}H_{54}O_{10}$ 538.718

(4S,6S,8S,10S,12S,14R,16R,18R,20R,22R)-form
Deca-Me ether: 4,6,8,10,12,14,16,18,20,22-Decamethoxy-1-heptacosene
[131487-90-6]
[72620-12-3]
$C_{37}H_{74}O_{10}$ 678.986
Isol. from *Tolypothrix conglutinata* var. *chlorata*.
Mynderse, J.S. *et al., Phytochemistry*, 1979, **18**, 1181-1183 (*isol*)
Mori, Y. *et al., J.O.C.*, 1991, **56**, 631-637 (*synth*)

26-Heptacosene-9,10-diol H-158

$H_2C{=}CH(CH_2)_{15}CH(OH)CH(OH)(CH_2)_7CH_3$
$C_{27}H_{54}O_2$ 410.722
9-(9-Octadecenoyl)(Z-): [168981-88-2]
$C_{45}H_{86}O_3$ 675.173
Constit. of *Botryococcus braunii*.
Metzger, P. *et al., Phytochemistry*, 1995, **40**, 543-554 (*isol, pmr, cmr, ms*)

20-Heptacosenoic acid H-159

$H_3C(CH_2)_5CH{=}CH(CH_2)_{18}COOH$
$C_{27}H_{52}O_2$ 408.707

(Z)-form [140197-98-4]
Constit. of the sponge *Amphimedon compressa*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1992, **55**, 333

14,16-Heptadecadiene-2,4-diyn-1-ol H-160

$H_2C{=}CHCH{=}CH(CH_2)_8C{\equiv}CC{\equiv}CCH_2OH$
$C_{17}H_{24}O$ 244.376

(Z)-form [156632-31-4]
Isol. from the eggs of the coral *Montipora digitata*.
Coll, J.C. *et al., Mar. Biol. (Berlin)*, 1994, **118**, 177-182 (*isol*)

3,16-Heptadecadiene-5,7-diyn-2-one H-161

$H_2C{=}CH(CH_2)_7C{\equiv}CC{\equiv}CCH{=}CHCOCH_3$
$C_{17}H_{22}O$ 242.36

(E)-form
Montiporyne C
Isol. from the stony coral *Montipora* sp. Cytotoxic agent. Yellow oil.

(Z)-form
Montiporyne D
Isol. from *Montipora* sp.
Pale yellow oil.
Bae, B.H. *et al., J. Nat. Prod.*, 2000, **63**, 1511-1514 (*isol*)
Fiandanese, V. *et al., Tetrahedron*, 2006, **62**, 5126-5132 (*synth*)

6,9-Heptadecadienoic acid H-162

$H_3C(CH_2)_6CH{=}CHCH_2CH{=}CH(CH_2)_4COOH$
$C_{17}H_{30}O_2$ 266.423

(Z,Z)-form [122576-58-3]
Isol. from the gorgonian *Leptogorgia piccola*.
Miralles, J. *et al., Lipids*, 1995, **30**, 459 (*isol, struct*)

2,4-Heptadecanedione, 9CI H-163

Tetradecanoylacetone. Myristoylacetone
[64042-18-8]
$H_3C(CH_2)_{12}COCH_2COCH_3$
$C_{17}H_{32}O_2$ 268.439
Acetogenin. Constit. of *Ruta graveolens* (rue) and the brown alga *Caulocystis cephalornithos*. Also found in various mammalian tissues. Oil.
Mp 42.5° (39°).
Morgan, G.T. *et al., J.C.S.*, 1925, **127**, 2891 (*synth*)
Douglas, D.E. *et al., Lipids*, 1977, **12**, 635 (*synth*)
Douglas, D.E. *et al., Can. J. Biochem.*, 1978, **56**, 691 (*occur*)
Tattje, D.H.E. *et al., Pharm. Weekbl.*, 1978, **113**, 1169 (*isol*)
Amico, V. *et al., J. Nat. Prod.*, 1990, **53**, 1379 (*isol*)

Heptadecanoic acid H-164

Margaric acid. Daturinic acid
[506-12-7]
$H_3C(CH_2)_{15}COOH$
$C_{17}H_{34}O_2$ 270.454
Constit. of *Erythrina crista-galli* trunkwood and bark. Common constit. of lipids, e.g. present in *Physalia physalis* (Portuguese-man-of-war). Used (with Stigmast-5-ene-3,7,20-triol) for amino acid sequencing in peptides. Cryst. (petrol).
Mp 62-63°.
▶ LD_{50} (mus, ivn) 36 mg/kg. MI3850000
Me ester: [1731-92-6]
$C_{18}H_{36}O_2$ 284.481
Cryst. (EtOH). Mp 30°. Bp_9 184-187°.
Et ester: [14010-23-2]
$C_{19}H_{38}O_2$ 298.508
Cryst. (EtOH aq.). Mp 28°. Bp_5 185°.
Chloride: [40480-10-2]
$C_{17}H_{33}ClO$ 288.9
d 0.88. Bp_4 176°. n_D^{20} 1.4530.
Amide: [25844-13-7]
$C_{17}H_{35}NO$ 269.47
Cryst. (EtOH). Mp 108°.
Nitrile: [5399-02-0]
$C_{17}H_{33}N$ 251.454
Cryst. (EtOH). Mp 34°. Bp_{10} 185°.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 485B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 757A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 577C; 630C (*ir*)
Fierz-David, H.E. *et al., Helv. Chim. Acta*, 1939, **22**, 82 (*chloride*)
Bricas, E. *et al., Biochemistry*, 1965, **4**, 2254 (*use*)
Buchta, E. *et al., Annalen*, 1966, **698**, 93 (*synth*)
Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*Physalia physalis constit*)
Imamura, H. *et al., Gifu Daigaku Nogakubu Kenkyu Hokoku*, 1981, 77; *CA*, **96**, 196524y (*occur*)
Bengsch, E. *et al., J. Magn. Reson.*, 1986, **68**, 1 (*cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HAS500

1-Heptadecanol H-165

Heptadecyl alcohol
[1454-85-9]
$H_3C(CH_2)_{15}CH_2OH$
$C_{17}H_{36}O$ 256.471
Cryst. (Me_2CO). Mp 54°. Bp 308°.

▶ Fl. p. 154° (oc).

O-*Sulfate:* [15416-78-1]
[5910-79-2 (Na salt)]
$C_{17}H_{36}O_4S$ 336.535
Isol. from the tunicate *Sidnyum turbinatum*. Amorph. solid (as Na salt).

Tridecanoyl: Heptadecyl tridecanoate
$C_{30}H_{60}O_2$ 452.803
Constit. of *Sesbania bispinosa*.

4-Nitrobenzyl: Mp 54°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 113B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 168B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 159C (*ir*)
Watanabe, A. *et al., Bull. Chem. Soc. Jpn.*, 1954, **32**, 1295 (*synth*)
Aiello, A. *et al., J. Nat. Prod.*, 2001, **64**, 219-221 (*sulfate, isol*)
Misra, L. *et al., Indian J. Chem., Sect. B*, 2005, **44**, 1915-1921 (*tridecanoyl*)

2-Heptadecanone H-166

[2922-51-2]
$H_3C(CH_2)_{14}COCH_3$
$C_{17}H_{34}O$ 254.455
Constit of the sponge *Spheciospongia vagabunda* and constit. of aroma compounds of white bread and ovine adipose tissue. Cryst. Mp 48°. Bp 319-320° Bp_{110} 246°.

Keskin, H. *et al., CA*, 1946, **40**, 1822^7 (*synth*)
Bente, P.F. *et al., J. Phys. Chem.*, 1975, **79**, 713-721 (*synth, ms*)
Caporaso, F. *et al., J. Agric. Food Chem.*, 1977, **25**, 1230-1234 (*ovine constit*)
Obretenov, T. *et al., Z. Lebensm.-Unters. -Forsch.*, 1977, **165**, 195-199 (*bread constits, glc, ms*)
Xiao, D. *et al., Fenxi Huaxue*, 2004, **32**, 1621-1623; *CA*, **143**, 23210 (*Spheciospongia vagabunda constit*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 828

8,11,14-Heptadecatrienal H-167

[112209-66-2]
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_6CHO$
$C_{17}H_{28}O$ 248.408

(*all-Z*)-*form* [56797-44-5]
Constit. of cucumber, tobacco and wheat. Also found in the algae *Enteromorpha* sp., *Scytosiphon lomentaria* and *Ulva pertusa*.

14,15-Dihydro: 8,11-Heptadecadienal
[56797-42-3]
$C_{17}H_{30}O$ 250.423
Constit. of cucumber and tobacco. Also from *Enteromorpha* sp., *Porphyra tenera*, *Scytosiphon lomentaria* and *Ulva pertusa*.

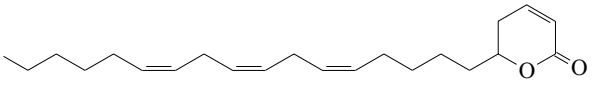
11,12,14,15-Tetrahydro: 8-Heptadecenal, 9CI
[56797-41-2]
$C_{17}H_{32}O$ 252.439
Constit. of cucumber and tobacco. Also from *Enteromorpha* sp., *Porphyra tenera*, *Scytosiphon lomentaria*, *Ulva pertusa* and *Cercospora arachidicola*. Oil.

[1191-86-2, 96360-10-0, 123350-64-1]

Kemp, T.R. *et al., J. Am. Oil Chem. Soc.*, 1975, **52**, 300-302 (*occur*)
Takagi, Y. *et al., Agric. Biol. Chem.*, 1981, **45**, 769
Stoessl, A. *et al., Can. J. Microbiol.*, 1985, **31**, 129 (*isol*)
Hamilton-Kemp, T.R. *et al., Phytochemistry*, 1986, **25**, 241 (*isol*)
Kajiwara, T. *et al., Phytochemistry*, 1989, **28**, 407; 1990, **29**, 745; 2193; 1991, **30**, 1805 (*isol*)
Poigny, S. *et al., J.C.S. Perkin 1*, 1997, 2175-2177 (*tetrahydro, synth, ir, pmr, cmr*)
Akakabe, Y. *et al., Biosci., Biotechnol., Biochem.*, 2005, **69**, 1348-1352 (*synth, pmr, cmr*)

6-(5,8,11-Heptadecatrienyl)-5,6-dihydro-2*H*-pyran-2-one, 9CI H-168

2,10,13,16-Docosatetraen-5-olide



$C_{22}H_{34}O_2$ 330.509

(*all-Z*)-*form* [81575-28-2]
Obt. from the red alga *Phacelocarpus labillardieri*.
Oil. $[\alpha]_D^{25}$ -51 (c, 0.7 in $CHCl_3$).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 113 (*ms, pmr, cmr*)

6-Heptadecene H-169

[103963-44-6]
[61140-71-4 (*E*-form)]
$H_3C(CH_2)_9CH{=}CH(CH_2)_4CH_3$
$C_{17}H_{34}$ 238.456

(*Z*)-*form* [74533-98-5]
Constit. of gizzard shad *Clupanodon punctatus* and sardine *Sardinops melanosticta*.

Sojak, L. *et al., J. Chromatogr., A*, 1980, **195**, 43-64 (*glc*)
Hoshita, N. *et al., Lipids*, 1982, **17**, 390-392 (*Z-form, isol, synth*)

7-Heptadecene H-170

[54290-12-9]
$H_3C(CH_2)_8CH{=}CH(CH_2)_5CH_3$
$C_{17}H_{34}$ 238.456
No phys. props. reported.

(*Z*)-*form* [65118-45-8]
Constit. of *Cladophora densa*, *Ulva pertusa* and gonads of sea urchins *Temnopleurus toreumaticus*, *Anthocidaris crassispina* and *Enteromorpha prolifera*.

(ξ)-*form*
Constit. of Argentine ant *Iridomyrmex humilis.*

[91454-74-9 (*E*-form)]

Cavill, G.W.K. *et al., J. Insect Physiol.*, 1974, **20**, 2049-2059 (*occur*)
Okano, M. *et al., Nippon Suisan Gakkaishi*, 1979, **45**, 389-393; 1982, **48**, 1485-1490 (*Z-form, occur*)
Sojak, L. *et al., J. Chromatogr., A*, 1980, **195**, 43-64 (*glc*)

14-Heptadecene-4,16-diynoic acid H-171

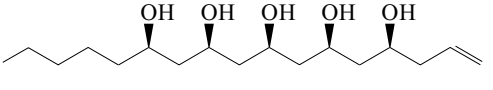
$HC{\equiv}CCH{=}CH(CH_2)_8C{\equiv}CCH_2CH_2COOH$
$C_{17}H_{24}O_2$

(*Z*)-*form*

2-Phenylethylamide: N-*(2-Phenylethyl)-14-heptadecene-4,16-diynamide.* ***Callyspongamide A***
[549494-83-9]
$C_{25}H_{33}NO$ 363.542
Alkaloid from the Red Sea sponge *Callyspongia fistularis.*
Cytotoxic. Light yellow oil. λ_{max} 216 (log ϵ 4.12) (MeOH).

Youssef, D.T.A. *et al., J. Nat. Prod.*, 2003, **66**, 861-862 (*isol, pmr, cmr*)

1-Heptadecene-4,6,8,10,12-pentol H-172



$C_{17}H_{34}O_5$ 318.453

(4S,6S,8R,10R,12R)-form

Penta-Me ether: 4,6,8,10,12-Pentamethoxy-1-heptadecene
[127999-45-5]
$C_{22}H_{44}O_5$ 388.587
Isol. from the blue-green algae *Scytonema burmanicum* and *Scytonema mirabile.*
$[\alpha]_D^{25}$ +7.39 (c, 0.77 in $CHCl_3$).
Mori, Y. *et al., J.O.C.*, 1991, **56**, 631 (*isol, synth, pmr, cmr, abs config*)

8-Heptadecenoic acid, 9CI H-173

Civetic acid
[1975-86-6]
[26265-99-6]
$H_3C(CH_2)_7CH{=}CH(CH_2)_6COOH$
$C_{17}H_{32}O_2$ 268.439
Constit. of cod liver oil and animal lipids.

(E)-form [69695-25-6]
No Mp reported.

(Z)-form [7432-41-9]
[28040-00-8]
Constit. of the sponge *Amphimedon complanata*.
Mp 5.5-7°.

Me ester: [65092-95-7]
$C_{18}H_{34}O_2$ 282.465
Liq. Bp_6 159-165°.

Weitkamp, A.W. *et al., J.A.C.S.*, 1947, **69**, 1938 (*isol*)
Gernot, G. *et al., Chem. Ber.*, 1963, **96**, 3370 (*synth*)
Boon, J.J. *et al., Lipids*, 1977, **12**, 717 (*synth, ms*)
Hase, T.A. *et al., Synth. Commun.*, 1979, **9**, 63 (*synth*)
Christie, W.W. *et al., Lipids*, 1986, **21**, 657 (*isol, chromatog*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 315-317 (*isol*)
Poigny, S. *et al., J.C.S. Perkin 1*, 1997, 2175-2177 (*synth, ir, pmr, cmr*)

9-Heptadecenoic acid H-174

[10136-52-4]
[26265-99-6]
$H_3C(CH_2)_6CH{=}CH(CH_2)_7COOH$
$C_{17}H_{32}O_2$ 268.439

(E)-form [76261-97-7]
Mp 38°.

Et ester:
$C_{19}H_{36}O_2$ 296.492
$Bp_{0.5}$ 150°.

(Z)-form [1981-50-6]
[28040-00-8]
Minor constit. of several animal and vegetable fats. Constit. of *Amphimedon complanata*. Prod. by *Sporothrix flocculosa*. Antifungal agent.
Mp 11.4-12.2° Mp 14.5°. $Bp_{0.5}$ 175°.

Me ester: [14101-91-8]
$C_{18}H_{34}O_2$ 282.465
Mp -26.3°. Bp_2 149-152°.

Et ester: $Bp_{0.1}$ 139°.

Ames, D.H. *et al., J.C.S.*, 1951, 1079
Vauer, V.A. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1966, 2241 (*synth, ir*)
Boon, J.J. *et al., Lipids*, 1977, **12**, 717 (*synth, ms*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 315-317 (*isol*)
Benyagoub, M. *et al., J. Chem. Ecol.*, 1996, **22**, 405 (*isol, activity*)

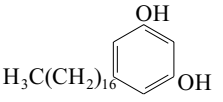
3-Heptadecen-2-one H-175

$H_3C(CH_2)_{12}CH{=}CHCOCH_3$
$C_{17}H_{32}O$ 252.439

(E)-form [75808-36-5]
Constit. of the alga *Caulocystis cephalornithos*. Isol. from *Ginkgo biloba*. Shows phospholipase Cγ1 inhibitory activity. Oil.
Kazlauskas, R. *et al., Aust. J. Chem.*, 1980, **33**, 2097 (*isol*)
Lee, J.S. *et al., Saengyak Hakhoechi*, 1999, **30**, 280; *CA*, **132**, 276641m (*activity*)

5-Heptadecyl-1,3-benzenediol, 9CI H-176

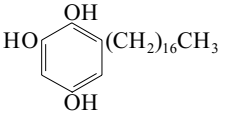
5-Heptadecylresorcinol
[41442-57-3]



$C_{23}H_{40}O_2$ 348.568
Isol. from *Grevillea* spp. and from cereal grains. Plates (cyclohexane).
Mp 91-93°.

*5′,6′,8′,9′,11′,12′,14′,15′-Octadehydro(*all-*Z-): **5-(5,8,11,14-Heptadecatetraenyl)-1,3-benzenediol, 9CI**. 5-(5,8,11,14-Heptadecatetraenyl)resorcinol*
[65341-45-9]
[114679-03-7, 117940-52-0]
$C_{23}H_{32}O_2$ 340.505
Isol. from the brown alga *Cystophora torulosa*. Oil. Darkens rapidly on exposure to air.
Gregson, R.P. *et al., Aust. J. Chem.*, 1977, **30**, 2527 (*octadehydro*)

6-Heptadecyl-1,2,4-benzenetriol H-177



$C_{23}H_{40}O_3$ 364.567

1,2-Di-Me ether: 3-Heptadecyl-4,5-dimethoxyphenol
[144078-16-0]
$C_{25}H_{44}O_3$ 392.621
Constit. of *Iris* spp.

*2,4-Di-Me ether: 2-Heptadecyl-4,6-dimethoxyphenol, 9CI. **Hierridin A**. Phaffiaol*
[144189-26-4]
$C_{25}H_{44}O_3$ 392.621
Prod. by the yeast *Phaffia rhodozyma* and the marine cyanobacterium *Phormidium ectocarpi*. Antioxidant. Antiplasmodial agent. Cryst. (MeOH).
Mp 77.7-79.1° (74.8-77.3). λ_{max} 222; 254; 263; 274 (MeOH). λ_{max} 289 (ε 3810) (EtOH).

*10′,11′-Didehydro(Z-), 1,2-di-Me ether: **Irisphenol***
[144078-15-9]
$C_{25}H_{42}O_3$ 390.605
Constit. of *Iris* spp. Viscous oil.

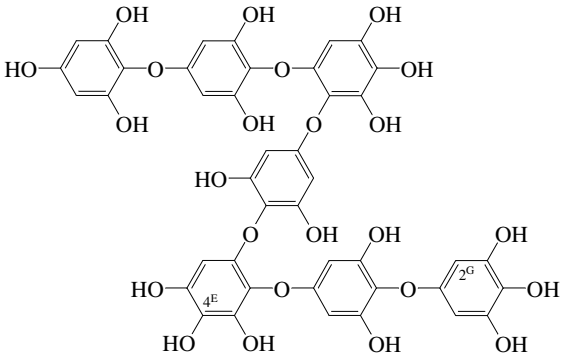
*10′,11′-Didehydro(Z-), 2,4-di-Me ether: 2-(10-Heptadecenyl)-4,6-dimethoxyphenol. **Belamcandaphenol P***
[163565-73-9]
$C_{25}H_{42}O_3$ 390.605
Constit. of the seeds of *Iris pallasii*. Oil.

*8′,9′,11′,12′-Tetradehydro(Z,Z-), 1-Ac: **Ardisiphenol C***
$C_{25}H_{38}O_4$ 402.573
Constit. of the fruit of *Ardisia colorata*. Cytotoxic. Oil. Darkens in air. λ_{max} 223 (log ε 3.89); 280 (log ε 3.45) (MeOH).

Marner, F.-J. *et al., Helv. Chim. Acta*, 1992, **75**, 1557-1562 (*isol, ms, pmr*)
Seki, K. *et al., Phytochemistry*, 1995, **38**, 965-973 (*Belamcandaphenol P, isol, pmr, cmr, uv*)
Jinno, S. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1688-1694 (*2,4-di-Me ether, synth, ir, uv, pmr, cmr*)
Jinno, S. *et al., J. Antibiot.*, 1998, **51**, 508-511 (*Phaffiaol*)
Papendorf, O. *et al., Phytochemistry*, 1998, **49**, 2383-2386 (*Hierridin A*)
Sumino, M. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1484-1487 (*Ardisiphenol C*)

Heptafuhalol A **H-178**

Heptafuhalol
[76265-30-0]



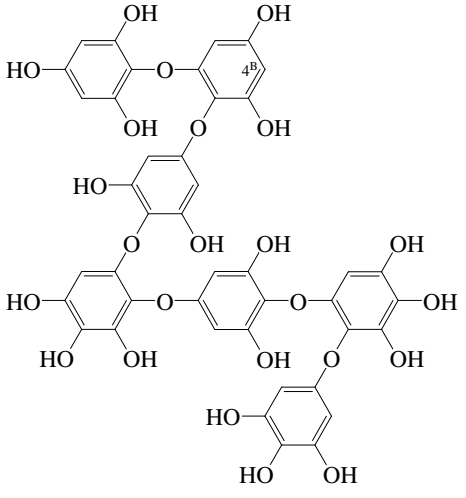
$C_{42}H_{30}O_{24}$ 918.685
Constit. of *Halidrys siliquosa*, *Carpophyllum maschalocarpum*, *Carpophyllum angustifolium* and *Sargassum spinuligerum*.

4^E-Deoxy: ***Deshydroxyheptafuhalol A***. *Dehydroxyheptafuhalol A*
[137809-94-0]
$C_{42}H_{30}O_{23}$ 902.685
Constit. of *Carpophyllum maschalocarpum*.

2^G-Hydroxy: ***Hydroxyheptafuhalol A***
$C_{42}H_{30}O_{25}$ 934.684
Isol. from *Sargassum spinuligerum*.

Sattler, E. *et al., Tetrahedron*, 1977, **33**, 1239-1244 (*isol, pmr*)
Glombitza, K.-W. *et al., Bot. Mar.*, 1980, **23**, 735 (*isol, pmr*)
Glombitza, K.-W. *et al., Phytochemistry*, 1991, **30**, 2741-2745; 1995, **38**, 975-985; 987-995 (*isol, Hydroxyheptafuhalol A*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

Heptafuhalol B **H-179**

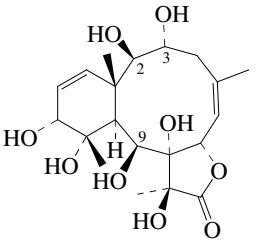


$C_{42}H_{30}O_{24}$ 918.685
Isol. from *Sargassum spinuligerum*.

4^B-Hydroxy: ***Hydroxyheptafuhalol B***
$C_{42}H_{30}O_{25}$ 934.684
Isol. from *Sargassum spinuligerum* and *Carpophyllum angustifolium*.

Keusgen, M. *et al., Phytochemistry*, 1995, **38**, 975-985 (*isol, struct*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

2,3,8,9,11,12,17-Heptahydroxy-5,13-briaradien-18,7-olide **H-180**



$C_{20}H_{30}O_9$ 414.452

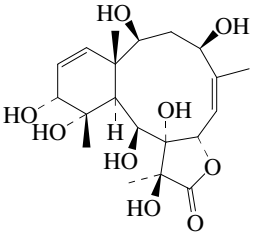
(2β,3α,5*Z*,7α,8α,9β,11α,12α,17β)-*form*

2,3,9-Tri-Ac: ***Violide M***
[252058-40-5]
$C_{26}H_{36}O_{12}$ 540.563
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ +4.83 (c, 0.29 in MeOH). λ_{max} 206 (log ϵ 3.86) (MeOH).

2,3,9,12-Tetra-Ac: ***Violide P***
[299926-26-4]
$C_{28}H_{38}O_{13}$ 582.6
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ -14.6 (c, 0.18 in MeOH). λ_{max} 206 (log ϵ 3.72) (MeOH).

Iwagawa, T. *et al., Heterocycles*, 1999, **51**, 2619-2625; 2000, **53**, 1789-1792

2,4,8,9,11,12,17-Heptahydroxy-5,13-briaradien-18,7-olide **H-181**



$C_{20}H_{30}O_9$ 414.452

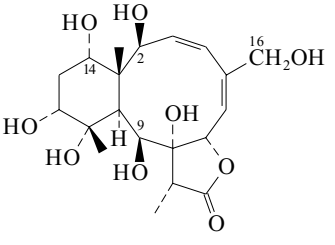
(2β,4β,5*Z*,7α,8α,9β,11α,12α,17β)-*form*

4-Butanoyl, 2,9-di-Ac: [851539-02-1]
$C_{28}H_{40}O_{12}$ 568.617
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ -6 (c, 0.14 in MeOH).

4-Octanoyl, 2,9-di-Ac: [851539-01-0]
$C_{32}H_{48}O_{12}$ 624.724
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ -5 (c, 0.15 in MeOH).

Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 607-617 (*Briareum constits*)

2,8,9,11,12,14,16-Heptahydroxy-3,5-briaradien-18,7-olide **H-182**



$C_{20}H_{30}O_9$ 414.452

(2β,3*Z*,5*E*,7α,8α,9β,11α,12α,14α)-*form*

2,9,14-Tri-Ac: ***Laboutein***
[90042-98-1]
$C_{26}H_{36}O_{12}$ 540.563
Constit. of *Pteroeides laboutei*. Cryst.
Mp 200-210° dec. $[\alpha]_D$ -6 (c, 0.36 in $CHCl_3$). Genus name sometimes spelt Pteroides.

2,9,12,14,16-Penta-Ac: ***Briarein H***
$C_{30}H_{40}O_{14}$ 624.638
Constit. of *Briareum asbestinum*. Semi-solid. $[\alpha]_D^{25}$ +18.3 (c, 1.5 in $CHCl_3$).

16-Butanoyl, 2,9,11,12,14-penta-Ac: ***Briarein L***
$C_{34}H_{46}O_{15}$ 694.728
Constit. of *Briareum asbestinum*. Semi-solid. $[\alpha]_D^{25}$ -19.8 (c, 2.3 in $CHCl_3$).

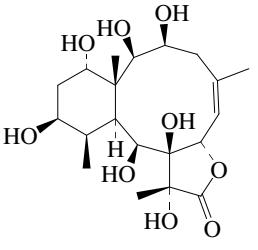
16-Octanoyl, 2,9,12,14-tetra-Ac: ***Briarein I***
$C_{36}H_{52}O_{14}$ 708.798
Constit. of *Briareum asbestinum*. Semi-solid. $[\alpha]_D^{25}$ +3.5 (c, 6 in $CHCl_3$).

12-Octanoyl, 16-butanoyl, 2,9,14-tri-Ac: ***Briarein K***
$C_{38}H_{56}O_{14}$ 736.852
Constit. of *Briareum asbestinum*. Semi-solid. $[\alpha]_D^{25}$ -1.6 (c, 1.9 in $CHCl_3$).

16-Deoxy, 16-chloro, 2,9,12,14-tetra-Ac: ***Briarein J***
$C_{28}H_{37}ClO_{12}$ 601.046
Constit. of *Briareum asbestinum*. Semi-solid. $[\alpha]_D^{25}$ +5.5 (c, 1.45 in $CHCl_3$).

Clastres, A. *et al., J. Nat. Prod.*, 1984, **47**, 155-161 (*Laboutein*)
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1996, **59**, 15 (*Briareins*)

2,3,8,9,12,14,17-Heptahydroxy-5-briaren-18,7-olide H-183



$C_{20}H_{32}O_9$ 416.467

(2β,3β,5*Z*,7α,8β,9β,12β,14α,17α*OH*)-*form*

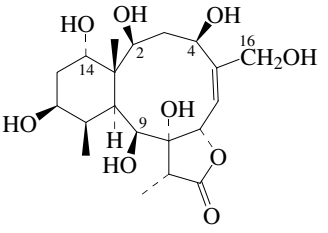
2,3,9,14-Tetra-Ac: ***Briaexcavatolide K***
[334831-89-9]
$C_{28}H_{40}O_{13}$ 584.616
Constit. of *Briareum excavatum*. Cryst.
Mp 270-273°. $[\alpha]_D^{27}$ -25 (c, 1 in $CHCl_3$).

3-Butanoyl, 2,9,14-tri-Ac: ***Briaexcavatolide L***
[334831-90-2]
$C_{30}H_{44}O_{13}$ 612.67
Constit. of *Briareum excavatum*. Powder.
Mp 164-166°. $[\alpha]_D^{27}$ -37 (c, 0.8 in $CHCl_3$).

3-Butanoyl, 2,9,12,14-tetra-Ac: ***Briaexcavatolide Z***
[782496-61-1]
$C_{32}H_{46}O_{14}$ 654.707
Constit. of *Briareum excavatum*. Powder.
Mp 147-148°. $[\alpha]_D^{25}$ -41 (c, 0.8 in $CHCl_3$).

Sung, P.-J. *et al., J. Nat. Prod.*, 2001, **64**, 318-323 (*isol, pmr, cmr, cryst struct*)
Sung, P.-J. *et al., Tetrahedron*, 2004, **60**, 8975-8979 (*Briaexcavatolide Z*)

2,4,8,9,12,14,16-Heptahydroxy-5-briaren-18,7-olide H-184

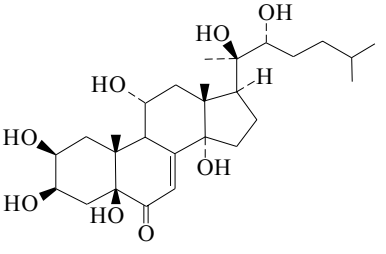


$C_{20}H_{32}O_9$ 416.467

(2β,4β,5*E*,7α,8α,9β,12β,14α)-*form*

2,4,9,14,16-Penta-Ac: ***16-Acetoxymilolide G***
[438552-10-4]
$C_{30}H_{42}O_{14}$ 626.653
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ +67.2 (c, 0.61 in CH_2Cl_2).
Kwak, J.H. *et al., J. Nat. Prod.*, 2002, **65**, 704-708 (*isol, pmr, cmr*)

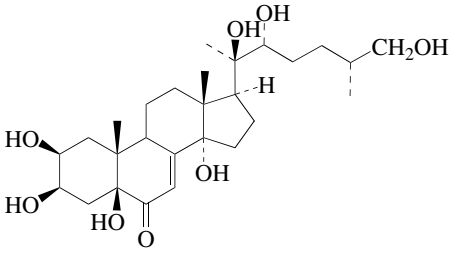
2,3,5,11,14,20,22-Heptahydroxycholest-7-en-6-one H-185



$C_{27}H_{44}O_8$ 496.64

(2β,3β,5β,11α,20*R*,22*R*)-*form*
Muristerone A
[38778-30-2]
Constit. of *Ipomoea calonyction*. Also isol. from the sponge *Ptilocaulis spiculifer*. Shows v. high insect moulting activity.
Cryst. (MeOH).
Mp 238-240°. $[\alpha]_D^{20}$ +49.6 (c, 1 in Py). λ_{max} 236 (ϵ 8900) (MeOH).
Canonica, L. *et al., Phytochemistry*, 1975, **14**, 525-527 (*isol, pmr*)
Canonica, L. *et al., Gazz. Chim. Ital.*, 1977, **107**, 123 (*struct*)
Krepinsky, J. *et al., Org. Magn. Reson.*, 1977, **10**, 255 (*cmr*)
West, R.R. *et al., J.O.C.*, 1989, **54**, 3234-3236 (*cmr*)
Diop, M. *et al., J. Nat. Prod.*, 1996, **59**, 271-272 (*Ptilocaulis, isol*)

2,3,5,14,20,22,26-Heptahydroxycholest-7-en-6-one H-186



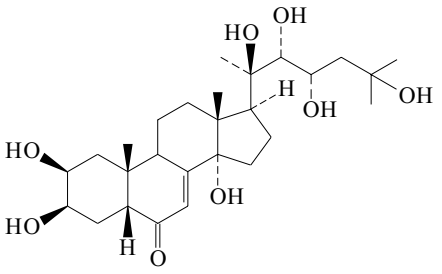
$C_{27}H_{44}O_8$ 496.64

(2β,3β,5β,14α,20*R*,22*R*,25*R*)-*form*
Palythoalone B
[220757-97-1]
Constit. of *Palythoa australiae*.

Amorph. solid. $[\alpha]_D^{28}$ +56 (c, 1 in MeOH). λ_{max} 245 (ϵ 11000) (MeOH).

Shigemori, H. *et al., J. Nat. Prod.*, 1999, **62**, 372-374 (*isol, pmr, cmr*)

2,3,14,20,22,23,25-Heptahydroxycholest-7-en-6-one H-187



$C_{27}H_{44}O_8$ 496.64

(2β,3β,5β,14α,20*R*,22*R*,23*S*)-*form*

Gerardiasterone

[102712-89-0]

Constit. of *Gerardia savaglia*.

Amorph. solid.

Mp 143-146°. $[\alpha]_D^{22}$ +52.3 (c, 0.35 in MeOH).

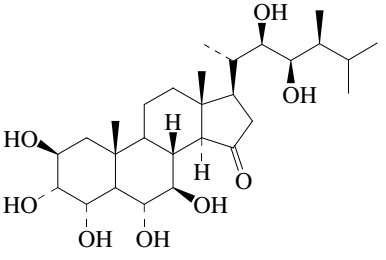
Guerriero, A. *et al., Chem. Comm.*, 1986, 40

Honda, T. *et al., Tet. Lett.*, 1993, **34**, 8275 (*synth, abs config*)

Tsubuki, M. *et al., Tetrahedron*, 1996, **52**, 14515 (*synth, abs config*)

2,3,4,6,7,22,23-Heptahydroxyergostan-15-one H-188

2,3,4,6,7,22,23-Heptahydroxy-24-methylcholestan-15-one



$C_{28}H_{48}O_8$ 512.682

(2β,3α,4α,6α,7β,14α,22*R*,23*R*,24*S*)-*form*

Tamosterone

2-Sulfate: ***Tamosterone sulfate***

[246516-37-0]

$C_{28}H_{48}O_{11}S$ 592.747

Constit. of an Oceanapiid sponge. Amorph. solid. $[\alpha]_D$ +34.4 (c, 0.3 in MeOH).

(2β,3α,4α,6α,7β,14β,22*R*,23*R*,24*S*)-*form*

14β-Tamosterone

2-Sulfate: ***14β-Tamosterone sulfate***

[246860-42-4]

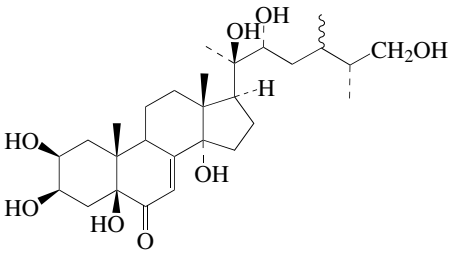
$C_{28}H_{48}O_{11}S$ 592.747

Constit. of an Oceanapiid sponge. Amorph. solid. $[\alpha]_D$ +5.7 (c, 0.81 in MeOH).

Fu, X. *et al., J.O.C.*, 1999, **64**, 6706-6709 (*isol, pmr, cmr*)

2,3,5,14,20,22,26-Heptahydroxyergost-7-en-6-one H-189

2,3,5,14,20,22,26-Heptahydroxy-24-methylcholest-7-en-6-one



$C_{28}H_{46}O_8$ 510.667

(2β,3β,5β,14α,20*R*,22*R*,24ξ,25*R*)-*form*

Palythoalone A

[220757-95-9]

Constit. of *Palythoa australiae*.

Amorph. solid. $[\alpha]_D^{26}$ +87 (c, 2.2 in MeOH). λ_{max} 243 (ϵ 10000) (MeOH).

Shigemori, H. *et al., J. Nat. Prod.*, 1999, **62**, 372-374 (*isol, pmr, cmr*)

Sepia officinalis Heptapeptide H-190

[368879-49-6]

H-Val-Tyr-Ser-Ala-Pro-Tyr-Gly-OH

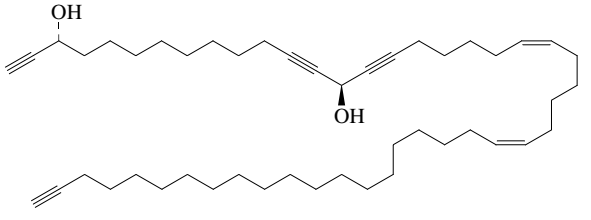
$C_{36}H_{49}N_7O_{11}$ 755.823

Heptapeptide. Isol. from the stellar ganglia of the mollusc cephalopod *Sepia officinalis*. Neuropeptide.

Marvin, L.F. *et al., Peptides (N.Y.)*, 2001, **22**, 1391-1396 (*isol*)

21,27-Heptatetracontadiene-1,12,15,46-tetrayne-3,14-diol H-191

Petrotetrayndiol F



$C_{47}H_{76}O_2$ 673.116

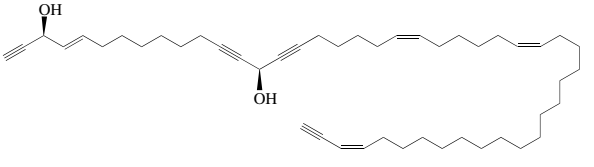
(3*R*,14*S*,21*Z*,27*Z*)-*form*

Isol. from the marine sponge *Petrosia* sp. Cytotoxic. Yellow oil.

Lim, Y.J. *et al., J. Nat. Prod.*, 2001, **64**, 1565-1567

4,21,27,44-Heptatetracontatetraene-1,12,15,46-tetrayne-3,14-diol H-192

Homopetrocortyne A



$C_{47}H_{72}O_2$ 669.085

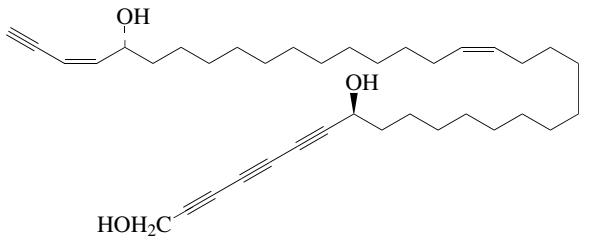
(3*S*,4*E*,14*S*,21*Z*,27*Z*,44*Z*)-*form*

Isol. from the sponge *Petrosia* sp.

Yellow oil.

Lim, Y.J. *et al., J. Nat. Prod.*, 2001, **64**, 46-53

20,34-Heptatriacontadiene-2,4,6,36-tetrayne-1,8,33-triol H-193



$C_{37}H_{56}O_3$ 548.848

(8*S*,20*Z*,33*R*,34*Z*)-*form*
Triangulyne H
[182314-14-3]
Isol. from the sponge *Pellina triangulata*. Cytotoxic agent. Oil. $[\alpha]_D$ -23.7 (c, 0.3 in $CHCl_3$). λ_{max} 203 (log ϵ 3.8); 223 (log ϵ 4.1); 255 (log ϵ 2.7) (MeOH).
Dai, J.-R. *et al., J. Nat. Prod.*, 1996, **59**, 860-865 (*isol, uv, ir, pmr, cmr, ms*)

15,22-Heptatriacontadien-2-one H-194

[81531-17-1]
$H_3C(CH_2)_{13}CH{=}CH(CH_2)_5CH{=}CH(CH_2)_{12}COCH_3$
$C_{37}H_{70}O$ 530.959
Found in sedimentary rocks and marine sediments. Constit. of *Emiliania huxleyi*. Biomarker for coccolithophorids.

[119650-08-7, 119650-09-8]

Volkman, J.K. *et al., Phytochemistry*, 1980, **19**, 2619
Rechka, J.A. *et al., Org. Geochem.*, 1988, **13**, 727
Rechka, J.A. *et al., Tet. Lett.*, 1988, **27**, 2599 (*synth*)
Marlowe, I.T. *et al., Chem. Geol.*, 1990, **88**, 349

1,15,22-Heptatriacontatriene H-195

$H_3C(CH_2)_{13}CH{=}CH(CH_2)_5CH{=}CH(CH_2)_{12}CH{=}CH_2$
$C_{37}H_{70}$ 514.96

(*E*,*E*)-*form* [211238-38-9]
Isol. from the haptophyte *Emiliania huxleyi*.
Rieley, G. *et al., Lipids*, 1998, **33**, 617-625 (*isol*)

3-Heptenal, 9CI H-196

[89896-73-1]
$H_3C(CH_2)_2CH{=}CHCH_2CHO$
$C_7H_{12}O$ 112.171
Bp 151° Bp_{15} 45-46°.

Oxime:
$C_7H_{13}NO$ 127.186
Mp 39°.

Semicarbazone: Mp 126°.

(*E*)-*form* [21662-20-4]
Constit. of *Scytosiphon lomentaria*.

(*Z*)-*form* [21662-18-0]
Oil.

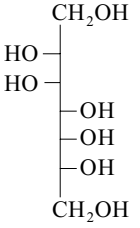
Di-Et acetal: 1,1-Diethoxy-3-heptene
$C_{11}H_{22}O_2$ 186.294
Bp_{15} 90-91°.

[21662-18-0, 21662-20-4, 72931-56-7]

Gouge, M. *et al., Ann. Chim. (Paris)*, 1951, **6**, 648 (*synth*)
Durand, M.H. *et al., Bull. Soc. Chim. Fr.*, 1961, 2396 (*synth*)
Battersby, A.R. *et al., J.C.S. Perkin 1*, 1979, 2550
Nomura, M. *et al., Yukagaku*, 1980, **29**, 755; *CA*, **94**, 120792 (*synth*)
Kajiwara, T. *et al., Phytochemistry*, 1991, **30**, 1805 (*isol*)

D-*glycero*-D-*manno*-Heptitol, 9CI, 8CI H-197

D-glycero-D-talo-*Heptitol. Volemitol. α-Sedoheptitol. β-Manno-heptitol*
[488-38-0]



$C_7H_{16}O_7$ 212.199
Occurs in the edible chichitake mushroom (*Lactarius volemus*), in roots of Primulae and in lipopolysaccharides from *Escherichia coli*. Also in red algae. Widely distributed in plants. Needles (EtOH).
Mp 152-153°. $[\alpha]_D^{20}$ +2.2 (H_2O).

Hepta-Ac: 1,2,3,4,5,6,7-Hepta-O-*acetyl*-D-glycero-D-manno-*heptitol*
$C_{21}H_{30}O_{14}$ 506.46
Mp 63°. $[\alpha]_D^{20}$ +36.1 (c, 2 in $CHCl_3$).

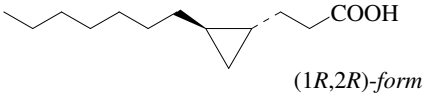
Tri-O-*benzylidene:*
$C_{28}H_{28}O_7$ 476.525
Needles. Mp 214-215°. $[\alpha]_D^{20}$ +1.7 ($CHCl_3$). Exact struct. apparently not detd.

[30635-52-0]

La Forge, F.B. *et al., J. Biol. Chem.*, 1917, **30**, 61; 1920, **42**, 375; 1928, **79**, 1 (*isol, tribenzylidene*)
Maclay, W.D. *et al., J.O.C.*, 1944, **9**, 293 (*occur, synth, hepta-Ac*)
Merrill, A.T. *et al., J.A.C.S.*, 1947, **69**, 70 (*synth, hepta-Ac*)
Adams, G.A. *et al., Can. J. Microbiol.*, 1967, **13**, 1605 (*isol, glc*)
Mills, J.A. *et al., Aust. J. Chem.*, 1974, **27**, 1433 (*conformn*)
Angyal, S. *et al., Carbohydr. Res.*, 1984, **126**, 15 (*cmr*)
Brimacome, J.S. *et al., Carbohydr. Res.*, 1986, **150**, 35 (*synth*)
Köll, P. *et al., Carbohydr. Res.*, 1991, **218**, 55; 1993, **247**, 111 (*cryst struct, hepta-Ac*)

2-Heptyl-1-cyclopropanepropanoic acid H-198

4,5-Methylenedodecanoic acid



(1*R*,2*R*)-*form*

$C_{13}H_{24}O_2$ 212.331

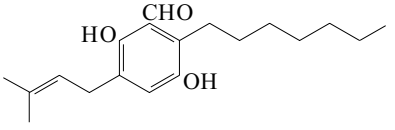
(1*R*,2*R*)-*form*
2-Phenylethylamide: ***Grenadamide***
[205521-84-2]
$C_{21}H_{33}NO$ 315.498
Isol. from *Lyngbya majuscula*. Toxic to brine shrimp, cannabinoid receptor antagonist. $[\alpha]_D$ -11 (c, 0.1 in $CHCl_3$). λ_{max} 206 (ϵ 2600) (MeOH).

(1*R*,2*R*)-*form*
(5-Acetoxy-4-bromo-1,3-pentadienyl) ester (Z,Z-): ***Grenadadiene***
[205521-82-0]
$C_{20}H_{31}BrO_4$ 415.367
Isol. from *Lyngbya majuscula*. Cytotoxic agent. $[\alpha]_D$ -8 (c, 0.1 in $CHCl_3$). λ_{max} 252 (ϵ 12200) (MeOH).
5-Acetoxy-1,3-pentadienyl ester (1Z,3E-): ***Debromogrenadadiene***
[205521-83-1]
$C_{20}H_{32}O_4$ 336.47
Isol. from *Lyngbya majuscula*. Toxic to brine shrimp. $[\alpha]_D$ +5 (c, 0.1 in $CHCl_3$). λ_{max} 232 (ϵ 8000) (hexane).
Sitachitta, N. *et al., J. Nat. Prod.*, 1998, **61**, 681-684 (*isol, uv, ir, pmr, cmr, ms*)

Al Dulayymi, J.R. *et al., Tetrahedron*, 2004, **60**, 341-345 (*Grenadamide, synth, abs config*)
Green, R. *et al., Tet. Lett.*, 2005, **46**, 7931-7934 (*Grenadamide, synth*)
Avery, T.D. *et al., Org. Biomol. Chem.*, 2006, **4**, 323-330 (*Grenadamide, synth*)

2-Heptyl-3,6-dihydroxy-5-prenylbenzaldehyde H-199

2-Heptyl-3,6-dihydroxy-5-(3-methyl-2-butenyl)benzaldehyde, 9CI. 6-Heptyl-3-(3-methyl-2-butenyl)gentisaldehyde, 9CI. ***Flavoglaucin***
[523-73-9]



$C_{19}H_{28}O_3$ 304.428
Isol. from *Aspergillus flavus*, other *Aspergillus* spp. and a marine-derived *Microsporum* sp. Mycotoxin. Pale yellow cryst.
Mp 103°. λ_{max} 236 (ϵ 70000); 274 (ϵ 7080); 394 (ϵ 4570) (MeOH) (Berdy). λ_{max} 270 (ϵ 68000); 394 (ϵ 5050) (EtOH) (Berdy).

Phenylhydrazone: Mp 137°. Rather unstable.

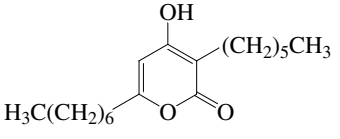
*(*E*)-2,4-Dinitrophenylhydrazone:*
Red cryst. Mp 179-181°.

*(*Z*)-2,4-Dinitrophenylhydrazone:*
Orange cryst. Mp 186-187°.

Raistrick, H. *et al., J.C.S.*, 1937, 80
Quilico, A. *et al., Gazz. Chim. Ital.*, 1953, **83**, 754
Podojil, M. *et al., Folia Microbiol. (Prague)*, 1978, **23**, 438 (*isol, props*)
Allen, J.K. *et al., J.C.S. Perkin 1*, 1978, 152 (*biosynth*)
Gatti, G. *et al., J. Chem. Res., Synop.*, 1979, 366 (*cmr*)
Nazar, M. *et al., Toxicol. Lett.*, 1984, **23**, 233 (*tox*)
Li, Y. *et al., Chem. Pharm. Bull.*, 2006, **54**, 882-883 (*marine, isol*)

6-Heptyl-3-hexyl-4-hydroxy-2*H*-pyran-2-one H-200

***Pseudopyronine B**. Antibiotic Sch 419560. Sch 419560*

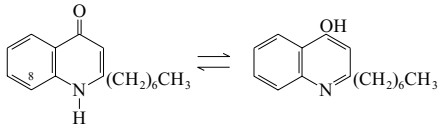


$C_{18}H_{30}O_3$ 294.433
Prod. by *Pseudomonas fluorescens* and a marine *Pseudomonas* sp. F92S91. Antibacterial agent. Pale yellow solid. λ_{max} 292 (ϵ 15200) (MeOH).

Chu, M. *et al., J. Antibiot.*, 2002, **55**, 215-218 (*isol, pmr, cmr*)
Singh, M.P. *et al., J. Antibiot.*, 2003, **56**, 1033-1044 (*isol, activity*)
Kong, F.-M. *et al., J. Nat. Prod.*, 2005, **68**, 920-923 (*isol, uv, pmr, cmr, ms*)

2-Heptyl-4-hydroxyquinoline H-201

*2-Heptyl-4(1*H*)-quinolinone, 9CI. 2-Heptyl-4-quinolinol.* ***Pyo Ib**. Pseudane VII. MY 12-62a. Antibiotic MY 12-62a*
[40522-46-1]



$C_{16}H_{21}NO$ 243.348
Alkaloid from a yellow marine pseudomonad. The terrestrial bacterium *Pseudomonas aeruginosa* also yields this compd. Shows antibiotic props. against a number of bacteria. 5-Lipoxygenase inhibitor and Streptomycin antagonist. Cryst. (Me_2CO aq.).
Mp 146-147°. $Bp_{0.2}$ 118-122°.

N-*Oxide: 2-Heptyl-4-hydroxyquinoline* N-*oxide.* ***Antibiotic KF 8940**. KF 8940*
[341-88-8]
$C_{16}H_{21}NO_2$ 259.347
Metab. of *Pseudomonas pyocyanea, Pseudomonas aeruginosa, Pseudomonas methanica* and *Pseudomonas* sp. KUH-001. Potent 5-lipoxygenase inhibitor. Active against *Staphylococcus aureus.* Synergistic with Vancomycin and Erythromycin. Cryst. (EtOH).
Mp 158-160°.
▶ LD_{50} (mus, ipr) 40 mg/kg. VC5890000

*1′,2′-Didehydro: 2-(1-Heptenyl)-4(1*H*)-quinolinone, 9CI. 2-(1-Heptenyl)-4-hydroxyquinoline.* ***Δ¹-Pseudene VII***
[60783-02-0]
$C_{16}H_{19}NO$ 241.332
Prod. by *Pseudomonas aeruginosa*. Antifungal agent.

*4′,5′-Didehydro: 2-(4-Heptenyl)-4(1*H*)-quinolinone.* ***Acutine***
[36150-05-7]
$C_{16}H_{19}NO$ 241.332
Alkaloid from the above-ground parts of *Haplophyllum acutifolium* (Rutaceae). Prisms (Me_2CO).
Mp 122-123°. Becomes pink on standing in the light.

NH-form

N-*Me: 2-Heptyl-1-methyl-4(1*H*)-quinolinone.* ***Schinifoline***†
$C_{17}H_{23}NO$ 257.375
Alkaloid from peel of *Zanthoxylum schinifolium* (Rutaceae). Cryst.
Mp 81-82°.

8-Methoxy, N-*Me:* ***2-Heptyl-8-methoxy-1-methyl-4(1H)-quinolinone***
$C_{18}H_{25}NO_2$ 287.401
Alkaloid from trunk bark of *Esenbeckia almawillia* (Rutaceae). Oil.

OH-form

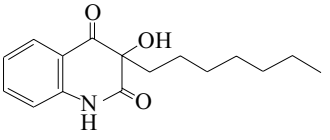
Me ether: 2-Heptyl-4-methoxyquinoline, 9CI
[80554-59-2]
$C_{17}H_{23}NO$ 257.375
Alkaloid from *Zanthoxylum avicennae.*
Mp 35-38°.

[2503-80-2]

Hays, E.E. *et al., J. Biol. Chem.*, 1945, **159**, 725 (*isol*)
Wells, I.C. *et al., J. Biol. Chem.*, 1952, **196**, 331 (*synth, uv, struct*)
Cornforth, J.W. *et al., Biochem. J.*, 1956, **63**, 124; 130 (*isol, props*)
Ames, D.E. *et al., J.C.S.*, 1956, 3079 (*synth*)
Luckner, M. *et al., Tet. Lett.*, 1965, 741 (*biosynth*)
Ritter, C. *et al., Eur. J. Biochem.*, 1971, **18**, 391
Razzakova, D.M. *et al., Khim. Prir. Soedin.*, 1973, **9**, 206; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 199 (*Acutine*)
Kozlovskii, A.G. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1976, 1146-1150 (*Δ¹-Pseudene VII*)
Wratten, S.J. *et al., Antimicrob. Agents Chemother.*, 1977, **11**, 411 (*isol*)
Budzikiewicz, H. *et al., Monatsh. Chem.*, 1979, **110**, 947 (*isol, uv*)
Somanathan, R. *et al., J. Het. Chem.*, 1981, **18**, 1077 (*synth, uv, ir, pmr*)
Kitamura, S. *et al., J. Antibiot.*, 1986, **39**, 1160 (*isol, struct, props*)
Liu, S.L. *et al., Yaoxue Xuebao*, 1991, **26**, 836; *CA*, **117**, 86638h (*Schinifoline*)
Wu, W. *et al., Zhongcaoyao*, 1992, **23**, 115; *CA*, **117**, 76305h (*isol, Me ether*)
Guilhon, G.M.S.P. *et al., Phytochemistry*, 1994, **37**, 1193 (*2-Heptyl-8-methoxy-1-methyl-4(1H)-quinolinone*)
Debitus, C. *et al., J. Mar. Biotechnol.*, 1998, **6**, 136-141 (*isol*)
Hwang, S.-Y. *et al., J. Microb. Biotechnol.*, 1998, **8**, 111-118 (*N-oxide, isol, activity*)

3-Heptyl-3-hydroxy-2,4(1*H*,3*H*)-quinolinedione H-202

MY 12-62c. Antibiotic MY 12-62c
[69808-30-6]

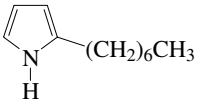


$C_{16}H_{21}NO_3$ 275.347
Prod. by *Pseudomonas methanica* and *Pseudomonas aeruginosa*. Also prod. by a bacterium isol. from the sponge *Suberea creba*. 5-Lipoxygenase inhibitor. Cryst. (EtOAc).
Mp 142°.

Neuenhaus, N. *et al., Z. Naturforsch., B*, 1979, **34**, 313 (*isol, struct, synth*)
Kitamura, S. *et al., J. Antibiot.*, 1986, **39**, 1160 (*isol, struct, props*)
Debitus, C. *et al., J. Mar. Biotechnol.*, 1998, **6**, 136-141 (*isol*)

2-Heptylpyrrole, 9CI H-203

[878-12-6]

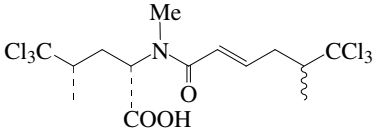


$C_{11}H_{19}N$ 165.278
Bp_{40} 160°.

N-*Sulfo: 2-Heptylpyrrole sulfamate*
[587875-52-3]
$C_{11}H_{19}NO_3S$ 245.342
Alkaloid from the marine annelid *Cirriformia tentaculata*. Glass (as Na salt).

Garrido, D.O.A. *et al., J.O.C.*, 1984, **49**, 2619-2622 (*synth*)
Barsby, T. *et al., J. Nat. Prod.*, 2003, **66**, 1110-1112 (*sulfamate*)

Herbacic acid H-204



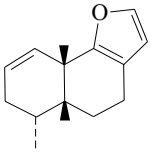
$C_{14}H_{19}Cl_6NO_3$ 462.025
Isol. from the sponge *Dysidea herbacea*. Prisms (MeCN).
Mp 182-184°. $[\alpha]_D$ -36.3 (c, 0.7 in MeOH). λ_{max} 211 (ϵ 14100) (MeCN).

Me ester: ***Herbaceamide****. Herbaceamide A*
[145873-83-2]
$C_{15}H_{21}Cl_6NO_3$ 476.052
Isol. from the sponge *Dysidea herbacea*. Oil. $[\alpha]_D$ -35.1 (c, 0.5 in MeOH). λ_{max} 212 (log ϵ 4.2) (MeOH).

Lee, G.M. *et al., Tet. Lett.*, 1992, **33**, 7671 (*Herbaceamide*)
Macmillan, J.B. *et al., J. Nat. Prod.*, 2000, **63**, 155-157 (*Herbacic acid*)

Herbacin† H-205

*4,5,5*a*,6,7,9*a*-Hexahydro-5*a*,6,9*a*-trimethylnaphtho[1,2-*b*]furan*
[106793-86-6]

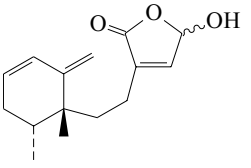


$C_{15}H_{20}O$ 216.322
The name Herbacin is also used for a flavonoid. Isol. from marine sponge *Dysidea herbacea*. Needles (C_6H_6).
Mp 40-41°. $[\alpha]_D$ +9.2 (c, 0.2 in $CHCl_3$). λ_{max} 252 (ϵ 19950); 270 (ϵ 30900) (hexane) (Derep).

Sarma, N.S. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 1001 (*isol, struct*)
Rambabu, M. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 1156

Herbacin hydroxybutenolide H-206

[158014-62-1]

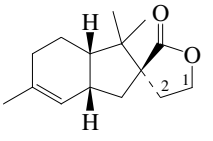


$C_{15}H_{20}O_3$ 248.321
Constit. of *Dysidea herbacea*. Oil.

Venkateswarlu, Y. *et al., J. Nat. Prod.*, 1994, **57**, 827 (*isol, pmr, cmr*)

Herbadysidolide H-207

[68299-90-1]



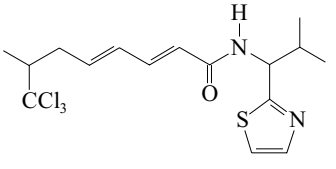
$C_{15}H_{22}O_2$ 234.338
Constit. of *Dysidea herbacea*. Cryst.
Mp 55-56°. $[\alpha]_D$ -47 (c, 0.42 in $CHCl_3$).

1,2-Didehydro: ***Dehydroherbadysidolide***
[292135-76-3]
$C_{15}H_{20}O_2$ 232.322
Constit. of *Dysidea* sp. 1524.
$[\alpha]_D$ -66 (c, 0.0004 in $CHCl_3$).

Charles, C. *et al., Bull. Soc. Chim. Belg.*, 1978, **87**, 481
Cameron, G.M. *et al., Tetrahedron*, 2000, **56**, 5247-5252 (*isol, pmr, cmr*)

Herbamide A H-208

[161503-26-0]

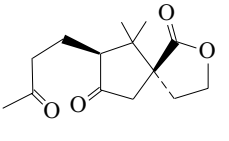


$C_{16}H_{21}Cl_3N_2OS$ 395.779
Isol. from the marine sponge *Dysidea herbacea*. Oil. $[\alpha]_D$ +13 (c, 0.013 in $CHCl_3$).

Clark, W.D. *et al., Tet. Lett.*, 1995, **36**, 1185 (*isol, uv, ir, pmr, cmr, struct*)

Herbasolide H-209

[68299-91-2]

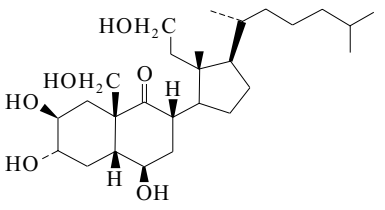


$C_{14}H_{20}O_4$ 252.31
Constit. of *Dysidea herbacea*. Cryst. (Et_2O/pentane).
Mp 97-98°. $[\alpha]_{436}$ +95 (c, 0.182 in $CHCl_3$).

Charles, C. *et al., Bull. Soc. Chim. Belg.*, 1978, **87**, 481
Ho, T.L. *et al., Chem. Comm.*, 1996, 1887 (*synth*)

Herbasterol H-210

2β,3α,6β,11,19-Pentahydroxy-9,11-secocholestan-9-one, 9CI
[98705-22-7]



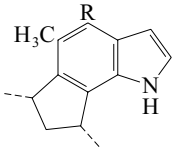
$C_{27}H_{48}O_6$ 468.673
Constit. of the sponge *Dysidea herbacea*. Shows ichthyotoxic and cytotoxic activities. Hygroscopic solid. Sol. MeOH, $CHCl_3$, CH_2Cl_2; poorly sol. H_2O.
Mp 113-115°. $[\alpha]_D$ +1.4 (c, 8.4 in MeOH).

3-Epimer: ***Stellettasterol***
[159736-50-2]
$C_{27}H_{48}O_6$ 468.673
Constit. of a *Stelletta* sp. Solid. $[\alpha]_D^{23}$ -18.5 (c, 0.35 in MeOH).

Capon, R.J. *et al., J.O.C.*, 1985, **50**, 4771 (*isol, activity*)
Li, H. *et al., Experientia*, 1994, **50**, 771 (*Stellettasterol*)

Herbindole A H-211

1,6,7,8-Tetrahydro-4,5,6,8-tetramethylcyclopent[g]indole, 9CI
[128397-78-4]



R = CH_3

$C_{15}H_{19}N$ 213.322
Alkaloid from the sponge *Axinella* sp. Cytotoxic and fish antifeedant. Needles (MeOH).
Mp 120-122°. λ_{max} 222 (ϵ 46800); 272 (ϵ 12300) (base in MeOH) (Derep). λ_{max} 210 (ϵ 55000); 226 (sh) (ϵ 47900); 272 (ϵ 8510) (acidic MeOH) (Derep).

Herb, R. *et al., Tetrahedron*, 1990, **46**, 3089 (*isol, pmr, cmr, struct*)
Muratake, H. *et al., Chem. Pharm. Bull.*, 1994, **42**, 854 (*synth, abs config*)

Herbindole B H-212

4-Ethyl-1,6,7,8-tetrahydro-5,6,8-trimethylcyclopent[g]indole, 9CI
[128397-79-5]
As Herbindole A, H-211 with
R = $–CH_2CH_3$

$C_{16}H_{21}N$ 227.349
Alkaloid from the sponge *Axinella* sp. Cytotoxic and fish antifeedant. Needles (MeOH).
Mp 118-120°. λ_{max} 222 (ϵ 46800); 272 (ϵ 12300) (base in MeOH) (Derep). λ_{max} 210 (ϵ 55000); 226 (sh) (ϵ 47900); 272 (ϵ 8510) (acidic MeOH) (Derep). λ_{max} 222 (ϵ 46773); 272 (ϵ 12300) (MeOH) (Berdy).

Herb, R. *et al., Tetrahedron*, 1990, **46**, 3089 (*isol, pmr, cmr, struct*)
Muratake, H. *et al., Chem. Pharm. Bull.*, 1994, **42**, 854 (*synth, abs config*)
Jackson, S.K. *et al., Org. Lett.*, 2005, **7**, 1215-1218 (*synth*)

Herbindole C H-213

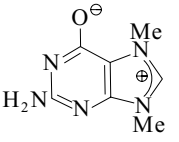
4-(1-Butenyl)-1,6,7,8-tetrahydro-5,6,8-trimethylcyclopent[g]indole, 9CI
[128397-80-8]
As Herbindole A, H-211 with
R = $–CH{=}CHCH_2CH_3$(*E*-)

$C_{18}H_{23}N$ 253.386
Alkaloid from the sponge *Axinella* sp. Cytotoxic and fish antifeedant. Oil. Regioisomer of Trikentrin B, T-697. λ_{max} 212 (ϵ 50100); 226 (ϵ 42700); 294 (ϵ 10000) (MeOH) (Derep).

Herb, R. *et al., Tetrahedron*, 1990, **46**, 3089 (*isol, pmr, cmr, struct*)
Muratake, H. *et al., Chem. Pharm. Bull.*, 1994, **42**, 854 (*synth, abs config*)

Herbipoline H-214

2-Amino-6,9-dihydro-7,9-dimethyl-6-oxo-1H-purinium hydroxide, inner salt, 9CI. 7,9-Dimethylguaninium betaine
[524-35-6]



$C_7H_9N_5O$ 179.181
Isol. from the giant silicious sponge *Geodia gigas*. Needles (EtOH aq.).
Mp 312°.

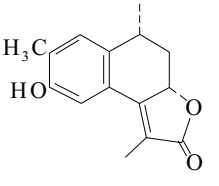
Picrate: Mp 292-295°.

N^1-*Me:* ***1-Methylherbipoline***
[97174-15-7]
$C_8H_{12}N_5O^{\oplus}$ 194.216
From the marine sponge *Jaspis* sp. Collagenase inhibitor. Sol. MeOH, Et_2O. Counterion in nat. prod. not characterised. λ_{max} 260 (ϵ 7600); 282 (ϵ 4460) (MeOH) (Berdy).

Ackermann, D. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1957, **308**, 270; **309**, 286 (*isol, ir*)
Bredereck, H. *et al., Chem. Ber.*, 1960, **93**, 1206 (*synth, struct*)
Pfleiderer, W. *et al., Annalen*, 1961, **647**, 167-173 (*synth*)
Yagi, H. *et al., J. Nat. Prod.*, 1994, **57**, 837-838 (*1-Methylherbipoline*)
Metzger, S. *et al., Chem. Eur. J.*, 1996, **35**, 1228 (*struct, props*)

Heritol H-215

15(4→3)-Abeo-4-hydroxy-1,3,5,7(11)-cadinatetraen-12,8-olide
[108295-47-2]

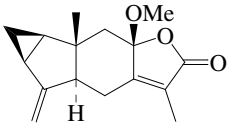


$C_{15}H_{16}O_3$ 244.29
Constit. of *Heritiera littoralis*. Ichthyotoxin. Needles (MeOH).
Mp 271-272°. $[\alpha]_D^{25}$ +261.3. λ_{max} 217 (ϵ 12600); 228 (ϵ 11950); 285 (ϵ 14215); 305 (ϵ 8076) (hexane) (Derep).

Miles, D.H. *et al., J.O.C.*, 1987, **52**, 2930-2932 (*isol, cryst struct*)
Irie, H. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1852 (*synth*)
Zubaidha, P.K. *et al., Tetrahedron*, 1991, **47**, 5759 (*synth*)
Chavan, S.P. *et al., Chem. Comm.*, 1994, 1101 (*synth*)

Heterogorgiolide H-216

[245062-24-2]

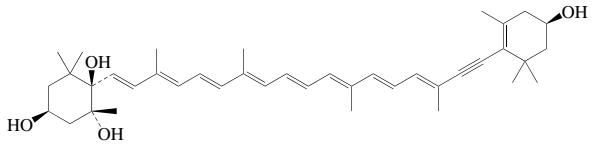


$C_{16}H_{20}O_3$ 260.332
Constit. of *Heterogorgia uatumami*. Amorph. solid.
Mp 149-151°. $[\alpha]_D^{25}$ +116 (c, 1 in $CHCl_3$). λ_{max} 207 (log ϵ 1.845) (MeOH).

Maia, L.F. *et al., J. Nat. Prod.*, 1999, **62**, 1322-1324 (*isol, pmr, cmr*)

Heteroxanthin H-217

7′,8′-Didehydro-5,6-dihydro-β,β-carotene-3,3′,5,6-tetrol
[29488-00-4]



$C_{40}H_{56}O_4$ 600.88
Constit. of *Vaucheria* and *Botrydium* spp. and *Mytilus edulis* (blue mussel). Cryst.

6-Epimer: ***6-Epiheteroxanthin***
[64023-28-5]
$C_{40}H_{56}O_4$ 600.88
Constit. of the corbicula clam (Shijimi), *Corbicula japonica*. λ_{max} 420; 443; 472 (Et_2O).

Strain, H.H. *et al., Tet. Lett.*, 1971, 733 (*struct*)
Buchecker, R. *et al., Phytochemistry*, 1977, **16**, 729-733 (*abs config*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1984, **67**, 2043 (*abs config*)
Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495 (*isol, pmr, uv, ms*)
Maoka, T. *et al., J. Nat. Prod.*, 2005, **68**, 1341-1344 (*6-Epiheteroxanthin*)

Hexaaquavanadium(*III*)(3+), 11CI H-218

*Hexaaquovanadium(*III*)*
[21374-21-0]
$[V(OH_2)_6]^{3\oplus}$
$H_{12}O_6V^{3\oplus}$ 159.033
The alums have the β-alum struct.: other salts contain the octahedral hexaaquo ion. A major form of vanadium in the marine organisms *Ascidia ceratodes* and *Phallusia nigra*.

*Trichloride: Vanadium(*III*) chloride hexahydrate*
[16901-56-7]
$Cl_3H_{12}O_6V$ 265.391
Synth. by electrolytic reduction of a soln. of V_2O_5 in conc. HCl which is kept satd. with HCl. Green solid. Paramagnetic, μ_{eff} = 2.787μ_B (300K), 2.666μ_B (77.8K). May be identical to chloride dihydrate of Tetraaquadichlorovanadium(*III*)(1+).

Caesium sulfate (1:1:2) hexahydrate: Caesium vanadium alum
[95246-80-3]
$CsH_{24}O_{20}S_2V$ 592.157
Synth. by electrolytic reduction of V(*V*) in H_2SO_4 soln. in the presence of a Cs salt. Green solid (dil. H_2SO_4).

Ammonium sulfate (1:1:2) hexahydrate: Ammonium vanadium alum
$H_{28}NO_{20}S_2V$ 477.289
Synth. by electrolytic reduction of NH_4VO_3 in H_2SO_4. Blue-violet air-stable solid.

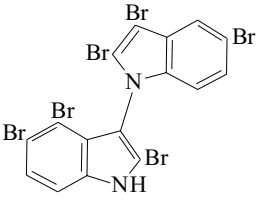
*Guanidinium sulfate (1:1:2): Guanidinium vanadium(*III*) disulfate hexahydrate*
[19497-65-5] Synth. by Zn reduction of V_2O_5 in aq. $H_2C_2O_4$ followed by addition of guanidinium sulfate.
Red-violet solid. Paramagnetic, μ_{eff} = 2.804μ_B (299K), 1.690μ_B (1.96K).

(Oxoniummonohydrate)tetrakis(trifluoromethanesulfonate):
$C_4H_{17}F_{12}O_{20}S_4V$ 792.353
Synth. from Bis(acetic acid)hexakis[μ-(acetato-*O*:*O*′)]-μ_3-oxo (tetrahydrofuran)trivanadium(*III*)(1+) loaded on a Dowex 50Wx2 column and eluting with 2*M* CF_3COOH. Blue-violet solid. Struct. determined by x-ray and not giving particularly precise struct.

Carlin, R.L. *et al., J. Chem. Phys.*, 1967, **47**, 4901 (*synth, magnetism*)
Beattie, J.K. *et al., J.C.S. Dalton*, 1981, 2105 (*cryst struct, alum*)
Lahiry, S. *et al., Chem. Phys. Lett.*, 1982, **89**, 159 (*magnetism*)
Ophardt, C.E. *et al., J. Chem. Educ.*, 1984, **61**, 1102 (*synth, alum*)
Cotton, F.A. *et al., J.A.C.S.*, 1984, **106**, 5319 (*synth, x-ray, nd, trifluoromethanesulfonate*)
Best, S.P. *et al., Chem. Phys. Lett.*, 1985, **122**, 401 (*Raman of ion*)
Frank, P. *et al., J. Inorg. Biochem.*, 2001, **86**, 635-648 (*occur, marine organisms*)
Frank, P. *et al., Coord. Chem. Rev.*, 2003, **237**, 31-39 (*occur, marine organisms*)

2,2′,3,4′,5,5′-Hexabromo-1,3′-bi-1*H*-indole H-219

[81387-87-3]

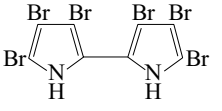


$C_{16}H_6Br_6N_2$ 705.661
Isol. from the marine blue-green alga *Rivularia firma*. Prisms (MeCN).
Mp 263-264°. $[\alpha]_D^{20}$ +18.7 (c, 1 in MeCN). Exhibits opt. activity owing to restricted rotn.

Norton, R.S. *et al., J.A.C.S.*, 1982, **104**, 3628-3635 (*isol, uv, ir, pmr, cmr*)

3,3′,4,4′,5,5′-Hexabromo-2,2′-bi-1*H*-pyrrole H-220

Bistribromopyrrole
[54705-15-6]

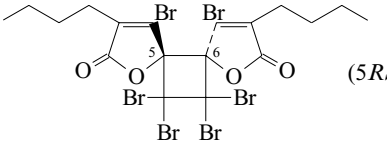


$C_8H_2Br_6N_2$ 605.541
Pyrrole antibiotic. Isol. from marine *Chromobacterium* sp. Active against *Chromobacterium* sp. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. λ_{max} 258 (MeOH) (Berdy). λ_{max} 272 (MeOH/NaOH) (Berdy).

*N,N′-Di-Me: 3,3′,4,4′,5,5′-Hexabromo-1,1′-dimethyl-2,2′-bi-1*H*-pyrrole*
[253798-63-9]
$C_{10}H_6Br_6N_2$ 633.595
Isol. from the eggs of various seabirds.
Mp 247-248°.

Andersen, R.J. *et al., Mar. Biol. (Berlin)*, 1974, **27**, 281 (*isol*)
Gribble, G.W. *et al., Chem. Comm.*, 1999, 2195-2196 (*synth, pmr, ms*)

4,10,11,11,12,12-Hexabromo-3,9-dibutyl-1,7-dioxadispiro[4.0.4.2]dodeca-3,9-diene-2,8-dione, 9CI H-221



(5*RS*,6*RS*)–*form*

$C_{18}H_{18}Br_6O_4$ 777.762

(5*RS*,6*RS*)-*form*
(±)-trans-*form*
[115721-45-4]
Constit. of the red alga *Delisea elegans*.
Needles.
Mp 102-104°.

(5*RS*,6*SR*)-*form*
(±)-cis-*form*
[115721-48-7]
Constit. of *Delisea elegans*.
Plates.
Mp 153-154°.

McCombs, J.D. *et al., Tetrahedron*, 1988, **44**, 1489

1,1,1,15,15,15-Hexachloro-3,12-pentadecadiyn-8-amine H-222

8-Amino-1,1,1,15,15,15-hexachloro-3,12-pentadecadiyne

$Cl_3CCH_2C{\equiv}C(CH_2)_3CH(NH_2)(CH_2)_3C{\equiv}CCH_2CCl_3$

$C_{15}H_{19}Cl_6N$ 426.038

(+)-*form*

N-*Ac: 8-Acetamido-1,1,1,15,15,15-hexachloro-3,12-pentadecadiyne*
[345261-10-1]
$C_{17}H_{21}Cl_6NO$ 468.075
Isol. from the cyanobacterium *Microcoleus lyngbyaceus*. Oil.

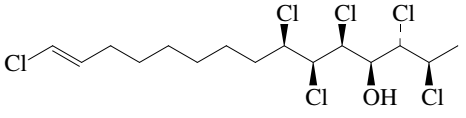
Dechloro, N-*Ac: 8-Acetamido-1,1,1,15,15-pentachloro-3,12-pentadecadiyne*
[345261-09-8]
$C_{17}H_{22}Cl_5NO$ 433.63
Isol. from the cyanobacterium *Microcoleus lyngbyaceus*. Pale yellow oil. $[\alpha]_D$ +36 (c, 0.08 in $CHCl_3$).

15-Dechloro, 3,3,4,4-tetrahydro, N-*Ac: 8-Acetamido-1,1,15,15,15-pentachloro-3-pentadecyne*
[345261-19-0]
$C_{17}H_{26}Cl_5NO$ 437.662
Isol. from the cyanobacterium *Microcoleus lyngbyaceus*. Oil. $[\alpha]_D$ +30 (c, 0.07 in $CHCl_3$).

1,15-Didechloro, 3,3,4,4-tetrahydro, N-*Ac: 8-Acetamido-1,1,15,15-tetrachloro-3-pentadecyne*
[345261-11-2]
$C_{17}H_{27}Cl_4NO$ 403.217
Isol. from the cyanobacterium *Microcoleus lyngbyaceus*. Oil. $[\alpha]_D$ +24 (0.08 in $CHCl_3$).

Orsini, M.A. *et al., J. Nat. Prod.*, 2001, **64**, 572-577 (*isol, ir, pmr, cmr*)

2,3,5,6,7,15-Hexachloro-14-pentadecen-4-ol H-223



$C_{15}H_{24}Cl_6O$ 433.07

(2*R*,3*S*,4*R*,5*S*,6*S*,7*R*,14*E*)-*form*

O-*Sulfate:*
$C_{15}H_{24}Cl_6O_4S$ 513.134
Isol. from Adriatic mussels (*Mytilus galloprovincialis*). Cytotoxic. $[\alpha]_D^{25}$ +20.4 (c, 0.0015 in MeOH).

Ciminiello, P. *et al., J.O.C.*, 2001, **66**, 578-582 (*isol, pmr, cmr, abs config*)

1,1,1,3,3,3-Hexachloro-2-propanone, 9CI H-224

Hexachloroacetone. HCA, WSSA
[116-16-5]
$Cl_3CCOCCl_3$
C_3Cl_6O 264.749
Constit. of *Osmanthus fragrans* (sweet osmanthus). Isol from the alga *Asparagopsis taxiformis*. Source of positive chlorine in enamine reactions. Herbicide, now superseded. Liq. Sl. sol. H_2O. d_{12}^{12} 1.74.
Fp -2. Bp 202-204° Bp_{26} 99-101.5°.
▶ LD_{50} (rat, orl) 1290 mg/kg; LD_{50} (rat, skn) 2980 mg/kg.
UC2100000

Tetrahydrate:
Unstable cryst. Mp 39.5-40.5° (incongruent). Unstable. Previously thought to be a covalent monohydrate.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 418A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 653C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 506C (*ir*)
Ambrus, T. *et al., Rev. Roum. Chim.*, 1963, **14**, 506; *CA*, **60**, 6739 (*manuf*)
Andersen, P. *et al., Acta Chem. Scand., Ser. A*, 1974, **28**, 239 (*struct*)
Hawkes, G.E. *et al., J.O.C.*, 1974, **39**, 1276 (*cmr*)
Japan. Pat., 1974, 7 424 909; *CA*, **80**, 145423b (*synth*)
Schulman, E.M. *et al., J.A.C.S.*, 1976, **98**, 3793 (*hydrate*)
Lee, E.K.C. *et al., Adv. Photochem.*, 1980, **12**, 1 (*rev*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 239 (*use*)
Ding, D. *et al., J. Essent. Oil Res.*, 1989, **1**, 295 (*isol*)
Pesticide Manual, 9th edn., 1991, No. 7060
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2642-2643 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HCL500

5,9-Hexacosadienoic acid H-225

[59708-84-8]
$H_3C(CH_2)_{15}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{26}H_{48}O_2$ 392.664

(5*Z*,9*Z*)-*form* [52715-55-6]
Isol. from *Axinella verrucosa*, *Petrosia ficiformis* and *Trikentrion loeve*. Other stereoisomers have been prepd.

[90913-50-1, 90913-54-5, 90913-61-4, 90913-68-1]

Ayanoglu, E. *et al., Lipids*, 1982, **17**, 617-625 (*isol*)
Lankelma, J. *et al., Lipids*, 1983, **18**, 853-858 (*isol*)
Mena, P.L. *et al., J.O.C.*, 1984, **49**, 3260-3264 (*synth, ir, pmr, ms*)
Hahn, S. *et al., J.A.C.S.*, 1988, **110**, 8117-8124 (*synth, pmr, ms*)
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol*)

9,19-Hexacosadienoic acid H-226

$H_3C(CH_2)_5CH{=}CH(CH_2)_8CH{=}CH(CH_2)_7COOH$
$C_{26}H_{48}O_2$ 392.664

(*Z*,*Z*)-*form* [143883-72-1]
Constit. of *Dysidea fragilis* and *Hymeniacidon sanguinea*.

Christie, W.W. *et al., Lipids*, 1992, **27**, 640-644 (*isol*)
Christie, W.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1994, **109**, 245-252 (*isol*)

15,19-Hexacosadienoic acid H-227

$H_3C(CH_2)_5CH{=}CHCH_2CH_2CH{=}CH(CH_2)_{13}COOH$
$C_{26}H_{48}O_2$ 392.664

(*Z*,*Z*)-*form* [187657-32-5]
Isol. from the sponge *Haliclona cinerea*.

Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*isol, ms*)

17,20-Hexacosadienoic acid H-228

[59708-85-9]
$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CH(CH_2)_{15}COOH$
$C_{26}H_{48}O_2$ 392.664

(*Z*,*Z*)-*form* [76014-34-1]
Found in the marine sponge *Microciona prolifera*.

Me ester:
$C_{27}H_{50}O_2$ 406.691
Ir ν_{CO} 1742 cm^{-1}.

Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206 (*isol*)
Kling, M.R. *et al., J.C.S. Perkin 1*, 1993, 1183 (*synth, ir, ms*)

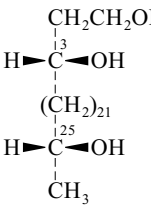
17,21-Hexacosadienoic acid H-229

$H_3C(CH_2)_3CH{=}CHCH_2CH_2CH{=}CH(CH_2)_{15}COOH$
$C_{26}H_{48}O_2$ 392.664

(*Z*,*Z*)-*form* [173866-86-9]
Constit. of the sponge *Pseudaxinella* cf. *lunaecharta*.

Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol, ms*)

1,3,25-Hexacosanetriol H-230



(3*R*,25*R*)–*form*

$C_{26}H_{54}O_3$ 414.711

(3*R*,25*R*)-*form* [142922-39-2]
Amorph. powder. $[\alpha]_D$ +7.7 (c, 0.13 in $CHCl_3$/MeOH).

1-O-α-D-*Glucopyranoside:* [142922-37-0]
$C_{32}H_{64}O_8$ 576.853
Isol. from *Anabaena cylindrica* and from the marine cyanobacterium *Nodularia harveyana*. Powder (EtOH).
Mp 112-114°. $[\alpha]_D$ +40.8 (c, 0.36 in $CHCl_3$/MeOH).

3-Ketone, 1-O-α-D-*glucopyranoside:* [142922-45-0]
$C_{32}H_{62}O_8$ 574.837
Isol. from *Anabaena cylindrica* and *Nodularia harveyana*. Powder. $[\alpha]_D$ +10.7 (c, 0.4 in $CHCl_3$/MeOH).

(3*S*,25*R*)-*form* [142922-40-5]
Amorph. powder. $[\alpha]_D$ +12 (c, 0.1 in $CHCl_3$/MeOH).

1-O-α-D-*Glucopyranoside:* [143004-36-8]
Isol. from *Nodularia harveyana* and the lichen *Solorina crocea*. Powder. $[\alpha]_D$ +40 (c, 0.3 in $CHCl_3$/MeOH).

1-O-β-D-*Glucopyranoside:*
$C_{32}H_{64}O_8$ 576.853
Constit. of *Solorina crocea*.

Soriente, A. *et al., Tetrahedron*, 1992, **48**, 5375-5384 (*Nodularia harveyana constits, isol, pmr, cmr*)
Mori, K. *et al., Annalen*, 1994, 35-39 (*synth, pmr, cmr*)
Soriente, A. *et al., Phytochemistry*, 1995, **38**, 641-645 (*Anabaena cylindrica constits*)
Gambacorta, A. *et al., Phytochemistry*, 1998, **48**, 801-805 (*isol*)

5,9,17-Hexacosatrienoic acid, 9CI H-231

[59708-88-2]
$H_3C(CH_2)_7CH{=}CH(CH_2)_6CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{26}H_{46}O_2$ 390.648

(*all-Z*)-*form*
Component of lipids of the sponge *Microciona prolifera*.
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206 (*occur*)

5,9,19-Hexacosatrienoic acid, 8CI H-232

[59708-89-3]
$H_3C(CH_2)_5CH{=}CH(CH_2)_8CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{26}H_{46}O_2$ 390.648

(5*Z*,9*Z*,19*E*)-*form* [129536-39-6]
Isol. from various freshwater sponges from Lake Baikal.

(5*Z*,9*Z*,19*Z*)-*form* [52715-56-7]
Constit. of marine sponge *Microciona prolifera*.
Jefferts, E. *et al., Lipids*, 1974, **9**, 244 (*ir, nmr, glc*)
Morales, R.W. *et al., Lipids*, 1977, **12**, 570
Vysotskii, M.V. *et al., Tet. Lett.*, 1990, **31**, 4367 (*isol*)

5,9,21-Hexacosatrienoic acid H-233

$H_3C(CH_2)_3CH{=}CH(CH_2)_{10}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{26}H_{46}O_2$ 390.648

(*all-Z*)-*form* [173866-87-0]
Constit. of the sponge *Pseudaxinella* cf. *lunaecharta*.
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol, ms*)

17,20,23-Hexacosatrienoic acid H-234

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_{15}COOH$
$C_{26}H_{46}O_2$ 390.648

(*all-Z*)-*form* [76014-33-0]
Isol. from the sponge *Halichondria panicea*.
Dembitskii, V.M. *et al., Bioorg. Khim.*, 1980, **6**, 1542 (*isol*)

19-Hexacosenal H-235

$H_3C(CH_2)_5CH{=}CH(CH_2)_{17}CHO$
$C_{26}H_{50}O$ 378.68

(*Z*)-*form* [140163-49-1]
Constit. of the sponge *Amphimedon compressa*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1992, **55**, 333

1-Hexacosene H-236

[18835-33-1]
$H_3C(CH_2)_{23}CH{=}CH_2$
$C_{26}H_{52}$ 364.697
Constit. of *Acanthopanax giraldii*, *Aralia elata* (Japanese angelica tree), *Hippophae rhamnoides* and various algae incl. *Chlorella* sp.

Dreisbach, R.R. *et al., Adv. Chem. Ser.*, 1959, **22**, 1 (*props*)
Streibl, M. *et al., Coll. Czech. Chem. Comm.*, 1964, **29**, 2522 (*synth*)
Watanabe, S. *et al., Z. Naturforsch., C*, 1975, **30**, 825 (*isol*)
Tembe, G.L. *et al., Ind. Eng. Chem. Res.*, 1991, **30**, 2247 (*synth*)
Nesterov, G.A. *et al., J. Mol. Catal.*, 1991, **66**, 367 (*synth*)

9-Hexacosenoic acid H-237

[59708-77-9]
$H_3C(CH_2)_{15}CH{=}CH(CH_2)_7COOH$
$C_{26}H_{50}O_2$ 394.68

(*Z*)-*form* [86901-41-9]
Isol. from the marine sponge *Microciona prolifera*.
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206 (*isol*)
Cervilla, M. *et al., Anal. Chem.*, 1983, **55**, 2100 (*ms*)
Lam, W. *et al., J.O.C.*, 1989, **54**, 3428 (*isol*)

11-Hexacosenoic acid H-238

$H_3C(CH_2)_{13}CH{=}CH(CH_2)_9COOH$
$C_{26}H_{50}O_2$ 394.68

(*Z*)-*form* [173866-84-7]
Constit. of the sponge *Pseudaxinella* cf. *lunaecharta*.
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol, ms*)

17-Hexacosenoic acid H-239

[544-84-3]
$H_3C(CH_2)_7CH{=}CH(CH_2)_{15}COOH$
$C_{26}H_{50}O_2$ 394.68

(*Z*)-*form*
Ximenic acid
[66274-43-9]
Isol. from seed fat of *Tropaeolum speciosum* and *Ximenia* spp. Also in fish oil lipids and sponges.
Mp 50.5-50.9°.

Me ester:
$C_{27}H_{52}O_2$ 408.707
Oil.

Lightelm, S.P. *et al., J. Sci. Food Agric.*, 1954, **5**, 281 (*isol, config, bibl*)
Litchfield, C. *et al., Lipids*, 1970, **5**, 144; 1978, **13**, 199 (*isol*)
Kling, M.R. *et al., J.C.S. Perkin 1*, 1993, 1183 (*synth, ir, ms*)

18-Hexacosenoic acid H-240

$H_3C(CH_2)_6CH{=}CH(CH_2)_{16}COOH$

$C_{26}H_{50}O_2$ 394.68

(*Z*)-*form* [128065-63-4]

Isol. from the sponge *Thalysias juniperina*.

Carballeira, N.M. *et al., Lipids*, 1990, **25**, 235 (*isol*)

19-Hexacosenoic acid H-241

[59708-79-1]

$H_3C(CH_2)_5CH{=}CH(CH_2)_{17}COOH$

$C_{26}H_{50}O_2$ 394.68

(*Z*)-*form* [117021-35-9]

Constit. of various sponges incl. *Cinachyrella kükenthali* and *Trikentrion loeve*.

Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol*)
Barnathan, G. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2003, **135**, 297-308 (*isol*)

21-Hexacosenoic acid H-242

$H_3C(CH_2)_3CH{=}CH(CH_2)_{19}COOH$

$C_{26}H_{50}O_2$ 394.68

(*Z*)-*form* [97761-96-1]

Isol. from the sponge *Haliclona cinerea*. Constit. of seed oil of *Grevillea decora*.

Kleiman, R. *et al., Lipids*, 1985, **20**, 373 (*isol*)
Joh, Y.-G. *et al., Lipids*, 1997, **32**, 13-17 (*isol*)

3,13-Hexadecadiene-1,15-diyne H-243

$HC{\equiv}CCH{=}CH(CH_2)_8CH{=}CHC{\equiv}CH$

$C_{16}H_{22}$ 214.35

(3*Z*,13*Z*)-*form*

Callydiyne

[137319-24-5]

Isol. from the sponge *Callyspongia flammea*.

Oil.

Miao, S. *et al., J. Nat. Prod.*, 1991, **54**, 1433 (*isol, pmr, cmr, ms, struct*)

13,15-Hexadecadiene-2,4-diyn-1-ol, 9CI H-244

[125906-54-9]

$H_2C{=}CHCH{=}CH(CH_2)_7C{\equiv}CC{\equiv}CCH_2OH$

$C_{16}H_{22}O$ 230.349

Isol. from hermatypic corals *Montipora* sp. and *Pectinia lactuca*. Shows ichthyotoxicity and antimicrobial activity. Sol. MeOH, Me_2CO.

Higa, T. *et al., Chem. Lett.*, 1990, 145 (*isol, struct*)

5,9-Hexadecadienoic acid H-245

[63317-99-7]

[25377-52-0]

$H_3C(CH_2)_5CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$

$C_{16}H_{28}O_2$ 252.396

Isol. from the sponges *Chondrilla nucula* and *Xestospongia muta* and the slime mold *Dictyostelium discoideum*.

[28933-88-2, 129596-72-1]

Carballeira, N.M. *et al., Lipids*, 1986, **21**, 470-471; 1988, **23**, 682 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2002, **65**, 1715-1718 (*synth, activity*)

6,9-Hexadecadienoic acid H-246

[4780-50-1]

[25377-52-0]

$H_3C(CH_2)_5CH{=}CHCH_2CH{=}CH(CH_2)_4COOH$

$C_{16}H_{28}O_2$ 252.396

(*Z,Z*)-*form*

[28933-88-2]

A minor component of rat liver lipids and of some fish lipids. Metab. of 9-Hexadecenoic acid, H-263.

Schmitte, B. *et al., Lipids*, 1977, **12**, 307
Moreno, V.J. *et al., Lipids*, 1979, **14**, 15

7,11-Hexadecadien-1-ol, 9CI H-247

[59741-58-1]

$H_3C(CH_2)_3CH{=}CHCH_2CH_2CH{=}CH(CH_2)_5CH_2OH$

$C_{16}H_{30}O$ 238.412

The acetate (mixt. of *E*- and *Z*-isomers) is known as Gossyplure. Sex pheromone of *Sitotroga cerealella*.

(*all-E*)-*form* [53963-09-0]

Constit. of *Lobophytum crassum*.

Ac: [53042-81-2]
$C_{18}H_{32}O_2$ 280.45
$Bp_{0.12}$ 97-99° $Bp_{0.05}$ 118°.

(7*Z*,11*E*)-*form* [56879-24-4]
$Bp_{0.35}$ 121-122°.

Ac: [51607-94-4]

Pheromone of the pink bollworm *Pectinophora gossypiella*. $Bp_{0.5}$ 135-136° $Bp_{0.08}$ 92-94°.

▶ ML7001000

(7*Z*,11*Z*)-*form* [53963-06-7]
$Bp_{0.2}$ 118°.

Ac: [52207-99-5]

Pheromone for the pink bollworm *Pectinophora gossypiella*. $Bp_{0.05}$ 86-89°.

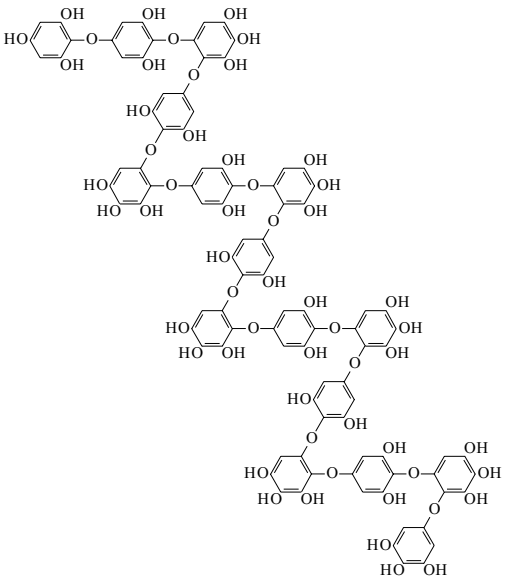
▶ ML7002000

[50933-33-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 636B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 969B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 667D (*ir*)
Mori, K. *et al., Agric. Biol. Chem.*, 1974, **38**, 1551 (*synth*)
Vick, K.W. *et al., Experientia*, 1974, **30**, 17
Mori, K. *et al., Tetrahedron*, 1975, **31**, 1846 (*synth, ir, pmr*)
Disselnkötter, H. *et al., Tetrahedron*, 1976, **32**, 1591 (*synth*)
Rossi, R. *et al., Tetrahedron*, 1982, **38**, 639 (*cmr*)
Michelot, D. *et al., Synthesis*, 1983, 130 (*synth*)
Andelic, I. *et al., Acta Chem. Scand., Ser. B*, 1985, **39**, 231 (*synth*)
Matveeva, E.D. *et al., Zh. Org. Khim.*, 1994, **30**, 961 (*synth*)
Odinokov, V.N. *et al., Khim. Prir. Soedin.*, 1998, **34**, 231-234; *Chem. Nat. Compd. (Engl. Transl.)*, 1998, **34**, 186-188 (*synth*)
Pesticide Manual, 12th edn., 2000, No. 408 (*gossyplure*)
Yin, S.-W. *et al., Helv. Chim. Acta*, 2006, **89**, 567-572 (*Lobophytum, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GJK000

Hexadecafuhalol A H-248

[164176-34-5]



$C_{96}H_{66}O_{56}$ 2115.544
Constit. of the brown alga *Sargassum spinuligerum*.

Glombitza, K.-W. *et al., Phytochemistry*, 1995, **38**, 987-995 (*isol, pmr, cmr, ms*)

Hexadecanoic acid H-249

Palmitic acid, USAN. Aethalic acid. FEMA 2832
[57-10-3]
$H_3C(CH_2)_{14}COOH$
$C_{16}H_{32}O_2$ 256.428
Occurs in the form of esters (glycerides) in oils and fats of vegetable and animal origin, e.g. present in lipids of *Physalia physalis* (Portuguese-man-of-war). Usually obt. from palm oil. Widely distributed in plants. Used in detn. of water hardness. Active ingredient of Levovist™, used in echo enhancement in sonographic Doppler B-mode imaging. Ultrasound contrast medium. Cryst.
Mp 63-64°. Bp 390° Bp_{100} 268.5° Bp_{15} 215°.
▶ Skin irritant. LD_{50} (mus, ivn) 57 mg/kg. RT4550000

[408-35-5, 542-42-7, 2624-31-9, 4991-47-3]

Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*Physalia physalis constit*)

1-Hexadecanol H-250

Cetyl alcohol, USAN. *Cetanol. Palmityl alcohol. Hexadecyl alcohol. Hyfatol 16. FEMA 2554*
[36653-82-4]
[29354-98-1]
$H_3C(CH_2)_{14}CH_2OH$
$C_{16}H_{34}O$ 242.444
Occurs chiefly in the form of esters in waxes of which spermaceti (from the head oil of the sperm whale) is the most important, also in many glycerides. Used in cosmetics industry as emulsifying and stiffening agent. Pharmaceutical aid.
Mp 50°. Bp 334° Bp_{12} 178-182°.
▶ Eye and skin irritant. LD_{50} (rat, orl) 6400 mg/kg. MM0225000

Hydrogen sulfate: Hexadecyl sulfate. Cetyl sulfate
[1120-01-0]
$C_{16}H_{34}O_4S$ 322.508
Detergent, wetting agent (as Na salt). Trimorphic cryst. (Na salt). Mp 25-26° Mp 30-31° Mp 40-41°. CAS no. refers to Na salt (sodium dodecyl sulfate).

O-*[2,3,4-Tri*-O-*acetyl-α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* ***Cupanioside***
$C_{34}H_{60}O_{13}$ 676.84
Constit. of the bark of *Cupania glabra*. Cytotoxic. Cryst. $[\alpha]_D^{26}$ -46.9.

O-*[β-D-Arabinopyranosyl-(1→4)-β-D-arabinopyranosyl-(1→4)-β-D-arabinopyranoside]:* ***Cervicoside***
[454234-57-2]
$C_{31}H_{58}O_{13}$ 638.791
Isol. from *Sinularia cervicornis*. Cytotoxic.

O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranosyl-(1→3)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:*
$C_{40}H_{74}O_{19}$ 859.013
Constit. of *Dimocarpus fumatus.*
$[\alpha]_D$ -37.2 (c, 0.49 in MeOH).

O-*[α-L-Rhamnopyranosyl-(1→2)[α-L-arabinopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→3)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:*
$C_{45}H_{82}O_{23}$ 991.129
Constit. of *Dimocarpus fumatus.*
$[\alpha]_D$ -26.7 (c, 0.22 in MeOH).

Ac: [629-70-9]
$C_{18}H_{36}O_2$ 284.481
Component of the hair pencil secretion of male butterflies *Lycorea ceres ceres*. Dimorph.
Mp 24.2°. Bp_{205} 220-225° Bp_{15} 200°.

4-Nitrobenzoyl: Mp 68.4°.

Vinyl ether: 1-(Ethenyloxy)hexadecane, 9CI. Hexadecyl vinyl ether, 8CI
[822-28-6]
$C_{18}H_{36}O$ 268.482
Liq. d_4^{20} 0.83. Bp_1 142°. n_D^{20} 1.4468.

[124-29-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 113A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 168A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 159B (*ir*)
Org. Synth., 1930, **10**, 62 (*synth*)
Rawlings, F.F. *et al., J.A.C.S.*, 1955, **77**, 870-872 (*sodium dodecyl sulfate, synth, cryst struct*)
Reppe, A. *et al., Annalen*, 1956, **601**, 84 (*vinyl ether*)
Meinwald, J. *et al., J.A.C.S.*, 1966, **88**, 1305
Dolejs, L. *et al., Org. Mass Spectrom.*, 1968, **1**, 563 (*ms*)
Geiseler, G. *et al., Spectrochim. Acta A*, 1968, **24**, 1007 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 683 (*rev, tox*)
Rossi, R. *et al., Tetrahedron*, 1982, **38**, 639 (*cmr*)
Kartha, V.B. *et al., Can. J. Chem.*, 1984, **62**, 128-132 (*sodium dodecyl sulfate, synth, ir, Raman*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HCP000
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 99-103
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 326
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1408
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1286-1288
Voutquenne, L. *et al., Phytochemistry*, 1999, **50**, 63-69 (*Dimocarpus glycosides*)
He, X.-X. *et al., Zhongshan Daxue Xuebao Ziran Kexueban*, 2002, **41**, 114-116; *CA*, **137**, 198514j (*Curvicoside*)
Setzer, W.N. *et al., Planta Med.*, 2005, **71**, 686-688 (*Cupanioside*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HCP000

Hexadecanol dehydrogenase H-251

E.C. 1.1.1.164. Hexadecanol:NAD⊕ oxidoreductase
[62213-59-6]
Oxidoreductase enzyme. Isol. from rat liver and *Euglena gracilis.* Catalyses the reversible reaction of 1-Hexadecanol, H-250 with $NAD^{\oplus}$ to give Hexadecanal and NADH. The rat liver enzyme acts on C_8-C_{16} primary alcohols; the *Euglena* enzyme oxidises the aldehyde to the carboxylic acid.

Kolattukudy, P.E. *et al., Biochemistry*, 1970, **9**, 1095-1102 (*isol, Euglena*)
Springer Handbook of Enzymes, (ed. Schomburg, D. *et al*), Springer-Verlag, 2004, **18**, 43-45 (*rev*)

2-Hexadecanone H-252

Methyl tetradecyl ketone
[18787-63-8]
$H_3C(CH_2)_{13}COCH_3$
$C_{16}H_{32}O$ 240.428
Isol. from hop oil (*Humulus lupulus*) and the marine sponge *Spheciospongia vagabunda*. Prod. by a marine bacterium. Cryst. Mp 43-43.5°. Bp_{100} 130-131°.

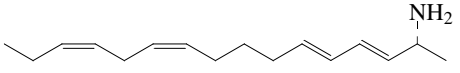
▶ MM0300000

Semicarbazone:
Cryst. (EtOH). Mp 117-118°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 642C (*nmr*)
Jahnsen, V.J. *et al., Nature (London)*, 1962, **196**, 474 (*isol*)
Klein, D.A. *et al., Appl. Microbiol.*, 1969, **17**, 676
Bailey, A.V. *et al., J. Chem. Eng. Data*, 1970, **15**, 542
Wyrick, S.D. *et al., J. Med. Chem.*, 1976, **19**, 219 (*synth*)
Villemin, D. *et al., Synth. Commun.*, 2002, **32**, 1501-1515 (*synth*)
Xiao, D. *et al., Fenxi Huaxue*, 2004, **32**, 1621-1623; *CA*, **143**, 23210 (*Spheciospongia vagabunda constit*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol*)

3,5,10,13-Hexadecatetraen-2-amine H-253

2-Amino-3,5,10,13-hexadecatetraene



$C_{16}H_{27}N$ 233.396

(2*R*,3*E*,5*E*,10*Z*,13*Z*)-*form* [356073-88-6]
Isol. from a *Pseudodistoma* sp.
Oil. $[\alpha]_D$ -6 (c, 0.05 in MeOH). λ_{max} 229 (log ϵ 3.38) (MeOH).
Rashid, M.A. *et al., Tetrahedron*, 2001, **57**, 5751-5755 (*Pseudodistoma constit, isol, ir, pmr, cmr, uv*)

4,7,10,13-Hexadecatetraenoic acid H-254

[3209-28-7]
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH_2COOH$
$C_{16}H_{24}O_2$ 248.364

(all-*Z*)-*form* [29259-52-7]
Isol. from *Chlorella* spp., *Euglena gracilis, Scenedesmus* spp. and *Ulva fasciata*.
Liq. $Bp_{0.0001}$ 76°.

[25377-57-5]

Paschke, R.F. *et al., J. Am. Oil Chem. Soc.*, 1954, **31**, 81 (*isol, struct*)
Klenk, E. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1959, **317**, 243 (*isol, struct*)
Alamsjah, M.A. *et al., Biosci., Biotechnol., Biochem.*, 2005, **69**, 2186-2192 (*isol, pmr, cmr*)

6,9,12,15-Hexadecatetraenoic acid, 9CI H-255

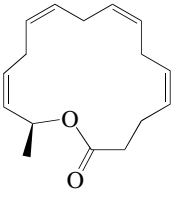
[74838-22-5]
$H_2C{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_4COOH$
$C_{16}H_{24}O_2$ 248.364

(6*Z*,9*Z*,12*Z*)-*form* [86995-95-1]
Isol. from fish oils, the diatoms *Navicula delognei*, *Pseudonitzschia multiseries* and *Pseudonitzschia pungens* and numerous other marine sources.
Liq.
Mp -57.4–56.6°. n_D^{16} 1.4888.
Me ester: [94035-78-6]
$C_{17}H_{26}O_2$ 262.391
Isol. from *Navicula delognei*. Oil.

Silk, M.H. *et al., Biochem. J.*, 1954, **57**, 574-577 (*isol*)
Findlay, J.A. *et al., J. Nat. Prod.*, 1984, **47**, 815-818 (*isol*)
Budge, S.M. *et al., Phytochemistry*, 1999, **52**, 561-566 (*isol*)
Pohnert, G. *et al., Chem. Phys. Lipids*, 2004, **131**, 159-166 (*synth*)

4,7,10,13-Hexadecatetraen-15-olide H-256

Aplyolide A†
[192935-65-2]



$C_{16}H_{22}O_2$ 246.349
Isol. from the marine mollusc *Aplysia depilans*. Ichthyotoxin. Oil. $[\alpha]_D^{25}$ -57.9 (c, 0.4 in $CHCl_3$).

Spinella, A. *et al., J.O.C.*, 1997, **62**, 5471-5475 (*isol, ir, pmr, cmr, ms*)

7,10,13-Hexadecatrienal H-257

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_5CHO$
$C_{16}H_{26}O$ 234.381

(*all-Z*)-*form*
Isol. from the marine red alga *Ulva pertusa*.
Oil.

Akakabe, Y. *et al., Biosci., Biotechnol., Biochem.*, 2005, **69**, 1348-1352 (*synth, pmr, cmr*)

6,10,14-Hexadecatrienoic acid H-258

Hiragonic acid
[4444-12-6]
[32839-24-0]
$H_3CCH{=}CHCH_2CH_2CH{=}CHCH_2CH_2CH{=}CH(CH_2)_4COOH$
$C_{16}H_{26}O_2$ 250.38
Constit. of *Clupea sprattus* and red alga *Hypnea musciformis*.

Viviani, R. *et al., CA*, 1969, **71**, 47002h (*isol*)
Siddiqui, S. *et al., Pak. J. Pharm. Sci.*, 1993, **6**, 45-51 (*occur, Hypnea*)

7,10,13-Hexadecatrienoic acid H-259

[2271-35-4]
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_5COOH$
$C_{16}H_{26}O_2$ 250.38

(*Z,Z,Z*)-*form* [7561-64-0]
[32839-24-0]
Present in a wide variety of angiosperm leaves, also in lipids of ferns and green algae. Isol. from the sponge *Dysidea fragilis*.

Heyes, J.K. *et al., Biochem. J.*, 1951, **49**, 503 (*struct*)
Radunz, A. *et al., Phytochemistry*, 1967, **6**, 399 (*isol*)
Jamieson, G.R. *et al., Phytochemistry*, 1971, **10**, 1837 (*occur, bibl*)
Christie, W.W. *et al., Lipids*, 1992, **27**, 640-644 (*Dysidea, isol*)
Mongrand, S. *et al., Phytochemistry*, 1998, **49**, 1049-1064 (*occur*)

8,11,14-Hexadecatrienoic acid H-260

$H_3CCH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_6COOH$
$C_{16}H_{26}O_2$ 250.38

(*all-Z*)-*form* [109031-12-1]
[32839-24-0]
Constit. of *Lemna trisulca* and the lipid fractions of *Dunaliella acidophila*.

Monaco, P. *et al., Phytochemistry*, 1987, **26**, 745 (*isol*)
Della Greca, M. *et al., Biochim. Biophys. Acta*, 1989, **1004**, 271 (*isol*)

3-Hexadecenoic acid, 9CI H-261

[25447-95-4]

$H_3C(CH_2)_{11}CH{=}CHCH_2COOH$

$C_{16}H_{30}O_2$ 254.412

(*E*)-*form* [1686-10-8]

Constit. of many plant systems including spinach leaves, red clover (*Trifolium pratense*) (as phosphatidylglycerol ester) and *Aster* spp. Other major sources are seed oils of *Grindelia oxylepis* and *Helenium bigelovii*. Also isol. from algae.

Mp 53-54°.

[28039-99-8]

Klenk, E. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1963, **334**, 44 (*isol*)
Weenik, R.O. *et al., Biochim. Biophys. Acta*, 1964, **84**, 613
Hopkins, C.Y. *et al., Can. J. Chem.*, 1964, **42**, 2224 (*isol*)
Haverkate, F. *et al., Experientia*, 1964, **20**, 511
Kleiman, R. *et al., Lipids*, 1966, **1**, 301 (*isol*)
Knipprath, W. *et al., Lipids*, 1966, **1**, 81 (*synth*)
Kannan, R. *et al., Fette, Seifen, Anstrichm.*, 1974, **76**, 344 (*pmr*)

6-Hexadecenoic acid, 9CI H-262

[2197-46-8]

[25447-95-4]

$H_3C(CH_2)_8CH{=}CH(CH_2)_4COOH$

$C_{16}H_{30}O_2$ 254.412

(*E*)-*form* [28290-76-8]

Constit. of seed oil of parsley and *Picramnia sellowii*. Also present in adipose tissue and skin. Widely distributed in marine animals, such as sunfish, *Mola mola*, spadefish *Chaetodipterus faber*, jellyfish *Physalia physalis* and *Aurelia aurita*, the frilled anemone *Metridium dianthus* and turtles *Demochelys coriacea coriacea*, *Coretta coretta coretta* and *Lepichelys olivacea*.

(*Z*)-*form* [17004-51-2]

[28039-99-8]

Present in seed oils of *Thunbergia alata* and *Picramnia sellowii*.

Spencer, G.F. *et al., Lipids*, 1971, **6**, 712-714 (*Z-form, isol*)
Hooper, S.N. *et al., Lipids*, 1972, **7**, 624-626; 1973, **8**, 509-551 (*E-form, isol, occur*)
Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*E-form, occur*)
Pearce, R.E. *et al., Lipids*, 1976, **11**, 247-249 (*E-form, occur*)

9-Hexadecenoic acid, 9CI H-263

Hypogaic acid

[2091-29-4]

[25447-95-4]

$H_3C(CH_2)_5CH{=}CH(CH_2)_7COOH$

$C_{16}H_{30}O_2$ 254.412

Present in lipids of *Physalia physalis* (Portuguese-man-of-war).

(*E*)-*form*

Palmitelaidic acid

[10030-73-6]

Constit. of many plant and animal systems, e.g. isol. from *Vespula pensylvanica*, *Sopubia delphinipholia*, *Saccharomyces cerevisiae*, *Phormidium tenue*, *Trichosporon* sp., *Kluyveromyces polysporus*, *Navicula* sp. Pheromone of hide beetle *Dermestes maculatus*. Germination inducer, blood vessel protectant, shows anticaries props, algicide.

Mp 32-33°.

▶ LD_{50} (mus, iabd) 300-700 mg/kg.

(*Z*)-*form*

Palmitoleic acid. Zoomaric acid. Physetoleic acid

[373-49-9]

[28039-99-8]

A major component of lipids of marine plants and animals, also found in plant oils, e.g. *Macadamia ternifolia* (small-fruited Macadamia nut) seed oil (20%).

Mp 0.5°. Bp_1 180-183° $Bp_{0.6}$ 162°. n_D^{20} 1.4582.

Me ester: [1120-25-8]

$C_{17}H_{32}O_2$ 268.439

Liq. Bp_5 140-141°.

Et ester: [56219-10-4]

$C_{18}H_{34}O_2$ 282.465

Constit. of labial gland of the bumblebee *Bombus lucarum*.

Isopropyl ester: Isopropyl 9-hexadecenoate

[68862-23-7]

$C_{19}H_{36}O_2$ 296.492

Sex pheromone for male *Aleochara curtula* and *Dermestes maculatus*.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 782B; 986C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 587D (*ir*)
Armstrong, E.F. *et al., J. Soc. Chem. Ind., London*, 1925, **44**, 182T
Bridge, R.E. *et al., J.C.S.*, 1950, 2396-2399 (*isol*)
Boughton, B.W. *et al., J.C.S.*, 1952, 671-677 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 734 (*occur*)
Suzuki, T. *et al., Agric. Biol. Chem.*, 1974, **38**, 2269-2271 (*occur, ir, ms*)
Batchelor, J.G. *et al., J.O.C.*, 1974, **39**, 1698-1705 (*cmr*)
Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*Physalia physalis constit*)
Francke, W. *et al., Angew. Chem., Int. Ed.*, 1979, **18**, 796-797 (*isopropyl ester, isol*)
Mannan, A. *et al., Chem. Ind. (London)*, 1984, 851 (*Z-form, isol*)
Peschke, K. *et al., Chemoecology*, 1999, **9**, 47-54 (*isopropyl ester, isol*)
Urbanova, K. *et al., Eur. J. Entomol.*, 2001, **98**, 111-115 (*Z-form, Et ester, isol*)

11-Hexadecenoic acid H-264

Lycopodiumoleic acid. Tanacetumoleic acid. Palmitvaccenic acid

[2271-34-3]

[25447-95-4]

$H_3C(CH_2)_3CH{=}CH(CH_2)_9COOH$

$C_{16}H_{30}O_2$ 254.412

(*E*)-*form* [73292-39-4]

Isol. from *Chrysanthemum vulgare* (tansy), *Lycopodium vulgare*, etc. Bp_{18} 235-240°.

(*Z*)-*form* [2416-20-8]

[28039-99-8]

Present as minor component in many bacterial and animal lipids. Constit. of *Plakortis halichondrioides* and other sponges. Surface-active agent, inhibitor of fruiting body formation in microorganisms. Sol. MeOH, hexane; poorly sol. H_2O.

Ackman, R.G. *et al., Lipids*, 1966, **1**, 341 (*occur*)
Walker, R.W. *et al., Lipids*, 1969, **4**, 15 (*occur*)
Nichols, P.D. *et al., J. Microbiol. Methods*, 1986, **5**, 49
Carballeira, N.M. *et al., Lipids*, 1990, **25**, 835-840 (*marine, isol*)

8-Hexadecen-2-one H-265

$H_3C(CH_2)_6CH{=}CH(CH_2)_5COCH_3$

$C_{16}H_{30}O$ 238.412

(*Z*)-*form*

Prod. by a marine bacterium.

Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol, synth, pmr, cmr, ms*)

10-Hexadecen-2-one H-266

$H_3C(CH_2)_4CH{=}CH(CH_2)_7COCH_3$

$C_{16}H_{30}O$ 238.412

(*Z*)-*form*

Prod. by a marine bacterium.

Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol, synth, pmr, cmr, ms*)

12-Hexadecen-2-one H-267

$H_3CCH_2CH_2CH{=}CH(CH_2)_9COCH_3$

$C_{16}H_{30}O$ 238.412

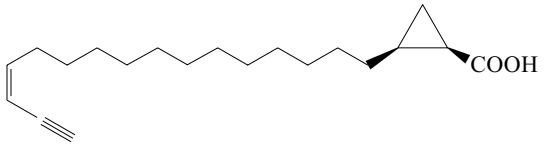
(Z)-form

Prod. by a marine bacterium.

Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol, pmr, cmr, ms, synth*)

2-(13-Hexadecen-15-ynyl)cyclopropanecarboxylic acid H-268

2,3-Methylene-16-nonadecen-18-ynoic acid. ***Cladocroic acid***



$C_{20}H_{32}O_2$ 304.472

(1R*,2S*,13Z)-form [148054-06-2]

Isol. from the sponge *Cladocroce incurvata*.

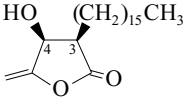
$[\alpha]_D$ +14.3.

D'Auria, M.V. *et al., J. Nat. Prod.*, 1993, **56**, 418 (*isol, pmr, cmr*)

3-Hexadecyldihydro-4-hydroxy-5-methylene-2(3*H*)-furanone, 9CI H-269

2-Hexadecyl-3-hydroxy-4-penten-4-olide

[81576-08-1]



$C_{21}H_{38}O_3$ 338.529

(3R*,4S*)-form

Isol. from the gorgonian *Plexaura flava*.

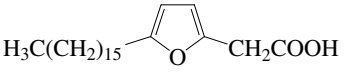
Wax. $[\alpha]_D^{20}$ +2.8 (c, 1.4 in CH_2Cl_2).

Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 105 (*isol, ir, pmr, ms*)

Dalla, V. *et al., Tet. Lett.*, 1994, **35**, 3525 (*synth*)

5-Hexadecyl-2-furanacetic acid H-270

3,6-Epoxy-3,5-docosadienoic acid. ***Plakorsin B***



$C_{22}H_{38}O_3$ 350.54

Isol. from *Plakortis simplex*. Cytotoxic. Amorph. solid. λ_{max} 221 (log ϵ 2.93); 242 (log ϵ 1.39); 283 (log ϵ 2.34) (MeOH).

Me ester: ***Plakorsin A***

$C_{23}H_{40}O_3$ 364.567

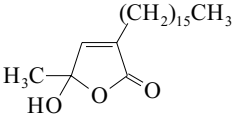
Isol. from *Plakortis simplex*. Oil. λ_{max} 220 (log ϵ 3.13); 281 (log ϵ 2.41) (MeOH).

Shen, Y.-C. *et al., J. Nat. Prod.*, 2001, **64**, 324-327

3-Hexadecyl-5-hydroxy-5-methyl-2(5*H*)-furanone H-271

2-Hexadecyl-4-hydroxy-4-methyl-2-buten-4-olide. ***Flavalactone 1***

[81346-95-4]



$C_{21}H_{38}O_3$ 338.529

Isol. from the Japanese gorgonian *Euplexaura flava*. Granulation inhibitor. Antiinflammatory agent. Needles (MeOH). Sol. MeOH, Me_2CO, EtOAc; poorly sol. H_2O.

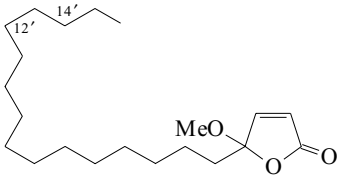
Mp 67°. λ_{max} 224 (ϵ 4500) (MeOH) (Derep).

Kituchi, H. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1172-1176 (*isol, ir, pmr, cmr*)

5-Hexadecyl-5-methoxy-2(5*H*)-furanone H-272

4-Methoxy-2-eicosen-4-olide

[131985-20-1]



$C_{21}H_{38}O_3$ 338.529

Constit. of the sponge *Plakortis lita*. Solid.

Mp 34.5-35.5° Mp 69° (synthetic). $[\alpha]_D$ -13.9 (c, 0.43 in CH_2Cl_2).

*14′,15′-Didehydro (*E-*): 5-(14-Hexadecenyl)-5-methoxy-2(5*H*)-furanone. 4-Methoxy-2,18-eicosadien-4-olide*

[131985-21-2]

$C_{21}H_{36}O_3$ 336.514

Constit. of *Plakortis lita*. Solid.

Mp 52-53°. $[\alpha]_D$ -13.7 (c, 0.71 in CH_2Cl_2).

*12′,13′,14′,15′-Tetradehydro (*E,E-*): 5-(12,14-Hexadecadienyl)-5-methoxy-2(5*H*)-furanone. 4-Methoxy-2,16,18-eicosatrien-4-olide*

[131985-22-3]

$C_{21}H_{34}O_3$ 334.498

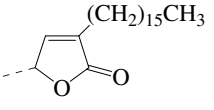
Constit. of *Plakortis lita*.

De Guzman, F.S. *et al., J. Nat. Prod.*, 1990, **53**, 926 (*isol, pmr, cmr, struct*)

Miller, M. *et al., J.O.C.*, 1993, **58**, 6779 (*synth*)

3-Hexadecyl-5-methyl-2(5*H*)-furanone H-273

2-Hexadecyl-2-penten-4-olide



$C_{21}H_{38}O_2$ 322.53

(R)-form

Isol. from the gorgonian *Pterogorgia anceps.*

Amorph. powder. $[\alpha]_D$ -12.7 (c, 1.9 in dioxan). $[\alpha]_D$ -11.9 (c, 2.5 in $CHCl_3$). λ_{max} 214 (ϵ 3800) (EtOH).

Guo, Y.-W. *et al., J. Nat. Prod.*, 1999, **62**, 1194-1196 (*isol, uv, pmr, cmr*)

7-Hexadecynoic acid, 9CI H-274

Palmitolic acid

[629-57-2]

$H_3C(CH_2)_7C{\equiv}C(CH_2)_5COOH$

$C_{16}H_{28}O_2$ 252.396

Found in some fish liver oils. Cryst.

Mp 38-39° Mp 47°. $Bp_{0.6}$ 160-163°.

Me ester: [39077-31-1]

$C_{17}H_{30}O_2$ 266.423

$Bp_{0.05}$ 102°.

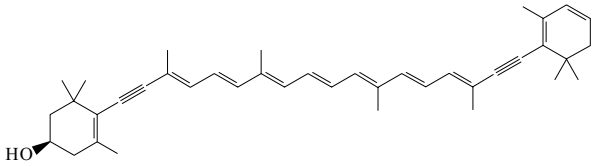
[73374-89-7]

Ames, D.E. *et al., J.C.S.*, 1963, 775-778 (*synth*)

Williams, J.L. *et al., Chem. Phys. Lipids*, 1972, **9**, 295-308; 320-331 (*Me ester, synth, pmr*)

3′,4′,7,7′,8,8′-Hexadehydro-β,β-caroten-3-ol H-275

[116107-37-0]



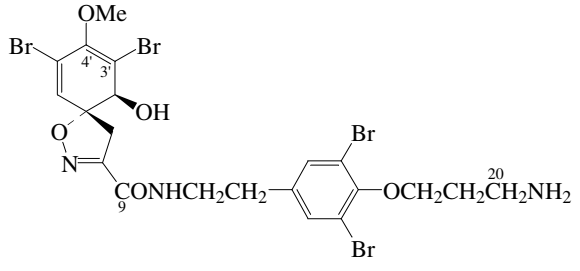
$C_{40}H_{50}O$ 546.834

Occurs as esters in *Euglena viridis*. λ_{max} 457 (no solvent reported).

Fiksdahl, A. *et al., Phytochemistry*, 1988, **27**, 1447 (*occur, uv, ms, pmr*)

Hexadellin B H-276

[121135-01-1]



$C_{21}H_{23}Br_4N_3O_5$ 717.046

Alkaloid from the deep water sponge *Hexadella* sp.

N^{20}-*Me:* ***Purealidin S***

$C_{22}H_{25}Br_4N_3O_5$ 731.073

Alkaloid from the Fijian sponge *Druinella* sp. Cytotoxic. Oil. λ_{max} 280 (log ϵ 3.28) (MeOH).

N^{20},N^{20}-*Di-Me:* ***Purealidin Q***

[167394-82-3]

$C_{23}H_{27}Br_4N_3O_5$ 745.099

Alkaloid from the Okinawan sponge *Psammaplysilla purea*. Cytotoxic agent. Enzyme inhibitor. Oil (as trifluoroacetate). Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{19}$ +9.1 (c, 0.39 in MeOH). λ_{max} 277 (ϵ 1700); 284 (ϵ 1380) (MeOH) (Berdy).

N^{20}-*(13-Methyltetradecanoyl):* ***Purpurealidin C***

[799246-88-1]

$C_{36}H_{51}Br_4N_3O_6$ 941.431

Isol. from *Psammaplysilla purpurea*. Oil. $[\alpha]_D^{28}$ +158.5 (c, 0.2 in $CHCl_3$). λ_{max} 218 (ϵ 2500); 282 (ϵ 10000) (MeOH).

N^{20}-*Hexadecanoyl:* ***Purpurealidin D***

[799246-89-2]

$C_{37}H_{53}Br_4N_3O_6$ 955.458

Isol. from *Psammaplysilla purpurea*. Oil. λ_{max} 218 (ϵ 2500); 282 (ϵ 10000) (MeOH).

3′ξ,4′ξ-Dihydro, N^{9},N^{20},N^{20}-*tri-Me:* ***Purpurealidin A***

[799246-86-9]

$C_{24}H_{31}Br_4N_3O_5$ 761.142

Isol. from the sponge *Psammaplysilla purpurea*. Oil. $[\alpha]_D^{28}$ +9.5 (c, 0.2 in MeOH). λ_{max} 277 (ϵ 1700); 284 (ϵ 1400) (MeOH).

Morris, S.A. *et al., Can. J. Chem.*, 1989, **67**, 677 (*isol, ir, pmr, cmr, ms, struct*)

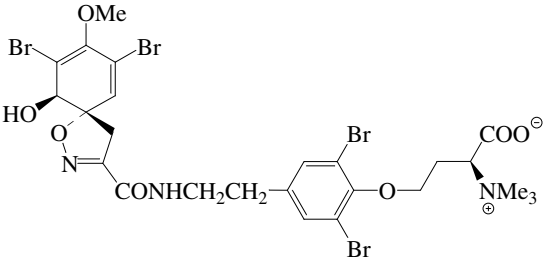
Kobayashi, J. *et al., Chem. Pharm. Bull.*, 1995, **43**, 403 (*Purealidin Q*)

Tabudravu, J.N. *et al., J. Nat. Prod.*, 2002, **65**, 1798-1801 (*Purealidin S*)

Tilvi, S. *et al., Tetrahedron*, 2004, **60**, 10207-10215 (*Purpurealidins A,C,D, Purealidin Q*)

Hexadellin C H-277

[245436-91-3]



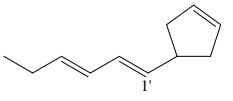
$C_{25}H_{29}Br_4N_3O_7$ 803.136

Zwitterionic. Isol. from the sponge *Aiolochroia crassa*. Amorph. solid. $[\alpha]_D$ +102 (c, 0.07 in MeOH). λ_{max} 207 (ϵ 8300); 284 (ϵ 1200) (EtOH).

Gao, H. *et al., Tetrahedron*, 1999, **55**, 9717-9726

4-(1,3-Hexadienyl)-1-cyclopentene H-278

1-(3-Cyclopenten-1-yl)-1,3-hexadiene



(1′*E*,3′*E*)-*form*

$C_{11}H_{16}$ 148.247

(1′E,3′E)-form [143520-77-8]

Constit. of the brown alga *Dictyopteris acrostichoides*.

3′,4′-Dihydro: ***4-(1-Hexenyl)-1-cyclopentene***. *1-(3-Cyclopenten-1-yl)-1-hexene*

[107531-28-2]

$C_{11}H_{18}$ 150.263

Constit. of *Dictyopteris* spp. and *Scytosiphon lomentaria*.

(1′E,3′Z)-form [143520-76-7]

Constit. of *Dictyopteris acrostichoides*.

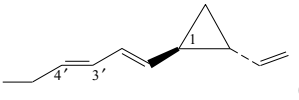
Kajiwara, T. *et al., Phytochemistry*, 1989, **28**, 636 (*isol, deriv*)

Wirth, D. *et al., Helv. Chim. Acta*, 1992, **34**, 734

1-(1,3-Hexadienyl)-2-vinylcyclopropane H-279

1-Ethenyl-2-(1,3-hexadienyl)cyclopropane, 9CI

[50265-58-2]



(1*R*,1′*E*,2*R*,3′*E*)–*form*

$C_{11}H_{16}$ 148.247

(1R,1′E,2R,3′E)-form [103833-89-2]

Isol. from *Dictyopteris acrostichoides*. Sol. MeOH, hexane; poorly sol. H_2O. λ_{max} 245 (sh); 254; 263; 274 (pentane) (Derep). λ_{max} 247 (EtOH) (Berdy).

3′,4′-Dihydro: 1-(1-Hexenyl)-2-vinylcyclopropane. ***Dictyopterene A***. *Predictyotene*

[25047-20-5]

$C_{11}H_{18}$ 150.263

Isol. from *Dictyopteris* spp. and from *Spermatochnus paradoxus*. Oil. $[\alpha]_D^{21}$ +77 (c, 0.5 in EtOH). λ_{max} 206 (ϵ 16000) (95% EtOH) (Derep).

(1R,1′E,2R,3′Z)-form

Dictyopterene B. *Hormosirene. Preectocarpene*

[29837-20-5]

Constit. of the essential oil of algae *Dictyopteris* spp.

Oil. $Bp_{0.3}$ 62°. $[\alpha]_D^{24}$ -43 (c, 10.1 in $CHCl_3$). The (*R,R*)-form is usually secreted exclusively by the female gametes, but both

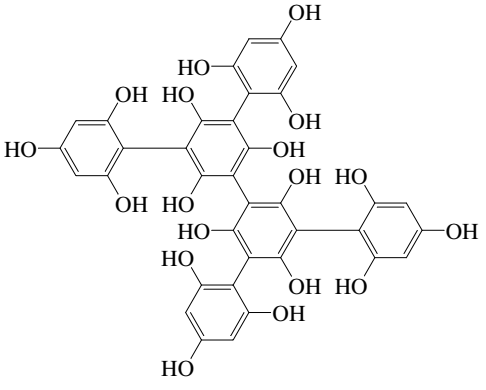
enantiomers are attractive to the male gametes of some species. λ_{max} 245 (sh); 254; 263; 274 (pentane) (Derep).

5′,6′-Didehydro: 1-(1,3,5-Hexatrienyl)-2-vinylcyclopropane. ***Predesmarestene***
$C_{11}H_{14}$ 146.232
Algal pheromone of *Desmarestia aculeata*. Thermolabile.

Weinstein, B. *et al., Chem. Comm.*, 1971, 940 (*synth*)
Moore, R.E. *et al., J.O.C.*, 1974, **39**, 2201 (*isol*)
Müller, D.G. *et al., Naturwissenschaften*, 1981, **67**, 476
Jaenicke, L. *et al., Angew. Chem., Int. Ed.*, 1982, **21**, 643 (*rev*)
Müller, D.G. *et al., Experientia*, 1984, **40**, 211 (*isol*)
Colobert, F. *et al., Tet. Lett.*, 1985, **26**, 2779 (*synth*)
Dorsch, D. *et al., Tet. Lett.*, 1985, **26**, 3319 (*synth*)
Abraham, W.D. *et al., J.A.C.S.*, 1991, **113**, 2313 (*synth*)
Grandjean, D. *et al., Tetrahedron*, 1991, **47**, 1215 (*synth*)
Wirth, D. *et al., Helv. Chim. Acta*, 1992, **34**, 734 (*occur*)
Narjes, F. *et al., J.O.C.*, 1993, **58**, 626 (*synth*)
Pohnert, G. *et al., Tetrahedron*, 1996, **52**, 10073 (*biosynth*)
Pohnert, G. *et al., Tetrahedron*, 1997, **53**, 13681-13694 (*synth*)
Itoh, T. *et al., Bull. Chem. Soc. Jpn.*, 2000, **73**, 409-416 (*Dictyopterene A*)

Hexafucol B H-280

[642487-14-7]

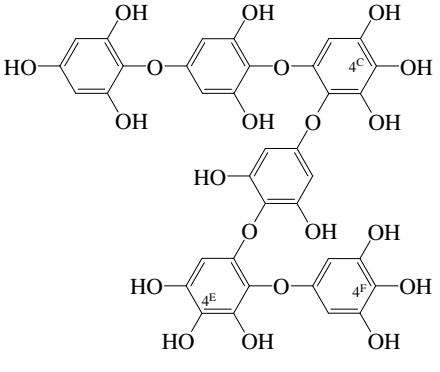


$C_{36}H_{26}O_{18}$ 746.591
Isol. from the brown alga *Scytothamnus australis*. Isol. as the octadeca-Ac to which the CAS no. refers.

Glombitza, K.-W. *et al., Bot. Mar.*, 2003, **46**, 315-320 (*isol, pmr, cmr*)

Hexafuhalol A H-281

Hexafuhalol
[83903-60-0]



$C_{36}H_{26}O_{21}$ 794.589
Constit. of *Carpophyllum maschalocarpum*, *Carpophyllum angustifolium* and *Sargassum spinuligerum*.

4^C-Deoxy: ***Deshydroxyhexafuhalol A***
$C_{36}H_{26}O_{20}$ 778.589
Isol. from *Sargassum spinuligerum* and *Carpophyllum angustifolium*.

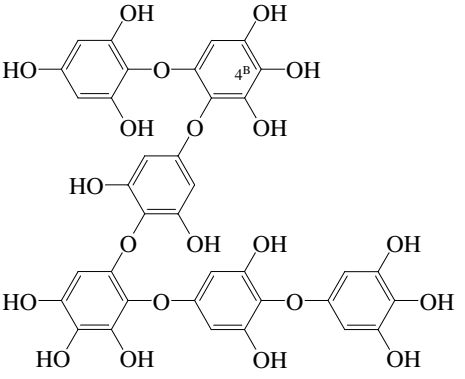
4^E-Deoxy: ***Deshydroxyhexafuhalol D***
$C_{36}H_{26}O_{20}$ 778.589
Isol. from *Sargassum spinuligerum*.

4^F-Deoxy: ***Deshydroxyhexafuhalol C***
$C_{36}H_{26}O_{20}$ 778.589
Isol. from *Sargassum spinuligerum*.

Glombitza, K.-W. *et al., Bot. Mar.*, 1982, **25**, 449-453 (*isol, pmr*)
Glombitza, K.-W. *et al., Phytochemistry*, 1991, **30**, 2741; 1995, **38**, 987-995 (*isol, Deshydroxyoctafuhalols*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

Hexafuhalol B H-282

[137830-18-3]



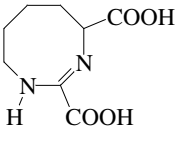
$C_{36}H_{26}O_{21}$ 794.589
Constit. of *Carpophyllum maschalocarpum* and *Carpophyllum angustifolium*.

4^B-Deoxy: ***Deshydroxyhexafuhalol B***
$C_{36}H_{26}O_{20}$ 778.589
Isol. from *Sargassum spinuligerum*.

Glombitza, K.-W. *et al., Phytochemistry*, 1991, **30**, 2741-2745; 1995, **38**, 975-985 (*isol, pmr, cmr*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

1,4,5,6,7,8-Hexahydro-1,3-diazocine-2,4-dicarboxylic acid, 9CI H-283

[203579-33-3]

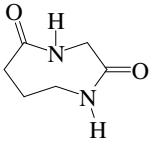


$C_8H_{12}N_2O_4$ 200.194
Zwitterionic with charge delocalisation over the two N's. Isol. from the sponge *Axinyssa terpnis*. Needles (MeOH). Mp 210-212°. $[\alpha]_D$ -66.3 (c, 0.9 in MeOH).

Li, C.-J. *et al., J. Nat. Prod.*, 1998, **61**, 387-389 (*isol, ir, pmr, cmr, ms*)

Hexahydro-1,4-diazocine-2,5-dione, 9CI H-284

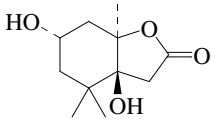
Cyclo(4-aminobutanoylglycyl)
[4345-52-2]



$C_6H_{10}N_2O_2$ 142.157
Prod. by a strain of *Ruegeria* sp. isol. from the sponge *Suberites domuncula*. Amorph. solid.

Guedez, T. *et al., J.C.S. Perkin 2*, 2002, 2078-2082 (*synth*)
Mitova, M. *et al., J. Nat. Prod.*, 2004, **67**, 1178-1181 (*isol*)

Hexahydro-3*a*,6-dihydroxy-4,4,7*a*-trimethyl-2(3*H*)-benzofuranone H-285



(3a*R**,6*R**,7a*R**)-*form*

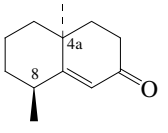
$C_{11}H_{18}O_4$ 214.261

(3*a*R,6*R*,7*aR*)-*form* [398119-19-2]
Constit. of *Undaria pinnatifida*.
Oil. $[\alpha]_D$ -64 (c, 0.013 in $CHCl_3$).

(3*aR*,6*S*,7*aR*)-*form* [398119-18-1]
Constit. of *Undaria pinnatifida*.
Oil. $[\alpha]_D$ +23 (c, 0.028 in $CHCl_3$).
Kimura, J. *et al., J. Nat. Prod.*, 2002, **65**, 57-58 (*isol, pmr, cmr*)

4,4*a*,5,6,7,8-Hexahydro-4*a*,8-dimethyl-2(3*H*)-naphthalenone, 9CI H-286

11,12,13-Trinor-5-eudesmen-7-one
[4071-63-0]



(4*aS*,8*S*)-form

$C_{12}H_{18}O$ 178.274

(4*aS*,8*S*)-*form* [39850-89-0]
[17990-00-0]
Constit. of the oil of *Vetiveria zizanioides* and metab. of *Chondromyces crocatus*.
Oil. $Bp_{0.05}$ 70°. $[\alpha]_D^{20}$ +201.7 (c, 2 in $CHCl_3$).

*1,8aβ-Dihydro: 3,4,4*a*,5,6,7,8,8*a*-Octahydro-4*a*,8-dimethyl-2(1*H*)-naphthalenone. 5,9-Dimethyl-2-decalone. 11,12,13-Trinor-7-eudesmanone*
[52305-17-6]
$C_{12}H_{20}O$ 180.289
Metab. of *Chondromyces crocatus*.

(4*a*ξ,8ξ)-*form*

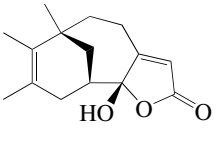
*1,8-Dihydro, 2-alcohol: Decahydro-4*a*,8-dimethyl-2-naphthalenol. 5,9-Dimethyl-2-decalol. 11,12,13-Trinor-7-eudesmanol*
[52252-50-3]
$C_{12}H_{22}O$ 182.305
Metab. of *Chondromyces crocatus*. Stereochem. not established.

[58407-30-0, 60102-91-2, 64281-61-4, 69460-62-4]

Maurer, B. *et al., Helv. Chim. Acta*, 1972, **55**, 2371
Schulz, S. *et al., Tetrahedron*, 2004, **60**, 3863-3872 (*isol, pmr, cmr, ms, synth*)

4,5,6,9,10,10*a*-Hexahydro-10*a*-hydroxy-6,7,8-trimethyl-6,10-methano-2*H*-cyclonona[*b*]furan-2-one, 9CI H-287

[174720-19-5]

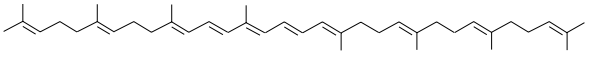


$C_{15}H_{20}O_3$ 248.321
Constit. of *Dysidea fragilis* from the Venice lagoon. Related to Nakafuran 9, N-15.

*Me ether: **4,5,6,9,10,10a-Hexahydro-10a-methoxy-6,7,8-trimethyl-6,10-methano-2H-cyclonona[b]furan-2-one, 9CI***
[79827-33-1]
$C_{16}H_{22}O_3$ 262.348
Constit. of *Hypselodoris* spp. and *Dysidea fragilis*. Oil. $[\alpha]_D$ +38 (c, 0.47 in MeOH).
Hochlowski, J.E. *et al., J.O.C.*, 1982, **47**, 88-91 (*Me ether*)
Aiello, A. *et al., Biochem. Syst. Ecol.*, 1996, **24**, 37-42 (*isol, pmr, cmr*)

7,7′,8,8′,11,12-Hexahydrolycopene H-288

7,7′,8,8′,11,12-Hexahydro-ψ,ψ-carotene
[540-05-6]



$C_{40}H_{62}$ 542.93
Constit. of *Neurospora* spp. and other microorganisms. Widespread in plants. Pale yellow oil with brilliant green fluorescence. The (all-*E*) and several mono- and di-*Z* isomers appear to occur naturally.

1,2-Epoxide: 1,2-Epoxy-1,2,7′,8,8′,11,12-octahydro-ψ,ψ-carotene
[51598-36-8]
$C_{40}H_{62}O$ 558.929
Isol. from tomatoes (*Lycopersicon esculentum*). Not separated from the 1′,2′-epoxide.

1′,2′-Epoxide: 1,2-Epoxy-1,2,7′,8,8′,11′,12′-octahydro-ψ,ψ-carotene
[51599-11-2]
$C_{40}H_{62}O$ 558.929
Isol. from tomatoes (*Lycopersicon esculentum*). λ_{max} 331; 348; 367 (petrol).

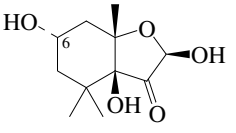
9*Z*-*form* [151767-13-4]
Constit. of *Dunaliella bardawil*. Branch point for the formation of 9-*cis*-β-carotene in *Dunaliella bardawil*.
Pale yellow liq. λ_{max} 332; 348; 367 (hexane).

15*Z*-*form*
Phytofluene
[27664-65-9]
Widespread in plants.
Pale yellow oil.

(15*Z*,9′*Z*)-*form* [72746-34-0]
Isol. from tomato (*Lycopersicon esculentum* var. 'Tangella'). Yellow oil with intense blue-green fluorescence. λ_{max} 249; 257; 331; 348; 367 (hexane).

Zechmeister, L. *et al., Arch. Biochem. Biophys.*, 1953, **47**, 160 (*occur*)
Jungawala, F.B. *et al., Arch. Biochem. Biophys.*, 1965, **110**, 291-299 (*config, Phytofluene*)
Davis, J.B. *et al., J.C.S.(C)*, 1966, 2154 (*isol, struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 1817 (*occur*)
Ben-Aziz, A. *et al., Phytochemistry*, 1973, **12**, 2759 (*epoxides*)
Brown, D.J. *et al., Biochem. Soc. Trans.*, 1975, **3**, 741 (*biosynth*)
Clough, J.M. *et al., J.C.S. Perkin 1*, 1983, 3011 (*15Z,9′Z-form, ir, pmr, cmr*)
Frecknall, E.A. *et al., Phytochemistry*, 1984, **23**, 1707 (*occur*)
Ebenezer, W.J. *et al., J.C.S. Perkin 1*, 1993, 1869 (*9Z-isomer*)

Hexahydro-2,3*a*,6-trihydroxy-4,4,7*a*-trimethyl-3(2*H*)-benzofuranone H-289

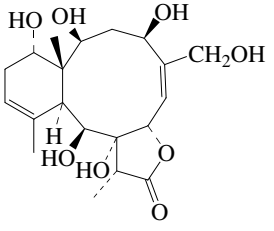


$C_{11}H_{18}O_5$ 230.26

(2R,3aS,6S,7aS)-form

6-Ac: [398119-17-0]
$C_{13}H_{20}O_6$ 272.297
Constit. of *Undaria pinnatifida*. Oil. $[\alpha]_D$ +33 (c, 0.078 in $CHCl_3$). Related to Loliolide, L-219.
Kimura, J. *et al., J. Nat. Prod.*, 2002, **65**, 57-58 (*isol, pmr, cmr*)

2,4,8,9,14,16-Hexahydroxy-5,11-briaradien-18,7-olide H-290



$C_{20}H_{30}O_8$ 398.452

(2β,4β,5Z,7α,8α,9β,14α)-form

2,4,9,14-Tetra-Ac: ***16-Hydroxymilolide M***
[438552-17-1]
$C_{28}H_{38}O_{12}$ 566.601
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ +49.6 (c, 0.27 in CH_2Cl_2).

2,4,9,14,16-Penta-Ac: ***16-Acetoxymilolide M***
[438552-18-2]
$C_{30}H_{40}O_{13}$ 608.638
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ +23.9 (c, 0.18 in CH_2Cl_2).

4-Butanoyl, 2,9,14,16-tetra-Ac: ***16-Acetoxymilolide N***
[438552-20-6]
$C_{32}H_{44}O_{13}$ 636.692
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ +22.2 (c, 0.17 in CH_2Cl_2).

4-O-(3-Acetoxybutanoyl), 2,9,14-tri-Ac: ***Erythrolide N***
[410096-44-5]
$C_{32}H_{44}O_{14}$ 652.691
Constit. of *Erythropodium caribaeorum*. Gum. $[\alpha]_D^{25}$ +20 (c, 0.32 in $CHCl_3$).

11,12-Epoxide: 11,12-Epoxy-2,4,8,9,14,16-hexahydroxy-5-briaren-18,7-olide

11β,12β-Epoxide, 2,4,9,14-tetra-Ac: ***16-Hydroxymilolide A***
[352273-94-0]
$C_{28}H_{38}O_{13}$ 582.6
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ +50.4 (c, 0.42 in CH_2Cl_2).

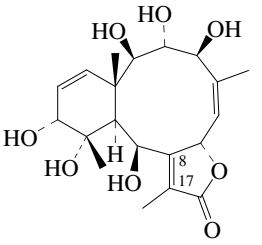
11β,12β-Epoxide, 2,4,9,14,16-penta-Ac: ***16-Acetoxymilolide A***
[352273-93-9]
$C_{30}H_{40}O_{14}$ 624.638
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ +44.2 (c, 0.6 in CH_2Cl_2).

16-Carboxylic acid: 2,4,8,9,14-Pentahydroxy-5,11-briaradien-18,7-olid-16-oic acid
Has 5*E*-config. (change of CIP priorities).

16-Carboxylic acid, 2,4,9,14-tetra-Ac, Me ester: [753001-79-5]
$C_{29}H_{38}O_{13}$ 594.611
Constit. of a *Pteroeides* sp. Solid. $[\alpha]_D^{26}$ +23 (c, 0.83 in $CHCl_3$).

Banjoo, D. *et al., J. Nat. Prod.*, 2002, **65**, 314-318 (*Erythrolide N*)
Kwak, J.H. *et al., J. Nat. Prod.*, 2002, **65**, 704-708 (*Hydroxymiliolides, Acetoxymiliolides*)
Tanaka, C. *et al., J. Nat. Prod.*, 2004, **67**, 1368-1373 (*Pteroeides constit*)

2,3,4,9,11,12-Hexahydroxy-5,8(17),13-briaratrien-18,7-olide H-291



$C_{20}H_{28}O_8$ 396.436

(2β,3α,4β,5Z,7α,9β,11α,12α)-form

2,3,4,9-Tetra-Ac: ***4-Acetoxybriviolide D***
[868281-78-1]
$C_{28}H_{36}O_{12}$ 564.585
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +44 (c, 0.05 in MeOH). λ_{max} 217 (ε 10100) (MeOH).

4-Octanoyl, 9-Ac: ***Briviolide E***
[868526-12-9]
$C_{30}H_{44}O_{10}$ 564.672
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ -24 (c, 0.04 in MeOH). λ_{max} 216 (ε 14300) (MeOH).

8,17-Epoxide: 8,17-Epoxy-2,3,4,9,11,12-hexahydroxy-5,13-briaradien-18,7-olide

8α,17α-Epoxide, 2,4,9-tri-Ac: ***Briarlide J***
[845641-20-5]
$C_{26}H_{34}O_{12}$ 538.547
Constit. of a *Briareum* sp. Amorph. solid. $[\alpha]_D$ +13 (c, 0.07 in MeOH).

8α,17α-Epoxide, 4,9,12-tri-Ac: ***Briarlide C***
[610311-46-1]
$C_{26}H_{34}O_{12}$ 538.547
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ -96 (c, 0.13 in MeOH).

8α,17α-Epoxide, 2,3,4,9-tetra-Ac: ***Violide B***
[207113-52-8]
$C_{28}H_{36}O_{13}$ 580.585
Constit. of a *Briareum* sp. and *Pachyclavularia violacea*. Ichthyotoxic. Amorph. solid. $[\alpha]_D$ +50.7 (c, 0.07 in MeOH). Error in CAS struct. λ_{max} 206 (ε 5800) (MeOH).

8α,17α-Epoxide, 2,4,9,12-tetra-Ac: ***Briarlide B***
[610311-45-0]
$C_{28}H_{36}O_{13}$ 580.585
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ -36.8 (c, 1.19 in MeOH).

8α,17α-Epoxide, 2,3,4,9,12-penta-Ac: ***Briarlide A***
[610311-44-9]
$C_{30}H_{38}O_{14}$ 622.622
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ -13 (c, 0.23 in MeOH).

8α,17α-Epoxide, 4-butanoyl, 9,12-di-Ac: ***Briarlide K***
[845641-21-6]
$C_{28}H_{38}O_{12}$ 566.601
Constit. of a *Briareum* sp. Amorph. solid. $[\alpha]_D$ -74 (c, 0.14 in MeOH).

8α,17α-Epoxide, 4-butanoyl, 2,3,9-tri-Ac: ***Violide E***
[230647-95-7]
$C_{30}H_{40}O_{13}$ 608.638
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ +76.2 (c, 0.3 in MeOH). λ_{max} 205 (ε 7600) (MeOH).

8α,17α-Epoxide, 4-hexanoyl, 2,9-di-Ac: [851539-00-9]
$C_{30}H_{42}O_{12}$ 594.655
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +26 (c, 0.13 in MeOH).

8α,17α-Epoxide, 4-hexanoyl, 2,3,9-tri-Ac: ***Violide D***
[243972-84-1]
$C_{32}H_{44}O_{13}$ 636.692
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ +74.3 (c, 0.15 in MeOH). λ_{max} 205 (ε 7100) (MeOH).

8α,17α-Epoxide, 4-hexanoyl, 2,9,12-tri-Ac: ***Briarlide D***
[610311-48-3]
$C_{32}H_{44}O_{13}$ 636.692
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ -34 (c, 0.13 in MeOH).

8α,17α-Epoxide, 3-octanoyl, 2,9-di-Ac: ***Violide Q***
[851723-71-2]
$C_{32}H_{46}O_{12}$ 622.708
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +44 (c, 0.17 in MeOH).

8α,17α-Epoxide, 3-octanoyl, 2,9,12-tri-Ac: ***Briarlide F***
[610311-49-4]
$C_{34}H_{48}O_{13}$ 664.745
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ -57 (c, 0.05 in MeOH).

8α,17α-Epoxide, 4-octanoyl, 9-Ac: ***Violide F***
[243972-85-2]
$C_{30}H_{44}O_{11}$ 580.671
Constit. of a *Briareum* sp. Cryst. (CH_2Cl_2/hexane).
Mp 149-152°. $[\alpha]_D$ -2.6 (c, 0.39 in MeOH). λ_{max} 205 (ϵ 8300) (MeOH).

8α,17α-Epoxide, 4-octanoyl, 2,9-di-Ac: ***Violide A***
[207113-50-6]
$C_{32}H_{46}O_{12}$ 622.708
Constit. of a *Briareum* sp. and *Pachyclavularia violacea*. Ichthyotoxic. Cryst. (EtOH).
Mp 183.8-184.1°. $[\alpha]_D$ +33 (c, 0.1 in MeOH). λ_{max} 206 (ϵ 5200) (MeOH).

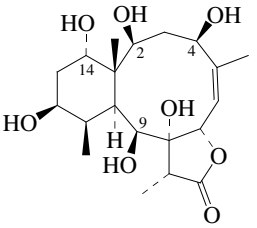
8α,17α-Epoxide, 4-octanoyl, 2,3,9-tri-Ac: ***Violide C***
[243972-83-0]
$C_{34}H_{48}O_{13}$ 664.745
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ +72.6 (c, 0.43 in MeOH). λ_{max} 205 (ϵ 7800) (MeOH).

8α,17α-Epoxide, 4-octanoyl, 2,9,12-tri-Ac: ***Briarlide E***
[610311-47-2]
$C_{34}H_{48}O_{13}$ 664.745
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ -24 (c, 0.12 in MeOH).

8α,17α-Epoxide, 4-octanoyl, 2,3,9,12-tetra-Ac: ***Briarlide I***
[845641-19-2]
$C_{36}H_{50}O_{14}$ 706.783
Constit. of a *Briareum* sp. Amorph. solid. $[\alpha]_D$ +27 (c, 0.06 in MeOH).

Iwagawa, T. *et al., Heterocycles*, 1998, **48**, 123-128; 1999, **51**, 1653-1659 (*Violides, cryst struct*)
Iwagawa, T. *et al., J. Nat. Prod.*, 2003, **66**, 1412-1415; 2005, **68**, 31-35 (*Briarlides*)
Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 607-617; 2083-2093 (*epoxide 4-hexanoyl-2,9-di-Ac, Violide Q, 4-Acetoxybriviolide D, Briviolide E*)

2,4,8,9,12,14-Hexahydroxy-5-briaren-18,7-olide H-292



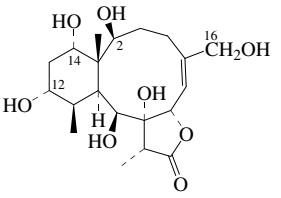
$C_{20}H_{32}O_8$ 400.468

(2β,4β,5*Z*,7α,8α,9β,12β,14α)-*form*

2,4,9,14-Tetra-Ac: ***Milolide G***
[438552-09-1]
$C_{28}H_{40}O_{12}$ 568.617
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ +53.6 (c, 0.38 in CH_2Cl_2).

Kwak, J.H. *et al., J. Nat. Prod.*, 2002, **65**, 704-708 (*isol, pmr, cmr*)

2,8,9,12,14,16-Hexahydroxy-5-briaren-18,7-olide H-293



(2β,5*E*,7α,8α,9β,12α,14α)-*form*

$C_{20}H_{32}O_8$ 400.468

(2β,5*E*,7α,8α,9β,12α,14α)-*form*

2,9,14-Tri-Ac: ***Briviolide A***
[868526-08-3]
$C_{26}H_{38}O_{11}$ 526.58
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ -23 (c, 0.04 in MeOH).

2,12,14,16-Tetra-Ac: ***Milolide H***
[438552-11-5]
$C_{28}H_{40}O_{12}$ 568.617
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ +8.6 (c, 0.62 in CH_2Cl_2).

(2β,5*E*,7α,8α,9β,12β,14α)-*form*

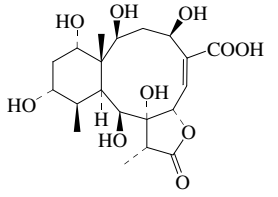
16-Carboxylic acid: 2,8,9,12,14-Pentahydroxy-5-briaren-18,7-olid-16-oic acid
$C_{20}H_{30}O_9$ 414.452

16-Carboxylic acid, 2,9,14-tri-Ac, Me ester: ***Milolide I***
[438552-12-6]
$C_{27}H_{38}O_{12}$ 554.59
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ +3.8 (c, 0.48 in CH_2Cl_2).

16-Carboxylic acid, 2,9,12,14-tetra-Ac, Me ester: ***Erythrolide O***
[410096-45-6]
$C_{29}H_{40}O_{13}$ 596.627
Constit. of *Erythropodium caribaeorum*. Gum. $[\alpha]_D^{25}$ +58.5 (c, 0.41 in $CHCl_3$). λ_{max} 216 (log ϵ 3.66) (MeOH).

Banjoo, D. *et al., J. Nat. Prod.*, 2002, **65**, 314-318 (*Erythrolide O*)
Kwak, J.H. *et al., J. Nat. Prod.*, 2002, **65**, 704-708 (*Milolides*)
Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 2083-2093 (*Briviolide A*)

2,4,8,9,12,14-Hexahydroxy-5-briaren-18,7-olid-16-oic acid H-294



(2β,4β,5*E*,7α,8α,9β,12α,14α)-*form*

$C_{20}H_{30}O_{10}$ 430.451

(2β,4β,5*E*,7α,8α,9β,12α,14α)-*form*

4-(3-Hydroxybutanoyl), 2,9,12,14-tetra-Ac, Me ester: ***Erythrolide S***
[627878-03-9]
$C_{33}H_{46}O_{16}$ 698.717
Constit. of *Erythropodium caribaeorum*. Amorph. solid. $[\alpha]_D^{25}$ +111. λ_{max} 224 (ϵ 3150) (MeOH).

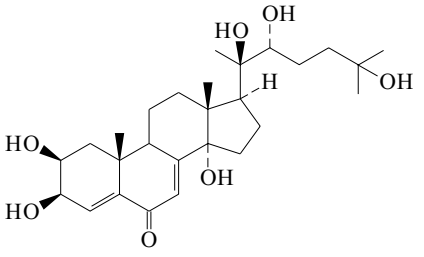
4-(3-Acetoxybutanoyl), 2,9,12,14-tetra-Ac, Me ester: ***Erythrolide J***
[151782-96-6]
$C_{35}H_{48}O_{17}$ 740.754
Constit. of *Erythropodium caribaeorum*. Amorph. solid. $[\alpha]_D$ +17.3 (c, 0.33 in $CHCl_3$).

(2β,4β,5*E*,7α,8α,9β,12β,14α)-*form*

2,4,9,14-Tetra-Ac, Me ester: ***Milolide J***

[438552-13-7]
$C_{29}H_{40}O_{14}$ 612.627
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ +34.5 (c, 0.2 in CH_2Cl_2).
Dookran, R. *et al., J. Nat. Prod.*, 1993, **56**, 1051-1056 (*Erythrolide J*)
Kwak, J.H. *et al., J. Nat. Prod.*, 2002, **65**, 704-708 (*Milolide J*)
Taglialatela-Scafati, O. *et al., Eur. J. Org. Chem.*, 2003, 3515-3523 (*Erythrolide S*)

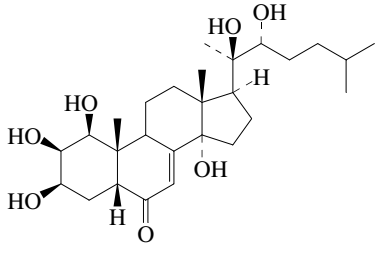
2,3,14,20,22,25-Hexahydroxycholesta-4,7-dien-6-one H-295



$C_{27}H_{42}O_7$ 478.625

(2β,3β,14α,20*R*,22*R*)-*form*
4-Dehydroecdysterone
[162830-29-7]
Constit. of a *Parazoanthus* sp.
Cryst. (MeCN).
Mp 236-238° dec. $[\alpha]_D$ -33 (c, 0.09 in MeOH).
Searle, P.A. *et al., J. Nat. Prod.*, 1995, **58**, 264 (*isol, pmr, cmr*)

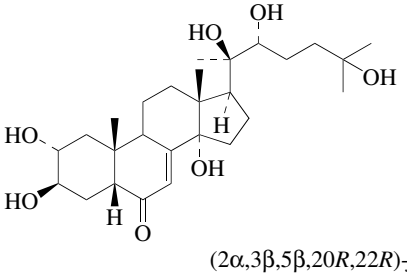
1,2,3,14,20,22-Hexahydroxycholest-7-en-6-one H-296



$C_{27}H_{44}O_7$ 480.64

(1β,2β,3β,5β,14α,20*R*,22*R*)-*form*
Zoanthusterone
[454476-11-0]
Constit. of a *Zoanthus* sp.
Amorph. solid.
Suksamrarn, A. *et al., J. Nat. Prod.*, 2002, **65**, 1194-1197 (*isol, pmr, cmr*)

2,3,14,20,22,25-Hexahydroxycholest-7-en-6-one, 9CI H-297



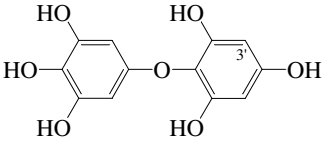
(2α,3β,5β,20*R*,22*R*)-*form*

$C_{27}H_{44}O_7$ 480.64

(2β,3β,5β,20*R*,22*R*)-*form*
Crustecdysone. *Commisterone. β-Ecdysone. Ecdysterone. 20-Hydroxy-α-ecdysone. Isoinokosterone. Polypodine A. Viticosterone*
[5289-74-7]
Isol. from the marine crayfish *Jasus lalandei* in low yield (2 mg/ton), saturniid oak-silk moth pupae, the silkworm, the wood of *Podocarpus elatus* and in *Polypodium vulgare* and many other plants. Crustacean moulting hormone. Exhibits antiinflammatory, antiarrhythmic and antiulcer props. Plates (EtOAc/THF).
Mp 237.5-239.5° (243°). $[\alpha]_D$ +61.8 ($CHCl_3$). Log P -1.91 (uncertain value) (calc).
► LD_{50} (mus, ipr) 6400 mg/kg. Exp. reprod. effects. FZ8060000
[35241-82-8]
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 574C (*nmr*)
Galbraith, M.N. *et al., Chem. Comm.*, 1966, 905-906 (*isol, Crustecdysone*)
Hüppi, G. *et al., J.A.C.S.*, 1967, **89**, 6790-6792 (*Crustecdysone, synth*)
Kerb, U. *et al., Tet. Lett.*, 1968, 4277-4280 (*20-Hydroxyecdysterone, synth*)
Dammeier, B. *et al., Chem. Ber.*, 1971, **104**, 1660-1673 (*Ecdysterone, struct, abs config*)
Kametani, T. *et al., Tet. Lett.*, 1980, 4855-4856 (*20-Hydroxyecdysterone, synth*)
Hedtmann, U. *et al., Tetrahedron*, 1991, **47**, 3753-3772 (*synth*)
Suksamrarn, A. *et al., Phytochemistry*, 1995, **38**, 473-476 (*pmr, cmr*)
Calcagno, M.-P. *et al., Tetrahedron*, 1996, **52**, 10137-10146 (*pmr, cmr*)

2,3′,4,4′,5′,6-Hexahydroxydiphenyl ether H-298

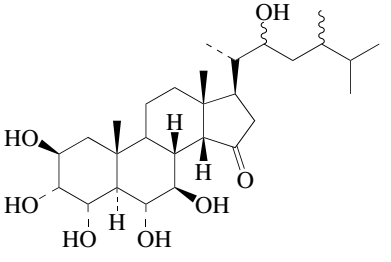
5-(2,4,6-Trihydroxyphenoxy)-1,2,3-benzenetriol, 9CI. ***Bifuhalol***
[53254-99-2]



$C_{12}H_{10}O_7$ 266.207
The name Bifuhalol is a combination of Bifurcaria and Halidrys and is not intended to have systematic connotations. Constit. of *Bifurcaria bifurcata*, *Halidrys* sp., *Carpophyllum angustifolium* and other brown algae.
Hexa-Ac: Mp 184-186°.
3′-Chloro: ***3′-Chlorobifuhalol***
$C_{12}H_9ClO_7$ 300.652
Isol. from *Carpophyllum angustifolium*. Called 3[A]-chloro in the lit. by analogy with other phlorotannins having a greater number of rings.
Glombitza, K.-W. *et al., Phytochemistry*, 1974, **13**, 1245-1247 (*isol, struct*)
Sattler, E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1975, **308**, 813-818 (*synth*)
Sattler, E. *et al., Tetrahedron*, 1977, **33**, 1239-1244 (*isol, struct*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*3′-Chlorobifuhalol*)

2,3,4,6,7,22-Hexahydroxyergostan-15-one H-299

2,3,4,6,7,22-Hexahydroxy-24-methylcholestan-15-one



$C_{28}H_{48}O_7$ 496.683

(2β,3α,4α,5α,6α,7β,14β,22ξ,24ξ)-*form*
Haliclostanone
2-Sulfate: ***Haliclostanone sulfate***
[185420-75-1]

$C_{28}H_{48}O_{10}S$ 576.747
Constit. of a *Haliclona* sp. Amorph. yellow solid. $[\alpha]_D$ +15.6 (c, 0.18 in MeOH).
Sperry, S. *et al., J. Nat. Prod.*, 1997, **60**, 29 (*isol, pmr, cmr*)

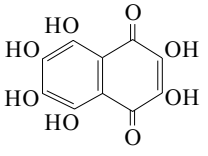
2,3,14,20,22,26-Hexahydroxyergost-7-en-6-one H-300

2,3,14,20,22,26-Hexahydroxy-24-methylcholest-7-en-6-one
$C_{28}H_{46}O_7$ 494.667

(2β,3β,5β,14α,20*R*,22*R*,24*R*,25ξ)-*form*
Makisterone B. *Callinecdysone B*
[20512-31-6]
Phytoecdysone from *Podocarpus macrophyllus*, also from the female marine crab *Callinectes sapidus*.
Cryst.
Mp 172-173° dec. The identity of Callinecdysone B with Makisterone B is based on CAS registry data.
Imai, S. *et al., Tet. Lett.*, 1968, 3887
Faux, A. *et al., Chem. Comm.*, 1969, 175

Hexahydroxy-1,4-naphthoquinone H-301

2,3,5,6,7,8-Hexahydroxy-1,4-naphthalenedione, 9CI. ***Spinochrome E***
[476-37-9]



$C_{10}H_6O_8$ 254.153
Isol. from sea urchins *Paracentrotus lividus, Psammechinus miliaris* and *Strongylocentrotus droebachiensis*. Brownish-red needles (MeOH). Sublimes at 300-320° without melting. λ_{max} 270 (ϵ 15200); 359 (ϵ 5000); 477 (ϵ 4370) (MeOH) (Berdy).

Hexa-Ac:
$C_{22}H_{18}O_{14}$ 506.376
Yellow cryst. Mp 192°.

2-Me ether: 2,3,5,6,8-Pentahydroxy-7-methoxy-1,4-naphthoquinone. ***Namakochrome***
[15308-24-4]
$C_{11}H_8O_8$ 268.179
Isol. from *Polycheira rufescens*. Cryst. (AcOH).
Mp 218°. Tautomeric to give the 7-Me ether struct.

2,6-Di-Me ether: 2,5,6,8-Tetrahydroxy-3,7-dimethoxy-1,4-naphthoquinone, 8CI
[15308-22-2]
$C_{12}H_{10}O_8$ 282.206
Isol. from spines of *Acanthaster planci*.

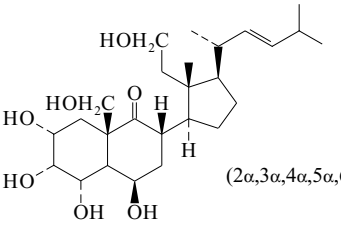
2,7-Di-Me ether: 2,5,7,8-Tetrahydroxy-3,6-dimethoxy-1,4-naphthoquinone, 8CI
[14090-99-4]
$C_{12}H_{10}O_8$ 282.206
Isol. from spines of *Acanthaster planci*.

2,3,6,7-Tetra-Me ether:
$C_{14}H_{14}O_8$ 310.26
Brown cryst. Mp 185°.

2,3-Di-Me, 6,7-methylene ether: 5,8-Dihydroxy-2,3-dimethoxy-6,7-methylenedioxy-1,4-naphthoquinone. 2,3-Dimethoxy-6,7-methylenedioxynaphthazarin. ***Tricrozarin A***. *4,9-Dihydroxy-6,7-dimethoxynaphtho[2,3-*d*]-1,3-dioxole-5,8-dione, 12CI*
[107817-60-7]
$C_{13}H_{10}O_8$ 294.217
Constit. of *Tritonia crocosmaeflora*. Deep red needles (MeOH). Sol. MeOH, C_6H_6, $CHCl_3$; poorly sol. H_2O.
Mp 187°. λ_{max} 236; 264; 341; 481 (MeOH) (Berdy). λ_{max} 235; 266; 342; 473 (MeOH/HCl) (Berdy). λ_{max} 242; 346; 547; 580 (MeOH/NaOH) (Berdy).

Lederer, E. *et al., Biochim. Biophys. Acta*, 1952, **9**, 92-100 (*isol*)
Mukai, T. *et al., Bull. Chem. Soc. Jpn.*, 1960, **33**, 453-456; 1234-1235 (*Namakochrome*)
Smith, J. *et al., J.C.S.*, 1961, 1008-1012 (*isol*)
Singh, I. *et al., J.A.C.S.*, 1965, **87**, 4023-4024 (*synth*)
Anderson, H.A. *et al., J.C.S.(C)*, 1966, 426-428 (*synth*)
Singh, H. *et al., Experientia*, 1967, **23**, 624-626 (*occur*)
Singh, H. *et al., Tetrahedron*, 1967, **23**, 3271-3305 (*Me ethers, synth*)
Kol'tsova, E.A. *et al., Khim. Prir. Soedin.*, 1977, **13**, 202-207; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 174-177 (*isol*)
Masuda, K. *et al., J. Nat. Prod.*, 1987, **50**, 418 (*Tricrozarin A*)

2,3,4,6,11,19-Hexahydroxy-24-nor-9,11-secocholest-22-en-9-one H-302



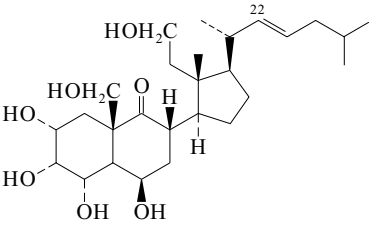
(2α,3α,4α,5α,6β,22*E*)–*form*

$C_{26}H_{44}O_7$ 468.629

(2α,3α,4α,5α,6β,22*E*)-*form*
Eurypongiol B5
[157085-55-7]
Constit. of an *Eurypongia* sp. Antihistamine. Antiallergic agent. $[\alpha]_D^{21}$ -45 (c, 0.002 in MeOH). λ_{max} 208 (MeOH) (Berdy).

(2α,3β,4α,5α,6β,22*E*)-*form*
Eurypongiol A5
[156980-10-8]
Costit. of an *Eurypongia* sp. Antihistamine. Antiallergic agent. $[\alpha]_D^{21}$ -48 (c, 0.0001 in MeOH). λ_{max} 208 (MeOH) (Berdy).
Dopeso, J. *et al., Tetrahedron*, 1994, **50**, 3813 (*isol, pmr, cmr*)

2,3,4,6,11,19-Hexahydroxy-9,11-secocholest-22-en-9-one H-303



$C_{27}H_{46}O_7$ 482.656

(2α,3α,4α,5α,6β,22*E*)-*form*
Eurypongiol B1
[156980-11-9]
Constit. of an *Eurypongia* sp. Antihistamine. Antiallergic agent. $[\alpha]_D^{21}$ -39 (c, 0.003 in MeOH). λ_{max} 208 (MeOH) (Berdy).

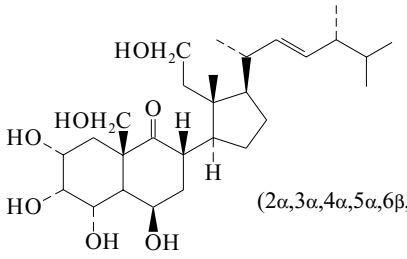
22,23-Dihydro: 2,3,4,6,11,19-Hexahydroxy-9,11-secocholestan-9-one. ***Eurypongiol B2***
[156980-12-0]
$C_{27}H_{48}O_7$ 484.672
Constit. of an *Eurypongia* sp. Antihistamine. Antiallergic agent. $[\alpha]_D^{21}$ -50 (c, 0.0006 in MeOH). λ_{max} 208 (MeOH) (Berdy).

(2α,3β,4α,5α,6β,22*E*)-*form*
Eurypongiol A1
[156980-08-4]
Constit. of an *Eurypongia* sp. Antihistamine. Antiallergic agent. $[\alpha]_D^{21}$ -42 (c, 0.001 in MeOH). λ_{max} 208 (MeOH) (Berdy).

22,23-Dihydro: ***Euryspongiol A2***
[156984-43-9]
$C_{27}H_{48}O_7$ 484.672
Constit. of an *Euryspongia* sp. Antihistamine. Antiallergic agent. $[\alpha]_D^{21}$ -22 (c, 0.001 in MeOH). λ_{max} 208 (MeOH) (Berdy).
Dopeso, J. *et al., Tetrahedron*, 1994, **50**, 3813 (*isol, pmr, cmr, ms*)

2,3,4,6,11,19-Hexahydroxy-9,11-secoergost-22-en-9-one H-304

2,3,4,6,11,19-Hexahydroxy-24-methyl-9,11-secocholest-22-en-9-one



(2α,3α,4α,5α,6β,22*E*,24*R*)–*form*

$C_{28}H_{48}O_7$ 496.683

(2α,3α,4α,5α,6β,22*E*,24*R*)-*form*
Euryspongiol B4
[157085-54-6]
Constit. of an *Euryspongia* sp. Antihistamine. Antiallergic agent. λ_{max} 208 (MeOH) (Berdy).

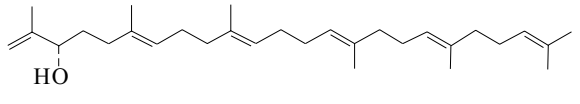
(2α,3α,4α,5α,6β,22*E*,24*S*)-*form*
Euryspongiol B3
[157085-53-5]
Constit. of an *Euryspongia* sp. Antihistamine. Antiallergic agent. λ_{max} 208 (MeOH) (Berdy).

(2α,3β,4α,5α,6β,22*E*,24*R*)-*form*
Euryspongiol A4
[157085-52-4]
Constit. of an *Euryspongia* sp. Antihistamine. Antiallergic agent. λ_{max} 208 (MeOH) (Berdy).

(2α,3β,4α,5α,6β,22*E*,24*S*)-*form*
Euryspongiol A3
[156980-09-5]
Constit. of an *Euryspongia* sp. Antihistamine. Antiallergic agent. λ_{max} 208 (MeOH) (Berdy).
Dopeso, J. *et al., Tetrahedron*, 1994, **50**, 3813 (*isol, pmr, cmr*)

2,6,10,15,19,23-Hexamethyl-1,6,10,14,18,22-tetracosahexaen-3-ol H-305

3-Isosqualenol



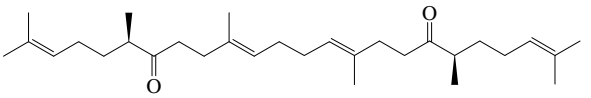
$C_{30}H_{50}O$ 426.724

(*S*, *all-E*)-*form* [82729-39-3]
Constit. of *Caulerpa prolifera*.
Oil. $[\alpha]_D^{20}$ -10 (c, 0.1 in $CHCl_3$).

[80225-55-4]

Buil, P. *et al., CA*, 1982, **96**, 40711w
De Napoli, L. *et al., Phytochemistry*, 1982, **21**, 782

2,6,10,15,19,23-Hexamethyl-2,10,14,22-tetracosatetraene-7,18-dione H-306



$C_{30}H_{50}O_2$ 442.724

(6*R*,10*E*,14*E*,19*R*)-*form* [224176-69-6]
Constit. of *Hyrtios erectus*.
Amorph. solid. $[\alpha]_D^{25}$ -371 (c, 0.055 in CH_2Cl_2). $[\alpha]_D^{24}$ -14.82 (c, 0.5 in $CHCl_3$). Discrepancy in αD noted by Enders.
Williams, D.E. *et al., J. Nat. Prod.*, 1999, **62**, 653-654 (*isol, pmr, cmr*)
Enders, D. *et al., Synthesis*, 2002, 2280-2288 (*synth, abs config, ir, pmr, cmr, ms*)

Hexane, 9CI H-307

[110-54-3]
$H_3C(CH_2)_4CH_3$
C_6H_{14} 86.177
Occurs in petroleum. Present in various plant spp. e.g. apple, orange, porcini (*Boletus edulis*), shiitake (*Lentinus edodes*), sage. Also present in scallops. Extraction solvent used in food production. Liq. d_4^{25} 0.66.
Fp -93.5. Bp 68.95°. n_D^{25} 1.3723.
▶ Highly flammable, fl. p. -23°, autoignition temp. 223°. Eye irritant. Symptoms of acute exposure incl. headache, drowsiness, dizziness and unconsciousness. Chronic exposure (and abuse) associated with development of peripheral neuropathies. OES: long-term 20 ppm. MN9275000

[21666-38-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 2B (*ir*)
Michael, A. *et al., Am. Chem. J.*, 1901, **25**, 421
Albright, M.J. *et al., J. Organomet. Chem.*, 1977, **125**, 1-8 (*cmr*)
Sato, F. *et al., J. Organomet. Chem.*, 1977, **142**, 71-79 (*synth*)
Gussoni, M. *et al., J. Mol. Struct.*, 1980, **61**, 355-359 (*ir*)
Mikaya, A.I. *et al., Org. Mass Spectrom.*, 1984, **19**, 428-432 (*ms*)
Riddick, J.A. *et al., Tech. Chem. (N.Y.)*, 4th edn., Wiley-Interscience, 1986, **2**, 92; 824 (*props, purifn*)
Battershill, J.M. *et al., HSE Toxicity Review 18: n-Hexane*, HMSO, London, 1987, (*rev, tox*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HEN000
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1103
Boese, R. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 988-992 (*cryst struct*)
Graham, D.G. *et al.*, , 1987, 327 (*rev, tox*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 670
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HEN000

2,3-Hexanedione, 9CI H-308

Methyl propyl diketone. Methyl propyl glyoxal. FEMA 2558
[3848-24-6]
$H_3CCOCO(CH_2)_2CH_3$
$C_6H_{10}O_2$ 114.144
Constit. of coffee, peach, roast chicken, beer, shoyu and clam. Minor component of the male pheromone of *Hylotrupes bajulus*. Flavour ingredient. Buttery, cheese tasting and creamy buttery odour. d_4^{19} 0.93. Bp 128°.
▶ Skin irritant. MO3140000

3-Oxime: [42563-83-7]
$C_6H_{11}NO_2$ 129.158
Cryst. (EtOH). Mp 49.5° Mp 60°.

► MO3350000

Dioxime: Methyl propyl glyoxime
[4481-42-9]
$C_6H_{12}N_2O_2$ 144.173
Needles (Et_2O). Mp 175°.

Bisphenylhydrazone:
Yellow needles (C_6H_6). Mp 137-138°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 424C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 510B (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 387B (*nmr*)
Dufraise, *et al., Bull. Soc. Chim. Fr.*, 1927, **41**, 1370
Bestman, H.-J. *et al., Chem. Ber.*, 1969, **102**, 2259 (*synth*)
Yamashita, M. *et al., Chem. Comm.*, 1977, 691 (*synth*)
Schroeder, F. *et al., Annalen*, 1994, 1211 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HEQ200

Hexanethioic acid H-309

[7530-91-8]
$H_3C(CH_2)_4COSH \Leftrightarrow H_3C(CH_2)_4C(S)OH$
$C_6H_{12}OS$ 132.226
Bp_9 62-63°.

SH-form

Me ester: S-*Methyl hexanethioate. Methanethiol caproate. FEMA 3862*
[2432-77-1]
$C_7H_{14}OS$ 146.253
Present in durian (*Durio zibethinus*) fruit volatiles and fish oils. Flavouring ingredient. Liq. with sulfurous odour. Bp_{15} 50°.

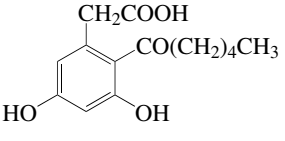
Propyl ester: [2432-78-2]
$C_9H_{18}OS$ 174.307
Present in leek oil. Characterised spectroscopically.

2-Propenyl ester: [156420-69-8]
$C_9H_{16}OS$ 172.291
Aroma constit. of fried garlic.
Characterised spectroscopically.

McFadden, W.H. *et al., Anal. Chem.*, 1965, **37**, 560-566 (*S-Me ester, synth, ms*)
Kobayashi, Y. *et al., Synthesis*, 1985, 671-672 (*synth, ir*)
Vinokurov, V.A. *et al., Zh. Org. Khim.*, 1987, **23**, 2250-2251; *J. Org. Chem. USSR (Engl. Transl.)*, 1987, **23**, 1990-1991 (*S-Me ester, synth, uv*)
Stephani, A. *et al., Z. Lebensm.-Unters. -Forsch.*, 1992, **194**, 21-25 (*S-Propyl ester*)
Shin, H.C. *et al., Lipids*, 1993, **28**, 73-74 (*synth*)
Weenen, H. *et al., J. Agric. Food Chem.*, 1996, **44**, 3291-3293 (*S-Me ester, occur, durian*)
Eri, S. *et al., J. Agric. Food Chem.*, 2000, **48**, 1140-1149 (*S-Me ester, occur, hops*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1134 (*S-Me ester, use*)
Hsu, J.P. *et al., CA*, **121**, 81405c (*S-2-propenyl ester*)

(2-Hexanoyl-3,5-dihydroxyphenyl)acetic acid H-310

3,5-Dihydroxy-2-(1-oxohexyl)benzeneacetic acid

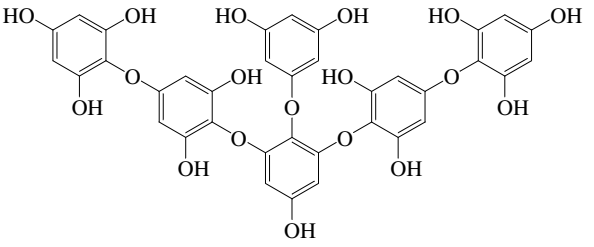


$C_{14}H_{18}O_5$ 266.293

Et ester: ***14,15-Secocurvularin***
$C_{16}H_{22}O_5$ 294.347
Prod. by an unidentified fungus derived from the sponge *Spirastrella vagabunda*.

Abrell, L.M. *et al., Tet. Lett.*, 1996, **37**, 8983-8984 (*isol, pmr, cmr, deriv*)

Hexaphlorethol A H-311

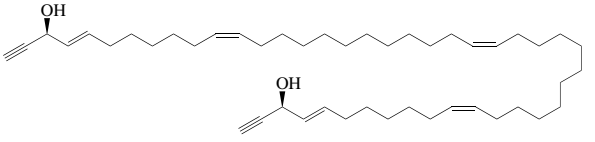


$C_{36}H_{26}O_{18}$ 746.591
Isol. from *Cystophora retroflexa*.

Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol, pmr, cmr, ms*)

4,11,23,35,42-Hexatetracontapentaene-1,45-diyne-3,44-diol H-312

Fulvinol
[183961-38-8]



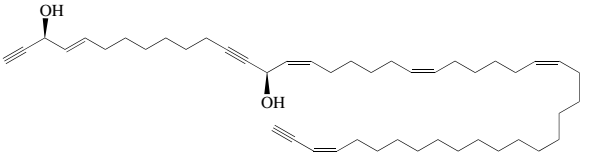
Absolute Configuration

$C_{46}H_{76}O_2$ 661.105
Isol. from the sponge *Reniera fulva*. Cytotoxic agent. Cryst. (petrol/EtOAc).
Mp 35-37°. $[\alpha]_D^{25}$ -14.8 (c, 0.4 in $CHCl_3$).

Ortega, M.J. *et al., J. Nat. Prod.*, 1996, **59**, 1069 (*isol, ir, pmr, cmr, ms*)

4,15,21,27,43-Hexatetracontapentaene-1,12,45-triyne-3,14-diol H-313

Petrotriyndiol A



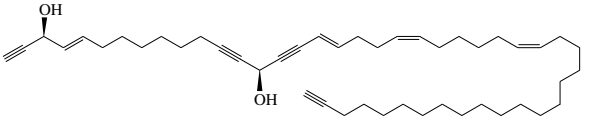
$C_{46}H_{72}O_2$ 657.074

(3S,4E,14R,15Z,21Z,27Z,43Z)-form
Isol. from the sponge *Petrosia* sp.
Yellow oil. $[\alpha]_D^{23}$ +7 (c, 0.05 in MeOH). λ_{max} 221 (log ϵ 3.7) (MeOH).

Lim, Y.J. *et al., J. Nat. Prod.*, 2001, **64**, 46-53

4,17,21,27-Hexatetracontatetraene-1,12,15,45-tetrayne-3,14-diol H-314

Petrotetrayndiol E



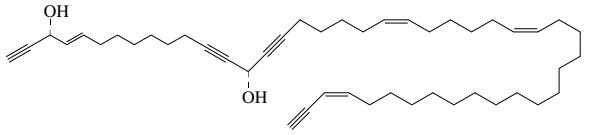
$C_{46}H_{70}O_2$ 655.058

(3S,4E,14S,17E,21Z,27Z)-form
Isol. from the sponge *Petrosia* sp.
Oil.

Lim, Y.J. *et al., J. Nat. Prod.*, 2001, **64**, 46-53 (*isol, pmr, cmr*)

4,21,27,43-Hexatetracontatetraene-1,12,15,45-tetrayne-3,14-diol H-315

Petrocortyne A



(3*R*,4*E*,14*R*,21*Z*,27*Z*,43*Z*)-*form*

$C_{46}H_{70}O_2$ 655.058

(3*R*,4*E*,14*R*,21*Z*,27*Z*,43*Z*)-*form* [201990-21-8]
Isol from the sponge *Petrosia* sp.
Gum. $[\alpha]_D^{25}$ +6.4 (c, 0.2 in MeOH). λ_{max} 223 (log ϵ 4.32) (MeOH).
λ_{max} 223 (ϵ 20900) (MeOH) (Berdy).

43,44-Dihydro: 4,21,27-Hexatetracontatriene-1,12,15,45-tetrayne-3,14-diol. ***Petrocortyne B***
[201990-67-2]
$C_{46}H_{72}O_2$ 657.074
Isol. from *Petrosia* sp. Gum. $[\alpha]_D^{25}$ +3.4 (c, 0.3 in MeOH).

(3*S*,4*E*,14*R*,21*Z*,27*Z*,43*Z*)-*form*

14-Ketone: 3-Hydroxy-4,21,27,43-hexatetracontatetraene-1,12,15,45-tetrayn-14-one. ***Petrotetraynol A***
$C_{46}H_{68}O_2$ 653.042
Isol. from a *Petrosia* sp. Yellow oil.

4,5-Dihydro: 21,27,43-Hexatetracontatriene-1,12,15,45-tetrayne-3,14-diol. ***Petrocortyne D***
[214553-84-1]
$C_{46}H_{72}O_2$ 657.074
Constit. of a Korean *Petrosia* sp. Gum. $[\alpha]_D^{25}$ -0.8 (c, 0.14 in MeOH). λ_{max} 223 (log ϵ 4.09) (MeOH).

(3*S*,4*E*,14*S*,21*Z*,27*Z*,43*Z*)-*form*

(3S,14S)-Petrocortyne A
[222178-88-3]
Isol. from a *Petrosia* sp. Cytotoxic agent. Yellow oil. $[\alpha]_D^{23}$ +10.8 (c, 1.9 in MeOH). λ_{max} 223 (log ϵ 3.9) (MeOH).

*17,18-Didehydro(*E-*): 4,17,21,27,43-Hexatetracontapentaene-1,12,15,45-tetrayne-3,14-diol.* ***Petrotetrayndiol A***
[222178-89-4]
$C_{46}H_{68}O_2$ 653.042
Isol. from a *Petrosia* sp. Cytotoxic agent. Yellow oil. $[\alpha]_D^{23}$ +7.3 (c, 0.12 in MeOH). λ_{max} 223 (log ϵ 3.3) (MeOH).

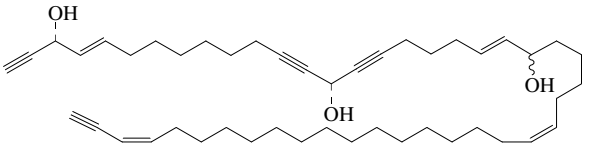
4,5-Dihydro: ***Petrotetrayndiol B***
[222178-90-7]
Isol. from a *Petrosia* sp. Cytotoxic agent. Oil. $[\alpha]_D^{23}$ +3.8 (c, 0.17 in MeOH). λ_{max} 223 (log ϵ 3.2) (MeOH).

43,44-Dihydro: ***(3S,14S)-Petrocortyne B***
Isol. from a *Petrosia* sp.
Yellow oil. $[\alpha]_D^{23}$ +2 (c, 0.6 in MeOH). λ_{max} 222 (log ϵ 3.6) (MeOH).

Shin, J. *et al., J. Nat. Prod.*, 1998, **61**, 1268-1273 (*Petrocortyne D*)
Seo, Y. *et al., Tetrahedron*, 1998, **54**, 447-462 (*isol, uv, ir, pmr, cmr, ms*)
Kim, J.S. *et al., J. Nat. Prod.*, 1999, **62**, 554-559 (*3S,4S-Petrocortyne A, Petrotetrayndiol A,B*)
Lim, Y.J. *et al., J. Nat. Prod.*, 2001, **64**, 46-53 (*3S,14S-Petrocortyne D, Petrotetraynol A*)

4,20,27,43-Hexatetracontatetraene-1,12,15,45-tetrayne-3,14,22-triol H-316

Petrocortyne F



(3*R*,4*E*,14*R*,20*E*,22ξ,27*Z*,43*Z*)-*form*

$C_{46}H_{70}O_3$ 671.057

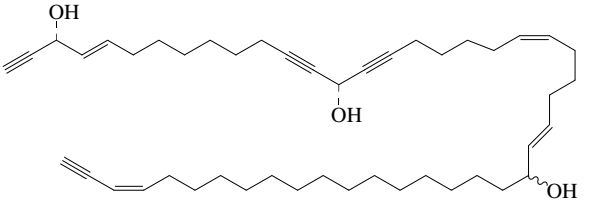
(3*R*,4*E*,14*R*,20*E*,22ξ,27*Z*,43*Z*)-*form* [214553-92-1]
Isol. from a Korean *Petrosia* sp.
Gum. $[\alpha]_D^{25}$ +8.5 (c, 0.03 in MeOH). λ_{max} 223 (log ϵ 4.14) (MeOH).

(3*S*,4*E*,14*R*,20*E*,22ξ,27*Z*,43*Z*)-*form*
Isol. from a *Petrosia* sp.
Oil.

Shin, J. *et al., J. Nat. Prod.*, 1998, **61**, 1268-1273 (*isol, uv, ir, pmr, cmr*)
Lim, Y.J. *et al., J. Nat. Prod.*, 2001, **64**, 1565-1567 (*isol, pmr, cmr, ms*)

4,21,26,43-Hexatetracontatetraene-1,12,15,45-tetrayne-3,14,28-triol H-317

Petrocortyne H



(3*R*,4*E*,14*R*,21*Z*,26*E*,28ξ,43*Z*)-*form*

$C_{46}H_{70}O_3$ 671.057

(3*R*,4*E*,14*R*,21*Z*,26*E*,28ξ,43*Z*)-*form* [214553-98-7]
Isol. from a Korean *Petrosia* sp.
Gum. $[\alpha]_D^{25}$ +4.4 (c, 0.07 in MeOH). λ_{max} 223 (log ϵ 4.17) (MeOH).

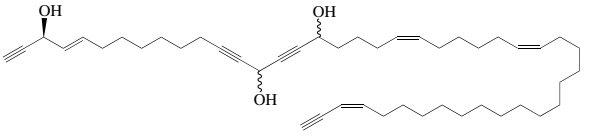
26,27-Dihydro, 28-ketone: 3,14-Dihydroxy-4,21,43-hexatetracontatriene-1,12,15,45-tetrayn-28-one. ***Petrotetrayndiol D***
$C_{46}H_{70}O_3$ 671.057
Isol. from a *Petrosia* sp. Yellow oil. C-3 and C-14 configs. not determined.

(3*S*,4*E*,14*R*,21*Z*,26*E*,28ξ,43*Z*)-*form*
Isol. from a *Petrosia* sp.
Oil.

Shin, J. *et al., J. Nat. Prod.*, 1998, **61**, 1268-1273 (*isol, uv, ir, pmr, cmr*)
Lim, Y.J. *et al., J. Nat. Prod.*, 2001, **64**, 46-53 (*Petrotetrayndiol D*)
Lim, Y.J. *et al., J. Nat. Prod.*, 2001, **64**, 1565-1567 (*isol, pmr, cmr, ms*)

4,21,27,43-Hexatetracontatetraene-1,12,15,45-tetrayne-3,14,17-triol H-318

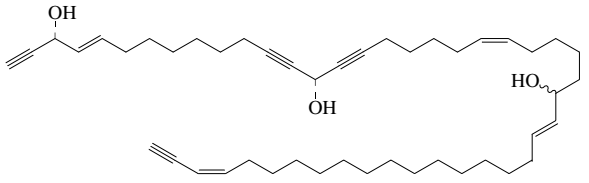
Petrotetrayntriol A



$C_{46}H_{70}O_3$ 671.057

(3*S*,4*E*,14ξ,17ξ,21*Z*,27*Z*,43*Z*)-*form*
Isol. from the sponge *Petrosia* sp.
Yellow oil. $[\alpha]_D^{23}$ +7.3 (c, 0.12 in MeOH). λ_{max} 223 (log ϵ 3.3) (MeOH).
Lim, Y.J. *et al., J. Nat. Prod.*, 2001, **64**, 46-53 (*isol*)

4,21,28,43-Hexatetracontatetraene-1,12,15,45-tetrayne-3,14,27-triol H-319
Petrocortyne G



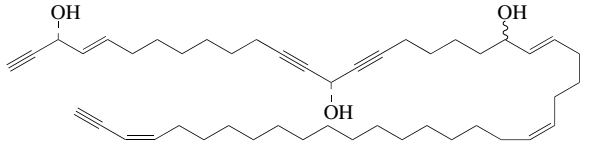
(3*R*,4*E*,14*R*,21*Z*,27ξ,28*E*,43*Z*)-*form*

$C_{46}H_{70}O_3$ 671.057

(3*R*,4*E*,14*R*,21*Z*,27ξ,28*E*,43*Z*)-*form* [214553-95-4]
Isol. from a Korean *Petrosia* sp.
Gum. $[\alpha]_D^{25}$ +8.3 (c, 0.04 in MeOH). λ_{max} 223 (log ϵ 4) (MeOH).

(3*S*,4*E*,14*R*,21*Z*,27ξ,28*E*,43*Z*)-*form*
Isol. from a *Petrosia* sp.
Oil.
Shin, J. *et al., J. Nat. Prod.*, 1998, **61**, 1268-1273 (*isol, uv, ir, pmr, cmr*)
Lim, Y.J. *et al., J. Nat. Prod.*, 2001, **64**, 1565-1567 (*isol, pmr, cmr, ms*)

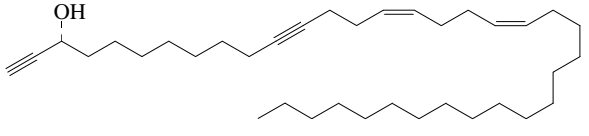
4,22,27,43-Hexatetracontatetraene-1,12,15,45-tetrayne-3,14,21-triol H-320
Petrocortyne E



$C_{46}H_{70}O_3$ 671.057

(3*R*,4*E*,14*R*,21ξ,22*E*,27*Z*,43*Z*)-*form* [214553-88-5]
Isol. from a Korean *Petrosia* sp.
Gum. $[\alpha]_D^{25}$ +3 (c, 0.15 in MeOH). λ_{max} 224 (log ϵ 4.15) (MeOH).
λ_{max} 224 (ϵ 14125) (MeOH) (Berdy).
Shin, J. *et al., J. Nat. Prod.*, 1998, **61**, 1268-1273 (*isol, uv, ir, pmr, cmr*)
Lim, Y.J. *et al., J. Nat. Prod.*, 2001, **64**, 46-53 (*isol,pmr,cmr*)

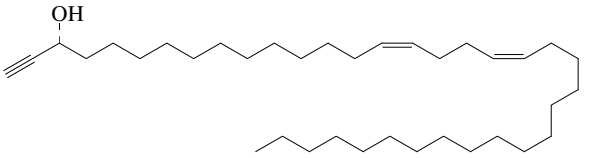
15,19-Hexatriacontadiene-1,11-diyn-3-ol H-321
Lembehyne A



$C_{36}H_{62}O$ 510.885

(3*R*,15*Z*,19*Z*)-*form*
Isol. from the sponge *Haliclona* sp. Neuritogenic agent. Powder.
$[\alpha]_D^{22}$ +1.9 (c, 0.5 in $CHCl_3$).
Aoki, S. *et al., Tetrahedron*, 2000, **56**, 9945-9948 (*isol*)
Murakami, N. *et al., Tet. Lett.*, 2001, **42**, 1941-1943 (*synth*)

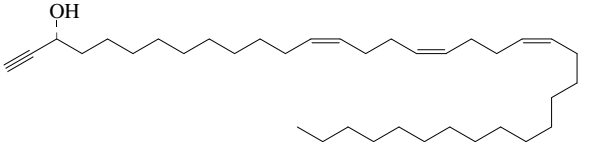
15,19-Hexatriacontadien-1-yn-3-ol H-322
Lembehyne B



$C_{36}H_{66}O$ 514.917

(3*R*,15*Z*,19*Z*)-*form*
Constit. of the sponge *Haliclona* sp. Neuritogenic agent. Powder.
$[\alpha]_D^{25}$ +0.4 (c, 0.2 in $CHCl_3$).
Aoki, S. *et al., Tetrahedron*, 2002, **58**, 5417-5422 (*isol, pmr, cmr*)

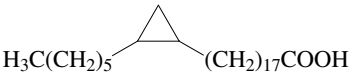
13,17,21-Hexatriacontatrien-1-yn-3-ol H-323
Lembehyne C



$C_{36}H_{64}O$ 512.901

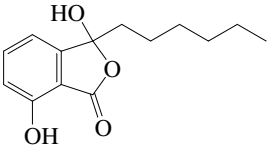
(3*R*,13*Z*,17*Z*,21*Z*)-*form*
Constit. of the sponge *Haliclona* sp. Neuritogenic agent. Powder.
$[\alpha]_D^{25}$ +0.7 (c, 0.2 in $CHCl_3$).
Aoki, S. *et al., Tetrahedron*, 2002, **58**, 5417-5422 (*isol, pmr, cmr*)

2-Hexylcyclopropaneoctadecanoic acid, 9CI H-324
19,20-Methylenehexacosanoic acid
[89188-19-2]



$C_{27}H_{52}O_2$ 408.707
Isol. from sponge *Calyx nicaensis.*
Lankelma, J. *et al., Lipids*, 1983, **18**, 853-858 (*isol*)

3-Hexyl-3,7-dihydroxy-1(3*H*)-isobenzofuranone, 9CI H-325
3-Hexyl-3,7-dihydroxyphthalide. ***Corollosporin***
[211441-46-2]

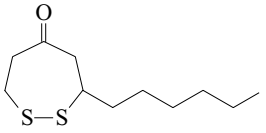


$C_{14}H_{18}O_4$ 250.294
λ_{max} 214 (log ϵ 4.44); 235 (log ϵ 4.2); 301 (log ϵ 3.95) (MeOH/HCl aq.).

(±)-*form*
Prod. by the marine fungus *Corollospora maritima*. Antibacterial agent. Cryst. (hexane/EtOAc).
Mp 79.5-81.5°.
Liberra, K. *et al., Pharmazie*, 1998, **53**, 578-581 (*isol*)
Ohzeki, T. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 172-175 (*synth, ir, pmr, cmr, ms*)

3-Hexyl-1,2-dithiepan-5-one, 9CI H-326

3-Hexyl-4,5-dithiacycloheptanone
[52354-00-4]

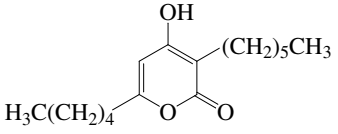


$C_{11}H_{20}OS_2$ 232.41

(-)-*form* [33783-83-4]
Constit. of the seaweed *Dictyopteris plagiogramma*, the green algae *Bryopsis pennata*, *Caulerpa prolifera* and *Cymopolia barbata* and other marine algae.
Oil. $[\alpha]_D$ -65 ($CHCl_3$).

Roller, P. *et al., Chem. Comm.*, 1971, 503 (*isol*)
Asato, A.E. *et al., Tet. Lett.*, 1973, 4941 (*synth*)
Mayer, A.M.S. *et al., Hydrobiologia*, 1993, **260**, 521-529; *CA*, **119**, 199280v (*isol*)

3-Hexyl-4-hydroxy-6-pentyl-2*H*-pyran-2-one H-327

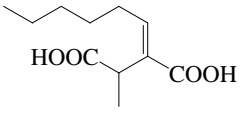


$C_{16}H_{26}O_3$ 266.38
Prod. by the marine *Pseudomonas* sp. F92S91. Antibacterial agent (incl. MRSA).

Singh, M.P. *et al., J. Antibiot.*, 2003, **56**, 1033-1044 (*isol, activity*)

2-Hexylidene-3-methylbutanedioic acid H-328

2-Hexylidene-3-methylsuccinic acid. 3-Nonene-2,3-dicarboxylic acid. ***Piliformic acid***



(+)-(*E*)-*form*

$C_{11}H_{18}O_4$ 214.261

(+)-(*E*)-*form* [98985-74-1]
Prod. by *Hypoxylon deustum*. Phytotoxin. $[\alpha]_D^{23}$ +31 (c, 1 in MeOH).

(-)-(*E*)-*form* [98985-75-2]
Prod. by *Poronia piliformis*, *Xylaria longipes* and *Xylaria polymorpha*.
Needles ($MeNO_2$).
Mp 132°. $[\alpha]_D^{23}$ -89 (c, 1 in MeOH).

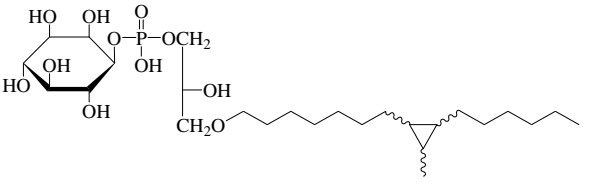
4-Me ester:
$C_{12}H_{20}O_4$ 228.288
Isol. from the marine fungus *Halorosellinia oceanica*. Oil. $[\alpha]_D^{29}$ -15.8 (c, 0.35 in MeOH). λ_{max} 212 (MeOH).

(±)-(*E*)-*form* [98985-76-3]
Prod. by *Xylaria hypoxylon* and *Xylaria mali*.
Needles ($MeNO_2$).
Mp 155°.

Anderson, J.R. *et al., J.C.S. Perkin 1*, 1985, 1481 (*isol, synth, pmr, ms*)
Chesters, N.C.J.E. *et al., J.C.S. Perkin 1*, 1997, 827 (*pmr, biosynth*)
Mangaleswaran, S. *et al., J.C.S. Perkin 1*, 2000, 3290-3291 (*synth*)
Chinworrungsee, M. *et al., Bioorg. Med. Chem. Lett.*, 2001, **11**, 1965-1969 (*Me ester*)

1-[7-(2-Hexyl-3-methylcyclopropyl)heptyl]lysoplasmanylinositol H-329

[351447-43-3]

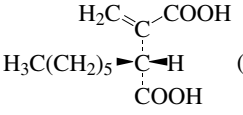


$C_{26}H_{51}O_{11}P$ 570.656
Isol. from the sponge *Theonella swinhoei*. Antimicrobial agent. Solid. $[\alpha]_D^{20}$ -10 (c, 0.03 in MeOH).

Matsunaga, S. *et al., J. Nat. Prod.*, 2001, **64**, 816-818

2-Hexyl-3-methylenebutanedioic acid H-330

Hexylmethylenebutanedioic acid, 9CI. 1-Nonene-2,3-dicarboxylic acid. ***Hexylitaconic acid***
[111430-51-4]



(*R*)-*form*

$C_{11}H_{18}O_4$ 214.261

(*R*)-*form* [94513-51-6]
Prod. by terrestrial and marine *Aspergillus niger*. Also from *Penicillium striatisporum*. Plant-growth regulator. Precursor of Canadensolide. Cryst. Sol. MeOH, $CHCl_3$, EtOAc.
Mp 46-47°. $[\alpha]_D$ +15.3 (c, 2 in MeOH). λ_{max} 207 (ϵ 5630) (MeOH).

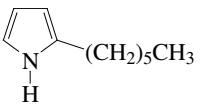
(*S*)-*form*
Isol. from the marine fungi *Apiospora montagnei* and *Arthrinium* sp. Inhibitor of p53-HDM2 interaction. Amorph. solid. $[\alpha]_D^{23}$ -17.9 (c, 0.5 in MeOH).

(±)-*form*
Thick oil.

Isogai, A. *et al., Agric. Biol. Chem.*, 1984, **48**, 2607-2609 (*isol, pmr, ms*)
Almassi, F. *et al., J. Nat. Prod.*, 1994, **57**, 833-836 (*isol*)
Varoglu, M. *et al., J. Nat. Prod.*, 2000, **63**, 41-43 (*isol*)
Kar, A. *et al., Tetrahedron*, 2003, **59**, 2991-2998 (*synth, pmr, cmr*)
Klemke, C. *et al., J. Nat. Prod.*, 2004, **67**, 1058-1063 (*isol, pmr, cmr*)
Stewart, M. *et al., J. Nat. Prod.*, 2005, **68**, 581-584 (*isol*)
Tsukamoto, S. *et al., Bioorg. Med. Chem. Lett.*, 2006, **16**, 69-71 (*isol, activity*)

2-Hexylpyrrole, 9CI H-331

[1551-14-0]



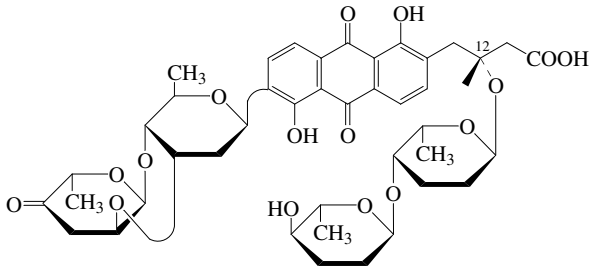
$C_{10}H_{17}N$ 151.251
$Bp_{1.5}$ 92°.

N-*Sulfo: 2-Hexylpyrrole sulfamate*
[587875-53-4]
$C_{10}H_{17}NO_3S$ 231.315
Alkaloid from the marine annelid *Cirriformia tentaculata*. Glass (as Na salt).

Utimoto, K. *et al., Tet. Lett.*, 1981, **22**, 4277-4288 (*synth*)
Garrido, D.O.A. *et al., J.O.C.*, 1984, **49**, 2619-2622 (*synth*)
Barsby, T. *et al., J. Nat. Prod.*, 2003, **66**, 1110-1112 (*sulfamate*)

Himalomycin A H-332

[701915-10-8]



$C_{43}H_{52}O_{16}$ 824.874

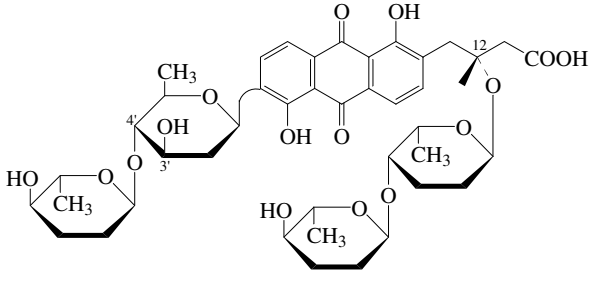
Prod. by the marine *Streptomyces* sp. B6921. Orange-yellow solid. $[\alpha]_D$ +30 (c, 0.07 in MeOH). λ_{max} 254 (log ϵ 4.32); 290 (log ϵ 3.95); 441 (log ϵ 3.88) (MeOH).

12-O-Deglycosyl: ***Fridamycin D***
[701915-09-5]
$C_{31}H_{32}O_{12}$ 596.587
Prod. by *Streptomyces parvulus* Tu1989. Yellow solid. $[\alpha]_D^{20}$ +40 (0.06 in MeOH). Anthracycline antibiotic. CAS no. not found 8-14CI. λ_{max} 254 (log ϵ 4.14); 293 (log ϵ 3.85); 443 (log ϵ 3.72) (MeOH).

Kricke, P. *et al., Ph.D. Thesis*, Univ. of Gottingen, 1984, (*Fridamycin D*)
Krohn, K. *et al., Tetrahedron*, 1988, **44**, 49-54 (*Fridamycin D*)
Maskey, R.P. *et al., J. Antibiot.*, 2003, **56**, 942-949 (*Himalomycin A*)

Himalomycin B H-333

[701915-11-9]



$C_{43}H_{56}O_{16}$ 828.906

Anthracycline antibiotic. Prod. by the marine *Streptomyces* sp. B6921. Yellow solid. $[\alpha]_D^{20}$ +30 (c, 0.07 in MeOH). λ_{max} 256 (log ϵ 4.36); 292 (log ϵ 3.96); 434 (log ϵ 3.97) (MeOH).

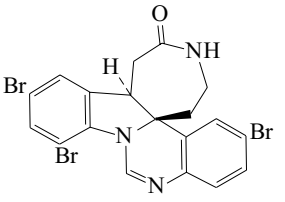
4′,12-Bis(deglycosyl): ***Fridamycin A***. *Vineomycinone B_2*
[30270-05-4]
$C_{25}H_{26}O_{10}$ 486.474
Prod. by *Streptomyces parvulus* Tu1989. Related to Vineomycin B_2, V-46.

4′,12-Bis(deglycosyl), 3′,4′-diepimer: ***Fridamycin B***
$C_{25}H_{26}O_{10}$ 486.474
Prod. by *Streptomyces parvulus* Tu1989.

Kricke, P. *et al., Ph.D. Thesis*, Univ. of Göttingen, 1984, (*Fridamycins*)
Krohn, K. *et al., Tetrahedron*, 1988, **44**, 49-54 (*Fridamycins*)
Maskey, R.P. *et al., J. Antibiot.*, 2003, **56**, 942-949 (*Himalomycin B*)
Chen, C.-L. *et al., J.A.C.S.*, 2006, **128**, 13696-13697 (*Fridamycin A, synth*)

Hinckdentine A H-334

[112663-91-9]



$C_{19}H_{14}Br_3N_3O$ 540.051

Alkaloid from the marine bryozoan *Hincksinoflustra denticulata*. Mp 196-197°. $[\alpha]_D^{25}$ +274 (solvent unspecified).

Blackman, A.J. *et al., Tet. Lett.*, 1987, **28**, 5561-5562 (*isol, uv, ir, pmr, ms, struct, abs config*)

Hipposin H-335

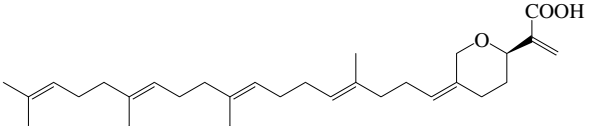
[518412-68-5]

Peptide containing 51 amino acid residues. Isol. from the skin mucus of the Atlantic halibut *Hippoglossus hippoglossus*. Antimicrobial agent.

Birkemo, G.A. *et al., Biochim. Biophys. Acta*, 2003, **1646**, 207-215 (*isol*)

Hippospongic acid A H-336

[183381-06-8]



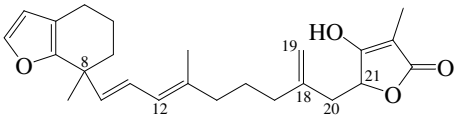
$C_{30}H_{46}O_3$ 454.692

Struct. revised in 1999. Constit. of a *Hippospongia* sp. $[\alpha]_D^{25}$ +37 (c, 0.22 in $CHCl_3$).

Ohta, S. *et al., Tet. Lett.*, 1996, **37**, 7765-7766 (*isol, pmr, cmr*)
Hioki, H. *et al., Tet. Lett.*, 1998, **39**, 7745-7746 (*synth, abs config*)
Tokumasu, M. *et al., J.C.S. Perkin 1*, 1999, 489-496 (*synth, struct*)
Takikawa, H. *et al., J.C.S. Perkin 1*, 1999, 2271-2275 (*synth*)
Ichihashi, M. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 2569-2572 (*synth*)
Hioki, H. *et al., Tetrahedron*, 2001, **57**, 1235-1246 (*synth, abs config*)
Trost, B.M. *et al., J.A.C.S.*, 2005, **127**, 7014-7024 (*synth*)

Hippospongin† H-337

[103538-55-2]



$C_{25}H_{32}O_4$ 396.525

Sesterterpene antibiotic. Isol. from *Hippospongia* sp. Shows antispasmodic activity. Also active against gram-positive bacteria. Oil. Sol. $CHCl_3$, Et_2O; poorly sol. C_6H_6, H_2O. $[\alpha]_D^{25}$ +15 (c, 5.4 in $CHCl_3$). λ_{max} 241 (ϵ 25100) (EtOH) (Derep).

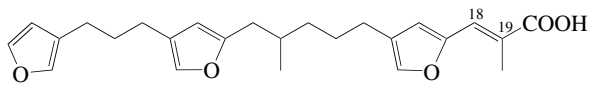
*8-Epimer, 18*S*,19-dihydro, 20,21-didehydro(*Z*-):* [501427-48-1]
$C_{25}H_{32}O_4$ 396.525
Constit. of an *Ircinia* sp. Oil. $[\alpha]_D^{30}$ +30.2 (c, 0.34 in $CHCl_3$). λ_{max} 240 (log ϵ 4.4); 310 (log ϵ 3.2) (MeOH).

*8*S*,12*Z*-Isomer, 18*S*,19-dihydro, 20,21-didehydro:* [501427-46-9]
$C_{25}H_{32}O_4$ 396.525
Constit. of an *Ircinia* sp. Oil. $[\alpha]_D^{25}$ +42 (c, 0.34 in $CHCl_3$). λ_{max} 240 (log ϵ 4.4); 310 (log ϵ 3.4) (MeOH).

Kobayashi, J. *et al., Tet. Lett.*, 1986, **27**, 2113-2116 (*isol, struct*)
Issa, H.H. *et al., J. Nat. Prod.*, 2003, **66**, 251-254 (*Ircinia constits*)

Hippospongin B H-338

[184301-91-5]

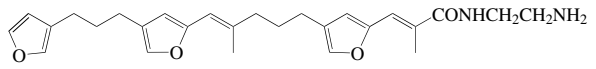


$C_{25}H_{30}O_5$ 410.509
Constit. of a *Hippospongia* sp. Pale yellow oil. $[\alpha]_D$ -5.1 (c, 0.9 in $CHCl_3$). λ_{max} 215 (log ϵ 4.17); 308 (log ϵ 4.38) (EtOH). λ_{max} 215 (ϵ 14800); 308 (ϵ 24000) (MeOH) (Berdy).

18,19-Dihydro: ***Hippospongin A***
[184301-90-4]
$C_{25}H_{32}O_5$ 412.525
Constit. of a *Hippospongia* sp. Pale yellow oil. $[\alpha]_D$ +0.4 (c, 0.9 in $CHCl_3$). λ_{max} 218 (log ϵ 4.54) (EtOH). λ_{max} 218 (ϵ 34670) (MeOH) (Berdy).
Rochfort, S.J. *et al., J. Nat. Prod.*, 1996, **59**, 1024-1028 (*isol, pmr, cmr, ms*)

Hippospongin C H-339

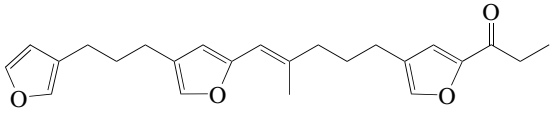
[184301-92-6]



$C_{27}H_{34}N_2O_4$ 450.577
Constit. of *Hippospongia* sp. Pale yellow oil. λ_{max} 206 (log ϵ 4.19); 276 (log ϵ 4.39); 287 (log ϵ 4.39); 303 (log ϵ 4.34) (EtOH). λ_{max} 206 (ϵ 13800); 276 (ϵ 24000); 287 (ϵ 24000); 303 (ϵ 21900) (MeOH) (Berdy).
Rochfort, S.J. *et al., J. Nat. Prod.*, 1996, **59**, 1024-1028 (*isol, pmr, cmr, ms*)

Hippospongin D H-340

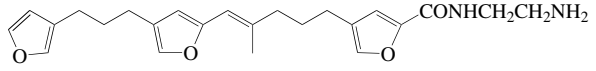
[184301-93-7]



$C_{24}H_{28}O_4$ 380.483
Constit. of a *Hippospongia* sp. Pale yellow oil. λ_{max} 214 (log ϵ 3.87); 277 (log ϵ 4.14) (EtOH). λ_{max} 214 (ϵ 7410); 303 (ϵ 23000) (MeOH) (Berdy).
Rochfort, S.J. *et al., J. Nat. Prod.*, 1996, **59**, 1024-1028 (*isol, pmr, cmr, ms*)

Hippospongin E H-341

[184301-94-8]

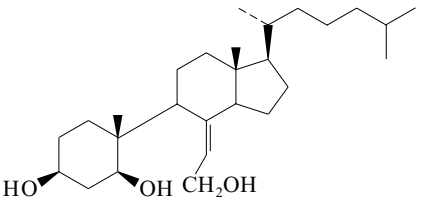


$C_{24}H_{30}N_2O_4$ 410.512
Constit. of a *Hippospongia* sp. Pale yellow oil. λ_{max} 279 (log ϵ 3.95) (EtOH). λ_{max} 279 (ϵ 8900) (MeOH) (Berdy).

ω-N-*Ac:* ***Hippospongin F***
[184301-95-9]
$C_{26}H_{32}N_2O_5$ 452.549
Constit. of a *Hippospongia* sp. Pale yellow oil. λ_{max} 265 (log ϵ 4.02) (EtOH). λ_{max} 265 (ϵ 10450) (MeOH) (Berdy).
Rochfort, S.J. *et al., J. Nat. Prod.*, 1996, **59**, 1024 (*isol, pmr, cmr, ms*)

Hipposterol H-342

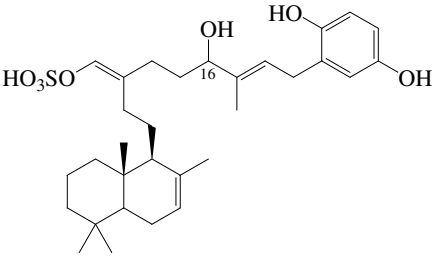
5,6-Secocholest-7-ene-3,5,6-triol
[119105-17-8]



$C_{27}H_{48}O_3$ 420.674
Constit. of *Hippospongia communis.* Cryst.
Mp 85-87°. $[\alpha]_D$ +71.9 (c, 0.3 in $CHCl_3$).
Madaio, A. *et al., Tet. Lett.*, 1988, **29**, 5999 (*struct, synth*)

Hipposulfate B H-343

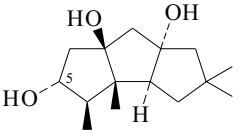
[331840-74-5]



$C_{31}H_{46}O_7S$ 562.766
Constit. of *Hippospongia* cf. *metachromia*. Oil. $[\alpha]_D$ +36.8 (c, 0.07 in MeOH). λ_{max} 205 (log ϵ 4.06); 293 (log ϵ 3.24) (MeOH).

16-Deoxy: ***Hipposulfate A***
[331840-72-3]
$C_{31}H_{46}O_6S$ 546.767
Constit. of *Hippospongia* cf. *metachromia*. Oil. $[\alpha]_D$ +8.1 (c, 0.31 in MeOH). λ_{max} 205 (log ϵ 4.08); 293 (log ϵ 3.23) (MeOH).
Musman, M. *et al., J. Nat. Prod.*, 2001, **64**, 350-352 (*isol, pmr, cmr*)

5,7,9-Hirsutanetriol H-344



$C_{15}H_{26}O_3$ 254.369

(5α,7β,9α)-*form*
Arthrosporol
[124724-99-8]
Metab. of an arthroconidial fungus (UMAH 4262). Antifungal agent. Cryst. (Et_2O). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 163-164°. $[\alpha]_D$ -29 (c, 2 in $CHCl_3$).

5-Ketone: 7,9-Dihydroxy-5-hirsutanone. ***Arthrosporone***
[124724-98-7]
$C_{15}H_{24}O_3$ 252.353
Metab. of fungus UAMH 4262. Antifungal agent. Cryst. (Et_2O/hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 139-141°. $[\alpha]_D$ -140.8 (c, 0.9 in $CHCl_3$). λ_{max} 232 (log ϵ 1.45); 283 (log ϵ 1.03) (MeCN). λ_{max} 280 (ϵ 650) (MeOH) (Berdy).

(3β,5β,7β,9α)-*form*
Gloeosteretriol
[141434-36-8]
Constit. of *Gloeostereum incarnatum*.
$[\alpha]_D^{22}$ +5.6 (c, 0.115 in MeOH).

ent*-(3β,5β,7β,9α)-*form

ent-*Gloeosteretriol*

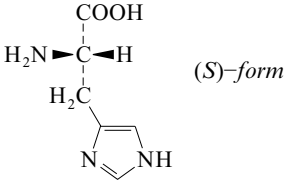
Metab. of an unidentified fungus isol. from a *Haliclona* sponge. $[\alpha]_D^{25}$ -1.5 (c, 1.33 in MeOH). λ_{max} 208 (ϵ 321) (MeOH).

Amouzou, E. *et al., J. Nat. Prod.*, 1989, **52**, 1042 (*isol, pmr*)
Gao, J. *et al., Acta Pharm. Sci.*, 1992, **27**, 33-36 (*Gloeosteretriol*)
Hellwig, V. *et al., Eur. J. Org. Chem.*, 1998, 73-79 (*isol, pmr, cmr, cryst struct*)
Wang, G.Y.S. *et al., Tetrahedron*, 1998, **54**, 7335-7342 (*Entgloeosteretriol*)

Histidine, INN, USAN H-345

*α-Amino-1*H*-imidazole-4-propanoic acid, 9CI. 2-Amino-3-imidazolylpropionic acid. 3-(1-Imidazolyl)alanine. His*

[7006-35-1]



(*S*)–*form*

$C_6H_9N_3O_2$ 155.156

The tautomerism of histidine in soln. does not appear very well documented. Both imidazole tautomers presumably present.

(*S*)-*form*

L-form. FEMA 3694

[71-00-1]

Constit. of most proteins, essential for infant growth. Dietary supplement, nutrient. Sol. H_2O (7.59 g per 100 cm^3 at 25°); sl. sol. EtOH.

Mp 277° dec. $[\alpha]_D^{25}$ -59.8 (-38.5) (H_2O). $[\alpha]_D^{25}$ +18.3 (+11.8) (5*M* HCl). Isoelectric point pH 7.59. Bitter taste.

▶ Exp. reprod. effects (large dose). MS3070000

N^{α}-*Ac:* N-*Acetylhistidine*

[2497-02-1]

[39145-52-3 (monohydrate)]

$C_8H_{11}N_3O_3$ 197.193

Constit. of the tissues of various fish, e.g. Atlantic salmon (*Salmo salar*), rainbow trout (*Salmo gairdneri*), Nile tilapia (*Oreochromis niloticus*) and amphibian spp., e.g. frogs (*Rana nigromaculata*, *Rana catesbiana* and *Bufo bufo japonicus*). Cryst. (H_2O).

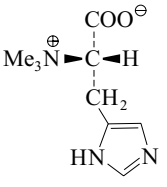
Mp 169° (157-159° (dec.)) Mp 187° (hydrate). $[\alpha]_D^{25}$ +46.8 (c, 1 in H_2O).

Kistenmacher, T.L. *et al., Acta Cryst. B*, 1972, **28**, 3352 (*N-Ac, cryst struct*)
Reddy, A.V. *et al., Synth. Commun.*, 1992, **22**, 257-264 (*N-Acetyhistidine*)
Togashi, M. *et al., Fish. Sci.*, 1998, **64**, 174-175 (*N^{α}-Ac, occur*)
Breck, O. *et al., Aquac. Nutr.*, 2005, **11**, 321-332 (*N^{α}-Ac, occur*)

Histidine trimethylbetaine H-346

α-Carboxy-N,N,N-*trimethyl-1*H*-imidazole-4-ethanaminium hydroxide inner salt, 9CI. (1-Carboxy-2-imidazol-4-ylethyl)trimethylammonium hydroxide inner salt, 8CI.* ***Hercynin****. Erzinine. Herzynine*

[507-29-9]



$C_9H_{15}N_3O_2$ 197.236

(*S*)-*form*

[534-30-5]

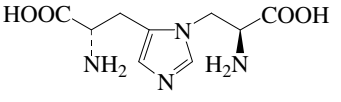
Occurs in rubber latex, prod. by fungi, e.g. *Boletus edulis* (porcini), *Agaricus bisporus* (button mushroom) and microorganisms. Shows fungal growth-regulating activity. Intermed. in biosynth. of Ergothioneine, E-781.

Mp 237-238° dec. $[\alpha]_D^{22}$ +44.5 (c, 1 in 5*M* HCl).

Barger, G. *et al., J.C.S.*, 1911, 2336 (*synth*)
Reinhold, V.N. *et al., J. Med. Chem.*, 1968, **11**, 258 (*synth*)
Tan, C.H. *et al., Phytochemistry*, 1968, **7**, 109 (*isol*)
Espersen, W.G. *et al., J. Phys. Chem.*, 1976, **80**, 741 (*cmr*)
Champavier, Y. *et al., Enzyme Microb. Technol.*, 2000, **26**, 243-251 (*activity*)

N^{π}-Histidinylalanine H-347

*α,α′-Diamino-1*H*-imidazole-1,5-dipropanoic acid.* N-*π-Histidinoalanine*



$C_9H_{14}N_4O_4$ 242.234

(*S,S*)-*form* [87047-17-4]

Isol. from the extrapallial fluid of the estuarine clam (*Rangia cuneata*). Characterised spectroscopically.

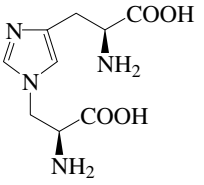
Sass, R.L. *et al., Biochem. Biophys. Res. Commun.*, 1983, **114**, 304-309 (*isol, clam, pmr, cmr*)
Henle, T. *et al., Z. Lebensm.-Unters. -Forsch.*, 1993, **197**, 114-117 (*occur, milk*)

N^{τ}-Histidinylalanine H-348

*α,α′-Diamino-1*H*-imidazole-1,4-dipropanoic acid.* N-*τ-Histidinoalanine. HAL*

[103974-26-1]

[141949-35-1]



$C_9H_{14}N_4O_4$ 242.234

(*S,S*)-*form* [65428-77-5]

Present in hydrolysates of human aorta, cataract lens, collagen, connective tissue, dentine and urine. Concentration increases with age and degree of tissue calcification. Also present in the extrapallial fluid of the estuarine clam (*Rangia cuneata*). Characterised spectroscopically.

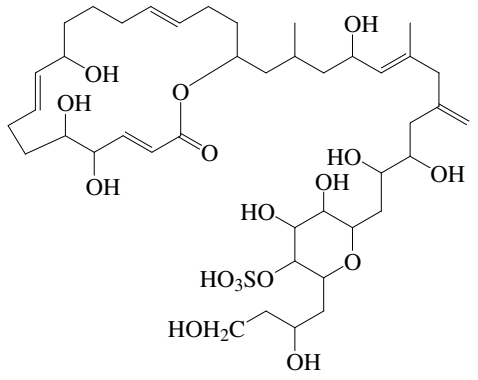
Fujimoto, D. *et al., Biochem. Biophys. Res. Commun.*, 1982, **104**, 1102-1106 (*S,S-form, occur, synth, pmr*)
Sass, R.L. *et al., Biochem. Biophys. Res. Commun.*, 1983, **114**, 304-309 (*isol, clam, pmr, cmr*)
Friedman, M. *et al., J. Agric. Food Chem.*, 1999, **47**, 1295-1319 (*rev, occur*)
Lauber, S. *et al., Nahrung*, 2001, **45**, 215-217 (*occur*)

HmT Toxin H-349

Peptide containing 177 amino acid residues lacking cysteine. Isol. from the sea anemone *Heteractis magnifica*. Cytolytic toxin.

Samejima, Y. *et al., Toxicon*, 2000, **38**, 259-264 (*isol*)

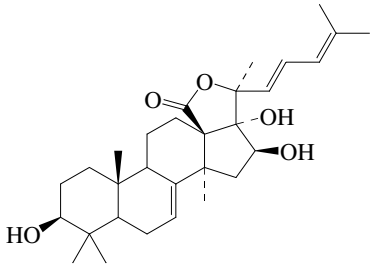
Hoffmanniolide H-350



$C_{42}H_{70}O_{17}S$ 879.071
Isol. from *Prorocentrum hoffmannianum*.

Hu, T. *et al., Tet. Lett.*, 1999, **40**, 3977-3980 (*isol, pmr, cmr*)

Holasta-7,22,24-triene-3,16,17-triol H-351



$C_{30}H_{44}O_5$ 484.675

(3β,16β,17α*OH*,22*E*)-*form*

*16-Ac, 3-*O*-[3-*O*-methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Intercedenside C***
[588728-83-0]
$C_{55}H_{84}O_{27}S$ 1209.318
Constit. of *Mensamaria intercedens*. Amorph. powder.
Mp 192-193°. $[\alpha]_D^{20}$ -32.3 (c, 0.54 in Py).

Zou, Z.-R. *et al., J. Nat. Prod.*, 2003, **66**, 1055-1060 (*isol, pmr, cmr*)

Holokinins H-352

Pro-Leu-Gly-Tyr-Met-Phe-Arg
Struct. of Holokinin 1 shown. Isol. from the body wall of the sea cucumber *Stichopus japonicus*. Controls the stiffness of the dermis.

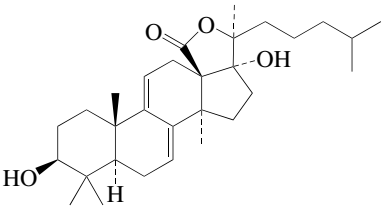
Holokinin 1 [169217-32-7]
$C_{42}H_{62}N_{10}O_9S$ 883.079

Holokinin 2 [169217-33-8]
$C_{42}H_{62}N_{10}O_{10}S$ 899.079
Struct. is that of Holokinin 1 with the methionine residue oxidised.

Iwakoshi, E. *et al., Pept. Chem.*, 1994, 261-264 (*isol*)
Birenheide, R. *et al., Biol. Bull. (Woods Hole, Mass.)*, 1998, **194**, 253-259 (*isol*)

Holosta-7,9(11)-diene-3,17-diol H-353

3,17-Dihydroxylanosta-7,9(11)-dien-18,20-olide



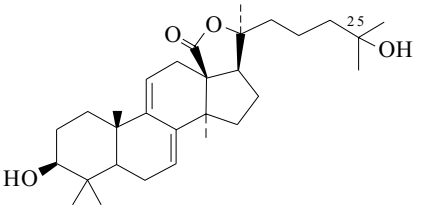
$C_{30}H_{46}O_4$ 470.691

3β-*form*

Holothurinogenin. *Nobilisdenol A*
[25495-63-0]
Constit. of *Holothuria nobilis*, *Holothuria polii*, *Holothuria atra*, *Holothuria scabra* and *Actinopyga flammea*.
Cryst. (MeOH).
Mp 277° dec. $[\alpha]_D$ +94.

Habermehl, G. *et al., Annalen*, 1970, **731**, 53-57 (*occur, pmr*)
Bhatnagar, S. *et al., Bull. Soc. Chim. Fr.*, 1985, 124-129 (*occur*)
Sarma, N.S. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 715-721 (*isol*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 666-668; 1996, **35**, 810-814 (*isol*)
Wu, J. *et al., Zhongguo Tianran Yaowu*, 2005, **3**, 276-279; *CA*, **144**, 209043c (*Nobilisidenol A*)

Holosta-7,9(11)-diene-3,25-diol H-354



$C_{30}H_{46}O_4$ 470.691

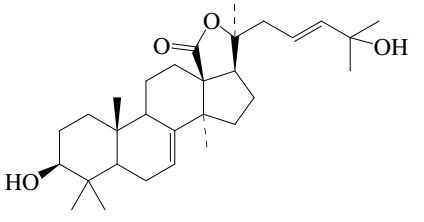
3β-*form*

17-Deoxy-25-hydroxyholothurinogenin. ***Koellikerigenin***
[24041-67-6]
Constit. of the sea cucumber *Bohadschia koellikeri* and *Holothuria polii*.
Cryst. (MeOH).
Mp 213-214°. $[\alpha]_D$ -8 ($CHCl_3$).

25-Me ether: ***Ternaygenin***
[24041-66-5]
$C_{31}H_{48}O_4$ 484.718
Constit. of *Bohadschia koellikeri*. Cryst.
Mp 239-242°. $[\alpha]_D$ +2 ($CHCl_3$). Artifact.

Roller, P. *et al., J.A.C.S.*, 1969, **91**, 4918 (*isol*)
Habermehl, G. *et al., Annalen*, 1970, 731; 53 (*isol*)

Holosta-7,23-diene-3,25-diol H-355

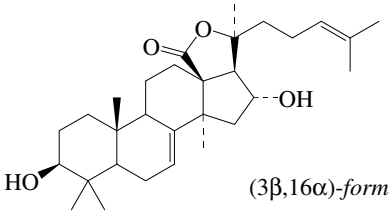


$C_{30}H_{46}O_4$ 470.691

(3β,23*E*)-*form*

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Frondoside A_2-3***
[852637-95-7]
$C_{59}H_{94}O_{29}S$ 1299.44
Constit. of *Cucumaria frondosa*. Powder.
Mp 213-215°. $[\alpha]_D^{20}$ -15 (c, 0.1 in Py).
Silchenko, A.S. *et al., Can. J. Chem.*, 2005, **83**, 21-27 (*Frondoside A_2-3*)

Holosta-7,24-diene-3,16-diol H-356



(3β,16α)-*form*

$C_{30}H_{46}O_4$ 470.691

(3β,16α)-*form*

16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Lefevreioside B***
[125850-46-6]
$C_{55}H_{86}O_{25}S$ 1179.335
Constit. of *Cucumaria lefevrei*.
$[\alpha]_D$ -25.4.

16-Ketone: 3-Hydroxyholosta-7,24-dien-16-one
$C_{30}H_{44}O_4$ 468.675

16-Ketone, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Frondoside A_2-1***
[852637-93-5]
$C_{59}H_{92}O_{29}S$ 1297.424
Constit. of *Cucumaria frondosa*. Powder.
Mp 218-220°. $[\alpha]_D^{20}$ -70 (c, 0.1 in Py).

(3β,16β)-*form*

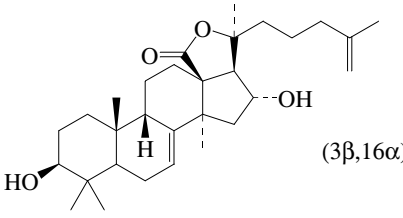
16-Ac: ***Philinopgenin C***
$C_{32}H_{48}O_5$ 512.728
Constit. of *Pentacta quadrangularis*. Powder.
Mp 216.5-217.5°.

16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Philinopside A***
[533936-25-3]
$C_{55}H_{86}O_{25}S$ 1179.335
Constit. of *Pentacta quadrangularis*. Amorph. powder.
Mp 222-225°. $[\alpha]_D^{20}$ -16.7 (c, 0.5 in Py).

16-Ac, 3-O-*[3*-O-*methyl-6*-O-*sulfo-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Intercedenside B***
[588728-81-8]
$C_{55}H_{86}O_{28}S_2$ 1259.4
Constit. of *Mensamaria intercedens*. Amorph. powder.
Mp 218-220°. $[\alpha]_D^{20}$ -14.2 (c, 0.5 in Py).

16-Ac, 3-O-*[3*-O-*methyl-6*-O-*sulfo-β-D-glucopyranosyl-(1→3)-6-O-sulfo-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Liouvilloside A***
[347894-53-5]
$C_{56}H_{88}O_{32}S_3$ 1369.49
Constit. of *Staurocucumis liouvillei*. Amorph. powder.
Mp 191-193°. $[\alpha]_D^{20}$ -4.9 (c, 0.5 in Py).
Rodriguez, J. *et al., J. Chem. Res., Synop.*, 1989, 342-343; *J. Chem. Res., Miniprint*, 1989, 2620 (*Lefevreioside B*)
Maier, M.S. *et al., J. Nat. Prod.*, 2001, **64**, 732-736 (*Liouvilloside A*)
Zou, Z.-R. *et al., J. Nat. Prod.*, 2003, **66**, 1055-1060 (*Intercedenside B*)
Zhang, S.-L. *et al., Mar. Drugs*, 2004, **2**, 185-191 (*Philinopgenin C*)
Silchenko, A.S. *et al., Can. J. Chem.*, 2005, **83**, 21-27 (*Frondoside A_2-1*)
Yi, Y.-H. *et al., Helv. Chim. Acta*, 2006, **89**, 54-63 (*Philinopside A*)

Holosta-7,25-diene-3,16-diol H-357



(3β,16α)-*form*

$C_{30}H_{46}O_4$ 470.691

(3β,16α)-*form*

Mp 247-249°. $[\alpha]_D^{20}$ -23.6 (c, 1.0 in Py).

16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Lefevreioside C***
[125850-47-7]
$C_{55}H_{86}O_{25}S$ 1179.335
Constit. of *Cucumaria lefevrei*.
$[\alpha]_D$ -13.6.

(3β,16β)-*form*

16-Ac: ***Cucumariogenin***
[86073-76-9]
$C_{32}H_{48}O_5$ 512.728
Genin from *Cucumaria fraudatrix*.

16-Ac, 3-O-*[3*-O-*methyl-β-D-xylopyranosyl-(1→4)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Thyonoside B***
[686347-82-0]
$C_{54}H_{84}O_{24}S$ 1149.309
Constit. of *Thyone aurea*. Amorph. powder.

16-Ac, 3-O-*[3*-O-*methyl-β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-β-D-fucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Cucumarioside G_1***
[81296-42-6]
$C_{55}H_{86}O_{25}S$ 1179.335
Constit. of *Cucumaria fraudatrix*. Cryst.
Mp 216-218°. $[\alpha]_D^{20}$ -21.8 (c, 3 in EtOH aq.).

16-Ac, 3-O-*[3*-O-*methyl-β-D-xylopyranosyl-(1→3)-6*-O-*sulfo-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Thyonoside A***
[686347-81-9]
$C_{55}H_{86}O_{28}S_2$ 1259.4
Constit. of *Thyone aurea*. Amorph. powder.

16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-2*-O-*sulfo-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Philinopside B***
[880496-30-0]
$C_{55}H_{86}O_{28}S_2$ 1259.4
Constit. of *Pentacta quadrangularis*. Amorph. powder.
Mp 218-220°. $[\alpha]_D^{20}$ -13.4 (c, 0.5 in Py).

16-Ac, 3-O-*[3*-O-*methyl-6*-O-*sulfo-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Neothyonidioside C***
[127506-67-6 (Na salt)]
$C_{55}H_{86}O_{28}S_2$ 1259.4
Constit. of *Neothyonidium magnum*. Cryst.
Mp 186° dec. (as Na salt). $[\alpha]_D^{20}$ -15 (c, 1 in Py) (Na salt).

16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-sulfo-β-D-xylopyranoside]:* ***Cucumarioside A_o-2***
[168433-96-3]
$C_{60}H_{94}O_{29}S$ 1311.451

Constit. of *Cucumaria japonica*. Cryst.
Mp 231-133°. $[\alpha]_D$ -44 (c, 0.1 in Py).

Di-Ac:
Cryst. (MeOH). Mp 213-215°. $[\alpha]_D^{20}$ +8 (c, 0.56 in $CHCl_3$).

16-Ketone: ***3-Hydroxyholosta-7,25-dien-16-one***
[79781-66-1]
$C_{30}H_{44}O_4$ 468.675
From *Cucumaria japonica*. Cryst.
Mp 225-257°. $[\alpha]_D^{20}$ -160 (c, 0.5 in $CHCl_3$).

*16-Ketone, 3-*O*-[3-*O*-methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Mollisoside B_2***
[857288-92-7]
$C_{53}H_{82}O_{25}S$ 1151.282
Constit. of *Australostichopus mollis*. Cryst.
Mp 240-242°. $[\alpha]_D^{20}$ -28 (c, 0.1 in Py).

*16-Ketone, 3-*O*-[3-*O*-methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Cucumarioside A_0-3***
[168433-97-4]
$C_{58}H_{90}O_{28}S$ 1267.398
Constit. of *Cucumaria japonica*. Cryst.
Mp 202° dec. $[\alpha]_D$ -100 (c, 0.1 in Py).

*16-Ketone, 3-*O*-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-sulfo-β-D-xylopyranoside]:* ***Cucumarioside A_4-2***
[133952-01-9]
$C_{58}H_{90}O_{29}S$ 1283.398
Constit. of *Cucumaria japonica*. Cryst.
Mp 205-207°. $[\alpha]_D^{20}$ -91 (c, 0.1 in Py).

*16-Ketone, 3-*O*-[6-*O*-acetyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-sulfo-β-D-xylopyranoside]:* ***Cucumarioside A_1-2***
[168433-94-1]
$C_{60}H_{92}O_{30}S$ 1325.435
Constit. of *Cucumaria japonica*.

*16-Ketone, 3-*O*-[3-*O*-methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Cucumarioside A_2-2***. *Frondoside E_1*
[95499-80-2]
$C_{59}H_{92}O_{29}S$ 1297.424
Constit. of *Cucumaria japonica* and *Cucumaria frondosa*. Cryst.
Mp 245-247°. $[\alpha]_D^{20}$ -68 (c, 0.2 in Py).

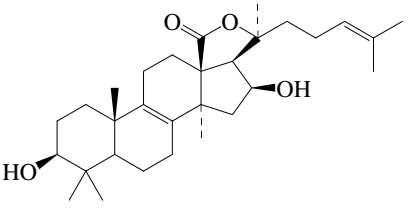
*16-Ketone, 3-*O*-[3-*O*-methyl-β-D-glucopyranosyl-(1→3)-6-*O*-sulfo-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Cucumarioside A_3***
[178209-19-3]
$C_{59}H_{92}O_{32}S_2$ 1377.489
Isol. from sea cucumbers *Cucumaria miniata* and *Cucumaria japonica*.
Mp 230-231° dec. (as Na/K salt). $[\alpha]_D^{20}$ -80 (c, 0.1 in Py) (Na/K salt).

*16-Ketone, 3-*O*-[3-*O*-methyl-6-*O*-sulfo-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Cucumarioside A_6-2***
[178209-18-2]
$C_{59}H_{92}O_{32}S_2$ 1377.489
Isol. from *Cucumaria miniata* and *Cucumaria japonica*.
Mp 230-232° dec. (as Na/K salt). $[\alpha]_D^{20}$ -80 (c, 0.1 in Py) (Na/K salt).

*16-Ketone, 3-*O*-[3-*O*-methyl-6-sulfo-β-D-glucopyranosyl-(1→3)-6-sulfo-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-sulfo-β-D-xylopyranoside]:* ***Cucumarioside A_7-1***
[172274-40-7]
$C_{59}H_{92}O_{35}S_3$ 1457.553
Constit. of *Cucumaria japonica*. Cryst.
Mp 223-225° dec. $[\alpha]_D$ -83 (c, 0.1 in aq. Py).

Afiyatullov, S.S. *et al., Khim. Prir. Soedin.*, 1983, **19**, 59-64; 1985, **21**, 244-248; *Chem. Nat. Compd. (Engl. Transl.)*, 1983, **19**, 55-59; 1985, **21**, 228-232 (*Cucumariogenin, Cucumarioside G1*)
Sharypov, V.F. *et al., Khim. Prir. Soedin.*, 1985, **21**, 55-59; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 51-56 (*16-ketone*)
Rodriguez, J. *et al., J. Chem. Res., Synop.*, 1989, 342-343; *J. Chem. Res., Miniprint*, 2620 (*Lefevreioside C*)
Avilov, S.A. *et al., Khim. Prir. Soedin.*, 1990, **26**, 55-57; 787-793; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 42-45; 670-675 (*Neothyonidioside C, Cucumariosides A4-2, A2-2*)
Drozdova, O.A. *et al., Khim. Prir. Soedin.*, 1992, **28**, 590-591; 1993, **29**, 242-248; 369-374; *Chem. Nat. Compd. (Engl. Transl.)*, 1992, **28**, 518-519; 1993, **29**, 200-205; 309-313 (*Cucumariosides*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508 (*biosynth*)
Drozdova, O.A. *et al., Liebigs Ann./Recl.*, 1997, 2351-2356 (*Cucumarioside A_3, Cucumarioside A_6-2*)
Yayli, N. *et al., Indian J. Chem., Sect. B*, 2001, **40**, 399-404 (*Frondoside E1*)
Bonnard, I. *et al., Tetrahedron*, 2004, **60**, 2987-2992 (*Thyonosides*)
Moraes, G. *et al., J. Nat. Prod.*, 2005, **68**, 842-847 (*Mollisoside B_2*)
Yi, Y.-H. *et al., Helv. Chim. Acta*, 2006, **89**, 54-63 (*Philinopside B*)

Holosta-8,24-diene-3,16-diol H-358

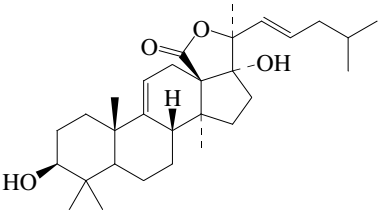


$C_{30}H_{46}O_4$ 470.691

(3β,16β)-*form*

16-Ac: ***Philinopgenin C***
[851625-07-5]
$C_{32}H_{48}O_5$ 512.728
Constit. of the sea cucumber *Pentacta quadrangularis*. Powder.
Mp 216.5-217.5°.
Zhang, S.-L. *et al., Mar. Drugs*, 2004, **2**, 185-191 (*Philinopgenin C*)

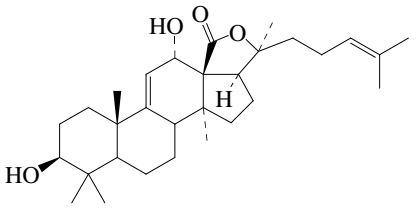
Holosta-9(11),22-diene-3,17-diol H-359



$C_{30}H_{46}O_4$ 470.691

(3β,5α,17α,22*E*)-*form*
Nobilisidenol B
[875627-67-1]
Constit. of *Holothuria nobilis*.
Wu, J. *et al., Zhongguo Tianran Yaowu*, 2005, **3**, 276-279; *CA*, **144**, 209043c (*Nobilisidenol B*)

Holosta-9(11),24-diene-3,12-diol H-360

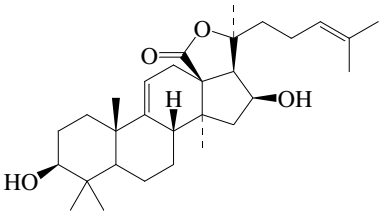


$C_{30}H_{46}O_4$ 470.691

(3β,12α)-*form*

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Pervicoside B***
[96157-95-8]
$C_{54}H_{86}O_{25}S$ 1167.324
Constit. of *Holothuria pervicax*. Sol. MeOH, H_2O, butanol; poorly sol. hexane.
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1230-1234

Holosta-9(11),24-diene-3,16-diol H-361

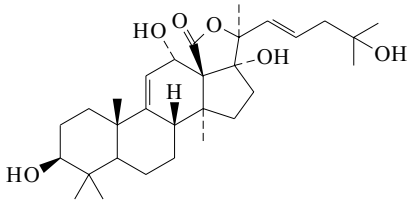


$C_{30}H_{46}O_4$ 470.691

(3β,16β)-*form*

16-Ac: ***Philinopgenin A***
[851625-05-3]
$C_{32}H_{48}O_5$ 512.728
Constit. of *Pentacta quadrangularis.* Powder.
Mp 208.5°.
Zhang, S.-L. *et al., Mar. Drugs*, 2004, **2**, 185-191 (*Philinopgenin A*)

Holosta-9(11),22-diene-3,12,17,25-tetrol H-362



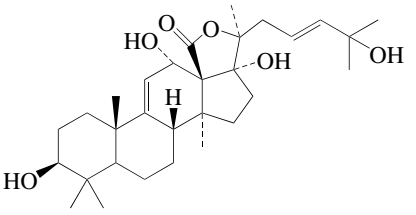
$C_{30}H_{46}O_6$ 502.69

(3β,12α,17α,20*S*,22*E*)-*form*

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***25-Hydroxydehydroechinoside A***
[97285-48-8]
$C_{54}H_{86}O_{27}S$ 1199.323
Constit. of *Actinopyga flammea*. Possibly Δ^{23}-isomer.

25-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Holothurinoside B***
[136005-73-7]
$C_{62}H_{98}O_{30}$ 1323.438
Constit. of echinoderm *Holothuria forskalii.* Cryst.
Mp 230-232°.
Bhatnagar, S. *et al., Bull. Soc. Chim. Fr.*, 1985, 124-129 (*25-Hydroxydehydroechinoside A*)
Rodriguez, J. *et al., Tetrahedron*, 1991, **47**, 4753-4762 (*Holothurinoside B*)

Holosta-9(11),23-diene-3,12,17,25-tetrol H-363

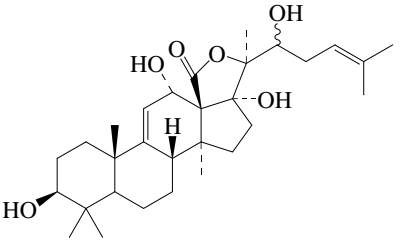


$C_{30}H_{46}O_6$ 502.69

(3β,12α,17α,23*E*)-*form*

3-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Holothurin B_4***
[852469-38-6]
$C_{41}H_{64}O_{17}S$ 861.012
Constit. of *Holothuria polii*. Cryst.
Mp 232-233°. $[\alpha]_D^{20}$ -12 (c, 0.1 in Py).
Silchenko, A.S. *et al., J. Nat. Prod.*, 2005, **68**, 564-567 (*Holothurin B_4*)

Holosta-9(11),24-diene-3,12,17,22-tetrol H-364

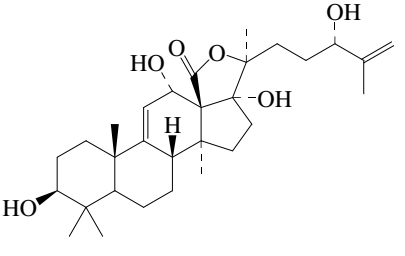


$C_{30}H_{46}O_6$ 502.69

(3β,12α,17α,22ξ)-*form*

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***22-Hydroxy-24-dehydroechinoside A***
[97243-48-6]
$C_{54}H_{86}O_{27}S$ 1199.323
Constit. of *Actinopyga flammea*.
Bhatnagar, S. *et al., Bull. Soc. Chim. Fr.*, 1985, 124-129 (*isol, pmr, cmr*)

Holosta-9(11),25-diene-3,12,17,24-tetrol H-365



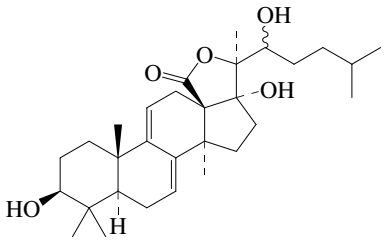
$C_{30}H_{46}O_6$ 502.69

(3β,12α,17α,24*S*)-*form*

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***24-Hydroxy-25-dehydroechinoside A***
[97243-47-5]
$C_{54}H_{86}O_{27}S$ 1199.323

Constit. of *Actinopyga flammea*.
Bhatnagar, S. *et al., Bull. Soc. Chim. Fr.*, 1985, 124-129 (*isol, pmr, cmr*)

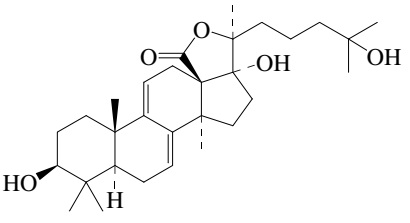
Holosta-7,9(11)-diene-3,17,22-triol H-366



$C_{30}H_{46}O_5$ 486.69

(3β,5α,22ξ): ***Griseogenin***. *22ξ-Hydroxyholothurinogenin*
[13855-03-3]
Constit. of *Holothuria polii* and *Halodeima grisea*.
Cryst. ($CHCl_3$/hexane).
Mp 285-287°. $[\alpha]_D^{26}$ -22 (c, 0.4 in $CHCl_3$).
Tursch, B. *et al., Tetrahedron*, 1967, **23**, 761-767 (*Griseogenin*)

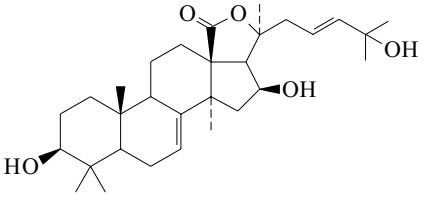
Holosta-7,9(11)-diene-3,17,25-triol H-367



$C_{30}H_{46}O_5$ 486.69

(3β,5α)-*form*
25-Me ether: 25-Methoxyholosta-7,9(11)-diene-3,17-diol. ***Praslinogenin***
[25495-64-1]
$C_{31}H_{48}O_5$ 500.717
Constit. of *Holothuria polii* and *Bohadschia koellikeri*. Cryst. (MeOH).
Mp 290-291.5°. Artifact.
Habermehl, G. *et al., Annalen*, 1970, **731**, 53-57 (*Praslinogenin*)

Holosta-7,23-diene-3,16,25-triol H-368



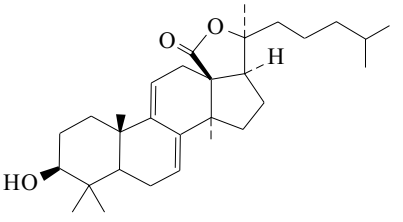
$C_{30}H_{46}O_5$ 486.69

(3β,16β,23*E*)-*form*
*16-Ac, 3-*O*-[3-*O*-methyl-β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]*: ***Cucumarioside G4***
[402741-14-4]
$C_{55}H_{86}O_{26}S$ 1195.335
Constit. of *Eupentacta fraudatrix*. Cryst.
Mp 211-213°. $[\alpha]_D$ -11 (c, 0.1 in Py).

*16-Ac, 3-*O*-[3-*O*-methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]*: ***Eximisoside A***
[193816-63-6]
$C_{55}H_{86}O_{24}$ 1131.27
Constit. of *Psolus eximius*. Cryst.
Mp 218-221°. $[\alpha]_D^{20}$ -25 (c, 0.1 in Py).

*16-Ac, 3-*O*-[3-*O*-methyl-6-*O*-sulfo-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]*: ***Calcigeroside E***
[298693-71-7]
$C_{62}H_{98}O_{35}S_2$ 1467.567
Isol. from sea cucumber *Pentamera calcigera*.
Mp 239-241° (as di-Na salt). $[\alpha]_D^{20}$ -20 (c, 0.1 in 50% Py aq.) (di-Na salt).
Kalinin, V.I. *et al., Khim. Prir. Soedin.*, 1992, **28**, 691-694; *Chem. Nat. Compd. (Engl. Transl.)*, 1992, **28**, 600-603 (*Cucumarioside G4*)
Kalinin, V.I. *et al., J. Nat. Prod.*, 1997, **60**, 817-819 (*Eximisoside A*)
Avilov, S.A. *et al., J. Nat. Prod.*, 2000, **63**, 1349-1356 (*Calcigeroside E*)

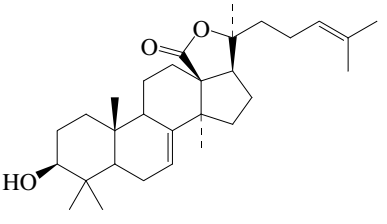
Holosta-7,9(11)-dien-3-ol H-369



$C_{30}H_{46}O_3$ 454.692

3β-*form*
Seychellogenin
[24041-68-7]
Constit. of the sea cucumber *Bohadschia koellikeri*.
Cryst.
Mp 234-238°. $[\alpha]_D$ -7 ($CHCl_3$). λ_{max} 236 (ϵ 12200); 243 (ϵ 12500); 252 (ϵ 8800) (MeOH) (Derep).
Roller, P. *et al., J.A.C.S.*, 1969, **91**, 4918 (*isol, struct*)
Milliet, A. *et al., Tet. Lett.*, 1974, 1939 (*synth*)
Habermehl, G. *et al., Naturwissenschaften*, 1978, **65**, 155 (*synth*)

Holosta-7,24-dien-3-ol H-370

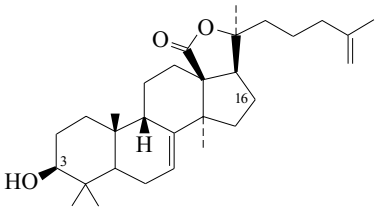


$C_{30}H_{46}O_3$ 454.692

3β-*form*
*3-*O*-[3-*O*-Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]*: ***Frondoside A_2-4***
[890152-27-9]
$C_{59}H_{94}O_{28}S$ 1283.441
Constit. of *Cucumaria frondosa*. Powder.
Mp 235-237°. $[\alpha]_D^{20}$ -90 (c, 0.1 in Py).
*3-*O*-[3-*O*-Methyl-β-D-glucopyranosyl-(1→3)-6-*O*-sulfo-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]*: ***Frondoside B***

[139069-40-2]
[139030-90-3]
$C_{59}H_{94}O_{31}S_2$ 1363.505
Constit. of *Cucumaria frondosa*. Amorph. solid.
Mp 216-218° dec. $[\alpha]_D^{23}$ -34.7 (c, 0.0017 in Py aq.).
Findlay, J.A. *et al., J. Nat. Prod.*, 1992, **55**, 93-101 (*Frondoside B*)
Silchenko, A.S. *et al., Can. J. Chem.*, 2005, **83**, 2120-2126 (*Frondoside A_2-4*)

Holosta-7,25-dien-3-ol H-371



$C_{30}H_{46}O_3$ 454.692

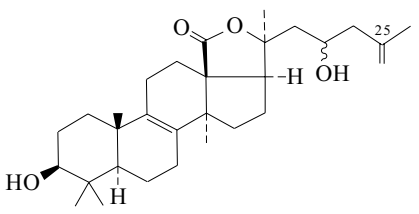
3β-*form* [97719-78-3]
Constit. of *Cucumaria japonica*.
Cryst.
Mp 188-190°. $[\alpha]_D^{20}$ -36 (c, 0.15 in $CHCl_3$).

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Cucumarioside A_2-4***
[133952-00-8]
$C_{59}H_{94}O_{28}S$ 1283.441
Constit. of *Cucumaria japonica*. Cryst.
Mp 203-205°. $[\alpha]_D^{20}$ -53 (c, 0.1 in Py).

3-O-*[3*-O-*Methyl-6*-O-*sulfo-β-D-glucopyranosyl-(1→3)-6*-O-*sulfo-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Cucumarioside A_7-3***
[172304-09-5]
$C_{59}H_{94}O_{34}S_3$ 1443.569
Constit. of *Cucumaria japonica*. Cryst.
Mp 238-240°. $[\alpha]_D$ -43 (c, 0.1 in Py aq.).
Avilov, S.A. *et al., Khim. Prir. Soedin.*, 1990, **26**, 787-793; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 670-675 (*Cucumarioside A_2-4*)
Drozdova, O.A. *et al., Khim. Prir. Soedin.*, 1993, **29**, 369-374; *Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 309-313 (*Cucumarioside A_7-3*)

Holosta-8,25-dien-3-ol H-372

*3,20,23-Trihydroxylanosta-8,25-dien-18-oic acid γ-lactone. 3β,23ξ-Dihydroxylanosta-8,25-diene-18,20*S*-lactone*



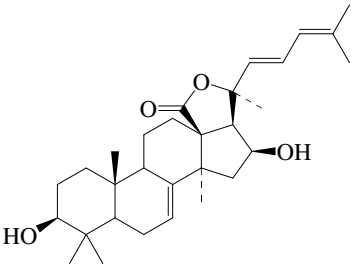
$C_{30}H_{46}O_4$ 470.691

(3β,23ξ)-*form*

23-Ac: ***23-Acetoxyholosta-8,25-dien-3-ol***
[62335-07-3]
$C_{32}H_{48}O_5$ 512.728
Aglycone from *Thelonota ananas*. Cryst.
Mp 196-198°.

25ξ,26-Dihydro, 23-Ac: ***23ξ-Acetoxyholost-8-en-3β-ol***
[62335-06-2]
$C_{32}H_{50}O_5$ 514.744
Aglycone from *Thelonota ananas*.
Mp 198-201°. $[\alpha]_D$ +13.8 (c, 0.5 in MeOH).
Kelecom, A. *et al., Tetrahedron*, 1976, **32**, 2313-2319 (*isol, pmr, cmr*)

Holosta-7,22,24-triene-3,16-diol H-373



(3β,16β,22*E*)-*form*

$C_{30}H_{44}O_4$ 468.675

(3β,16β,22*E*)-*form*

16-Ac, 3-O-*[3*-O-*methyl-β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Cucumarioside C_2***
[114129-89-4]
$C_{60}H_{92}O_{26}$ 1229.371
Constit. of *Cucumaria fraudatrix*. Cryst.
Mp 192-194°. $[\alpha]_D^{20}$ -48 (c, 0.1 in Py).

16-Ac, 3-O-*[3*-O-*methyl-β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Cucumarioside H***
[116524-58-4]
$C_{60}H_{92}O_{29}S$ 1309.435
Constit. of *Cucumaria fraudatrix*. Cryst.
Mp 205-208°. $[\alpha]_D^{20}$ -71 (c, 0.1 in Py).

16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Intercedenside A***
[588728-73-8]
$C_{55}H_{84}O_{25}S$ 1177.32
Constit. of *Mensamaria intercedens*. Amorph. powder.
Mp 184-186°. $[\alpha]_D^{20}$ -27.3 (c, 0.6 in Py).

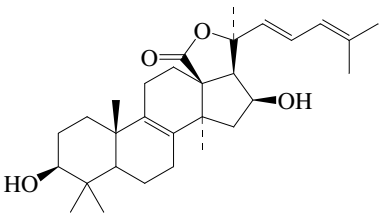
(3β,16β,22*Z*)-*form*

16-Ac, 3-O-*[3*-O-*methyl-β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Cucumarioside G_3***
[402824-98-0]
$C_{54}H_{82}O_{24}S$ 1147.293
Constit. of *Eupentacta fraudatrix*. Cryst.
Mp 208-211°. $[\alpha]_D$ -85 (c, 0.1 in Py).

16-Ac, 3-O-*[3*-O-*methyl-β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Cucumarioside C_1***
[114054-66-9]
$C_{60}H_{92}O_{26}$ 1229.371
Constit. of *Cucumaria fraudatrix*. Cryst.
Mp 196-199°. $[\alpha]_D^{20}$ -12 (c, 0.323 in MeOH).

16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-xylopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Intercedenside G***
[852637-24-2]
$C_{54}H_{82}O_{25}S$ 1163.293
Constit. of *Mensamaria intercedens*. Amorph. powder.
Mp 241.5-243°. $[\alpha]_D^{20}$ -41.9 (c, 0.46 in Py).
Afiyatullov, S.S. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 691-695 (*Cucumariosides C_1,C_2*)
Kalinin, V.I. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1988, **24**, 187-189 (*Cucumarioside H*)
Kalinin, V.I. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1992, **28**, 635-636 (*Cucumarioside G_3*)
Zou, Z.-R. *et al., J. Nat. Prod.*, 2003, **66**, 1055-1060 (*Intercedenside A*)
Zou, Z. *et al., J. Nat. Prod.*, 2005, **68**, 540-546 (*Intercedenside G*)

Holosta-8,22,24-triene-3,16-diol H-374

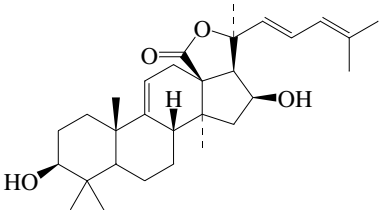


$C_{30}H_{44}O_4$ 468.675

(3β,16β,22*E*)-*form*

16-Ac: ***Intercedenol B***
[717890-68-1]
$C_{32}H_{46}O_5$ 510.712
Constit. of *Mensamaria intercedens.* Powder.
Mp 203.5-205.4°.
Zou, Z.R. *et al., Chin. Chem. Lett.*, 2004, **15**, 309-312 (*isol, pmr, cmr*)

Holosta-9(11),22,24-triene-3,16-diol H-375

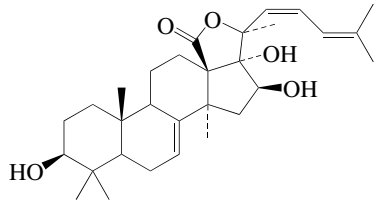


$C_{30}H_{44}O_4$ 468.675

(3β,16β,22*E*)-*form*

16-Ac: ***Intercedenol A***
[717890-67-0]
$C_{32}H_{46}O_5$ 510.712
Constit. of *Mensamaria intercedens.* Powder.
Mp 212.5-213.4°.
Zou, Z.R. *et al., Chin. Chem. Lett.*, 2004, **15**, 309-312 (*isol, pmr, cmr*)

Holosta-7,22,24-triene-3,16,17-triol H-376



$C_{30}H_{44}O_5$ 484.675

(3β,16β,17α,22*Z*)-*form*

16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Intercedenside D***
[852636-81-8]
$C_{55}H_{84}O_{27}S$ 1209.318
Constit. of *Mensamaria intercedens.* Amorph. powder.
Mp 214-216°. $[\alpha]_D^{20}$ -36.3 (c, 0.54 in Py).

16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-xylopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Intercedenside E***
[852636-82-9]
$C_{54}H_{82}O_{26}S$ 1179.292
Constit. of *Mensamaria intercedens.* Amorph. powder.
Mp 242-244°. $[\alpha]_D^{20}$ -39.4 (c, 0.43 in Py).

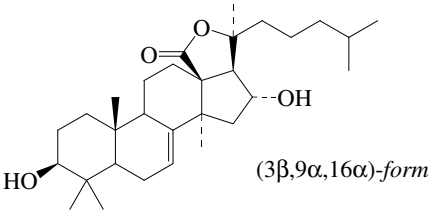
16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Intercedenside H***
[852637-25-3]
$C_{55}H_{84}O_{26}S$ 1193.319
Constit. of *Mensamaria intercedens.* Amorph. powder.
Mp 188-190°.

22,23-Dihydro: Holosta-7,24-diene-3,16,17-triol
$C_{30}H_{46}O_5$ 486.69

22,23-Dihydro, 16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Intercedenside F***
[852636-83-0]
$C_{55}H_{86}O_{27}S$ 1211.334
Constit. of *Mensamaria intercedens.* Amorph. powder.
Mp 226-228°. $[\alpha]_D^{20}$ -33.2 (c, 0.39 in Py).

22,23-Dihydro, 16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Intercedenside I***
[852637-26-4]
$C_{55}H_{86}O_{26}S$ 1195.335
Constit. of *Mensamaria intercedens.* Amorph. powder.
Mp 221-223°. $[\alpha]_D^{20}$ -17 (c, 0.47 in Py).
Zou, Z. *et al., J. Nat. Prod.*, 2005, **68**, 540-546 (*Intercedensides D-F and H-I*)

Holost-7-ene-3,16-diol H-377



$C_{30}H_{48}O_4$ 472.707

(3β,9α,16α)-*form*

16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Lefevreioside A$_1$***
[125850-44-4]
$C_{55}H_{88}O_{22}$ 1101.287
Constit. of *Cucumaria lefevrei.*
$[\alpha]_D$ -17.7.

16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Lefevreioside A$_2$***
[125850-45-5]
$C_{55}H_{88}O_{25}S$ 1181.351
Constit. of *Cucumaria lefevrei.*
$[\alpha]_D$ -18.3.

(3β,9α,16β)-*form*

16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-sulfo-β-D-xylopyranoside]:* ***Frondoside A$_1$***
[169219-21-0]
$C_{60}H_{96}O_{29}S$ 1313.467
Constit. of *Cucumaria frondosa.* Cryst.
Mp 242-244°. $[\alpha]_D$ -14 (c, 0.1 in Py).

16-Ac, 3-O-*[3*-O-*methyl-6*-O-*sulfo-β-D-glucopyranosyl-(1→3)-6*-O-*sulfo-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Liouvilloside B***
[347894-57-9]
$C_{56}H_{90}O_{32}S_3$ 1371.506
Constit. of *Staurocucumis liouvillei.* Amorph. powder.
Mp 192-194°. $[\alpha]_D^{20}$ -10.5 (c, 0.4 in Py).

16-Ketone, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Cucumarioside A$_2$-3***
[133951-99-2]
$C_{59}H_{94}O_{29}S$ 1299.44
Constit. of *Cucumaria japonica*. Cryst.
Mp 211-212°. $[\alpha]_D^{20}$ -62.5 (c, 0.16 in Py).

16-Ketone, 3-O-*[3*-O-*methyl-6-sulfo-β-D-glucopyranosyl-(1→3)-6-sulfo-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-sulfo-β-D-xylopyranoside]:* ***Cucumarioside A$_7$-2***
[172274-41-8]
$C_{59}H_{94}O_{35}S_3$ 1459.569
Constit. of *Cucumaria japonica*.

(3β,9β,16α)-*form*

16-Ac: Frondogenin
[90706-52-8]
$C_{32}H_{50}O_5$ 514.744
Sapogenin from *Cucumaria frondosa*.

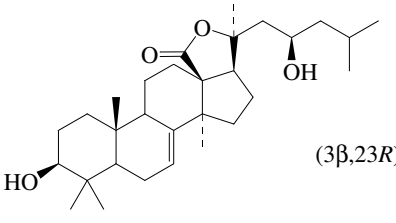
16-Ac, 3-O-*[β-D-xylopyranosyl-(1→4)-xylopyranoside]:* [90706-56-2]
$C_{42}H_{66}O_{13}$ 778.976
Constit. of *Cucumaria frondosa*. Amorph.

(3β,9β,16β)-*form*

16-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-sulfo-β-D-xylopyranoside], 16-Ac:* ***Frondoside A***
[127367-76-4]
$C_{60}H_{96}O_{29}S$ 1313.467
Constit. of *Cucumaria frondosa*. Cryst.
Mp 234-236°. $[\alpha]_D$ -31 (c, 0.1 in Py). $[\alpha]_D$ -13 (c, 26 in H_2O).
Findlay, J.A. *et al., J. Nat. Prod.*, 1984, **47**, 320-324 (*Frondogenin, 16-Ac 3-dixyloside*)
Rodriguez, J. *et al., J. Chem. Res., Synop.*, 1989, 342-343; *J. Chem. Res., Miniprint*, 1989, 2620-2636 (*Lefevreiosides*)
Girard, M. *et al., Can. J. Chem.*, 1990, **68**, 11-18 (*Frondoside A*)
Avilov, S.A. *et al., Khim. Prir. Soedin.*, 1990, **26**, 787-793; 1993, **29**, 260-263; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 670-675; 1993, **29**, 216-218 (*Cucumarioside A2-3, Frondosides*)
Drozdova, O.A. *et al., Khim. Prir. Soedin.*, 1993, **29**, 369-374; *Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 309-313 (*Cucumarioside A7-2*)
Maier, M.S. *et al., J. Nat. Prod.*, 2001, **64**, 732-736 (*Liouvilloside B*)

Holost-7-ene-3,23-diol H-378

3,23-Dihydroxylanost-7-en-18,20-olide



(3β,23*R*)-*form*

$C_{30}H_{48}O_4$ 472.707

(3β,23*R*)-*form*

23-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Stichoposide C***
[37341-38-1]
$C_{68}H_{110}O_{32}$ 1439.598
Constit. of *Stichopus variegatus*. Cryst.
Mp 260°. $[\alpha]_D^{20}$ -40.8 (c, 0.45 in Py).

(3β,23*S*)-*form*
Stichlorogenol
[78183-30-9]
Isol. from the sea cucumber *Stichopus chloronotus*.
Cryst. (MeOH).
Mp 225-226°. $[\alpha]_D^{20}$ -42 ($CHCl_3$).

23-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Thelenotoside A***
[84897-09-6]
$C_{55}H_{88}O_{22}$ 1101.287
Constit. of *Thelenota ananas*. Cryst. (EtOH). Sol. MeOH, butanol; fairly sol. H_2O.
Mp 241-242°. $[\alpha]_D^{20}$ -50.3 (c, 2.7 in Py).

23-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Thelenotoside B***
[72175-95-2]
$C_{55}H_{88}O_{23}$ 1117.286
Constit. of the echinoderm *Thelenota ananas*. Cryst. (EtOH). Sol. MeOH, butanol; fairly sol. H_2O.
Mp 208-210°. $[\alpha]_D^{20}$ -45.7 (c, 1.4 in Py).

23-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl (1→2)-[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Stichloroside C$_1$***
[78244-73-2]
$C_{68}H_{110}O_{32}$ 1439.598
Constit. of echinoderm *Stichopus chloronotus*. Antifungal agent. Cryst. Poorly sol. hexane.
Mp 251-253°. $[\alpha]_D^{15}$ -50 (Py).

23-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-β-D-xylopyranosyl (1→2)-[3*-O-*methyl-β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Stichloroside A$_1$****. Stichoposide E*
[78244-75-4]
$C_{68}H_{110}O_{33}$ 1455.597
Constit. of *Stichopus chloronotus*. Antifungal agent. Cryst.
Mp 213-215°. $[\alpha]_D^{15}$ -47 (Py).

23-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-glucopyranosyl (1→2)-[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Stichloroside B$_1$****. Stichoposide D*
[78244-74-3]
$C_{68}H_{110}O_{33}$ 1455.597
Constit. of *Stichopus chloronotus*. Antifungal agent. Cryst.
Mp 270-271°. $[\alpha]_D^{15}$ -44 (Py).

25,26-Didehydro: Holosta-7,25-diene-3,23-diol. 3,23-Dihydroxylanosta-7,25-dien-18,20-olide. Dehydrostichlorogenol
[78183-29-6]
Cryst. Mp 239-240°. $[\alpha]_D^{17}$ -35 ($CHCl_3$).

25,26-Didehydro, 23-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Synallactoside A$_1$***
[478696-84-3]
$C_{55}H_{86}O_{22}$ 1099.271
Constit. of *Synallactes nozawai*. Cryst.
Mp 220-222°. $[\alpha]_D^{20}$ -54 (c, 0.1 in Py).

25,26-Didehydro, 23-Ac, 3-O-*[3*-O-*methyl-β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Synallactoside B$_2$***
[478700-16-2]
$C_{60}H_{94}O_{26}$ 1231.387
Constit. of *Synallactes nozawai*. Cryst.
Mp 196-197°. $[\alpha]_D^{20}$ -40 (c, 0.1 in Py).

25,26-Didehydro, 23-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Synallactoside C***
[478700-32-2]
$C_{61}H_{96}O_{27}$ 1261.413
Constit. of *Synallactes nozawai*. Cryst.
Mp 190-192°. $[\alpha]_D^{20}$ -35 (c, 0.1 in Py).

25,26-Didehydro, 23-Ac, 3-O-*[3*-O-*methyl-β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[3*-O-*methyl-β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Synallactoside A₂***
[478698-80-5]
$C_{66}H_{104}O_{30}$ 1377.53
Constit. of *Synallactes nozawai*. Cryst.
Mp 184-186°. $[\alpha]_D^{20}$ -52 (c, 0.1 in Py).

25,26-Didehydro, 23-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[3*-O-*methyl-β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Synallactoside B₁***
[478699-47-7]
$C_{67}H_{106}O_{31}$ 1407.556
Constit. of *Synallactes nozawai*. Cryst.
Mp 177-179°. $[\alpha]_D^{20}$ -39 (c, 0.1 in Py).

25,26-Didehydro, 23-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Stichloroside C₂***. *Astichoposide C*
[78244-70-9]
$C_{68}H_{108}O_{32}$ 1437.582
Constit. of *Stichopus chloronotus*. Cryst. Poorly sol. hexane.
Mp 250-251°. $[\alpha]_D^{15}$ -45 (Py).

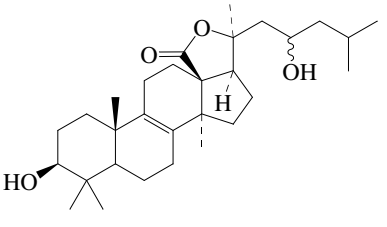
25,26-Didehydro, 23-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-β-D-xylopyranosyl (1→2)-[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Stichloroside A₂***
[78244-72-1]
$C_{68}H_{108}O_{33}$ 1453.581
Constit. of *Stichopus chloronotus*. Antifungal agent. Cryst. Poorly sol. hexane.
Mp 205-207°. $[\alpha]_D^{15}$ -33 (Py).

25,26-Didehydro, 23-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-glucopyranosyl (1→2)-[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Stichloroside B₂***
[78244-71-0]
$C_{68}H_{108}O_{33}$ 1453.581
Constit. of *Stichopus chloronotus*. Antifungal agent. Cryst. Poorly sol. hexane.
Mp 265-266°. $[\alpha]_D^{15}$ -37 (Py).

Kiitagawa, I. *et al., Chem. Pharm. Bull.*, 1981, **29**, 1189-1192; 2387 (*Stichlorosides, cryst struct*)
Stonik, V.A. *et al., Khim. Prir. Soedin.*, 1982, 200-204; *Chem. Nat. Compd. (Engl. Transl.)*, 1982, **18**, 182-186 (*Stichoposide D*)
Stonik, V.A. *et al., Khim. Prir. Soedin.*, 1982, **18**, 194-199 (*Astichoposide C, Stichoposide C*)
Stonik, V.A. *et al., Khim. Prir. Soedin.*, 1982, **18**, 624; *Chem. Nat. Compd. (Engl. Transl.)*, 1982, **18**, 590 (*Thelenotosides*)
Mal'tsev, I.I. *et al., Khim.-Farm. Zh.*, 1985, **19**, 54-56; *CA*, **102**, 146003z (*Thelelenotoside A*)
Ilin, S.G. *et al., Bioorg. Khim.*, 1991, **17**, 1123-1128 (*23-Ac, cryst struct*)
Silchenko, A.S. *et al., J. Nat. Prod.*, 2002, **65**, 1802-1808 (*Synallactosides*)

Holost-8-ene-3,23-diol H-379

3,23-Dihydroxylanost-8-en-18,20-olide



$C_{30}H_{48}O_4$ 472.707

(3β,23ξ)-*form*

23-Ac:
$C_{32}H_{50}O_5$ 514.744
Aglycone from *Thelonota ananas*. Cryst.
Mp 198-201°. $[\alpha]_D$ +13.8 (c, 0.5 in MeOH).

23-Ac, 3-glycoside: ***Thelothurin A***
Constit. of *Thelonota ananas*. Sol. MeOH, butanol. Struct. not fully known. Not obt. pure.

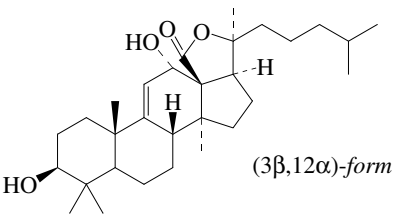
25,26-Didehydro: Holosta-8,25-diene-3,23-diol
$C_{30}H_{46}O_4$ 470.691

25,26-Didehydro, 23-Ac:
$C_{32}H_{48}O_5$ 512.728
Aglycone from *Thelonota ananas*. Cryst.
Mp 196-198°.

25,26-Didehydro, 23-Ac, 3-glycoside: ***Thelothurin B***
Constit. of *Thelonota ananas*. Sol. MeOH, butanol. Struct. not fully known. Not obt. pure.

Kelecom, A. *et al., Tetrahedron*, 1976, **32**, 2313-2319; 2353-2359

Holost-9(11)-ene-3,12-diol H-380



(3β,12α)-*form*

$C_{30}H_{48}O_4$ 472.707

(3β,12α)-*form*

3-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Bivittoside A***
[77394-03-7]
$C_{41}H_{66}O_{12}$ 750.965
Constit. of echinoderm *Bohadschia bivittata*. Cryst. Sol. MeOH, butanol.
Mp 267-268°. $[\alpha]_D$ +9 (Py).

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranoside]:* ***Bivittoside B***
[77394-04-8]
$C_{54}H_{88}O_{22}$ 1089.276
Constit. of *Bohadschia bivittata*. Cryst. Sol. MeOH, butanol.
Mp 270-273°. $[\alpha]_D$ +6 (Py).

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Bivittoside D***
[77394-06-0]
$C_{67}H_{110}O_{32}$ 1427.587
Constit. of *Bohadschia bivittata* and *Thelenota ananas*. Cryst. Sol. MeOH, butanol.
Mp 219-221°. $[\alpha]_D$ -7 (Py). Genus name given as Telenota.

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Pervicoside C***
[96157-96-9]
$C_{54}H_{88}O_{25}S$ 1169.34
Constit. of echinoderm *Holothuria pervicax*. Sol. MeOH, H_2O, butanol; poorly sol. hexane.

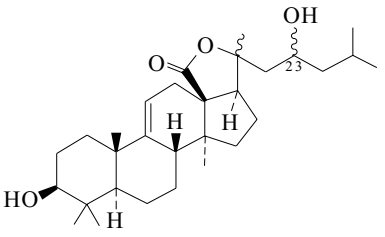
(3β,12β)-*form*

Isol. from sea cucumber *Bohadschia vitiensis* after hydrol. Prob. an artifact since hydrol. of the glycosides causes epimerisation at C-12.

Clastres, A. *et al., Experientia*, 1978, **34**, 973-974 (*isol*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1981, **29**, 282; 1989, **37**, 61-67 (*Bivittosides*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1230-1234 (*Pervicoside C*)
Hegde, V.R. *et al., Bioorg. Med. Chem. Lett.*, 2002, **12**, 3203-3205 (*Thelenota ananas glycoside*)

Holost-9(11)-ene-3,23-diol H-381

3,23-Dihydroxylanost-9(11)-en-18,20-olide. 17-Deoxy-7,8-dihydro-23-hydroxyholothurinogenin

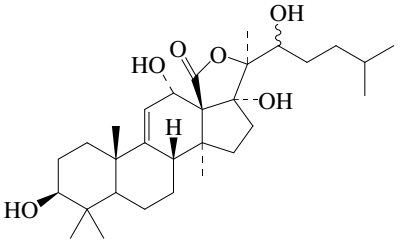


$C_{30}H_{48}O_4$ 472.707

(3β,20ξ,23ξ)-*form* [36872-80-7]
Cryst. (MeOH aq.). Mp 233-236°. $[\alpha]_D^{20}$ -1.4 (c, 0.4 in $CHCl_3$).

23-Ac: [36872-76-1]
$C_{32}H_{50}O_5$ 514.744
Constit. of *Stichopus chloronotus.* Cryst. (MeOH).
Mp 223-224°. $[\alpha]_D^{20}$ -20 (c, 0.74 in $CHCl_3$).
Rothberg, I. *et al., J.O.C.*, 1973, **38**, 209

Holost-9(11)-ene-3,12,17,22-tetrol H-382



$C_{30}H_{48}O_6$ 504.706

(3β,12α,17α*OH*,20*S*,22ξ)-*form*

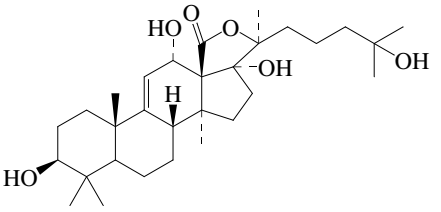
3-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Holothurin B_2***
[852469-36-4]
$C_{41}H_{66}O_{17}S$ 863.028
Constit. of *Holothuria polii*. Cryst.
Mp 243°. $[\alpha]_D^{20}$ -7 (c, 0.1 in Py).

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Holothurin A_1****. 22-Hydroxyechinoside A*
[78206-64-1]
$C_{54}H_{88}O_{27}S$ 1201.339
Isol. from the holothurians *Holothuria floridana* and *Holothuria grisea*, and from the sponge *Actinopyga flammea*. Cryst. (EtOH).
Mp 261-264°. $[\alpha]_D^{20}$ -9.22 (c, 0.03 in EtOH).

22-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***22-Acetoxyechinoside A***
[97243-49-7]
$C_{56}H_{90}O_{28}S$ 1243.376
Constit. of *Actinopyga flammea.*

Oleinikova, G.K. *et al., Khim. Prir. Soedin.*, 1981, 101-102; 1982, 464-469; *Chem. Nat. Compd. (Engl. Transl.)*, 1982, **18**, 430-434 (*Holothurin A_1*)
Bhatnagar, S. *et al., Bull. Soc. Chim. Fr.*, 1985, 124-129 (*22-Acetoxyechinoside A*)
Silchenko, A.S. *et al., J. Nat. Prod.*, 2005, **68**, 564-567 (*Holothurin B_2*)

Holost-9(11)-ene-3,12,17,25-tetrol H-383

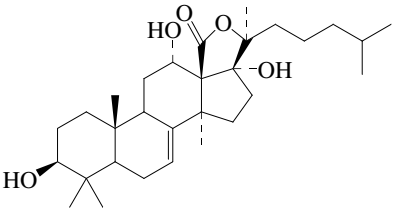


$C_{30}H_{48}O_6$ 504.706

(3β,12α,17α)-*form*

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Ananaside D***
[854520-05-1]
$C_{54}H_{88}O_{26}S$ 1185.34
Constit. of *Thelenota ananas.* Cryst.
Mp 203-205°. $[\alpha]_D^{20}$ -12.3 (c, 0.2 in MeOH).
Wu, J. *et al., Zhongguo Tianran Yaowu*, 2005, **3**, 34-37; *CA*, **143**, 56803c (*Ananaside D*)

Holost-7-ene-3,12,17-triol H-384

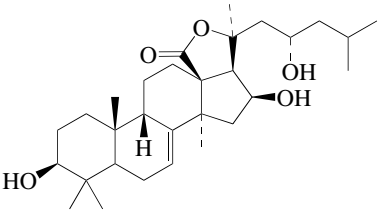


$C_{30}H_{48}O_5$ 488.706

(3β,12α,17α*OH*)-*form*

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-6*-O-*sulfo-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Patagonicoside A***
[392689-55-3]
$C_{54}H_{88}O_{29}S_2$ 1265.404
Constit. of *Psolus patagonicus.* Amorph. powder.
Mp 204-206°. $[\alpha]_D^{20}$ -30 (c, 0.5 in MeOH).
Murray, A.P. *et al., Tetrahedron*, 2001, **57**, 9563-9568 (*isol, pmr, cmr*)

Holost-7-ene-3,16,23-triol H-385



$C_{30}H_{48}O_5$ 488.706

(3β,16β,23*S*)-*form*

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-sulfo-β-D-xylopyranoside], 16-Ac:* ***Frondoside D***
[221040-26-2]
$C_{60}H_{96}O_{30}S$ 1329.466
Constit. of *Cucumaria frondosa.* Cryst.
Mp 217-220°. $[\alpha]_D^{23}$ -22.9 (c, 0.0013 in Py aq.).

16,23-Diketone: 3-Hydroxyholost-7-ene-16,23-dione

*16,23-Diketone, 3-*O*-[3-*O*-methyl-β-D-glucopyranosyl-(1→3)-6-*O*-sulfo-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Cucumechinoside A***
[125640-30-4]
$C_{54}H_{84}O_{29}S_2$ 1261.372
Constit. of echinoderm *Cucumaria echinata*. Powder. Sol. MeOH, butanol.
Mp 224-225°. $[\alpha]_D$ -59.5 (c, 0.9 in MeOH).

*16,23-Diketone, 3-*O*-[3-*O*-methyl-β-D-glucopyranosyl-(1→3)-2-*O*-sulfo-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Cucumechinoside B***
[125640-31-5]
$C_{53}H_{82}O_{28}S_2$ 1231.346
Constit. of *Cucumaria echinata*. Powder. Sol. MeOH, butanol.
Mp 204-206°. $[\alpha]_D$ -85.5 (c, 0.3 in MeOH).

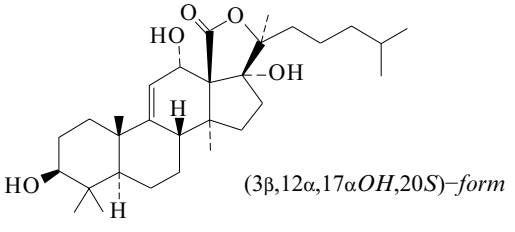
*16,23-Diketone, 3-*O*-[3-*O*-methyl-6-*O*-sulfo-β-D-glucopyranosyl-(1→3)-6-*O*-sulfo-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Cucumechinoside D***
[125640-33-7]
$C_{54}H_{84}O_{32}S_3$ 1341.436
Constit. of *Cucumaria echinata*. Powder. Sol. MeOH, butanol.
Mp 256-258°. $[\alpha]_D$ -58.3 (c, 0.2 in H_2O).

*16,23-Diketone, 3-*O*-[3-*O*-methyl-6-*O*-sulfo-β-D-glucopyranosyl-(1→3)-2-*O*-sulfo-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Cucumechinoside E***
[125640-34-8]
$C_{53}H_{82}O_{31}S_3$ 1311.41
Constit. of *Cucumaria echinata*. Powder. Sol. MeOH, butanol.
Mp 240-242°. $[\alpha]_D$ -28.5 (c, 0.2 in H_2O).

Miyamoto, T. *et al., Annalen*, 1990, 453-460 (*Cucumechinosides*)
Yayli, N. *et al., Phytochemistry*, 1999, **50**, 135-138 (*Frondoside D*)

Holost-9(11)-ene-3,12,17-triol H-386

3,12,17-Trihydroxylanost-9(11)-en-18,20-olide



(3β,12α,17α*OH*,20*S*)–*form*

$C_{30}H_{48}O_5$ 488.706

(3β,12α,17αOH,20*S*)-*form*

*3-*O*-[3-*O*-Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Echinoside A***†. *Holothurin A_2*
[75410-53-6]
$C_{54}H_{88}O_{26}S$ 1185.34
Isol. from the sea cucumbers *Actinopyga echinites* and *Actinopyga flammea*, also from *Bohadschia graeffei*. Needles (MeOH aq.) (as Na salt). Sol. Py, H_2O, MeOH.
Mp 228-230° (Na salt). $[\alpha]_D^{12}$ -6 (c, 1.36 in Py). CAS no. refers to Na salt.

*3-*O*-[6-Deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Echinoside B***
[75410-52-5]
$C_{41}H_{66}O_{16}S$ 847.029
Isol. from *Actinopyga echinites* and *Actinopyga mauritiana*.
Needles + $1H_2O$ (MeOH aq.) (as Na salt).
Mp 203.5-204.5°. $[\alpha]_D^{12}$ -2.2 (c, 0.88 in Py). CAS no. refers to Na salt.

▶ Extremely toxic to mice and other organisms.

*3-*O*-[α-L-Rhamnopyranosyl-(1→2)-β-D-xylopyranoside]:*
[180047-97-6]
$C_{41}H_{66}O_{13}$ 766.965
Isol. from *Holothuria atra*. Amorph. powder (MeOH).
Mp 234-236°.

24,25-Didehydro: Holosta-9(11),24-diene-3,12,17-triol. 3,12,17-Trihydroxylanosta-9(11),24-dien-18,20-olide
$C_{30}H_{46}O_5$ 486.69

*24,25-Didehydro, 3-*O*-[3-*O*-methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***24-Dehydroechinoside A***
[83175-58-0]
$C_{54}H_{86}O_{26}S$ 1183.324
Constit. of *Actinopyga agassizi* and *Actinopyga flammea*. Not obt. pure.

*24,25-Didehydro, 3-*O*-[6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***24-Dehydroechinoside B***
$C_{41}H_{64}O_{16}S$ 845.013
Constit. of *Actinopyga mauritiana*. Not obt. pure.

(3β,12β,17α*OH*,20*S*)-*form*

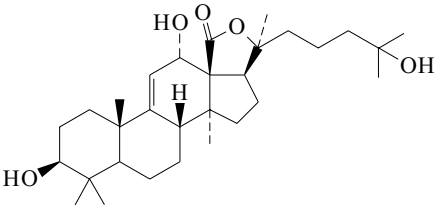
7,8-Dihydro-12β-hydroxyholothurinogenin

12-Me ether: 12-Methoxyholost-9(11)-ene-3,17-diol. 3,17-Dihydroxy-12-methoxylanost-9(11)-en-18,20-olide
$C_{31}H_{50}O_5$ 502.733
Aglycone from *Holothuria atra* and *Holothuria scabra*. Cryst. (MeOH)(as Ac).
Mp 264-268° (Ac). $[\alpha]_D$ -26 (Ac).

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2045-2050; 1985, **33**, 5214-5224; 1991, **39**, 2282-2287 (*Echinosides, Dehydroechinosides*)
Sarma, N.S. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 715 (*isol*)
Parameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 1991, **30**, 375-376 (*Echinoside B*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 810 (*3-rhamnosylxyloside*)

Holost-9(11)-ene-3,12,25-triol H-387

3,12,25-Trihydroxylanost-9(11)-en-18,20-olide



$C_{30}H_{48}O_5$ 488.706

(3β,12α)-*form*

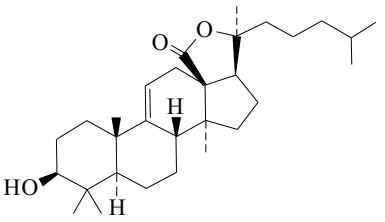
*3-*O*-[3-*O*-Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-β-D-quinovopyranosyl-(1→2)-4-*O*-sulfonato-β-D-xylopyranoside], 25-Ac:* ***Neothyoside A***. *Pervicoside A*
[96157-94-7]
$C_{56}H_{90}O_{27}S$ 1227.377
Constit. of *Neothyone gibbosa* and *Holothuria pervicax*. Solid. Sol. MeOH, H_2O, butanol; poorly sol. hexane.
Mp 204-206° dec. $[\alpha]_D$ -5 (c, 0.8 in EtOH aq.). λ_{max} (MeOH) (Berdy).

*3-*O*-[β-D-Quinovopyranosyl-(1→2)-4-*O*-sulfonato-β-D-xylopyranoside], 25-Ac:* ***Neothyoside B***
[182064-70-6]
$C_{43}H_{68}O_{17}S$ 889.066
Constit. of *Neothyone gibbosa*. Solid.

Kitagawa, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1230-1234 (*Pervicoside A*)
Encarnación, D.R. *et al., J. Nat. Prod.*, 1989, **52**, 248-251 (*Neothyoside A*)
Encarnación, D.R. *et al., Acta Chem. Scand.*, 1996, **50**, 848-849 (*Neothyoside B, pmr, cmr*)

Holost-9(11)-en-3-ol H-388

3-Hydroxylanost-9(11)-en-18,20-olide



$C_{30}H_{48}O_3$ 456.707

(3β,20*S*)-*form*

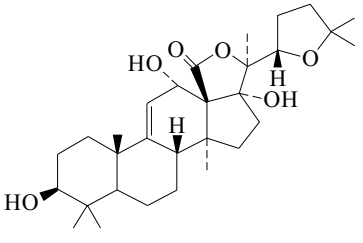
Deoxybivittogenin. *Synaptogenin R*
[77394-02-6]
Sapogenin from sea cucumber *Bohadschia bivittata*. Hydrol. prod. of Synaptosides S2 and S3 from *Synapta maculata* and of Bivittoside C below.
Cryst. (MeOH).
Mp 231-233°. $[\alpha]_D$ -16 (c, 1.0 in $CHCl_3$).

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranoside]:* ***Bivittoside C***
[77394-05-9]
$C_{67}H_{110}O_{31}$ 1411.587
Constit. of *Bohadschia bivittata*. Cryst. Sol. MeOH, butanol.
Mp 216-218°. $[\alpha]_D$ -31 (Py).

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1981, **29**, 282 (*Bivittoside C*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1982, **29**, 282 (*isol*)
Habermehl, G.G. *et al., Tet. Lett.*, 1983, **24**, 2981 (*synth*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1989, **37**, 61-67 (*Bivittoside C*)

Holothurigenol H-389

22,25-Epoxyholost-9(11)-ene-3,12,17-triol
[72244-90-7]



$C_{30}H_{46}O_6$ 502.69
Mp 274-275°. $[\alpha]_D^{20}$ +1.5 (c, 0.5 in $CHCl_3$).

3-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-4-sulfo-β-D-xylopyranoside]:* ***Holothurin B***
[11052-32-7]
$C_{41}H_{64}O_{17}S$ 861.012
Constit. of sea cucumber *Holothuria leucospilota*, also of *Holothuria lubrica* , *Holothuria floridiana*, *Holothuria edulis*, *Holothuria atra*, *Stichopus chloronotus*, *Actinopyga flammea*, *Actinopyga agassizi* and *Thelenota ananas*. Haemolytic agent, piscicide. Needles (EtOH aq.) (as Na salt). Sol. H_2O; poorly sol. MeOH, EtOH, hexane.
Mp 224-226° (Na salt). $[\alpha]_D^{17}$ -11 (c, 0.3 in MeOH).
▶ LD_{50} (mus, ipr) 14 mg/kg (Na salt). OE3420000

3-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:*
$C_{47}H_{74}O_{19}$ 943.09
Isol. from the sea cucumber *Thelenota ananas*. Genus name given as Telenata.

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Desholothurin A***
[137252-03-0]
$C_{54}H_{86}O_{24}$ 1119.259
Constit. of *Holothuria forskolii*. Shows antitumour activity.

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4-sulfo-β-D-xylopyranoside]:* ***Holothurin A***
[38-26-6]
$C_{54}H_{86}O_{27}S$ 1199.323
Constit. of sea cucumber *Holothuria leucospilota* and sponge *Actinopyga flammea*. Needles (EtOH aq.) (as Na salt).
Mp 228-230° (Na salt). $[\alpha]_D^{18}$ -14.9 (c, 0.1 in H_2O).
▶ OE3450000

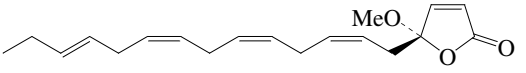
3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Holothurinoside A***
[136005-72-6]
$C_{60}H_{96}O_{29}$ 1281.401
Constit. of *Holothuria forskolii*. Shows antitumour and antiviral activity. Glass.
Mp 232-233°. $[\alpha]_D$ -0.9 (c, 0.0135 in MeOH).

Glycoside: ***Stychoposide A***
Glycoside from *Stychopus japonicus*.
Mp 215-217°. $[\alpha]_D^{25}$ -62.3 (c, 5.01 in Py). Conts. glycose, xylose and 3-methylglucose. Holothurigenol not proved to be the aglycone. Stychoposide C also isol., no details given.

Elyakov, G.B. *et al., Khim. Prir. Soedin.*, 1968, **4**, 253-254; 1979, **15**, 522-527; *Chem. Nat. Compd. (Engl. Transl.)*, 1968, **4**, 217-218; 1979, **15**, 453-457 (*Stychoposide A, Holothurin B*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1981, **29**, 1942-1950; 1951-1956 (*struct*)
Ivanova, N.S. *et al., Khim. Prir. Soedin.*, 1984, 448-451; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 424-426 (*Holothurin B*)
Bhatnagar, S. *et al., Bull. Soc. Chim. Fr.*, Part II, 1985, 124-129 (*Holothurins, isol, pmr, cmr*)
Rodriguez, J. *et al., Tetrahedron*, 1991, **47**, 4753-4762 (*Holothurinoside A, Desholothurin*)
Kerr, R.G. *et al., J. Nat. Prod.*, 1995, **58**, 172 (*biosynth*)
Hegde, V.R. *et al., Bioorg. Med. Chem. Lett.*, 1992, **12**, 3203-3205 (*Telenata ananas glycoside*)

Homaxinolide C H-390

*5-Methoxy-5-(2,5,8,11-tetradecatetraenyl)-2(5*H*)-furanone*



$C_{19}H_{26}O_3$ 302.413

(*S*)-*form*

Isol. from the marine sponge *Homaxinella* sp.
Pale yellow oil. $[\alpha]_D^{21}$ +14 (c, 0.43 in MeOH). λ_{max} 203 (log ε 1.4); 228 (log ε 0.3); 278 (log ε 0.2) (MeOH).

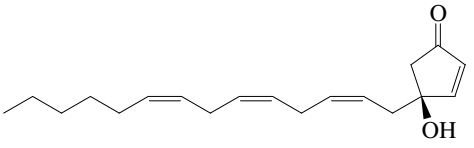
5-Epimer, 11′Z-isomer: ***Homaxinolide B***
$C_{19}H_{26}O_3$ 302.413
Isol. from a *Homaxinella* sp. Light yellow oil. $[\alpha]_D^{21}$ -10 (c, 0.27 in MeOH). λ_{max} 203 (log ε 1.1); 226 (log ε 0.3); 270 (log ε 0.2) (MeOH).

*11′,12′-Dihydro: 5-Methoxy-5-(2,5,8-tetradecatrienyl)-2(5*H*)-furanone.* ***Homaxinolide A***
$C_{19}H_{28}O_3$ 304.428
Isol. from a *Homaxinella* sp. Light yellow oil. $[\alpha]_D^{21}$ +20 (c, 0.33 in MeOH). λ_{max} 203 (log ε 1.3); 230 (log ε 0.8); 270 (log ε 0.2) (MeOH).

Mansoor, T.A. *et al., J. Nat. Prod.*, 2004, **67**, 721-724 (*isol, cd, pmr, cmr*)

Homaxinone A H-391

4-Hydroxy-4-(2,5,8-tetradecatrienyl)-2-cyclopenten-1-one, 9CI



$C_{19}H_{28}O_2$ 288.429

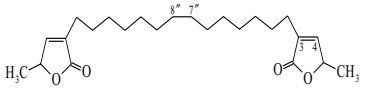
(S)-form

Isol. from the sponge *Homaxinella* sp.
Light yellow oil. $[\alpha]_D^{21}$ +22 (c, 0.48 in MeOH). λ_{max} 204 (log ϵ 1.3); 226 (log ϵ 1); 266 (log ϵ 0.37); 313 (log ϵ 0.03) (MeOH).

Mansoor, T.A. *et al., J. Nat. Prod.*, 2004, **67**, 721-724 (*isol, cd, pmr, cmr*)

Homoancepsenolide H-392

*3,3′-(Tetradecane-1,14-diyl)bis(5-methyl-2(5*H*)-furanone)*
[156116-46-0]



$C_{24}H_{38}O_4$ 390.562

Trivial names in this series are misleading. Numbering systems vary. Constit. of the gorgonian *Pterogorgia citrina*. Solid. Mp 99.6-101.6°. $[\alpha]_D^{25}$ +16.7 (c, 2 in $CHCl_3$). λ_{max} 214 (ϵ 11800) (MeOH).

3,4-Dihydro, 4-acetoxy: ***Homoancepsenolide acetate***
[156116-47-1]
$C_{26}H_{42}O_6$ 450.614
Constit. of *Pterogorgia citrina*. Semisolid. $[\alpha]_D^{25}$ -5.4 (c, 3.2 in $CHCl_3$). λ_{max} 212 (ϵ 13200) (MeOH).

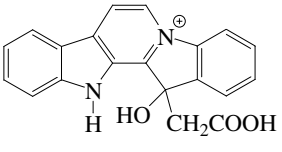
3,4-Dihydro, 4-acetoxy, 3,4-diepimer: ***Hydroxyhomoancepsenolide acetate***
$C_{26}H_{42}O_6$ 450.614
Constit. of *Pterogorgia citrina*. Semisolid. $[\alpha]_D^{25}$ +16.9 (c, 1.7 in $CHCl_3$). λ_{max} 212 (ϵ 7300) (MeOH).

7″,8″-Didehydro (Z-): ***Dehydrohomoancepsenolide***
[156116-48-2]
$C_{24}H_{36}O_4$ 388.546
Constit. of *Pterogorgia citrina*. Oil. $[\alpha]_D^{25}$ +29.7 (c, 2 in $CHCl_3$). Called 13,13′-didehydro in the ref. λ_{max} 214 (ϵ 14800) (MeOH).

7″,8″-Didehydro, 3,4-dihydro, 4-acetoxy: ***Dehydrohomoancepsenolide acetate***
[156116-49-3]
$C_{26}H_{40}O_6$ 448.598
Prod. by *Pterogorgia citrina*. Oil. $[\alpha]_D^{25}$ -12.9 (c, 3 in $CHCl_3$). Called 13,14-Dehydro in the ref. λ_{max} 214 (ϵ 8400) (MeOH).

Rodriguez, A.D. *et al., J. Nat. Prod.*, 1994, **57**, 339 (*isol, uv, ir, pmr, cmr*)

Homofascaplysate A H-393

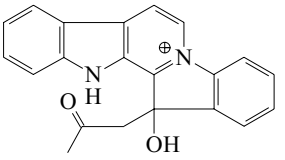


$C_{20}H_{15}N_2O_3^{\oplus}$ 331.35
Quaternary alkaloid isol. from the sponge *Fascaplysinopsis reticulata*. Yellow solid (as chloride). $[\alpha]_D^{25}$ +14 (c, 0.25 in MeOH) (chloride).

Segraves, N.L. *et al., J. Nat. Prod.*, 2004, **67**, 783-792 (*isol, pmr, cmr*)

Homofascaplysin A H-394

[132911-50-3]



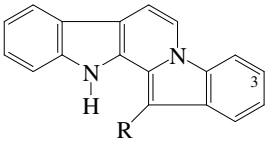
$C_{21}H_{17}N_2O_2^{\oplus}$ 329.377
Isol. from the sponge *Hyrtios erecta* and from *Fascaplysinopsis reticulata*. Inhibits HIV reverse transcriptase (HIV-rt). Shows cytotoxic, antibacterial and antiplasmodial activities. Inhibits $p56^{ICK}$ tyrosine kinase. Brown oil. λ_{max} 202 (ϵ 11300); 220 (ϵ 11200); 264 (ϵ 8100); 334 (ϵ 5250) (MeOH) (Derep). λ_{max} 256 (ϵ 2010); 314 (ϵ 838) (EtOH) (Berdy).

Salt with Dehydroluffariellolide diacid, D-60:
$C_{46}H_{54}N_2O_6$ 730.942
Alkaloid-sesterterpene salt from the sponge *Fascaplysinopsis reticulata*. Red viscous oil. $[\alpha]_D^{20}$ -9.36 (c, 0.0064 in MeOH).

Jimènez, C. *et al., J.O.C.*, 1991, **56**, 3403 (*isol, uv, ir, pmr, cmr, ms, struct, activity*)
Kirsch, G. *et al., J. Nat. Prod.*, 2000, **63**, 825-829 (*isol, activity*)

Homofascaplysin B H-395

[132938-12-6]



R = COCOOMe

$C_{21}H_{14}N_2O_3$ 342.353
Alkaloid from the sponge *Fascaplysinopsis reticulata*. Red oil. λ_{max} 268 (ϵ 12100); 294 (ϵ 5980); 330 (ϵ 7690) (MeOH) (Derep).

3-Bromo: ***3-Bromohomofascaplysin B***
[693790-73-7]
$C_{21}H_{13}BrN_2O_3$ 421.249
Isol. from a *Didemnum* sp. Yellow solid.

Jimenez, C. *et al., J.O.C.*, 1991, **56**, 3403-3410 (*isol, uv, ir, pmr, cmr, struct*)
Gribble, G.W. *et al., J.O.C.*, 1992, **57**, 3636-3642 (*synth*)
Segraves, N.L. *et al., J. Nat. Prod.*, 2004, **67**, 783-792 (*3-Bromohomofascaplysin B*)

Homofascaplysin B1 H-396

[694436-61-8]
As Homofascaplysin B, H-395 with
R = -COCOOEt
$C_{22}H_{16}N_2O_3$ 356.38
Isol. from a *Didemnum* sp. Red oil.

3-Bromo: ***3-Bromohomofascaplysin B1***
[693790-74-8]
$C_{22}H_{15}BrN_2O_3$ 435.276
Isol. from a *Didemnum* sp. Yellow solid.

Segraves, N.L. *et al., J. Nat. Prod.*, 2004, **67**, 783-792 (*isol, pmr, cmr*)

Homofascaplysin C H-397

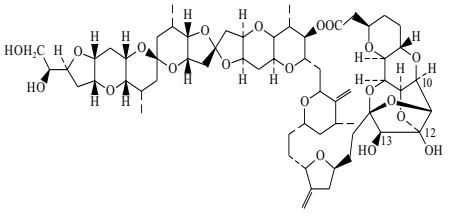
*12*H*-Pyrido[1,2-a:3,4-*b*′]diindole-13-carboxaldehyde, 9CI*
[132911-52-5]
As Homofascaplysin B, H-395 with
R = CHO
$C_{19}H_{12}N_2O$ 284.317
Alkaloid from *Didemnum* sp. and *Fascaplysinopsis reticulata*. Yellow oil. λ_{max} 266 (ϵ 7810); 292 (ϵ 2980) (MeOH) (Derep).

3-Bromo: ***3-Bromohomofascaplysin C***
[193790-75-9]
$C_{19}H_{11}BrN_2O$ 363.213
Isol. from a *Didemnum* sp. Yellow solid.

Jimenez, C. *et al., J.O.C.*, 1991, **56**, 3403-3410 (*isol, uv, ir, pmr, cmr, struct*)
Gribble, G.W. *et al., J.O.C.*, 1992, **57**, 3636-3642 (*synth*)
Carter, D.S. *et al., J.O.C.*, 1999, **64**, 8537-8545 (*synth*)
Segraves, N.L. *et al., J. Nat. Prod.*, 2004, **67**, 783-792 (*3-Bromohomofascaplysin C*)

Homohalichondrin A H-398

[101383-40-8]



$C_{61}H_{86}O_{21}$ 1155.338
Polyether macrolide. Isol. from the marine sponges *Halichondria okadai* and *Axinella* sp. Cytotoxic. Sol. MeOH, butanol, Py; poorly sol. H_2O. $[\alpha]_D$ -97.1 (c, 1.23 in MeOH).

13-Deoxy: ***Homohalichondrin C***
[101383-41-9]
$C_{61}H_{86}O_{20}$ 1139.338
Isol. from *Halichondria okadai*. Sol. MeOH, butanol, Py; poorly sol. H_2O.

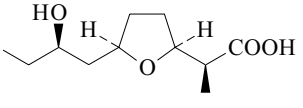
12,13-Dideoxy: ***Homohalichondrin B***
[101383-39-5]
$C_{61}H_{86}O_{19}$ 1123.339
Isol. from *Halichondria okadai*, *Axinella carteri*, *Phakellia carteri*, *Lissodendoryx* sp. Tubulin interactive macrolide. Antimitotic agent. Sol. MeOH, butanol, Py; poorly sol. H_2O.

12,13-Dideoxy, 10-hydroxy: ***Halistatin 2***
[151013-33-1]
$C_{61}H_{86}O_{20}$ 1139.338
Isol. from *Axinella carteri*. Tubulin polymerisation inhibitor.

Hirata, Y. *et al., Pure Appl. Chem.*, 1986, **58**, 701 (*isol, struct*)
Aicher, T.D. *et al., J.A.C.S.*, 1992, **114**, 3162 (*synth, abs config*)
Pettit, G.R. *et al., Gazz. Chim. Ital.*, 1993, **123**, 371 (*Halistatin 2*)

Homononactic acid H-399

Tetrahydro-5-(2-hydroxybutyl)-α-methyl-2-furanacetic acid, 9CI
[35986-06-2]



Absolute configuration

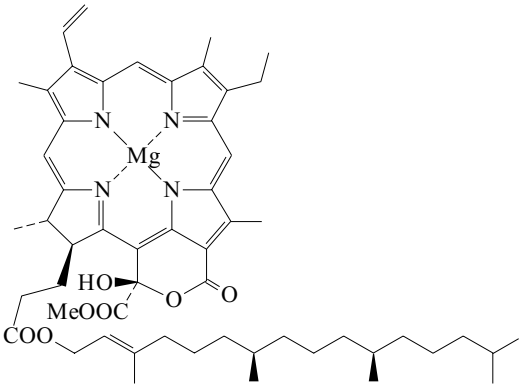
$C_{11}H_{20}O_4$ 216.277
Hydrol. prod. of Monactin, Dinactin and Trinactin and many *Streptomyces* spp.

Me ester:
$Bp_{0.04}$ 90°. $[\alpha]_D$ +12.9 (c, 5.51 in $CHCl_3$).

Beck, J. *et al., Helv. Chim. Acta*, 1962, **45**, 620 (*ir, pmr*)
Gerlach, H. *et al., Annalen*, 1963, **669**, 121 (*config*)
Schmidt, U. *et al., Synthesis*, 1986, 986 (*synth*)
Rezanka, T. *et al., Tetrahedron*, 2004, **60**, 4781-4787 (*Me ester, pmr, cmr, ms*)

13^1-A-Homo-13^1-A-oxa-13^2-hydroxychlorophyll a H-400

[71699-06-4]



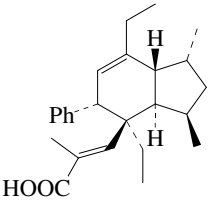
$C_{55}H_{72}MgN_4O_7$ 925.501
Isol. from the blue-green alga *Anacystis nidulans.*

[91656-50-7]

Wu, S.M. *et al., Phytochemistry*, 1988, **27**, 353 (*isol, pmr, ms*)

Homoplakotenin H-401

[246245-14-7]

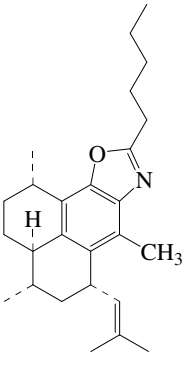


$C_{25}H_{34}O_2$ 366.542
Constit. of *Plakortis lita*. Oil. $[\alpha]_D$ +183 (c, 0.5 in MeOH). λ_{max} 217 (ϵ 22000) (hexane).

Qureshi, A. *et al., J. Nat. Prod.*, 1999, **62**, 1205-1207 (*isol, pmr, cmr*)

Homopseudopteroxazole H-402

[549520-74-3]

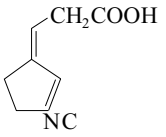


$C_{26}H_{37}NO$
Homologue of Pseudopteroxazole, P-681. Alkaloid from *Pseudopterogorgia elisabethae.* Active against *Mycobacterium tuberculosis.* Yellowish oil. $[\alpha]_D^{25}$ +103.2 (c, 0.9 in $CHCl_3$). λ_{max} 204 (ϵ 25500); 244 (ϵ 9000); 279 (ϵ 3500) (MeOH).

Rodriguez, I.I. *et al., J. Nat. Prod.*, 2003, **66**, 855-857 (*isol, pmr, cmr*)

Homothallin H-403

3-(3-Isocyanocyclopenten-1-ylidene)propanoic acid, 9CI
[73372-49-3]



$C_9H_9NO_2$ 163.176

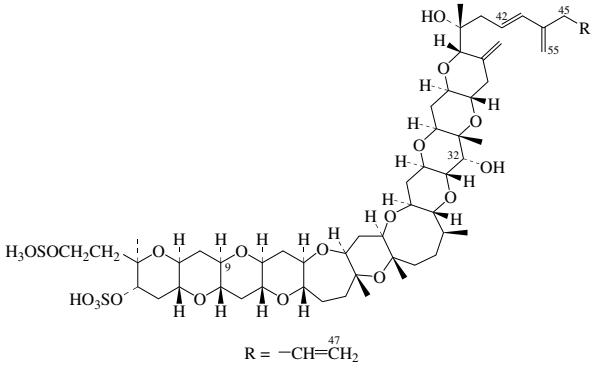
Isonitrile antibiotic. Prod. by *Trichoderma hamatum* and *Trichoderma harzianum*. Also isol. from *Plexaura homomalla*. Shows antibacterial props. Inhibits Rumen organisms which digest cellulose. Unstable prisms. Related to Trichoviridin and Isonitrin A. λ_{max} 270 (Et_2O).

[82470-75-5]

Baldwin, J.E. *et al., Chem. Comm.*, 1981, 1227 (*biosynth*)
Brewer, D. *et al., Can. J. Microbiol.*, 1982, **28**, 1252 (*isol*)
Parry, R.J. *et al., Tet. Lett.*, 1982, **23**, 1438 (*biosynth*)
Scheuer, P.J. *et al., Science (Washington, D.C.)*, 1990, **248**, 173-177 (*occur*)
Lee, C.H. *et al., J. Antibiot.*, 1997, **50**, 469 (*isol*)

41*a*-Homoyessotoxin H-404

[809234-27-3]



$C_{56}H_{84}O_{21}S_2$ 1157.399
Isol. from *Protoceratium reticulatum*.

44,55-Dihydro, 44,55-dihydroxy: ***44,55-Dihydroxy-41a-homoyessotoxin***
[862783-87-7]
$C_{56}H_{86}O_{23}S_2$ 1191.414
Isol. from *Protoceratium reticulatum*.

9-Methyl: ***9-Methyl-41a-homoyessotoxin***
[809234-28-4]
$C_{57}H_{86}O_{21}S_2$ 1171.426
Isol. from *Protoceratium reticulatum*.

9-Methyl, 44,55-dihydro, 44,55-dihydroxy: ***44,55-Dihydroxy-9-methyl-41a-homoyessotoxin***
[862783-88-8]
$C_{57}H_{88}O_{23}S_2$ 1205.44
Isol. from *Protoceratium reticulatum*.

45,46,47-Trinor, 44,55-dihydro, 44-oxo: ***45,46,47-Trinor-44-oxo-41a-homoyessotoxin***
$C_{53}H_{80}O_{22}S_2$ 1133.334
Isol. from *Protoceratium reticulatum*. Tentative struct. assigned.

Miles, C.O. *et al., Chem. Res. Toxicol.*, 2004, **17**, 1414-1422 (*isol, struct*)
Finch, S.C. *et al., Toxicon*, 2005, **45**, 160-170 (*44,45-Dihydroxy-41a-homoyessotoxin*)
Miles, C.O. *et al., Toxicon*, 2006, **47**, 229-240 (*Trinoroxohomoyessotoxin*)

41*a*-Homoyessotoxin amide H-405

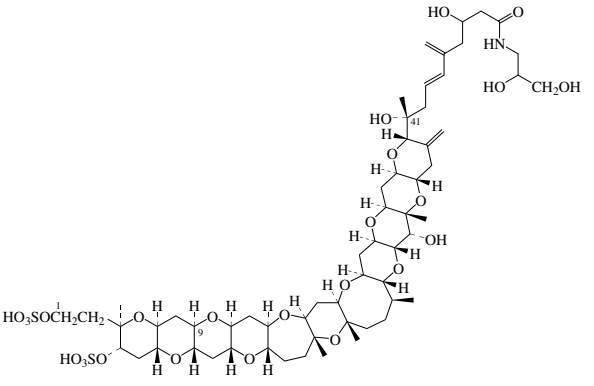
As 41*a*-Homoyessotoxin, H-404 with
R = -CH(OH)CH_2CONHCH_2CH(OH)CH_2OH

$C_{60}H_{93}NO_{25}S_2$ 1292.518
Isol. from *Protoceratium reticulatum*.

9-Methyl: ***9-Methyl-41a-homoyessotoxin amide***
$C_{61}H_{95}NO_{25}S_2$ 1306.545
Isol. from *Protoceratium reticulatum*.

Miles, C.O. *et al., Toxicon*, 2005, **45**, 61-71 (*isol, pmr, cmr, ms*)

41*a*-Homoyessotoxin tetrahydroxyamide H-406



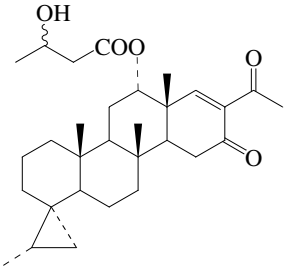
$C_{60}H_{93}NO_{25}S_2$ 1292.518
Isol. from *Protoceratium reticulatum*.

9-Me: ***9-Methyl-41a-homoyessotoxin tetrahydroxyamide***
$C_{61}H_{95}NO_{25}S_2$ 1306.545
Isol. from *Protoceratium reticulatum*.

Miles, C.O. *et al., Toxicon*, 2005, **45**, 61-71 (*isol, pmr, cmr, ms*)

Honuenone H-407

[306997-39-7]



$C_{30}H_{44}O_5$ 484.675
Constit. of *Strepsichordaia aliena*. Solid. $[\alpha]_D$ +16 (c, 0.4 in CH_2Cl_2).

Jiménez, J.I. *et al., J. Nat. Prod.*, 2000, **63**, 1388-1392 (*isol, pmr, cmr*)

Hopkinsiaxanthin H-408

[12708-31-5]

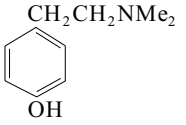
$C_{31}H_{38}O_3$ 458.639

Full struct. unknown. Alkali treatment gives Hopkinsianone. Isol. from the sea slug *Triopha carpenteri*, the nudibranch *Hopkinsia rosacea* and its food organism, the bryozoan *Eurystomella bilabiata*. λ_{max} 438; 462; 493 (hexane).

McBeth, J.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1972, **41**, 69-77 (*isol*)

Hordenine H-409

4-(2-Dimethylaminoethyl)phenol, 9CI. 4-Hydroxy-N,N-*dimethylphenethylamine.* N,N-*Dimethyltyramine. Peyocactine. Anhaline. Cactine. Eremursine*
[539-15-1]



$C_{10}H_{15}NO$ 165.235
Alkaloid from *Anhalonium fissuratum, Hordeum vulgare* (barley), a very wide range of plant spp. esp. in the Cactaceae. Also present in the Amaryllidaceae, Gramineae, Leguminosae and a few algae and fungi including marine alga *Phyllophora nervosa*. Diuretic, disinfectant, antihypotensive (in large doses) agent. Used for treatment of dysentery. Feeding repellant for grasshoppers. Shows similar actions to 2-(Methylamino)-1-phenyl-1-propanol.
Mp 118°. Bp_{11} 173-174°. Log P 1.17 (calc).

Hydrochloride: Mp 176-177°.

Sulfate (2:1): [622-64-0]
Mp 207-208°.

O-*β-D-Glucopyranoside:* ***Hordenine* O-*glucoside***
[93710-65-7]
$C_{16}H_{25}NO_6$ 327.377
Alkaloid from *Pancratium biflorum*. Solid.
Mp 100-108° dec. $[\alpha]_D^{20}$ -55.4 (c, 0.5 in EtOH). λ_{max} 225 (log ϵ 3.92); 266 (sh) (log ϵ 3.61); 275 (log ϵ 3.52); 305 (sh) (log ϵ 2.98) (MeOH).

O-*α-L-Rhamnopyranoside:* ***Hordenine* O-*α-L-rhamnopyranoside***
$C_{16}H_{25}NO_5$ 311.377
Alkaloid from *Selaginella doederleinii* (Selaginellaceae).
Amorph. solid. $[\alpha]_D^{20}$ -96 (c, 1 in MeOH).

O-*[6-O-Cinnamoyl-β-D-glucopyranosyl-(1→3)-α-L-rhamnopyranoside]:* ***Hordenine* O-*(6″-O-trans-cinnamoyl-3′-O-β-D-glucopyranosyl-α-L-rhamnopyranoside)***
[111537-51-0]
$C_{31}H_{41}NO_{11}$ 603.665
Alkaloid from *Selaginella doederleinii* (Selaginellaceae). Amorph. solid. $[\alpha]_D^{20}$ -84 (c, 1 in MeOH).

O-*[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranosyl-(1→3)-α-L-rhamnopyranoside]:* ***Hordenine* O-*(6″-O-p-coumaroyl-3′-O-β-D-glucopyranosyl-α-L-rhamnopyranoside)***
[130748-25-3]
$C_{31}H_{41}NO_{12}$ 619.664
Alkaloid from *Selaginella doederleinii* (Selaginellaceae). Amorph. $[\alpha]_D^{20}$ -81 (c, 0.2 in MeOH).

N-*Me:* ***Candicine***. *Maltoxin*
[6656-13-9]
$C_{11}H_{18}NO^{\oplus}$ 180.269
Quaternary alkaloid from *Trichocereus candicans, Trichocereus lamprochlorus, Trichocereus spachianus*, several *Desmodium* spp. (Cactaceae, Leguminosae) and several other spp. in different families. Also from mescal (*Lophophora williamsii*). Ganglionic blocker and vasoconstrictor with nicotine-like action. Curarising in large doses.
▶ Toxic, LD_{50} (rat) 50 mg/kg. BR1574700

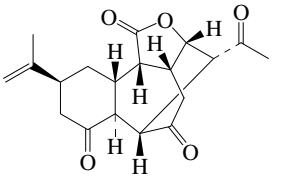
N-*Me, chloride:*
$C_{11}H_{18}ClNO$ 215.722
Mp 285° dec.

N-*Me, iodide:* [1976-98-3]
$C_{11}H_{18}INO$ 307.174
Mp 230-231°.

Voswinckel, H. *et al., Ber.*, 1912, **45**, 1004 (*synth*)
Buck, J.S. *et al., J.A.C.S.*, 1938, **60**, 1789 (*synth, deriv*)
Badger, G.M. *et al., Aust. J. Chem.*, 1963, **16**, 734 (*isol, pmr*)
Rao, G.S. *et al., J. Pharm. Pharmacol.*, 1970, **22**, 545
Güven, K.C. *et al., Phytochemistry*, 1970, **9**, 1893 (*isol, Phyllophora*)
Cherayil, G.D. *et al., J. Pharm. Sci.*, 1973, **62**, 2054 (*synth*)
Rao, K.V. *et al., Planta Med.*, 1975, **27**, 31 (*isol, deriv*)
Srinivasan, P.R. *et al., Org. Magn. Reson.*, 1976, **8**, 198 (*cmr*)
Kruger, T.L. *et al., J.O.C.*, 1977, **42**, 4161 (*ms*)
Smith, T.A. *et al., Phytochemistry*, 1977, **16**, 9 (*occur*)
Meyer, B.N. *et al., J. Nat. Prod.*, 1983, **46**, 688 (*O-Methylcandicine*)
Ghosal, S. *et al., Phytochemistry*, 1984, **23**, 1167 (*glucoside*)
Lin, R.C. *et al., J. Nat. Prod.*, 1990, **53**, 882 (*glycosides*)
Parvez, M. *et al., Acta Cryst. C*, 1991, **47**, 1450 (*cryst struct*)

Horiolide H-410

[436807-33-9]

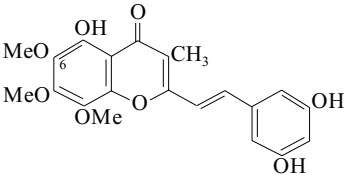


$C_{19}H_{22}O_5$ 330.38
Constit. of a *Sinularia* soft coral. Cryst.
Mp 210-212°. $[\alpha]_D$ +81 (c, 0.037 in MeOH). λ_{max} 270 (ϵ 5400) (MeOH).

Radhika, P. *et al., J. Nat. Prod.*, 2002, **65**, 737-739 (*isol, pmr, cmr*)

Hormothamnione H-411

*2-[2-(3,5-Dihydroxyphenyl)ethenyl]-5-hydroxy-6,7,8-trimethoxy-3-methyl-4*H*-1-benzopyran-4-one, 9CI. 2-(3,5-Dihydroxystyryl)-5-hydroxy-6,7,8-trimethoxy-3-methylchromone*
[103654-49-5]



$C_{21}H_{20}O_8$ 400.384
Chromone antibiotic. Isol. from the marine cryptophyte *Chrysophaeum taylori* and *Hormothamnion enteromorphoides*. Potent cytotoxin with anticancer potential. Inhibits RNA synthesis. Yellow solid.
Mp 270° dec. λ_{max} 295 (ϵ 11200); 353 (ϵ 19800) (MeOH) (Derep).

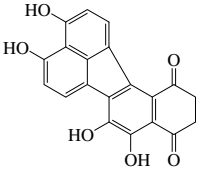
6-Demethoxy: ***6-Desmethoxyhormothamnione***
[111574-76-6]
$C_{20}H_{18}O_7$ 370.358
Constit. of *Chrysophaeum taylori*. Cytotoxic agent. Light yellow solid. λ_{max} 270 (ϵ 1340); 342 (ϵ 3000) (MeOH) (Derep).

6-Demethoxy, tri-Ac:
Cryst. Mp 184-186°.

Gerwick, W.H. *et al., Tet. Lett.*, 1986, **27**, 1979 (*cryst struct*)
Gerwick, W.H. *et al., J. Nat. Prod.*, 1989, **52**, 252 (*isol, deriv*)

Hortein H-412

10,11-Dihydro-3,4,7,8-tetrahydroxybenzo[j]fluoranthene-9,12-dione

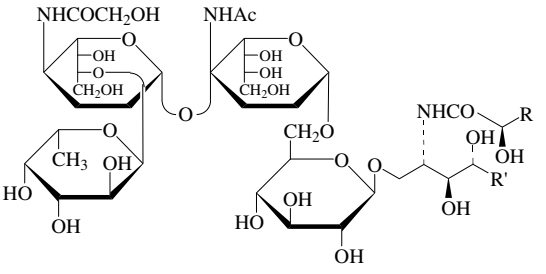


$C_{20}H_{12}O_6$ 348.311

Prod. by the fungus *Hortaea werneckii* isol. from the sponge *Aplysina aerophoba*. Brown powder. λ_{max} 204; 257; 358; 444 (MeOH).

Brauers, G. *et al., J. Nat. Prod.*, 2001, **64**, 651-652

HPG 1 H-413



R = mostly *n*-C_{22}
R' = various, major component 10-methyldodecyl

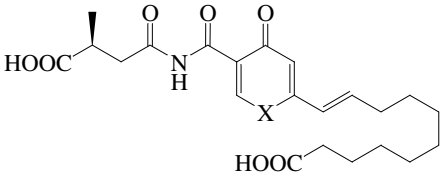
Isol. from polar lipids of the sea cucumber *Holothuria pervicax*. Amorph. powder.
Mp 261-270°.

O-*Defucosyl:* ***HPG 3***
Isol. from *Holothuria pervicax*.
Amorph. powder.
Mp > 300°.

O-*De(fucosyl*-N-*glycolylneuraminic acid):* ***HPG 8***
Isol. from *Holothuria pervicax*.
Amorph. powder.
Mp 200-205°.

Yamada, K. *et al., Eur. J. Org. Chem.*, 1998, 2519-2525 (*isol, cmr, ms, struct*)

Humeic acid A H-414



X = O

$C_{22}H_{29}NO_8$ 435.473
Prod. by a marine-derived *Aspergillus* sp. Ubiquitin-activating enzyme inhibitor. $[\alpha]_D^{26}$ -15 (c, 0.14 in MeOH). λ_{max} 234 (log ϵ 4.5); 254 (log ϵ 4.4) (MeOH).

N-*Deacyl:* ***Humeic acid B***
$C_{17}H_{23}NO_5$ 321.372
Isol. from a marine-derived *Aspergillus* sp. λ_{max} 227 (log ϵ 4.3); 266 (log ϵ 4.1) (MeOH).

Tsukamoto, S. *et al., Bioorg. Med. Chem. Lett.*, 2005, **15**, 191-194 (*isol, pmr, cmr*)

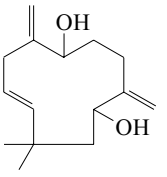
Humeic acid C H-415

As Humeic acid A, H-414 with
X = NH

$C_{22}H_{30}N_2O_7$ 434.488
Prod. by a marine-derived *Aspergillus* sp.
$[\alpha]_D^{26}$ -9.8 (c, 0.32 in MeOH). λ_{max} 252 (log ϵ 4.4) (MeOH).

Tsukamoto, S. *et al., Bioorg. Med. Chem. Lett.*, 2005, **15**, 191-194 (*isol, pmr, cmr*)

3(15),7(14),9-Humulatriene-2,6-diol H-416



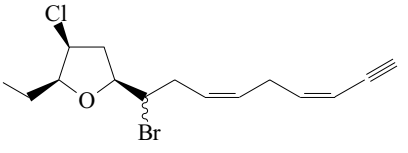
$C_{15}H_{24}O_2$ 236.353
Metab. of red alga *Laurencia obtusa*. Cryst.
Mp 104.5-107°. Occurs as racemate resolvable into enantiomers.

[127760-78-5, 127760-79-6, 127760-80-9]

Takeda, S. *et al., Chem. Lett.*, 1990, 155 (*isol, struct*)

Hurgadenyne H-417

[132412-60-3]

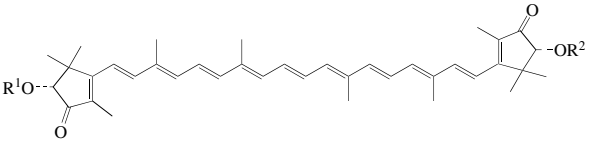


$C_{15}H_{20}BrClO$ 331.679
Metab. of *Laurencia obtusa*. Oil. $[\alpha]_D^{24}$ -110 (c, 5 in $CHCl_3$). λ_{max} 225 (ϵ 13500); 270 (sh) (Et_2O).

Ayyad, S.-E.N. *et al., Phytochemistry*, 1990, **29**, 3193-3196 (*isol, pmr, cmr, ms*)

Hurghadin H-418

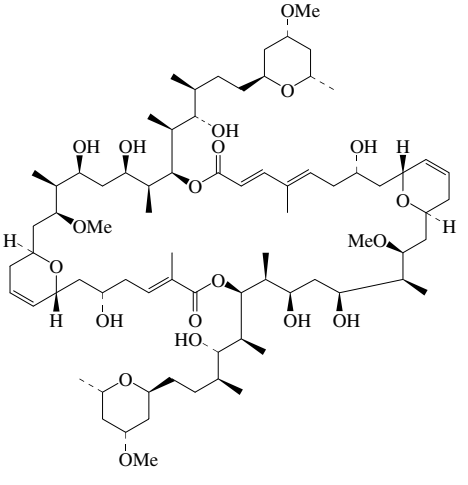
[207410-14-8]



R^1 and R^2 are a mixture of fatty acids ($C_{18:0}$, $C_{18:1}$, $C_{19:0}$, $C_{20:1}$, $C_{20:2}$, $C_{27:2}$). Constit. of *Hexabranchus sanguineus*. Defensive agent. Deep red powder. λ_{max} 498 (ϵ 50000) (Me_2CO).

Guo, Y. *et al., Tet. Lett.*, 1998, **39**, 2635-2638 (*isol, pmr, cmr*)

Hurghadolide A H-419



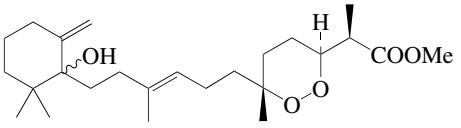
$C_{76}H_{130}O_{20}$ 1363.851

Related to Swinholide A, S-548. Isol. from *Theonella swinhoei*. Cytotoxic. Light yellow solid. $[\alpha]_D^{25}$ -29.4 (c, 0.08 in MeOH). λ_{max} 274 (log ϵ 4.95) (MeOH).

Youssef, D.T.A. *et al., J. Nat. Prod.*, 2006, **69**, 154-157 (*isol, pmr, cmr*)

Hurghaperoxide H-420

[189388-82-7]



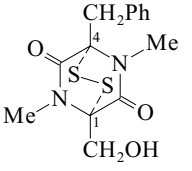
$C_{25}H_{42}O_5$ 422.604

Constit. of a Red Sea sponge. Oil. $[\alpha]_D^{21}$ -41 (c, 0.44 in $CHCl_3$).

Guo, Y. *et al., Nat. Prod. Lett.*, 1996, **9**, 105-112 (*isol, pmr, cmr*)

Hyalodendrin H-421

1-(Hydroxymethyl)-5,7-dimethyl-4-(phenylmethyl)-2,3-dithia-5,7-diazabicyclo[2.2.2]octane-6,8-dione, 9CI. 3-Benzyl-6-hydroxymethyl-1,4-dimethyl-3,6-epidithio-2,5-piperazinedione. A 26771A. Antibiotic A 26771A



(+)–*form*

$C_{14}H_{16}N_2O_3S_2$ 324.424

Epithiodioxopiperazine antibiotic. Antibiotic A 26771A was the (-)-form. λ_{max} 255 (sh) (ϵ 1000) (EtOH) (Derep).

(+)-*form* [51920-94-6]

Fungitoxic metab. from *Hyalodendron* spp. Used to treat Dutch elm disease. Prisms (Et_2O). Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 100.5-101.5°. $[\alpha]_D^{22}$ +26 (c, 1.06 in $CHCl_3$). λ_{max} 260 (ϵ 1000) (EtOH) (Berdy).

▶ LD_{50} (mus, ipr) 75 mg/kg. JO4990000

Trisulfide analogue: ***Hyalodendrin trisulfide. Hyalodendrin II***
[40380-25-4]
$C_{14}H_{16}N_2O_3S_3$ 356.49
Prod. by a *Hyalodendron* sp. Yellow oil. Tentative stereochem.

▶ LD_{50} (mus, ipr) 24-40 mg/kg.

Tetrasulfide analogue: See 3-Benzyl-6-hydroxymethyl-1,4-dimethyl-3,6-epitetrathia-2,5-piperazinedione in *The Combined Chemical Dictionary.*

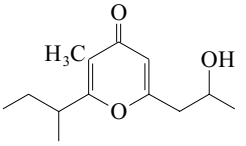
(-)-*form* [40380-24-3]
[51773-88-7]
Prod. by *Penicillium turbatum*.
Yellow cryst. (Me_2CO/Et_2O/pentane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{277}$ -88 (c, 0.15 in MeOH). λ_{max} 200 (EtOH).

(±)-*form* [53777-19-8]
Pale yellow cryst. (CH_2Cl_2/Et_2O). Mp 131-134°.

De Vault, R.L. *et al., J. Antibiot.*, 1973, **26**, 532-534 (*Hyalodendrin II*)
Strunz, G.M. *et al., J.C.S. Perkin 1*, 1973, 2600 (*struct*)
Strunz, G.M. *et al., Experientia*, 1974, **30**, 719 (*synth*)
Michel, K.H. *et al., J. Antibiot.*, 1974, **27**, 57-64 (*A 26771A*)
Williams, R.M. *et al., J.O.C.*, 1980, **45**, 2625 (*synth, ir, pmr, ms*)
Fukuyama, T. *et al., Tetrahedron*, 1981, **37**, 2045 (*synth*)
Pita Boente, M.I. *et al., J.C.S. Perkin 1*, 1991, 1283-1290
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 577

Hyalopyrone H-422

6-(2-Hydroxypropyl)-3-methyl-2-(1-methylpropyl)-4H-pyran-4-one
[140671-27-8]



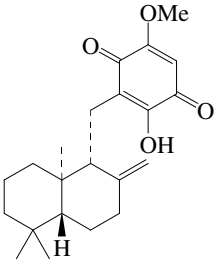
$C_{13}H_{20}O_3$ 224.299

Metab. of *Ascochyta hyalospora*, *Sporormiella teretispora* and the marine-derived *Ascochyta salicorniae*. Phytotoxin. Pale yellow syrup. $[\alpha]_D^{27}$ -16.6 (c, 1 in MeOH). λ_{max} 215 (ϵ 8700); 255 (ϵ 22500) (MeOH).

Venkatasubbaiah, P. *et al., J. Nat. Prod.*, 1992, **55**, 461-467 (*isol, pmr, cmr*)
Seibert, S.F. *et al., Org. Biomol. Chem.*, 2006, **4**, 2233-2240 (*marine, isol*)

Hyatellaquinone H-423

[151751-74-5]



Absolute Configuration

$C_{22}H_{30}O_4$ 358.477

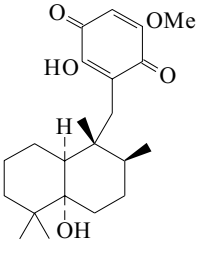
Constit. of *Hyatella intestinalis* and *Spongia* sp. Isol. from red algae. HIV reverse transcriptase (HIV-rt) inhibitor. Oil. $[\alpha]_D^{25}$ +15.6 (c, 0.5 in $CHCl_3$). λ_{max} 205 (ϵ 17800); 287 (ϵ 1180) (MeOH) (Berdy).

O-*De-Me: De*-O-*methylhyatellaquinone.* ***Antibiotic F 12509A. F 12509A***
$C_{21}H_{28}O_4$ 344.45
Prod. by the discomycete, *Trichopezizella barbata*. Sphingosine kinase inhibitor. Pale orange powder. $[\alpha]_D^{25}$ -96 (c, 0.25 in MeOH). λ_{max} 290 (ϵ 14700); 477 (ϵ 500) (MeOH).

Capon, R.J. *et al., Aust. J. Chem.*, 1993, **46**, 1245-1253 (*isol*)
Talpir, R. *et al., Tetrahedron*, 1994, **50**, 4179 (*isol, pmr, cmr, activity*)
Poigny, S. *et al., J.O.C.*, 1999, **64**, 9318-9320 (*synth, abs config*)
Kono, K. *et al., J. Antibiot.*, 2000, **53**, 459-466 (*F 12509A*)
Bernet, A. *et al., Helv. Chim. Acta*, 2003, **86**, 2009-2020 (*synth*)

Hyatoquinone H-424

Chiatoquinone
[114019-14-6]



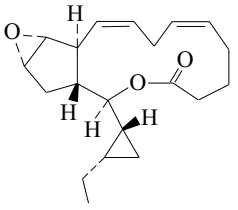
$C_{22}H_{32}O_5$ 376.492

Hyatoquinone and Chiatoquinone are transliteration equivalents. Constit. of a *Hyatella* sp. Orange needles (EtOH aq.). Mp 68.5-69.5°. $[\alpha]_D^{18}$ +34 (c, 1 in EtOH).

Rebachuk, N.M. *et al., Khim. Prir. Soedin.*, 1987, **23**, 793; *Chem. Nat. Compd. (Engl. Transl.)*, 656 (*isol, pmr, cmr*)
Il'in, S.G. *et al., Khim. Prir. Soedin.*, 1991, **27**, 467; *Chem. Nat. Compd. (Engl. Transl.)*, 407 (*cryst struct*)

Hybridalactone H-425

[81892-88-8]

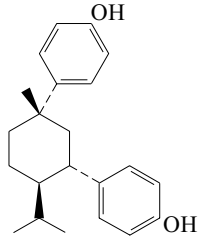


$C_{20}H_{28}O_3$ 316.439
Constit. of red alga *Laurencia hybrida*. Semisolid. $[\alpha]_D^{20}$ -56 (c, 4.9 in MeOH).

Higgs, M.D. *et al., Tetrahedron*, 1981, **37**, 4259
Corey, E.J. *et al., Tet. Lett.*, 1984, **25**, 1015 (*cryst struct*)

Hydrallmanol A H-426

[121079-02-5]

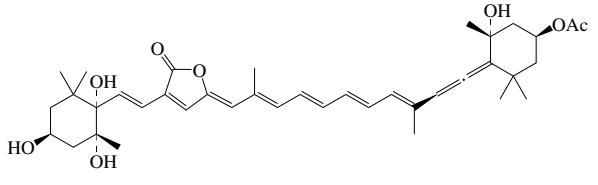


$C_{22}H_{28}O_2$ 324.462
Metab. of *Hydrallmania falcata*. Cytotoxic agent. Pale yellow oil.

Pathirana, C. *et al., Tet. Lett.*, 1989, **30**, 1487

Hydratoperidinin H-427

[866025-63-0]

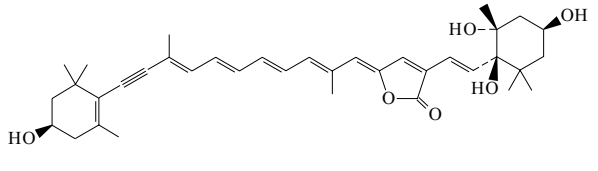


$C_{39}H_{52}O_8$ 648.835
Constit. of the corbicula clam (Shijimi), *Corbicula japonica*. λ_{max} 455; 475 (Et_2O).

Maoka, T. *et al., J. Nat. Prod.*, 2005, **68**, 1341-1344 (*Hydratoperdimin*)

Hydratopyrrhoxanthinol H-428

[120416-68-4]

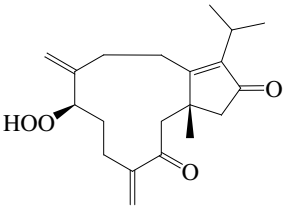


$C_{37}H_{48}O_6$ 588.783

Struct. incorrectly drawn in paper. Abs. config. based on comparison with Heteroxanthin, H-217. Constit. of the edible mussel *Mytilus edulis*. λ_{max} 452 (Me_2CO).

Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495 (*isol, pmr, uv, ms*)

7-Hydroperoxy-4(16),8(17),11-dolabellatriene-3,13-dione H-429



$C_{20}H_{28}O_4$ 332.439

7β-*form* [359415-70-6]
Constit. of *Clavularia inflata*.
Oil. $[\alpha]_D^{25}$ +95.6 (c, 0.12 in $CHCl_3$). λ_{max} 230 (log ϵ 4.24) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2001, **64**, 1028-1031 (*isol, pmr, cmr*)

12-Hydroperoxy-5,8,10,14-eicosatetraenoic acid H-430

12-HPETE
$H_3C(CH_2)_4CH{=}CHCH_2CH(OOH)(CH{=}CH)_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{20}H_{32}O_4$ 336.47

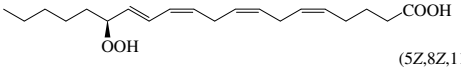
(5*Z*,8*Z*,10*E*,12*S*,14*Z*)-*form*
Biosynthetic intermed. isol. from the brown alga *Laminaria angustata*.

(5*Z*,8*Z*,10*E*,12*RS*,14*Z*)-*form* [71030-35-8]
[71774-10-2]
Obt. from arachidonic acid by photooxygenation. A metab. of arachidonic acid (presumably in chiral form).

Porter, N.A. *et al., J.O.C.*, 1979, **44**, 3177 (*synth, ms*)
Corey, E.J. *et al., J.A.C.S.*, 1980, **102**, 1433 (*synth*)
Porter, N.A. *et al., J.A.C.S.*, 1980, **102**, 5912; 1981, **103**, 6447 (*synth*)
Boeynaems, J.M. *et al., Prostaglandins*, 1980, **19**, 87 (*synth*)
Terao, J. *et al., Agric. Biol. Chem.*, 1981, **45**, 587 (*synth*)
Boonprab, K. *et al., Phytochemistry*, 2003, **63**, 669-678 (*isol*)

15-Hydroperoxy-5,8,11,13-eicosatetraenoic acid H-431

15-HPETE



(5*Z*,8*Z*,11*Z*,13*E*,15*S*)-*form*

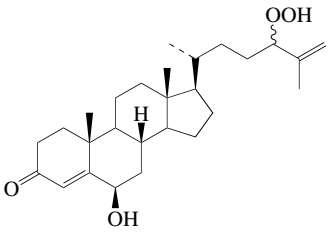
$C_{20}H_{32}O_4$ 336.47

(5*Z*,8*Z*,11*Z*,13*E*,15*S*)-*form* [70981-96-3]
[69371-38-6]
Metab. of arachidonic acid. Biosynthetic intermed. isol. from the brown alga *Laminaria angustata*. Prostacyclin synthase inhibitor. $[\alpha]_D$ -4.6 (MeOH).
Me ester: [77026-90-5]
$C_{21}H_{34}O_4$ 350.497
$[\alpha]_D$ -3.5 (MeOH).

(5*Z*,8*Z*,11*Z*,13*E*,15*RS*)-*form* [73804-66-7]
[69371-38-6]
Obt. from arachidonic acid by autoxidn. or photooxygenation.

Baldwin, J.E. *et al., J.C.S. Perkin 1*, 1979, 115 (*synth*)
Porter, N.A. *et al., J.O.C.*, 1979, **44**, 3177 (*synth, ms*)
Corey, E.J. *et al., J.A.C.S.*, 1980, **102**, 1433 (*synth*)
Boeynaems, J.M. *et al., Prostaglandins*, 1980, **19**, 87 (*synth*)
Terao, J. *et al., Agric. Biol. Chem.*, 1981, **45**, 587 (*synth*)
Porter, N.A. *et al., J.A.C.S.*, 1981, **103**, 6447 (*synth*)
Dussault, P. *et al., J.O.C.*, 1992, **57**, 1952 (*synth*)
Boonprab, K. *et al., Phytochemistry*, 2003, **63**, 669-678 (*isol, biosynth*)

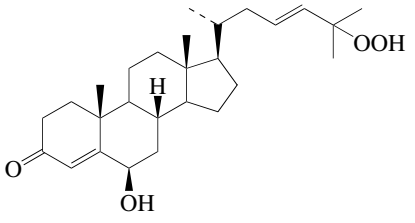
24-Hydroperoxy-6-hydroxycholesta-4,25-dien-3-one H-432



$C_{27}H_{42}O_4$ 430.626

(6β,24ξ)-*form* [196500-76-2]
Constit. of *Galaxaura marginata*.
Powder.
Mp 166-167°. $[\alpha]_D^{28}$ +9 (c, 0.11 in $CHCl_3$). λ_{max} 237 (log ϵ 3.92) (EtOH).
6-Ketone: ***24-Hydroperoxycholesta-4,25-diene-3,6-dione***
[196500-78-4]
$C_{27}H_{40}O_4$ 428.611
Constit. of *Galaxaura marginata*.
Sheu, J.-H. *et al., J. Nat. Prod.*, 1997, **60**, 900-903 (*isol, pmr, cmr*)

25-Hydroperoxy-6-hydroxycholesta-4,23-dien-3-one H-433

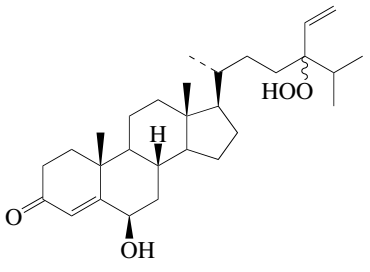


$C_{27}H_{42}O_4$ 430.626

(6β,23*E*)-*form* [196500-77-3]
Constit. of *Galaxaura marginata*.
Powder.
Mp 159-160°. $[\alpha]_D^{30}$ +6 (c, 0.07 in $CHCl_3$). λ_{max} 237 (log ϵ 4.07) (EtOH).
6-Ketone: ***25-Hydroperoxycholesta-4,23-diene-3,6-dione***
[196500-80-8]
$C_{27}H_{40}O_4$ 428.611
Constit. of *Galaxaura marginata*.
Sheu, J.-H. *et al., J. Nat. Prod.*, 1997, **60**, 900-903 (*isol, pmr, cmr*)

24-Hydroperoxy-6-hydroxystigmasta-4,28-dien-3-one H-434

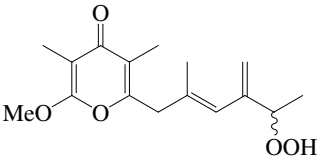
24-Ethenyl-24-hydroperoxy-6-hydroxycholest-4-en-3-one



$C_{29}H_{46}O_4$ 458.68

(6β,24ξ)-*form* [219832-38-9]
Constit. of *Turbinaria conoides*.
Cryst.
Mp 151-152°. $[\alpha]_D^{27}$ +16 (c, 0.34 in $CHCl_3$). λ_{max} 238 (log ϵ 4.09) (EtOH).
6-Ketone: ***24-Hydroperoxystigmasta-4,28-diene-3,6-dione****. 24-Ethenyl-24-hydroperoxycholest-4-ene-3,6-dione*
[219832-36-7]
$C_{29}H_{44}O_4$ 456.664
Constit. of *Turbinaria conoides*. Gum. $[\alpha]_D^{34}$ -9 (c, 0.075 in $CHCl_3$). λ_{max} 249 (log ϵ 3.89) (EtOH).
Sheu, J.-H. *et al., J. Nat. Prod.*, 1999, **62**, 224-227 (*isol, pmr, cmr*)

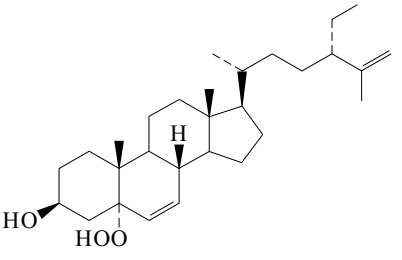
2-(5-Hydroperoxy-2-methyl-4-methylene-2-hexenyl)-6-methoxy-3,5-dimethyl-4*H*-pyran-4-one H-435



$C_{16}H_{22}O_5$ 294.347
Related to Cyercene A, C-1090. Isol. from *Placida dendritica*.
Amorph. solid.
Cutignano, A. *et al., J. Nat. Prod.*, 2003, **66**, 1399-1401 (*isol, pmr, cmr*)
Zuidema, D.R. *et al., J. Nat. Prod.*, 2005, **68**, 481-486 (*synth, pmr, cmr*)

5-Hydroperoxystigmasta-6,25-dien-3-ol H-436

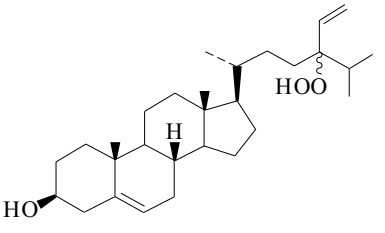
24-Ethyl-5-hydroperoxycholesta-6,25-dien-3-ol



$C_{29}H_{48}O_3$ 444.696

(3β,5α,24*S*)-*form* [173681-53-3]
Constit. of *Codium arabicum*.
Amorph. powder. $[\alpha]_D^{24}$ -9.1 (c, 0.07 in $CHCl_3$).
Sheu, J.-H. *et al., J. Nat. Prod.*, 1995, **58**, 1521 (*isol, pmr, cmr*)

24-Hydroperoxystigmasta-5,28-dien-3-ol H-437



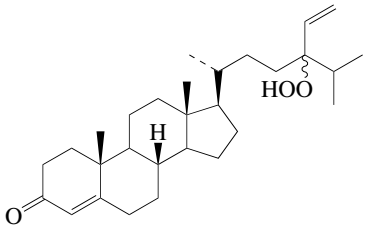
$C_{29}H_{48}O_3$ 444.696

(3β,24ξ)-*form*
24-Hydroperoxy-24-vinylcholesterol
[82780-53-8]
Obt. from tunicates *Phallusia mamillata*, *Ciona intestinalis*, *Turbinaria conoides* and *Padina pavonica* as well as brown algae.
Shows cytotoxic activity. Cryst.
Mp 140-145°. $[\alpha]_D^{23}$ -28.9 (c, 1.33 in $CHCl_3$).
Guyot, M. *et al., Tet. Lett.*, 1982, **23**, 1905

Sheu, J.-H. *et al., J. Chin. Chem. Soc. (Taipei)*, 1991, **38**, 501 (*isol, pmr, cmr*)
Ktari, L. *et al., J. Appl. Phycol.*, 1999, **11**, 511-513 (*activity, isol*)

24-Hydroperoxystigmasta-4,28-dien-3-one H-438

24-Ethenyl-24-hydroperoxycholest-4-en-3-one

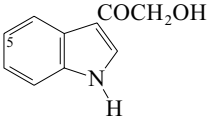


$C_{29}H_{46}O_3$ 442.681

24ξ-*form* [219832-34-5]
Constit. of *Turbinaria conoides*.
Gum. λ_{max} 242 (log ϵ 4.06) (EtOH).
Sheu, J.-H. *et al., J. Nat. Prod.*, 1999, **62**, 224-227 (*isol, pmr, cmr*)

3-(Hydroxyacetyl)-1*H*-indole H-439

*2-Hydroxy-1-(1*H*-indol-3-yl)ethanone, 9CI*
[2400-51-3]



$C_{10}H_9NO_2$ 175.187
Alkaloid from the red marine alga *Prionitis lanceolata*. Also isol. from the sponge *Tedania ignis* and from liquid cultures of the fungus *Lactarius deliciosus*. Plant growth regulator. CNS stimulant. Needles (EtOAc); cryst. (H_2O or C_6H_6).
Mp 162-163° Mp 173-174°. λ_{max} 212 (ϵ 10232); 240 (ϵ 5500); 294 (ϵ 4466) (MeOH) (Berdy).

▶ KM5779000

Oxime:
$C_{10}H_{10}N_2O_2$ 190.201
Mp 116-118°.

O-*Ac:* [27536-15-8]
$C_{12}H_{11}NO_3$ 217.224
Cryst. (H_2O). Mp 140°.

O-*Benzoyl:* [2400-52-4]
$C_{17}H_{13}NO_3$ 279.295
Cryst. (MeOH). Mp 187-189°.

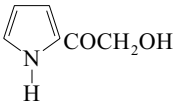
N,O-*Di-Ac:*
$C_{14}H_{13}NO_4$ 259.261
Oil. Mp 0° approx.

*5-Hydroxy: 5-Hydroxy-3-(hydroxyacetyl)-1*H*-indole.* ***Hyrtiosin A***†
[132922-98-6]
$C_{10}H_9NO_3$ 191.186
Alkaloid from the marine sponge *Hyrtios erecta*. Needles.
Mp 196-197°. λ_{max} 215 (ϵ 59200); 252 (ϵ 35000); 270 (ϵ 22400); 303 (ϵ 23300) (MeOH) (Berdy).

[34951-71-8, 34951-79-6]

Suvorov, N.N. *et al., Khim. Geterotsikl. Soedin.*, 1965, 265; 1971, 778; *Chem. Heterocycl. Compd.*, 1965, 173; 1971, 725 (*synth, oxime, ir*)
U.K. Pat., 1970, 1 183 919; *CA*, **72**, 132517v (*synth, O-Ac*)
Vereshchagin, A.L. *et al., Khim. Geterotsikl. Soedin.*, 1983, 46; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1983, 40 (*O-Ac*)
Tsujii, S. *et al., J.O.C.*, 1988, **53**, 5446 (*synth*)
Bernart, M. *et al., Phytochemistry*, 1990, **29**, 3697 (*isol*)
Kobayashi, J. *et al., Tetrahedron*, 1990, **46**, 7699 (*Hyrtiosin A*)
Dillman, R.L. *et al., J. Nat. Prod.*, 1991, **54**, 1056 (*isol, uv, pmr, cmr, ms*)
Ayer, W.A. *et al., J. Nat. Prod.*, 1994, **57**, 839 (*isol, pmr, ms, struct*)
Böhlendorf, B. *et al., Annalen*, 1996, 49 (*isol, ir, pmr, cmr, ms*)

2-(Hydroxyacetyl)-1*H*-pyrrole H-440



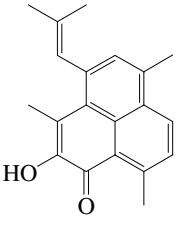
$C_6H_7NO_2$ 125.127

N-*(2-Acetoxyethyl)*, O-*Ac:* ***2-(Acetoxyacetyl)-1-(2-acetoxyethyl)-1*H*-pyrrole***
[136396-66-2]
$C_{12}H_{15}NO_5$ 253.254
Constit. of the red alga *Gracilariopsis lemaneiformis*. Oil.

N-*(2-Acetoxypropyl)*, O-*Ac:* ***2-(Acetoxyacetyl)-1-(2-acetoxypropyl)-1*H*-pyrrole***
[136396-64-0]
$C_{13}H_{17}NO_5$ 267.281
Constit. of red alga *Gracilariopsis lemaneiformis*. Oil. $[\alpha]_D^{23}$ -47.2 (c, 0.29 in MeOH).
Jiang, Z.D. *et al., J. Nat. Prod.*, 1991, **54**, 403-407 (*isol, uv, ir, pmr, cmr, ms, struct, derivs*)

10-Hydroxy-1,3,5,7,10,12,14-amphilectaheptaen-9-one H-441

Elisabatin B
[237749-85-8]

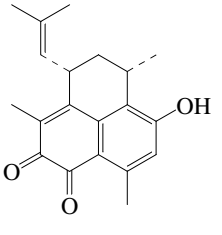


$C_{20}H_{20}O_2$ 292.377
Constit. of *Pseudopterogorgia elisabethae*. Orange oil. λ_{max} 246; 286 (sh); 348; 374 (sh); 450 (MeOH).

Rodriguez, A.D. *et al., J. Nat. Prod.*, 1999, **62**, 997-999 (*isol, pmr, cmr*)
Shi, Y.-P. *et al., Bopuxue Zazhi*, 2002, **19**, 395-400; *CA*, 2002, **138**, 304417 (*pmr, cmr*)
Baran, P. *et al., J. Chem. Crystallogr.*, 2003, **33**, 711-718 (*cryst struct*)

5-Hydroxy-4,6,8(13),11,14-amphilectapentaene-9,10-dione H-442

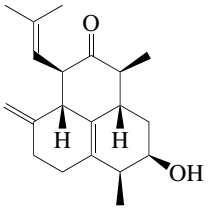
Elisabatin A
[237749-84-7]



$C_{20}H_{22}O_3$ 310.392
Constit. of *Pseudopterogorgia elisabethae*. Yellow oil. $[\alpha]_D^{24}$ +59 (c, 0.56 in $CHCl_3$). λ_{max} 218 (ϵ 17000); 276 (ϵ 10000); 406 (ϵ 3000) (MeOH).

Rodriguez, A.D. *et al., J. Nat. Prod.*, 1999, **62**, 997-999 (*isol, pmr, cmr*)

6-Hydroxy-8(13),11(20),14-amphilectatrien-2-one H-443



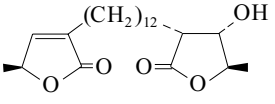
$C_{20}H_{28}O_2$ 300.44

6β-*form*

Ac: ***Sinulobatin A***
[189455-83-2]
$C_{22}H_{30}O_3$ 342.477
Constit. of *Sinularia nanolobata*. Cryst. (hexane).
Mp 126-128°. $[\alpha]_D^{25}$ +115.6 (c, 0.43 in $CHCl_3$).
Yamada, K. *et al., Tetrahedron*, 1997, **53**, 4569-4578 (*isol, pmr, cmr, cryst struct*)

Hydroxyancepsenolide H-444

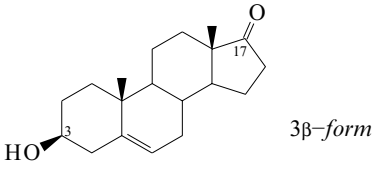
*3-[12-(2,5-Dihydro-5-methyl-2-oxo-3-furanyl)dodecyl]dihydro-4-hydroxy-5-methyl-2(3*H*)-furanone, 9CI*
[18634-45-2]



$C_{22}H_{36}O_5$ 380.523
Constit. of the gorgonian *Pterogorgia anceps*. Plates (2-propanol).
Mp 122.5-123.7°. $[\alpha]_D^{24}$ +3.4. λ_{max} 209 nm (ϵ 15 800) (EtOH).

Ac: [18634-46-3]
Mp 68.3-70.3°.
Schmitz, F.J. *et al., J.O.C.*, 1969, **34**, 1989 (*ms, ir, pmr*)

3-Hydroxyandrost-5-en-17-one, 9CI H-445



3β–*form*

$C_{19}H_{28}O_2$ 288.429

3α-*form*

Dehydroandrosterone
[2283-82-1]
Bile and urine constit. Cryst. (EtOAc). Mp 221°. $[\alpha]_D$ 0 ($CHCl_3$).

Oxime:
$C_{19}H_{29}NO_2$ 303.444
Cryst. (EtOH). Mp 204-206°.

Me ether: 3α-Methoxyandrost-5-en-17-one
$C_{20}H_{30}O_2$ 302.456
Cryst. (petrol). Mp 140-142°.

Ac:
$C_{21}H_{30}O_3$ 330.466
Cryst. (MeOH). Mp 173.5-174.5°.
Phase III clin. trials (2004) for the treatment of lupus erythematosus. Orphan drug designated (2003) for replacement therapy in people with adrenal insufficiency

3β-*form*

Dehydroisoandrosterone. ***Prasterone, INN.*** *Cetovister. 17-Chetovis. Dastonil S. Deandros. Diandrone. Hormobago. 17-Hormoforin. 17-Ketovis. Mentalormen. Psicosterone. Dehydroepiandrosterone. DHEA. Prestara. Fidelin*
[53-43-0]
Male sex hormone. Constit. of human adrenal cortex and testicular tissue, found in urine. Sterol identified in sponge *Damiriana hawaiiana*. Reported to possess antidepressant and psychotonic props.; shows anti-HIV activity. Used in the treatment of lupus erythematosus. Needles or leaflets.
Mp 140-141° (needles) Mp 152-153° (leaflets). $[\alpha]_D^{23}$ -3 ($CHCl_3$).
Log P 3.07 (uncertain value) (calc). Dimorphic.
▶ BV8396000

3-Sulfate: 3-(Sulfooxy)androst-5-en-17-one, 9CI
[651-48-9]
$C_{19}H_{28}O_5S$ 368.493
Psychotropic. Log P 3.01 (uncertain value) (calc).

3-Sulfate, Na salt: ***Prasterone sodium sulfate****. Mylis. DHEAS. Astenile*
[1099-87-2]
Mp 154° dec.
▶ LD_{50} (rat, ipr) 523 mg/kg. Exp. reprod. and teratogenic effects.
BV8397400

3-Heptanoyl: Dehydroepiandrosterone enanthate. ***Prasterone enanthate****. EDHEA*
[23983-43-9]
$C_{26}H_{40}O_3$ 400.6
Adrenocortical hormone, antidepressant, psychotonic. Log P 6.66 (uncertain value) (calc).

Oxime: [2830-48-0]
Cryst. (CH_2Cl_2/MeOH). Mp 201-203°.

Ac: [853-23-6]
Cryst. (Me_2CO/hexane). Mp 169-171°. $[\alpha]_D^{23}$ -1.3 ($CHCl_3$).

(3β,13α)-*form* [571-35-7]
Needles (EtOH aq.). Mp 187.5-189°. $[\alpha]_D^{20}$ -162.9 (c, 0.528 in EtOH).

Ac: [18462-31-2]
Mp 143-144°. $[\alpha]_D^{20}$ -149 (c, 1.362 in EtOH).

Me ether: 3β-Methoxyandrost-5-en-17-one
[56085-46-2]
$C_{20}H_{30}O_2$ 302.456
Leaflets (MeOH aq.). Mp 118-120°. $[\alpha]_D^{25}$ -133 (c, 0.11 in $CHCl_3$).

(3β,14β)-*form* [24357-33-3]
Mp 160-162°. $[\alpha]_D^{14}$ +72.6 (c, 0.05 in $CHCl_3$).

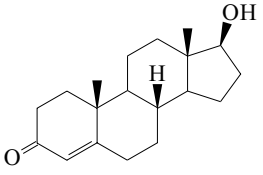
Ac: [33203-18-8]
Cryst. (MeOH). Mp 167-168°. $[\alpha]_D^{23}$ +39 (c, 0.5 in $CHCl_3$).

[1232-19-5, 2497-74-7, 10457-69-9, 13996-45-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1050D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 573B (*nmr*)
Ruzicka, L. *et al., Helv. Chim. Acta*, 1936, **19**, 1407; 1410 (*synth*)
Testa, E. *et al., Gazz. Chim. Ital.*, 1957, **87**, 971 (*3β-form, synth*)
Romo, J. *et al., J.A.C.S.*, 1957, **79**, 1118 (*3β-form, synth, ir*)
Jones, R.N. *et al., J.A.C.S.*, 1958, **80**, 6121 (*3β-form, synth*)
Bots, J.P.L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1958, **77**, 1010 (*3β13α-form, synth*)
Muller, G. *et al., Bull. Soc. Chim. Fr.*, 1962, 296 (*3β13β-form, synth*)
Birmingham, M.K. *et al., Steroids*, 1963, **1**, 463 (*3β-form, ir*)
Weinman, J. *et al., Steroids*, 1965, **6**, 683 (*3α-form, ir*)
Siddall, J.B. *et al., Chem. Ind. (London)*, 1966, 25 (*3β-form, synth*)
Weinman, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1967, **264**, 1352 (*3α-form, ir*)
Nambara, T. *et al., Chem. Pharm. Bull.*, 1969, **17**, 1782 (*3β14β-form, synth*)
Reich, H.J. *et al., J.A.C.S.*, 1969, **91**, 7445 (*3β-form, cmr*)
Oertel, G.W. *et al., Arzneim.-Forsch.*, 1971, **21**, 543 (*pharmacol*)
U.K. Pat., 1971, (*Schering*)1 246 639; *CA*, **75**, 130020r (*deriv*)
Portheine, J.C. *et al., Acta Cryst. B*, 1972, **28**, 849 (*cryst struct*)
Meinwald, J. *et al., J.A.C.S.*, 1973, **95**, 7663 (*3β13α-form, synth*)
Hosoda, H. *et al., J.O.C.*, 1973, **38**, 4209 (*3β-form, synth*)
Gyory, G. *et al., Magy. Noorv. Lapja*, 1974, **37**, 451 (*isol*)
Baehring-Kuhlmey, S.R. *et al., Drugs of Today (Barcelona)*, 1976, **12**, 459 (*rev, sulfate*)
Boar, R.B. *et al., J.C.S. Perkin 1*, 1977, 2163 (*3β13α-form, synth*)
Holland, H.L. *et al., Can. J. Chem.*, 1978, **56**, 3121 (*cmr*)

Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1420-1476 (*isol, sponge*)
Pulver, K.P.J. *et al., Diss. Abstr. Int., B*, 1981, **42**, 611 (*metab*)
Colebrook, L.D. *et al., Org. Magn. Reson.*, 1983, **21**, 532 (*3β-form, pmr*)
Gramain, J.C. *et al., Magn. Reson. Chem.*, 1986, **24**, 938 (*3β-form, cmr*)
Preti, G. *et al., J. Chem. Ecol.*, 1987, **13**, 717
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1194
Thijssen, J.H.H. *et al., DHEA: A Comprehensive Review*, Parthenon Publishing, 1999, (*book*)
Hinson, J.P. *et al., Curr. Opin. Invest. Drugs*, 2003, **4**, 1205-1208 (*DHEA, rev*)
Ramsey-Goldman, R. *et al., Curr. Rheumatol. Rep.*, 2003, **5**, 347; 348-349 (*prasterone, rev*)
Merrill, J.T. *et al., Expert Opin. Invest. Drugs*, 2003, **12**, 1017-1025 (*prasterone, rev*)
Petri, M.A. *et al., Arthritis Rheum.*, 2004, **50**, 2858-2868 (*3β-form, pharmacol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AOO450; SJK400; SJK410

17-Hydroxyandrost-4-en-3-one H-446



17β-*form*

$C_{19}H_{28}O_2$ 288.429

17β-*form*

Testosterone, BAN, INN, USAN. *Andropatch. Atmos. Many other names*

[58-22-0]

Male sex hormone. Pheromone for domestic sheep and precocious male Atlantic salmon *Salmo salar*. Androgen. Used in the treatment of male hypogonadism (transdermal administration). Cryst. (Me_2CO aq.).

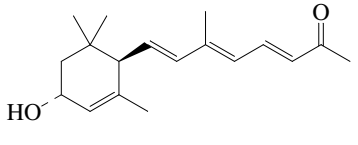
Mp 155°. $[\alpha]_D$ +109 (c, 4 in EtOH).

▶ Adverse effects reported when used therapeutically (and for ester derivatives). Exp. neoplastic agent. Human teratogen, exp. reprod. effects. XA3030000

[1159-27-9, 4069-10-7, 6891-35-6, 14958-66-8, 14958-67-9]

Shoolery, J.N. *et al., J.A.C.S.*, 1958, **80**, 5121 (*17β-form, pmr*)
Bots, J.P.L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1958, **77**, 1010 (*synth, uv, ir*)
Johnson, W.S. *et al., J.A.C.S.*, 1960, **82**, 3409 (*synth, uv, ir*)
Chinn, L.J. *et al., J.O.C.*, 1962, **27**, 54 (*synth*)
Birmingham, M.K. *et al., Steroids*, 1963, **1**, 463 (*ir*)
Idler, D.R. *et al., Can. J. Biochem.*, 1964, **42**, 211-218 (*17β-form, isol*)
Idler, D.R. *et al., Gen. Comp. Endocrinol.*, 1971, **16**, 257-267 (*17β-form, isol*)
Highet, R.J. *et al., Steroids*, 1980, **35**, 119 (*17β-form, cmr*)
Aristoff, P.A. *et al., J.O.C.*, 1985, **50**, 1765 (*17β-form, ir, pmr, cmr, synth*)

3-Hydroxy-13-apo-β-caroten-13-one H-447



$C_{18}H_{26}O_2$ 274.402

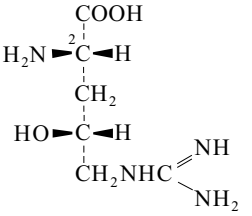
(3*R*,6*R*)-*form* [761409-24-9]

Constit. of *Chenopodium album* and *Chaetomorpha basiretorsa*. $[\alpha]_D^{25}$ +251 (c, 0.006 in $CHCl_3$). λ_{max} 329 (log ϵ 4.3) ($CHCl_3$).

DellaGreca, M. *et al., J. Nat. Prod.*, 2004, **67**, 1492-1495 (*Chenopodium album constit*)
Shi, D.Y. *et al., Chin. Chem. Lett.*, 2005, **16**, 777-780 (*Chaetomorpha basiretorsa cinstit*)

4-Hydroxyarginine, 9CI H-448

2-Amino-5-guanidino-4-hydroxypentanoic acid. γ-Hydroxyarginine



(2*S*,4*R*)–*form*

$C_6H_{14}N_4O_3$ 190.202

(2*S*,4*R*)-*form*

L-erythro-*form*

[61370-10-3]

Occurs in *Vicia* spp., in the sea-cucumber (*Polycheira rufescens*), in the sea anemone (*Anthopleura japonica*) and in lentil seeds (*Lens culinaris*). Cryst. (EtOH aq.) (as hydrochloride). Mp 190-191° dec. (hydrochloride). $[\alpha]_D^{18}$ +6.3 (c, 2 in 5*M* HCl) (hydrochloride).

Lactone:

$C_6H_{12}N_4O_2$ 172.186

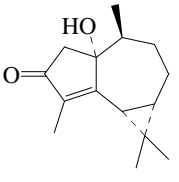
Constit. of *Vicia sativa*. Needles + $1H_2O$ (EtOH aq.) (as dihydrochloride). Mp 158° (dihydrochloride).

(±)-*form*

Hygroscopic powder. Mp 184-188°. Mixt. of diastereoisomers.

Bell, E.A. *et al., Biochem. J.*, 1965, **97**, 104 (*occur*)
Sulser, H. *et al., Lebensm.-Wiss. Technol.*, 1974, **7**, 327 (*synth, config*)
Mizusaki, K. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 470 (*synth*)
Bell, E.A. *et al., Phytochemistry*, 1999, **50**, 1201-1204 (*isol, pmr, cmr, cryst struct, abs config*)

1-Hydroxy-4-aromadendren-3-one H-449



(1α,6β*H*,7β*H*,10β)-*form*

$C_{15}H_{22}O_2$ 234.338

(1α,6β*H*,7β*H*,10β)-*form*

1-Hydroxycyclocolorenone

[67594-83-6]

Constit. of a *Nephthea* sp. Cryst. ($CHCl_3$/MeOH). Mp 169-171°. $[\alpha]_D^{27}$ +15.2 (c, 0.3 in $CHCl_3$).

(1β,6β*H*,7β*H*,10β)-*form* [276684-22-1]

Constit. of the liverwort *Heteroscyphus coalitus*.

$[\alpha]_D^{25}$ +2.4 (c, 0.11 in $CHCl_3$).

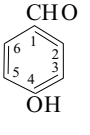
Jong, J.-R. *et al., J. Chin. Chem. Soc. (Taipei)*, 2000, **47**, 359-362 (*isol, pmr, ms*)
Rao, C.B. *et al., Indian J. Chem., Sect. B*, 2004, **43**, 1329-1331 (*1-Hydroxycyclocolorenone*)

4-Hydroxybenzaldehyde H-450

p-*Formylphenol*

[123-08-0]

[28777-87-9]



$C_7H_6O_2$ 122.123

Present in sulfite liquor. Occurs naturally combined in many glycosides. Isol. in free state from opium poppy (*Papaver somniferum*) and found in chlorophyte alga *Boodlea composita* and microorganisms. Found in *Gelasinospora kobi*, *Alternaria porri*, *Phycomyces blakesleeanus*, *Sirodesmium diversum*, *Ceratocystis clavigera*, *Tedania anhelans*, *Isodictya erinacea*. Constit. of wing gland and abdominal hairpencils of the male African sugarcane borer *Eldana saccharina*. Reagent for the colorimetric detn. of shikimic acid. Shows immunosuppressive and phytotoxic props. Needles (H_2O). Mp 115-116°. pK_a 7.62 (25°, H_2O). λ_{max} 221 (ϵ 12000); 284 (ϵ 14800); 291 (MeOH) (Berdy). λ_{max} 220 (ϵ 14800); 280 (ϵ 18700); 330 (ϵ 6600) (EtOH) (Berdy).

▶ CU6475000

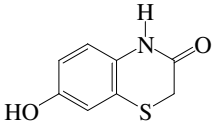
O-*(3-Phenylpropanoyl): 4-(3-Phenylpropanoyloxy)benzaldehyde*
$C_{16}H_{14}O_3$ 254.285
Isol. from the sponge *Sigmadocia pumila*. Mp 98°.

[60221-52-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 111C; 111D; 112A; 132B; 132C; 314B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 941B; 941C; 942A; 943A; 975B; 975C; 1291C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1290D; 1291A; 1291B; 1291C; 1311B; 1311C; 1382B (*ir*)
Gattermann, L. *et al., Ber.*, 1898, **31**, 1765
Gattermann, L. *et al., Annalen*, 1907, **357**, 313
Magnusen, L.B. *et al., J.A.C.S.*, 1963, **85**, 1711
Beistel, D.W. *et al., J. Phys. Chem.*, 1976, **80**, 2023 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **13**, 70 (*rev*)
Venkateswarlu, Y. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 1264-1268 (*3-phenylpropanoyl*)

7-Hydroxy-2*H*-1,4-benzothiazin-3(4*H*)-one, 9CI H-451

[91375-75-6]

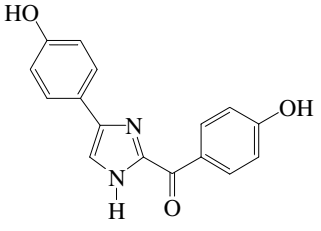


$C_8H_7NO_2S$ 181.215
Prod. by the marine-derived *Halomonas* sp. RK377. Cryst. (Me_2CO). Mp 217°.

Jones, G.H. *et al., J. Med. Chem.*, 1987, **30**, 295-303 (*synth*)
Crescenzi, O. *et al., Gazz. Chim. Ital.*, 1990, **120**, 21-24 (*synth*)
Liang, L. *et al., Dissertation*, Univ. of Göttingen, 2003, (*isol, pmr, cmr, ms*)

2-(4-Hydroxybenzoyl)-4(5)-(4-hydroxyphenyl)-1*H*-imidazole H-452

[251907-19-4]

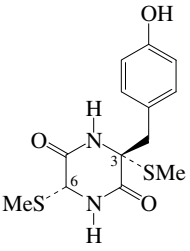


1*H-form*

$C_{16}H_{12}N_2O_3$ 280.282
Alkaloid from the red ascidian *Botryllus leachi*. Amorph. yellow solid. λ_{max} 248 (ϵ 7600); 305 (ϵ 6000); 360 (ϵ 13700) (MeOH).

Duran, R. *et al., Tetrahedron*, 1999, **55**, 13225-13232 (*isol*)
Mahboobi, S. *et al., Monatsh. Chem.*, 2004, **135**, 333-342 (*synth, pmr, tautom*)

3-(4-Hydroxybenzyl)-3,6-bis(methylthio)-2,5-piperazinedione H-453



(3*R*,6*R*)-*form*

$C_{13}H_{16}N_2O_3S_2$ 312.413

(3*R*,6*R*)-*form*

1,4-N-*Di-Me:* ***3-(4-Hydroxybenzyl)-1,4-dimethyl-3,6-bis(methylthio)-2,5-piperazinedione***
[77053-26-0]
$C_{15}H_{20}N_2O_3S_2$ 340.467
Biogenetically related to Gliotoxin, G-94. Prod. by *Gliocladium virens* and *Fusarium chlamydosporum*. Obt. as CH_2Cl_2 adduct. Mp 68-69°. $[\alpha]_D$ -55.6 (c, 1.06 in $CHCl_3$).

O-*(3-Methyl-2-butenyl), 1,4*-N-*di-Me: 1,4-Dimethyl-3-[(4-(γ,γ-dimethylallyloxy)phenyl)methyl]-3,6-bis(methylthio)-2,5-piperazinedione.* ***Bis(methylthio)silvatin***
[77053-25-9]
$C_{20}H_{28}N_2O_3S_2$ 408.585
Prod. by *Gliocladium virens* and *Fusarium chlamydosporum*. Oil. $[\alpha]_D^{16}$ -43.9 (c, 0.41in $CHCl_3$).

O-*(3-Hydroxymethyl-2-butenyl), 1,4*-N-*di-Me:* [112926-39-3]
$C_{20}H_{28}N_2O_4S_2$ 424.584
Prod. by *Gliocladium virens*. Gum.

(3*R*,6*S*)-*form*

O-*(3-Methyl-2-butenyl):* ***Antibiotic Sch 54796***. *Sch 54796*
$C_{18}H_{24}N_2O_3S_2$ 380.531
Prod. by *Tolypocladium* sp. and *Fusarium chlamydosporum*. Amorph. solid.
Mp 210°. $[\alpha]_D^{25}$ -25 (c, 0.1 in DMSO). λ_{max} 277; 281 (MeOH) (Berdy).

(3*S*,6*S*)-*form*

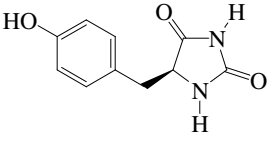
Fusaperazine A
Prod. by *Fusarium chlamydosporum* OUPS-N124.
Needles. $[\alpha]_D^{16}$ -110.8 (c, 0.2 in DMSO). λ_{max} 226 (log ϵ 4.25); 278 (log ϵ 3.83); 285 (log ϵ 3.81) (EtOH).

O-*(3-Methyl-2-butenyl):* ***Antibiotic Sch 54794***. *Sch 54794*
$C_{18}H_{24}N_2O_3S_2$ 380.531
Prod. by *Tolypocladium* sp. and *Fusarium chlamydosporum*. Platelet activating factor (PAF) inhibitor. Needles(CH_2Cl_2). Mp 200-203° (180-182°). $[\alpha]_D^{28}$ -70.4 (c, 0.43 in DMSO). λ_{max} 277; 281 (MeOH) (Berdy).

Hanson, J.R. *et al., J.C.S. Perkin 1*, 1981, 218
Kirby, G.W. *et al., J.C.S. Perkin 1*, 1988, 301 (*derivs, isol*)
Chu, M. *et al., Tet. Lett.*, 1993, **34**, 7537 (*Sch 54794, Sch 54796*)
Yonezawa, Y. *et al., Heterocycles*, 1997, **45**, 1151 (*synth, ir, pmr, cmr*)
Usami, Y. *et al., J. Antibiot.*, 2002, **55**, 655-659 (*Fusaperazine A*)

5-(4-Hydroxybenzyl)-2,4-imidazolidinedione H-454

*5-(*p-*Hydroxybenzyl)hydantoin*
[58942-04-4]
[98819-07-9]



(*S*)-*form*

$C_{10}H_{10}N_2O_3$ 206.201

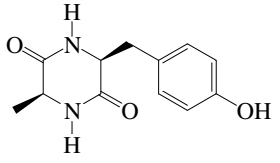
(*S*)-*form* [40856-79-9]
$[\alpha]_D$ -165 (EtOH). $[\alpha]_D$ -292 (1*M* NaOH).

(±)-*form* [67337-72-8]
Cryst. (EtOH). Mp 258-259°.

(ξ)-*form*
Isol. from a marine endophytic fungus No. 1893. No details are given for its isol. from the fungus.
Suzuki, T. *et al., Agric. Biol. Chem.*, 1973, **37**, 411-416; 1976, **40**, 225-226 (*synth ord pmr*)
Marton, J. *et al., J. Agric. Food Chem.*, 1993, **41**, 148-152 (*synth*)
Chen, G. *et al., Tetrahedron*, 2003, **59**, 4907-4909 (*isol*)

3-(4-Hydroxybenzyl)-6-methyl-2,5-piperazinedione H-455

Cyclo(alanyltyrosyl). Cyclo(tyrosylalanyl)
[21754-26-7]
[15266-80-5, 19943-32-9, 35590-93-3, 56390-14-8]

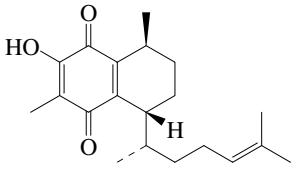


$C_{12}H_{14}N_2O_3$ 234.254

(3*S*,6*S*)-*form*
L-L-form
Isol. from the mangrove endophytic fungus No. 1839. Constit. of the rhizomes of *Pinellia pedatisecta*.
Needles.
Mp 264-265° dec.
Kopple, K.D. *et al., J.A.C.S.*, 1967, **89**, 6193-6200; 1969, **91**, 962-970 (*pmr, conformn*)
Szafranek, J. *et al., Org. Magn. Reson.*, 1976, **11**, 920-930 (*ms*)
Göktürk, A.K. *et al., J.C.S. Perkin 1*, 1982, 953-959 (*synth*)
Qin, W.J. *et al., Zhongcaoyao*, 1995, **26**, 3-6; *CA*, **122**, 298789m (*isol*)
Chen, G. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2006, **42**, 138-141 (*isol, pmr*)

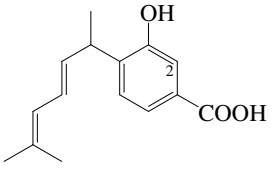
3-Hydroxy-1(6),3,15-bifloratriene-2,5-dione H-456

Elisabethadione
[433717-71-6]



$C_{20}H_{28}O_3$ 316.439
Constit. of *Pseudopterogorgia elisabethae.*
$[\alpha]_D^{20}$ +93.3 (MeOH). λ_{max} 248; 326 (MeOH).
Ata, A. *et al., Tetrahedron*, 2003, **59**, 4215-4222 (*isol, pmr, cmr*)
Davies, H.M.L. *et al., Tetrahedron*, 2006, **62**, 10477-10484 (*synth*)

1-Hydroxy-1,3,5,8,10-bisabolapentaen-15-oic acid H-457

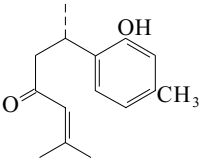


$C_{15}H_{18}O_3$ 246.305

(*E*)-*form*
Me ether: 1-Methoxy-1,3,5,8,10-bisabolapentaen-15-oic acid. ***Parahigginic acid***
[224176-21-0]
$C_{16}H_{20}O_3$ 260.332
Constit. of a *Parahigginsia* sp. Oil. $[\alpha]_D$ -29.2 (c, 0.15 in $CHCl_3$). λ_{max} 216 (log ϵ 4); 249 (log ϵ 3.6); 257 (log ϵ 3.6); 264 (log ϵ 3.5); 299 (log ϵ 3.2) (MeOH).
2-Hydroxy, 15-aldehyde: 1,2-Dihydroxy-1,3,5,8,10-bisabolapentaen-15-al. ***Parahigginol D***
[224176-20-9]
$C_{15}H_{18}O_3$ 246.305
Constit. of a *Parahigginsia* sp. Oil. $[\alpha]_D$ -73.5 (c, 0.225 in $CHCl_3$).
Chen, C.-Y. *et al., J. Nat. Prod.*, 1999, **62**, 573-576 (*isol, pmr, cmr*)

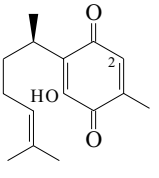
1-Hydroxy-1,3,5,10-bisabolatetraen-9-one H-458

Parahigginone. ***Turmeronol B***
[131651-38-2]
[139085-15-7]



$C_{15}H_{20}O_2$ 232.322
Constit. of turmeric (*Curcuma longa*). Isol. from the marine sponge *Parahigginsia* sp. Oil. $[\alpha]_D^{23}$ +79 (c, 0.1 in $CHCl_3$). λ_{max} 224 (log ϵ 4.1); 241 (log ϵ 4); 276 (log ϵ 3.4); 284 (log ϵ 3.4) (MeOH) (Derep).
Imai, S. *et al., Agric. Biol. Chem.*, 1990, **54**, 2367 (*isol, pmr, cmr*)
Sharma, M.L. *et al., Tet. Lett.*, 1996, **37**, 2275 (*synth*)
Tanaka, K. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1053-1055 (*synth*)
Shen, Y.-C. *et al., J. Chin. Chem. Soc. (Taipei)*, 1999, **46**, 201-204 (*isol, pmr, cmr, ms*)
Du, Z.-T. *et al., J. Chin. Chem. Soc. (Taipei)*, 2004, **51**, 571-574 (*synth*)

5-Hydroxy-2,5,10-bisabolatriene-1,4-dione H-459



$C_{15}H_{20}O_3$ 248.321
Possesses laxative props. Log P 3.77 (calc).

(*R*)-*form*
Perezone. *Pipitzahoic acid*
[3600-95-1]
Constit. of *Trixis piptzhuac, Perezia* spp., *Acourtia thurberi, Jungia spectabilis, Jungia malvaefolia, Coreopsis mitica* and *Bidens andicola* (sometimes as isovalerate or angelate).
Golden-yellow leaflets (H_2O).
Mp 104-106°. $[\alpha]_D^{20}$ -17 (Et_2O). Pharmacol. active isomer.
Me ether: [33418-02-9]
$C_{16}H_{22}O_3$ 262.348
Constit. of *Coreopsis* spp. Yellow oil.
5-Deoxy: 2,5,10-Bisabolatriene-1,4-dione. ***Curcuquinone.*** *6-Deoxyperezone*
[69301-26-4]
$C_{15}H_{20}O_2$ 232.322
Constit. of *Wyethia helenioides, Bidens* spp. and the gorgonian *Pseudopterogorgia rigida*. Yellow oil. $[\alpha]_D^{24}$ -33.5 (c, 0.93 in $CHCl_3$) (-1.3). λ_{max} 253 (ϵ 10200) (MeOH) (Derep). λ_{max} 205 (ϵ 6920); 253 (ϵ 10200) (MeOH) (Berdy).

5-Deoxy, 2-acetoxy: ***2-Acetoxycurcuquinone***
[89913-50-8]
$C_{17}H_{22}O_4$ 290.358
Isol. from aerial parts of *Coreopsis fasciculata*. Yellow oil.

Hydroquinone: 1,3,5,10-Bisabolatetraene-1,4,5-triol. Leucoperezone
[27678-50-8]
$C_{15}H_{22}O_3$ 250.337
No phys. props. reported.

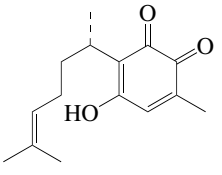
Hydroquinone, 5-Ac: ***5-Acetoxycurcuquinol***
[97763-20-7]
$C_{17}H_{24}O_4$ 292.374
Constit. of *Coreopsis senaria*. Oil.

Hydroquinone, tri-Ac: Leucotriacetyl perezone
[18142-26-2]
$C_{21}H_{28}O_6$ 376.449
$Bp_{0.15}$ 145-150°.

[78964-28-0, 100761-40-8]

Arigoni, D. *et al., Helv. Chim. Acta*, 1954, **37**, 881 (*abs config*)
Joseph-Nathan, P. *et al., Org. Magn. Reson.*, 1971, **3**, 23 (*cmr*)
Joseph-Nathan, P. *et al., Rev. Soc. Quim. Mex.*, 1974, **18**, 226 (*rev*)
Joseph-Nathan, P. *et al., Tetrahedron*, 1977, **33**, 1573 (*struct, bibl*)
McEnroe, F.J. *et al., Tetrahedron*, 1978, **34**, 1661 (*Curcuquinone*)
Sánchez, I.H. *et al., J.O.C.*, 1981, **46**, 4666; 1985, **50**, 5077 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 2245; 1983, **22**, 1286; 2858 (*derivs*)
Bohlmann, F. *et al., Phytochemistry*, 1985, **24**, 1295 (*5-Acetoxycurcuquinol*)
Garcá, G.E. *et al., J. Nat. Prod.*, 1987, **50**, 1055 (*synth*)
Saa, J.M. *et al., Tet. Lett.*, 1987, **28**, 5045 (*synth*)
Enksen, A. *et al., J.O.C.*, 1990, **55**, 1177 (*synth*)
Ono, M. *et al., Heterocycles*, 1994, **37**, 181 (*synth*)
Ono, M. *et al., Chem. Pharm. Bull.*, 1995, **43**, 553 (*synth*)
Yoshimura, T. *et al., ARKIVOC*, 2003, **viii**, 247-255 (*synth*)
Vyvyan, J.R. *et al., J.O.C.*, 2004, **69**, 2461-2468 (*synth*)
Minatti, A. *et al., J.O.C.*, 2005, **70**, 3745-3748 (*synth*)

5-Hydroxy-3,5,10-bisabolatriene-1,2-dione H-460

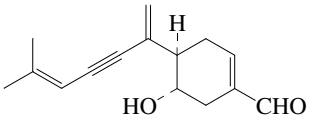


$C_{15}H_{20}O_3$ 248.321

(*S*)-*form*
Rigidone
[186344-35-4]
Constit. of *Pseudopterogorgia rigida*.
Pale red powder. $[\alpha]_D$ +8.3 (c, 0.37 in $CHCl_3$). λ_{max} 210; 264; 408 (MeOH). λ_{max} 264; 408 (MeOH) (Berdy).

Freyer, A.J. *et al., J. Nat. Prod.*, 1997, **60**, 309-311 (*isol, pmr, cmr*)

1-Hydroxy-3,7(14),10-bisabolatrien-8-yn-15-al H-461



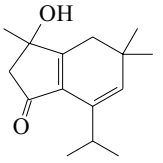
$C_{15}H_{18}O_2$ 230.306

(1α,6β)-*form*
Volvatellin
[234112-45-9]
Constit. of a *Volvatella* sp.
Pale yellow oil. $[\alpha]_D$ -88.3 (c, 0.04 in Et_2O). λ_{max} 229 (ϵ 15630); 263 (ϵ 9430); 277 (ϵ 8700) (EtOH).

Cimino, G. *et al., Curr. Org. Chem.*, 1999, **3**, 327-372
Fontana, A. *et al., J. Nat. Prod.*, 1999, **62**, 931-933 (*isol, pmr, cmr*)
Mancini, I. *et al., Helv. Chim. Acta*, 2000, **83**, 694-701 (*synth*)

9-Hydroxy-1(6),4-brasiladien-7-one H-462

[135448-13-4]

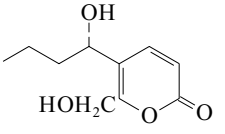


$C_{15}H_{22}O_2$ 234.338
Metab. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ -1 (c, 0.5 in EtOH).

Amico, V. *et al., Phytochemistry*, 1991, **30**, 1921 (*isol, pmr, cmr*)

5-(1-Hydroxybutyl)-6-hydroxymethyl-2*H*-pyran-2-one, 9CI H-463

Taiwapyrone



$C_{10}H_{14}O_4$ 198.218

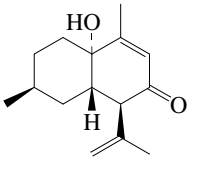
(*S*)-*form* [60031-98-3]
Metab. of *Cercospora taiwanensis* strain 139.35 and the marine-derived *Microsphaeropsis* sp. Stamm 6288.
Oil. $[\alpha]_D^{20}$ -48.5 (c, 0.33 in MeOH). λ_{max} 211 (sh) (log ϵ 3.86); 296 (log ϵ 3.8) (MeOH). λ_{max} 212 (sh) (log ϵ 3.74); 298 (log ϵ 3.71) (MeOH/HCl). λ_{max} 224 (sh) (log ϵ 3.43); 364 (log ϵ 4.18) (MeOH/NaOH).

*1′-Ketone: 5-Butanoyl-6-hydroxymethyl-2*H*-pyran-2-one.* ***Dehydrotaiwapyrone***
$C_{10}H_{12}O_4$ 196.202
Prod. by *Microsphaeropsis* sp. Stamm 6288. Amorph. solid. Mp 134°. λ_{max} 268 (log ϵ 3.83) (MeOH). λ_{max} 277 (log ϵ 3.86) (MeOH/HCl). λ_{max} 264 (log ϵ 3.8) (MeOH/NaOH).

*5ξ,6ξ-Dihydro: 5,6-Dihydro-5-(1-hydroxybutyl)-6-hydroxymethyl-2*H*-pyran-2-one.* ***5,6-Dihydrotaiwapyrone***
$C_{10}H_{16}O_4$ 200.234
Prod. by *Microsphaeropsis* sp. Stamm 6288. Oil. λ_{max} 291 (log ϵ 3.29) (MeOH). λ_{max} 315 (log ϵ 3.39) (MeOH/HCl). λ_{max} 291 (log ϵ 3.67) (MeOH/NaOH).

Camarda, L. *et al., Phytochemistry*, 1976, **15**, 537-539 (*isol, pmr, cmr, abs config*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol, cd, uv, pmr, cmr, ms*)

1-Hydroxy-9,11-cadinadien-8-one H-464



(1α,4β,6β,7β)-*form*

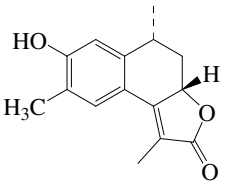
$C_{15}H_{22}O_2$ 234.338

(1α,4β,6β,7β)-*form*
Xenitorin E
[479199-48-9]
Constit. of *Xenia puerto-galerae*.
Oil. $[\alpha]_D^{25}$ -10 (c, 0.18 in $CHCl_3$). λ_{max} 237 (log ϵ 3.6) (MeOH).

(1β,4β,6β,7β)-*form*
Xenitorin F
[479199-49-0]
Constit. of *Xenia puerto-galerae*.

Oil. $[\alpha]_D^{25}$ +65 (c, 0.22 in $CHCl_3$). λ_{max} 239 (log ε 3.9) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1853-1856 (*isol, pmr, cmr*)

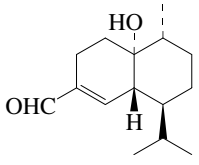
3-Hydroxy-1,3,5,7(11)-cadinatetraen-12,8-olide H-465



$C_{15}H_{16}O_3$ 244.29

(8α,10α)-*form*
*Me ether: 3-Methoxy-1,3,5,7(11)-cadinatetraen-12,8-olide. 4,5-Dihydro-7-methoxy-1,5,8-trimethylnaphtho[2,1-*b*]furan-2(3*aH*)-one, 9CI.* ***Heritonin***
[123514-48-7]
Isol. from *Heritiera littoralis.* Piscicide. Cryst. (C_6H_6/Et_2O). Mp 115-116°. λ_{max} 220; 226; 284; 304 (cyclohexane).
Miles, P.H. *et al., J. Nat. Prod.*, 1989, **52**, 896-898 (*isol, pmr*)
Chavan, S.P. *et al., Chem. Comm.*, 1994, 1101 (*synth*)
Silveira, C.C. *et al., Tet. Lett.*, 2004, **45**, 4077-4080 (*synth*)

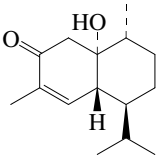
1-Hydroxy-4-cadinen-15-al H-466



$C_{15}H_{24}O_2$ 236.353

(1α,6β,10α)-*form* [785793-98-8]
Constit. of *Dictyopteris divaricata*.
Gum. $[\alpha]_D^{20}$ -33 (c, 0.1 in MeOH).
Song, F. *et al., J. Nat. Prod.*, 2004, **67**, 1644-1649 (*isol, pmr, cmr*)

1-Hydroxy-4-cadinen-3-one H-467

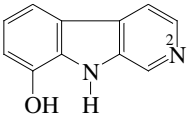


$C_{15}H_{24}O_2$ 236.353

(1α,6β,7β,10α)-*form*
Cubenol-3-one
[162522-29-4]
Constit. of *Dictyopteris delicatula*. Cryst. Mp 98° (subl.). $[\alpha]_D^{25}$ -78.4 (c, 0.55 in $CHCl_3$).
König, G.M. *et al., Magn. Reson. Chem.*, 1995, **33**, 178-183 (*isol, pmr, cmr*)

8-Hydroxy-β-carboline H-468

*9*H*-Pyrido[3,4-*b*]indol-8-ol*
[334709-41-0]



$C_{11}H_8N_2O$ 184.197

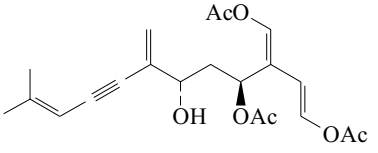
Cryst. (toluene or Me_2CO). Mp 250°.

N^2-Me: 8-Hydroxy-2-methyl-β-carbolinium
[356073-89-7]
$C_{12}H_{11}N_2O^{\oplus}$ 199.232
Quaternary alkaloid from a *Pseudodistoma* sp. Gum. Counterion not specified. λ_{max} 228 (log ε 3.68); 268 (log ε 3.56); 317 (log ε 3.23); 389 (log ε 2.7) (MeOH).

*Me ether: 8-Methoxy-9*H*-pyrido[3,4-*b*]indole, 9CI. 8-Methoxy-β-carboline*
[30684-48-1]
$C_{12}H_{10}N_2O$ 198.224
Cryst. (xylene). Mp 204-205°. λ_{max} 216; 243; 268; 278; 287; 343; 354 (sh) (EtOH).
Ho, B.T. *et al., J. Pharm. Sci.*, 1970, **59**, 1445-1448 (*Me ether, synth*)
Rocco, P. *et al., J. Het. Chem.*, 1995, **32**, 1171-1175 (*synth, ir, pmr*)
Rashid, M.A. *et al., Tetrahedron*, 2001, **57**, 5751-5755 (N^2*-Me, isol*)

6-Hydroxy-$\Delta^{7,(14)}$-caulerpenyne H-469

[149183-81-3]

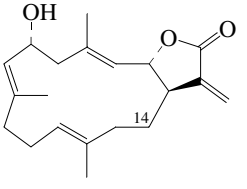


$C_{21}H_{26}O_7$ 390.432
Constit. of *Caulerpa taxifolia*. Mutagen. Oil. $[\alpha]_D^{20}$ -53.7 (c, 0.095 in EtOH). λ_{max} 242 (ε 21500) (EtOH) (Berdy).

[149183-83-5]

Guerriero, A. *et al., Helv. Chim. Acta*, 1993, **76**, 855 (*isol, pmr, cmr*)

6-Hydroxy-3,7,11,15(17)-cembratetraen-16,2-olide H-470



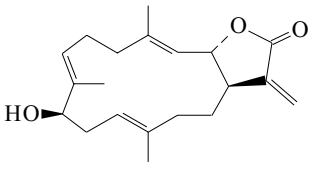
Absolute Configuration

$C_{20}H_{28}O_3$ 316.439

(1*R*,2*S*,3*E*,6*R*,7*E*,11*E*)-*form*
Ac: [314776-57-3]
Constit. of *Clavularia koellikeri*.
Oil. $[\alpha]_D^{25}$ +102.3 (c, 0.13 in $CHCl_3$). λ_{max} 229 (log ε 3.39) (EtOH).

(1*R*,2*S*,3*E*,6*S*,7*E*,11*E*)-*form*
Cytotoxic.
Ac: ***Kericembrenolide A***
[104992-94-1]
$C_{22}H_{30}O_4$ 358.477
Constit. of soft coral *Clavularia koellikeri*. Cytotoxin. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{22}$ -88 ($CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 2306-2309 (*Kericembrenolide A*)
Iwashima, M. *et al., J. Nat. Prod.*, 2000, **63**, 1647-1652 (*Clavularia koellikeri constit*)

9-Hydroxy-3,7,11,15(17)-cembratetraen-16,2-olide H-471

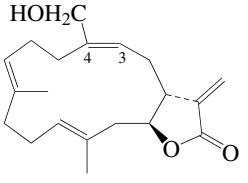


$C_{20}H_{28}O_3$ 316.439

(3*E*,7*E*,9*R*,11*E*)-*form*

Ac: ***Kericembrenolide B***
[104992-93-0]
$C_{22}H_{30}O_4$ 358.477
Constit. of the soft coral *Clavularia koellikeri*. Cytotoxic. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{22}$ +97 ($CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 2306

18-Hydroxy-3,7,11,15(17)-cembratetraen-16,14-olide H-472



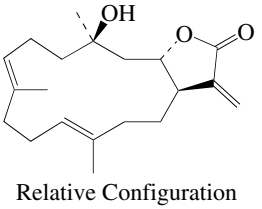
$C_{20}H_{28}O_3$ 316.439

(1*R*,3*E*,7*E*,11*E*,14*S*)-*form* [852469-29-5]
[86302912 (1ξ,3ξ,7ξ,11ξ,14ξ)-*form]*
Constit. of Lobophytum crassum.
Oil.

Ac: [86302-92-3]
$C_{22}H_{30}O_4$ 358.477
From *Lobophytum crassum.* Oil.

*3*R*,4*S*-Epoxide: 3,4-Epoxy-18-hydroxy-7,11,15(17)-cembratrien-16,14-olide.* ***Sinularolide D***
[852469-27-3]
$C_{20}H_{28}O_4$ 332.439
Constit. of *Sinularia gibberosa.* Oil. $[\alpha]_D^{25}$ -31.6 (c, 0.04 in $CHCl_3$).
Kashman, Y. *et al., J.O.C.*, 1981, **46**, 3592-3596 (*Lobophytum crassum constit*)
Kinamoni, Z. *et al., Tetrahedron*, 1983, **39**, 1643-1648 (*Lobophytum crassum constits*)
Li, G. *et al., J. Nat. Prod.*, 2005, **68**, 649-652 (*Sinularolide D*)

4-Hydroxy-7,11,15(17)-cembratrien-16,2-olide H-473

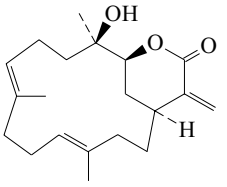


Relative Configuration

$C_{20}H_{30}O_3$ 318.455

(1R*,2S*,4R*,7*E*,11*E*)-*form* [179985-61-6]
Isol. from the soft coral *Sinularia hirta*.
Oil. λ_{max} 213 ($CHCl_3$).
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 815-818 (*isol, uv, ir, pmr, cmr*)

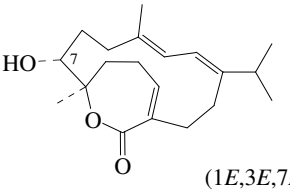
4-Hydroxy-7,11,15(17)-cembratrien-16,3-olide H-474



$C_{20}H_{30}O_3$ 318.455

(1*S*,3*S*,4*R*,7*E*,11*E*)-*form*
14-Deoxycrassin
[148149-82-0]
Constit. of *Pseudoplexaura porosa*.
Oil. $[\alpha]_D^{26}$ +29.6 (c, 0.24 in $CHCl_3$). λ_{max} 220 (ϵ 2500) (MeOH) (Berdy).
Rodríguez, A.D. *et al., Experientia*, 1993, **49**, 179 (*isol, pmr, cmr*)
Li, S.H. *et al., Chin. Chem. Lett.*, 2002, **13**, 820-823 (*synth*)

7-Hydroxy-1,3,11-cembratrien-20,8-olide H-475



(1*E*,3*E*,7*R*,8*S*,11*Z*)-*form*

$C_{20}H_{30}O_3$ 318.455

(1*E*,3*E*,7*R*,8*S*,11*Z*)-*form* [81745-39-3]
Constit. of soft coral *Sarcophyton glaucum*.
Oil. $[\alpha]_D$ +161 (c, 0.5 in $CHCl_3$). λ_{max} 234 (ϵ 5424); 251 (sh) (ϵ 4855); 292 (sh) (ϵ 1301) (EtOH).

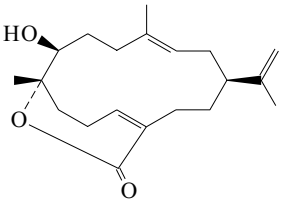
Ac: [81754-67-8]
$C_{22}H_{32}O_4$ 360.492
Constit. of a *Sarcophyton* sp.

7-Ketone: 7-Oxo-1,3,11-cembratrien-20,8-olide. ***Sarcophytolide***†
[81499-72-1]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Sarcophyton glaucum* and *Sarcophyton elegans.* Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +177 (c, 0.1 in $CHCl_3$). $[\alpha]_D$ +201.4 (c, 1.43 in $CHCl_3$). λ_{max} 238 (ϵ 20700) (EtOH) (Berdy).

(1*E*,3*Z*,7*S*,8*S*,11*Z*)-*form* [714252-49-0]
Constit. of a *Sarcophyton* sp.
Oil. $[\alpha]_D^{23}$ +84 (c, 0.2 in CH_2Cl_2). λ_{max} 234 (ϵ 8767); 253 (sh) (ϵ 6261); 290 (sh) (ϵ 2040) (EtOH).

7-Ketone: [714252-50-3]
$C_{20}H_{28}O_3$ 316.439
Constit. of a *Sarcophyton* sp. Oil. $[\alpha]_D^{23}$ +147.9 (c, 0.1 in CH_2Cl_2). λ_{max} 224 (ϵ 12849); 251 (sh) (ϵ 6847); 288 (sh) (ϵ 1313) (EtOH).
Bowden, B.F. *et al., Aust. J. Chem.*, 1982, **35**, 621
Uchio, Y. *et al., Chem. Lett.*, 1983, 613
Gross, H. *et al., Org. Biomol. Chem.*, 2004, **2**, 1133-1138 (*isol, pmr, cmr*)

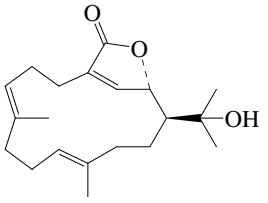
7-Hydroxy-3,11,15-cembratrien-20,8-olide H-476



$C_{20}H_{30}O_3$ 318.455

(3*E*,7*S*,8*S*,11*Z*)-*form* [169211-83-0]
Constit. of *Eunicea tourneforti*.
Glass. $[\alpha]_D^{24}$ +3 (c, 0.1 in $CHCl_3$). $[\alpha]_D$ +196.5 (c, 2.1 in $CHCl_3$).
Govindan, M. *et al., J. Nat. Prod.*, 1995, **58**, 1174-1184 (*isol, pmr, cmr*)
Marville, K.I. *et al., J. Nat. Prod.*, 2003, **66**, 1284-1287 (*isol, pmr, cmr*)

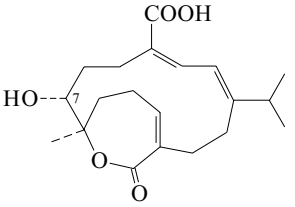
15-Hydroxy-3,7,11-cembratrien-18,2-olide H-477



$C_{20}H_{30}O_3$ 318.455

(1*R*,2*S*,7*E*,11*E*)-*form*
Brassicolide
[249731-33-7]
Constit. of *Nephthea brassica*.
Cryst.
Mp 115-116°. $[\alpha]_D^{25}$ +50.3 (c, 3.7 in $CHCl_3$). λ_{max} 236 (log ϵ 4.1) (MeOH).
Ac: ***Brassicolide acetate***
[249731-34-8]
$C_{22}H_{32}O_4$ 360.492
Constit. of *Nephthea brassica*. Oil. $[\alpha]_D^{25}$ +101 (c, 0.25 in MeOH). λ_{max} 234 (log ϵ 4.4) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 1999, **62**, 1518-1521 (*isol, pmr, cmr, cryst struct*)

7-Hydroxy-1,3,11-cembratrien-20,8-olid-18-oic acid H-478

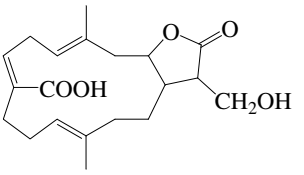


Relative configuration

$C_{20}H_{28}O_5$ 348.438

(1*E*,3*Z*,7*R,8*R**,11*Z*)-*form***
7-Ac, Me ester: ***Emblide***
[77249-87-7]
$C_{23}H_{32}O_6$ 404.502
Constit. of *Sarcophyton glaucum*. Cryst. (MeOH).
Mp 119-120°. $[\alpha]_D^{25}$ +92 (c, 1.3 in CCl_4).
7-Ketone, Me ester: ***Ketoemblide***
[81499-21-0]
$C_{21}H_{28}O_5$ 360.449
Isol. from *Sarcophyton elegans*. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +51.5 (c, 1.7 in $CHCl_3$). λ_{max} 207 (ϵ) (MeOH) (Derep). λ_{max} 284 (ϵ 12000) (EtOH) (Berdy).
Toth, J.A. *et al., Tetrahedron*, 1980, **36**, 1307 (*cryst struct*)
Uchio, Y. *et al., Chem. Lett.*, 1983, 613 (*Ketoemblide*)

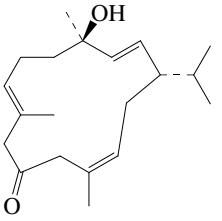
17-Hydroxy-4,7,11-cembratrien-16,2-olid-19-oic acid H-479



$C_{20}H_{28}O_5$ 348.438

17-Me ether, 19-Me ester: [159646-74-9]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Lobophytum strictum*. Cryst. (Me_2CO/hexane).
Mp 119-120°. $[\alpha]_D^{25}$ +78.3 (c, 0.3 in $CHCl_3$). λ_{max} 217 ($CHCl_3$).
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 1165-1169 (*isol, pmr, cmr*)

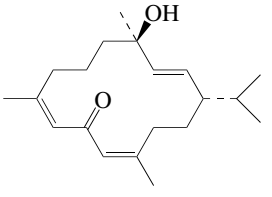
4-Hydroxy-2,7,12-cembratrien-10-one H-480



$C_{20}H_{32}O_2$ 304.472

(1*S*,2*E*,4*R*,7*E*,12*Z*)-*form*
Sartone E
[237755-19-0]
Constit. of a *Sarcophyton* sp.
Oil. $[\alpha]_D$ +50.7 (c, 0.18 in MeOH). λ_{max} 208 (log ϵ 3.58) (MeOH).
Iwagawa, T. *et al., J. Nat. Prod.*, 1999, **62**, 1046-1049 (*isol, pmr, cmr*)

4-Hydroxy-2,8,11-cembratrien-10-one H-481

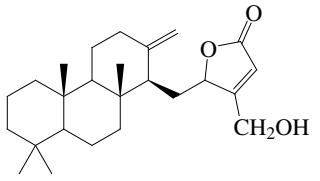


$C_{20}H_{32}O_2$ 304.472

(1*S*,2*E*,4*R*,8*Z*,11*Z*)-*form*
Sartone D
[185117-90-2]
Constit. of *Sarcophyton* sp.
Oil. $[\alpha]_D^{27}$ +39.6 (c, 0.13 in MeOH). λ_{max} 272 (ϵ 7500) (MeOH). λ_{max} 272 (ϵ 7500) (MeOH) (Berdy).
Iwagawa, T. *et al., Bull. Chem. Soc. Jpn.*, 1996, **69**, 3543-3549 (*isol, pmr, cmr*)

25-Hydroxy-13(24),17-cheilanthadien-19,16-olide H-482

[334491-26-8]

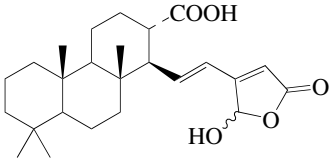


$C_{25}H_{38}O_3$ 386.573

Constit. of an *Ircinia* sponge. Amorph. solid. $[\alpha]_D^{25}$ -8.53 (c, 0.23 in $CHCl_3$). λ_{max} 210 (log ϵ 3.47) (EtOH).

Buchanan, M.S. *et al., J. Nat. Prod.*, 2001, **64**, 300-303 (*isol, pmr, cmr*)

25-Hydroxy-15,17-cheilanthadien-19,25-olid-24-oic acid H-483



$C_{25}H_{36}O_5$ 416.556

(15*E*,25ξ)-*form*

Petrosaspongiolide R

[209408-76-4]

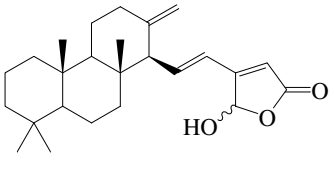
Constit. of *Petrosaspongia nigra*.

Amorph. solid. $[\alpha]_D$ -15.6 (c, 0.003 in MeOH). λ_{max} 264 (log ϵ 4.15) (MeOH). λ_{max} 264 (ϵ 14125) (MeOH) (Berdy).

Randazzo, A. *et al., J. Nat. Prod.*, 1998, **61**, 571-575 (*isol, pmr, cmr*)

25-Hydroxy-13(24),15,17-cheilanthatrien-19,25-olide H-484

[334491-25-7]

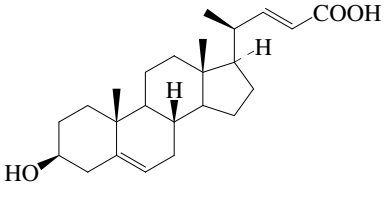


$C_{25}H_{36}O_3$ 384.558

Constit. of an *Ircinia* sponge. Amorph. solid. $[\alpha]_D$ -36.09 (c, 0.53 in $CHCl_3$). λ_{max} 202 (log ϵ 3.56); 264 (log ϵ 3.79) (EtOH).

Buchanan, M.S. *et al., J. Nat. Prod.*, 2001, **64**, 300-303 (*isol, pmr, cmr*)
Basabe, P. *et al., J.O.C.*, 2005, **70**, 9480-9485 (*synth*)

3-Hydroxychola-5,22-dien-24-oic acid H-485



$C_{24}H_{36}O_3$ 372.547

(3β,20*R*,22*E*)-*form*

Me ester:
$C_{25}H_{38}O_3$ 386.573
Constit. of *Ptilosarcus gurneyi*.

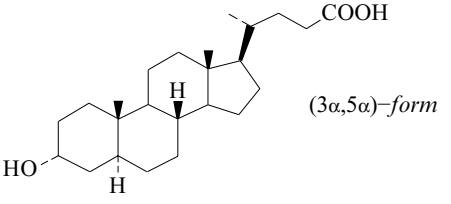
3-Ac, Me ester: [63814-49-3]
$C_{27}H_{40}O_4$ 428.611
Cryst. (MeOH). Mp 151-151.5°. $[\alpha]_D$ -85 (c, 0.14 in $CHCl_3$). λ_{max} 218 (ϵ 13000) (EtOH).

Vanderah, D.J. *et al., J.O.C.*, 1978, **43**, 1442-1448 (*isol, pmr, synth, abs config*)

3-Hydroxycholan-24-oic acid H-486

3-Hydroxycholanic acid

[35498-67-0]



(3α,5α)–*form*

$C_{24}H_{40}O_3$ 376.578

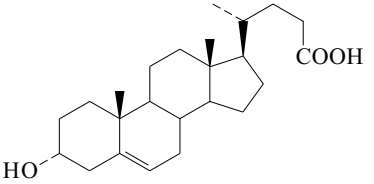
(3β,5α,20*S*)-*form*

Me ester: [63814-53-9]
Constit. of *Ptilosarcus gurneyi*.

Vanderah, D.J. *et al., J.O.C.*, 1978, **43**, 1442-1448 (*Ptilosarcus gurneyi constit, synth, abs config*)

3-Hydroxychol-5-en-24-oic acid H-487

3-Hydroxychol-5-enic acid



$C_{24}H_{38}O_3$ 374.562

3α-*form* [474-57-7]
Cryst. (MeOH). Mp 199-200°. $[\alpha]_D^{21}$ -25.5 (c, 1 in $CHCl_3$).

Me ester: [14956-24-2]
$C_{25}H_{40}O_3$ 388.589
Mp 127°. $[\alpha]_D^{21}$ -30 (c, 1 in $CHCl_3$).

Me ester, Ac: [3633-72-5]
$C_{27}H_{42}O_4$ 430.626
Cryst. (MeOH). Mp 109-111°. $[\alpha]_D^{21}$ -18.5 (c, 1 in $CHCl_3$).

3β-*form* [5255-17-4]
Needles (EtOAc or MeOH aq.). Mp 240-242° (218-221°). $[\alpha]_D^{20}$ -36 (c, 0.116 in EtOH).

Me ester: [20231-57-6]
Needles (CH_2Cl_2/hexane). Mp 147-148.5°. $[\alpha]_D$ -39.6 (c, 1 in $CHCl_3$).

Me ester, Ac: [31823-53-7]
Mp 159-161°. $[\alpha]_D$ -45.2 (c, 0.55 in $CHCl_3$).

3-Ac: [19462-13-6]
$C_{26}H_{40}O_4$ 416.6
Needles (MeOH). Mp 95-97°. $[\alpha]_D^{20}$ -42.9 (c, 0.238 in $CHCl_3$).

Hydrazide: Mp 220-222°.

(3β,20*S*)-*form*

Me ester: [63865-06-5]
Isol. from *Ptilosarcus gurneyi*.

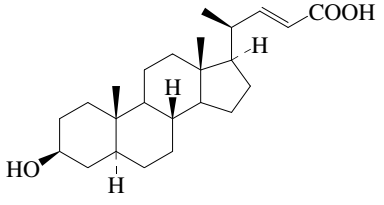
Me ester, Ac: [63814-50-6]
Cryst. (MeOH). Mp 119-120°. $[\alpha]_D$ -54 (c, 0.9 in $CHCl_3$).

3-O-β-D-Glucopyranoside, Me ester:
$C_{31}H_{50}O_8$ 550.731
Isol. from *Sparganium stoloniferum*. Cryst. Mp 201-205°.

3-O-(α-L-Rhamnopyranosyl-β-D-glucuronopyranoside), Me ester:
$C_{37}H_{58}O_{13}$ 710.857
Isol. from *Sparganium stoloniferum*. Cryst. Mp 215-219°.

Wallis, E.S. *et al., J.A.C.S.*, 1935, **57**, 1504 (*synth*)
Ruzicka, L. *et al., Helv. Chim. Acta*, 1942, **25**, 435 (*synth*)
Bergstroem, S. *et al., Acta Chem. Scand.*, 1955, **9**, 699 (*synth*)
Bharucha, K.R. *et al., Can. J. Chem.*, 1956, **34**, 982 (*synth*)
Lehmann, G. *et al., Annalen*, 1967, **703**, 176 (*synth, 3α-form*)
Gottarelli, G. *et al., J.C.S.(C)*, 1967, 1370 (*ord*)
Burton, G. *et al., J. Steroid Biochem.*, 1977, **8**, 69 (*synth*)
Vanderah, D.J. *et al., J.O.C.*, 1978, **43**, 1442 (*isol, synth, epimer*)
Shaw, R. *et al., J. Chromatogr.*, 1980, **202**, 347 (*hplc*)
Lin, Y.Y. *et al., Lipids*, 1980, **15**, 756 (*ms*)
Javitt, N.B. *et al., Falk Symp.*, 1981, **29**, 93 (*rev, metab*)
Fukumoto, K. *et al., Tetrahedron*, 1982, **38**, 3701 (*synth*)
Byon, C.Y. *et al., J. Labelled Compd. Radiopharm.*, 1984, **21**, 65 (*synth*)
Miyamoto, K. *et al., Synth. Commun.*, 1986, **16**, 513 (*synth*)
Iida, T. *et al., Magn. Reson. Chem.*, 1993, **31**, 421 (*cmr*)
Zhang, W. *et al., Zhongcaoyao*, 1996, **27**, 643; *CA*, **126**, 197396h (*glycosides*)

3-Hydroxychol-22-en-24-oic acid H-488



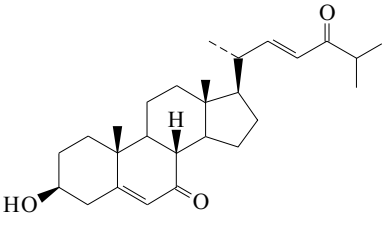
$C_{24}H_{38}O_3$ 374.562

(3β,5α,20*R*,22*E*)-*form*
Me ester:
$C_{25}H_{40}O_3$ 388.589
Constit. of *Ptilosarcus gurneyi*.

3-Ac, Me ester: [65166-02-1]
$C_{27}H_{42}O_4$ 430.626
Cryst. (MeOH). Mp 122-123°. $[\alpha]_D$ +18 (c, 0.57 in $CHCl_3$). λ_{max} 219 (ε 6500) (EtOH).

Vanderah, D.J. *et al., J.O.C.*, 1978, **43**, 1442-1448 (*isol, pmr, synth, abs config*)

3-Hydroxycholesta-5,22-diene-7,24-dione H-489

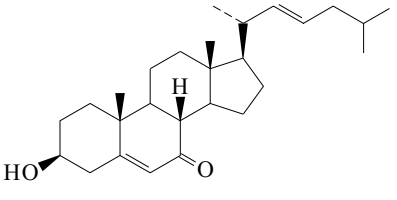


$C_{27}H_{40}O_3$ 412.611

(3β,22*E*)-*form* [147641-71-2]
Constit. of *Stelodoryx chlorophylla*. $[\alpha]_D$ -40 (c, 0.2 in $CHCl_3$).

De Riccardis, F. *et al., J. Nat. Prod.*, 1993, **56**, 282 (*isol, pmr, ms*)

3-Hydroxycholesta-5,22-dien-7-one H-490

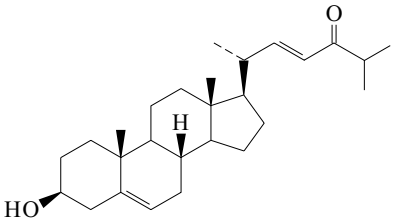


$C_{27}H_{42}O_2$ 398.628

(3β,22*E*)-*form* [118964-36-6]
Constit. of *Calliblepharis lanceolata*, *Laurencia pinnatifida* and *Lithophyllum incrustans*. Isol. from *Cliona capiosa* and *Stelodoryx chlorophylla*.

Quiñoa, E. *et al., An. Quim., Ser. C*, 1988, **84**, 267-269 (*isol, pmr*)
Notaro, G. *et al., J. Nat. Prod.*, 1992, **55**, 1588-1594 (*isol, pmr, ms*)
De Riccardis, F. *et al., J. Nat. Prod.*, 1993, **56**, 282-287 (*Stelodoryx, isol*)

3-Hydroxycholesta-5,22-dien-24-one H-491

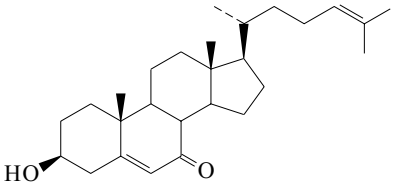


$C_{27}H_{42}O_2$ 398.628

3β-*form* [89495-47-6]
Constit. of a sponge, *Hyrtios* sp.

Koch, P. *et al., Helv. Chim. Acta*, 1983, **66**, 2431

3-Hydroxycholesta-5,24-dien-7-one H-492



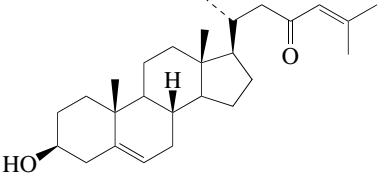
$C_{27}H_{42}O_2$ 398.628

3β-*form*
7-Oxodesmosterol
[64907-26-2]
Constit. of the red alga *Palmaria palmata*.
Cryst. (MeOH).
Mp 155-156°.

Ac: [64907-24-0]
$C_{29}H_{44}O_3$ 440.665
Mp 145-146°. $[\alpha]_D$ -107 (c, 1.4 in $CHCl_3$).

Nagano, H. *et al., J. Chem. Res., Synop.*, 1977, 218-219 (*synth, ir, Raman, ms*)
Ma, Y.-C. *et al., Bot. Mar.*, 1995, **38**, 133 (*isol, pmr, cmr, ms*)

3-Hydroxycholesta-5,24-dien-23-one H-493



$C_{27}H_{42}O_2$ 398.628

3β-*form* [201800-61-5]
Constit. of *Gersemia fruticosa*. Apoptosis inducer. Plates.
Mp 103-104°. $[\alpha]_D$ +12.8 (c, 1.9 in MeOH). λ_{max} 237 (EtOH). λ_{max} 237 (MeOH) (Berdy).

Koljak, R. *et al., Tetrahedron*, 1998, **54**, 179-186 (*isol, pmr, cmr*)

3-Hydroxycholesta-5,25-dien-24-one H-494

$C_{27}H_{42}O_2$ 398.628

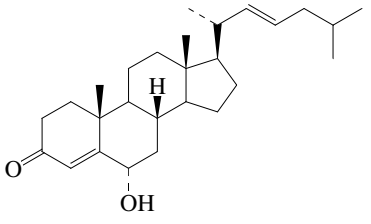
3β-*form* [96886-12-3]
Constit. of *Haliclona oculata* and *Haliclona chilensis*.
Findlay, J.A. *et al., Can. J. Chem.*, 1985, **63**, 2406 (*isol*)
Seldes, A.M. *et al., Experientia*, 1985, **41**, 34 (*isol*)

3-Hydroxycholesta-8,14-dien-23-one H-495

$C_{27}H_{42}O_2$ 398.628

(3β,5α)-*form* [68654-93-3]
Constit. of *Echinaster sepositus*.
Cryst. (MeOH).
Mp 96-98°. $[\alpha]_D$ -2.3 (c, 1 in $CHCl_3$).
Minale, L. *et al., Tet. Lett.*, 1978, 2609; 1979, 645 (*isol, cmr*)

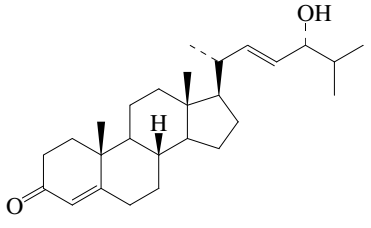
6-Hydroxycholesta-4,22-dien-3-one H-496



$C_{27}H_{42}O_2$ 398.628

(6α,22*E*)-*form* [452082-60-9]
Constit. of *Hypnea musciformis*.
Bultel-Poncé, V. *et al., Bioorg. Med. Chem. Lett.*, 2002, **12**, 1715-1718 (*isol, pmr, cmr*)

24-Hydroxycholesta-4,22-dien-3-one H-497



$C_{27}H_{42}O_2$ 398.628

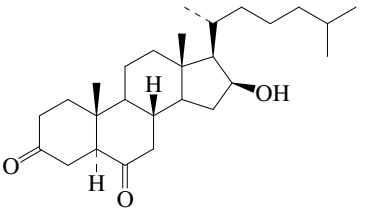
(22*E*,24*R*)-*form* [745075-24-5]
Constit. of *Dasystenella acanthina*.
Amorph. powder. $[\alpha]_D^{25}$ +47.6 (c, 0.2 in $CHCl_3$). λ_{max} 240 (ϵ 13200) (MeOH).
Mellado, G.G. *et al., Steroids*, 2004, **69**, 291-299 (*isol, pmr, cmr*)

11-Hydroxycholestane-3,6-dione H-498

$C_{27}H_{44}O_3$ 416.643

(5α,11α)-*form* [124727-07-7]
Constit. of *Acanthophora spicifera*.
Cryst. (MeOH).
Mp 145°. $[\alpha]_D^{25}$ -11.1. Genus name given as Acantophora.
Prakash, O. *et al., J. Nat. Prod.*, 1989, **52**, 686-692 (*isol, cmr, pmr*)

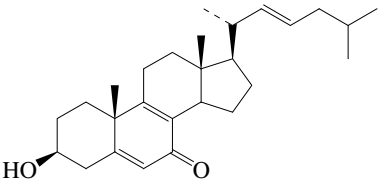
16-Hydroxycholestane-3,6-dione H-499



$C_{27}H_{44}O_3$ 416.643

(5α,16β)-*form* [318294-27-8]
Constit. of *Jania rubens*. Cytotoxic agent. Powder.
Mp 125-126°. $[\alpha]_D$ -2 (c, 0.1 in CH_2Cl_2).
Ktari, L. *et al., Bioorg. Med. Chem. Lett.*, 2000, **10**, 2563-2565 (*isol, pmr, cmr*)
Denancé, M. *et al., Steroids*, 2006, **71**, 599-602 (*synth*)

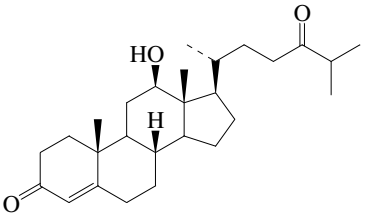
3-Hydroxycholesta-5,8,22-trien-7-one H-500



$C_{27}H_{40}O_2$ 396.612

(3β,22*E*)-*form* [121714-74-7]
Isol. from the Mediterranean sponge *Clathrina clathrus* and from *Ircinia fasciculata*. λ_{max} 246 (ϵ 14200); 322 (ϵ 98) (no solvent reported).
Aiello, A. *et al., Steroids*, 1988, **52**, 533-542 (*isol, ir, pmr, ms, struct*)

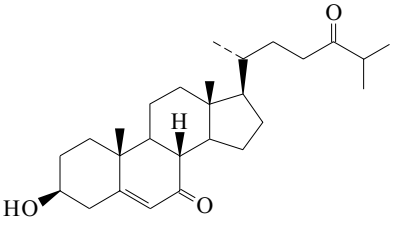
12-Hydroxycholest-4-ene-3,24-dione H-501



$C_{27}H_{42}O_3$ 414.627

12β-*form*
12-Ac: [745075-26-7]
$C_{29}H_{44}O_4$ 456.664
Constit. of *Dasystenella acanthina*. Amorph. powder. $[\alpha]_D^{25}$ +68.7 (c, 0.1 in $CHCl_3$). λ_{max} 239 (ϵ 9380) (MeOH).
Mellado, G.G. *et al., Steroids*, 2004, **69**, 291-299 (*isol, pmr, cmr*)

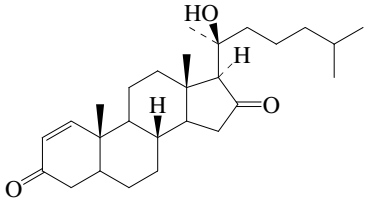
3-Hydroxycholest-5-ene-7,24-dione H-502



$C_{27}H_{42}O_3$ 414.627

3β-*form* [147641-72-3]
Constit. of *Stelodoryx chlorophylla*.
$[\alpha]_D$ -27.5 (c, 0.1 in $CHCl_3$).
De Riccardis, F. *et al., J. Nat. Prod.*, 1993, **56**, 282 (*isol, pmr, ms*)

20-Hydroxycholest-1-ene-3,16-dione H-503



$C_{27}H_{42}O_3$ 414.627

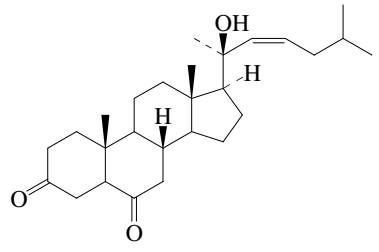
(20*S*)-*form* [257904-95-3]
Constit. of *Leptogorgia sarmentosa*.
Solid. $[\alpha]_D$ -48.3 (c, 0.06 in $CHCl_3$). λ_{max} 228 (ϵ 4900) (MeOH).
Garrido, L. *et al., Steroids*, 2000, **65**, 85-88 (*isol, pmr, cmr*)

20-Hydroxycholest-1-ene-7,11-dione H-504

$C_{27}H_{42}O_3$ 414.627

(5β,20ξ)-*form*
Constit. of *Hypnea musciformis*.
Babu, J.M. *et al., Phytochemistry*, 1990, **29**, 2029 (*isol, pmr, cmr, ms*)

20-Hydroxycholest-22-ene-3,6-dione H-505



$C_{27}H_{42}O_3$ 414.627

(5α,20*S*,22*Z*)-*form* [452082-59-6]
Constit. of *Hypnea musciformis*.
Powder. $[\alpha]_D$ +17 (c, 0.09 in CH_2Cl_2).
Bultel-Poncé, V. *et al., Bioorg. Med. Chem. Lett.*, 2002, **12**, 1715-1718 (*isol, pmr, cmr*)

3-Hydroxycholest-5-en-7-one H-506

[600-85-1]

$C_{27}H_{44}O_2$ 400.643

3α-*form* [59042-88-5]
Mp 169-171°. $[\alpha]_D^{20}$ -90 ($CHCl_3$).

3β-*form*
7-Oxocholesterol
[566-28-9]
Constit. of *Cliona copiosa* and *Damiriana hawaiiana*. Shows antitumour activity. Cryst. ($CHCl_3$/Et_2O).
Mp 157° and 170° (double Mp). $[\alpha]_D$ -108 (c, 0.9 in $CHCl_3$).
▶FZ8708000
3-Sulfate: ***3-Sulfooxycholest-5-en-7-one***
[53216-02-7]
$C_{27}H_{44}O_5S$ 480.708
Constit. of *Leptasterias alaskensis asiatica* and *Leptasterias fisheri*.

E-*Oxime:* [31220-44-7]
$C_{27}H_{45}NO_2$ 415.658
Cryst. (MeOH). Mp 239-241°. $[\alpha]_D$ -204 (c, 1.0 in $CHCl_3$).
2,4-Dinitrophenylhydrazone: Mp 246-247°. $[\alpha]_D$ -600 ($CHCl_3$).
Ac: [809-51-8]
$C_{29}H_{46}O_3$ 442.681
Cryst. (Me_2CO). Mp 156-158°. $[\alpha]_D$ -96 (c, 1.0 in $CHCl_3$).
Me ether: 3-Methoxycholest-5-en-7-one
[41336-65-6]
$C_{28}H_{46}O_2$ 414.67
Cryst. (Me_2CO). Mp 121-123°.

[66899-84-1]

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 574B (*nmr*)
Windaus, A. *et al., Annalen*, 1940, **543**, 240
Oppenauer, R.V. *et al., An. Quim.*, 1949, **37**, 246
Fieser, L.F. *et al., J.A.C.S.*, 1949, **71**, 2226
Milburn, A.H. *et al., J.C.S.*, 1956, 1740 (*synth, 3β-form*)
Shoppee, C.W. *et al., J.C.S.(C)*, 1968, 981 (*synth, uv, ir, 3β-form*)
Chicoye, E. *et al., Lipids*, 1968, **3**, 551 (*synth, 3β-form*)
Matkovics, B. *et al., Acta Chim. Acad. Sci. Hung.*, 1970, **66**, 333 (*synth, ir, 3β-form*)
Smith, L.L. *et al., Steroids*, 1973, **22**, 627 (*synth, uv, ir, 3β-form*)
Kolek, T. *et al., Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1975, **23**, 963 (*synth, ir, 3α-form*)
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476 (*isol, Damiriana*)
Dayal, B. *et al., Steroids*, 1980, **35**, 81 (*cd, 3β-form*)
Aringer, L. *et al., Biomed. Mass Spectrom.*, 1981, **8**, 183 (*ms*)
Suginome, H. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 517 (*synth, pmr, 3β-form*)
Parish, E.J. *et al., J.O.C.*, 1983, **48**, 4766 (*synth, uv, ir, pmr, ms, 3β-form*)
Kumar, V. *et al., Synth. Commun.*, 1987, **17**, 1279 (*synth, 3β-form, derivs*)
Notaro, G. *et al., J. Nat. Prod.*, 1992, **55**, 1588 (*isol, pmr, cmr, ms*)
Kapustina, I.I. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2001, **37**, 515-519 (*3-sulfate*)
Zhang, Q. *et al., CA*, **127**, 117125b (*3β-form, activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ONO000

3-Hydroxycholest-5-en-24-one, 9CI H-507

[17752-17-9]

$C_{27}H_{44}O_2$ 400.643

3β-*form*
24-Oxocholesterol
[17752-16-8]
Isol. from various plants and animals incl. marine organisms, e.g. the sponge *Damiriana hawaiiana*.
Needles (MeOH).
Mp 138-139°. $[\alpha]_D^{25}$ -37.4 (c, 1.23 in $CHCl_3$).
2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 147-148°.
Ac: [20981-59-3]
Cryst. (MeOH). Mp 115-116° and 128° (double Mp). $[\alpha]_D^{24}$ -40 (c, 0.3 in $CHCl_3$).
Me ether: 3-Methoxycholest-5-en-24-one
[58497-29-3]
Cryst. (MeOH). Mp 129-130°. $[\alpha]_D^{20}$ -45.4 (c, 1.2 in $CHCl_3$).
Vinyl enol ether (23Z-): 24-Vinyloxycholesta-5,23-dien-3-ol
[99499-81-7]
$C_{29}H_{46}O_2$ 426.681
Constit. of brown alga *Sargassum thumbergii*.
Riegel, B. *et al., J.A.C.S.*, 1944, **66**, 723 (*synth*)
Hey, D.H. *et al., J.C.S.*, 1950, 2881 (*synth*)
Bergmann, W. *et al., Annalen*, 1957, **603**, 36 (*synth, ir*)
Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095 (*synth, deriv*)
Ochi, K. *et al., Steroids*, 1977, **30**, 795 (*synth*)
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476 (*isol, sponge*)
Aringer, L. *et al., Biomed. Mass Spectrom.*, 1981, **8**, 183 (*synth, ms*)
Koch, P. *et al., Bull. Soc. Chim. Fr.*, 1983, 189 (*synth*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1985, **33**, 4012-4013 (*vinyl enol ether*)

6-Hydroxycholest-4-en-3-one, 9CI H-508

$C_{27}H_{44}O_2$ 400.643

6α-*form* [570-90-1]
Constit. of *Hypnea musciformis*.
Needles (MeOH).
Mp 163.5-164°. $[\alpha]_D^{14}$ +80 (c, 1.00 in $CHCl_3$). Genus name given as Hypnaea.

Ac: [18883-26-6]
$C_{29}H_{46}O_3$ 442.681
Mp 105-106°.

Me ether: 6α-Methoxycholest-4-en-3-one
$C_{28}H_{46}O_2$ 414.67
Cryst. (MeOH). Mp 94°. $[\alpha]_D$ +59 (c, 0.37 in $CHCl_3$).

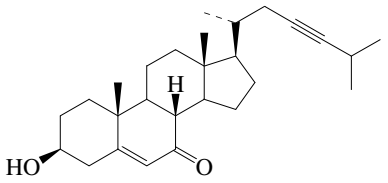
6β-*form* [570-89-8]
Constit. of *Iotrochota birotulata*.
Needles (MeOH).
Mp 194-195°. $[\alpha]_D^{22}$ +31.8 (c, 0.22 in $CHCl_3$). Genus name given, apparently incorrectly, as Iotrichoto.

Ac: [2326-51-4]
Needles (MeOH). Mp 103.5-104.5°.

Me ether: 6β-Methoxycholest-4-en-3-one
[13163-81-0]
Cryst. (MeOH). Mp 115-116°. $[\alpha]_D$ +44 (c, 0.90 in $CHCl_3$).

Djerassi, C. *et al., J.A.C.S.*, 1956, **78**, 6377 (*ord*)
Morita, K. *et al., Bull. Chem. Soc. Jpn.*, 1959, **32**, 227 (*synth*)
Miyake, A. *et al., J.C.S. Perkin 1*, 1972, 663 (*synth, uv, ir, pmr*)
Houminer, Y. *et al., J.C.S. Perkin 1*, 1975, 1663 (*synth, uv, ir, pmr*)
Aringer, L. *et al., Biomed. Mass Spectrom.*, 1981, **8**, 183 (*ms*)
Akihisa, T. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 680 (*pmr*)
Sakamaki, H. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 5023 (*synth*)
Bultel-Poncé, V. *et al., Bioorg. Med. Chem. Lett.*, 2002, **12**, 1715-1718 (*isol, pmr, cmr*)
Li, L.-Y. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 115-120 (*Iotrochoto birotulata constit*)

3-Hydroxycholest-5-en-23-yn-7-one H-509



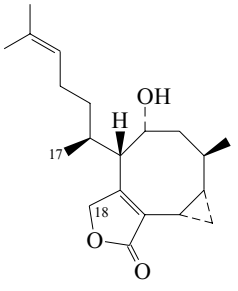
$C_{27}H_{40}O_2$ 396.612

3β-*form*
Gelliusterol C
[351198-08-8]
Constit. of a *Gellius* sponge.
$[\alpha]_D$ -36.6 (c, 0.28 in MeOH). λ_{max} 238 (ε 4767) (MeOH).

Gallimore, W.A. *et al., J. Nat. Prod.*, 2001, **64**, 741-744 (*isol, pmr, cmr*)

4-Hydroxycrenulide H-510

4-Hydroxy-1,13-crenuladien-19,18-olide. 9-Hydroxycrenulide. Crenulide (incorr.)
[83845-31-2]



$C_{20}H_{30}O_3$ 318.455

Incorrectly called Crenulide in CAS. The abs. config. appears to be as shown. This is as given in the more recent papers including chiral syntheses, but is not explicitly stated. Constit. of *Aplysia vaccaria* and *Dictyota volubilis*. Oil. $[\alpha]_D$ +17.6 (c, 1.64 in $CHCl_3$). λ_{max} 209 (ε 4310); 231 (ε 5790) (MeOH) (Derep).

4-Ac: ***4-Acetoxycrenulide***. *Acetoxycrenulatin. Crenullactone*
[65043-52-9]
[173658-98-5]
$C_{22}H_{32}O_4$ 360.492
Constit. of *Dictyota crenulata*, *Dictyota dichotoma*, *Aplysia vaccaria* and *Glossophora kunthii*. Ichthyotoxic, vermifuge. Oil. Sol. MeOH. $[\alpha]_D$ +13 (c, 0.67 in $CHCl_3$). λ_{max} 265 (ε 6500) (EtOH/NaOH) (Derep). λ_{max} 208 (ε 6610); 225 (ε 6450) (EtOH) (Derep). λ_{max} 227 (ε 12500) (MeOH) (Berdy). λ_{max} 208 (ε 5162); 227 (ε 6195) (EtOH) (Berdy).

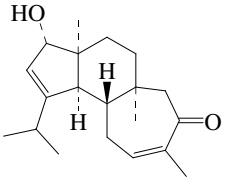
18α-Hydroxy: ***4,18-Dihydroxycrenulide***. *4,18-Dihydroxy-1,13-crenuladien-19,18-olide*
[85443-36-3]
$C_{20}H_{30}O_4$ 334.455
Constit. of *Aplysia vaccaria*. Cryst. (Et_2O).
Mp 114-115°. $[\alpha]_D$ +25.9 (c, 1.19 in $CHCl_3$). λ_{max} (MeOH/NaOH) (Derep). λ_{max} 209 (ε 4310); 231 (ε 5790) (MeOH) (Derep).

18α-Hydroxy, 4-Ac: ***4-Acetoxy-18-hydroxycrenulide***
[85443-37-4]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Aplysia vaccaria*. Oil. $[\alpha]_D$ +26.53 (c, 1.93 in $CHCl_3$). λ_{max} 265 (ε 6500) (EtOH/NaOH) (Derep). λ_{max} 208 (ε 6610); 225 (ε 6450) (EtOH) (Derep).

17-Acetoxy: ***17-Acetoxy-4-hydroxycrenulide***
[133585-92-9]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Dictyota divaricata*. Oil. $[\alpha]_D$ +45 (c, 0.06 in $CHCl_3$). λ_{max} 229 (ε 12200) (MeOH) (Berdy).

Sun, H.H. *et al., J.O.C.*, 1983, **48**, 1903-1906 (*isol, struct*)
Midland, S.L. *et al., J.O.C.*, 1983, **48**, 1906-1909 (*isol, struct*)
König, G.M. *et al., Tetrahedron*, 1991, **47**, 1399-1410 (*17-acetoxy*)
Guella, G. *et al., Chem. Comm.*, 1993, 1539 (*synth*)
Wang, T.-Z. *et al., J.A.C.S.*, 1996, **118**, 1309-1318 (*synth*)

1-Hydroxy-2,11-cyathadien-13-one H-511

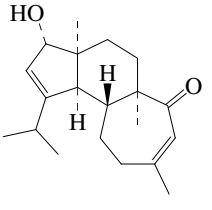


$C_{20}H_{30}O_2$ 302.456

(1α,9α)-*form*
Cyanthiwigin Y
[481643-60-1]
Constit. of *Myrmekioderma styx*.
Gum. $[\alpha]_D$ +24 (c, 0.1 in MeOH). λ_{max} 238 (ε 6914) (MeOH).

Peng, J. *et al., Tetrahedron*, 2002, **58**, 7809-7819 (*isol, pmr, cmr*)

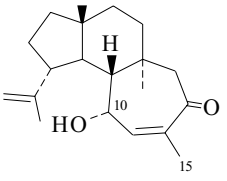
1-Hydroxy-2,12-cyathadien-14-one H-512



$C_{20}H_{30}O_2$ 302.456

(1α,9α)-*form*
Cyanthiwigin Z
[481643-61-2]
Constit. of *Myrmekioderma styx*.
Gum. $[\alpha]_D$ -160 (c, 0.03 in MeOH). λ_{max} 238 (ϵ 13828) (MeOH).
Peng, J. *et al., Tetrahedron*, 2002, **58**, 7809-7819 (*isol, pmr, cmr*)

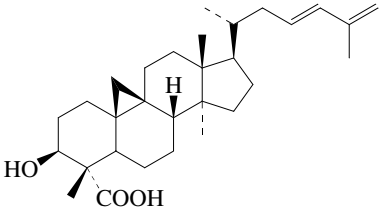
10-Hydroxy-11-cyathen-13-one H-513



$C_{20}H_{30}O_2$ 302.456

10α-*form* [99235-04-8]
Constit. of a *Higginsia* sp.
Oil. $[\alpha]_D$ +35 (c, 4.2 in $CHCl_3$).
15-Hydroxy: ***10α,15-Dihydroxy-11-cyathen-13-one***
[99235-02-6]
$C_{20}H_{30}O_3$ 318.455
From a *Higginsia* sp. Cryst. (EtOAc).
Mp 104-105°. $[\alpha]_D$ +58.8 (c, 1.1 in $CHCl_3$).
15-Acetoxy: ***15-Acetoxy-10α-hydroxy-11-cyathen-13-one***
[99235-03-7]
$C_{22}H_{32}O_4$ 360.492
From a *Higginsia* sp. Oil. $[\alpha]_D$ +35 (c, 4.2 in $CHCl_3$).
Cassidy, M.P. *et al., Aust. J. Chem.*, 1985, **38**, 1187

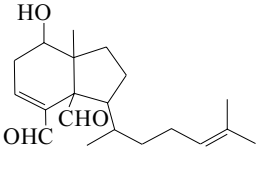
3-Hydroxycycloarta-23,25-dien-28-oic acid H-514



$C_{30}H_{46}O_3$ 454.692

(3β,23*E*)-*form*
Me ester: ***Galaxaurol C***
[859501-79-4]
$C_{31}H_{48}O_3$ 468.718
Constit. of a *Galaxaura* red alga sp. Powder.
Mp 157-158°. $[\alpha]_D^{25}$ +32.8 (c, 0.024 in $CHCl_3$). λ_{max} 248 (log ϵ 2.5) ($CHCl_3$).
Zhang, W.-H. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 59-65 (*Galaxaurol C*)

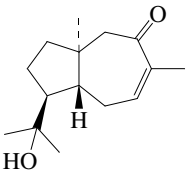
7-Hydroxy-2,6-cyclo-9,13-xenicadiene-18,19-dial H-515



$C_{20}H_{30}O_3$ 318.455
Constit. of *Dictyota dichotoma*. Oil.

Ac:
$C_{22}H_{32}O_4$ 360.492
Constit. of *Dictyota dichotoma*. Oil.
Blount, J.F. *et al., Aust. J. Chem.*, 1982, **35**, 145

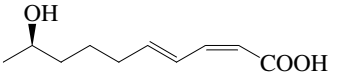
11-Hydroxy-7-daucen-9-one H-516



$C_{15}H_{24}O_2$ 236.353

(1α,4β,5β)-*form*
Styxone B
[498552-76-4]
Constit. of *Myrmekioderma styx*.
Oil. $[\alpha]_D$ +48 (c, 0.1 in MeOH). λ_{max} 238 (ϵ 4289) (no solvent reported).
Peng, J. *et al., Tet. Lett.*, 2002, **43**, 9699-9702 (*isol, pmr, cmr*)

9-Hydroxy-2,4-decadienoic acid H-517

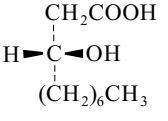


$C_{10}H_{16}O_3$ 184.235

(2*Z*,4*E*,9*R*)-*form*
Et ester: ***Modiolin***
$C_{12}H_{20}O_3$ 212.288
Isol. from the fungus *Paraphaeosphaeria* sp. (N-119) obt. from the mussel *Modiolus auriculatus*. Oil. λ_{max} 260 (ϵ 17500) (MeOH).
Tsuda, M. *et al., J. Nat. Prod.*, 2003, **66**, 412-415 (*isol, pmr, cmr*)

3-Hydroxydecanoic acid H-518

Myrmicacin
[14292-26-3]
[33044-91-6]



(*R*)–*form*

$C_{10}H_{20}O_3$ 188.266

(R)-form [19525-80-5]
Constit. of the secretion of the metathoracic glands of Myrmicine ants. Occurs in bacterial lipids, residue present in the antibiotic viscosin.
Mp 48-49°. $[\alpha]_D^{20}$ -20.8 (c, 1 in $CHCl_3$).
Me ester: [56618-58-7]
$C_{11}H_{22}O_3$ 202.293
Oil. $[\alpha]_D^{20}$ -4.5 (neat).
O-*[α-L-Rhamnopyranosyl-(1→2)-α-L-rhamnopyranoside]:*
[95932-09-5]
$C_{22}H_{40}O_{11}$ 480.551
Prod. by *Pseudomonas aeruginosa*. Solid. $[\alpha]_D$ -44.6 (c, 1 in $CHCl_3$).
O-*[3-(β-D-Glucopyranosyloxy)tetradecanoyl]:* ***Rubiwettin RG1***
[129039-46-9]
$C_{30}H_{56}O_{10}$ 576.766
Prod. by *Serratia rubidaea*. Biosurfactant.

(S)-form [19526-23-9]
Me ester: $Bp_{0.05}$ 74-76°. $[\alpha]_D^{20}$ +25.8 (c, 1 in cyclohexane).

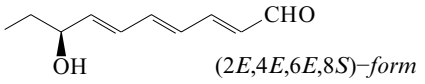
(±)-*form* [5561-87-5]
Mp 54.6-56.6°.

Succinimide: See 1-[(3-Hydroxy-1-oxodecyl)oxy]-2,5-pyrrolidinedione in *The Combined Chemical Dictionary.*

Skogh, M. *et al., Acta Chem. Scand.*, 1952, **6**, 809-817 (*synth*)
Serck-Hanssen, K. *et al., Acta Chem. Scand.*, 1955, **9**, 866 (*synth*)
Bishop, D.G. *et al., Biochem. Biophys. Res. Commun.*, 1962, **7**, 337-341 (*isol*)
Shemyakin, M.M. *et al., Tet. Lett.*, 1964, 47-54 (*synth*)
Schildknecht, H. *et al., Angew. Chem., Int. Ed.*, 1971, **10**, 124-125 (*isol*)
Tahara, S. *et al., Agric. Biol. Chem.*, 1978, **42**, 879-883 (*synth*)
Kawahara, K. *et al., Biochim. Biophys. Acta*, 1979, **572**, 1-8 (*biosynth*)
Ketelaar, P.E.F. *et al., Tet. Lett.*, 1985, **26**, 4665-4668 (*synth*)
Matsuyama, T. *et al., J. Bacteriol.*, 1990, **172**, 3015-3022 (*Rubiwettin RG1*)
Duynstee, H.I. *et al., Eur. J. Org. Chem.*, 1998, 303-307 (*dirhamnoside*)
Franklin, A.F. *et al., J.O.C.*, 1999, **64**, 1512-1519 (*S-form, Me ester, synth, pmr, cmr, ms, ir*)
Sugimura, T. *et al., Bull. Chem. Soc. Jpn.*, 2002, **75**, 355-363 (*R-form, Me ester*)

8-Hydroxy-2,4,6-decatrienal H-519

Coalital



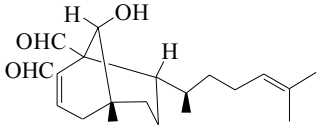
(2*E*,4*E*,6*E*,8*S*)–*form*

$C_{10}H_{14}O_2$ 166.219

(2*E*,4*E*,6*E*,8*S*)-*form* [151310-55-3]
Isol. from the alga *Acrosiphonia coalita.*
Unstable oil. Sol. hexane. Possible artifact. λ_{max} 312 (ϵ 43000) (MeOH) (Berdy).

(2*E*,4*Z*,6*E*,8*S*)-*form* [147292-95-3]
Isol. from *Acrosiphonia coalita*. Isomerises easily to (*all-E*)-form.
Bernart, M.W. *et al., J. Nat. Prod.*, 1993, **56**, 245 (*isol*)

9-Hydroxy-2,14-dichotomadiene-19,20-dial H-520



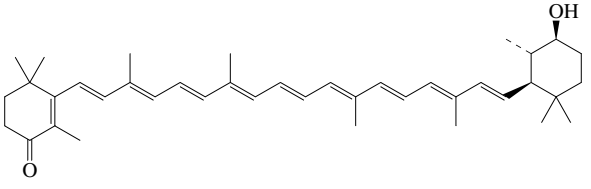
$C_{20}H_{30}O_3$ 318.455

(9*R*)-*form* [81574-88-1]
Constit. of *Dictyota dichotoma.*
Cryst. (hexane).
Mp 129-131°. $[\alpha]_D^{25}$ +4.5 (c, 1 in $CHCl_3$).

Ac: [81574-89-2]
$C_{22}H_{32}O_4$ 360.492
Constit. of *Dictyota dichotoma.* Cryst.
Mp 35-39°. $[\alpha]_D^{25}$ +10.2 (c, 1.7 in CH_2Cl_2).
Blount, J.F. *et al., Aust. J. Chem.*, 1982, **35**, 145-163 (*Dictyota dichotoma constits*)

4′-Hydroxy-5′,6′-dihydro-β,β-caroten-4-one H-521

4′-Hydroxy-5′,6′-dihydroechinone

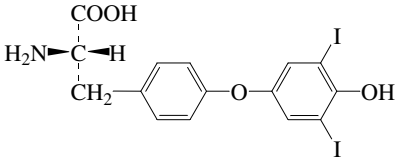


$C_{40}H_{56}O_2$ 568.881

(4′*S*,5′*S*,6′*S*)-*form* [98509-02-5]
Isol. from the spindle shell *Fusinus perplexus.* λ_{max} 414 (sh); 451; 472 (Et_2O).
Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **81**, 905-908
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 297
Tsushima, M. *et al., J. Nat. Prod.*, 2001, **64**, 1139-1142 (*isol, pmr, abs config*)

O-(4-Hydroxy-3,5-diiodophenyl)tyrosine, 9CI H-522

*3-[*p*-(4-Hydroxy-3,5-diiodophenoxy)phenyl]alanine, 8CI. 3′,5′-Diiodothyronine*
[1955-17-5]



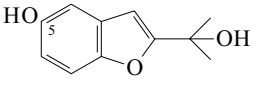
(*S*)-*form*

$C_{15}H_{13}I_2NO_4$ 525.081

(*S*)-*form*
L-form
[4192-14-7]
Constit. of *Porphyra umbilicalis* and *Enteromorpha intestinalis.*
Cryst.
Mp 205° dec. $[\alpha]_D^{21}$ +10.5 (c, 1 in HCl/EtOH).

(±)-*form* [60363-25-9]
Cryst. Mp 206° dec.
Block, P. *et al., J.A.C.S.*, 1942, **64**, 1070-1074 (*synth*)
Coulson, C.B. *et al., Chem. Ind. (London)*, 1953, 997-998 (*occur*)
Varcoe, J.S. *et al., J.C.S.*, 1960, 2711-2715 (*S-form, synth*)
Ong, R.L. *et al., Biochem. Int.*, 1985, **10**, 803-811 (*pmr*)

5-Hydroxy-α,α-dimethyl-2-benzofuranmethanol, 9CI H-523



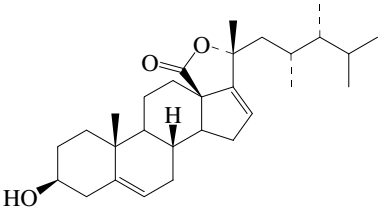
$C_{11}H_{12}O_3$ 192.214

5-Me ether: 2-(1-Hydroxy-1-methylethyl)-5-methoxybenzofuran
[86360-38-5]
$C_{12}H_{14}O_3$ 206.241
Isol. from *Lactarius fuliginosus* and *Lactarius picinus.*
Mp 44-45°.

2,3-Dihydro: 2,3-Dihydro-5-hydroxy-α,α-dimethyl-2-benzofuranmethanol. 2,3-Dihydro-5-hydroxy-2-(1-hydroxy-1-methylethyl)-benzofuran. ***Antibiotic F 11334A$_2$****. F 11334A$_2$*
$C_{11}H_{14}O_3$ 194.23
Prod. by the marine-derived *Acremonium murorum*. Powder.
$[\alpha]_D$ +49.8 (c, 1 in MeOH). λ_{max} 216 (sh) (ϵ 4020); 229 (ϵ 4310); 303 (ϵ 3670) (MeOH).
De Bernardi, M. *et al., Tetrahedron*, 1992, **48**, 7331
Tanaka, M. *et al., J. Antibiot.*, 1999, **52**, 827-830 (*F 11334A2*)
Abdel-Lateff, A. *et al., J. Nat. Prod.*, 2002, **65**, 1605-1611 (*F 11334A2*)

3-Hydroxy-23,24-dimethylcholesta-5,16-dien-18,20-olide H-524

3-Hydroxy-23-methylergosta-5,16-dien-18,20-olide

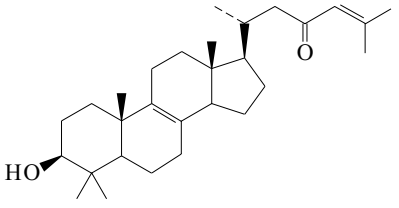


$C_{29}H_{44}O_3$ 440.665

(3β,20*R*,23*R*,24*R*)-*form*
Dissectolide
[862279-42-3]
Constit. of *Sinularia dissecta*.
Gum. $[\alpha]_D^{20}$ +15 (c, 0.14 in $CHCl_3$).
Jin, P. *et al., Steroids*, 2005, **70**, 487-493 (*Dissectolide*)

3-Hydroxy-4,4-dimethylcholesta-8,24-dien-23-one H-525

3-Hydroxy-30-norlanosta-8,24-dien-23-one



$C_{29}H_{46}O_2$ 426.681

(3β,5α)-*form* [114550-75-3]
Sapogenin from *Asteropus sarasinosum*.
Cryst. ($CHCl_3$/hexane).
Mp 153-154°.

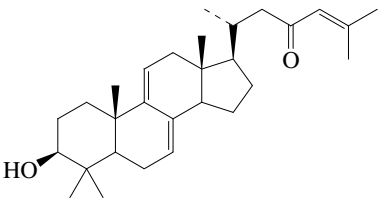
3-O-*[β-D-Xylopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Sarasinoside C₁***
[114066-51-2]
$C_{55}H_{88}N_2O_{20}$ 1097.302
Constit. of *Asteropus sarasinosum*. Cryst. (MeOH).
Mp 194-197°. $[\alpha]_D^{25}$ -22 (c, 2.65 in MeOH). λ_{max} 237 (ε 13600) (MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Sarasinoside A₁***
[114099-54-6]
$C_{62}H_{100}N_2O_{26}$ 1289.47
Constit. of *Asteropus sarasinosum*. Shows cytotoxic activity. Ichthyotoxic agent. Powder ($CHCl_3$/MeOH).
Mp 208-212°. $[\alpha]_D$ -7.4 (c, 0.3 in MeOH). λ_{max} 237 (ε 13500) (MeOH) (Derep). λ_{max} 237 (ε 10192) (MeOH) (Berdy).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Sarasinoside B₁***
[114066-50-1]
$C_{61}H_{98}N_2O_{25}$ 1259.444
Constit. of *Asteropus sarasinosum*. Ichthyotoxic agent. Cryst. (MeOH).
Mp 197-199°. $[\alpha]_D^{20}$ -16 (c, 0.99 in MeOH). λ_{max} 239 (ε 13600) (MeOH). λ_{max} 237 (MeOH) (Berdy).
Schmitz, F.J. *et al., J.O.C.*, 1988, **53**, 5941 (*isol, pmr, cmr*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2867-2877 (*Sarasinosides*)
Lee, H.-S. *et al., J. Nat. Prod.*, 2000, **63**, 915-919 (*Sarasinoside A_1, activity*)

3-Hydroxy-4,4-dimethylcholesta-7,9(11),24-trien-23-one H-526

3-Hydroxy-30-norlanosta-7,9(11),24-trien-23-one



$C_{29}H_{44}O_2$ 424.665

3β-*form*

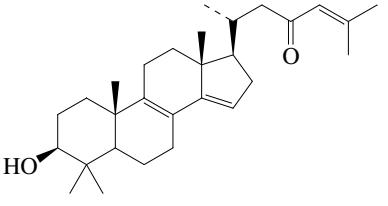
3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Sarasinoside A₂***
[116237-56-0]
$C_{62}H_{98}N_2O_{26}$ 1287.454
Constit. of *Asteropus sarasinosum*. Cryst. (MeOH aq.).
Mp 205-208°. $[\alpha]_D^{23}$ -5.5 (c, 0.5 in MeOH). λ_{max} 239 (sh) (ε 22000); 243 (ε 23500); 251 (sh) (ε 16500) (MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Sarasinoside B₂***
[116237-58-2]
$C_{61}H_{96}N_2O_{25}$ 1257.428
Constit. of *Asteropus sarasinosum*. Cryst. (MeOH aq.).
Mp 192-195°. $[\alpha]_D$ -10 (c, 0.3 in MeOH). λ_{max} 239 (sh) (ε 21700); 243 (ε 22800); 251 (sh) (ε 16200) (MeOH).

3-O-*[β-D-Xylopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Sarasinoside C₂***
[116237-60-6]
$C_{55}H_{86}N_2O_{20}$ 1095.286
Constit. of *Asteropus sarasinosum*. Cryst. (MeOH aq).
Mp 188-191°. $[\alpha]_D^{25}$ -11 (c, 0.3 in MeOH). λ_{max} 239 (sh) (ε 22500); 243 (ε 23800); 251 (sh) (ε 16800) (MeOH).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2867-2877 (*isol, pmr, cmr*)

3-Hydroxy-4,4-dimethylcholesta-8,14,24-trien-23-one H-527

3-Hydroxy-30-norlanosta-8,14,24-trien-23-one



$C_{29}H_{44}O_2$ 424.665

3β-*form*

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Sarasinoside A₃***
[116237-57-1]
$C_{62}H_{98}N_2O_{26}$ 1287.454
Constit. of *Asteropus sarasinosum*. Cryst.
Mp 205-208°. $[\alpha]_D^{23}$ -22 (c, 1.2 in MeOH). λ_{max} 245 (ε 22000) (MeOH).

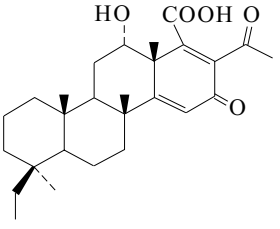
3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Sarasinoside B₃***
[116237-59-3]
$C_{61}H_{96}N_2O_{25}$ 1257.428
Constit. of *Asteropus sarasinosum*. Cryst. (MeOH aq.).
Mp 190-193°. $[\alpha]_D^{25}$ -23 (c, 0.4 in MeOH). λ_{max} 243 (ε 21600) (MeOH).

3-O-*[β-D-Xylopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Sarasinoside C₃***
[116237-61-7]
$C_{55}H_{86}N_2O_{20}$ 1095.286

Constit. of *Asteropus sarasinosum*. Cryst. (MeOH aq.). Mp 187-190°. $[\alpha]_D^{25}$ -31 (c, 0.9 in MeOH). λ_{max} 244 (ϵ 25900) (MeOH).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2867-2877 (*isol, pmr, cmr*)

12-Hydroxy-20,24-dimethyl-16,24-dioxo-14,17-scalaradien-25-oic acid H-528



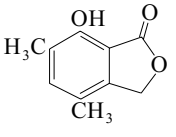
$C_{27}H_{38}O_5$ 442.594

12α-*form*

Ac: ***12α-Acetoxy-20,24-dimethyl-16,24-dioxo-14,17-scalaradien-25-oic acid***
[99631-21-7]
$C_{29}H_{40}O_6$ 484.631
Constit. of sponge *Carteriospongia foliascens*. Cryst. (as Me ester). $[\alpha]_D$ +95 (c, 1.5 in $CHCl_3$) (Me ester).

Declercq, J.P. *et al., Acta Cryst. C*, 1985, **41**, 1222-1224 (*cryst struct*)
Braekman, J.C. *et al., Tetrahedron*, 1985, **41**, 4603 (*isol, struct*)

7-Hydroxy-4,6-dimethyl-1(3*H*)-isobenzofuranone, 9CI H-529
7-Hydroxy-4,6-dimethylphthalide, 8CI
[10088-77-4]

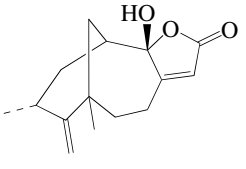


$C_{10}H_{10}O_3$ 178.187
Prod. *Penicillium gladioli* and *Penicillium megasporum*. Needles. Mp 156-158°.

*Me ether: 7-Methoxy-4,6-dimethyl-1(3*H*)-isobenzofuranone. 7-Methoxy-4,6-dimethylphthalide*
$C_{11}H_{12}O_3$ 192.214
Prod. by a marine *Diaporthe* sp. Cytotoxic. Prisms.

Raistrick, H. *et al., Biochem. J.*, 1952, **50**, 635 (*synth*)
Duncanson, L.A. *et al., J.C.S.*, 1953, 1331 (*ir*)
Birch, A.J. *et al., J.C.S.*, 1962, 370 (*biosynth*)
Asaoka, M. *et al., Chem. Lett.*, 1977, **2**, 167 (*synth*)
Wang, J.F. *et al., Acta Cryst. E*, 2003, **59**, 1235-1236 (*Me ether, cryst struct*)
Lin, X. *et al., FEMS Microbiol. Lett.*, 2005, **251**, 53-58 (*Me ether, isol*)

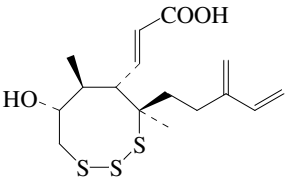
2-Hydroxy-9,11-dimethyl-10-methylene-3-oxatricyclo[7.3.1.0^{2,6}]tridec-5-en-4-one H-530
[221315-53-3]



$C_{15}H_{20}O_3$ 248.321
Constit. of *Dysidea herbacea*. Antifouling agent. Solid. $[\alpha]_D^{24}$ +0.23 (c, 0.35 in MeOH). Related to Nakafuran 9, N-15.

Sera, Y. *et al., J. Nat. Prod.*, 1999, **62**, 395-396 (*isol, pmr, cmr*)

3-[7-Hydroxy-4,6-dimethyl-4-(3-methylene-4-pentenyl)-1,2,3-trithiocan-5-yl]-2-propenoic acid H-531

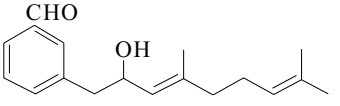


Absolute Configuration

$C_{16}H_{24}O_3S_3$ 360.562
Isol. from the Atlantic tunicate *Perophora viridis*. Amorph. solid. $[\alpha]_D^{24}$ +121.5 (c, 0.15 in EtOH). λ_{max} 205 (log ϵ 1.05); 258 (log ϵ 3.24) (EtOH).

Rezanka, T. *et al., Eur. J. Org. Chem.*, 2002, 2400-2404 (*isol, pmr, cmr, ms*)

3-(2-Hydroxy-4,8-dimethyl-3,7-nonadienyl)benzaldehyde H-532

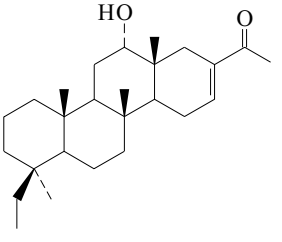


$C_{18}H_{24}O_2$ 272.386

Ac:
$C_{20}H_{26}O_3$ 314.424
Constit. of green algae *Halimeda scabra, Halimeda macroloba* and *Halimeda discoidea*. Oil. $[\alpha]_D^{25}$ +2.4 (c, 0.5 in $CHCl_3$). λ_{max} 249 (ϵ 6700); 286 (ϵ 3500) (MeOH) (Derep).

Paul, V.J. *et al., Tetrahedron*, 1984, **40**, 3053

12-Hydroxy-20,24-dimethyl-25-nor-16-scalaren-24-one H-533



$C_{26}H_{42}O_2$ 386.617

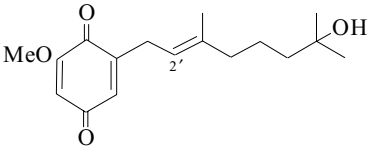
12α-*form*

Phyllofenone A
Constit. of *Phyllospongia foliascens*.

Ac:
$C_{28}H_{44}O_3$ 428.654
Isol. from sponge *Carteriospongia foliascens*. Foam.

Quinn, R.J. *et al., Aust. J. Chem.*, 1989, **42**, 751-755 (*Ac*)
Zeng, L. *et al., J. Nat. Prod.*, 1991, **54**, 421 (*cmr*)

2-(7-Hydroxy-3,7-dimethyl-2-octenyl)-6-methoxy-1,4-benzoquinone H-534



(*E*)*-form*

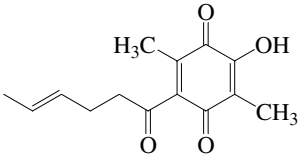
$C_{17}H_{24}O_4$ 292.374

(*E*)-*form*
Verapliquinone C
[109954-47-4]
Constit. of an *Aplidium* sp. λ_{max} 265 (ϵ 9800); 342 (ϵ 1200) ($CHCl_3$).

(*Z*)-*form*
Verapliquinone D
[109954-46-3]
Constit. of an *Aplidium* sp. λ_{max} 265 (ϵ 9800); 342 (ϵ 1200) ($CHCl_3$).
Guella, G. *et al., Helv. Chim. Acta*, 1987, **70**, 621-626 (*isol, pmr, cmr, uv*)

2-Hydroxy-3,6-dimethyl-5-(1-oxo-4-hexenyl)-1,4-benzoquinone H-535

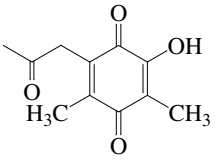
2-Hydroxy-3,6-dimethyl-5-(1-oxo-4-hexenyl)-2,5-cyclohexadiene-1,4-dione



$C_{14}H_{16}O_4$ 248.278
Prod. by a marine-derived *Penicillium terrestre*. Orange needles. Mp 127-129°. λ_{max} 211 (log ϵ 4.23); 269 (log ϵ 4.1) (MeOH).
Liu, W. *et al., J. Antibiot.*, 2005, **58**, 441-446 (*isol, pmr, cmr*)

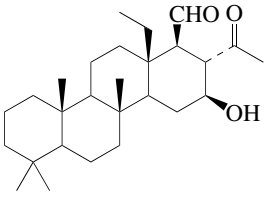
2-Hydroxy-3,5-dimethyl-6-(2-oxopropyl)-1,4-benzoquinone H-536

2-Hydroxy-3,5-dimethyl-6-(2-oxopropyl)-2,5-cyclohexadiene-1,4-dione



$C_{11}H_{12}O_4$ 208.213
Prod. by a marine-derived *Penicillium terrestre*. Orange needles. Mp 118° dec. λ_{max} 267 (log ϵ 4.08) (MeOH).
Liu, W. *et al., J. Antibiot.*, 2005, **58**, 441-446 (*isol, pmr, cmr*)

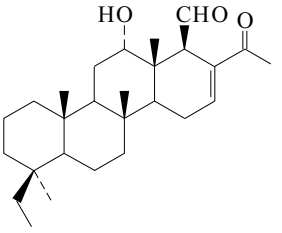
16-Hydroxy-23,24-dimethyl-24-oxo-25-scalaranal H-537



$C_{27}H_{44}O_3$ 416.643

(16β,17β*H*)-*form* [209268-01-9]
Constit. of *Cacospongia scalaris*.
Cryst. (hexane).
Mp 123-125°. $[\alpha]_D$ +60.4 (c, 0.5 in $CHCl_3$).
De Rosa, S. *et al., Tetrahedron*, 1998, **54**, 6185-6190 (*isol, pmr, cmr*)

12-Hydroxy-20,24-dimethyl-24-oxo-16-scalaren-25-al H-538

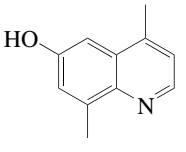


$C_{27}H_{42}O_3$ 414.627

(12α)-*form*
12-(3-Hydroxypentanoyl):
$C_{32}H_{50}O_5$ 514.744
Constit. of *Strepsichordaia lendenfeldi*. Needles (Me_2CO/hexane).
Mp 155-156°. $[\alpha]_D$ +43 (c, 0.57 in $CHCl_3$).
12-(3-Acetoxybutanoyl):
$C_{33}H_{50}O_6$ 542.754
Constit. of *Strepsichordaia lendenfeldi*. Glass. $[\alpha]_D$ +47.7 (c, 0.27 in $CHCl_3$). λ_{max} 234 (ϵ 8200) (EtOH) (Berdy).
12-(3-Acetoxypentanoyl):
$C_{34}H_{52}O_6$ 556.781
Constit. of *Strepsichordaia lendenfeldi*. Glass. $[\alpha]_D$ +44.6 (c, 0.33 in $CHCl_3$). λ_{max} 233 (ϵ 7800) (EtOH) (Berdy).
12-(3-Propanoyloxybutanoyl): [221163-31-1]
$C_{34}H_{52}O_6$ 556.781
Constit. of *Strepsichordaia lendenfeldi*. Oil. $[\alpha]_D^{25}$ +56.5 (c, 1.25 in $CHCl_3$). λ_{max} 232 (ϵ 18650) (MeOH).
12-(3-Propanoyloxypentanoyl):
$C_{35}H_{54}O_6$ 570.808
Constit. of *Strepsichordaia lendenfeldi*. Oil. $[\alpha]_D$ +37.4 (c, 0.46 in $CHCl_3$). λ_{max} 233 (ϵ 8150) (EtOH) (Berdy).
Bowden, B.F. *et al., J. Nat. Prod.*, 1992, **55**, 1234 (*isol, pmr, cmr*)
Jahn, T. *et al., J. Nat. Prod.*, 1999, **62**, 375-377 (*3-propanoyloxybutanoyl*)

6-Hydroxy-4,8-dimethylquinoline H-539

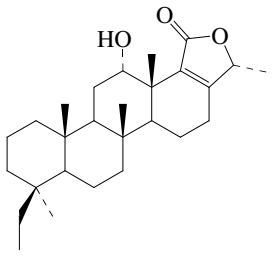
4,8-Dimethyl-6-quinolinol, 9CI
[194143-58-3]



$C_{11}H_{11}NO$ 173.214
Alkaloid from the marine cyanobacterium *Lyngbya majuscula*. Amorph. powder. λ_{max} 234 (log ϵ 4.47); 283 (log ϵ 3.51); 322 (log ϵ 3.28); 333 (log ϵ 3.28) (MeOH).

O-*(2,4-Di-O-methyl-β-D-xylopyranoside):* [194143-57-2]
$C_{18}H_{23}NO_5$ 333.383
From *Lyngbya majuscula*. Amorph. powder. $[\alpha]_D^{25}$ -56.7 (c, 0.15 in $CHCl_3$). λ_{max} 236 (log ϵ 4.65); 286 (log ϵ 3.57); 316 (log ϵ 3.44); 328 (log ϵ 3.44) (MeOH).
Orjala, J. *et al., Phytochemistry*, 1997, **45**, 1087-1090 (*isol, uv, ir, pmr, cmr, ms, struct*)

12-Hydroxy-20,24-dimethyl-17-scalaren-25,24-olide H-540



(12α,24*R*)-*form*

$C_{27}H_{42}O_3$ 414.627

(12α,24*R*)-*form*

12-(3-Hydroxybutanoyl): ***Phyllofolactone I***
[306997-41-1]
$C_{31}H_{48}O_5$ 500.717
Constit. of *Strepsichordaia aliena*. Amorph. solid. $[\alpha]_D$ +61.9 (c, 0.93 in CH_2Cl_2).

12-(3-Hydroxypentanoyl): ***Phyllofolactone K***
[306997-43-3]
$C_{32}H_{50}O_5$ 514.744
Constit. of *Strepsichordaia aliena*. Amorph. solid. $[\alpha]_D$ +53.8 (c, 0.8 in CH_2Cl_2).

(12α,24*S*)-*form*

Phyllofolactone B
[134985-08-3]
Constit. of *Phyllospongia foliascens*.
Cryst. (Me_2CO).
Mp 232-234°. $[\alpha]_D^{20}$ +61.9 (c, 0.0042 in $CHCl_3$).

Ac: ***12-Acetoxy-20,24-dimethyl-17-scalaren-25,24-olide***
[136118-96-2]
$C_{29}H_{44}O_4$ 456.664
Constit. of *Carteriospongia foliascens*. Cryst. (MeOH).
Mp 217-219°.

12-Ketone: 20,24-Dimethyl-12-oxo-17-scalaren-25,24-olide. ***Phyllofolactone C***
[222960-89-6]
$C_{27}H_{40}O_3$ 412.611
Constit. of *Phyllospongia foliascens*. Amorph. solid. $[\alpha]_D$ +133.5 (c, 0.2 in CH_2Cl_2).

12-(3-Hydroxybutanoyl): ***Phyllofolactone H***
[306997-40-0]
$C_{31}H_{48}O_5$ 500.717
Constit. of *Strepsichordaia aliena*. Amorph. solid. $[\alpha]_D$ +78.5 (c, 1.3 in CH_2Cl_2).

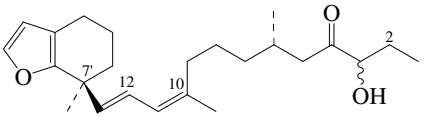
12-(3-Hydroxypentanoyl): ***Phyllofolactone J***
[306997-42-2]
$C_{32}H_{50}O_5$ 514.744
Constit. of *Strepsichordaia aliena*. Amorph. solid. $[\alpha]_D$ +55.3 (c, 0.8 in CH_2Cl_2).

(12β,24*R*)-*form*

12-Epiphyllofolactone B
[154067-31-9]
Constit. of *Phyllospongia foliascens*.
Needles.
Mp 233-235°. $[\alpha]_D$ +3.4 (c, 0.23 in $CHCl_3$).

Barron, P.F. *et al., Aust. J. Chem.*, 1991, **44**, 995 (*isol, pmr, cmr*)
Zeng, L. *et al., J. Nat. Prod.*, 1991, **54**, 421 (*Phyllofolactone B*)
Venkata, M. *et al., Indian J. Chem., Sect. B*, 1993, **32**, 1196 (*12-Epiphyllofolactone B*)
Fu, X. *et al., J. Nat. Prod.*, 1999, **62**, 644-646 (*Phyllofolactone C*)
Jiménez, J.I. *et al., J. Nat. Prod.*, 2000, **63**, 1388-1392 (*Phyllofolactones H - K*)

3-Hydroxy-6,10-dimethyl-13-(4,5,6,7-tetrahydro-7-methyl-7-benzofuranyl)-10,12-tridecadien-4-one H-541



$C_{24}H_{36}O_3$ 372.547

(3ξ,7′*S*,10*Z*,12*E*)-*form* [501445-47-2]
Constit. of an *Ircinia* sp.
Pale yellow oil. $[\alpha]_D^{30}$ +12.2 (c, 0.2 in $CHCl_3$). λ_{max} 242 (log ϵ 4.4) (MeOH).

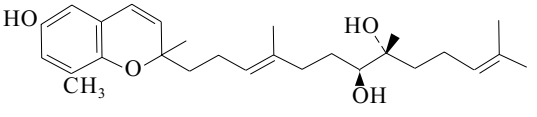
2-Chloro (stereoisomer 1): ***2-Chloro-3-hydroxy-6,10-dimethyl-13-(4,5,6,7-tetrahydro-7-methyl-7-benzofuranyl)-10,12-tridecadien-4-one***
[501445-48-3]
$C_{24}H_{35}ClO_3$ 406.991
Constit. of an *Ircinia* sp. Pale yellow oil. $[\alpha]_D^{30}$ +3.3 (c, 0.3 in $CHCl_3$). λ_{max} 242 (log ϵ 4.3) (MeOH).

2-Chloro (stereoisomer 2): [501445-49-4]
$C_{24}H_{35}ClO_3$ 406.991
Constit. of an *Ircinia* sp. Pale yellow oil. $[\alpha]_D^{30}$ +2.5 (c, 0.85 in $CHCl_3$). λ_{max} 242 (log ϵ 4.3) (MeOH).

Issa, H.H. *et al., J. Nat. Prod.*, 2003, **66**, 251-254 (*isol, pmr, cmr*)

6-Hydroxy-2,8-dimethyl-2-(4,8,12-trimethyl-7,8-dihydroxy-3,11-tridecadienyl)-2*H*-chromene H-542

*13-(6-Hydroxy-2,8-dimethyl-2*H*-1-benzopyran-2-yl)-2,6,10-trimethyl-2,10-tridecadiene-6,7-diol*



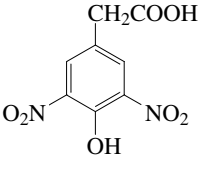
Relative configuration

$C_{27}H_{40}O_4$ 428.611
Constit. of brown alga *Cystoseira caespitosa*. Oil. $[\alpha]_D^{20}$ +11.2.

Amico, V. *et al., J. Chem. Res., Synop.*, 1982, 262

4-Hydroxy-3,5-dinitrophenylacetic acid H-543

4-Hydroxy-3,5-dinitrobenzeneacetic acid, 9CI
[10463-37-3]



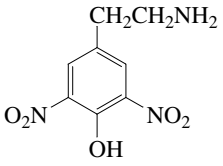
$C_8H_6N_2O_7$ 242.145
Isol. from the marine-derived *Flavobacterium* sp. T436. Cryst.
Mp 176-177°.

Me ester:
$C_9H_8N_2O_7$ 256.171
Isol. from *Flavobacterium* sp. T436.

Wilkinson, J.H. *et al., Biochem. J.*, 1956, **63**, 601-605 (*synth*)
Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*isol*)

2-(4-Hydroxy-3,5-dinitrophenyl)ethylamine H-544

4-(2-Aminoethyl)-2,6-dinitrophenol, 9CI. 4-Hydroxy-2,6-dinitrophenethylamine. 3,5-Dinitrotyramine

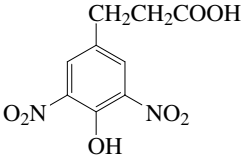


$C_8H_9N_3O_5$ 227.176

N-*Ac:* N-*2-[(4-Hydroxy-3,5-dinitrophenyl)ethyl]acetamide.*
N-*Acetyl-3,5-dinitrotyramine*
$C_{10}H_{11}N_3O_6$ 269.213
Isol. from the marine-derived *Flavobacterium* sp. T436.
Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*isol*)

3-(4-Hydroxy-3,5-dinitrophenyl)propanoic acid H-545

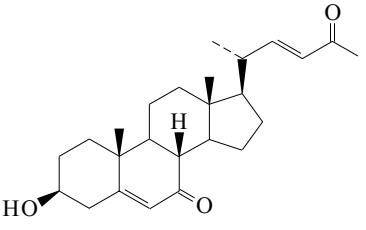
4-Hydroxy-3,5-dinitrobenzenepropanoic acid. 4-Hydroxy-3,5-dinitrohydrocinnamic acid



$C_9H_8N_2O_7$ 256.171
Isol. from the marine-derived *Flavobacterium* sp. T436.
Mp 135-136°.

3-Chloro: 3-Chloro-3-(4-hydroxy-3,5-dinitrophenyl)propanoic acid
$C_9H_7ClN_2O_7$ 290.616
Isol. from *Flavobacterium* sp. T436. Isol. as Me ester.
Kharasch, N. *et al., J.O.C.*, 1956, **21**, 925-928 (*synth*)
Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*isol*)

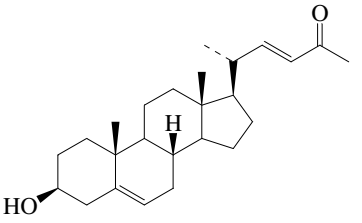
3-Hydroxy-26,27-dinorcholesta-5,22-diene-7,24-dione H-546



$C_{25}H_{36}O_3$ 384.558

(3β,22*E*)-*form* [147641-73-4]
Constit. of *Stelodoryx chlorophylla*.
$[\alpha]_D$ -60 (c, 0.3 in $CHCl_3$).
De Riccardis, F. *et al., J. Nat. Prod.*, 1993, **56**, 282 (*isol, pmr, cmr, ms*)

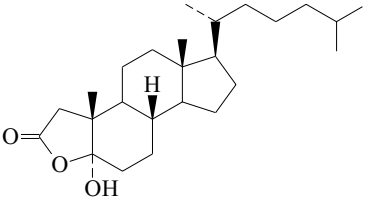
3-Hydroxy-26,27-dinorcholesta-5,22-dien-24-one H-547



$C_{25}H_{38}O_2$ 370.574

(3β,22*E*)-*form* [67230-06-2]
Isol. from sponge *Damiriana hawaiiana*.
Mp 163-165°. λ_{max} 225 (ϵ 15000) (MeOH).
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476

5-Hydroxy-3,4-dinorcholestane-2,5-olide H-548

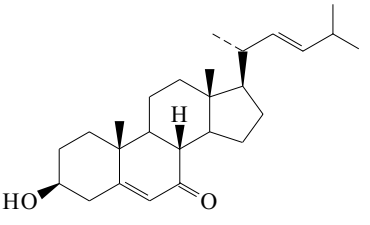


$C_{25}H_{42}O_3$ 390.605

(5α*OH*)-*form* [140384-70-9]
Constit. of *Laurencia obtusa*.
Cryst.
Mp 162-165°. $[\alpha]_D$ +28 (c, 0.8 in $CHCl_3$).
Kobayashi, M. *et al., Tet. Lett.*, 1992, **33**, 519 (*isol, pmr, cmr*)

3-Hydroxy-26,27-dinorergosta-5,22-dien-7-one, 9CI H-549

3-Hydroxy-24-norcholesta-5,22-dien-7-one

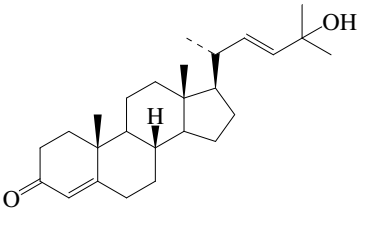


$C_{26}H_{40}O_2$ 384.601

(3β,22*E*)-*form* [145075-01-0]
Constit. of *Cliona copiosa*.
Notaro, G. *et al., J. Nat. Prod.*, 1992, **55**, 1588 (*isol, pmr, cmr*)

24-Hydroxy-26,27-dinorergosta-4,22-dien-3-one H-550

25-Hydroxy-24-norcholesta-4,22-dien-3-one

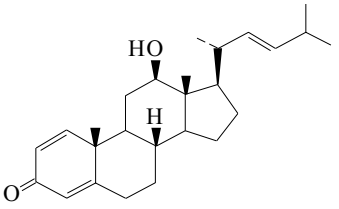


$C_{26}H_{40}O_2$ 384.601

(22*E*)-*form* [745075-28-9]
Constit. of *Dasystenella acanthina*.
Amorph. powder. $[\alpha]_D^{25}$ +45.9 (c, 0.07 in $CHCl_3$). λ_{max} 240 (ϵ 14900) (MeOH).
Mellado, G.G. *et al., Steroids*, 2004, **69**, 291-299 (*isol, pmr, cmr*)

12-Hydroxy-26,27-dinorergosta-1,4,22-trien-3-one, 9CI H-551

12-Hydroxy-24-norcholesta-1,4,22-trien-3-one

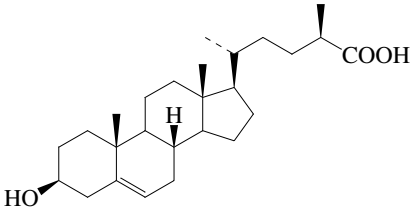


$C_{26}H_{38}O_2$ 382.585

(12β,22*E*)-*form*
Constit. of *Gersemia rubiformis*.
Ac:
$C_{28}H_{40}O_3$ 424.622
Constit. of *Gersemia rubiformis*.
Kingston, J.F. *et al., Can. J. Chem.*, 1982, **60**, 820

3-Hydroxy-26,27-dinorergost-5-en-25-oic acid H-552

3-Hydroxy-24-norcholest-5-en-26-oic acid

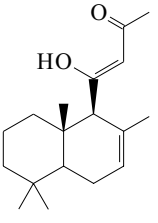


$C_{26}H_{42}O_3$ 402.616

(3β,24*R*)-*form*
3-Hydroxy-26,27-dinorcampest-5-en-25-oic acid
[874918-04-4]
Constit. of a *Euryspongia* sp.
Amorph. powder. $[\alpha]_{365}^{25}$ -47 (c, 1.6 in $CHCl_3$).
Mandeau, A. *et al., Steroids*, 2005, **70**, 873-878

11-Hydroxy-14,15-dinor-7,11-labdadien-13-one H-553

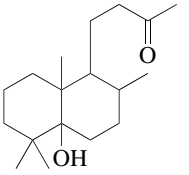
Sollasin F
[149298-02-2]



$C_{18}H_{28}O_2$ 276.418
Enolised β-diketone. Constit. of *Poecillastra sollasi*. Oil. $[\alpha]_D^{24}$ +92.5 (c, 0.28 in $CHCl_3$).
Killday, K.B. *et al., J. Nat. Prod.*, 1993, **56**, 500-507 (*isol, pmr, cmr*)

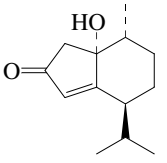
5-Hydroxy-14,15-dinor-13-labdanone H-554

[205382-27-0]



$C_{18}H_{32}O_2$ 280.45
Constit. of a *Mycale* sp. Oil. $[\alpha]_D$ -19 (c, 1.1 in $CHCl_3$).
Capon, R.J. *et al., J. Nat. Prod.*, 1998, **61**, 525-528 (*isol, pmr, cmr*)

1-Hydroxy-4,15-dinor-5-oplopen-3-one H-555



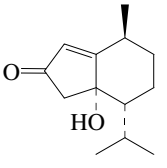
(1α,7β,10α)-*form*

$C_{13}H_{20}O_2$ 208.3

(1α,7β,10α)-*form* [865723-17-7]
Constit. of *Dictyopteris divaricata*.
Cryst. (Me_2CO).
Mp 146-147.5°. $[\alpha]_D^{20}$ +23 (c, 0.1 in MeOH).

(1β,7β,10α)-*form* [865723-18-8]
Constit. of *Dictyopteris divaricata*.
Gum. $[\alpha]_D^{20}$ -16 (c, 0.1 in MeOH).
Song, F. *et al., J. Nat. Prod.*, 2005, **68**, 1309-1313 (*Dictyopteris divaricata constits, cryst struct, abs config*)

6-Hydroxy-4,15-dinor-1-oplopen-3-one H-556

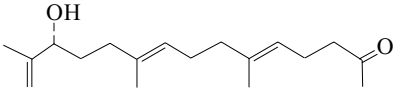


$C_{13}H_{20}O_2$ 208.3

(6α,7α,10β)-*form* [865723-19-9]
Constit. of *Dictyopteris divaricata*.
Gum. $[\alpha]_D^{20}$ +102 (c, 0.12 in MeOH).
Song, F. *et al., J. Nat. Prod.*, 2005, **68**, 1309-1313 (*Dictyopteris divaricata constit*)

14-Hydroxy-1,2-dinor-6,10,15-phytatrien-3-one H-557

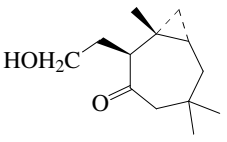
13-Hydroxy-6,10,14-trimethyl-5,9,14-pentadecatrien-2-one



$C_{18}H_{30}O_2$ 278.434

(6*E*,10*E*,14*R*)-*form* [81373-97-9]
Isol. from *Cystophora moniliformis*.
Oil. $[\alpha]_D^{22}$ -8.3 (c, 1 in $CHCl_3$).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 171

4-Hydroxy-3,15-dinor-2,3-seco-2-africanone H-558

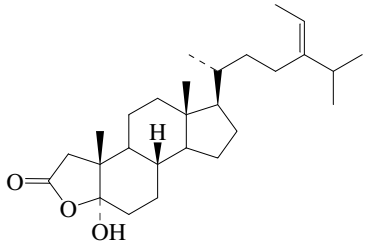


$C_{13}H_{22}O_2$ 210.316

Ac:
$C_{15}H_{24}O_3$ 252.353
Constit. of *Sinularia dissecta*.

Ramesh, P. *et al., J. Crystallogr. Spectrosc. Res.*, 2000, 48-50 (*isol, pmr, cmr*)

5-Hydroxy-3,4-dinor-2,3-secostigmast-24(28)-en-2,5-olide H-559

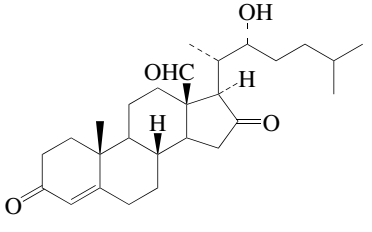


$C_{27}H_{44}O_3$ 416.643

(5α*OH*,24(28)*E*)-*form* [477885-38-4]
Constit. of *Sargassum carpophyllum*.
Amorph. solid.
Mp 130-133°.

Tang, H.-F. *et al., J. Asian Nat. Prod. Res.*, 2002, **4**, 95-101 (*isol, pmr, cmr*)

22-Hydroxy-3,16-dioxocholest-4-en-18-al H-560

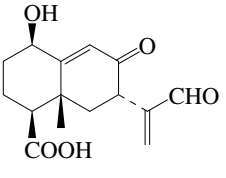


$C_{27}H_{40}O_4$ 428.611

(22*R*)-*form* [176704-07-7]
Constit. of a *Ctenocella* sp. Antiproliferative agent. Isol. as a mixt. of 18-epimeric (18→22)-hemiacetals. λ_{max} 242 (ε 17400) (MeOH) (Berdy).

Fretté, X.C. *et al., Tet. Lett.*, 1996, **37**, 2959-2962 (*isol, pmr, cmr*)

1-Hydroxy-8,12-dioxo-9,11(13)-eremophiladien-15-oic aid H-561



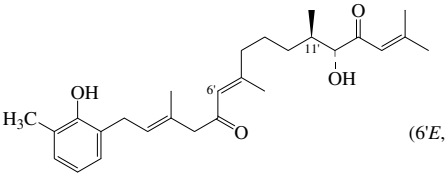
$C_{15}H_{18}O_5$ 278.304

(1β,7β*H*)-*form*
1-O-*(2,4ξ-Dimethyl-2*E*-octenoyl):* ***Integric acid***
[215866-65-2]
$C_{25}H_{34}O_6$ 430.54
Prod. by a *Xylaria* sp. ATCC 74397. HIV-1 integrase inhibitor.
Powder.
Mp 172-175°. $[\alpha]_D^{25}$ +38.3 (c, 0.63 in MeOH). λ_{max} 216 (ε 29500) (MeOH).

[215866-66-3, 215866-67-4, 215866-69-6]

Singh, S.B. *et al., Tet. Lett.*, 1999, **40**, 8775-8779 (*isol, pmr, cmr*)
Singh, S.B. *et al., Bioorg. Med. Chem. Lett.*, 2000, **10**, 235-238 (*activity*)

12-Hydroxy-5,13-dioxoisohalidrol H-562



(6′*E*,11′*R**,12′*R**)-*form*

$C_{28}H_{40}O_5$ 456.621

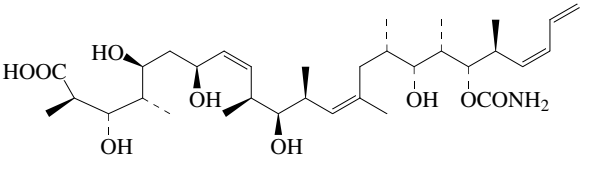
(6′*E*,11′*R,12′*R**)-*form***
12α-Hydroxy-5,13-dioxoisohalidrol
[80756-07-6]
Found in the brown alga *Halidrys siliquosa*.
Oil. $[\alpha]_D^{20}$ +43 (c, 3.7 in MeOH).

(6′*E*,11′*R,12′*S**)-*form***
12β-Hydroxy-5,13-dioxoisohalidrol
[80756-08-7]
Constit. of *Halidrys siliquosa*.
Oil. $[\alpha]_D^{20}$ -9.6 (c, 5 in MeOH).

(6′*Z*,11′*R,12′*R**)-*form***
12α-Hydroxy-5,13-dioxohalidrol
[80756-06-5]
Constit. of *Halidrys siliquosa*.
Oil. $[\alpha]_D^{20}$ +49 (c, 4.7 in MeOH).

Higgs, M.D. *et al., Tetrahedron*, 1981, **37**, 3209-3213

5-Hydroxydiscodermolic acid H-563

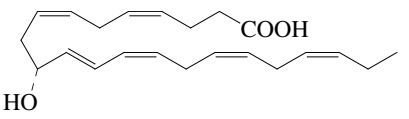


$C_{33}H_{57}NO_9$ 611.815
Ring-opened form of Discodermolide, D-1077.

Me ester: Methyl 5-hydroxydiscodermolate. 5-Hydroxymethyldiscodermolate
[358968-13-5]
$C_{34}H_{59}NO_9$ 625.841
Isol. from a *Discodermia* sp. Solid. $[\alpha]_D^{21}$ +14.6 (c, 0.1 in MeOH).

Gunasekera, S.P. *et al., J. Nat. Prod.*, 2002, **65**, 1643-1648 (*isol, pmr, cmr*)

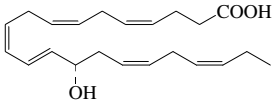
10-Hydroxy-4,7,11,13,16,19-docosahexaenoic acid H-564



$C_{22}H_{32}O_3$ 344.493

(-)-(4*Z*,7*Z*,11*E*,13*Z*,16*Z*,19*Z*)-*form* [229316-81-8]
Isol. from the coral *Madrepora oculata*.
$[\alpha]_D^{20}$ -8 (c, 0.1 in EtOH) (as Me ester). λ_{max} 234 (ϵ 24700) (EtOH) (Me ester).
Mancini, I. *et al., Helv. Chim. Acta*, 1999, **82**, 677-684

14-Hydroxy-4,7,10,12,16,19-docosahexaenoic acid H-565



(4*Z*,7*Z*,10*Z*,12*E*,14*S*,16*Z*,19*Z*)-*form*

$C_{22}H_{32}O_3$ 344.493

(4*Z*,7*Z*,10*Z*,12*E*,14*S*,16*Z*,19*Z*)-*form* [119433-37-3]
Formed by blood platelets in humans and other animals. Metab. of 4,7,10,13,16,19-Docosahexaenoic acid, D-1113. Also found in the sponge *Echinochalina mollis*.
Oil (as Me ester). $[\alpha]_D^{20}$ +7.2 (c, 0.3 in Me_2CO) (Me ester).

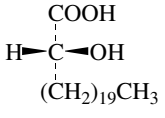
(4*Z*,7*Z*,10*Z*,12*E*,14ξ,16*Z*,19*Z*)-*form* [87042-40-8]
Constit. of the sponge *Echinochalina mollis*.
Oil (as Me ester). $[\alpha]_D^{20}$ +7.2 (c, 0.3 in Me_2CO) (Me ester).
19,20-Dihydro: See 14-Hydroxy-4,7,10,12,16-docosapentaenoic acid, H-568

[100838-25-3, 131485-68-2]

Van Rollins, M. *et al., J. Lipid Res.*, 1984, **25**, 507
Guerriero, A. *et al., J. Nat. Prod.*, 1990, **53**, 57 (*isol, uv, pmr, cmr, ms*)
Kim, H.Y. *et al., Prostaglandins Ser.*, 1990, **40**, 473 (*isol, props, struct*)

2-Hydroxydocosanoic acid H-566

2-Hydroxybehenic acid
[13980-14-8]



(*R*)-*form*

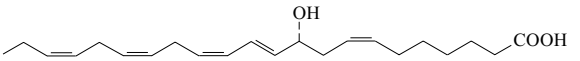
$C_{22}H_{44}O_3$ 356.588

(*R*)-*form*
Me ether: 2-Methoxydocosanoic acid
[88416-35-7]
$C_{23}H_{46}O_3$ 370.615
Constit. of the sponge *Higginsia tethyoides*.

(±)-*form*
Constit. of cork.
Cryst. ($CHCl_3$).
Mp 97°.
Me ester: [13980-17-1]
$C_{23}H_{46}O_3$ 370.615
Cryst. (Et_2O/petrol). Mp 75°.
Et ester:
$C_{24}H_{48}O_3$ 384.641
Cryst. Mp 70-71°.
Ac:
$C_{24}H_{46}O_4$ 398.625
Cryst. (EtOH). Mp 79°.

(ξ)-*form*
Constit. of various sponges incl. *Amphimedon compressa* and *Callyspongia fallax*.
Zetzsche, F. *et al., Helv. Chim. Acta*, 1931, **14**, 632
Ansari, A.A. *et al., J. Am. Oil Chem. Soc.*, 1976, **53**, 118 (*synth, pmr*)
Ayanoglu, E. *et al., Lipids*, 1983, **18**, 830-836 (*Me ether*)
Barnathan, G. *et al., J. Nat. Prod.*, 1993, **56**, 2104-2113 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*isol*)

10-Hydroxy-7,11,13,16,19-docosapentaenoic acid H-567



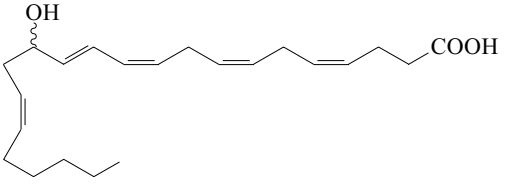
$C_{22}H_{34}O_3$ 346.509

(7*Z*,10*R*,11*E*,13*Z*,16*Z*,19*Z*)-*form*
Leiopathic acid
[117332-99-7]
Isol. from the antipatharian hexacoral, *Leiopathes* sp.
$[\alpha]_D^{20}$ +3.1 (c, 1.85 in $CHCl_3$).
Et ester: [117333-00-3]
$C_{24}H_{38}O_3$ 374.562
Isol. from *Leiopathes* sp.
$[\alpha]_D^{20}$ +5.3 (c, 0.53 in $CHCl_3$).

(7*Z*,10*S*,11*E*,13*Z*,16*Z*,19*Z*)-*form*
Isol. from the coral *Madrepora oculata*.
$[\alpha]_D^{20}$ -7.4 (c, 0.05 in EtOH) (as Me ester). 10*S*-Config. tentative.
λ_{max} 231 (ϵ 40700) (EtOH) (Me ester).
Guerriero, A. *et al., Helv. Chim. Acta*, 1988, **71**, 1094 (*isol, struct, uv, pmr, cmr, ms, abs config*)
Mancini, I. *et al., Helv. Chim. Acta*, 1999, **82**, 677-684 (*isol*)

14-Hydroxy-4,7,10,12,16-docosapentaenoic acid H-568

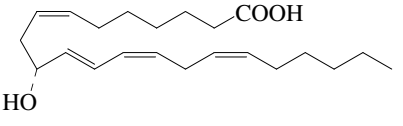
[104854-39-9]



$C_{22}H_{34}O_3$ 346.509
λ_{max} 236 (24500) (MeOH).

(4*Z*,7*Z*,10*Z*,12*E*,14ξ,16*Z*)-*form* [99312-72-8]
Isol. from the sponge *Echinochalina mollis*.
Oil (as Me ester). $[\alpha]_D^{20}$ +8 (c, 0.1 in Me_2CO) (Me ester).
Guerriero, A. *et al., J. Nat. Prod.*, 1990, **53**, 57; 1181 (*isol*)

10-Hydroxy-7,11,13,16-docosatetraenoic acid H-569



$C_{22}H_{36}O_3$ 348.525

(7*Z*,10*R*,11*E*,13*Z*,16*Z*)-*form* [229316-82-9]
Isol. from the coral *Madrepora oculata*. λ_{max} 232 (ϵ 18000) (EtOH) (as Me ester).
Mancini, I. *et al., Helv. Chim. Acta*, 1999, **82**, 677-684

2-Hydroxy-13-docosenoic acid H-570

$H_3C(CH_2)_7CH{=}CH(CH_2)_{10}CH(OH)COOH$
$C_{22}H_{42}O_3$ 354.572

(*Z*)-*form* [156576-70-4]
Constit. of the sea urchin *Tripneustes esculentus*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1994, **57**, 614 (*isol, ms*)

12-Hydroxy-5,8,10-dodecatrienoic acid H-571

$HOH_2CCH{=}CHCH{=}CHCH_2CH{=}CH(CH_2)_3COOH$
$C_{12}H_{18}O_3$ 210.272

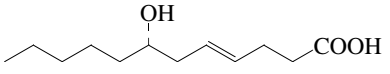
(5*Z*,8*E*,10*E*)-*form* [135378-22-2]
Isol. from the red alga *Gracilariopsis lemaneiformis*.
[135378-20-0]
Jiang, Z.D. *et al., Phytochemistry*, 1991, **30**, 1187

12-Hydroxy-6,9,11-dodecatrienoic acid H-572

$HOCH{=}CHCH{=}CHCH_2CH{=}CH(CH_2)_4COOH$
$C_{12}H_{18}O_3$ 210.272

(6*Z*,9*Z*,11*E*)-*form*
1,3-Hexadienyl ether(Z,Z-): 12-(1,3-Hexadienyloxy)-6,9,11-dodecatrienoic acid
[151675-35-3]
$C_{18}H_{26}O_3$ 290.402
Constit. of the brown alga *Laminaria* sp. Isol. as Me ester to which registry numbers refers.
6,7-Dihydro, 1,3-hexadienyl ether(Z,Z-): 12-(1,3-Hexadienyloxy)-9,11-dodecadienoic acid
[151675-37-5]
$C_{18}H_{28}O_3$ 292.417
Constit. of the brown alga *Laminaria* sp. Isol. as Me ester to which registry number refers.
Proteau, P.J. *et al., Lipids*, 1993, **28**, 783-787 (*isol, struct*)

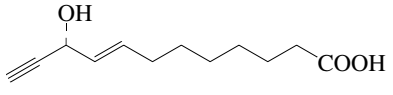
7-Hydroxy-4-dodecenoic acid H-573



$C_{12}H_{22}O_3$ 214.304

(4*E*,7*S*)-*form*
Me ether: 7-Methoxy-4-dodecenoic acid
$C_{13}H_{24}O_3$ 228.331
Isol. from *Lyngbya majuscula*. Pale yellow oil. $[\alpha]_D^{20}$ -8 (c, 1.8 in $CHCl_3$).
Mesguiche, V. *et al., Tet. Lett.*, 1999, **40**, 7473-7476 (*isol, synth, ir, pmr, cmr, ms*)

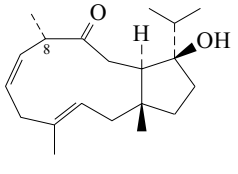
10-Hydroxy-8-dodecen-11-ynoic acid H-574



$C_{12}H_{18}O_3$ 210.272

(8*E*,10*R*)-*form*
Me ester: ***Petrynol***
[219917-20-1]
$C_{13}H_{20}O_3$ 224.299
Constit of the sponge, *Petrosia* sp.
$[\alpha]_D^{25}$ +15.3 (c, 0.08 in $CHCl_3$).
Seo, Y. *et al., J. Nat. Prod.*, 1999, **62**, 122-126 (*isol, ir, pmr, cmr*)

12-Hydroxy-3,6-dolabelladien-9-one H-575



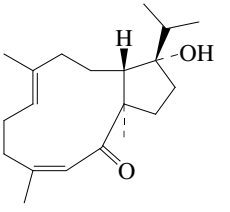
(3*E*,6*Z*,8α)–*form*

$C_{20}H_{32}O_2$ 304.472

(3*E*,6*Z*,8α)-*form*
Constit. of *Dictyota dichotoma* and *Dictyota pardalis* f. *pseudohamata*.
Oil. $[\alpha]_D$ +17.9 (c, 0.79 in $CHCl_3$).

(3*E*,6*Z*,8β)-*form*
From *Dictyota dichotoma* and *Dictyota pardalis* f. *pseudohamata*.
Oil. $[\alpha]_D$ -17.8 (c, 0.37 in $CHCl_3$).
Rao, C.B. *et al., J.O.C.*, 1986, **51**, 2736
König, G.M. *et al., J. Nat. Prod.*, 1994, **57**, 1529 (*isol, pmr, cmr, struct*)

12-Hydroxy-3,7-dolabelladien-2-one H-576



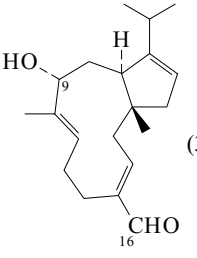
(3*Z*,7*E*)-*form*

$C_{20}H_{32}O_2$ 304.472

(3*Z*,7*E*)-*form*
Metab. of *Dictyota divaricata*.
Oil. $[\alpha]_D$ +37 (c, 0.65 in $CHCl_3$).

(3*Z*,7*Z*)-*form* [135650-24-7]
Metab. of *Dictyota divaricata*.
Oil. $[\alpha]_D$ +35.5 (c, 0.34 in $CHCl_3$).
Rao, C.B. *et al., Phytochemistry*, 1991, **30**, 1971 (*isol, pmr, cmr*)

9-Hydroxy-3,7,12-dolabellatrien-16-al H-577



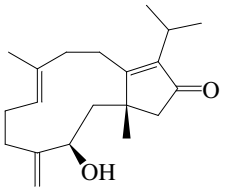
(3*E*,7*E*,9α)–*form*

$C_{20}H_{30}O_2$ 302.456

(3*E*,7*E*,9α)-*form*
9-Ac: ***9-Acetoxy-3,7,12-dolabellatrien-16-al***
$C_{22}H_{32}O_3$ 344.493
Constit. of *Dictyota dichotoma*. Cryst. ($CHCl_3$/petrol).
Mp 163-165°. $[\alpha]_D$ +10 (c, 0.5 in $CHCl_3$). λ_{max} 229 (ϵ 5950) (MeOH) (Derep).
16-Carboxylic acid, 9-Ac: ***9-Acetoxy-3,7,12-dolabellatrien-16-oic acid***
$C_{22}H_{32}O_4$ 360.492
From *Dictyota dichotoma*. Cryst. ($CHCl_3$/petrol).
Mp 152-154°. $[\alpha]_D$ +60.2 (c, 2.56 in $CHCl_3$). λ_{max} 222 (ϵ 5700) (MeOH) (Derep).

(3*Z*,7*E*,9ξ)-*form*
9-Ac:
$C_{22}H_{32}O_3$ 344.493
Constit. of *Dictyota bartayresiana*. Oil. $[\alpha]_D$ +6.6 (c, 0.53 in $CHCl_3$). Error in struct. diagram in ref.
Rao, C.B. *et al., J.O.C.*, 1986, **51**, 2736 (*isol, struct*)
Rao, C.B. *et al., Phytochemistry*, 1994, **37**, 509-513 (*Dictyota bartayresiana constit*)

3-Hydroxy-4(16),7,11-dolabellatrien-13-one H-578

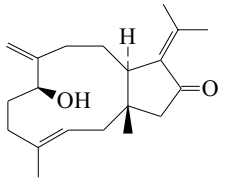


$C_{20}H_{30}O_2$ 302.456

(3β,7*E*)-*form* [359415-69-3]
Constit. of *Clavularia inflata*.
Oil. $[\alpha]_D^{25}$ +76.1 (c, 0.08 in $CHCl_3$). λ_{max} 228 (log ϵ 4.28) (MeOH).

3-Ketone: ***4(16),7,11-Dolabellatriene-3,13-dione***
[359415-68-2]
$C_{20}H_{28}O_2$ 300.44
Constit. of *Clavularia inflata*. Oil. $[\alpha]_D^{25}$ -264.5 (c, 0.11 in $CHCl_3$). λ_{max} 232 (log ϵ 4.16) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 2001, **64**, 1028-1031 (*isol, pmr, cmr*)

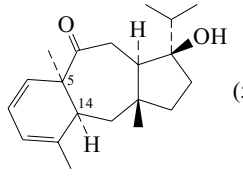
7-Hydroxy-3,8(17),12(18)-dolabellatrien-13-one H-579



$C_{20}H_{30}O_2$ 302.456

Ac: ***Dolabellane 7***
[133523-27-0]
$C_{22}H_{32}O_3$ 344.493
Constit. of *Eunicea laciniata*. Cryst. (Me_2CO).
Mp 103-104°. $[\alpha]_D$ +170 (c, 0.7 in $CHCl_3$).
Shin, J. *et al., J.O.C.*, 1991, **56**, 3392 (*isol, pmr, cmr*)

9-Hydroxy-1,3-dolastadien-6-one H-580



(5α,8α,9β,12β,14α)–*form*

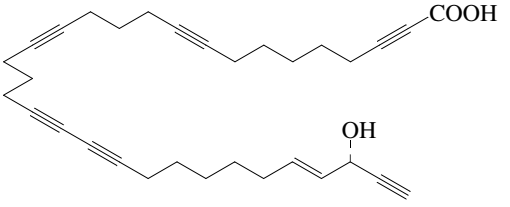
$C_{20}H_{30}O_2$ 302.456
λ_{max} 204 (ϵ 1600); 261 (ϵ 3500) (MeOH) (Derep).

(5α,8α,9β,12β,14α)-*form*
Constit. of *Dictyota dichotoma* and *Dictyota pardalis* f. *pseudohamata*.
Oil. $[\alpha]_D$ +160 (c, 0.76 in $CHCl_3$).

(5β,8α,9β,12β,14β)-*form*
Constit. of *Dictyota pardalis* f. *pseudohamata* and *Dictyota bartayresiana*.
Cryst.
Mp 121-124°. $[\alpha]_D^{25}$ -87 (c, 0.85 in $CHCl_3$). $[\alpha]_D$ -148 (c, 0.35 in $CHCl_3$).
Rao, C.B. *et al., J.O.C.*, 1986, **51**, 2736
König, G.M. *et al., J. Nat. Prod.*, 1994, **57**, 1529-1538 (*Dictyota pardalis constits*)
Rao, C.B. *et al., Phytochemistry*, 1994, **37**, 509-513 (*Dictyota bartayresiana constit*)

30-Hydroxy-28-dotriacontene-2,9,14,19,21,31-hexaynoic acid H-581

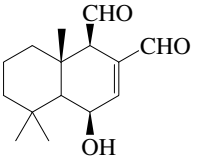
Callyspongynic acid



$C_{32}H_{38}O_3$ 470.65

(*S,E*)-*form*
Isol. from the marine sponge *Callyspongia truncata*. α-Glucosidase inhibitor. Oil. $[\alpha]_D$ +5.4 (c, 0.5 in EtOH). λ_{max} 204 (ϵ 6890) (MeOH).
Nakao, Y. *et al., J. Nat. Prod.*, 2002, **65**, 922-924 (*isol, pmr, cmr*)

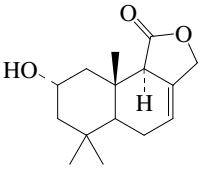
6-Hydroxy-7-drimene-11,12-dial H-582



$C_{15}H_{22}O_3$ 250.337

6β-*form*
Ac: ***6β-Acetoxypolygodial***
[231605-91-7]
$C_{17}H_{24}O_4$ 292.374
Constit. of *Dendrodoris arborescens.*
Fontana, A. *et al., Tetrahedron*, 1999, **55**, 5937-5946 (*isol, pmr, cmr*)

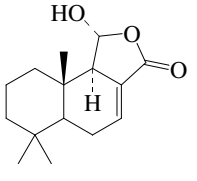
2-Hydroxy-7-drimen-11,12-olide H-583



$C_{15}H_{22}O_3$ 250.337

2α-*form*
Dendocarbin B
[350986-75-3]
Constit. of *Dendrodoris carbunculosa*.
Oil. $[\alpha]_D^{25}$ -88 (c, 0.03 in $CHCl_3$). λ_{max} 220 (ϵ 10000) (MeOH).
Sakio, Y. *et al., J. Nat. Prod.*, 2001, **64**, 726-731 (*isol, pmr, cmr*)

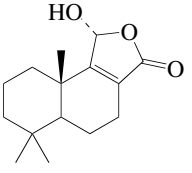
11-Hydroxy-7-drimen-12,11-olide H-584



$C_{15}H_{22}O_3$ 250.337

11α-*form*
Dendocarbin A
[350986-74-2]
Constit. of *Dendrodoris carbunculosa*.
Oil. $[\alpha]_D^{25}$ -10 (c, 0.14 in $CHCl_3$). λ_{max} 220 (ϵ 10000) (MeOH).
Ac:
$C_{17}H_{24}O_4$ 292.374
Constit. of a *Dysidea* sp. Oil. $[\alpha]_D^{25}$ -40.1 (c, 0.1 in MeOH). λ_{max} 223 (log ϵ 3.78) (MeOH).
Et ether: ***11α-Ethoxycinnamolide***
$C_{17}H_{26}O_3$ 278.391
Constit. of *Polygonum hydropiper*. Cryst.
Mp 45-47°.
Fukuyama, T. *et al., Phytochemistry*, 1985, **24**, 1521 (*Et ether*)
Paul, V.J. *et al., J. Nat. Prod.*, 1997, **60**, 1115-1120 (*Ac*)
Sakio, Y. *et al., J. Nat. Prod.*, 2001, **64**, 726-731 (*Dendocarbin A*)

11-Hydroxy-8-drimen-12,11-olide H-585



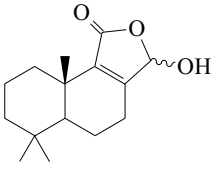
11α-*form*

$C_{15}H_{22}O_3$ 250.337

11α-*form*
Valdiviolide
[24173-70-4]
Constit. of *Drimys winteri* bark.
Cryst. (C_6H_6).
Mp 177-178°. $[\alpha]_D$ +111 (c, 1.18 in $CHCl_3$).
Ac:
$C_{17}H_{24}O_4$ 292.374
Constit. of a *Dysidea* sp. Na/K-ATPase inhibitor. Oil. $[\alpha]_D^{25}$ -7.2 (c, 0.1 in MeOH). λ_{max} 221 (log ϵ 3.65) (MeOH).

11β-*form*
Constit. of *Dysidea fusca*.
Oil. $[\alpha]_D$ +87 (c, 0.5 in $CHCl_3$).
Appel, H.H. *et al., Tetrahedron*, 1963, **19**, 635 (*Valdiviolide*)
Ley, S.V. *et al., J.C.S. Perkin 1*, 1983, 1379 (*synth*)
Montagnac, A. *et al., J. Nat. Prod.*, 1996, **59**, 866 (*isol, pmr, cmr, 11β-form*)
Paul, V.J. *et al., J. Nat. Prod.*, 1997, **60**, 1115-1120 (*Ac*)
Nakano, T. *et al., J. Chem. Res., Synop.*, 1998, 560-561 (*synth*)

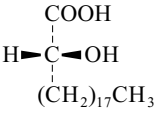
12-Hydroxy-8-drimen-11,12-olide H-586
12-Hydroxyisodrimenin



$C_{15}H_{22}O_3$ 250.337

12ξ-*form* [81369-50-8]
Constit. of *Dysidea fusca*.
Oil. $[\alpha]_D$ +74 (c, 0.4 in $CHCl_3$).
Montagnac, A. *et al., J. Nat. Prod.*, 1996, **59**, 866-868 (*isol, pmr, cmr*)
Nakano, T. *et al., J. Chem. Res., Synop.*, 1998, 560-561 (*synth*)

2-Hydroxyeicosanoic acid H-587
2-Hydroxyarachidic acid



(*R*)–*form*

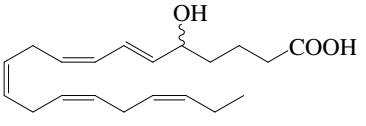
$C_{20}H_{40}O_3$ 328.534

(R)-form [26632-14-4]
Constit. of brain cerebrosides.
Me ether: 2-Methoxyeicosanoic acid
[88416-34-6]
$C_{21}H_{42}O_3$ 342.561
Constit. of the sponge *Higginsia tethyoides*.

(±)-*form* [16742-48-6]
Cryst. (C_6H_6/petrol). Mp 91-92°.
Me ester: [16742-49-7]
$C_{21}H_{42}O_3$ 342.561
Mp 62-64°.
Et ester:
$C_{22}H_{44}O_3$ 356.588
Mp 62-63°.

(ξ)-*form*
Constit. of the sponges *Aplysina archeri* and *Verongula gigantea*.
Hammarström, S. *et al., FEBS Lett.*, 1969, **5**, 192 (*config*)
Ayanoglu, E. *et al., Lipids*, 1983, **18**, 830-836 (*Me ether*)
Carballeira, N.M. *et al., Lipids*, 1989, **24**, 229-232 (*isol*)

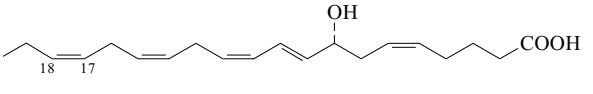
5-Hydroxy-6,8,11,14,17-eicosapentaenoic acid H-588
5-HEPE
[112572-25-5]



$C_{20}H_{30}O_3$ 318.455

(5ξ,6*E*,8*Z*,11*Z*,14*Z*,17*Z*)-*form*
Constit. of the red alga *Rhodymenia pertusa*. λ_{max} 236 (ϵ 23000) (no solvent reported).
[83952-40-3, 92008-51-0]
Hammarstrom, S. *et al., J. Biol. Chem.*, 1983, **258**, 1427 (*synth, uv, gc-ms*)
Jiang, Z.D. *et al., Phytochemistry*, 2000, **53**, 129-133

8-Hydroxy-5,9,11,14,17-eicosapentaenoic acid, 9CI H-589



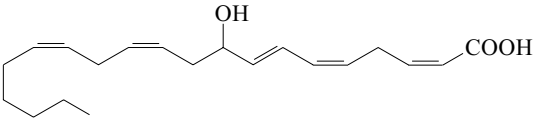
$C_{20}H_{30}O_3$ 318.455

(5*Z*,8*R*,9*E*,11*Z*,14*Z*,17*Z*)-*form*
8-HEPE
[117407-06-4]
Constit. of the antipatharian hexacoral *Leiopathes* sp. Also isol. from *Balanus balanoides*, *Patiria miniata* and *Elimineus modestus*. Induces the hatching of barnacles. Oil. $[\alpha]_D^{24}$ +33.4 (c, 2 in $CHCl_3$) (86% ee).
Et ester: [117333-01-4]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Leiopathes* sp.
$[\alpha]_D^{20}$ +3.7 (c, 0.33 in $CHCl_3$).

17,18-Dihydro: See 8-Hydroxy-5,9,11,14-eicosatetraenoic acid, H-595

D'Auria, M.V. *et al., Experientia*, 1988, **44**, 719-720
Guerriero, A. *et al., Helv. Chim. Acta*, 1988, **71**, 1094 (*isol, struct, uv, pmr, cmr, abs config*)
Shing, T.K.M. *et al., Tet. Lett.*, 1994, **35**, 1067

9-Hydroxy-2,5,7,11,14-eicosapentaenoic acid H-590

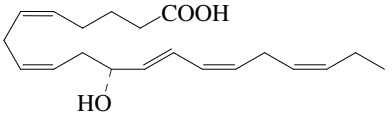


$C_{20}H_{30}O_3$ 318.455

(2*Z*,5*Z*,7*E*,11*Z*,14*Z*)-*form*
Isol. from the red alga *Laurencia hybrida*. Antimicrobial. Poorly sol. hexane. λ_{max} 236 (ϵ 9968) (MeOH) (Berdy).

Me ester: [81892-93-5]
$[\alpha]_D^{20}$ -4.5 (c, 0.65 in MeOH).
Higgs, M.D. *et al., Tetrahedron*, 1981, **37**, 4255 (*isol, pmr, ms*)

11-Hydroxy-5,8,12,14,17-eicosapentaenoic acid, 9CI H-591

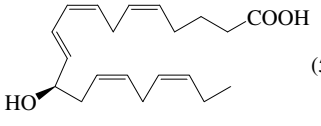


$C_{20}H_{30}O_3$ 318.455

(5*Z*,8*Z*,11*R*,12*E*,14*Z*,17*Z*)-*form* [109430-11-7]
Isol. from eggs of the sea urchin, *Strongylocentrotus purpuratus.*
Hawkins, D.J. *et al., J. Biol. Chem.*, 1987, **262**, 7629-7634 (*isol*)

12-Hydroxy-5,8,10,14,17-eicosapentaenoic acid H-592

12-HEPE
[74838-73-6]



(5*Z*,8*Z*,10*E*,12*R*,14*Z*,17*Z*)-*form*

$C_{20}H_{30}O_3$ 318.455
Formed by blood platelets from eicosapentaenoic acid in humans. Metab. of 5,8,11,14-Eicosatetraenoic acid in humans.

(5*Z*,8*Z*,10*E*,12*R*,14*Z*,17*Z*)-*form* [109430-12-8]
Isol. from eggs of the sea urchin *Strongylocentrotus purpuratus.* λ_{max} 237 (ϵ 23000) (no solvent reported).

(5*Z*,8*Z*,10*E*,12*S*,14*Z*,17*Z*)-*form* [116180-17-7]
Constit. of *Constantinea simplex, Echinochalina mollis, Gracilariopsis lemaneiformis* and *Murrayella periclados.* H.K- and Na,K-ATPase inhibitor. Neutrophil degranulation inhibitor. λ_{max} 238 (ϵ 23900) (MeOH) (Berdy).

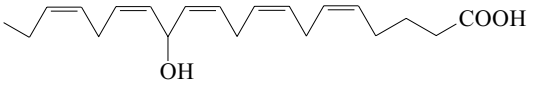
Me ester: [116084-98-1]
$C_{21}H_{32}O_3$ 332.482
Constit. of *Murrayella periclados.*
$[\alpha]_D$ -11 (c, 0.5 in Me_2CO).

[81187-21-5, 100838-24-2]

Hashimoto, Y. *et al., Thromb. Res.*, 1985, **40**, 307
Hawkins, D.J. *et al., J. Biol. Chem.*, 1987, **262**, 7629-7634 (*isol*)
Hawkins, D.J. *et al., Anal. Biochem.*, 1988, **173**, 456-462 (*chiral hplc*)
Bernart, M.W. *et al., Tet. Lett.*, 1988, **29**, 2015
Guerriero, A. *et al., J. Nat. Prod.*, 1990, **53**, 57; 1181 (*isol*)
Nagle, D.G. *et al., Tet. Lett.*, 1990, **31**, 2995 (*isol*)
Jiang, Z.D. *et al., Phytochemistry*, 1991, **30**, 1187 (*isol*)
Bernart, M.W. *et al., Phytochemistry*, 1994, **36**, 1233 (*isol, pmr*)

13-Hydroxy-5,8,11,14,17-eicosapentaenoic acid H-593

13-Hydroxytimnodonic acid

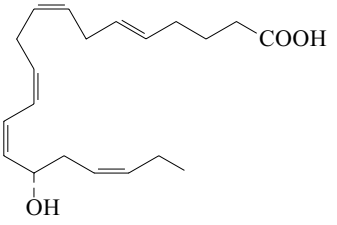


$C_{20}H_{30}O_3$ 318.455

(all-Z)-form
Et ester: [132705-45-4]
$C_{22}H_{34}O_3$ 346.509
Isol. from a mixture of the algae *Lithothamnion calcareum* and *Lithothamnion corallioides.*
$[\alpha]_D^{20}$ +2.1 (c, 0.33 in EtOH).
Guerriero, A. *et al., Helv. Chim. Acta*, 1990, **73**, 2183

15-Hydroxy-5,8,11,13,17-eicosapentaenoic acid H-594

15-HEPE
[97850-14-1]



$C_{20}H_{30}O_3$ 318.455

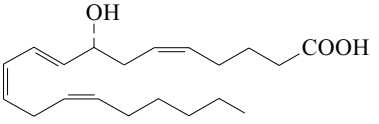
(5*E*,8*Z*,11*Z*,13*Z*,15*S*,17*Z*)-*form* [86282-92-0]
Prod. by *Skeletonema costatum*. Autoinhibitor. Sol. MeOH, EtOAc. λ_{max} 235 (MeOH) (Berdy).

[88852-33-9, 104758-12-5]

Mitchell, P.D. *et al., Biochem. Soc. Trans.*, 1984, **12**, 839
Fogh, K. *et al., Biomed. Environ. Mass Spectrom.*, 1988, **17**, 459 (*synth, ms*)
Imada, N. *et al., CA*, 1992, **117**, 229789; 248273 (*isol, pmr, cmr*)

8-Hydroxy-5,9,11,14-eicosatetraenoic acid, 9CI H-595

8-HETE
[69845-60-9]



(5*Z*,8*R*,9*E*,11*Z*,14*Z*)–*form*

$C_{20}H_{32}O_3$ 320.471

(5*Z*,8*R*,9*E*,11*Z*,14*Z*)-*form* [105500-09-2]
Isol. from the black coral *Leiopathes* sp. and from the starfish *Patiria miniata* and horseshoe crab *Limulus polyphemus.* Modulator of immune response in *Limulus polyphemus.* $[\alpha]_D^{20}$ +4 (c, 0.48 in $CHCl_3$). λ_{max} 237 (ϵ 21150) (95% EtOH).

Et ester: [117333-02-5]
$C_{22}H_{36}O_3$ 348.525
Isol. from *Leiopathes* sp.

$[\alpha]_D^{20}$ +4.5 (c, 0.32 in $CHCl_3$).

8-Ketone: 8-Oxo-5,9,11,14-eicosatetraenoic acid. 8-Oxo-ETE. 8-KETE
[116539-62-9]
$C_{20}H_{30}O_3$ 318.455
Arachidonic acid metab.

(5*Z*,8*S*,9*E*,11*Z*,14*Z*)-*form* [98462-03-4]
Metab. of 5,8,11,14-Eicosatetraenoic acid. This enantiomer predominates in mammalian tisues.

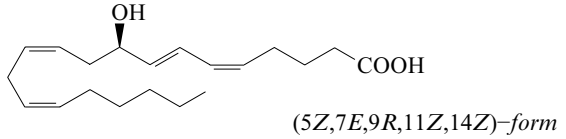
Me ester:
$C_{21}H_{34}O_3$ 334.498
Oil. $[\alpha]_D^{22}$ -4.75 (c, 0.4 in $CHCl_3$).

[70968-93-3, 79495-84-4, 100896-77-3]

Porter, N.A. *et al., J.O.C.*, 1979, **44**, 3177 (*synth, ms*)
Boeynaems, J.M. *et al., Anal. Biochem.*, 1980, **104**, 259 (*synth*)
Rabinovitch, H. *et al., Lipids*, 1981, **16**, 518 (*metab*)
Adams, J. *et al., Tet. Lett.*, 1984, **25**, 35 (*synth*)
Just, G. *et al., J.O.C.*, 1986, **51**, 4796 (*synth, ms, pmr*)
Yadagiri, P. *et al., Tet. Lett.*, 1986, **27**, 6039 (*synth*)
Wiseman, J.S. *et al., Biochem. Biophys. Res. Commun.*, 1988, **154**, 544 (*synth*)
D'Auria, M.V. *et al., Experientia*, 1988, **44**, 719-720 (*isol, Patiria*)
Guerriero, A. *et al., Helv. Chim. Acta*, 1988, **71**, 1094 (*synth, uv, ir, pmr, cmr*)
Kuehn, H. *et al., Eicosanoids*, 1991, **4**, 9 (*biosynth*)
MacPherson, J.C. *et al., Biochim. Biophys. Acta*, 1996, **1303**, 127-136 (*occur, Limulus*)

9-Hydroxy-5,7,11,14-eicosatetraenoic acid H-596

9-HETE
[69845-60-9]



(5*Z*,7*E*,9*R*,11*Z*,14*Z*)–*form*

$C_{20}H_{32}O_3$ 320.471

(5*Z*,7*E*,9*R*,11*Z*,14*Z*)-*form* [107656-14-4]
Metab. of arachidonic acid.

(5*Z*,7*E*,9*S*,11*Z*,14*Z*)-*form* [70968-92-2]
Metab. of arachidonic acid. Isol. from rat brain. The nat. prod. may be the 9*R*-enantiomer.

Me ester: [70968-96-6]
$C_{21}H_{34}O_3$ 334.498
Isol. from the red alga *Polyneura latissima*. Oil. $[\alpha]_D^{23}$ +11.1 (c, 0.56 in MeOH). λ_{max} 236 (ϵ 21500) (MeOH).

(5*Z*,7*E*,11*Z*,14*Z*)-*form*

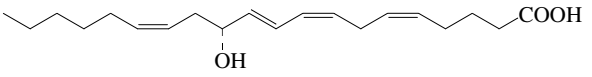
9-Ketone: 9-Oxo-5,7,11,14-eicosatetraenoic acid. 9-KETE. 9-Oxo-ETE
[135200-66-7]
$C_{20}H_{30}O_3$ 318.455
Metab. of arachidonic acid.

[117957-82-1]

Porter, N.A. *et al., J.O.C.*, 1977, **44**, 3177 (*synth, ms*)
Boeynaems, J.M. *et al., Anal. Biochem.*, 1980, **104**, 259 (*synth*)
Rabinovitch, M. *et al., Lipids*, 1981, **16**, 518 (*metab*)
Capdevila, J. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1982, **79**, 767 (*synth, ms*)
Adams, J. *et al., Tet. Lett.*, 1984, **25**, 35 (*synth*)
Capdevila, J. *et al., Biochem. Biophys. Res. Commun.*, 1986, **141**, 1007 (*biosynth*)
Just, G. *et al., J.O.C.*, 1986, **51**, 4796 (*synth, pmr, uv, ms*)
Saniere, M. *et al., Tetrahedron*, 1989, **45**, 7317 (*synth, pmr*)
Kuehn, H. *et al., Eicosanoids*, 1991, **4**, 9 (*biosynth*)
Jiang, Z.-D. *et al., Lipids*, 1997, **32**, 231-235 (*Me ester, isol*)
Yadev, J.S. *et al., Tetrahedron*, 1998, **54**, 3929-3934 (*9S-form, Me ester, synth, pmr*)

12-Hydroxy-5,8,10,14-eicosatetraenoic acid, 9CI H-597

12-HETE
[59985-28-3]
[69845-60-9]



(5*Z*,8*Z*,10*E*,12*R*,14*Z*)-*form*

$C_{20}H_{32}O_3$ 320.471

(5*Z*,8*Z*,10*E*,12*R*,14*Z*)-*form*
[71030-37-0]
Metab. of arachidonic acid. Biochem. diff. from 12*S*-form.

Me ester:
Oil. $[\alpha]_D^{20}$ -1.25 (c, 0.25 in $CHCl_3$).

(5*Z*,8*Z*,10*E*,12*S*,14*Z*)-*form* [54397-83-0]
[71030-37-0]
Metab. of arachidonic acid. Isol. from rat brain. Also found in the red alga *Murrayella periclados* and sponge *Echinochalina mollis*. Immunohormone. Cell growth inhibitor. Proinflammatory agent. Toxic to brine shrimp. Sol. MeOH, Et_2O; poorly sol. H_2O.

Me ester: [57872-14-7]
$C_{21}H_{34}O_3$ 334.498
$[\alpha]_D^{22}$ +1.3 (c, 0.3 in $CHCl_3$).

12-Oxo: 12-Keto-5,8,10,14-eicosatetraenoic acid. 12-Oxo-ETE. 12-KETE
[108437-64-5]
$C_{20}H_{30}O_3$ 318.455
Formed in the nervous system of *Aplysia* spp. Metab. of arachidonic acid.

(5*Z*,8*Z*,10*Z*,12*S*,14*Z*)-*form*
$[\alpha]_D^{21}$ -1.87 (c, 6.1 in $CHCl_3$).

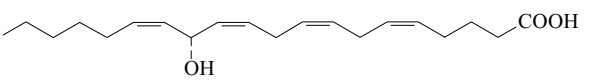
Me ester: [81623-72-5]
$[\alpha]_D^{23}$ -2.06 (c, 5.4 in $CHCl_3$).

[108437-55-4]

Corey, E.J. *et al., J.A.C.S.*, 1978, **100**, 1942 (*synth, pmr*)
McGuire, J.C. *et al., Prep. Biochem.*, 1978, **8**, 147 (*metab*)
Porter, N.A. *et al., J.O.C.*, 1979, **44**, 3177 (*synth, ms*)
Boeynaems, J.M. *et al., Anal. Biochem.*, 1980, **104**, 259 (*synth*)
Corey, E.J. *et al., J.A.C.S.*, 1980, **102**, 1433 (*synth*)
Rabinovitch, H. *et al., Lipids*, 1981, **16**, 518 (*metab*)
Russell, S.W. *et al., J.C.S. Perkin 1*, 1982, 545 (*synth*)
Corey, E.J. *et al., Tet. Lett.*, 1984, **25**, 5115 (*synth*)
Woollard, P.M. *et al., Biochem. Biophys. Res. Commun.*, 1986, **136**, 169
Just, G. *et al., J.O.C.*, 1986, **51**, 4796 (*deriv, synth, pmr, ir, ms*)
Nicolaou, K.C. *et al., Synthesis*, 1986, 344 (*synth*)
Yadagiri, P. *et al., Tet. Lett.*, 1986, **27**, 6039 (*synth*)
Fruteau de Laclos, B. *et al., Prostaglandins*, 1987, **33**, 315 (*synth, ms*)
Taffer, I.M. *et al., Tet. Lett.*, 1987, **28**, 6543 (*synth*)
Saniere, M. *et al., Angew. Chem., Int. Ed.*, 1989, **28**, 614 (*synth*)
Piomelli, D. *et al., Ann. N.Y. Acad. Sci.*, 1989, **559**, 202 (*rev*)
Nicolaou, K.C. *et al., Synthesis*, 1989, 898 (*synth, ir, uv, pmr, bibl*)
Guerriero, A. *et al., J. Nat. Prod.*, 1990, **53**, 57-61 (*Echinochalina, isol*)
Bernart, M.W. *et al., Phytochemistry*, 1994, **36**, 1233 (*Murrayella, isol*)
Benkouider, A. *et al., J. Chem. Res., Synop.*, 1999, 104-105 (*synth*)
Rodriguez, A. *et al., Tetrahedron*, 2001, **57**, 25-27 (*synth*)

13-Hydroxy-5,8,11,14-eicosatetraenoic acid H-598

13-Hydroxyarachidonic acid. 13-HETE
[69845-60-9]



$C_{20}H_{32}O_3$ 320.471

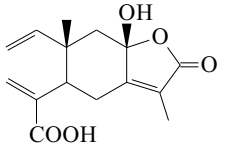
(*R*)-(*all-Z*)-*form*
Constit. of the red alga *Lithothamnion corallioides*. Isol. as Et ester.

Et ester: [132679-88-0]
$[\alpha]_D^{20}$ +1.5 (c, 0.6 in EtOH).

[96349-53-0, 96349-55-2]

Guerriero, A. *et al., Helv. Chim. Acta*, 1990, **73**, 2183 (*isol, deriv*)
Gerwick, W.H. *et al., Phytochemistry*, 1993, **34**, 1029 (*biosynth, abs config*)

8-Hydroxy-1,3,7(11)-elematrien-12,8-olid-15-oic acid H-599

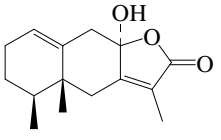


$C_{15}H_{18}O_5$ 278.304

8β*OH-form*

Me ester: ***Edwardsolide B***
[158515-37-8]
$C_{16}H_{20}O_5$ 292.331
Constit. of *Maasella edwardsi*.
$[\alpha]_D$ -6.4 (c, 0.5 in MeOH).
Bifulco, G. *et al., Nat. Prod. Lett.*, 1993, **3**, 167 (*isol, pmr, cmr*)

8-Hydroxy-1(10),7(11)-eremophiladien-12,8-olide H-600



8α*OH-form*

$C_{15}H_{20}O_3$ 248.321

8α*OH-form*

Palmosalide A
[128255-36-7]
Constit. of *Coelogorgia palmosa*.
Cryst.
Mp 172-174°. $[\alpha]_D$ +155 (c, 1.1 in $CHCl_3$).

1β,10β-Epoxide: ***1,10-Epoxy-8-hydroxy-7(11)-eremophilen-12,8-olide***
[849700-47-6]
$C_{15}H_{20}O_4$ 264.321
Isol. from *Senecio aegypticus* var. *discoideus*. Oil. $[\alpha]_D^{25}$ -12.25 (c, 2.92 in $CHCl_3$).

Me ether, 1α,10α-epoxide: ***1,10-Epoxy-8-methoxy-7(11)-eremophilen-12,8-olide***
[261164-38-9]
$C_{16}H_{22}O_4$ 278.347
Constit. of *Senecio flavus*. Cryst. (hexane).
Mp 102-103°. $[\alpha]_D$ -87.5 (c, 1 in $CHCl_3$).

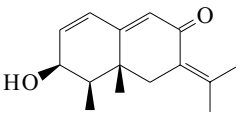
Me ether, 1β,10β-epoxide: [849700-48-7]
Isol. from *Senecio aegypticus* var. *discoideus*.
Cryst.

8β*OH-form*

1β,10β-Epoxide: ***Tsoongianolide F***
[849347-28-0]
$C_{15}H_{20}O_4$ 264.321
Constit. of *Senecio tsoongianus*. Gum. $[\alpha]_D^{25}$ +19 (c, 0.26 in $CHCl_2$).

Weimer, D.F. *et al., Tet. Lett.*, 1990, **31**, 1973 (*isol, struct*)
Torres, P. *et al., Phytochemistry*, 1999, **52**, 1507-1513 (*deriv*)
Zhao, Y. *et al., Chem. Biodiversity*, 2004, **1**, 1546-1559 (*Tsoongianolide F*)
Zhang, Q.J. *et al., Chin. Chem. Lett.*, 2005, **16**, 362-364 (*Tsoongianolide F*)
Mohamed, A.E.H. *et al., J. Nat. Prod.*, 2005, **68**, 439-442 (*Senecio aegypticus constits, cryst struct*)

3-Hydroxy-1,7(11),9-eremophilatrien-8-one H-601



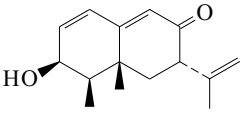
$C_{15}H_{20}O_2$ 232.322

3β-*form*

Oil. $[\alpha]_D^{20}$ +225 (c, 0.1 in $CHCl_3$).

3-(6-Methyl-2,4-octadienoyl): ***Dendryphiellin E2***
[133562-52-4]
$C_{24}H_{32}O_3$ 368.515
Constit. of *Dendryphiella salina*. Oil. $[\alpha]_D^{20}$ +617.6 (c, 0.18 in EtOH).
Guerriero, A. *et al., Helv. Chim. Acta*, 1990, **73**, 2090 (*isol, pmr, cmr*)

3-Hydroxy-1,9,11-eremophilatrien-8-one H-602



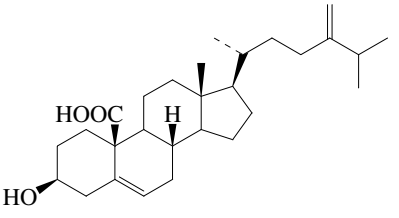
$C_{15}H_{20}O_2$ 232.322

(3β,7β*H*)-*form*

3-(6-Methyl-2,4-octadienoyl): ***Dendryphiellin E1***
[133562-51-3]
$C_{24}H_{32}O_3$ 368.515
Constit. of *Dendryphiella salina*. Oil. $[\alpha]_D^{20}$ +725.8 (c, 0.18 in EtOH).
Guerriero, A. *et al., Helv. Chim. Acta*, 1990, **73**, 2090 (*isol, pmr, cmr*)

3-Hydroxyergosta-5,24(28)-dien-19-oic acid H-603

3-Hydroxy-24-methylenecholest-5-en-19-oic acid



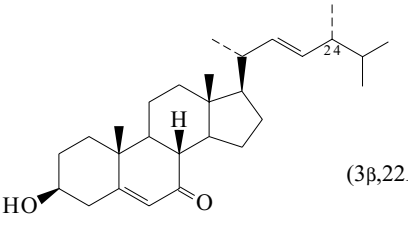
$C_{28}H_{44}O_3$ 428.654

3β-*form*

3-Sulfate:
$C_{28}H_{44}O_6S$ 508.718
Constit. of *Toxadocia zumi*.
Nakatsu, T. *et al., Experientia*, 1983, **39**, 759-761 (*isol, pmr*)

3-Hydroxyergosta-5,22-dien-7-one H-604

3-Hydroxy-24-methylcholesta-5,22-dien-7-one



(3β,22*E*,24*R*)−*form*

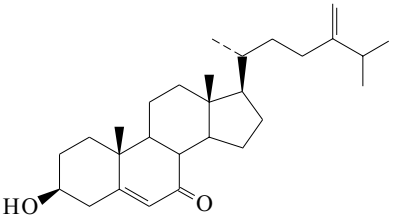
$C_{28}H_{44}O_2$ 412.654

(3β,22*E*,24*R*)-*form* [145163-96-8]
Constit. of *Cliona copiosa*.

(3β,22*E*,24*S*)-*form* [99081-78-4]
Constit. of *Cliona copiosa*.
Notaro, G. *et al., J. Nat. Prod.*, 1992, **55**, 1588 (*isol, pmr, ms*)

3-Hydroxyergosta-5,24(28)-dien-7-one H-605

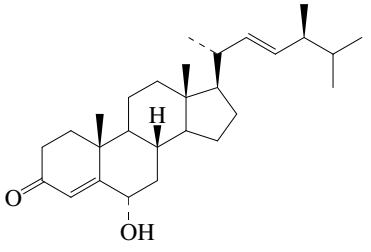
3-Hydroxy-24-methylenecholest-5-en-7-one



$C_{28}H_{44}O_2$ 412.654

3β-*form* [99081-76-2]
Constit. of *Haliclona oculata* and *Corallistes undulatus*.
Findlay, J.A. *et al., Can. J. Chem.*, 1985, **63**, 2406-2410 (*isol*)
Guerriero, A. *et al., J. Nat. Prod.*, 1993, **56**, 1962-1970 (*isol, pmr, cmr*)

6-Hydroxyergosta-4,22-dien-3-one H-606

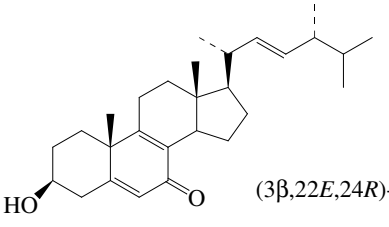


$C_{28}H_{44}O_2$ 412.654

(6α,22*E*,24*S*)-*form* [851610-90-7]
Constit. of *Iotrochota birotulata*.
Cryst.
Mp 129-132°. $[\alpha]_D^{20}$ +156 (c, 0.43 in MeOH). Genus name given, apparently incorrectly, as Iotrichoto. λ_{max} 245 (MeOH).
Li, L.-Y. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 115-120

3-Hydroxyergosta-5,8,22-trien-7-one H-607

3-Hydroxy-24-methylcholesta-5,8,22-trien-7-one



(3β,22*E*,24*R*)-*form*

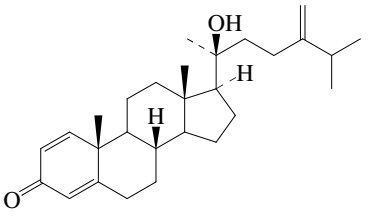
$C_{28}H_{42}O_2$ 410.639

(3β,22*E*,24*R*)-*form* [200942-18-3]
Constit. of *Grifola frondosa* (maitake).
Amorph. powder. $[\alpha]_D^{24}$ -28.3 (c, 0.1 in $CHCl_3$). λ_{max} 246 (log ε 4) (MeOH).

(3β,22*E*,24ξ)-*form*
Isol. from Mediterranean sponge *Clathrina clathrus*.
Aiello, A. *et al., Steroids*, 1988, **52**, 533-542 (*isol, pmr, ms, Clathrina*)
Ishizuka, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1756-1760 (*isol, pmr, cmr*)

20-Hydroxyergosta-1,4,24(28)-trien-3-one H-608

20-Hydroxy-24-methylenecholesta-1,4-dien-3-one



$C_{28}H_{42}O_2$ 410.639

(20*S*)-*form* [862286-71-3]
Constit. of *Anthomastus bathyproctus*.
Amorph. powder. $[\alpha]_D^{25}$ +5.6 (c, 0.08 in $CHCl_3$). λ_{max} 246 (log ε 4.03) (MeOH).
Mellado, G.G. *et al., J. Nat. Prod.*, 2005, **68**, 1111-1115 (*Anthomastus bathyproctus constit*)

3-Hydroxyergost-5-en-21-oic acid H-609

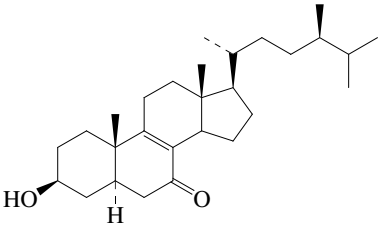
3-Hydroxy-24-methylcholest-5-en-21-oic acid

$C_{28}H_{46}O_3$ 430.67

(3β,24*S*)-*form*
Constit. of a *Sclerophytum* coral.
Needles.
Mp 269-271°. $[\alpha]_D^{21}$ -30 (c, 0.3 in Py).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 233 (*isol, pmr, cmr*)

3-Hydroxyergost-8-en-7-one H-610

3-Hydroxy-24-methylcholest-8-en-7-one

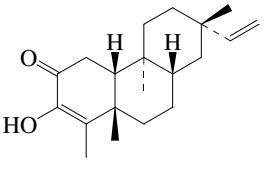


$C_{28}H_{46}O_2$ 414.67

(3β,5α,24*R*)-*form*
Me ether: 3-Methoxyergost-8-en-7-one
[139765-35-8]
$C_{29}H_{48}O_2$ 428.697
Constit. of the sponge *Jereicopsis graphidiophora*.
D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*isol, pmr, cmr, ms*)

3-Hydroxy-3,15-erythroxyladien-2-one H-611

3-Hydroxy-3,15-dolabradien-2-one



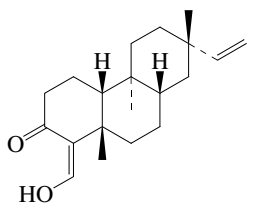
$C_{20}H_{30}O_2$ 302.456
Enolised α-diketone.

(*ent*-5α)-*form*
Tagalsin G
[862588-85-0]
Constit. of the mangrove *Ceriops tagal*.

Oil. $[\alpha]_D^{25}$ +55.97 (c, 0.09 in $CHCl_3$).
Zhang, Y. *et al., Phytochemistry*, 2005, **66**, 1465-1471 (*Tagalsin G*)

18-Hydroxy-4(18),15-erythroxyladien-3-one H-612

18-Hydroxy-4(18),15-dolabradien-3-one

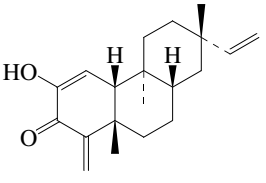


$C_{20}H_{30}O_2$ 302.456
Enolised β-ketoaldehyde.

(*ent*-4(18)*Z*,5α)-*form*
Tagalsin F
[862588-84-9]
Constit. of the mangrove *Ceriops tagal*.
Solid.
Mp 98-99°. $[\alpha]_D^{25}$ +34.86 (c, 0.072 in $CHCl_3$).
Zhang, Y. *et al., Phytochemistry*, 2005, **66**, 1465-1471 (*Tagalsin F*)

2-Hydroxy-1,4(18),15-erythroxylatrien-3-one H-613

2-Hydroxy-1,4(18),15-dolabratrien-3-one



$C_{20}H_{28}O_2$ 300.44
Enolised α-diketone.

(*ent*-5α)-*form*
Tagalsin C
[862588-81-6]
Constit. of the mangrove *Ceriops tagal*.
Yellow oil. $[\alpha]_D^{25}$ +92.3 (c, 0.05 in $CHCl_3$).

*4α,18-Epoxide (*ent-*4β): 4,18-Epoxy-2-hydroxy-1,15-erythroxyladien-3-one. 4,18-Epoxy-2-hydroxy-1,15-dolabradien-3-one.* ***Tagalsin B***
[862588-80-5]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Ceriops tagal*. Solid.
Mp 66-68°. $[\alpha]_D^{25}$ +165 (c, 0.06 in $CHCl_3$).

*4β,18-Epoxide (*ent-*4α): **Tagalsin A***
[862588-79-2]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Ceriops tagal*. Yellow cryst.
Mp 67-69°. $[\alpha]_D^{25}$ +69.26 (c, 0.054 in $CHCl_3$).
Zhang, Y. *et al., Phytochemistry*, 2005, **66**, 1465-1471 (*Tagalsins A-C*)

2-Hydroxy-1-ethanesulfonic acid, 9CI, 8CI H-614

2-Sulfoethyl alcohol. ***Isethionic acid***
[107-36-8]
$HOCH_2CH_2SO_3H$
$C_2H_6O_4S$ 126.133
Metab. of 2-Mercaptoethanol in rats. Constit. of *Ceramium flaccidum*, *Grateloupia doryphora* and other red algae and squid. Derivs. are used to make detergents. Syrup. Misc. H_2O, EtOH.
▶ Eye, skin and mucous membrane irritant. LD_{50} (mus, ipr) 50 mg/kg. KI7700000

Na salt: [1562-00-1]
Mp 191-194°.

NH_4 salt: [57267-78-4]
Hygroscopic. Mp 139-141°.
▶ KI7750000

O-*Sulfate:* See Ethionic acid in *The Combined Chemical Dictionary.*

Chloride: [78303-70-5]
$C_2H_5ClO_3S$ 144.578
Syrup. n_D^{25} 1.4902.

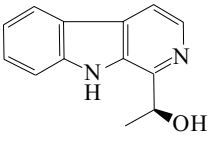
Ac, chloride: [78303-71-6]
$C_4H_7ClO_4S$ 186.616
Bp_{14} 130-132°.

Et ether: 2-Ethoxy-1-ethanesulfonic acid
$C_4H_{10}O_4S$ 154.187
Syrup. d^{21} 1.36.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 889A; 889B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1432A (*nmr*)
Aschütz, R. *et al., Annalen*, 1918, **415**, 89 (*synth*)
Goldberg, A.A. *et al., J.C.S.*, 1942, 716-718 (*synth*)
Challenger, F. *et al., Biochem. J.*, 1970, **117**, 65p-66p (*occur*)
Wooton, D.L. *et al., J.O.C.*, 1974, **39**, 2112-2114 (*synth*)
Hoskin, F.C.G. *et al., Arch. Biochem. Biophys.*, 1977, **180**, 583-586 (*biosynth*)
King, J.F. *et al., Can. J. Chem.*, 1983, **61**, 1583 (*chloride*)
Barrow, K.D. *et al., Phytochemistry*, 1993, **34**, 1429-1430 (*isol, pmr, cmr*)
Simon-Colin, C. *et al., Phycol. Res.*, 2002, **50**, 125-128 (*isol*)
Simon-Colin, C. *et al., Phytochem. Rev.*, 2005, **3**, 367-370 (*isol, purif*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANL100; HKI500

1-(1-Hydroxyethyl)-β-carboline H-615

α-*Methyl-9*H-*pyrido[3,4-*b*]indole-1-methanol, 9CI*



$C_{13}H_{12}N_2O$ 212.251
λ_{max} 211 (ε 6030); 234 (ε 9770); 287 (sh) (ε 6170); 337 (ε 1020) (EtOH) (Derep).

(*S*)-*form* [110282-66-1]
Alkaloid from the marine bryozoan *Costaticella hastata*.
Mp 163-169° dec. $[\alpha]_D^{25}$ -11.4 (MeOH).
Blackman, A.J. *et al., J. Nat. Prod.*, 1987, **50**, 494 (*isol, uv, ir, pmr, ms, struct*)
Bracher, F. *et al., Annalen*, 1993, 837 (*synth*)

(2-Hydroxyethyl)dimethylsulfoxonium(1+) H-616

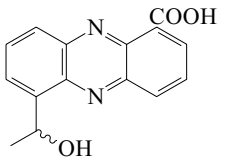
$Me_2S(O)CH_2CH_2OH$
$C_4H_{11}O_2S^{\oplus}$ 123.196
Prod. by the marine bryozoan *Alcyonidium gelatinosum*. Also isol. from sponge *Theonella* aff. *mirabilis*. Dermatitic agent. Causative agent of Dogger Bank itch. Sol. H_2O.
▶ Dermatitic agent.
Carlé, J.S. *et al., Bull. Soc. Chim. Belg.*, 1980, **89**, 1087-1091 (*isol*)
Carlé, J.S. *et al., J.A.C.S.*, 1980, **102**, 5107-5108 (*isol, struct*)
Warabi, K. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2001, **128**, 27-30 (*isol, sponge*)

N-(2-Hydroxyethyl)glycine, 9CI H-617

Petalonine
[5835-28-9]
$HOCH_2CH_2NHCH_2COOH$
$C_4H_9NO_3$ 119.12
Constit. of *Petalonia fascia*. Cryst. (EtOH aq.). Sol. H_2O.
Mp 186-188°.
Takagi, N. *et al., Yakugaku Zasshi*, 1970, **90**, 899-902; *CA*, **73**, 127782u (*isol*)
Lowe, G. *et al., J.C.S. Perkin 1*, 1997, 539-546 (*synth, pmr, cmr*)
Greiner, B. *et al., Helv. Chim. Acta*, 1999, **82**, 2151-2159 (*synth, pmr*)

6-(1-Hydroxyethyl)-1-phenazinecarboxylic acid H-618

Saphenic acid. *DC 86Y. Antibiotic DC 86Y*
[94448-14-3]



$C_{15}H_{12}N_2O_3$ 268.271

Phenazine antibiotic. Prod. by *Streptomyces luteogriseus* and *Streptomyces antibioticus*. Biol. inactive. Yellow needles. Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 223-225°. $[\alpha]_D^{20}$ +55.8 (c, 1.0 in DMSO). λ_{max} 252 (ε 79000); 363 (ε 14000) (MeOH) (Derep). λ_{max} 253 (ε 84000); 367 (ε 16000) (MeOH) (Berdy). λ_{max} 255 (ε 58100); 365 (ε 13200) (EtOH) (Berdy).

▶ LD_{50} (mus, ipr) 300 mg/kg.

6-Deoxy-α-L-glucopyranose-2-yl ester: 2′-L-Quinovosyl saphenate
[137570-43-5]
$C_{21}H_{22}N_2O_7$ 414.414
Isol. from a *Streptomyces* sp. Amorph. yellow solid. $[\alpha]_D$ -35 (c, 0.49 in MeOH). λ_{max} 252 (ε 74100); 365 (ε 14200) (EtOH) (Derep).

6-Deoxy-α-L-glucopyranose-3-yl ester: 3′-L-Quinovosyl saphenate
[137570-42-4]
$C_{21}H_{22}N_2O_7$ 414.414
Isol. from a *Streptomyces* sp. Amorph. yellow solid. $[\alpha]_D$ -40 (c, 0.73 in MeOH). λ_{max} 252 (ε 74100); 365 (ε 14200) (EtOH) (Derep).

Me ester: [73634-72-7]
$C_{16}H_{14}N_2O_3$ 282.298
Prod. by *Streptomyces* sp. Phosphodiesterase inhibitor.

O-*(Hydroxyacetyl):* ***Antibiotic DC 86M***. *DC 86M*
[94448-15-4]
$C_{17}H_{14}N_2O_5$ 326.308
Prod. by *Streptomyces luteogriseus*. Active against gram-positive and -negative bacteria and murine sarcoma. Yellow needles. Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 185-187°. $[\alpha]_D^{20}$ -43.8 (c, 0.5 in $CHCl_3$). λ_{max} 252 (ε 79000); 363 (ε 14000) (MeOH) (Derep).

▶ LD_{50} (mus, ipr) 20 mg/kg.

O-*(Chloroacetyl): Antibiotic DC 86C. DC 86C*
$C_{17}H_{13}ClN_2O_4$ 344.753
Semisynth., prod. from DC 86Y. Shows strong antibacterial activity. Yellow solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 154-156°. $[\alpha]_D^{25}$ -54 (c, 0.6 in $CHCl_3$). λ_{max} 254; 364 (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 40 mg/kg.

O-*(*tert*-Butoxyacetyl): Antibiotic DC 86R. DC 86R*
$C_{21}H_{22}N_2O_5$ 382.415
Semisynthetic. Biol. inactive. Yellow needles. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 189-192°. $[\alpha]_D^{25}$ -34.6 (c, 0.5 in $CHCl_3$). λ_{max} 252; 364 (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 250 mg/kg.

O-*(12-Methyltridecanoyl):* [120464-89-3]
$C_{29}H_{38}N_2O_4$ 478.63
From *Streptomyces antibioticus*.

O-*Tetradecanoyl:* [120482-16-8]
$C_{29}H_{38}N_2O_4$ 478.63
From *Streptomyces antibioticus*.

O-*(12-Methyltetradecanoyl):* [120464-90-6]
$C_{30}H_{40}N_2O_4$ 492.657
From *Streptomyces antibioticus*.

O-*(14-Methylpentadecanoyl):* [120464-91-7]
$C_{31}H_{42}N_2O_4$ 506.684
From *Streptomyces antibioticus*.

O-*Hexadecanoyl:* [120464-92-8]
$C_{31}H_{42}N_2O_4$ 506.684
From *Streptomyces antibioticus*.

O-*(14-Methylhexadecanoyl):*
$C_{32}H_{44}N_2O_4$ 520.711
From *Streptomyces antibioticus*.

O-*(16-Methylheptadecanoyl):* [120464-94-0]
$C_{33}H_{46}N_2O_4$ 534.737
From *Streptomyces antibioticus*.

O-*Benzoyl:* O-*Benzoylsaphenic acid*. ***Shisen 1***
[221300-00-1]
$C_{22}H_{16}N_2O_4$ 372.379
Prod. by *Streptoplanospora viridis*. Active against MRSA. Yellow powder. λ_{max} 254; 364 (no solvent reported).

O-*(2-Hydroxy-6-methylbenzoyl):* ***Saphenamycin***. *A 32256. Antibiotic A 32256*
[83198-27-0]
$C_{23}H_{18}N_2O_5$ 402.406
From *Streptomyces canarius* and other *Streptomyces* spp. Active against gram-positive and -negative bacteria. Weak antitumour props. Mosquito larvicide. Yellow prisms ($CHCl_3$/hexane).
Mp 200-202°. λ_{max} 254 (ε 95000); 300 (ε 15000); 348 (ε 17000); 364 (ε 22000) (EtOH/NaOH) (Derep). λ_{max} 207 (ε 51000); 255 (ε 86700); 365 (ε 13700) (EtOH) (Derep).

▶ SG1576540

Me ether, Me ester: [73634-71-6]
$C_{17}H_{16}N_2O_3$ 296.325
From *Streptomyces* sp. Phosphodiesterase inhibitor.

Me ether: 6-(1-Methoxyethyl)-1-phenazinecarboxylic acid. ***Saphenic acid methyl ether***
[120464-87-1]
$C_{16}H_{14}N_2O_3$ 282.298
From *Streptomyces antibioticus*. Yellow needles (Me_2CO/hexane).
Mp 158-159° dec. $[\alpha]_D^{24}$ +9.1 (c, 0.54 in $CHCl_3$).

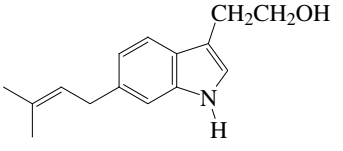
Ketone: ***6-Acetyl-1-phenazinecarboxylic acid***
[120464-88-2]
$C_{15}H_{10}N_2O_3$ 266.256
From *Streptomyces antibioticus*. Yellow needles (Me_2CO).
Mp 219-221°. Turns brown in light.

[137570-44-6, 137570-45-7]

Japan. Pat., 1980, 80 3 737; *CA*, **92**, 213541 (*isol, struct, props*)
Kitahara, M. *et al., J. Antibiot.*, 1982, **35**, 1412 (*Saphenamycin*)
Asano, K. *et al., J. Antibiot.*, 1986, **39**, 619 (*isol*)
Takahashi, K. *et al., J. Antibiot.*, 1986, **39**, 624 (*struct, uv, pmr, ms, props*)
Geiger, A. *et al., J. Antibiot.*, 1988, **41**, 1542 (*derivs*)
Pathirana, C. *et al., J.O.C.*, 1992, **57**, 740 (*glycosyl esters*)
Van't Land, C.W. *et al., J.O.C.*, 1993, **58**, 6576 (*Saphenamycin, biosynth*)
Yue, H. *et al., CA*, 1999, **130**, 234411q (*Shisen 1*)
Petersen, L. *et al., Synthesis*, 1999, 1763-1766 (*synth, cmr*)
Laursen, J.B. *et al., Bioorg. Med. Chem.*, 2003, **11**, 723-731 (*Saphenamycin, synth*)

3-(2-Hydroxyethyl)-6-prenylindole H-619

*6-(3-Methyl-2-butenyl)-1*H*-indole-3-ethanol, 9CI. 3-(2-Hydroxyethyl)-6-(3-methyl-2-butenyl)indole. 6-Prenyltryptophol*
[583060-24-6]



$C_{15}H_{19}NO$ 229.321
Alkaloid from a marine *Streptomyces* sp. (BL-49-58-005). Cytotoxic. λ_{max} 226; 282 (MeOH).

*Carboxylic acid, nitrile: 6-(3-Methyl-2-butenyl)-1*H*-indole-3-acetonitrile. 3-Cyanomethyl-6-prenylindole*
[583060-26-8]
$C_{15}H_{16}N_2$ 224.305
Prod. by a marine *Streptomyces* sp. (BL-49-58-005). λ_{max} 226; 278 (MeOH).

Aldehyde, oxime: [583060-25-7]
$C_{15}H_{18}N_2O$ 242.32

Prod. by a marine *Streptomyces* sp. (BL-49-58-005). Cytotoxic. λ_{max} 226; 280 (MeOH).

Sánchez López, J.M. *et al., J. Nat. Prod.*, 2003, **66**, 863-864 (*isol, pmr, cmr*)

(2-Hydroxyethyl)trimethylarsonium(1+) H-620

Arsenocholine
[39895-81-3]
$[Me_3AsCH_2CH_2OH]^{\oplus}$
$C_5H_{14}AsO^{\oplus}$ 165.087
Claimed isolation from marine crustacea (prawns). Nat. occurrence doubtful. Largely excreted unchanged within 3d when administered orally to small mammals. Main metab. is Arsenobetaine, A-683.

Chloride: [84796-08-7]
$C_5H_{14}AsClO$ 200.539
Hygroscopic white cryst. (pentanol/Et_2O). Mp 230°.

Bromide: [71802-31-8]
$C_5H_{14}AsBrO$ 244.991
Synth. from $AsMe_3$ + $BrCH_2CH_2OH$ at 75° for 3 d. V. hygroscopic white cryst. (MeCN). Mp 227° Mp 238-241°.

Iodide: [86947-37-7]
$C_5H_{14}AsIO$ 291.991
Synth. from the bromide + NaI in MeCN for 2 h in the dark at r.t. White cryst. (MeCN). Mp 213-215°. Must be stored in the dark.

Nitrate: [115195-57-8] Synth. from the bromide and $AgNO_3$. Cryst. (MeCN). Mp 119-121°.

Hydroxide: [86947-42-4]
$C_5H_{15}AsO_2$ 182.094
Stable only in soln.

4-Methylbenzenesulfonate: [115195-62-5]
Hygroscopic white cryst. (Me_2CO). Mp 104°.

Tetraphenylborate:
Cryst. (Me_2CO aq.). Mp 262°.

O-*Ac, bromide: Acetylarsenocholine bromide*
[51860-39-0]
$C_7H_{16}AsBrO_2$ 287.028
Cryst. (EtOAc). Mp 107°.

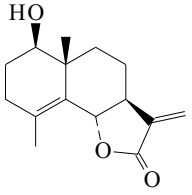
O-*Ac, iodide:*
$C_7H_{16}AsIO_2$ 334.028
Hygroscopic white cryst. (MeCN/EtOAc). Mp 103°.

O-*Ac, picrate:*
Yellow cryst. (EtOH). Mp 123°.

[115195-61-4]

Kunz, H. *et al., Annalen*, 1973, 2001 (*synth*)
Bollino, N.R. *et al., ACS Symp. Ser.*, 1978, **82**, 116
Norin, H. *et al., Chemosphere*, 1982, **11**, 287 (*isol, pmr, ms*)
Hedlund, B. *et al., J. Neurochem.*, 1982, **39**, 871
Marafante, E. *et al., Sci. Total Environ.*, 1984, **34**, 223 (*metab*)
Irgolic, K.J. *et al., Appl. Organomet. Chem.*, 1987, **1**, 403 (*synth, pmr, cmr*)
Siu, K.W. *et al., Rapid Commun. Mass Spectrom.*, 1988, **2**, 69 (*ms*)
Kostick, A. *et al., Acta Cryst. C*, 1989, **45**, 1306 (*synth, pmr, cmr, cryst struct*)
Cullen, W.R. *et al., Appl. Organomet. Chem.*, 1989, **3**, 401
Momplaisir, G.M. *et al., J. Agric. Food Chem.*, 1991, **39**, 1448 (*synth, hplc*)
Francesconi, K.A. *et al., Appl. Organomet. Chem.*, 1992, **6**, 247 (*formn, isol*)
Edmonds, J.S. *et al., Nat. Prod. Rep.*, 1993, **10**, 421 (*rev*)
Minhas, R. *et al., Adv. Organomet. Chem.*, 1998, **12**, 635-641 (*synth, pmr, cmr, ms*)

1-Hydroxy-4,11(13)-eudesmadien-12,6-olide H-621



(1β,6α)–*form*

$C_{15}H_{20}O_3$ 248.321

(1β,6α)-*form*
Magnolialide. *Splendolide. 10-Hydroxycichopumilide (incorr.)*
[72145-13-2]
Constit. of *Artemisia splendens*, *Magnolia grandiflora* and *Cichorium pumilum*. Shows differentiation inducing effect on leukaemia cells. Cryst. (hexane/Et_2O).
Mp 152-153°. $[\alpha]_D^{25}$ +74 (c, 0.23 in EtOH). Struct. of the compd. formerly called 10-Hydroxycichopumilide revised in 2001.

11β,13-Dihydro: 1-Hydroxy-4(15)-eudesmen-12,6-olide. ***Dihydromagnolialide***
$C_{15}H_{22}O_3$ 250.337
Isol. from *Artemisia tridentata* ssp. *wyomingensis* and *Cichorium pumilum*. Cryst. (Et_2O/petrol).
Mp 173-175° (130-131°). $[\alpha]_D^{31}$ +37 (c, 2.07 in $CHCl_3$). Struct. of isolate from *C. pumilum* revised in 2001.

(1α,6α)-*form*
11β,13-Dihydro: [82292-50-0]
$C_{15}H_{22}O_3$ 250.337
Constit. of *Artemisia spicigera*. Oil. $[\alpha]_D$ +56 (c, 1.9 in $CHCl_3$).

11β,13-Dihydro, Ac:
$C_{17}H_{24}O_4$ 292.374
Constit. of *Artemisia hugueti*. Oil. $[\alpha]_D$ +93.5 (c, 4.36 in $CHCl_3$).

11β,13-Dihydro, 1-ketone: ***1-Oxo-4(15)-eudesmen-12,6-olide***
[66321-33-3]
$C_{15}H_{20}O_3$ 248.321
Constit. of *Artemisia canariensis*.

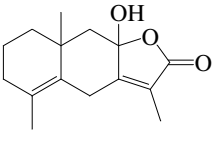
(*ent*-1β,6α)-*form*
1-Hydroxy-4,11(13)-steiractinadien-12,6β-olide
[125356-46-9]
Isol. from *Geigeria rigida*.
Gum.

(1α,5β,6β,10α)-*form*
11β,13-Dihydro: [865668-53-7]
$C_{15}H_{22}O_3$ 250.337
Constit. of a *Eunicea* sp. Oil. $[\alpha]_D^{25}$ +25.8 (c, 1.1 in $CHCl_3$).

Shafizadeh, F. *et al., Phytochemistry*, 1971, **10**, 2745
Ando, M. *et al., Tetrahedron*, 1977, **33**, 2785 (*synth*)
El-Feraly, F.S. *et al., Phytochemistry*, 1979, **18**, 881 (*Magnolialide*)
El-Masry, S. *et al., Phytochemistry*, 1984, **23**, 183-185 (*Chicorium pumilum constits*)
Van Hijfte, L. *et al., Tetrahedron*, 1984, **40**, 4371 (*synth*)
Zdero, C. *et al., Phytochemistry*, 1989, **28**, 3105 (*1-Hydroxysteiractinadienolide*)
Serkerov, S.V. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1991, **27**, 173-175 (*Splendolide*)
Marco, J.A. *et al., Phytochemistry*, 1993, **32**, 460; 1994, **37**, 477 (*dihydro, dihydro Ac, isol, pmr, cmr*)
Mansilla, H. *et al., Phytochemistry*, 1999, **51**, 995-997 (*dihydro 1-ketone*)
Lee, K.-T. *et al., Biol. Pharm. Bull.*, 2000, **23**, 1005-1007 (*Magnolialide, activity*)
Kisiel, W. *et al., Phytochemistry*, 2001, **57**, 523-527 (*struct*)
Garzón, S.P. *et al., J. Nat. Prod.*, 2005, **68**, 1354-1359 (*Eunicea constit*)

8-Hydroxy-4,7(11)-eudesmadien-12,8-olide H-622

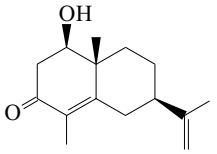
[139742-34-0]



$C_{15}H_{20}O_3$ 248.321
Isol. from the gorgonian *Leptogorgia piccola*.
$[\alpha]_D$ +134 (c, 0.003 in $CHCl_3$). Prob. artifact of oxidn. λ_{max} 204 (ϵ 5500); 215 (ϵ 3100); 220 (ϵ 5100) (MeOH).

Roussis, V. *et al., New J. Chem.*, 1991, **15**, 959-961 (*isol, pmr, cmr, struct*)

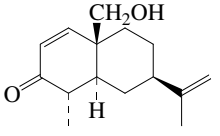
1-Hydroxy-4,11-eudesmadien-3-one H-623



$C_{15}H_{22}O_2$ 234.338

1β-*form*
Ligucyperonol. *1β-Hydroxy-α-cyperone*
Constit. of *Artemisia caerulescens*, *Ligularia dentata* and *Senecio bracteolatus*. Also isol. from the soft coral, *Sinularia* sp. Cytotoxic agent. Needles (Et_2O/pentane).
Mp 121-123°. $[\alpha]_D^{23}$ -75 (c, 0.94 in $CHCl_3$). $[\alpha]_D^{22}$ +85 (c, 1.1 in $CHCl_3$). The opposite opt. rotns. reported are unexplained.
Bohlmann, F. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 707 (*isol, pmr*)
Naya, K. *et al., Bull. Chem. Soc. Jpn.*, 1990, **63**, 2239
Sanz, J.F. *et al., Phytochemistry*, 1990, **29**, 2913 (*isol, pmr, cmr*)
Sheu, J.-H. *et al., J. Chin. Chem. Soc. (Taipei)*, 1999, **46**, 253-257 (*isol, activity*)

14-Hydroxy-1,11-eudesmadien-3-one H-624



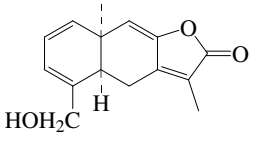
4α-form

$C_{15}H_{22}O_2$ 234.338

4α-*form* [181130-69-8]
Constit. of an Antarctic sponge.

(4α,5β,10α)-*form*
Ainigmaptilone A
[553641-40-0]
Constit. of *Ainigmaptilon antarcticus*.
Oil. $[\alpha]_D^{24}$ +26.8 (c, 0.23 in $CHCl_3$). λ_{max} 244 (ϵ 8000) (MeOH).
Urban, S. *et al., Nat. Prod. Lett.*, 1995, **6**, 187 (*isol, pmr, cmr*)
Iken, K.B. *et al., J. Nat. Prod.*, 2003, **66**, 888-890 (*Ainigmaptilone A*)

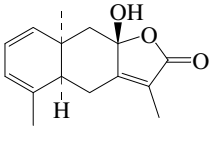
15-Hydroxy-1,3,7(11),8-eudesmatetraen-12,8-olide H-625



$C_{15}H_{16}O_3$ 244.29

(5α,10α)-*form*
Ac: ***Tubipolide G***
[385793-37-3]
$C_{17}H_{18}O_4$ 286.327
Constit. of *Tubipora musica*. Oil. $[\alpha]_D^{25}$ +22.6 (c, 0.02 in $CHCl_3$). λ_{max} 246 (log ϵ 4.24); 263 (log ϵ 3.27) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 2001, **64**, 1430-1433 (*isol, pmr, cmr*)

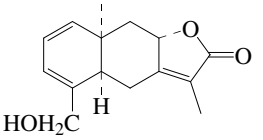
8-Hydroxy-1,3,7(11)-eudesmatrien-12,8-olide H-626



$C_{15}H_{18}O_3$ 246.305

(5α,8β*OH*,10α)-*form*
Tubipolide D
[385793-35-1]
Constit. of *Tubipora musica*.
Oil. $[\alpha]_D^{25}$ -29.6 (c, 0.04 in $CHCl_3$). λ_{max} 235 (log ϵ 4.29); 262 (log ϵ 3.16) (MeOH).
Duh, C.Y. *et al., J. Nat. Prod.*, 2001, **64**, 1430-1433 (*isol, pmr, cmr*)

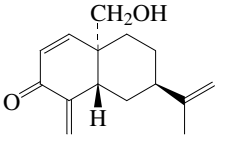
15-Hydroxy-1,3,7(11)-eudesmatrien-12,8-olide H-627



$C_{15}H_{18}O_3$ 246.305

(5α,8α,10α)-*form*
Ac: ***Tubipolide A***
[385793-32-8]
$C_{17}H_{20}O_4$ 288.343
Constit. of *Tubipora musica*. Oil. $[\alpha]_D^{25}$ -72.4 (c, 0.03 in $CHCl_3$). λ_{max} 226 (log ϵ 4.26); 262 (log ϵ 3.08) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 2001, **64**, 1430-1433 (*isol, pmr, cmr*)

14-Hydroxy-1,4(15),11-eudesmatrien-3-one H-628

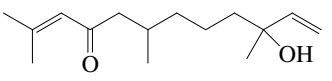


$C_{15}H_{20}O_2$ 232.322

(5β,10α)-*form*
Ainigmaptilone B
[553641-42-2]
Constit. of *Ainigmaptilon antarcticus*.
Oil. $[\alpha]_D^{24}$ -63.1 (c, 0.23 in $CHCl_3$).
Iken, K.B. *et al., J. Nat. Prod.*, 2003, **66**, 888-890 (*isol, pmr, cmr*)

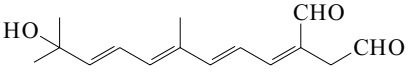
3-Hydroxy-1,10-farnesadien-9-one H-629

3-Hydroxy-3,7,11-trimethyl-1,10-dodecadien-9-one. ***Mucronatone***
[771533-64-3]



$C_{15}H_{26}O_2$ 238.369
Constit. of fruits of *Rhizophora mucronata*. Oil. $[\alpha]_D^{27}$ -16.66 (c, 0.04 in $CHCl_3$). λ_{max} 223 (log ϵ 4.16) (MeOH).
Laphookhie, S. *et al., Chem. Pharm. Bull.*, 2004, **52**, 883-885 (*isol, pmr, cmr*)

11-Hydroxy-3,5,7,9-farnesatetraene-1,15-dial H-630

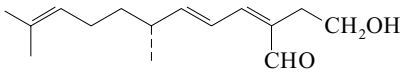


$C_{15}H_{20}O_3$ 248.321

(3*Z*,5*E*,7*E*,9*E*)-*form*
Rhipocephenal
[71135-77-8]
Constit. of *Rhipocephalus phoenix*. Fish antifeedant.
Oil. λ_{max} 350 (ϵ 45000) (MeOH) (Berdy).
Sun, H.H. *et al., Tet. Lett.*, 1979, 685

1-Hydroxy-3,5,10-farnesatrien-15-al H-631

2-(2-Hydroxyethyl)-6,10-dimethyl-2,4,9-undecatrienal



$C_{15}H_{24}O_2$ 236.353

(3Z,5E,7R)-form

Preraikovenal

[159736-49-9]

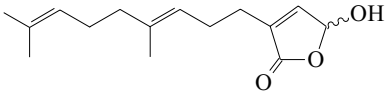
Constit. of *Euplotes raikovi*. Putative biogenetic precursor of Raikovenal, R-2.

Guella, G. *et al., Chem. Comm.*, 1994, 2585 (*isol, pmr, cmr*)
Snider, B.B. *et al., Synth. Commun.*, 1997, **27**, 1583-1600 (*synth, pmr, cmr*)

1-Hydroxy-2,6,10-farnesatrien-15,1-olide H-632

Dictyodendrillin C

[170717-27-8]



$C_{15}H_{22}O_3$ 250.337

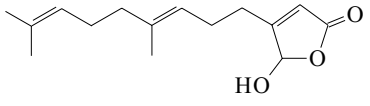
Constit. of a *Dictyodendrilla* sp.

Tran, N.H. *et al., Aust. J. Chem.*, 1995, **48**, 1757 (*isol, pmr, cmr*)

15-Hydroxy-2,6,10-farnesatrien-1,15-olide H-633

Dictyodendrillin B

[170557-40-1]

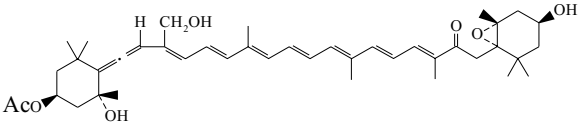


$C_{15}H_{22}O_3$ 250.337

Constit. of a *Dictyodendrilla* sp.

Tran, N.H. *et al., Aust. J. Chem.*, 1995, **48**, 1757 (*isol, pmr, cmr*)

19′-Hydroxyfucoxanthin H-634



$C_{42}H_{58}O_7$ 674.916

19′-Hexanoyl: ***19′-Hexanoyloxyfucoxanthin***

[60147-85-5]

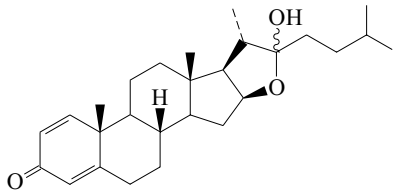
$C_{48}H_{68}O_8$ 773.06

Isol. from *Coccolithus huxleyi* and other marine organisms. λ_{max} 423; 450 (Me_2CO).

Arpin, N. *et al., Phytochemistry*, 1976, **15**, 529 (*occur, ir, pmr, ms*)
Hertzberg, S. *et al., Phytochemistry*, 1977, **16**, 587 (*struct*)
Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495 (*occur*)

22-Hydroxyfurosta-1,4-dien-3-one H-635

[161776-74-5]



$C_{27}H_{40}O_3$ 412.611

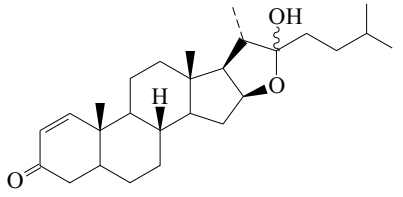
22ξ-form

Constit. of *Alcyonium gracillimum*.
Cryst.
Mp 123-124°. $[\alpha]_D$ -10.2 (c, 0.5 in $CHCl_3$). λ_{max} 236 (ϵ 13000) (MeCN) (Berdy).

Seo, Y. *et al., Tetrahedron*, 1995, **51**, 2497 (*isol, pmr, cmr*)

22-Hydroxyfurost-1-en-3-one H-636

[161776-73-4]



$C_{27}H_{42}O_3$ 414.627

22ξ-form

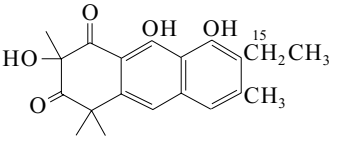
Constit. of *Alcyonium gracillimum*.
Solid.
Mp 43-45°. $[\alpha]_D$ -3.8 (c, 0.5 in $CHCl_3$). λ_{max} 225 (ϵ 11100) (MeCN) (Berdy).

Seo, Y. *et al., Tetrahedron*, 1995, **51**, 2497 (*isol, pmr, cmr*)

2-Hydroxygarveatin B H-637

7-Ethyl-2,8,9-trihydroxy-2,4,4,6-tetramethyl-1,3(2H,4H)-anthracenedione, 9CI

[109894-11-3]



$C_{20}H_{22}O_5$ 342.391

Constit. of *Garveia annulata*. Yellow solid.

15-Oxo: ***2-Hydroxygarveatin A***

[109894-10-2]

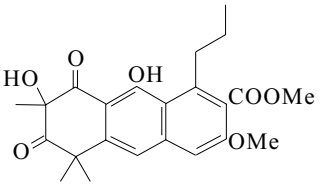
$C_{20}H_{20}O_6$ 356.374

Constit. of *Garveia annulata*. Orange solid. Sol. MeOH, hexane; poorly sol. H_2O. λ_{max} 226; 278; 318; 332; 385 (MeOH) (Berdy).

Fahy, E. *et al., Can. J. Chem.*, 1987, **65**, 376

2-Hydroxygarvin A H-638

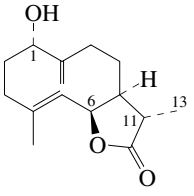
[99457-97-3]



$C_{23}H_{26}O_7$ 414.454
Metab. of *Garveia annulata*. Yellow needles (Et_2O).
Mp 195°. $[\alpha]_D$ +5.5 (c, 1.2 in $CHCl_3$). λ_{max} 226 (ϵ); 278 (ϵ); 318 (ϵ); 332 (ϵ); 385 (ϵ) (MeOH) (Derep).

Fahy, E. *et al., J.O.C.*, 1986, **51**, 57

1-Hydroxy-4,10(14)-germacradien-12,6-olide H-639



(1α,4*E*,6β,11β*H*)-*form*

$C_{15}H_{22}O_3$ 250.337

(1α,4*E*,6β,11β*H*)-*form* [865668-54-8]
Constit. of a *Eunicea* sp.
Oil. $[\alpha]_D^{25}$ +24.6 (c, 1.1 in $CHCl_3$).

(1β,4*E*,6α,11α*H*)-*form*
Constit. of *Artemisia herba*.
Oil.

11,13-Didehydro: 1β-Hydroxy-4,10(14),11(13)-germacratrien-12,6α-olide. ***Artemorin****. Deoxyperoxycostunolide*
[64845-92-7]
$C_{15}H_{20}O_3$ 248.321
Constit. of *Artemisia verlotorum* and others. Cryst. (CH_2Cl_2/Et_2O).
Mp 120-121°. $[\alpha]_D$ +89.

1-Ketone: ***1-Oxo-4(10),14-germacradien-12,6α-olide***
[69075-68-9]
$C_{15}H_{20}O_3$ 248.321
Isol. from *Artemisia herba-alba*. Oil. $[\alpha]_D^{23}$ +83 (c, 0.2 in $CHCl_3$).

11,13-Didehydro, 1-ketone: 1-Oxo-4,10(14),11(13)-germacratrien-12,6α-olide. ***Anhydroverlotorin***
[32619-90-2]
$C_{15}H_{18}O_3$ 246.305
Constit. of *Artemisia verlotorum*. Cryst. (Et_2O).
Mp 123-124°.

(1β,4*E*,6α,11β*H*)-*form*
Gallicin†
[69075-77-0]
Constit. of *Artemisia maritima*.
Mp 114-116°. $[\alpha]_D$ +121 (c, 0.3 in $CHCl_3$).

1-Ketone: [125675-20-9]
$C_{15}H_{20}O_3$ 248.321
From *Artemisia maritima*. Cryst.
Mp 132°.

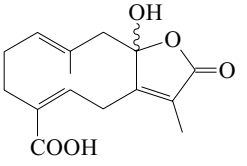
1-Ketone, 10α,14-dihydro: ***1-Oxo-4-germacren-12,6α-olide***
$C_{15}H_{22}O_3$ 250.337
Isol. from *Artemisia maritima*. Oil.

11,13-Didehydro, 1-hydroperoxide: 1β-Hydroperoxy-4,10(14),11(13)-germacratrien-12,6-olide. ***Verlotorin****. Peroxycostunolide*
[31105-79-0]
$C_{15}H_{20}O_4$ 264.321
Constit. of *Magnolia grandiflora*. Cryst. (Et_2O/EtOH).
Mp 141°. $[\alpha]_D^{25}$ +171 (c, 0.2 in Me_2CO).

[81679-95-0]

Geissman, T.A. *et al., Phytochemistry*, 1970, **9**, 2377 (*Anhydroverlotorin, Artemorin*)
Gonzalez, A.G. *et al., J.C.S. Perkin 1*, 1978, 1243 (*Gallicin*)
El-Feraly, F.S. *et al., J.O.C.*, 1979, **44**, 3952 (*Verlotorin*)
Gonzalez, A.G. *et al., Tet. Lett.*, 1979, 3769 (*conformn, Gallicin*)
Gordon, M.M. *et al., J. Nat. Prod.*, 1981, **44**, 432 (*isol*)
Shimizu, T. *et al., Heterocycles*, 1982, **17**, 53 (*synth*)
Pathak, V.P. *et al., Phytochemistry*, 1987, **26**, 2103 (*isol, derivs*)
Marco, J.A. *et al., Phytochemistry*, 1989, **28**, 3121 (*isol, pmr*)
Garzón, S.P. *et al., J. Nat. Prod.*, 2005, **68**, 1354-1359 (*Eunicea constit*)

8-Hydroxy-1(10),4,7(11)-germacratrien-12,8-olid-15-oic acid H-640

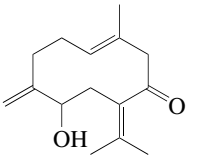


$C_{15}H_{18}O_5$ 278.304

(1(10)*E*,4*Z*,8ξ)-*form*
Me ester: ***Edwardsolide A***
[158446-28-7]
$C_{16}H_{20}O_5$ 292.331
Constit. of *Maasella edwardsi*.
$[\alpha]_D$ -0.9 (c, 0.5 in MeOH).

Bifulco, G. *et al., Nat. Prod. Lett.*, 1993, **3**, 167 (*isol, pmr, cmr*)

5-Hydroxy-1(10),4(15),7(11)-germacratrien-8-one H-641

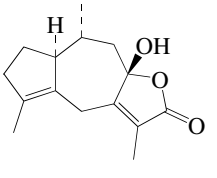


$C_{15}H_{22}O_2$ 234.338

(1(10)*E*, 5ξ)-*form* [222850-09-1]
Constit. of *Phyllogorgia dilatata*.
Pale yellow oil. $[\alpha]_D^{20}$ -8.78 (c, 0.026 in MeOH). λ_{max} 249 (3.17) ($CHCl_3$).

Martins, D.L. *et al., J. Braz. Chem. Soc.*, 1998, **9**, 586-590; *CA*, **130**, 279449z (*isol, pmr, cmr*)

8-Hydroxy-4,7(11)-guaiadien-12,8-olide H-642



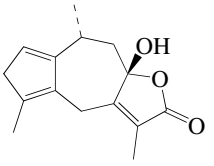
$C_{15}H_{20}O_3$ 248.321

(1α,8β*OH*,10α)-*form*
Americanolide E
[185614-64-6]
Constit. of *Pseudopterogorgia americana*.
Unstable yellow oil.

Me ether: 8-Methoxy-4,7(11)-guaiadien-12,8-olide. **O-*Methyla-mericanolide E***. *Methoxyamericanolide E (incorr.)*

[185614-67-9]
$C_{16}H_{22}O_3$ 262.348
Constit. of *Pseudopterogorgia americana*. Yellow oil. $[\alpha]_D^{23}$ -44 (c, 0.5 in $CHCl_3$). λ_{max} 208 (ϵ 10066) (MeOH).
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 207-211 (*isol, pmr, cmr*)

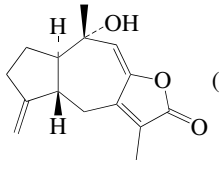
8-Hydroxy-1,4,7(11)-guaiatrien-12,8-olide H-643



$C_{15}H_{18}O_3$ 246.305

(8β*OH*,10α)-*form*
Me ether: 8-Methoxy-1,4,7(11)-guaiatrien-12,8-olide. ***Methoxyamericanolide G***
[185614-69-1]
$C_{16}H_{20}O_3$ 260.332
Constit. of *Pseudopterogorgia americana*. Yellow oil. $[\alpha]_D^{23}$ -60 (c, 1 $CHCl_3$). λ_{max} 212 (ϵ 10458); 254 (ϵ 2679); 282 (ϵ 1132) (MeOH). λ_{max} 212 (ϵ 10458); 254 (ϵ 2679) (MeOH) (Berdy).
Rodríguez, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 207-211 (*isol, pmr, cmr*)

10-Hydroxy-4(15),7(11),8-guaiatrien-12,8-olide H-644



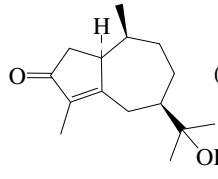
(1α,5β,10α)-form

$C_{15}H_{18}O_3$ 246.305

(1α,5β,10α)-*form*
Menverin B
[838862-36-5]
Constit. of *Menella verrucosa*.
Oil. $[\alpha]_D^{20}$ -53 (c, 0.08 in $CHCl_3$). λ_{max} 273 (log ϵ 3.69) (MeOH).

(1α,5β,10β)-*form*
Menverin A
[838862-35-4]
Constit. of *Menella verrucosa*.
Oil. $[\alpha]_D^{20}$ -160 (c, 0.09 in $CHCl_3$). λ_{max} 273 (log ϵ 4.06) (MeOH).
Zhang, W. *et al., Helv. Chim. Acta*, 2004, **87**, 2919-2925 (*Menverins A and B*)

11-Hydroxy-4-guaien-3-one H-645



(1α,7β,10β)-*form*

$C_{15}H_{24}O_2$ 236.353

(1α,7β,10β)-*form*
Hydroxycolorenone
[20482-28-4]
Constit. of *Euryops pedunculatus* and the coral *Nephthea chabrolii*. Insecticide. Oil. $[\alpha]_D^{24}$ +18 (c, 0.2 in $CHCl_3$). $[\alpha]_D$ +58.6 (c, 0.46 in $CHCl_3$). λ_{max} 248 (ϵ 17000) (MeOH).

Me ether: ***Methoxycolorenone***
[191212-40-5]
$C_{16}H_{26}O_2$ 250.38
Constit. of *Nephthea chabrolii*. Oil. $[\alpha]_D$ +57.4 (c, 0.31 in $CHCl_3$). λ_{max} 250 (ϵ 15000) (MeOH).

(1β,7β,10β)-*form*
Ac: [401892-69-1]
$C_{17}H_{26}O_3$ 278.391
Constit. of *Torilis japonica*.

[191212-39-2]

Jakupovic, J. *et al., Phytochemistry*, 1987, **26**, 1049-1052
Handayani, D. *et al., J. Nat. Prod.*, 1997, **60**, 716-718 (*Me ether, activity*)
Labbé, C. *et al., Phytochemistry*, 1998, **49**, 793-795 (*pmr, cmr*)
Ryu, J.-H. *et al., Arch. Pharmacal Res.*, 2001, **24**, 532-535; *CA*, **136**, 213620r (*Ac*)
Blay, G. *et al., Tetrahedron*, 2001, **57**, 9719-9725 (*synth*)

2-Hydroxyheneicosanoic acid H-646

[93361-62-7]
$H_3C(CH_2)_{18}CH(OH)COOH$
$C_{21}H_{42}O_3$ 342.561

(*R*)-*form*
Me ether: 2-Methoxyheneicosanoic acid
[88416-43-7]
$C_{22}H_{44}O_3$ 356.588
Constit. of the sponge *Higginsia tethyoides*.

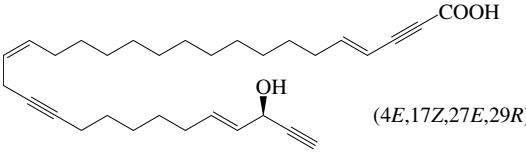
(ξ)-*form*
Constit. of the sponge *Verongula gigantea* and various microalgae. Also found as constit. of phospholipids and sphingolipids.
Ayanoglu, E. *et al., Lipids*, 1983, **18**, 830-836 (*Me ether*)
Matsumoto, G.I. *et al., Phytochemistry*, 1984, **23**, 1421 (*occur*)
Carballeira, N.M. *et al., Lipids*, 1989, **24**, 229-232 (*isol*)
Hayashi, A. *et al., Biochim. Biophys. Acta*, 1991, **1083**, 179 (*occur*)
Yasugi, E. *et al., J. Biochem. (Tokyo)*, 1991, **110**, 202

13-Hydroxyheneicosanoic acid H-647

$H_3C(CH_2)_7CH(OH)(CH_2)_{11}COOH$
$C_{21}H_{42}O_3$ 342.561

Me ether: 13-Methoxyheneicosanoic acid
$C_{22}H_{44}O_3$ 356.588
Constit. of the red alga *Schizymenia dubyi*.
Barnathan, G. *et al., Phytochemistry*, 1998, **47**, 761-765 (*isol, ms*)

29-Hydroxy-4,17,27-hentriacontatriene-2,20,30-triynoic acid H-648



(4*E*,17*Z*,27*E*,29*R*)-*form*

$C_{31}H_{44}O_3$ 464.687

(4*E*,17*Z*,27*E*,29*R*)-*form*
Corticatic acid B
[160333-32-4]
Isol. from the marine sponge *Petrosia corticata*. Antifungal agent. Oil. $[\alpha]_D^{23}$ +9 (c, 0.04 in $CHCl_3$). λ_{max} 226 (ϵ 12200); 245 (ϵ 11800); 255 (ϵ 8300) (MeOH) (Berdy).

(4*Z*,17*Z*,27*E*,29*R*)-*form*
Corticatic acid A
[160219-89-6]

From *Petrosia corticata*. Antifungal agent. Oil. $[\alpha]_D^{23}$ +28 (c, 0.1 in $CHCl_3$). λ_{max} 227 (ϵ 11500); 246; 253 (MeOH) (Berdy).

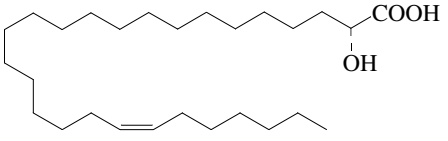
20,21-Dihydro (20Z-): 29-Hydroxy-4,17,20,27-hentriacontatetraene-2,30-diynoic acid. ***Corticatic acid E***
$C_{31}H_{46}O_3$ 466.703
Isol. from *Petrosia corticata*. Oil. $[\alpha]_D^{20}$ -3.1 (c, 0.1 in $CHCl_3$). Possesses 20*Z*-config. λ_{max} 250 (ϵ 6800) (MeOH).
Li, H.-Y. *et al., J. Nat. Prod.*, 1994, **57**, 1464-1467 (*isol, pmr*)
Nishimura, S. *et al., J. Nat. Prod.*, 2002, **65**, 1353-1356 (*isol, ms, abs config*)

2-Hydroxyheptacosanoic acid H-649

[139729-95-6]
$H_3C(CH_2)_{24}CH(OH)COOH$
$C_{27}H_{54}O_3$ 426.722

(ξ)-form
Constit. of the sponges *Aplysina* sp. and *Pseudosuberites* sp. and from earthworm lipids (*Lumbricus terrestris*).
Albro, P.W. *et al., Lipids*, 1992, **27**, 136-143 (*isol*)
Carballeira, N.M. *et al., Lipids*, 1992, **27**, 681-685 (*isol*)
Barnathan, G. *et al., J. Nat. Prod.*, 1993, **56**, 2104-2113 (*isol*)

2-Hydroxy-20-heptacosenoic acid H-650



$C_{27}H_{52}O_3$ 424.706

(2R,20Z)-form
Me ether: 2-Methoxy-20-heptacosenoic acid
[88416-45-9]
$C_{28}H_{54}O_3$ 438.733
Constit. of the sponge *Higginsia tethyoides*.
Ayanoglu, E. *et al., Lipids*, 1983, **18**, 830-836 (*isol*)

2-Hydroxyheptadecanoic acid H-651

[25022-78-0]
$H_3C(CH_2)_{14}CH(OH)COOH$
$C_{17}H_{34}O_3$ 286.454

(ξ)-form
Constit. of the sponges *Aplysina* sp. and *Pseudosuberites* sp. and from earthworm lipids (*Lumbricus terrestris*).
Albro, P.W. *et al., Lipids*, 1992, **27**, 136-143 (*isol*)
Carballeira, N.M. *et al., Lipids*, 1992, **27**, 681-685 (*isol*)
Barnathan, G. *et al., J. Nat. Prod.*, 1993, **56**, 2104-2113 (*isol*)

9-Hydroxyheptadecanoic acid H-652

$H_3C(CH_2)_7CH(OH)(CH_2)_7COOH$
$C_{17}H_{34}O_3$ 286.454

Me ether: 9-Methoxyheptadecanoic acid
$C_{18}H_{36}O_3$ 300.481
Constit. of the red alga *Schizymenia dubyi*.
Barnathan, G. *et al., Phytochemistry*, 1998, **47**, 761-765 (*isol, ms*)

4-Hydroxy-16-heptadecene-5,7-diyn-2-one H-653

Montiporyne K
$H_2C{=}CH(CH_2)_7C{\equiv}CC{\equiv}CCH(OH)CH_2COCH_3$
$C_{17}H_{24}O_2$ 260.375

(ξ)-form
Isol. from the coral *Montipora* sp.
Light yellow oil. λ_{max} 256 (ϵ 479); 293 (ϵ 1134); 309 (ϵ 1145) (MeOH).
Alam, N. *et al., J. Nat. Prod.*, 2001, **64**, 1059-1063

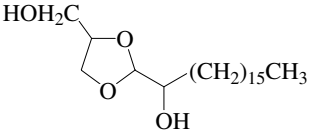
2-Hydroxy-6-heptadecenoic acid H-654

$H_3C(CH_2)_9CH{=}CH(CH_2)_3CH(OH)COOH$
$C_{17}H_{32}O_3$ 284.438

(2ξ,6Z)-form
Me ether: 2-Methoxy-6-heptadecenoic acid
$C_{18}H_{34}O_3$ 298.465
Isol. from *Spheciospongia cuspidifera*.
Carballeira, N.M. *et al., Lipids*, 2002, **37**, 305-308 (*isol, ms*)

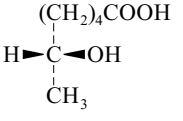
2-(1-Hydroxyheptadecyl)-4-hydroxymethyl-1,3-dioxolane H-655

1,2-O-(2-Hydroxyoctadecyl)glycerol



$C_{21}H_{42}O_4$ 358.56
Constit. of the gorgonian *Junceella juncea*. Powder.
Qi, S.-H. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1476-1478 (*isol, pmr, cmr, ms*)

6-Hydroxyheptanoic acid H-656



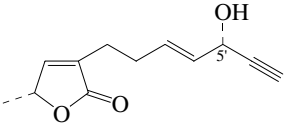
(R)–form

$C_7H_{14}O_3$ 146.186

(R)-form
*3,6-Dideoxy-α-L-*arabino*-hexopyranoside:* ***Daumone***
$C_{13}H_{24}O_6$ 276.329
Isol. from the nematode *Caenorhabditis elegans*. Induces a dauer stage in *C. elegans*. Syrup. $[\alpha]_D$ -85 (c, 0.1 in MeOH).
Lactone: 7-Methyl-2-oxepanone, 9CI. 6-Heptanolide
[69765-34-0]
$C_7H_{12}O_2$ 128.171
$[\alpha]_D^{20}$ +25 (c, 1.8 in $CHCl_3$).

(±)-form
Et ester:
[55099-47-3]
$C_9H_{18}O_3$ 174.239
Liq. $Bp_{0.75}$ 91°.
Lactone: [69854-30-4]
Liq. $Bp_{0.08}$ 46-47°.
[2549-61-3]
Starcher, R.S. *et al., J.A.C.S.*, 1958, **80**, 4079 (*synth*)
Pirkle, W.H. *et al., J.O.C.*, 1979, **44**, 2169 (*synth, ir, pmr*)
Fouque, E. *et al., Synthesis*, 1989, 661 (*synth, pmr, cmr, ms*)
Hester, J.B. *et al., J. Med. Chem.*, 2001, **44**, 1099-1115 (*Et ester*)
Viney, M.F. *et al., Naturwissenschaften*, 2004, **91**, 123-124 (*Daumone, isol*)
Jeong, P.-Y. *et al., Nature (London)*, 2005, **433**, 541-545 (*Daumone, synth, abs config, struct*)
Guo, H. *et al., Org. Lett.*, 2005, **7**, 3921-3924 (*Daumone, synth*)

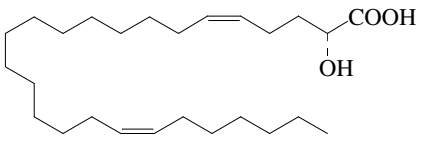
3-(5-Hydroxy-3-hepten-6-ynyl)-5-methyl-2(5*H*)-furanone H-657



$C_{12}H_{14}O_3$ 206.241

(5*R*,5′*S*)-*form*
Isol. from *Sarcophyton trocheliophorum*.
Oil. $[\alpha]_D$ -27.6 (c, 0.07 in EtOH). λ_{max} 212 (log ϵ 3.17) (EtOH).
Rezanka, T. *et al., Tetrahedron*, 2001, **57**, 8743-8749

2-Hydroxy-5,19-hexacosadienoic acid H-658

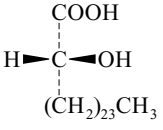


$C_{26}H_{48}O_3$ 408.663

(2*R*,5*Z*,19*Z*)-*form*
Me ether: 2-Methoxy-5,19-hexacosadienoic acid
[88416-39-1]
$C_{27}H_{50}O_3$ 422.69
Constit. of the sponge *Higginsia tethyoides*.
Ayanoglu, E. *et al., Lipids*, 1983, **18**, 830-836 (*isol*)

2-Hydroxyhexacosanoic acid H-659

[14176-13-7]

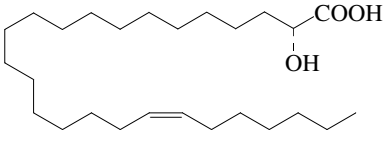


$C_{26}H_{52}O_3$ 412.695

(*R*)-*form* [26631-99-2]
Major component of yeast cerebrin. Also found in brain cerebrosides. Mp 104-105°. $[\alpha]_D^{20}$ +2.1 (c, 2.8 in Py).
Ac:
$C_{28}H_{54}O_4$ 454.732
Cryst. (Me_2CO/petrol). Mp 84.85°.

(ξ)-*form*
Constit. of *Aplysina* sp. and *Pseudosuberites* sp.
[72741-91-4]
Chibnall, A.C. *et al., Biochem. J.*, 1953, **55**, 711 (*isol*)
Hammarström, S. *et al., FEBS Lett.*, 1969, **5**, 192 (*resoln*)
Nurminen, T. *et al., Biochem. J.*, 1971, **125**, 963 (*isol*)
Muralidharan, F.N. *et al., Chem. Phys. Lipids*, 1984, **34**, 257 (*synth*)
Carballeira, N.M. *et al., Lipids*, 1992, **27**, 681-685 (*isol*)
Barnathan, G. *et al., J. Nat. Prod.*, 1993, **56**, 2104-2113 (*isol*)

2-Hydroxy-19-hexacosenoic acid H-660

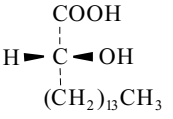


$C_{26}H_{50}O_3$ 410.679

(2*R*,19*Z*)-*form*
Me ether: 2-Methoxy-19-hexacosenoic acid
[88416-40-4]
$C_{27}H_{52}O_3$ 424.706
Constit. of the sponge *Higginsia tethyoides*.
Ayanoglu, E. *et al., Lipids*, 1983, **18**, 830-836 (*isol*)

2-Hydroxyhexadecanoic acid, 9CI H-661

2-Hydroxypalmitic acid
[764-67-0]



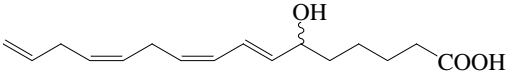
(*R*)–*form*

$C_{16}H_{32}O_3$ 272.427

(*R*)-*form* [16452-51-0]
Occurs in wool fat. Metab. of *Hansenula sydowiorum*.
Mp 93.3-93.6°. $[\alpha]_D$ -3.2 ($CHCl_3$).
Me ether: 2-Methoxyhexadecanoic acid
[94908-25-5]
$C_{17}H_{34}O_3$ 286.454
Isol. from the sponge *Amphimedon compressa*. Isol. as Me ester. Probable config. assigned.

(ξ)-*form*
Constit. of the sponges *Pseudosuberites* sp. and *Suberites massa*.
Barnathan, G. *et al., J. Nat. Prod.*, 1993, **56**, 2104-2113 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1998, **61**, 675-676 (*2-Methoxyhexadecanoic acid*)

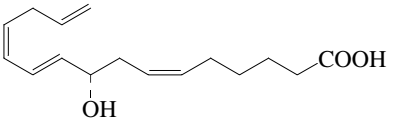
6-Hydroxy-7,9,12,15-hexadecatetraenoic acid H-662



$C_{16}H_{24}O_3$ 264.364

(6ξ,7*E*,9*Z*,12*Z*)-*form* [872050-17-4]
Isol. from the marine diatom *Thalassiosira rotula*. Isol. as Me ester.
Ketone: ***6-Oxo-7,9,12,15-hexadecatetraenoic acid***
[872050-16-3]
$C_{16}H_{22}O_3$ 262.348
Isol. from *Thalassiosira rotula*. Isol. as Me ester.
15,16-Dihydro: ***6-Hydroxy-7,9,12-hexadecatrienoic acid***
[872050-20-9]
$C_{16}H_{26}O_3$ 266.38
Isol. from *Thalassiosira rotula*. Isol. as Me ester.
15,16-Dihydro, ketone: ***6-Oxo-7,9,12-hexadecatrienoic acid***
[872050-19-6]
$C_{16}H_{24}O_3$ 264.364
Isol. from *Thalassiosira rotula*. Isol. as Me ester.
D'Ippolito, G. *et al., Org. Biomol. Chem.*, 2005, **3**, 4065-4070 (*isol, pmr, cmr*)

9-Hydroxy-6,10,12,15-hexadecatetraenoic acid H-663



$C_{16}H_{24}O_3$ 264.364

(6*Z*,9*S*,10*E*,12*Z*)-*form* [872050-18-5]
Isol. from the marine diatom *Thalassiosira rotula*. Isol. as Me ester.
15,16-Dihydro: 9-Hydroxy-6,10,12-hexadecatrienoic acid
[872050-15-2]
$C_{16}H_{26}O_3$ 266.38
Isol. from *Thalassiosira rotula*. Isol. as Me ester.
D'Ippolito, G. *et al., Org. Biomol. Chem.*, 2005, **3**, 4065-4070 (*isol, pmr, cmr, abs config*)

4-Hydroxy-15-hexadecene-5,7-diyn-2-one H-664

$H_2C{=}CH(CH_2)_6C{\equiv}CC{\equiv}CCH(OH)CH_2COCH_3$

$C_{16}H_{22}O_2$ 246.349

(ξ)-*form*

Homomontiporyne J

Isol. from the coral *Montipora* sp.

Light yellow oil.

Alam, N. *et al., Chem. Pharm. Bull.*, 2002, **50**, 661-662 (*isol, pmr, cmr*)

3-[(7-Hydroxy-1-hexadecene-3,5-diynyl)oxy]-1,2-propanediol H-665

1-O-*(7-Hydroxy-1-hexadecene-3,5-diynyl)glycerol*

[129602-15-9]

$H_3C(CH_2)_8CH(OH)C{\equiv}CC{\equiv}CCH{=}CHOCH_2CH(OH)CH_2OH$

$C_{19}H_{30}O_4$ 322.444

Isol. from a New Zealand sponge *Petrosia hebes*. Brown oil. λ_{max} 223 (ϵ 19500); 262 (ϵ 7940); 276 (ϵ 11200); 292 (ϵ 9330) (MeOH) (Derep). λ_{max} 223 (ϵ 19700); 262 (ϵ 8000); 276 (ϵ 11300); 292 (ϵ 9600) (MeOH) (Berdy).

Perry, N.B. *et al., J. Nat. Prod.*, 1990, **53**, 732 (*isol, struct, pmr, cmr, ms, ir, uv*)

2-Hydroxy-5-hexadecenoic acid H-666

$H_3C(CH_2)_9CH{=}CHCH_2CH_2CH(OH)COOH$

$C_{16}H_{30}O_3$ 270.411

(2ξ,5*Z*)-*form*

Me ether: 2-Methoxy-5-hexadecenoic acid

[139742-37-3]

$C_{17}H_{32}O_3$ 284.438

Isol. from the phospholipids of the sponge *Mycale laxissima*.

Carballeira, N.M. *et al., Tetrahedron*, 1992, **48**, 1053-1058 (*isol*)

Carballeira, N.M. *et al., J. Nat. Prod.*, 1994, **57**, 1152-1159; 1998, **61**, 1543-1546 (*isol, synth, pmr, cmr*)

2-Hydroxy-6-hexadecenoic acid H-667

$H_3C(CH_2)_8CH{=}CH(CH_2)_3CH(OH)COOH$

$C_{16}H_{30}O_3$ 270.411

(2ξ,6*Z*)-*form*

Me ether: 2-Methoxy-6-hexadecenoic acid

[139742-38-4]

$C_{17}H_{32}O_3$ 284.438

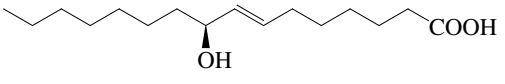
Isol. from the phospholipids of the sponge *Spheciospongia cuspidifera*.

Carballeira, N.M. *et al., Tetrahedron*, 1992, **48**, 1053-1058 (*isol*)

Carballeira, N.M. *et al., J. Nat. Prod.*, 1998, **61**, 1543-1546 (*synth, pmr, cmr*)

Soderquist, J.A. *et al., Tet. Lett.*, 1998, **39**, 3115-3116 (*synth*)

9-Hydroxy-7-hexadecenoic acid H-668



$C_{16}H_{30}O_3$ 270.411

(7*E*,9*S*)-*form* [872050-14-1]

Isol. from the marine diatom *Thalassiosira rotula*. Isol. as Me ester.

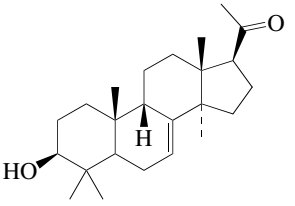
Ketone: ***9-Oxo-7-hexadecenoic acid***

$C_{16}H_{28}O_3$ 268.395

Isol. from *Thalassiosira rotula*. Isol. as Me ester.

D'Ippolito, G. *et al., Org. Biomol. Chem.*, 2005, **3**, 4065-4070 (*isol, pmr, cmr, abs config*)

3-Hydroxy-22,23,24,25,26,27-hexanorlanost-7-en-20-one H-669



$C_{24}H_{38}O_2$ 358.563

(3β,9β)-*form*

3-O-*[6*-O-*Sulfo-3*-O-*methyl-β-D-glucopyranosyl-(1→3)-6*-O-*sulfo-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Koreoside A***

[192213-04-0]

$C_{53}H_{86}O_{33}S_3$ 1347.441

Constit. of *Cucumaria koraiensis*.

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-6*-O-*sulfo-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Cucumarioside A_3-2***

[583028-65-3]

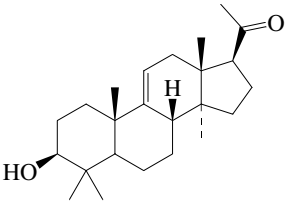
$C_{53}H_{86}O_{30}S_2$ 1267.376

Constit. of *Cucumaria conicospermium*.

Avilov, S.A. *et al., J. Nat. Prod.*, 1997, **60**, 808-810 (*Koreoside A*)

Avilov, S.A. *et al., J. Nat. Prod.*, 2003, **66**, 910-916 (*Cucumarioside A_3-2*)

3-Hydroxy-22,23,24,25,26,27-hexanorlanost-9(11)-en-20-one H-670



$C_{24}H_{38}O_2$ 358.563

3β-*form*

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-6*-O-*sulfo-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Cucumarioside A_3-3***

[583028-88-0]

$C_{53}H_{86}O_{30}S_2$ 1267.376

Constit. of *Cucumaria conicospermium*.

3-O-*[3*-O-*Methyl-6*-O-*sulfo-β-D-glucopyranosyl-(1→3)-6*-O-*sulfo-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Isokoreoside A***

[583028-89-1]

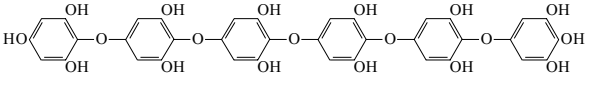
$C_{53}H_{86}O_{33}S_3$ 1347.441

Constit. of *Cucumaria conicospermium*.

Avilov, S.A. *et al., J. Nat. Prod.*, 2003, **66**, 910-916 (*isol, pmr, cmr*)

Hydroxyhexaphlorethol H-671

[137809-93-9]



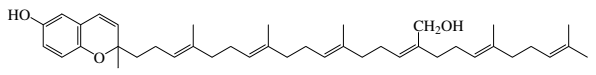
$C_{36}H_{26}O_{19}$ 762.59

Constit. of *Carpophyllum maschalocarpum*.

Glombitza, K.-W. *et al., Phytochemistry*, 1991, **30**, 2741 (*isol, pmr*)

2-(28-Hydroxyhexaprenyl)-2-methyl-2*H*-1-benzopyran-6-ol H-672

[868850-46-8]



$C_{41}H_{60}O_3$ 600.923

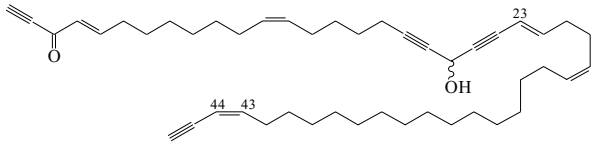
Constit. of *Ircinia spinosula*. λ_{max} 267 (ϵ 1046) (hexane).

Tzivelelta, L.-A. *et al., Chem. Biodiversity*, 2005, **2**, 901-909 (*Ircinia spinosula constit*)

20-Hydroxy-4,12,23,27,43-hexatetracontapentaene-1,18,21,45-tetrayn-3-one, 9CI H-673

Petroformyne 7

[128855-12-9]



$C_{46}H_{66}O_2$ 651.026

Minor metab. isol. from *Petrosia ficiformis*.

$[\alpha]_D$ +3. λ_{max} 232 (ϵ 15600) (MeOH) (Berdy).

23Z-Isomer: ***Isopetroformyne 7***

$C_{46}H_{66}O_2$ 651.026

Constit. of *Petrosia ficiformis*. Oil. $[\alpha]_D^{21}$ +2.5 (c, 0.1 in $CHCl_3$).

23,24-Dihydro: 20-Hydroxy-4,12,27,43-hexatetracontatetraene-1,18,21,45-tetrayn-3-one. ***23,24-Dihydropetroformyne 7***

$C_{46}H_{68}O_2$ 653.042

Constit. of *Petrosia ficiformis*. Pale yellow oil. $[\alpha]_D^{21}$ -16.1 (c, 0.2 in $CHCl_3$). λ_{max} 230 (ϵ 22300) (MeOH) (Berdy).

43,44-Dihydro: 20-Hydroxy-4,12,23,27-hexatetracontatetraene-1,18,21,45-tetrayn-3-one, 9CI. ***Petroformyne 6***

[128855-11-8]

$C_{46}H_{68}O_2$ 653.042

Minor metab. from *Petrosia ficiformis*.

$[\alpha]_D$ +2.9. λ_{max} 228 (ϵ 14500) (MeOH) (Berdy).

43,44-Dihydro, 23Z-Isomer: ***Isopetroformyne 6***

$C_{46}H_{68}O_2$ 653.042

Constit. of *Petrosia ficiformis*. Oil. $[\alpha]_D^{21}$ +2.6 (c, 0.3 in $CHCl_3$).

23,24,43,44-Tetrahydro: 20-Hydroxy-4,12,27-hexatetracontatriene-1,18,21,45-tetrayn-3-one. ***23,24-Dihydropetroformyne 6***

$C_{46}H_{70}O_2$ 655.058

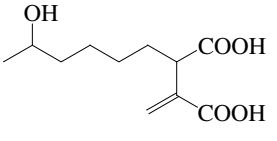
Constit. of *Petrosia ficiformis*. Pale yellow oil. $[\alpha]_D^{21}$ -3.8 (c, 0.4 in $CHCl_3$).

Cimino, G. *et al., J. Nat. Prod.*, 1990, **53**, 345 (*isol, struct*)

Guo, Y.-W. *et al., J. Nat. Prod.*, 1995, **58**, 712 (*isol, pmr, cmr*)

2-(5-Hydroxyhexyl)-3-methylenebutanedioic acid H-674

9-Hydroxyhexylitaconic acid. 8-Hydroxy-1-nonene-2,3-dicarboxylic acid



$C_{11}H_{18}O_5$ 230.26

(-)-form

1-Me ester:

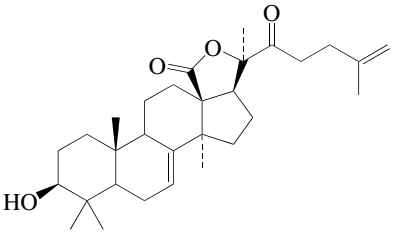
$C_{12}H_{20}O_5$ 244.287

Isol. from the marine fungus *Apiospora montagnei*. Oil.

$[\alpha]_D^{22}$ -4.8 (c, 0.24 in MeOH). λ_{max} 205 (log ϵ 4) (MeOH).

Klemke, C. *et al., J. Nat. Prod.*, 2004, **67**, 1058-1063 (*isol, pmr, cmr*)

3-Hydroxyholosta-7,25-dien-22-one H-675



$C_{30}H_{44}O_4$ 468.675

3β-form

3-O-[3-O-Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-βD-glucopyranosyl-(1→2)-4-O-sulfo-β-D-xylopyranoside]: ***Mollisoside A***

[857288-90-5]

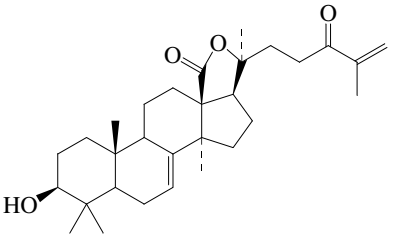
$C_{54}H_{84}O_{25}S$ 1165.309

Constit. of *Australostichopus mollis*. Cryst.

Mp 233-235°. $[\alpha]_D^{20}$ -37 (c, 0.1 in Py).

Moraes, G. *et al., J. Nat. Prod.*, 2005, **68**, 842-847 (*Mollisoside A*)

3-Hydroxyholosta-7,25-dien-24-one H-676



$C_{30}H_{44}O_4$ 468.675

3β-form

3-O-[3-O-Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-O-sulfo-β-D-xylopyranoside]: ***Frondoside A2-2***

[852637-94-6]

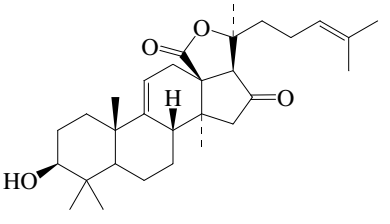
$C_{59}H_{92}O_{29}S$ 1297.424

Constit. of *Cucumaria frondosa*. Powder.

Mp 198-200°. $[\alpha]_D^{20}$ -36 (c, 0.1 in Py).

Silchenko, A.S. *et al., Can. J. Chem.*, 2005, **83**, 21-27 (*Frondoside A2-2*)

3-Hydroxyholosta-9(11),24-dien-16-one H-677



$C_{30}H_{44}O_4$ 468.675

3β-form

Stichopogenin A2

[23518-98-1]

Constit. of *Stychopus japonicus*.

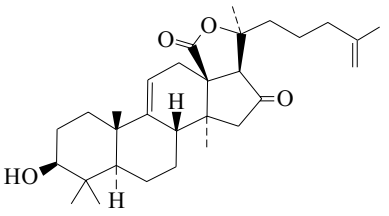
Cryst. (MeOH).

Mp 238-240°. $[\alpha]_D^{25}$ -48 (c, 2.5 in $CHCl_3$).

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Frondoside E₂***
[349544-12-3]
[349498-92-6]
$C_{59}H_{92}O_{29}S$ 1297.424
Constit. of *Cucumaria frondosa*.

Elyakov, G.B. *et al., Tet. Lett.*, 1969, 1151 (*Stichopogenin A_2, isol*)
Tan, W.L. *et al., J.O.C.*, 1975, **40**, 466 (*Stichopogenin A_2, struct*)
Yayli, N. *et al., Indian J. Chem., Sect. B*, 2001, **40**, 399-404 (*Frondoside E_2*)

3-Hydroxyholosta-9(11),25-dien-16-one H-678



$C_{30}H_{44}O_4$ 468.675

3β-*form*
Holotoxigenol

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Neothyonidioside***
$C_{53}H_{82}O_{24}S$ 1135.282
Isol. from the sea cucumber *Neothyonidium magnum*. Cryst. (EtOH aq.).
Mp 241-243°. $[\alpha]_D$ -73 (c, 0.49 in Py).

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Cladoloside A***
[92340-60-8]
$C_{53}H_{82}O_{21}$ 1055.218
Constit. of a *Cladolabes* sp. from Zanzibar. No phys. props. reported.

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Mollisoside B_1***
[857288-91-6]
$C_{53}H_{82}O_{25}S$ 1151.282
Constit. of *Australostichopus mollis*. Cryst.
Mp 245-247°. $[\alpha]_D^{20}$ -51 (c, 0.1 in Py).

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-6*-O-*sulfo-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Hemoiedemoside A***
[443791-82-0]
$C_{54}H_{84}O_{28}S_2$ 1245.373
Constit. of *Hemoiedema spectabilis*. Amorph. powder.
Mp 225-227°. $[\alpha]_D^{20}$ -29.6 (c, 0.4 in Py).

3-O-*[3*-O-*Methyl-6*-O-*sulfo-β-D-glucopyranosyl-(1→3)-6*-O-*sulfo-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Psolusoside A***
[90077-71-7]
$C_{54}H_{84}O_{28}S_2$ 1245.373
Isol. from *Psolus fabricii*. Cryst. (EtOH) (as di-Na salt).
Mp 208-211° (di-Na salt). $[\alpha]_D^{25}$ -73 (c, 0.01 in Py) (di-Na salt).
CAS number refers to di-Na salt.

3-O-*[3*-O-*Methyl-6*-O-*sulfo-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→3)-6*-O-*sulfo-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Psoluthurin A***
[87081-42-3]
$C_{54}H_{84}O_{28}S_2$ 1245.373
Isol. from *Psolus fabricii*. Cryst. (EtOH aq.) (as di-Na salt).
Mp 259-263° dec. (di-Na salt). $[\alpha]_D^{23}$ -32.6 (c, 0.4 in Py) (di-Na salt). CAS number refers to di-Na salt.

3-O-*[3*-O-*Methyl-6*-O-*sulfo-β-D-glucopyranosyl-(1→3)-6*-O-*sulfo-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Hemoiedemoside B***
[443791-83-1]
$C_{54}H_{84}O_{31}S_3$ 1325.437
Constit. of *Hemoiedema spectabilis*. Amorph. powder.
Mp 230-232°. $[\alpha]_D^{20}$ -28.9 (c, 0.5 in Py).

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Cladoloside B***
[92355-85-6]
$C_{59}H_{92}O_{26}$ 1217.36
Constit. of a *Cladolabes* sp. No phys. props. reported.

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***DS-Penaustroside C***
[143572-17-2]
$C_{59}H_{92}O_{26}$ 1217.36
Desulfated saponin from *Pentacta australis*. Powder.
Mp 254-260°. $[\alpha]_D^{23}$ -77.4 (c, 0.4 in Py).

3-O-*[3-Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Frondoside A_2-6***
[852637-96-8]
$C_{59}H_{92}O_{29}S$ 1297.424
Constit. of *Cucumaria frondosa*. Powder.
Mp 220-222°. $[\alpha]_D^{20}$ -51 (c, 0.1 in Py).

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Holotoxin B1***
[92340-59-5]
$C_{65}H_{102}O_{31}$ 1379.502
Constit. of *Stichopus japonicus*. Cryst. (EtOH).
Mp 223-224°. $[\alpha]_D^{20}$ -74 (c, 1 in Py).

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Holotoxin A1***. *Stichoposide A*
[85344-35-0]
$C_{66}H_{104}O_{31}$ 1393.529
Isol. from echinoderm *Stichopus japonicus*. Cryst. (EtOH).
Mp 258-260°. $[\alpha]_D^{20}$ -69.2 (c, 1.2 in Py).

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Holotoxin B***
[55892-88-1]
$C_{66}H_{104}O_{32}$ 1409.528
Constit. of echinoderm *Stichopus japonicus*. Cryst. ($CHCl_3$/MeOH/H_2O). Sol. MeOH.
Mp 252-253°. $[\alpha]_D^{23}$ -78 (c, 0.28 in Py). Struct. revised in 1978.

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]:* ***Holotoxin A***
[55762-47-5]
$C_{67}H_{106}O_{32}$ 1423.555
Constit. of *Stichopus japonicus* and *Holothuria pervicax*. Haemolytic agent. Cryst. ($CHCl_3$/MeOH/H_2O). Sol. MeOH, EtOH; poorly sol. H_2O, EtOAc, hexane.
Mp 250-253°. $[\alpha]_D^{23}$ -76 (c, 0.43 in Py). Struct. revised in 1978.

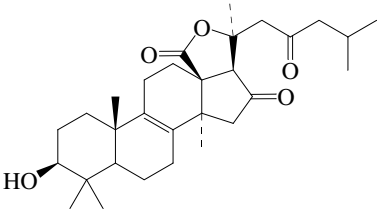
Glycoside: ***Holotoxin C***
Constit. of echioderm *Stichopus japonicus*. Full struct. unknown. Hydrol. gives xylose, 6-deoxyglucose, glucose and 3-methylglucose.

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1976, **24**, 275-284; 1978, **26**, 3722-3731 (*Holotoxins*)
Elyakov, G.B. *et al., Bioorg. Khim.*, 1983, **9**, 280-282 (*Holotoxin A1*)

Garneau, F.X. *et al., Can. J. Chem.*, 1983, **61**, 1465-1471 (*Psolothurin A*)
Kalinin, V.I. *et al., Khim. Prir. Soedin.*, 1983, 789-790; 1985, 212-217 (*Psolusoside A*)
Maltsev, I.I. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1984, **78**, 421-426 (*Holotoxins A1,B1*)
Zurita, M.B. *et al., J. Nat. Prod.*, 1986, **49**, 809-813 (*Neothyonidioside*)
Avilov, S.A. *et al., Khim. Prir. Soedin.*, 1988, **24**, 764-765; *Chem. Nat. Compd. (Engl. Transl.)*, 1988, **24**, 656 (*Cladolosides*)
Miyamoto, T. *et al., J. Nat. Prod.*, 1992, **55**, 940-946 (*DS-Penaustroside C*)
Chludil, H.D. *et al., J. Nat. Prod.*, 2002, **65**, 860-865 (*Hemoiedemosides*)
Silchenko, A.S. *et al., Can. J. Chem.*, 2005, **83**, 21-27 (*Frondoside A_2-6*)
Moraes, G. *et al., J. Nat. Prod.*, 2005, **68**, 842-847 (*Mollisoside B_1*)

3-Hydroxyholost-8-ene-16,23-dione H-679

3-Hydroxy-16,23-dioxolanost-8-en-18,20-olide



$C_{30}H_{44}O_5$ 484.675

3β-*form*

Cucumechinol C

[122970-14-3]

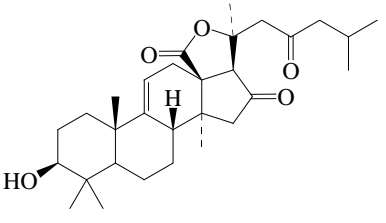
Formed on acid hydrol. of saponins from *Cucumaria echinata*. Needles.

Mp 206-207°. $[\alpha]_D$ -87.3 (c, 0.3 in $CHCl_3$).

Miyamoto, T. *et al., Annalen*, 1990, 39-42 (*isol, pmr, cmr*)

3-Hydroxyholost-9(11)-ene-16,23-dione H-680

3-Hydroxy-16,23-dioxolanost-9(11)-en-18,20-olide



$C_{30}H_{44}O_5$ 484.675

3β-*form*

Cucumechinol A

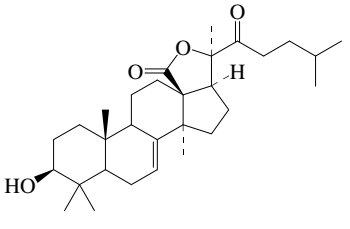
[122970-13-2]

Formed on acid hydrol. of saponins from *Cucumaria echinata*. Needles (C_6H_6).

Mp 233-243°. $[\alpha]_D$ -132.1 (c, 1.4 in $CHCl_3$).

Miyamoto, T. *et al., Annalen*, 1990, 39-42 (*isol, pmr, cmr*)

3-Hydroxyholost-7-en-22-one H-681



$C_{30}H_{46}O_4$ 470.691

3β-*form*

Urupogenin

*3-*O*-[3-*O*-Methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Pseudostichoposide A***

[125362-41-6]

$C_{53}H_{84}O_{24}S$ 1137.298

Main glycoside of the holothurian *Pseudostichopus trachus*. Cryst. (as Na salt).

Mp 200-202° (Na salt). $[\alpha]_D^{20}$ -23 (c, 0.1 in Py) (Na salt). Struct. incorr. descr. in the ref. as having terminal quinovosyl.

*3-*O*-[3-*O*-Methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-3-*O*-sulfo-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Pseudostichoposide B***

[859842-53-8]

$C_{53}H_{84}O_{27}S_2$ 1217.362

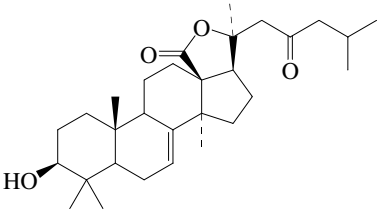
Constit. of *Pseudostichopus trachus*. Cryst.

Mp 269-271°. $[\alpha]_D^{20}$ -50 (c, 0.1 in Py aq.).

Kalinin, V.I. *et al., Khim. Prir. Soedin.*, 1989, 678-684; *Chem. Nat. Compd. (Engl. Transl.)*, 1989, **25**, 577-582 (*Pseudostichoposide A*)
Silchenko, A.S. *et al., Nat. Prod. Res.*, 2004, **18**, 565-570 (*Pseudostichoposide B*)

3-Hydroxyholost-7-en-23-one H-682

3-Hydroxy-23-oxolanost-7-en-18,20-olide



$C_{30}H_{46}O_4$ 470.691

3β-*form*

Synaptogenin

*3-*O*-[3-*O*-Methyl-β-D-glucopyranosyl-(1→3)-6-*O*-sulfo-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Cucumechinoside C***

[125640-32-6]

$C_{54}H_{86}O_{28}S_2$ 1247.389

Constit. of *Cucumaria echinata*. Powder. Sol. MeOH, butanol.

Mp 235-238°. $[\alpha]_D$ -21.9 (c, 0.8 in MeOH).

*3-*O*-[3-*O*-Methyl-6-*O*-sulfo-β-D-glucopyranosyl-(1→3)-6-*O*-sulfo-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Cucumechinoside F***

[125640-35-9]

$C_{54}H_{86}O_{31}S_3$ 1327.453

Constit. of *Cucumaria echinata*. Powder. Sol. MeOH, butanol.

Mp 236-240°. $[\alpha]_D$ -65 (c, 0.2 in H_2O).

*3-*O*-[3-*O*-Methyl-β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Calcigeroside C_2***

[253678-31-8]

$C_{59}H_{94}O_{29}S$ 1299.44

Constit. of *Pentamera calcigera*. Cryst.

Mp 226-228°. $[\alpha]_D^{20}$ -39 (c, 0.1 in Py).

*3-*O*-[3-*O*-Methyl-β-D-xylopyranosyl-(1→3)-6-*O*-sulfo-β-D-glucopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-*O*-sulfo-β-D-xylopyranoside]:* ***Calcigeroside D_2***

[298693-65-9]

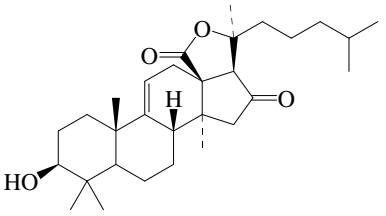
$C_{59}H_{94}O_{32}S_2$ 1379.504

Constit. of *Pentamera calcigera*.

Mp 242-244° (as di-Na salt). $[\alpha]_D^{20}$ -22 (c, 0.1 in 50% Py aq.) (di-Na salt).

Miyamoto, T. *et al., Annalen*, 1990, 39-42 (*Cucumechinosides*)
Avilov, S.A. *et al., J. Nat. Prod.*, 2000, **63**, 65-71; 1349-1355 (*Calcigerosides*)

3-Hydroxyholost-9(11)-en-16-one H-683



$C_{30}H_{46}O_4$ 470.691

3β-*form*

3-O-[3-O-Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]: ***DS-Penaustroside D***
[143572-18-3]
$C_{59}H_{94}O_{26}$ 1219.376
Desulfated saponin from *Pentacta australis*. Powder.
Mp 278-281°. $[\alpha]_D^{22}$ -64.6 (c, 0.12 in Py).

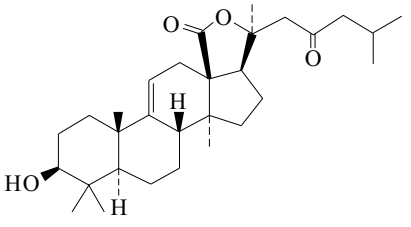
3-O-[3-O-Methyl-β-D-glucopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]: ***Parvimoside B***
[872131-53-8]
$C_{65}H_{104}O_{31}$ 1381.518
Constit. of *Stichopus parvimensis*. Amorph. solid.
Mp 215-218°.

3-O-[3-O-Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]: ***Parvimoside A***
[872131-52-7]
$C_{66}H_{106}O_{32}$ 1411.544
Constit. of *Stichopus parvimensis*. Amorph. solid.
Mp 270-275°.

Miyamoto, T. *et al., J. Nat. Prod.*, 1992, **55**, 940-946 (*DS-Penaustroside D*)
Iñiguez-Martinez, A.M. de M. *et al., J. Nat. Prod.*, 2005, **68**, 1669-1673 (*Parvimosides*)

3-Hydroxyholost-9(11)-en-23-one H-684

3-Hydroxy-23-oxolanost-9(11)-en-18,20-olide



$C_{30}H_{46}O_4$ 470.691

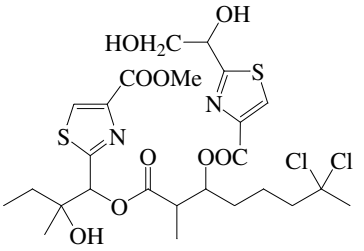
3β-*form*

Synaptogenin B. *Cucumechinol B*
[101247-83-0]
Pseudoaglycone formed by acid hydrol. of Synaptoside S2, S-554 and Synaptoside S3, S-555 from *Synapta maculata* and the Cucumechinosides from *Cucumaria echinata*.
Cryst. (C_6H_6).
Mp 244-245°. $[\alpha]_D$ -14.2 (c, 1.5 in $CHCl_3$).

Kuznetsova, J.A. *et al., Khim. Prir. Soedin.*, 1985, **21**, 667-670; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 626-629 (*Synaptogenin B, struct*)
Miyamoto, T. *et al., Annalen*, 1990, 39-42 (*isol, pmr, cmr*)

Hydroxyhomodolabellin H-685

Homohydroxydolabellin

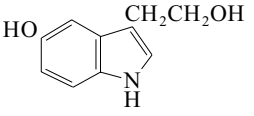


$C_{25}H_{34}Cl_2N_2O_9S_2$ 641.589
Isol. from a *Lyngbya* sp. Cytotoxic. Amorph. solid. $[\alpha]_D^{25}$ -10 (c, 0.05 in $CHCl_3$). CAS no. not found to CA 138. λ_{max} 203 (log ϵ 4.47); 238 (log ϵ 4.06) (MeOH).

Luesch, H. *et al., Tetrahedron*, 2002, **58**, 7959-7966 (*isol, pmr, cmr*)

5-Hydroxy-3-(2-hydroxyethyl)-1*H*-indole H-686

*5-Hydroxy-1*H*-indole-3-ethanol, 9CI. 5-Hydroxytryptophol*
[154-02-9]



$C_{10}H_{11}NO_2$ 177.202
Serotonin metab. in rat. Present in bovine pineal tissue and *Bufo alvarius*. Isol. from the sponge *Hyrtios erectus*. Prisms.
Mp 105-107°. λ_{max} 210 (ϵ 14400); 276 (ϵ 4940); 300 (sh) (ϵ 3450) (MeOH).

▶ Exp. reprod. effects. NL8512500

Picrate: Mp 150-152°.

5-Me ether: 3-(2-Hydroxyethyl)-5-methoxyindole. 5-Methoxytryptophol
[712-09-4]
$C_{11}H_{13}NO_2$ 191.229
Present in bovine pineal tissue and *Bufo alvarius*.

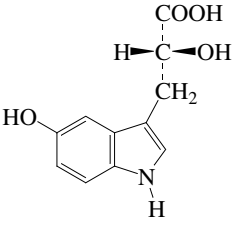
▶ Human and exp. reprod. effects. NL8513000

5-Benzyl ether: [41339-61-1]
$C_{17}H_{17}NO_2$ 267.327
Cryst. (C_6H_6). Mp 93-95°.

Kveder, S. *et al., Biochem. J.*, 1962, **85**, 447 (*synth*)
McIsaac, W.M. *et al., Science (Washington, D.C.)*, 1965, **148**, 102
Salmoun, M. *et al., J. Nat. Prod.*, 2002, **65**, 1173-1176 (*isol, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MFT300

2-Hydroxy-3-(5-hydroxy-1*H*-indol-3-yl)propanoic acid H-687

*α,5-Dihydroxy-1*H*-indole-3-propanoic acid, 9CI. 3-(5-Hydroxy-3-indolyl)lactic acid.* ***Hyrtioerectine C***

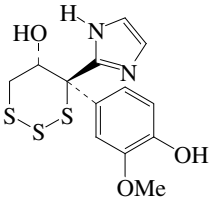


$C_{11}H_{11}NO_4$ 221.212

(*S*)-*form* [151764-92-0]
Alkaloid from the sponge *Hyrtios erectus*.
Amorph. solid. $[\alpha]_D^{25}$ -31.3 (c, 0.13 in MeOH). λ_{max} 229 (log ε 3.76); 276 (log ε 3.56); 301 (log ε 3.44) (MeOH).
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2005, **68**, 1416-1419 (*isol, pmr, cmr*)

5-Hydroxy-4-(4-hydroxy-3-methoxyphenyl)-4-(2-imidazolyl)-1,2,3-trithiane H-688

*4-(4-Hydroxy-3-methoxyphenyl)-4-(1*H*-imidazol-2-yl)-1,2,3-trithian-5-ol, 9CI*



Relative Configuration

$C_{13}H_{14}N_2O_3S_3$ 342.463

(+)-*form* [383191-04-6]
Isol. from the ascidian *Aplidium* sp. D. Cytotoxic. Yellow gum. $[\alpha]_D^{20}$ +26 (c, 0.1 in MeOH). λ_{max} 216 (ε 13750); 255 (ε 8100); 290 (ε 5800) (MeOH/KOH) (Derep). λ_{max} 283 (ε 3900) (MeOH) (Derep).

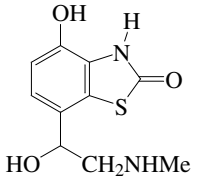
(-)-*form* [383191-01-3]
Isol. from the ascidian *Hypsistozoa fasmeriana*. Cytotoxic. $[\alpha]_D^{20}$ -26 (c, 0.1 in MeOH).

[123060-45-7, 123060-46-8]

Copp, B.R. *et al., Tet. Lett.*, 1989, **30**, 3703-3706 (*isol, struct*)
Pearce, A.N. *et al., J.O.C.*, 2001, **66**, 8257-8259 (*isol, cd, pmr, cmr*)

4-Hydroxy-7-[1-hydroxy-2-(methylamino)ethyl]-2(3*H*)-benzothiazolone H-689

S 1319
[220752-37-4]

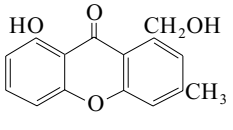


$C_{10}H_{12}N_2O_3S$ 240.282
Isol. from the marine sponge *Dysidea* sp. β_2-Adrenoceptor agonist.

Suzuki, H. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 1361-1364 (*isol, pmr, cmr, activity*)
Fairhurst, R.A. *et al., Org. Lett.*, 2005, **7**, 4697-4700 (*synth*)

8-Hydroxy-1-hydroxymethyl-3-methylxanthone H-690

[60883-98-9]

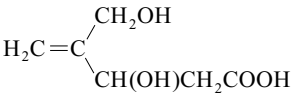


$C_{15}H_{12}O_4$ 256.257
Prod. by *Ascodesmis sphaerospora*, *Cyathus intermediuisol s* and the sponge-derived fungus *Ulocladium botrytis*. Antifungal agent. Yellow needles.
Mp 176-178°.

Ayer, W.A. *et al., Can. J. Chem.*, 1976, **54**, 1703-1707 (*isol, synth, uv, ir, pmr, ms*)
Hein, S.M. *et al., J. Nat. Prod.*, 1998, **61**, 1566-1567 (*isol, cmr*)
Höller, U. *et al., Eur. J. Org. Chem.*, 1999, 2949-2955 (*isol*)

3-Hydroxy-4-hydroxymethyl-4-pentenoic acid H-691

3,5-Dihydroxy-4-methylenepentanoic acid



$C_6H_{10}O_4$ 146.143
Metabolite of the marine sponge *Plakortis zygompha*.

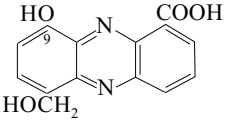
Et ester: [74403-51-3]
$C_8H_{14}O_4$ 174.196
Metabolite of *Plakortis zygompha*.

Et ester, di-Ac:
$C_{12}H_{18}O_6$ 258.271
Metabolite of *Plakortis zygompha*.

Faulkner, D.J. *et al., Tet. Lett.*, 1980, 23-26 (*isol, spectra*)

9-Hydroxy-6-hydroxymethyl-1-phenazinecarboxylic acid, 9CI H-692

Antibiotic T 41348. *T 41348*
[60160-03-4]



$C_{14}H_{10}N_2O_4$ 270.244
Phenazine antibiotic. Isol. from *Streptomyces recifensis*. Active against gram-positive and -negative bacteria. Orange-red cryst. Sol. MeOH. λ_{max} 267 (ε 42000); 368 (ε 8700) (MeOH) (Berdy).

9-Me ether: 6-Hydroxymethyl-9-methoxy-1-phenazinecarboxylic acid. ***Griseoluteic acid***. *B 4607B. Antibiotic B 4607B*
[489-76-9]
$C_{15}H_{12}N_2O_4$ 284.271
From *Streptomyces griseoluteus*. Degradation prod. of Griseolutein A and Griseolutein B. Active against HeLa cells and Ehrlich carcinoma. Reddish-yellow cryst. Sol. H_2O, MeOH. λ_{max} 263; 350; 365 (MeOH) (Berdy).

9-Me ether, Me ester:
Orange-yellow needles. Mp 189°.

*9-Me ether, 1′-*O*-aminoacetyl:* ***Pelagiomicin C***. *2088C. Antibiotic 2088C. B 4607A. Antibiotic B 4607A*. O*-Glycylgriseoluteic acid*
[173485-82-0]
$C_{17}H_{15}N_3O_5$ 341.323
Prod. by the marine bacterium *Pelagiomonas variabilis* and by a *Vibrio* sp. Active against gram-positive and -negative bacteria. Cytotoxic agent. Red-orange solid. λ_{max} 210 (log ε 4.67); 267 (log ε 4.65); 369 (log ε 4.09) (EtOH).

*9-Me ether, 1′-*O*-(2-aminopropanoyl):* **O-*Alanylgriseoluteic acid***. *B 4607C. Antibiotic B 4607C*
$C_{18}H_{17}N_3O_5$ 355.349
Prod. by *Vibrio* sp. Yellow powder. Sol. H_2O, MeOH. $[\alpha]_D$ -3.7 (MeOH). Not found in CAS. λ_{max} 263; 365 (MeOH) (Berdy).

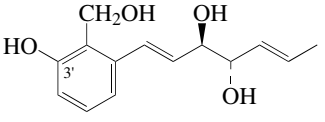
*9-Me ether, 1′-*O*-(2-amino-3-methylbutanoyl)(*S*-):* ***Pelagiomicin B***. *2088B. Antibiotic 2088B*
[173485-81-9]
$C_{20}H_{21}N_3O_5$ 383.403
Prod. by *Pelagiomonas variabilis*. Red-orange needles. Sol. MeOH, butanol, $CHCl_3$. λ_{max} 210 (log ε 4.7); 267 (log ε 4.66); 369 (log ε 4.1) (EtOH). λ_{max} 210 (ε 50118); 267 (ε 45710); 369 (ε 12590) (MeOH) (Berdy).

*9-Me ether, 1′-*O*-(2-amino-3-hydroxy-3-methylbutanoyl)(*S*-):* ***Pelagiomicin A***. *2088A. Antibiotic 2088A*. O*-(3-Hydroxyvalyl)griseoluteic acid*

[173485-80-8]
$C_{20}H_{21}N_3O_6$ 399.402
Prod. by *Pelagiomonas variabilis*. Antitumour agent. Red-orange needles.
Mp 130° dec. $[\alpha]_D$ +19.8 (c, 1 in $CHCl_3$). λ_{max} 209 (log ϵ 4.59); 265 (log ϵ 4.62); 368 (log ϵ 3.96) (EtOH).
Nakamura, S. *et al., Chem. Pharm. Bull.*, 1958, **6**, 539; 543; 547 (*synth, props*)
Nakamura, S. *et al., J. Antibiot., Ser. A*, 1959, **12**, 26; 55; 133 (*synth, props*)
Yagishita, K. *et al., J. Antibiot., Ser. A*, 1960, **13**, 83 (*isol*)
Holliman, F.G. *et al., Chem. Comm.*, 1970, 1423 (*synth, bibl*)
Ueda, K. *et al., Chem. Pharm. Bull.*, 1970, **18**, 1931 (*synth*)
Japan. Pat., 1976, 76 32 790; *CA*, **85**, 107461 (*isol, props*)
Japan. Pat., 1995, 95 330 741; *CA*, **124**, 315159s (*Antibiotic 2088A*)
Imamura, N. *et al., CA*, 1996, **124**, 170245e (*Pelagiomicins*)
Japan. Pat., 1996, 96 217 760; *CA*, **125**, 273725m
Imamura, N. *et al., J. Antibiot.*, 1997, **50**, 8 (*Pelagiomicins*)

1-[3-Hydroxy-4-(hydroxymethyl)phenyl]-1,5-heptadiene-3,4-diol, 9CI H-693

2-(3,4-Dihydroxy-1,5-heptadienyl)-6-hydroxybenzyl alcohol



(1*E*,3*R*,4*S*,5*E*)-*form*

$C_{14}H_{18}O_4$ 250.294

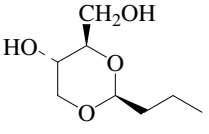
(1*E*,3*R*,4*S*,5*E*)-*form*
Dihydropyriculol
[112848-72-3]
Prod. by *Pyricularia oryzae*. Phytotoxin.
3′-Me ether, 5β,6β-epoxide: ***Varioxirane***
[419368-68-6]
$C_{15}H_{20}O_5$ 280.32
Isol. from a marine-derived *Emericella variecolor*. Antimicrobial agent. Oil (as tri-Ac). $[\alpha]_D^{25}$ -28 (c, 0.31 in $CHCl_3$) (tri-Ac). Rel. config. given as (3*R**,4*R**,5*S**,6*S**)-. λ_{max} 212 (log ϵ 5.5); 294 (log ϵ 4.4) (EtOH).

(1*E*,3*S*,4*S*,5*E*)-*form*
Epidihydropyriculol
Prod. by *Pyricularia oryzae*.
Gum. $[\alpha]_D$ -19 (c, 0.4 in EtOH). λ_{max} 219 (ϵ 16500); 252 (ϵ 7300); 295 (ϵ 1500) (MeOH).

(1*E*,3ξ,4ξ,5*E*)-*form*
3′-Me ether: 1-[2-(Hydroxymethyl)-3-methoxyphenyl]-1,5-heptadiene-3,4-diol, 9CI. 2-(3,4-Dihydroxy-1,5-heptadienyl)-6-methoxybenzyl alcohol
[72330-50-8]
$C_{15}H_{20}O_4$ 264.321
Prod. by *Aspergillus versicolor*. Cryst. ($CHCl_3$).
Mp 132-133°.
Dunn, A.W. *et al., J.C.S. Perkin 1*, 1979, 2122 (*Me ether*)
Kono, Y. *et al., Agric. Biol. Chem.*, 1991, **55**, 2785-2791 (*isol, uv, pmr, cmr*)
Nukina, M. *et al., Recent Res. Dev. Agric. Biol. Chem.*, 1998, **2**, 411 (*activity*)
Nukina, M. *et al., J. Pestic. Sci. (Int. Ed.)*, 1999, **24**, 293 (*rev*)
Malmstrom, J. *et al., J. Nat. Prod.*, 2002, **65**, 364-367 (*Varioxirane*)

5-Hydroxy-4-hydroxymethyl-2-propyl-1,3-dioxane H-694

5-Hydroxy-2-propyl-1,3-dioxane-4-methanol

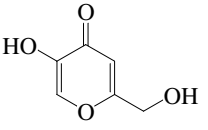


$C_8H_{16}O_4$ 176.212

(2*RS*,4*SR*,5*RS*)-*form*
1,3-Butylideneerythritol. ***Coruscol A***
Prod. by a *Penicillium* sp. derived from the marine bivalve *Mytilus coruscus*.
Amorph. solid.
Bonner, T.G. *et al., J.C.S.*, 1965, 7453-7458 (*synth*)
Kagata, T. *et al., J. Nat. Prod.*, 2000, **63**, 886-887 (*isol*)

5-Hydroxy-2-(hydroxymethyl)-4*H*-pyran-4-one, 9CI H-695

Kojic acid
[501-30-4]

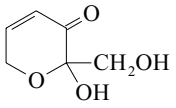


$C_6H_6O_4$ 142.111
Prod. by the action of microorganisms, esp. *Aspergillus* spp. but also *Penicillium* and *Acetobacter*, on carbohydrates, e.g. dextrose. Isol. from a marine-derived *Alternaria* sp. Synthetic intermed. for prodn. of food additives. Used as aq. soln. for photometric detn. of V, U. Forms chelates with many metals. in cosmetics. Shows weak antibacterial action. Skin whitening agent. Cryst. (H_2O). Sol. H_2O, AcOH; fairly sol. Py, EtOAc, $CHCl_3$, Et_2O; poorly sol. C_6H_6.
Mp 161° (152°). λ_{max} 227 (ϵ 20700); 313 (ϵ 5250) (MeOH/KOH) (Derep). λ_{max} 217 (ϵ 18200); 269 (ϵ 8320) (MeOH) (Berdy). λ_{max} 319 (ϵ 6020) (MeOH/NaOH) (Berdy).
▶ LD_{50} (mus, ipr) 250 mg/kg. UQ0875000
1′-O-β-D-Glucopyranoside: [149056-78-0]
$C_{12}H_{16}O_9$ 304.253
Prod. by *Aspergillus albus*. Inhibitor of tyrosine and melanine formation. Sol. H_2O.
*5-Me ether: 2-(Hydroxymethyl)-5-methoxy-4*H*-pyran-4-one*
$C_7H_8O_4$ 156.138
Isol. from a marine-derived *Alternaria* sp. Amorph. solid.
λ_{max} 222 (log ϵ 4); 283 (log ϵ 2.3) (MeOH).
*Di-Me ether: 5-Methoxy-2-(methoxymethyl)-4*H*-pyran-4-one*
$C_8H_{10}O_4$ 170.165
Isol. from a marine-derived *Alternaria* sp. Amorph. solid.
λ_{max} 216 (log ϵ 3.57); 294 (log ϵ 3.68) (MeOH).
5-Benzyl ether: [15771-06-9]
$C_{13}H_{12}O_4$ 232.235
Solid. Mp 132-133°.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 457B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 724C (*nmr*)
Yabuta, T. *et al., J.C.S.*, 1924, **125**, 575 (*struct*)
Beélik, A. *et al., Adv. Carbohydr. Chem.*, 1956, **11**, 145 (*rev*)
Becker, H.D. *et al., Acta Chem. Scand.*, 1962, **16**, 78 (*synth*)
Satyanarayana, D. *et al., Chemist-Analyst*, 1965, **54**, 4 (*detn, V*)
Sommer, L. *et al., Coll. Czech. Chem. Comm.*, 1966, **31**, 1288 (*detn, U*)
Lichtenthaler, F.W. *et al., Angew. Chem., Int. Ed.*, 1969, **8**, 978
Kingsbury, C.A. *et al., J.O.C.*, 1976, **41**, 2777 (*pmr*)
Bajpai, P. *et al., J. Sci. Ind. Res.*, 1982, **41**, 185 (*rev*)
Lokaj, J. *et al., Acta Cryst. C*, 1991, **47**, 193 (*cryst struct*)
Japan. Pat., 1993, 93 221 846; *CA*, **120**, 14652x (*glucoside*)
Li, X. *et al., Arch. Pharmacal Res.*, 2003, **26**, 532-534 (*isol, Me ethers*)
Ma, Y. *et al., J. Med. Chem.*, 2004, **47**, 6349-6362 (*benzyl ether*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 759
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HLH500

2-Hydroxy-2-(hydroxymethyl)-2*H*-pyran-3(6*H*)-one H-696

Microthecin

[73033-01-9]



$C_6H_8O_4$ 144.127

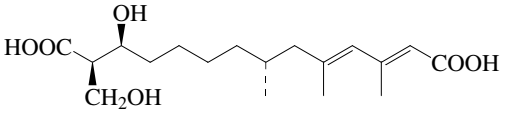
Prod. by *Melanospora ornata* and *Microthecium* spp. Isol. from *Morchella vulgaris* (morel) and from the red alga *Gracilariopsis lemaneiformis*. Platelet aggregation inhibitor. Cryst. (EtOAc). Sol. EtOAc. λ_{max} 225 (MeOH) (Berdy). λ_{max} 230 (ϵ 4365); 345 (ϵ 23) (dioxan) (Berdy).

Japan. Pat., 1979, 79 122 796; *CA*, **92**, 126906 (*isol, struct*)
Deffieux, G. *et al., Phytochemistry*, 1987, **26**, 1391-1393; 1395-1397 (*biosynth*)
Broberg, A. *et al., Phytochemistry*, 1996, **41**, 151-154 (*isol, biosynth, pmr, cmr*)
Broberg, A. *et al., Anal. Biochem.*, 1999, **268**, 35-42 (*anal*)

12-Hydroxy-13-(hydroxymethyl)-3,5,7-trimethyl-2,4-tetradecadiene-1,14-dioic acid, 9CI H-697

Antibiotic 1233B. 1233B

[34668-58-1]
[34668-61-6]



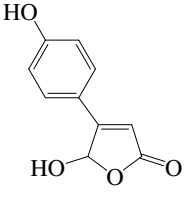
$C_{18}H_{30}O_6$ 342.431

Metab. of *Cephalosporium* spp. and the marine-derived *Scopulariopsis candida*. Shows antibiotic props. Cryst. (Et_2O). Poorly sol. H_2O.

Mp 88-94°.

Aldridge, D.C. *et al., J.C.S.(C)*, 1971, 3888-3891 (*isol, uv, ir, ms, pmr*)
Höller, U. *et al., Mycol. Res.*, 2000, **104**, 1354-1365 (*isol, pmr, cmr*)

5-Hydroxy-4-(4-hydroxyphenyl)-2(5*H*)-furanone H-698



$C_{10}H_8O_4$ 192.171

(-)-*form* [123564-56-7]

Constit. of *Sphagnum* spp.

Needles (H_2O).

Mp 228°. $[\alpha]_D^{20}$ -3.5 (c, 0.55 in MeOH).

(±)-*form* [161810-67-9]

Cryst. (2-propanol). Mp 231-233°.

(ξ)-*form*

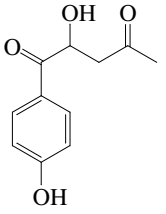
Isol. from the sponge *Iotrochota birotulata*.

Mp 205-207°. Genus name given, apparently incorrectly, as Iotrichoto. λ_{max} 310 (MeOH).

Wilschke, J. *et al., Phytochemistry*, 1989, **28**, 1725-1727; 3581 (*(-)-form, isol*)
Eicher, T. *et al., J. Prakt. Chem.*, 1996, **338**, 706-710 (*synth, ir, pmr, cmr, ms, uv*)
Li, L. *et al., Pharmazie*, 2003, **58**, 680-681 (*ξ-form, isol, pmr, cmr*)

2-Hydroxy-1-(4-hydroxyphenyl)-1,4-pentanedione H-699

[656822-88-7]



$C_{11}H_{12}O_4$ 208.213

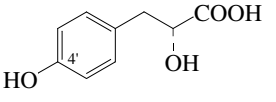
Constit. of *Isis hippuris*. Cryst. (hexane). $[\alpha]_D^{25}$ -6.2 (c, 0.4 in MeOH).

Chang, Y.-T. *et al., Chin. Pharm. J. (Taipei)*, 2003, **55**, 129-133 (*isol, pmr, cmr*)

2-Hydroxy-3-(4-hydroxyphenyl)propanoic acid H-700

α,4-Dihydroxybenzenepropanoic acid, 9CI. 3-(4-Hydroxyphenyl)-lactic acid, 8CI

[306-23-0]



(*R*)-*form*

$C_9H_{10}O_4$ 182.176

► Tumorigenic. OD5500000

(*R*)-*form* [89919-57-3]

Isol. from the heartwood of *Pterocarpus marsupium*.

Mp 169-170° (164-165°). $[\alpha]_D^{26}$ -19.6 (c, 1.3 in H_2O).

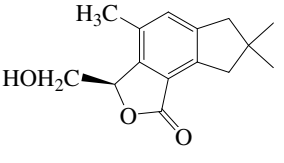
2-O-Sulfate: 3-(4-Hydroxyphenyl)-2-(sulfooxy)propanoic acid. ***Tichocarpol A***

$C_9H_{10}O_7S$ 262.24

Isol. from the red alga *Tichocarpus crinitus*. Amorph. solid. $[\alpha]_D^{26}$ +2.7 (c, 0.4 in H_2O).

Danifshefsky, S. *et al., J.A.C.S.*, 1979, **101**, 7013 (*synth, pmr*)
Lohaus, E. *et al., Z. Naturforsch., C*, 1983, **38**, 524 (*occur*)
Gowal, H. *et al., Helv. Chim. Acta*, 1985, **68**, 2132 (*synth*)
Ishii, T. *et al., J. Nat. Prod.*, 2004, **67**, 1764-1766 (*Tichocarpol A*)

4-Hydroxy-2,6,8-illudalatrien-15,5-olide H-701



$C_{15}H_{18}O_3$ 246.305

(*R*)-*form*

Nitrate ester: ***Alcyopterosin E***

[288851-31-0]

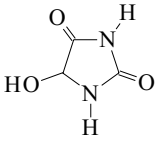
$C_{15}H_{17}NO_5$ 291.303

Constit. of *Alcyonium paessleri*. Oil. $[\alpha]_D^{25}$ -31.28 (c, 2.35 in $CHCl_3$). λ_{max} 242 (log ϵ 3.96); 302 (log ϵ 3.63) (CH_2Cl_2).

Palermo, J. *et al., J.O.C.*, 2000, **65**, 4482-4486 (*isol, pmr, cmr*)
Witulski, B. *et al., Chem. Comm.*, 2002, 2984-2985 (*synth*)

5-Hydroxy-2,4-imidazolidinedione H-702

5-Hydroxyhydantoin
[29410-13-7]



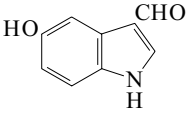
$C_3H_4N_2O_3$ 116.076
Isol. from the tunicate *Botryllus schlosseri*.

(±)-form
Cryst. (AcOH). Mp 140-142°. Compd. descr. in early ref. had different props.

Biltz, H. *et al., Ber.*, 1921, **54**, 1802 (*synth*)
Abblard, J. *et al., Bull. Soc. Chim. Fr.*, 1971, 942 (*synth, pmr*)
Usov, A.I. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2002, **28**, 147-151 (*isol*)

5-Hydroxy-1*H*-indole-3-carboxaldehyde, 9CI H-703

3-Formyl-5-hydroxyindole
[3414-19-5]



$C_9H_7NO_2$ 161.16
Alkaloid from the marine sponge *Hyrtios erecta*. Needles. Mp 220-221°. λ_{max} 215 (ϵ 12500); 252 (ϵ 11300); 270 (ϵ 9000); 298 (ϵ 1500) (MeOH) (Berdy).

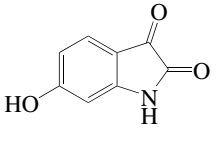
*Me ether: 5-Methoxy-1*H*-indole-3-carboxaldehyde*
[10601-19-1]
$C_{10}H_9NO_2$ 175.187
Cryst. (CH_2Cl_2/petrol). Mp 174-175°.

Me ether, N*-Me: 5-Methoxy-1-methyl-1*H*-indole-3-carboxaldehyde*
[39974-94-2]
$C_{11}H_{11}NO_2$ 189.213
Needles (EtOH). Mp 134°.

Reimann, E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1988, **321**, 823-826 (*Me ether N-Me, synth, ms, pmr, anal*)
Kobayashi, J. *et al., Tetrahedron*, 1990, **46**, 7699
Moody, C.J. *et al., J.C.S. Perkin 1*, 1993, 2561 (*Me ether, synth, ir, pmr, cmr, ms*)
Naylor, M.A. *et al., J. Med. Chem.*, 1997, **40**, 2335-2346 (*Me ether N-Me, synth, pmr*)

6-Hydroxy-1*H*-indole-2,3-dione, 9CI H-704

6-Hydroxyisatin
[116569-08-5]



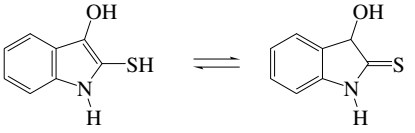
$C_8H_5NO_3$ 163.132
Prod. by the marine-derived *Streptomyces* sp. B1848. Orange cryst. (MeOH). Dec. >325° without melting. λ_{max} 263; 280 (sh); 349 (sh); 420 (sh) (MeOH).

*Me ether: 6-Methoxy-1*H*-indole-2,3-dione. 6-Methoxyisatin*
[52351-75-4]
$C_9H_7NO_3$ 177.159
Yellow needles (H_2O). Mp 233-235°.

Giovannini, E. *et al., Helv. Chim. Acta*, 1948, **31**, 1381-1391 (*synth, Me ether*)
Pavlidis, V.H. *et al., Synth. Commun.*, 1994, **24**, 533 (*synth*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*isol, pmr, cmr, ms*)

3-Hydroxy-1*H*-indole-2-thiol H-705

*1,3-Dihydro-3-hydroxy-2*H*-indole-2-thione. 3-Hydroxy-2-mercaptoindole*



C_8H_7NOS 165.215

SH-form

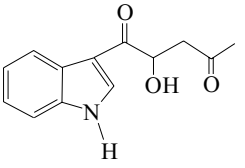
S-*Me,* O-*sulfate:*
$C_9H_9NO_4S_2$ 259.306
Isol. from *Murex trunculus*.

O,S-*Di-β-D-glucopyranoside:* ***Calanthoside***
$C_{20}H_{27}NO_{11}S$ 489.499
Alkaloid from *Calanthe discolor*. Powder. $[\alpha]_D^{25}$ -12 (c, 0.2 in MeOH). λ_{max} 222 (log ϵ 3.5); 290 (log ϵ 2.7) (MeOH).

Baker, J.T. *et al., Tet. Lett.*, 1968, 43 (*S-Me sulfate*)
Fouquet, H. *et al., Angew. Chem., Int. Ed.*, 1971, **10**, 816-817 (*S-Me sulfate, isol*)
Baker, J.T. *et al., Tet. Lett.*, 1976, 1233-1234 (*S-Me sulfate, occur*)
Murakami, T. *et al., Heterocycles*, 2001, **54**, 957-966 (*Calanthoside*)
Cooksey, C.J. *et al., Molecules*, 2001, **6**, 736-769 (*S-Me sulfate, rev*)

2-Hydroxy-1-(1*H*-indol-3-yl)-1,4-pentanedione, 9CI H-706

3-(2-Hydroxy-1,4-dioxopentyl)indole. 4-Hydroxy-5-(3-indolyl)-5-oxo-2-pentanone
[107749-00-8]



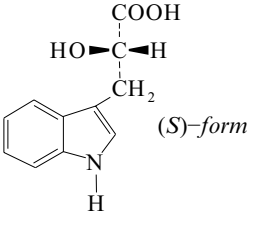
$C_{13}H_{13}NO_3$ 231.251

(±)-form
Alkaloid from the sponges *Dysidea etheria* and *Ulosa ruetzleri*. Possesses plant growth regulatory activity. Off-white solid. Sol. Me_2CO, MeOH.

Cardellina, J.H. *et al., J. Nat. Prod.*, 1986, **49**, 1065-1067 (*isol, ir, pmr, ms, struct*)

2-Hydroxy-3-(3-indolyl)propanoic acid H-707

*α-Hydroxy-1*H*-indole-3-propanoic acid, 9CI. 3-(3-Indolyl)lactic acid*
[1821-52-9]
[101312-07-6]



$C_{11}H_{11}NO_3$ 205.213

(*S*)-*form* [7417-65-4]
Cryst. (Et_2O/petrol). Mp 100-101° (99°). $[\alpha]_D^{20}$ -5.36 (H_2O).

N-*Me: α-Hydroxy-1-methyl-1*H-*indole-3-propanoic acid. 2-Hydroxy-3-(1-methylindolyl)propanoic acid*
$C_{12}H_{13}NO_3$ 219.24
Constit. of the skins of peanuts (*Arachis hypogaea*). Needles (MeOH).
Mp 216° dec. $[\alpha]_D^{25}$ +32.2 (c, 0.13 in MeOH).

*Me ether: α-Methoxy-1*H-*indole-3-propanoic acid. 2-Methoxy-3-(3-indolyl)propanoic acid*
$C_{12}H_{13}NO_3$ 219.24
Constit. of the skins of peanuts (*Arachis hypogaea*). Needles (MeOH).
Mp 252° dec. $[\alpha]_D^{25}$ +22.2 (c, 0.1 in MeOH).

(±)-*form* [832-97-3]
Mp 144-145°.

(ξ)-*form*
Metab. of various bacteria *Agrobacterium* spp., *Acetobacter* spp., *Aspergillus* spp. and *Streptomyces* spp. incl. the marine *Streptomyces* sp. B2150.

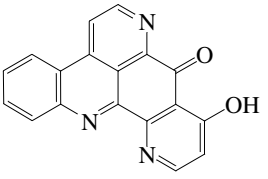
Et ester, O-*β-D-glucopyranoside:* [143884-93-9]
$C_{19}H_{25}NO_8$ 395.408
Constit. of grapes (Riesling wine).

*Me ether, dimethylamide: α-Methoxy-*N,N*-dimethyl-1*H-*indole-3-propanamide, 9CI. 3-(1*H-*Indol-3-yl)-2-methyl-*N,N*-dimethylpropanamide*
[201284-05-1]
$C_{14}H_{18}N_2O_2$ 246.308
Alkaloid from the seeds of *Erythrina brucei*.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 669B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 140C (*nmr*)
Ehrlich, F. *et al., Ber.*, 1911, **44**, 888
Bauguess, L.C. *et al., J. Biol. Chem.*, 1934, **104**, 679
Ratusky, J. *et al., Chem. Listy*, 1957, **51**, 109; *CA*, **51**, 13843 (*synth*)
Marinos, V.A. *et al., Phytochemistry*, 1992, **31**, 2755-2759; 4399 (*isol*)
Bugge, J. *et al., Pharm. Pharmacol. Lett.*, 1997, **7**, 155-156 (*Me ether dimethylamide*)
Lou, H. *et al., Planta Med.*, 2001, **67**, 345-349 (*N-Me, Me ether*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)
Irlinger, B. *et al., Helv. Chim. Acta*, 2005, **88**, 1472-1485 (*isol, pmr, cmr, ms*)

9-Hydroxyisoascididemnin H-708

*9-Hydroxy-8*H-*benzo[*b*]pyrido[4,3,2-*de*][1,10]phenanthrolin-8-one, 9CI*
[215590-37-7]

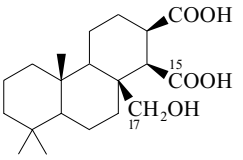


$C_{18}H_9N_3O_2$ 299.288
Alkaloid from the sponge *Biemna fortis*. Neuronal differentiation inducer. Amorph. yellow solid.
Mp 293-295° dec. (as Me ether). Possible artifact. λ_{max} 227 (ε 15000); 277 (ε 10600); 365 (ε 5270) (MeOH).

*9-Deoxy, 9-amino: 9-Amino-8*H-*benzo[*b*]pyrido[4,3,2-*de*][1,10]-phenanthrolin-8-one, 9CI.* ***9-Aminoisoascididemnin***
[191849-14-6]
$C_{18}H_{10}N_4O$ 298.303
Alkaloid from the sponge *Biemna fortis*. Neuronal differentiation inducer. Amorph. yellow solid (natural). Red powder ($CHCl_3$/petrol) (synthetic).
Mp > 250° (synthetic). λ_{max} 231 (ε 20000); 282 (ε 14100); 373 (ε 7020) (MeOH).

Kitahara, Y. *et al., Tetrahedron*, 1998, **54**, 8421-8432 (*synth, pmr, cmr*)
De la Fuente, J.A. *et al., Bioorg. Med. Chem.*, 2001, **9**, 1807-1814 (*synth, pmr, cmr*)
Aoki, S. *et al., Bioorg. Med. Chem.*, 2003, **11**, 1969-1973 (*isol, pmr, cmr*)

17-Hydroxy-15,16-isocopalanedioic acid H-709

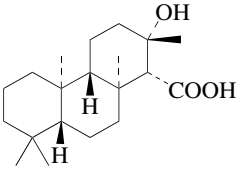


$C_{20}H_{32}O_5$ 352.47

(13α*H*,14α*H*)-*form*
15→17 Lactone, Me ester: Methyl 15,17-isocopalanolid-16-oate. ***Dendrillol 3***
[106019-61-8]
$C_{21}H_{32}O_4$ 348.481
Constit. of *Dendrilla rosea* and *Chromodoris obsoleta*. Cryst. Mp 162-164°.

Karuso, P. *et al., Aust. J. Chem.*, 1986, **39**, 1643
Miyamoto, T. *et al., Tetrahedron*, 1996, **52**, 8187-8198 (*isol, cmr*)

13-Hydroxy-15-isocopalanoic acid H-710



$C_{20}H_{34}O_3$ 322.487

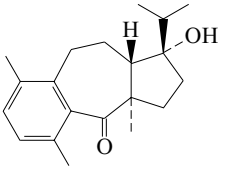
(*ent*-13β,14α*H*)-*form*
2-Acetoxy-3-hydroxypropyl ester: ***Anisodorin 4***
[220866-42-2]
$C_{25}H_{42}O_6$ 438.603
Constit. of *Anisodoris fontaini*.
$[\alpha]_D$ +17.9 (c, 0.2 in $CHCl_3$).

3-Acetoxy-2-hydroxypropyl ester: ***Anisodorin 3***
[220866-41-1]
$C_{25}H_{42}O_6$ 438.603
Constit. of *Anisodoris fontaini*.
$[\alpha]_D$ +2.9 (c, 0.13 in $CHCl_3$).

Gavagnin, M. *et al., J. Nat. Prod.*, 1999, **62**, 269-274 (*isol, pmr, cmr*)

9-Hydroxy-1,3,5(14)-isodolastatrien-13-one H-711

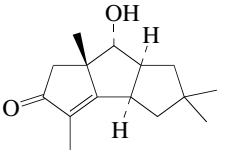
[135650-28-1]



$C_{20}H_{28}O_2$ 300.44
Metab. of *Dictyota divaricata*. Oil.

Rao, C.B. *et al., Phytochemistry*, 1991, **30**, 1971 (*isol, pmr, cmr*)

8-Hydroxy-3-isohirsuten-5-one H-712



$C_{15}H_{22}O_2$ 234.338

8α-*form*

Hirsutanol D

[210897-96-4]

Metab. of the marine fungus *Coriolus consors*.

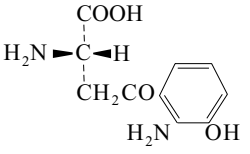
$[\alpha]_D^{25}$ -36 (c, 0.13 in $CHCl_3$). λ_{max} 248 (ϵ 2316) (MeOH).

Wang, G.-Y.-S. *et al., Tetrahedron*, 1998, **54**, 7335-7342 (*isol, pmr, cmr*)

3-Hydroxykynurenine H-713

α,2-Diamino-3-hydroxy-γ-oxobenzenebutanoic acid, 9CI. 3-(3-Hydroxyanthraniloyl)alanine

[484-78-6]



(*S*)–*form*

$C_{10}H_{12}N_2O_4$ 224.216

▶AY6475000

(*S*)-*form*

L-form

[606-14-4]

Yellow pigment found in the pupae of *Calliphora* and silkworms (*Bombyx mori*) and in the wings of butterflies. Also found as a urinary metab. from patients with severe tuberculosis and haemoblastosis. Constit. of the lens of *Sepia officinalis*. Crustacean moult inhibitor. Pale-yellow needles.

Mp 185-190° dec. $[\alpha]_D^{20}$ -45 (c, 0.9 in MeOH).

▶AY6650000

O-*Sulfate:* ***Rhodnitin***

$C_{10}H_{12}N_2O_7S$ 304.28

Fluorescent pigment from *Rhodnius prelixus*. Yellow powder (as NH_4 salt). Sol. H_2O. $[\alpha]_D^{25}$ -19.6 (H_2O, as NH_4 salt). Shows blue fluor.

O-*Glucoside:* [32342-57-7]

$C_{16}H_{22}N_2O_9$ 386.358

Isol. from *Bombyx mori* and from human eye lens.

(±)-*form* [2147-61-7]

Yellow needles (H_2O). Dec. at 223°.

Hydrobromide (1:2):

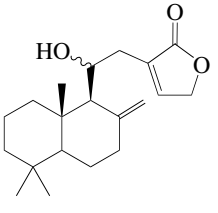
Cryst. Mp 233° dec.

Me ether, hydrochloride (1:2):

Prisms + H_2O. Mp 160°.

Butenandt, A. *et al., Chem. Ber.*, 1957, **90**, 1120 (*synth*)
Visconti, M. *et al., Helv. Chim. Acta*, 1963, **46**, 2509 (*Rhodnitin*)
Witkop, B. *et al., J.A.C.S.*, 1967, **89**, 1017 (*struct, ms*)
Brown, K.S. *et al., Tet. Lett.*, 1967, 1721 (*ms*)
Kuznezova, L.E. *et al., Nature (London)*, 1969, **222**, 484 (*tox*)
Van Heyningen, R. *et al., Nature (London)*, 1971, **230**, 393 (*isol*)
Shashar, N. *et al., Biol. Bull. (Woods Hole, Mass.)*, 1998, **195**, 187-188 (*marine, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HJD000; HJD500

11-Hydroxy-8(17),13-labdadien-16,15-olide H-714



$C_{20}H_{30}O_3$ 318.455

(11ξ)-*form*

Ac: ***Lutenolide***

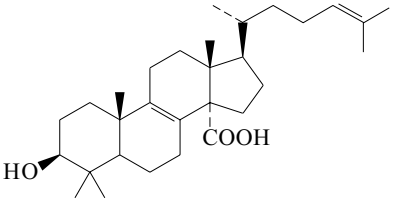
[194020-43-4]

$C_{22}H_{32}O_4$ 360.492

Constit. of *Cadlina luteomarginata*. Oil.

Dumdei, E.J. *et al., Can. J. Chem.*, 1997, **75**, 773-789 (*isol, pmr, cmr*)

3-Hydroxylanosta-8,24-dien-30-oic acid H-715



$C_{30}H_{48}O_3$ 456.707

3β-*form*

Penasterol

[116424-94-3]

Constit. of a *Penares* sp. sponge. Possesses antileukaemic props. Needles (EtOAc/hexane). Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 197-201°. $[\alpha]_D^{26}$ -54.5 (c, 0.1 in MeOH). λ_{max} 205 (ϵ 8000) (MeOH) (Berdy).

3-O-[β-D-Galactopyranosyl-(1→2)-α-L-arabinopyranoside]: ***Eryloside F***

[269055-90-5]

$C_{41}H_{66}O_{12}$ 750.965

Constit. of *Erylus formosus*. Thrombin receptor antagonist activity. Amorph. solid.

3-O-[α-L-Arabinopyranosyl-(1→3)-β-D-galacturonopyranosyl-(1→4)-β-D-glucuronopyranoside]: ***Nobiloside***

[415707-49-2]

$C_{47}H_{72}O_{19}$ 941.074

Constit. of *Erylus nobilis*. Powder. $[\alpha]_D^{24}$ -41.6 (c, 0.1 in MeOH).

3-O-[β-D-Galactopyranosyl-(1→3)-β-D-arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-arabinopyranoside]: ***Formoside***†

[160436-09-9]

$C_{52}H_{84}O_{21}$ 1045.223

Constit. of *Erylus formosus*. Amorph. solid.

3-O-[2-Acetamido-2-deoxy-β-D-galactopyranosyl-(1→2)-[β-D-galactopyranosyl-(1→3)-α-L-arabinopyranosyl-(1→3)]-α-L-arabinopyranoside]: ***Formoside B***

[336812-54-5]

$C_{54}H_{87}NO_{21}$ 1086.275

Constit. of *Erylus formosus*. Fish antifeedant. Amorph. solid. $[\alpha]_D^{20}$ -10.3 (c, 0.13 in MeOH). λ_{max} 211 (log ϵ 3.7) (MeOH).

Ac: ***Acetylpenasterol***

[145525-34-4]

$C_{32}H_{50}O_4$ 498.745

Constit. of the sponge *Penares incrustans*. Histamine release inhibitor. Cryst.

Mp 185-187°. $[\alpha]_D^{25}$ -44.7 (c, 0.59 in $CHCl_3$).

3-Ketone: 3-Oxolanosta-8,24-dien-30-oic acid. ***Penasterone***

[145525-33-3]

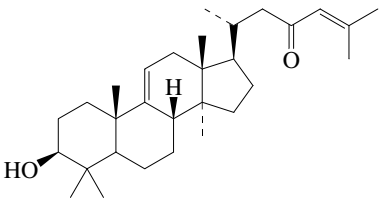
$C_{30}H_{46}O_3$ 454.692

Constit. of *Penares incrustans*. Histamine release inhibitor. Cryst. (MeOH).

Mp 126-130°. $[\alpha]_D^{25}$ -18.2 (c, 0.6 in $CHCl_3$).

Cheng, J.-F. *et al., J.C.S. Perkin 1*, 1988, 2403 (*isol, pmr, cmr*)
Shoji, N. *et al., J. Nat. Prod.*, 1992, **55**, 1682 (*isol, pmr, cmr, cryst struct*)
Jaspars, M. *et al., Tet. Lett.*, 1994, **35**, 7501-7504 (*Formoside*)
Stead, P. *et al., Bioorg. Med. Chem. Lett.*, 2000, **10**, 661-664 (*Eryloside F*)
Kubanek, J. *et al., Marine Ecol.: Progr. Ser.*, 2000, **207**, 69-77 (*Formoside B*)
Kubanek, J. *et al., Nat. Prod. Lett.*, 2001, **15**, 275-285 (*Formoside B*)
Takada, K. *et al., J. Nat. Prod.*, 2002, **65**, 411-413 (*Nobiloside*)

3-Hydroxylanosta-9(11),24-dien-23-one H-716

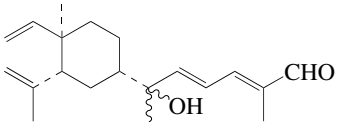


$C_{30}H_{48}O_2$ 440.708

3β-*form*

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]: ***Sarasinoside G***
[147769-50-4]
$C_{62}H_{100}N_2O_{25}$ 1273.47
Constit. of *Asteropus sarasinosum*. Protein kinase C inhibitor. Cryst. Sol. MeOH, butanol; fairly sol. $CHCl_3$; poorly sol. H_2O. Mp 203-206°. $[\alpha]_D^{20}$ -29.9 (MeOH).
Espada, A. *et al., Tetrahedron*, 1992, **48**, 8685-8696 (*isol, pmr, cmr*)

13-Hydroxy-8,10,15,17-lobatetraen-19-al H-717



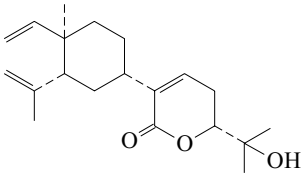
$C_{20}H_{30}O_2$ 302.456

(13ξ,15*E*,17*E*)-*form* [161536-22-7]
Constit. of *Lobophytum hirsutum*.
Oil. $[\alpha]_D$ +19 (c, 0.7 in $CHCl_3$). λ_{max} 264 (MeOH).

19-Carboxylic acid: ***13-Hydroxy-8,10,15,17-lobatetraen-19-oic acid***
$C_{20}H_{30}O_3$ 318.455
Isol. from soft coral *Lobophytum microlobulatum* from the Andaman Islands. Oil. $[\alpha]_D^{25}$ +23.4 (c, 0.8 in $CHCl_3$). λ_{max} 252 ($CHCl_3$).
Raja, B.L. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 221-226 (*isol, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 45-48 (*carboxylic acid*)

18-Hydroxy-8,10,13(15)-lobatrien-14,17-olide H-718

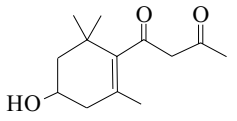
Lobatrienolide
[139579-31-0]



$C_{20}H_{30}O_3$ 318.455
Constit. of *Simularia flexibilis*. Oil. $[\alpha]_D^{25}$ +89.3 (c, 0.63 in $CHCl_3$).
Hamada, T. *et al., Chem. Lett.*, 1992, 33 (*isol, pmr, cmr*)
Kato, M. *et al., J.C.S. Perkin 1*, 1999, 783-788 (*synth*)

3-Hydroxy-5-megastigmene-7,9-dione H-719

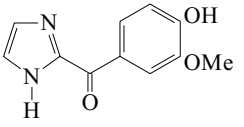
1-(2,6,6-Trimethyl-4-hydroxycyclohexenyl)-1,3-butanedione
[72726-22-8]



$C_{13}H_{20}O_3$ 224.299
Constit. of dinoflagellate *Prorocentrum minimum*. Oil. Sol. MeOH, hexane; poorly sol. H_2O. $[\alpha]_D^{25}$ -35 (c, 0.5 in MeOH). λ_{max} 299 (ε 11900) (MeOH/KOH) (Derep). λ_{max} 287 (ε 11000) (MeOH) (Derep). λ_{max} 287 (ε 11000) (MeOH) (Berdy). λ_{max} 299 (ε 1900) (MeOH-NAOH) (Berdy).
Andersen, R.J. *et al., J.O.C.*, 1980, **45**, 1169

2-(4-Hydroxy-3-methoxybenzoyl)imidazole H-720

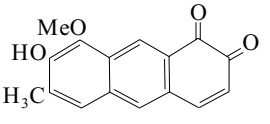
2-Vanilloylimidazole
[114703-13-8]



$C_{11}H_{10}N_2O_3$ 218.212
Metab. from the Australian ascidian *Aplydium pliciferum*. Also obt. from aged extracts of an undescribed New Zealand *Aplydium* sp. (not detected in freshly-prepared ascidian extracts).
Mp 226°. Prob. not a naturally occurring metab. λ_{max} 369 (ε 4300) (MeOH/KOH) (Derep). λ_{max} 240 (ε 2300); 291 (ε 2400); 324 (ε 2600) (MeOH) (Derep).
Arabshahi, L. *et al., Tet. Lett.*, 1988, **29**, 1099 (*isol, pmr, struct*)
Copp, B.R. *et al., Tet. Lett.*, 1989, **30**, 3703 (*uv, ir, cmr, cryst struct*)

7-Hydroxy-8-methoxy-6-methyl-1,2-anthraquinone H-721

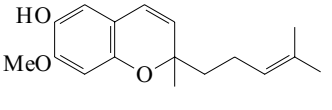
7-Hydroxy-8-methoxy-6-methyl-1,2-anthracenedione, 9CI. ***Hallachrome***
[38393-67-8]



$C_{16}H_{12}O_4$ 268.268
Pigment from the sea worms *Halla parthenopeia* and *Lumbriconereis impatiens*. Red prisms.
Mp 224-226°. λ_{max} 249 (log ε 4.61); 312 (log ε 4.47); 497 (log ε 4.3) (MeOH).
Bu'Lock, J.D. *et al., Biochem. J.*, 1950, **47**, 32 (*isol*)
Prota, G. *et al., J.C.S. Perkin 1*, 1972, 1614-1616 (*isol, struct*)
Krohn, K. *et al., Annalen*, 1993, 905 (*synth, pmr, cmr*)
Cameron, D.W. *et al., Aust. J. Chem.*, 1999, **52**, 833-836 (*synth*)

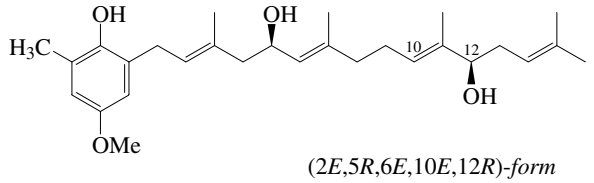
6-Hydroxy-7-methoxy-2-methyl-2-(4-methyl-3-pentenyl)-2*H*-1-benzopyran H-722

[124609-39-8]



$C_{17}H_{22}O_3$ 274.359
Metab. of *Amaroucium multiplicatum*. Oil.
Sato, A. *et al., J. Nat. Prod.*, 1989, **52**, 975-981 (*isol, synth, pmr, cmr*)

1-(2-Hydroxy-5-methoxy-3-methylphenyl)-3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraene-5,12-diol, 9CI H-723



(2*E*,5*R*,6*E*,10*E*,12*R*)-*form*

$C_{28}H_{42}O_4$ 442.637

(2*E*,5*R*,6*E*,10*E*,12*R*)-*form* [197355-29-6]
Constit. of *Cystoseira adriatica*.
Oil. $[\alpha]_D^{20}$ +2.8 (c, 1.6 in EtOH). λ_{max} 221 (ϵ 13400); 288 (ϵ 3800) (EtOH).

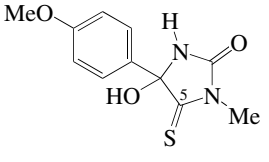
12-Ketone: ***5-Hydroxy-1-(2-hydroxy-5-methoxy-3-methylphenyl)-3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraen-12-one***
[121389-75-1]
$C_{28}H_{40}O_4$ 440.622
Constit. of a *Cystoseira* sp. Oil. $[\alpha]_D^{20}$ +8 (c, 0.6 in EtOH). λ_{max} 221 (ϵ 16400); 242 (ϵ 10500); 288 (ϵ 3550) (EtOH).

10,11-Dihydro, 12-ketone: ***5-Hydroxy-1-(2-hydroxy-5-methoxy-3-methylphenyl)-3,7,11,15-tetramethyl-2,6,14-hexadecatrien-12-one***
[80756-09-8]
$C_{28}H_{42}O_4$ 442.637
Constit. of a *Cystoseira* sp. and *Halidrys siliquosa*. Oil. $[\alpha]_D^{20}$ +11.3 (c, 2.1 in EtOH). λ_{max} 222 (ϵ 11100); 288 (ϵ 3800) (EtOH).

(2*E*,5ξ,6*E*,10*E*,12ξ)-*form* [85873-08-1]
Constit. of *Cytoseira elegans*.
$[\alpha]_D$ -1.9 (c, 9.3 in MeOH). Mixt. of C-12 epimers.

Banaigs, B. *et al., Tetrahedron*, 1983, **39**, 629-638 (*isol, struct*)
Amico, V. *et al., Gazz. Chim. Ital.*, 1988, **118**, 193-195 (*isol, pmr, cmr*)
Amico, V. *et al., J. Nat. Prod.*, 1997, **60**, 1088-1093 (*abs config*)

4-Hydroxy-4-(4-methoxyphenyl)-1-methyl-5-thioxo-2-imidazolidinone, 9CI H-724



$C_{11}H_{12}N_2O_3S$ 252.293

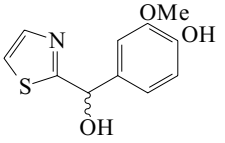
(±)-*form*
Metab. from the Indian ocean ascidian *Polycarpa clavata*.
Amorph. solid. Prob. an artifact. CAS no. not found 8-14CI.
λ_{max} 202 (log ϵ 3.99); 220 (log ϵ 3.91); 278 (log ϵ 3.88) (MeOH).

Me ether: 4-Methoxy-4-(4-methoxyphenyl)-1-methyl-5-thioxo-2-imidazolidinone
$C_{12}H_{14}N_2O_3S$ 266.32
Metab. from the ascidians *Polycarpa clavata* and *Polycarpa aurata*. Inosine monophosphate dehydrogenase inhibitor.
Needles.
Mp 127-129°. Prob. an artifact. CAS no. not found 8-14CI.
λ_{max} 203 (log ϵ 4.14); 222 (log ϵ 4.17); 279 (log ϵ 4.1) (MeOH).
λ_{max} 224 (ϵ 8822); 282 (ϵ 7640) (MeOH) (Berdy).

Abas, S.A. *et al., J.O.C.*, 1996, **61**, 2709-2712 (*Me ether, isol, uv, pmr, cmr, ms, struct*)
Kang, H. *et al., Tet. Lett.*, 1996, **37**, 2369-2372 (*Me ether, isol, ir, uv, pmr, cmr, struct*)

α-(4-Hydroxy-3-methoxyphenyl)-2-thiazolemethanol, 9CI H-725

[110281-34-0]



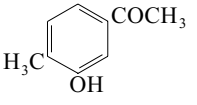
$C_{11}H_{11}NO_3S$ 237.279
Minor metab. from the Australian ascidian *Aplydium pliciferum*.
Mp 154-155°.

Ketone: (4-Hydroxy-3-methoxyphenyl)-2-thiazolylmethanone, 9CI. 2-(4-Hydroxy-3-methoxybenzoyl)thiazole
[110281-33-9]
$C_{11}H_9NO_3S$ 235.263
Metab. from *Aplydium pliciferum*. Mp 104°. λ_{max} 233 (ϵ 4900); 300 (ϵ 4800); 341 (ϵ 5600) (EtOH) (Derep).

Arabshahi, L. *et al., Tet. Lett.*, 1988, **29**, 1099-1102 (*isol, uv, ir, pmr, cmr, ms, struct*)

3′-Hydroxy-4′-methylacetophenone H-726

1-(3-Hydroxy-4-methylphenyl)ethanone. 5-Acetyl-o-cresol
[33414-49-2]



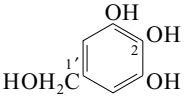
$C_9H_{10}O_2$ 150.177
Constit. of *Laurencia chilensis*. Cryst. ($CHCl_3$). Poorly sol. hexane. Mp 105-107°. λ_{max} 240; 270; 352 (MeOH/NaOH) (Derep). λ_{max} 214 (ϵ 7500); 222 (ϵ 8470); 260 (ϵ 5120); 310 (ϵ 1590) (MeOH) (Derep). λ_{max} 217 (ϵ 7500); 222 (ϵ 8470); 250 (ϵ 5118); 310 (ϵ 1588) (MeOH) (Berdy).

Me ether: 3′-Methoxy-4′-methylacetophenone
[3556-81-8]
$C_{10}H_{12}O_2$ 164.204
Liq. $Bp_{0.25}$ 74-75°.

Bisanz, T. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1973, **47**, 2279
Valdebenito, H. *et al., Phytochemistry*, 1982, **21**, 1456 (*isol*)
Fuganti, C. *et al., J.C.S. Perkin 1*, 2000, 3758-3764 (*Me ether, synth, ir, pmr, ms*)

5-(Hydroxymethyl)-1,2,3-benzenetriol H-727

α,3,4,5-Tetrahydroxytoluene. 3,4,5-Trihydroxybenzyl alcohol. Gallyl alcohol
[68325-64-4]



$C_7H_8O_4$ 156.138
Unstable, readily polymerises.

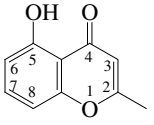
1′-Me ether: 5-(Methoxymethyl)-1,2,3-benzenetriol
[119188-78-2]
$C_8H_{10}O_4$ 170.165
Isol. from *Grateloupia filicina*. Needles ($CHCl_3$/Me_2CO). Sol. MeOH, EtOAc. Mp 176-178°. λ_{max} 274 (ϵ 580) (EtOH).

[119188-79-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1143D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 367C (*nmr*)
Nozaki, H. *et al., Agric. Biol. Chem.*, 1988, **52**, 3229-3230 (*1′-Me ether*)

5-Hydroxy-2-methyl-4*H*-1-benzopyran-4-one, 9CI H-728

5-Hydroxy-2-methylchromone
[1130-62-7]



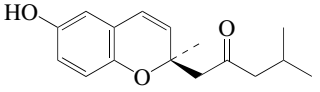
$C_{10}H_8O_3$ 176.171
Prod. by *Daldinia concentrica* and *Hypoxylon macrocarpum*. Used as 0.02*M* MeOH soln. for extraction-fluorimetric detn. of Ti (λ_{max} 511 nm, 40% MeOH, CCl_4). Yellow needles. Sol. MeOH.
Mp 82-84° Mp 92°.

*Me ether: 5-Methoxy-2-methyl-4*H*-1-benzopyran-4-one. 5-Methoxy-2-methylchromone*
[22105-23-3]
$C_{11}H_{10}O_3$ 190.198
Cryst. Mp 105°.

Allport, D.C. *et al., J.C.S.*, 1960, 654 (*isol, uv*)
Murray, R.D.H. *et al., Tetrahedron*, 1969, **25**, 5819 (*synth, ir*)
Ito, T. *et al., Anal. Chim. Acta*, 1980, **113**, 343 (*detn, Ti*)
Nagasawa, K. *et al., Heterocycles*, 1988, **27**, 1159 (*synth*)
Muhlbauer, A. *et al., Mycol. Prog.*, 2002, **1**, 235-248 (*occur*)
Okombi, S. *et al., Chem. Pharm. Bull.*, 2005, **53**, 1460-1462 (*synth*)

1-(6-Hydroxy-2-methyl-2*H*-1-benzopyran-2-yl)-4-methyl-2-pentanone H-729

*6-Hydroxy-2-methyl-2-(4-methyl-2-oxopentyl)-2*H*-1-benzopyran*

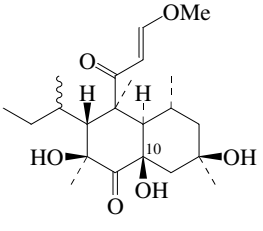


$C_{16}H_{20}O_3$ 260.332

(*R*)-*form* [185839-22-9]
Isol. from the tunicate *Aplidium solidum*. Yellow oil. $[\alpha]_D$ -17.1 (c, 0.8 in $CHCl_3$). λ_{max} 246 (ϵ 4000); 330 (ϵ 1650) (EtOH).

Rochfort, S.J. *et al., Aust. J. Chem.*, 1996, **49**, 1217 (*isol, uv, ir, pmr, cmr, ms*)

10-Hydroxy-18-*O*-methylbetaenone C H-730

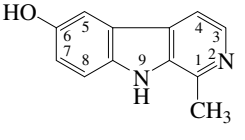


$C_{22}H_{36}O_6$ 396.523
Prod. by a *Microsphaeropsis* sp. isol. from the sponge *Aplysina aerophoba*. Inhibitor of protein kinases. Powder. $[\alpha]_D$ +16.6 (c, 1.25 in EtOH). λ_{max} 265 (MeOH).

Brauers, G. *et al., J. Nat. Prod.*, 2000, **63**, 739-745,

6-Hydroxy-1-methyl-β-carboline H-731

*1-Methyl-9*H*-pyrido[3,4-*b*]indol-6-ol, 9CI. **6-Hydroxyharman***
[67767-19-5]



$C_{12}H_{10}N_2O$ 198.224

Alkaloid from the roots of *Grewia mollis* and from *Ophiorrhiza japonica*. Also from the bryozoan *Cribricellina cribraria*. Pale-yellow prisms. Mp 276-278°.

Hydrochloride:
Cryst. (MeOH). Mp 320° dec.

*Me ether: 6-Methoxy-1-methyl-β-carboline. 6-Methoxyharman. **Isoharmine**. Coharmine*
[3589-72-8]
$C_{13}H_{12}N_2O$ 212.251
Alkaloid from *Mucuna pruriens* and leaves and stems of *Virola cuspidata* (Myristicaceae, Leguminosae). Also isol. from *Peganum harmala* (Zygophyllaceae). Prisms (MeOH).
Mp 275-276° dec. λ_{max} 232 (ϵ 33800); 246 (sh) (ϵ 29400); 257 (sh) (ϵ 21900); 285 (sh) (ϵ 15000); 290 (ϵ 15600); 296 (ϵ 25000); 354 (ϵ 7500) (EtOH).
▶ UV0168000

*3,4-Dihydro, Me ether: **3,4-Dihydro-6-methoxy-1-methyl-β-carboline. 6-Methoxyharmalan***
[3589-73-9]
$C_{13}H_{14}N_2O$ 214.266
Alkaloid from the leaves and stems of *Virola cuspidata* (Myristicaceae).
▶ UU9802000

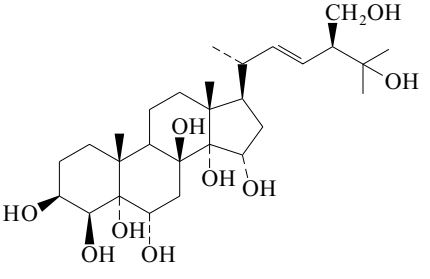
Cook, J.W. *et al., J.C.S.*, 1951, 1203-1207 (*synth*)
Cassady, J.M. *et al., J. Nat. Prod.*, 1971, **34**, 161-162 (*6-Methoxyharman, 6-Methoxyharmalan*)
Ghosal, S. *et al., Planta Med.*, 1972, **21**, 200-203 (*6-Methoxyharman, occur*)
Rosler, H. *et al., J. Nat. Prod.*, 1978, **41**, 383-384 (*isol, uv, ir, pmr, ms, struct*)
Aimi, N. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3064-3066 (*isol*)
Ayoub, M.T. *et al., Phytochemistry*, 1991, **30**, 1046-1047 (*Isoharmine*)
Rocca, P. *et al., Tet. Lett.*, 1994, **35**, 2003-2004 (*synth*)
Harwood, D.T. *et al., Nat. Prod. Res.*, 2003, **17**, 15-19 (*isol, pmr, cmr*)

8-Hydroxy-1-methyl-β-carboline H-732

*1-Methyl-9*H*-pyrido[3,4-*b*]indol-8-ol, 9CI. **8-Hydroxyharman***
[521305-60-2]
$C_{12}H_{10}N_2O$ 198.224
Alkaloid from the bryozoan *Cribricellina cribraria*. Yellow oil. λ_{max} 216 (ϵ 4000); 242 (ϵ 6500); 277 (ϵ 1300); 286 (ϵ 1500); 340 (ϵ 800) (EtOH).

Harwood, D.T. *et al., Nat. Prod. Res.*, 2003, **17**, 15-19 (*isol, pmr, cmr, ms*)

24-Hydroxymethylcholest-22-ene-3,4,5,6,8,14,15,25-octol H-733

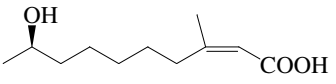


$C_{28}H_{48}O_9$ 528.682

(3β,4β,5α,6α,15α,22*E*,24*S*)-*form*
Campest-22-ene-3,4,5,6,8,14,15,25-octol
[123050-81-7]
Metab. of *Archaster typicus*.
Glass. $[\alpha]_D$ +18.4 (c, 0.4 in MeOH).

Riccio, R. *et al., J.C.S. Perkin 1*, 1989, 823-826 (*isol, pmr, cmr*)

9-Hydroxy-3-methyl-2-decenoic acid H-734



$C_{11}H_{20}O_3$ 200.277

(2*Z*,9*R*)-*form*

O-*(15Z-Docosenoyl), 2-sulfoethyl ester:* ***Irciniasulfonic acid A_1***
$C_{35}H_{64}O_7S$ 628.952
Isol. from the sponge *Ircinia* sp. Multidrug resistance modulator. Isol. as a mixt. with other Irciniasulfonic acids A, to which data refers. λ_{max} 220 (ϵ 6100) (MeOH).

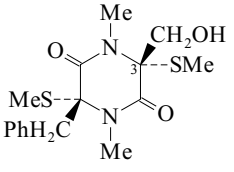
O-*Tricosanoyl, 2-sulfoethyl ester:* ***Irciniasulfonic acid A_3***
$C_{36}H_{68}O_7S$ 644.995
Isol. from *Ircinia* sp.

O-*(5Z,9Z-Tetracosadienoyl), 2-sulfoethyl ester:* ***Irciniasulfonic acid A_2***
$C_{37}H_{66}O_7S$ 654.99
Isol. from *Ircinia* sp.

Kawakami, A. *et al., Tet. Lett.*, 2001, **42**, 3335-3337 (*isol, pmr, cmr*)
Dobbs, A.P. *et al., Synlett*, 2005, 652-654 (*synth*)

3-(Hydroxymethyl)-1,4-dimethyl-3,6-bis(-methylthio)-6-(phenylmethyl)-2,5-piperazinedione, 9CI H-735

Bisdethiodi(methylthio)hyalodendrin
[50655-20-4]



(3*R*,6*R*)–*form*

$C_{16}H_{22}N_2O_3S_2$ 354.493
Epithiodioxopiperazine antibiotic.
▶ LD_{50} (mus, ipr) >200 mg/kg. TL6375030

(3*R*,6*R*)-*form*

(+)-cis-*form*. ***Gliovictin***. *Antibiotic A 26771E. A 26771E*
[52080-06-5]
Isol. from *Gliocladium virens*, *Helminthosporium victoriae* and *Penicillium turbatum* and the marine-derived *Asteromyces cruciatus*.
Cryst.
Mp 134°. $[\alpha]_D^{25}$ -65 ($CHCl_3$). λ_{max} 255 (sh) (ϵ 1000) (EtOH) (Derep).

N^4-*De-Me:*
$C_{15}H_{20}N_2O_3S_2$ 340.467
Prod. by *Verticillium hemipterigenum* BCC 1449. Cryst.
Mp 154-157°. $[\alpha]_D^{26}$ -70 (c, 0.21 in $CHCl_3$). Abs. config. revised in 2005. λ_{max} 205 (log ϵ 4.35); 258 (log ϵ 2.94) (EtOH).

N,N-*Di-de-Me:* ***Bis*-N-*norgliovictin***. *Di*-N-*norgliovictin*
[112900-75-1]
$C_{14}H_{18}N_2O_3S_2$ 326.44
Isol. from *Gliocladium virens* and *Verticillium hemipterigenum* BCC 1449. Needles.
Mp 231° dec. $[\alpha]_D$ -32 (c, 0.1 in MeOH).

(3*S*,6*S*)-*form*

(-)-cis-*form*
[52021-97-3]
Isol. from *Hyalodendron* spp.
Cryst. (CH_2Cl_2/cyclohexane).
Mp 141.5-142.5°. $[\alpha]_D^{24}$ +63.5 (c, 2.5 in $CHCl_3$).

(3*RS*,6*RS*)-*form*

(±)-cis-*form*
[71772-59-3]
Cryst. Mp 118-120°.

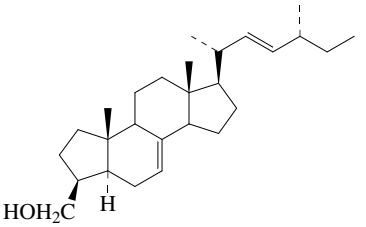
(3*RS*,6*SR*)-*form*

(±)-trans-*form*
[71772-60-6]
Cryst. (CH_2Cl_2/Et_2O). Mp 163-165.5°.

DeVault, R.L. *et al., J. Antibiot.*, 1973, **26**, 532-534 (*isol*)
Strunz, G.M. *et al., Can. J. Chem.*, 1974, **52**, 325-326 (*isol*)
Dorn, F. *et al., Experientia*, 1974, **30**, 134-135 (*isol, pmr, ms*)
Michel, K.H. *et al., J. Antibiot.*, 1974, **27**, 57-64 (*isol*)
Williams, R.M. *et al., J.O.C.*, 1980, **45**, 2625-2631 (*synth, ir, pmr, ms*)
Shin, J. *et al., Phytochemistry*, 1987, **26**, 3347 (*Asteromyces, isol*)
Kirby, G.W. *et al., J.C.S. Perkin 1*, 1988, 301-304 (*Bis-N-norgliovictin*)
Pita Boente, M.I. *et al., J.C.S. Perkin 1*, 1991, 1283-1290 (*isol, biosynth, pmr, cmr*)
Nilanonta, C. *et al., J. Antibiot.*, 2003, **56**, 647-651 (*4-N-de-Me*)
Isaka, M. *et al., Org. Lett.*, 2005, **7**, 2257-2260 (*4-N-de-Me, Bis-N-norgliovictin*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 583

3-Hydroxymethyl-*A*,27-dinorergosta-7,22-diene H-736

A,*27-Dinorergosta-7,22-diene-3-methanol*



(3β,5α,22*E*,24*R*)-*form*

$C_{27}H_{44}O$ 384.644

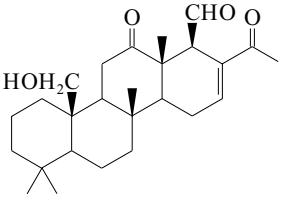
(3β,5α,22*E*,24*R*)-*form* [123165-79-7]
Isol. from the sponge *Phakellia aruensis.*

(3β,5α,22*E*,24*S*)-*form* [83704-11-4]
Isol. from *Acanthella aurantiaca*.

Bohlin, L. *et al., J.O.C.*, 1982, **47**, 5309-5314 (*isol*)
Malik, S. *et al., Steroids*, 1989, **53**, 271-284 (*isol*)

22-Hydroxy-24-methyl-12,24-dioxo-16-scalaren-25-al H-737

[75587-67-6]

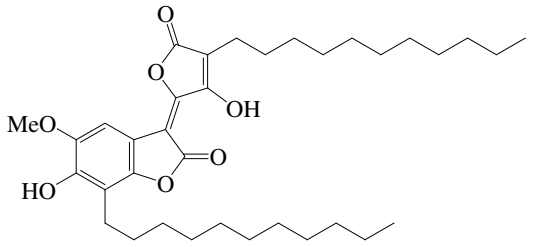


$C_{26}H_{38}O_4$ 414.584
Constit. of a *Phyllospongia* sp. Cryst. (EtOAc/petrol). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 204° dec. $[\alpha]_D^{21}$ +110 (c, 1 in $CHCl_3$). λ_{max} 231 (ϵ 8590) (MeOH) (Berdy).

Ac: [75587-68-7]
$C_{28}H_{40}O_5$ 456.621
Constit. of a *Phyllospongia* sp. Cryst. (EtOAc/petrol).
Mp 193.5-194.1°. $[\alpha]_D$ +95.4 (c, 1.27 in $CHCl_3$).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1980, **33**, 1783 (*isol, pmr, cryst struct*)

10-Hydroxy-4-*O*-methyl-2,11-diundecylgomphilactone H-738

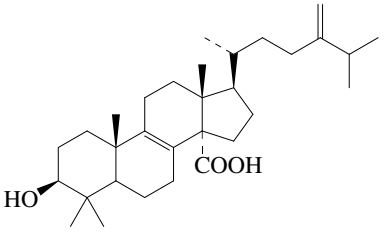


$C_{35}H_{52}O_7$ 584.792
Constit. of the mangrove plant *Aegiceras corniculatum*. Orange solid ($CHCl_3$).
Mp 103-105°. λ_{max} 220 (log ϵ 3.81); 273 (log ϵ 3.67); 453 (log ϵ 3.58) (MeOH).
Xu, M. *et al., J. Nat. Prod.*, 2004, **67**, 762-766 (*isol, pmr, cmr, ms*)

2-Hydroxy-21-methyldocosanoic acid H-739

[144465-60-1]
$(H_3C)_2CH(CH_2)_{18}CH(OH)COOH$
$C_{23}H_{46}O_3$ 370.615
Constit. of the sponge *Smenospongia aurea*.
Carballeira, N.M. *et al., Lipids*, 1992, **27**, 681 (*isol*)

3-Hydroxy-24-methylenelanost-8-en-30-oic acid H-740



$C_{31}H_{50}O_3$ 470.734

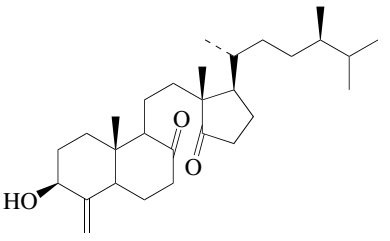
3β-*form*

3-O-*[2-Acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[α-L-arabinopyranosyl-(1→3)]-β-D-galactopyranoside]*: ***Eryloside G***
[350678-22-7]
$C_{50}H_{81}NO_{17}$ 968.186
Constit. of *Erylus nobilis*. Amorph. solid.
Mp 187-191° dec. $[\alpha]_D^{25}$ -18.8 (c, 0.09 in MeOH).

3-O-*[2-Acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[α-L-arabinopyranosyl-(1→3)]-α-L-arabinopyranoside]*: ***Eryloside H***
[350678-23-8]
$C_{49}H_{79}NO_{16}$ 938.16
Constit. of *Erylus nobilis*. Amorph. solid.
Mp 208-210°. $[\alpha]_D^{25}$ -12.4 (c, 0.07 in MeOH).
Shin, J. *et al., J. Nat. Prod.*, 2001, **64**, 767-771 (*isol, pmr, cmr*)

3-Hydroxy-4-methylene-8,14-secoergostane-8,14-dione H-741

3-Hydroxy-24-methyl-4-methylene-8,14-secocholestane-8,14-dione

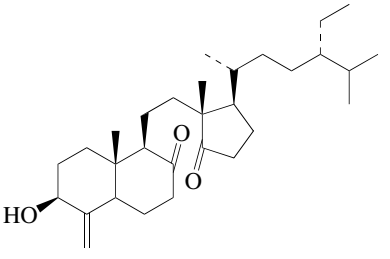


$C_{29}H_{48}O_3$ 444.696

(3β,5α,24*R*)-*form*

Swinhosterol B
[186312-99-2]
Constit. of *Theonella swinhoei*.
Oil. $[\alpha]_D^{25}$ -50 (c, 1 in $CHCl_3$).
Sugo, Y. *et al., Steroids*, 1995, **60**, 738-742 (*isol, pmr, cmr*)
Umeyama, A. *et al., J. Nat. Prod.*, 1997, **60**, 296-298 (*isol, pmr, cmr*)

3-Hydroxy-4-methylene-8,14-secostigmastane-8,14-dione H-742

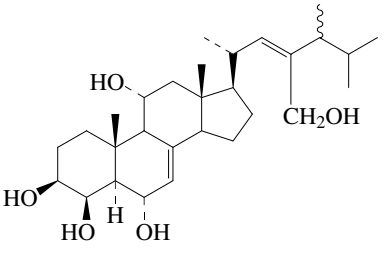


$C_{30}H_{50}O_3$ 458.723

(3β,24*S*)-*form*

Swinhosterol A
[186312-98-1]
Constit. of *Theonella swinhoei*.
Oil. $[\alpha]_D^{25}$ -50 (c, 1.67 in $CHCl_3$).
Umeyama, A. *et al., J. Nat. Prod.*, 1997, **60**, 296-298 (*isol, pmr, cmr*)

23-(Hydroxymethyl)ergosta-7,22-diene-3,4,6,11-tetrol H-743



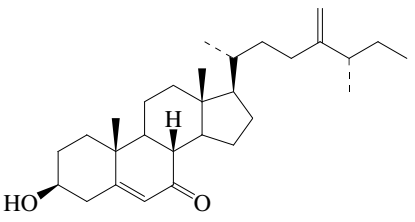
$C_{29}H_{48}O_5$ 476.695

(3β,4β,5α,6α,11α,22*Z*,24ξ)-*form*

3,4,6-Tri-Ac: ***Agosterol A*$_5$**
[255832-08-7]
$C_{35}H_{54}O_8$ 602.807
Constit. of a *Spongia* sp.
$[\alpha]_D$ +8.2 (c, 0.3 in $CHCl_3$).
Aoki, S. *et al., Tetrahedron*, 1999, **55**, 13965-13972 (*isol, pmr, cmr*)

3-Hydroxy-26-methylergosta-5,24(28)-dien-7-one H-744

3-Hydroxy-26-methyl-24-methylenecholest-5-en-7-one. 25-Ethyl-3-hydroxy-27-norergosta-5,24(28)-dien-7-one

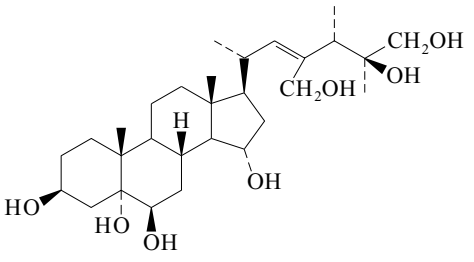


$C_{29}H_{46}O_2$ 426.681

(3β,25*S*)-*form* [385815-30-5]
Constit. of *Geodia japonica*.
Cryst.
Mp 50-51°. $[\alpha]_D^{25}$ -79 (c, 0.006 in MeOH). λ_{max} 234 (log ε 3.38) (MeOH).
Zhang, W.-H. *et al., J. Nat. Prod.*, 2001, **64**, 1489-1492 (*isol, pmr, cmr*)

23-(Hydroxymethyl)ergost-22-ene-3,5,6,15,25,26-hexol H-745

23-(Hydroxymethyl)-24-methylcholest-22-ene-3,5,6,15,25,26-hexol

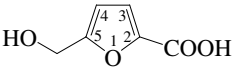


$C_{29}H_{50}O_7$ 510.71

(3β,5α,6β,15α,22*Z*,24*S*,25*S*)-*form*
26-Sulfate: [160538-76-1]
$C_{29}H_{50}O_{10}S$ 590.774
Constit. of *Styracaster caroli*.
$[\alpha]_D$ -3.3 (MeOH).
Iorizzi, M. *et al., J. Nat. Prod.*, 1994, **57**, 1361 (*isol, pmr, cmr*)

5-(Hydroxymethyl)-2-furancarboxylic acid, 9CI H-746

Sumiki's acid
[6338-41-6]



$C_6H_6O_4$ 142.111
Prod. by *Aspergillus* spp., *Gibberella fujikuroi*, *Helminthosporium maydis* and *Pyricularia grisea*. Also from the marine-derived fungi *Epicoccum* sp. and *Wardomyces anomalus*. Found in human urine. Shows some antitumour activity. Cryst. Sol. Py, DMSO; fairly sol. MeOH; poorly sol. hexane.
Mp 165-167°.

Me ester: [36802-01-4]
$C_7H_8O_4$ 156.138
Liq. $Bp_{5.4}$ 86°. n_D^{20} 1.5013.

Ac: 5-(Acetoxymethyl)-2-furancarboxylic acid
[90345-66-7]
[99114-85-9]
$C_8H_8O_5$ 184.148
Isol. from the marine-derived fungi *Cladosporium herbarum* and *Epicoccum* sp. λ_{max} 217 (log ε 4.6); 247 (log ε 3.7) (MeOH).

Ac, Me ester:
$C_9H_{10}O_5$ 198.175
Solid. Mp 39-40°. $Bp_{5.1}$ 136-139°.

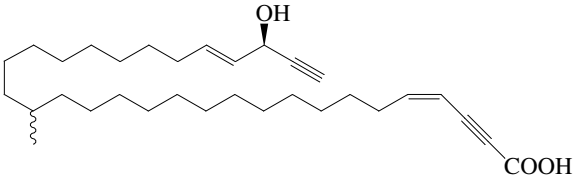
Me ether: 5-(Methoxymethyl)-2-furancarboxylic acid
$C_7H_8O_4$ 156.138
Cryst. (Et_2O). Mp 72-73°.

Me ether, Me ester:
$C_8H_{10}O_4$ 170.165
Liq. $Bp_{0.05}$ 61° approx.

Haworth, W.N. *et al., J.C.S.*, 1927, 1525 (*synth, deriv*)
Curtis, R.F. *et al., J.C.S.(C)*, 1968, 85 (*isol, ir, pmr, uv*)
Mrochek, J.E. *et al., Clin. Chem. (Winston-Salem, N.C.)*, 1972, **18**, 821 (*isol*)
Charon, S. *et al., J.C.S. Perkin 1*, 1973, 1175 (*synth, ms*)
Munekata, M. *et al., Agric. Biol. Chem.*, 1981, **45**, 2149 (*isol, ms, props*)
Moore, J.A. *et al., Org. Prep. Proced. Int.*, 1985, **17**, 203-205 (*Ac, synth*)
Nielek, S. *et al., J. Prakt. Chem.*, 1998, **330**, 825-829 (*Ac Me ester*)
Jadulco, R. *et al., J. Nat. Prod.*, 2001, **64**, 527-530 (*Ac, isol*)
Abdel-Lateff, A. *et al., Planta Med.*, 2003, **69**, 831-834 (*isol*)
Raimundo, B.C. *et al., J. Med. Chem.*, 2004, **47**, 3111-3130 (*Me ester*)

29-Hydroxy-18-methyl-4,27-hentriacontadiene-2,30-diynoic acid H-747

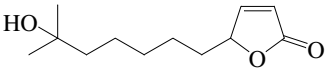
Aztequynol A



$C_{32}H_{52}O_3$ 484.761
Isol. from the sponge *Petrosia* sp.

27,28-Dihydro: 29-Hydroxy-18-methyl-4-hentriacontene-2,30-diynoic acid. ***Aztequynol B***
$C_{32}H_{54}O_3$ 486.777
Isol. from a *Petrosia* sp.
Guerriero, A. *et al., Tet. Lett.*, 1998, **39**, 6395-6398 (*isol, pmr, cmr, ms*)

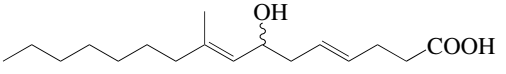
5-(6-Hydroxy-6-methylheptyl)-2(5*H*)-furanone H-748



$C_{12}H_{20}O_3$ 212.288

(+)-*form*
Antibiotic MKN 003B. *MKN 003B*
Prod. by a marine *Streptomyces* strain MO2750.
$[\alpha]_D^{25}$ +19.4 (c, 0.42 in MeOH). λ_{max} 208 (log ε 3.61) (MeOH).
Cho, M.W. *et al., J. Nat. Prod.*, 2001, **64**, 664-667

7-Hydroxy-9-methyl-4,8-hexadecadienoic acid H-749



$C_{17}H_{30}O_3$ 282.422

(4*E*,7ξ,8*E*)-*form*
Me ether: 7-Methoxy-9-methyl-4,8-hexadecadienoic acid
[73631-04-6]
[73631-05-7]
$C_{18}H_{32}O_3$ 296.449
Isol. from the blue-green alga *Lyngbya majuscula*. Oil (as Me ester).
Loui, M.S.M. *et al., Phytochemistry*, 1979, **18**, 1733-1734 (*isol, pmr, cmr, ms*)

2-Hydroxy-14-methylhexadecanoic acid H-750

$H_3CCH_2CH(CH_3)(CH_2)_{11}CH(OH)COOH$

$C_{17}H_{34}O_3$ 286.454

(2ξ,14ξ)-*form*

Me ether: 2-Methoxy-14-methylhexadecanoic acid

$C_{18}H_{36}O_3$ 300.481

Isol. from the sponge *Agelas dispar*.

Carballeira, N.M. *et al., Lipids*, 2002, **37**, 1033-1037 (*isol, synth, pmr, cmr, ms*)

5-Hydroxy-5-methyl-3-hexen-2-one H-751

$(H_3C)_2C(OH)CH{=}CHCOCH_3$

$C_7H_{12}O_2$ 128.171

(ξ)-*form*

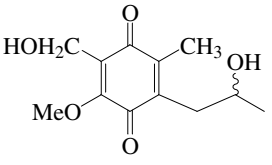
Prod. by the marine isolate *Streptomyces* sp. B5525.

Oil.

Maskey, R.P. *et al., Z. Naturforsch., B*, 2002, **57**, 823-829 (*isol, pmr, cmr, ms*)

2-Hydroxymethyl-5-(2-hydroxypropyl)-3-methoxy-6-methyl-1,4-benzoquinone H-752

Hydroxymethylanserinone B

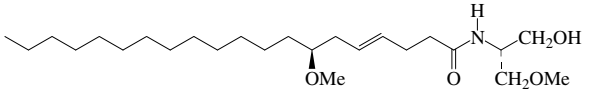


$C_{12}H_{16}O_5$ 240.255

Isol. from a mixt. of strains of the marine *Penicillium corylophilum*. Not obt. pure.

Gautschi, J.T. *et al., J. Nat. Prod.*, 2004, **67**, 362-367 (*isol, pmr, cmr*)

***N*-(1-Hydroxymethyl-2-methoxyethyl)-7-methoxy-4-eicosenamide** H-753



$C_{25}H_{49}NO_4$ 427.666

(1′*R*,4*E*,7*S*)-*form* [253443-61-7]

Isol. from an Australian cyanobacterium.

Plates.

Mp 32-34°. $[\alpha]_D^{20}$ -3 (c, 0.33 in $CHCl_3$).

2′-Ac: N-*(1-Acetoxymethyl-2-methoxyethyl)-7-methoxy-4-eicosenamide*

[253443-58-2]

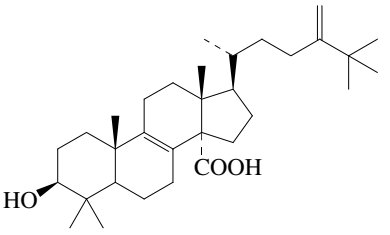
$C_{27}H_{51}NO_5$ 469.704

Isol. from an Australian cyanobacterium. Needles.

Mp 39-40.5°. $[\alpha]_D^{20}$ -6.1 (c, 0.58 in $CHCl_3$).

Wan, F. *et al., J. Nat. Prod.*, 1999, **62**, 1696-1699 (*isol, ir, pmr, cmr*)

3-Hydroxy-25-methyl-24-methylenelanost-8-en-30-oic acid H-754



$C_{32}H_{52}O_3$ 484.761

3β-*form*

3-O-*[2-Acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[α-L-arabinopyranosyl-(1→3)]-β-D-galactopyranoside]:* ***Eryloside I***

[350678-24-9]

$C_{51}H_{83}NO_{17}$ 982.213

Constit. of *Erylus nobilis*. Amorph. solid.

Mp 203-206°. $[\alpha]_D^{25}$ -18 (c, 0.06 in MeOH).

3-O-*[2-Acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[α-L-arabinopyranosyl-(1→3)]-α-L-arabinopyranoside]:* ***Eryloside J***

[350678-25-0]

$C_{50}H_{81}NO_{16}$ 952.187

Constit. of *Erylus nobilis*. Amorph. solid.

Mp 193-196°. $[\alpha]_D^{25}$ -16.9 (c, 0.06 in MeOH).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-galactopyranosyl-(1→3)]-β-D-galactopyranoside]:* ***Eryloside C***

[139933-53-2]

$C_{50}H_{82}O_{18}$ 971.187

Constit. of a Pacific sponge of *Erylus* sp. Amorph. powder.

3-O-*[β-D-Galactopyranosyl-(1→4)-β-D-galactopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-galactopyranoside]:* ***Eryloside D***

[139933-54-3]

$C_{56}H_{92}O_{23}$ 1133.329

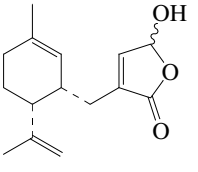
Constit. of an *Erylus* sp. Amorph. powder.

D'Auria, M.V. *et al., Tetrahedron*, 1992, **48**, 491-498

Shin, J. *et al., J. Nat. Prod.*, 2001, **64**, 767-771 (*isol, pmr, cmr*)

5-Hydroxy-3-[1-methyl-4-(1-methylethenyl)-1-cyclohexen-3-yl]-2(5*H*)-furanone H-755

[103202-18-2]



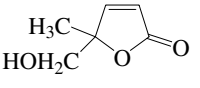
$C_{15}H_{20}O_3$ 248.321

Isol. from mollusc *Chromodoris funerea*.

Carté, B. *et al., J.O.C.*, 1986, **51**, 3528-3532 (*isol, pmr*)

5-Hydroxymethyl-5-methyl-2(5*H*)-furanone H-756

5-Hydroxy-4-methyl-2-penten-4-olide



$C_6H_8O_3$ 128.127

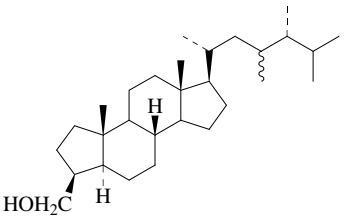
(+)-*form* [681143-75-9]

Isol. from *Sinularia nanolobata*.

Oil. $[\alpha]_D^{25}$ +9.8 (c, 1.02 in $CHCl_3$).

Ac: [681143-76-0]
$C_8H_{10}O_4$ 170.165
Isol. from *Sinularia nanolobata*. Oil. $[\alpha]_D^{25}$ +21.5 (c, 0.28 in $CHCl_3$).
Ahmed, A.F. *et al., J. Nat. Prod.*, 2004, **67**, 592-597 (*isol, pmr, cmr, ms*)

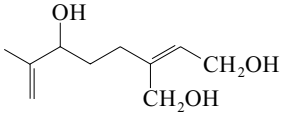
3-Hydroxymethyl-23-methyl-*A*-norergostane **H-757**
23-Methyl-A-*norergostane-3-methanol*



$C_{29}H_{52}O$ 416.729

(3β,5α,23ξ,24*R*)-*form* [83704-14-7]
Constit. of the sponge *Acanthella aurantiaca*.
Bohlin, L. *et al., J.O.C.*, 1982, **47**, 5309-5314 (*isol*)

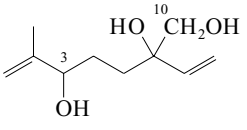
3-Hydroxymethyl-7-methyl-2,7-octadiene-1,6-diol **H-758**



$C_{10}H_{18}O_3$ 186.25

(*Z*)-*form* [125538-00-3]
Constit. of *Chondrococcus hornemanni*.
Oil. $[\alpha]_D$ -17.9 (c, 0.001 in $CHCl_3$).
Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1983 (*isol, pmr, cmr*)
Ahmed, A.A. *et al., Phytochemistry*, 1990, **29**, 3658 (*isol, pmr*)

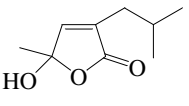
6-Hydroxymethyl-2-methyl-1,7-octadiene-3,6-diol **H-759**



$C_{10}H_{18}O_3$ 186.25

3,10-Dimethyl ether: 6-Methoxy-3-(methoxymethyl)-7-methyl-1,7-octadien-3-ol, 9CI
[136980-52-4]
$C_{12}H_{22}O_3$ 214.304
Constit. of *Portieria hornemannii*. Oil. $[\alpha]_D^{25}$ +4.7 (c, 0.7 in $CHCl_3$).
λ_{max} 217 (EtOH) (Berdy).
Wright, A.D. *et al., Tetrahedron*, 1991, **47**, 5717 (*isol, pmr, cmr*)

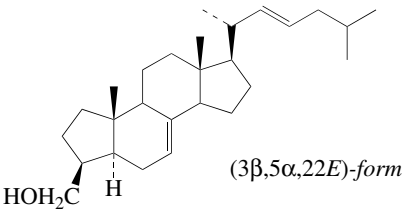
5-Hydroxy-5-methyl-3-(2-methylpropyl)-2(5*H*)-furanone **H-760**
Styxlactone



$C_9H_{14}O_3$ 170.208

(+)-*form* [498552-77-5]
Isol. from a Jamaican sponge *Myrmekioderma styx*.
Oil. $[\alpha]_D$ +10 (c, 0.1 in MeOH). λ_{max} 235 (ε 2770) (MeOH).
Peng, J. *et al., Tet. Lett.*, 2002, **43**, 9699-9702 (*isol, cd, pmr, cmr*)

3-Hydroxymethyl-*A*-norcholesta-7,22-diene **H-761**
A-*Norcholesta-7,22-diene-3-methanol*

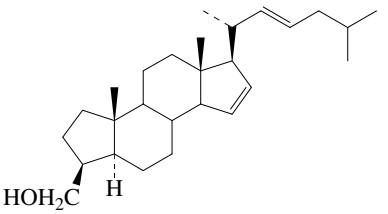


$C_{27}H_{44}O$ 384.644

(3β,5α,22*E*)-*form* [123116-05-2]
Constit. of *Phakellia aruensis.*

(3β,5α,22*Z*)-*form* [123116-06-3]
Constit. of *Phakellia aruensis.*
Malik, S. *et al., Steroids*, 1989, **53**, 271-284 (*isol*)

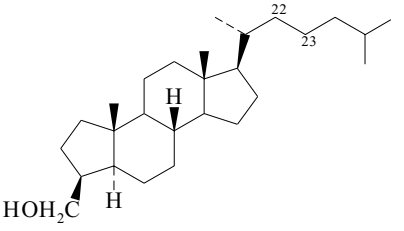
3-Hydroxymethyl-*A*-norcholesta-15,22-diene **H-762**
A-*Norcholesta-15,22-diene-3-methanol*



$C_{27}H_{44}O$ 384.644

(3β,5α,22*E*)-*form* [123116-03-0]
Constit. of the sponge *Phakellia aruensis.*
22,23-Dihydro: A-*Norcholest-15-ene-3-methanol. 3-Hydroxymethyl*-A-*norcholest-15-ene*
[83681-79-2]
$C_{27}H_{46}O$ 386.66
Constit. of *Acanthella aurantiaca* and *Homaxinella trachys.*
Mp 151-153°. $[\alpha]_D$ -37 (c, 0.0006 in $CHCl_3$).
Eggersdorfer, M.L. *et al., J.O.C.*, 1982, **47**, 5304-5309 (*isol, pmr, ms*)
Bohlin, L. *et al., J.O.C.*, 1982, **47**, 5309-5314 (*isol*)
Malik, S. *et al., Steroids*, 1989, **53**, 271-284 (*isol*)

3-Hydroxymethyl-*A*-norcholestane **H-763**
A-Norcholestane-3-methanol, 9CI

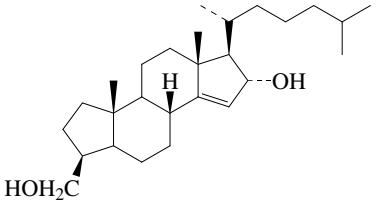


$C_{27}H_{48}O$ 388.676

(3β,5α)-*form* [3963-37-9]
Constit. of *Axinella verrucosa* and *Hymeniacidon aldis.*
Ac: [55081-43-1]
Needles (MeOH). Mp 52-54°.
22,23-Didehydro: 3β-Hydroxymethyl-A-nor-5α-cholest-22-ene
$C_{27}H_{46}O$ 386.66
From *Axinella verrucosa.*
22,23-Didehydro, Ac:
Cryst. (MeOH). Mp 64-65°. $[\alpha]_D$ +23 (c, 0.5 in $CHCl_3$).

Minale, L. *et al., J.C.S. Perkin 1*, 1974, 2380-2384 (*Axinella verrucosa constits*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2321-2328 (*Hymeniacidon aldis constit*)

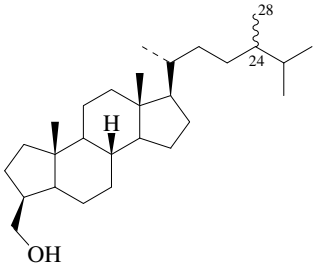
3-Hydroxymethyl-*A*-norcholest-14-en-16-ol H-765



$C_{27}H_{46}O_2$ 402.659

(3β,16α)-*form* [178326-54-0]
Isol. from sponge *Axinella proliferans.*
Aknin, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1996, **113**, 845-848

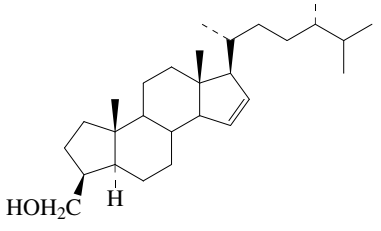
3-Hydroxymethyl-*A*-norergostane H-766
A-Norergostane-3-methanol, 9CI. 3-Hydroxymethyl-24-methyl-A-norcholestane



$C_{28}H_{50}O$ 402.702

(3β,5α,24ξ)-*form* [55088-75-0]
Constit. of *Axinella verrucosa* and *Hymeniacidon perlevis.*
Ac: [55081-44-2]
Cryst. (MeOH). Mp 84-86°. $[\alpha]_D$ +40 (c, 1.7 in $CHCl_3$).
24,28-Didehydro: 24-Methylene-A-norcholestane-3-methanol. 3-Hydroxymethyl-A-norergost-24(28)-ene
[76907-63-6]
[76907-64-7 (Ac)]
$C_{28}H_{48}O$ 400.687
Isol. from the triton *Charonia tritonis* and sponges *Homaxinella trachys* and *Phakellia aruensis.*
Minale, L. *et al., J.C.S. Perkin 1*, 1974, 2380-2384 (*isol*)
Teshima, S. *et al., Nippon Suisan Gakkaishi*, 1980, **46**, 1517-1520; *CA*, **94**, 136426 (*didehydro*)
Eggersdorfer, M.L. *et al., J.O.C.*, 1982, **47**, 5304-5309 (*isol*)
Bohlin, L. *et al., J.O.C.*, 1982, **47**, 5309-5314 (*isol*)

3-Hydroxymethyl-*A*-norergost-15-ene H-767
A-Norergost-15-ene-3-methanol. 3-Hydroxymethyl-24-methyl-A-norcholest-15-ene

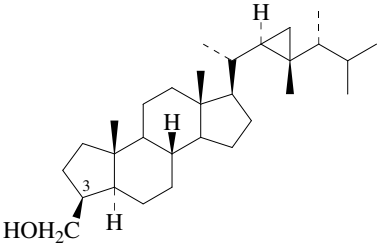


$C_{28}H_{48}O$ 400.687

(3β,5α)-*form* [123116-04-1]
Constit. of the sponges *Axinella tenuidigitata* and *Phakellia aruensis.*
Mp 104° (as Ac).

(3β,5α,24*R*)-*form* [123165-78-6]
Constit. of *Phakellia aruensis.*
Malik, S. *et al., Steroids*, 1989, **53**, 271-284 (*isol*)
Reddy, N.S. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 1145-1147 (*isol, pmr, cmr*)

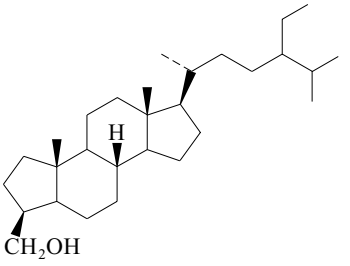
3-Hydroxymethyl-*A*-norgorgostane H-768
A-*Norgorgostane-3-methanol, 9CI*



$C_{30}H_{52}O$ 428.74

(3β,5α)-*form* [83730-43-2]
[74017-15-5]
Constit. of the sponges *Acanthella aurantiaca* and *Stylotella agminata.*
Cryst. (MeOH).
Mp 170-174.5°.
Bohlin, L. *et al., Steroids*, 1980, **35**, 295-304 (*isol*)
Bohlin, L. *et al., J.O.C.*, 1982, **47**, 5309-5314 (*isol*)

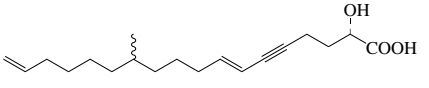
3-Hydroxymethyl-*A*-norstigmastane H-769
24-Ethyl-3-hydroxymethyl-A-norcholestane. A-Norstigmastane-3-methanol, 9CI



$C_{29}H_{52}O$ 416.729

(3β,5α)-*form* [55081-39-5]
[83709-58-4]
Constit. of *Acanthella aurantiaca*, *Axinella verrucosa* and *Homaxinella trachys.*
Ac: [55081-45-3]
Cryst. (MeOH). Mp 86-88°. $[\alpha]_D$ +24 (c, 0.7 in $CHCl_3$).
Minale, L. *et al., J.C.S. Perkin 1*, 1974, 2380-2384 (*isol, ms*)
Bohlin, L. *et al., J.O.C.*, 1982, **47**, 5309-5314 (*isol*)

2-Hydroxy-12-methyl-7,17-octadecadien-5-ynoic acid H-770



(2*S*,7*E*,12ξ)-*form*

$C_{19}H_{30}O_3$ 306.444

(2*S*,7*E*,12ξ)-*form*

Me ether: 2-Methoxy-12-methyl-7,17-octadecadien-5-ynoic acid.
(*E*)-Stellettic acid B
[502487-42-5]
$C_{20}H_{32}O_3$ 320.471
Isol. from the marine sponge *Stelletta* sp. Pale yellow oil. $[\alpha]_D^{21}$ -6 (c, 0.09 in MeOH).

7,8-Dihydro, Me ether: 2-Methoxy-12-methyl-17-octadecen-5-ynoic acid. ***Stellettic acid A***
[502487-40-3]
$C_{20}H_{34}O_3$ 322.487
Isol. from *Stelletta* sp. Pale yellow oil or gum. $[\alpha]_D^{21}$ -16 (c, 0.11 in MeOH). $[\alpha]_D^{25}$ -4.6 (c, 0.04 in MeOH).

Anhydride, 7,8-dihydro, Me ether: 4-(10-Methyl-15-hexen-3-ynyl)-2-oxetanone
[539827-45-7]
$C_{40}H_{66}O_5$ 626.958
Isol. from *Stelletta* sp. Gum. $[\alpha]_D^{25}$ -2.7 (c, 0.04 in MeOH).

(2*S*,7*Z*,12ξ)-*form*

Me ether: ***(Z)-Stellettic acid B***
[502487-41-4]
$C_{20}H_{32}O_3$ 320.471
Isol. from *Stelletta* sp. Pale yellow oil. $[\alpha]_D^{21}$ -18 (c, 0.14 in MeOH).

Zhao, Q. *et al., J. Nat. Prod.*, 2003, **66**, 408-411 (*Stellettic acid A, E-Stellettic acid A, Z-Stellettic acid B*)
Lee, H.-S. *et al., J. Nat. Prod.*, 2003, **66**, 566-568 (*7,8-dhydro derivs*)

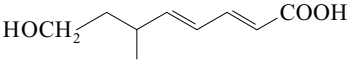
2-Hydroxy-17-methyloctadecanoic acid H-771

[144465-59-8]
$(H_3C)_2CH(CH_2)_{14}CH(OH)COOH$
$C_{19}H_{38}O_3$ 314.507
Constit. of the sponge *Smenospongia aurea*. No phys. props. reported.

Carballeira, N.M. *et al., Lipids*, 1992, **27**, 681 (*isol*)

8-Hydroxy-6-methyl-2,4-octadienoic acid, 9CI H-772

Dendryphiellic acid B
[121839-27-8]



$C_9H_{14}O_3$ 170.208
Metab. of *Dendryphiella salina*. Oil.

Guerriero, A. *et al., Helv. Chim. Acta*, 1989, **72**, 438 (*isol, pmr, cmr*)

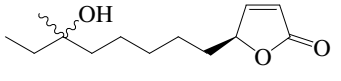
5-Hydroxy-7-methyl-3-octanone H-773

$(H_3C)_2CHCH_2CH(OH)CH_2COCH_2CH_3$
$C_9H_{18}O_2$ 158.24

(ξ)-*form*
Isol. from the sponge *Plakortis zygompha*.
No phys. props. reported.
Faulkner, D.J. *et al., Tet. Lett.*, 1980, 23-26 (*isol, pmr, cmr*)

5-(6-Hydroxy-6-methyloctyl)-2(5*H*)-furanone H-774

4,10-Dihydroxy-10-methyl-2-dodecen-4-olide



(5*S*,6′ξ)-*form*

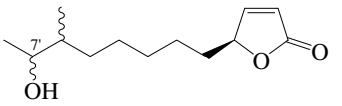
$C_{13}H_{22}O_3$ 226.315

(5*S*,6′ξ)-*form*
Prod. by a marine *Streptomyces* sp. B 5632.
$[\alpha]_D^{22}$ +44 (c, 0.07 in MeOH). λ_{max} 207 (log ϵ 3.63) (MeOH).

(5ξ,6′ξ)-*form*
Antibiotic MKN 003C*. MKN 003C*
Prod. by a marine *Streptomyces* strain M02750.
$[\alpha]_D^{25}$ +20.3 (c, 0.16 in MeOH). λ_{max} 206 (log ϵ 3.58) (MeOH).
Mukku, V.J.R.V. *et al., J. Nat. Prod.*, 2000, **63**, 1570-1572 (*isol, uv, cd, pmr, cmr*)
Cho, M.W. *et al., J. Nat. Prod.*, 2001, **64**, 664-667 (*MKN 003C*)

5-(7-Hydroxy-6-methyloctyl)-2(5*H*)-furanone H-775

4,11-Dihydroxy-10-methyl-2-dodecen-4-olide



$C_{13}H_{22}O_3$ 226.315
Prod. by marine *Streptomyces* sp. B 5632.
$[\alpha]_D^{22}$ +84.5 (c, 0.12 in MeOH). Mixt. of C-7′ epimers. λ_{max} 200 (log ϵ 3.8) (MeCN).

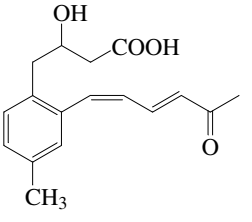
*7′-Ketone: 5-(6-Methyl-7-oxooctyl)-2(5*H*)-furanone. 4-Hydroxy-10-methyl-11-oxo-2-dodecen-4-olide. MKN 003A. Antibiotic MKN 003A*
$C_{13}H_{20}O_3$ 224.299
Prod. by a marine *Streptomyces* sp. B 3497 and by a marine *Streptomyces* strain M02750.
$[\alpha]_D^{22}$ +45 (c, 0.12 in MeOH). $[\alpha]_D^{25}$ +18.4 (c, 0.18 in MeOH). The two isolates may be stereoisomeric. λ_{max} 200 (log ϵ 4.13); 250 (log ϵ 3.47) (MeCN).

*6′-Hydroxy: 5-(6,7-Dihydroxy-6-methyloctyl)-2(5*H*)-furanone*
$C_{13}H_{22}O_4$ 242.314
Prod. by a marine-derived *Streptomyces* sp.

*6′-Hydroxy, 7′-ketone: 5-(6-Hydroxy-6-methyl-7-oxooctyl)-2(5*H*)-furanone*
$C_{13}H_{20}O_4$ 240.299
Prod. by a marine-derived *Streptomyces* sp.

Mukku, V.J.R.V. *et al., J. Nat. Prod.*, 2000, **63**, 1570-1572 (*isol, uv, pmr, cmr, cd*)
Cho, M.W. *et al., J. Nat. Prod.*, 2001, **64**, 664-667 (*isol, pmr, cmr*)
Laatsch, H. *et al., Dissertation*, Univ. of Göttingen, 2005, (*isol*)

3-Hydroxy-4-[4-methyl-2-(5-oxo-1,3-hexadienyl)-phenyl]butanoic acid H-776

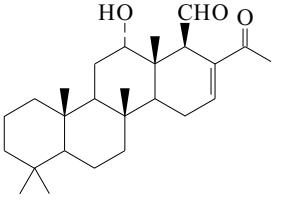


$C_{17}H_{20}O_4$ 288.343

Me ester.
$C_{18}H_{22}O_4$ 302.369
Isol. from a marine-derived fungus.

Grzeganek, P. *et al., Dissertation*, Univ. of Göttingen, 2003,

12-Hydroxy-24-methyl-24-oxo-16-scalaren-25-al H-777



$C_{26}H_{40}O_3$ 400.6

12α-*form*

Ac: [75605-86-6]

$C_{28}H_{42}O_4$ 442.637

Constit. of a *Phyllospongia* sp. Unstable yellow foam. $[\alpha]_D$ +32 (c, 0.35 in MeOH).

12β-*form* [75795-89-0]

3-Hydroxybutanoyl: ***Dendalone***

[75605-85-5]

$C_{30}H_{46}O_5$ 486.69

Constit. of a *Phyllospongia* sp. Antiinflammatory agent. Glass. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D$ +12 (c, 0.4 in $CHCl_3$). λ_{max} 232 (ϵ 8950) (MeOH) (Berdy).

▶ MT0800190

Buckle, P.J. *et al., Agents Actions*, 1980, **10**, 361 (*pharmacol*)
Kazlauskas, R. *et al., Aust. J. Chem.*, 1980, **33**, 1783 (*isol, pmr*)

2-Hydroxy-23-methylpentacosanoic acid H-778

[144465-62-3]

$H_3CCH_2CH(CH_3)CH_2(CH_2)_{19}CH(OH)COOH$

$C_{26}H_{52}O_3$ 412.695

Constit. of the sponge *Smenospongia aurea*. No phys. props. reported.

Carballeira, N.M. *et al., Lipids*, 1992, **27**, 681 (*isol*)

2-Hydroxy-24-methylpentacosanoic acid H-779

[144465-61-2]

$(H_3C)_2CH(CH_2)_{21}CH(OH)COOH$

$C_{26}H_{52}O_3$ 412.695

Constit. of the sponge *Smenospongia aurea*. No phys. props. reported.

Carballeira, N.M. *et al., Lipids*, 1992, **27**, 681 (*isol*)

2-Hydroxy-13-methylpentadecanoic acid H-780

$H_3CCH_2CH(CH_3)(CH_2)_{10}CH(OH)COOH$

$C_{16}H_{32}O_3$ 272.427

(2ξ,13ξ)-*form*

Me ether: 2-Methoxy-13-methylpentadecanoic acid

$C_{17}H_{34}O_3$ 286.454

Isol. from the sponge *Amphimedon complanata*.

Carballeira, N.M. *et al., Lipids*, 2001, **36**, 83-87 (*isol, ms*)

2-Hydroxy-14-methylpentadecanoic acid H-781

$(H_3C)_2CH(CH_2)_{11}CH(OH)COOH$

$C_{16}H_{32}O_3$ 272.427

(ξ)-*form*

Constit. of a *Pseudosuberites* sp.

Me ether: 2-Methoxy-14-methylpentadecanoic acid

$C_{17}H_{34}O_3$ 286.454

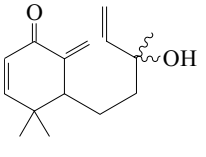
Isol. from the sponges *Amphimedon complanata* and *Agelas dispar*.

Barnathan, G. *et al., J. Nat. Prod.*, 1993, **56**, 2104-2113 (*isol*)
Carballeira, N.M. *et al., Lipids*, 2001, **36**, 83-87; 2002, **37**, 1033-1037 (*Me ether, isol, synth*)

5-(3-Hydroxy-3-methyl-4-pentenyl)-4,4-dimethyl-6-methylene-2-cyclohexen-1-one H-782

Debromo-3-dehydro-4-oxo-β-snyderol. Debromo-10-dehydro-8-oxo-β-snyderol

[134788-19-5]

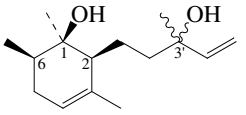


$C_{15}H_{22}O_2$ 234.338

Constit. of *Laurencia caespitosa*. Oil. $[\alpha]_D$ +13.6 (c, 0.77 in $CHCl_3$).

Norte, M. *et al., Can. J. Chem.*, 1991, **69**, 518 (*isol, pmr, cmr*)

2-(3-Hydroxy-3-methyl-4-pentenyl)-1,3,6-trimethyl-3-cyclohexen-1-ol H-783



(1*R**,2*S**,3'ξ,6*R**)-*form*

$C_{15}H_{26}O_2$ 238.369

(1*R,2*S**,3'ξ,6*R**)-*form*** [539824-90-3]

Isol. from *Aplysia punctata*.

Oil. $[\alpha]_D$ +10.4 (c, 0.001 in $CHCl_3$).

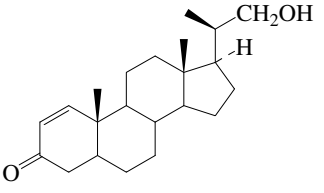
(1*R,2*S**,3'ξ,6*S**)-*form*** [539824-91-4]

Isol. from *Aplysia punctata*.

Oil. $[\alpha]_D$ +31.1 (c, 0.002 in $CHCl_3$).

Findlay, J.A. *et al., Can. J. Chem.*, 2002, **80**, 1697-1707 (*isol, pmr, cmr, ms*)

21-Hydroxy-20-methylpregn-1-en-3-one H-784



$C_{22}H_{34}O_2$ 330.509

(5α,20*R*)-*form*

Ac: [813436-40-7]

$C_{24}H_{36}O_3$ 372.547

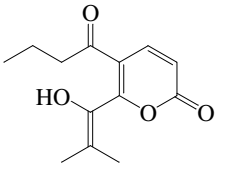
Constit. of a *Scleronephthya* sp. Cryst.

Mp 187-189°. $[\alpha]_D$ +78 (c, 0.34 in $CHCl_3$).

Yan, X.-H. *et al., Youji Huaxue*, 2004, **24**, 1233-1238; *CA*, **142**, 71702 (*isol, pmr, cmr*)

6-(1-Hydroxy-2-methyl-1-propenyl)-5-(1-oxobutyl)-2*H*-pyran-2-one H-785

7-(Methylethylidene)taiwapyrone

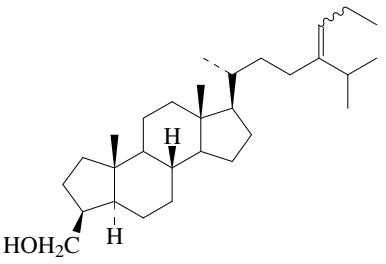


$C_{13}H_{16}O_4$ 236.267

Misleading synonym. Prod. by the marine-derived *Microsphaeropsis* strain 6288. Oil. λ_{max} 267 (log ϵ 3.87) (MeOH). λ_{max} 272 (log ϵ 3.94) (MeOH/HCl). λ_{max} 268 (log ϵ 3.95); 304 (sh) (log ϵ 3.55) (MeOH/NaOH).

Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*isol, uv, pmr, cmr, ms*)

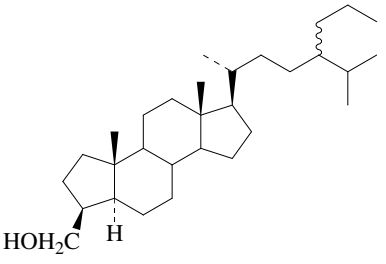
3-Hydroxymethyl-24-propylidene-*A*-norcholestane H-786
28-Ethyl-3-hydroxymethyl-A-*norergost-24(28)-ene*



$C_{30}H_{52}O$ 428.74

(3β,5α,24(28)ξ)-*form* [123165-80-0]
Isol. from *Phakellia aruensis.*
Malik, S. *et al., Steroids*, 1989, **53**, 271-284 (*isol*)

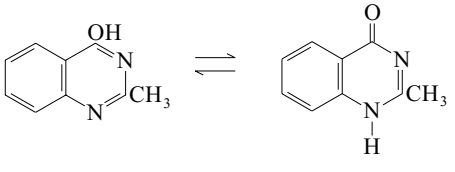
3-Hydroxymethyl-24-propyl-*A*-norcholestane H-787
28-Ethyl-3-hydroxymethyl-A-*norergostane. 24-Propyl*-A-*norcholestane-3-methanol*



$C_{30}H_{54}O$ 430.756

(3β,5α,24ξ)-*form* [83704-15-8]
Isol. from the sponge *Acanthella aurantiaca*.
Bohlin, L. *et al., J.O.C.*, 1982, **47**, 5309-5314 (*isol*)

4-Hydroxy-2-methylquinazoline H-788
*2-Methyl-4(1*H*)-quinazolinone, 9CI. 2-Methyl-4-quinazolinol*
[1769-24-0]



$C_9H_8N_2O$ 160.175

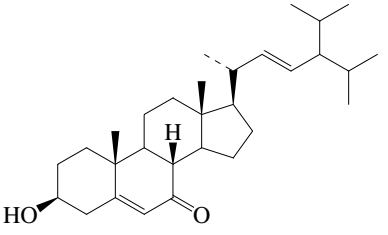
NH-form predominates. 3*H*- and di-*NH*-forms also possible.
Prod. by *Bacillus cereus*. Inhibitor of poly(ADP-ribose) synthetase. Needles (EtOH). Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane.
Mp 240-242° (232-234°). λ_{max} 232 (ϵ 38900); 269 (ϵ 10200); 291 (ϵ 7240); 302 (ϵ 5750) (MeOH/HCl) (Derep). λ_{max} 229 (ϵ 38000); 280 (ϵ 14500); 309 (ϵ 9120) (MeOH/NaOH) (Derep). λ_{max} 225 (ϵ 40700); 263 (ϵ 12900); 303 (ϵ 7080); 314 (ϵ 5890) (MeOH) (Derep). λ_{max} 225 (ϵ 40700); 263 (ϵ 12900); 303 (ϵ 7100); 314 (ϵ 5900) (MeOH) (Berdy). λ_{max} 232 (ϵ 39000); 269 (ϵ 10080); 291 (ϵ 7250); 302 (ϵ 5750) (MeOH-HCl) (Berdy). λ_{max} 229 (ϵ 38000); 280 (ϵ 14400); 309 (ϵ 9200) (MeOH-NaOH) (Berdy).
▶ LD_{50} (mus, orl) 859 mg/kg. VA3677000
Hydrochloride: [29378-39-0]
Cryst. (MeOH). Dec. >320°.

1*H-form*
N^1-*Me: 1,2-Dimethyl-4(1*H*)-quinazolinone.* ***Glomerine***
[7471-65-0]
$C_{10}H_{10}N_2O$ 174.202
Alkaloid from the defensive secretion of the arthropod *Glomeris marginata*. Yellow needles (EtOAc).
Mp 209-211°.

[86030-13-9, 92442-54-1, 110287-94-0, 132305-21-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 882A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 467A (*nmr*)
Bogert, M.T. *et al., J.A.C.S.*, 1900, **22**, 523; 1902, **24**, 1031 (*synth*)
Schildknecht, H. *et al., Z. Naturforsch., B*, 1966, **21**, 121; 552 (*Glomerine, isol, uv, ir, pmr, ms, struct, synth*)
Schildknecht, H. *et al., Tet. Lett.*, 1967, 1815 (*biosynth*)
Goncalves, H. *et al., Bull. Soc. Chim. Fr.*, 1970, 2599 (*synth*)
Kametani, T. *et al., J.C.S. Perkin 1*, 1977, 2347 (*synth*)
Kirmani, M.Z. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 526 (*ms*)
Naik, N.R. *et al., J. Indian Chem. Soc.*, 1979, **56**, 708 (*Glomerine, synth*)
Bhattacharrya, J. *et al., Heterocycles*, 1980, **14**, 1469 (*cmr*)
Etter, M.C. *et al., J.C.S. Perkin 2*, 1983, 115 (*synth, cryst struct*)
Gupton, J.T. *et al., Synth. Commun.*, 1984, **14**, 1013 (*synth, ir, pmr*)
Spasov, S. *et al., Magn. Reson. Chem.*, 1985, **23**, 795 (*pmr, cmr*)
Bajardi, M.L. *et al., Heterocycles*, 1986, **24**, 1367 (*synth*)
Singh, H. *et al., Tetrahedron*, 1986, **42**, 1449 (*synth*)
Shishoo, C.J. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 1039 (*synth*)
Yoshida, S. *et al., J. Antibiot.*, 1991, **44**, 111 (*isol, props*)
Smith, K. *et al., Zh. Org. Khim.*, 2003, **39**, 452-462; *Russ. J. Org. Chem. (Engl. Transl.)*, 2003, **39**, 430-435 (*synth, ir, pmr, cmr, ms*)
Rocco, S.A. *et al., Synthesis*, 2004, 429-435 (*synth, ir, pmr*)

3-Hydroxy-28-methylstigmasta-5,22-dien-7-one H-789
3-Hydroxy-24-isopropylcholesta-5,22-dien-7-one



$C_{30}H_{48}O_2$ 440.708

(3β,22*E*)-*form*
Polasterol A
[290353-68-3]
Constit. of a Japanese *Epipolasis* sp.
Amorph. powder.
Mp 122-125°. $[\alpha]_D^{21}$ -73.7 (c, 0.43 in $CHCl_3$). λ_{max} 238 (log ϵ 3.87) (MeOH).
Umeyama, A. *et al., J. Nat. Prod.*, 2000, **63**, 1175-1177 (*isol, pmr, cmr*)

2-Hydroxy-22-methyltetracosanoic acid H-790
[52900-16-0]
$H_3CCH_2CH(CH_3)CH_2(CH_2)_{18}CH(OH)COOH$
$C_{25}H_{50}O_3$ 398.668
Constit. of the sponge *Smenospongia aurea*. Also found in lanolin wool fat. No phys. props. reported.
Fawaz, F. *et al., Ann. Pharm. Fr.*, 1974, **32**, 59 (*occur*)
Carballeira, N.M. *et al., Lipids*, 1992, **27**, 681 (*isol*)

2-Hydroxy-23-methyltetracosanoic acid H-791
$(H_3C)_2CH(CH_2)_{20}CH(OH)COOH$
$C_{25}H_{50}O_3$ 398.668

(ξ)-*form* [120903-52-8]
Constit. of the sponge *Aplysina archeri*.
Carballeira, N.M. *et al., Lipids*, 1989, **24**, 229-232 (*isol*)

2-Hydroxy-13-methyltetradecanoic acid H-792

$(H_3C)_2CH(CH_2)_{10}CH(OH)COOH$

$C_{15}H_{30}O_3$ 258.4

(ξ)-*form*

Me ether: 2-Methoxy-13-methyltetradecanoic acid
$C_{16}H_{32}O_3$ 272.427
Isol. from the sponge *Amphimedon complanata*. Cytotoxic.
Carballeira, N.M. *et al., Lipids*, 2001, **36**, 83-87 (*isol, ms*)
Carballeira, N.M. *et al., Chem. Phys. Lipids*, 2003, **126**, 149-153 (*synth*)

2-Hydroxy-13-methyl-6-tetradecenoic acid H-793

$(H_3C)_2CH(CH_2)_5CH{=}CH(CH_2)_3CH(OH)COOH$

$C_{15}H_{28}O_3$ 256.384

(2ξ,6*Z*)-*form*

Me ether: 2-Methoxy-13-methyl-6-tetradecenoic acid
[340156-68-5]
$C_{16}H_{30}O_3$ 270.411
Isol. from the sponge *Callyspongia fallax*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*isol*)

2-Hydroxy-22-methyltricosanoic acid H-794

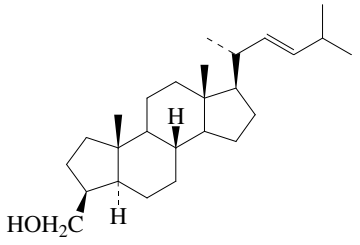
[52900-13-7]

$(H_3C)_2CH(CH_2)_{19}CH(OH)COOH$

$C_{24}H_{48}O_3$ 384.641
Constit. of the sponge *Smenospongia aurea*. Also found in lanolin wool fat. No phys. props. reported.
Fawaz, F. *et al., Ann. Pharm. Fr.*, 1974, **32**, 59 (*occur*)
Carballeira, N.M. *et al., Lipids*, 1992, **27**, 681 (*isol*)

3-Hydroxymethyl-*A*-26,27-trinorergost-22-ene H-795

A*,26,27-Trinorergost-22-ene-3-methanol.* A*,24-Dinorcholest-22-ene-3-methanol*

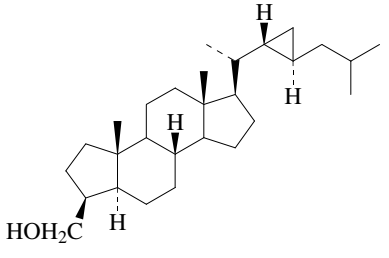


$C_{26}H_{44}O$ 372.633

(3β,5α,22*E*)-*form* [83704-10-3]
Constit. of *Acanthella aurantiaca*.
Bohlin, L. *et al., J.O.C.*, 1982, **47**, 5309-5314 (*isol*)

3-Hydroxymethyl-*A*-28,33-trinorgorgostane H-796

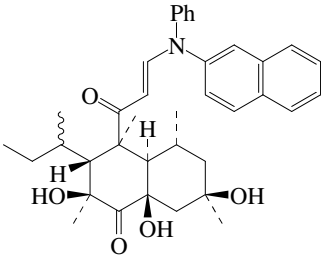
A*,28,33-Trinorgorgostane-3-methanol, 9CI*



$C_{28}H_{48}O$ 400.687

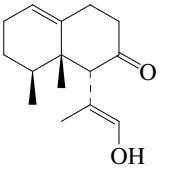
(3β,5α,22*R*,23*R*)-*form* [83704-13-6]
Constit. of the sponge *Acanthella aurantiaca*.
Bohlin, L. *et al., J.O.C.*, 1982, **47**, 5309-5314 (*isol*)

10-Hydroxy-18-(*N*-naphthalenyl-*N*-phenylamino)-betaenone C H-797



$C_{37}H_{45}NO_5$ 583.766
Prod. by a *Microsphaeropsis* sp. isol. from the sponge *Aplysina aerophoba*. Powder. $[\alpha]_D$ -44.4 (c, 1 in EtOH). λ_{max} 221; 350 (MeOH).
Brauers, G. *et al., J. Nat. Prod.*, 2000, **63**, 739-745,

12-Hydroxy-1(10),11-nardosinadien-7-one H-798

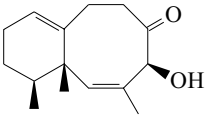


$C_{15}H_{22}O_2$ 234.338
Enolised aldehyde.

(6β*H*,11*E*)-*form*

12-Ac: [75222-53-6]
$C_{17}H_{24}O_3$ 276.375
Constit. of *Paralemnalia thyrsoides*. Cryst.
Mp 84-85°. $[\alpha]_D$ -288 (c, 0.15 in $CHCl_3$). λ_{max} 225 (ε 6400) (EtOH).
Bowden, B.F. *et al., Aust. J. Chem.*, 1980, **33**, 885-890 (*isol, pmr, cmr*)

4-Hydroxy-2,8-neolemnadien-5-one H-799



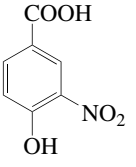
$C_{15}H_{22}O_2$ 234.338

4β-*form*

Ac: [148371-04-4]
$C_{17}H_{24}O_3$ 276.375
Constit. of *Lemnalia africana*. Oil. $[\alpha]_D$ +441 (c, 0.2 in $CHCl_3$). Related to Neolemnane, N-67.
Jurek, J. *et al., J. Nat. Prod.*, 1993, **56**, 508 (*isol, pmr, cmr*)

4-Hydroxy-3-nitrobenzoic acid H-800

[616-82-0]



$C_7H_5NO_5$ 183.12

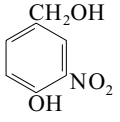
Isol. from the marine bacterium *Flavobacterium* sp. T436. Needles or leaflets (H_2O).
Mp 186-187°. pK_a 6.41 (25°).

[88071-93-6, 135328-57-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 222D; 223B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1129A; 1535A (*nmr*)
Cavill, G.W.K. *et al., J. Soc. Chem. Ind., London*, 1945, **64**, 212-215 (***synth, bibl***)
Frazier, T.C. *et al., J.O.C.*, 1961, **26**, 2223-2225 (*synth*)
Kondo, S. *et al., Chem. Pharm. Bull.*, 1994, **42**, 768-773 (***synth, pmr, uv***)
Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

4-Hydroxy-3-nitrobenzyl alcohol, 8CI H-801

4-Hydroxy-3-nitrobenzenemethanol, 9CI. α,4-Dihydroxy-3-nitrotoluene. 2-Nitro-4-(hydroxymethyl)phenol
[41833-13-0]



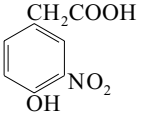
$C_7H_7NO_4$ 169.137
Metab. of *Pyricularia oryzae*. Also isol. from the bryozoan *Phidolopora pacifica*. Cryst. (H_2O).
Mp 97°.

4-Me ether: 4-Methoxy-3-nitrobenzenemethanol, 9CI
[41870-24-0]
$C_8H_9NO_4$ 183.163
Cryst. (H_2O). Mp 69°.

Hart, M.C. *et al., J.A.C.S.*, 1920, **42**, 2683 (*synth*)
Wakselman, M. *et al., Bull. Soc. Chim. Fr.*, 1973, 1179 (*synth*)
Ouertani, M. *et al., Tet. Lett.*, 1982, **23**, 4315 (*synth*)
Tischler, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **84**, 43-45 (*isol*)
Sviridov, S.I. *et al., Khim. Prir. Soedin.*, 1990, 811 (*isol*)
Myers, J.K. *et al., J.A.C.S.*, 1995, **117**, 11049 (*synth, pmr, cmr, ir*)
Touzeau, F. *et al., J. Med. Chem.*, 2003, **46**, 1962-1979 (*synth, ir, pmr*)
Bouvier, E. *et al., Bioorg. Med. Chem.*, 2004, **12**, 969-977 (*synth, pmr, cmr*)

(4-Hydroxy-3-nitrophenyl)acetic acid H-802

4-Hydroxy-3-nitrobenzeneacetic acid, 9CI. T 0007B_1. Antibiotic T 0007B_1
[10463-20-4]



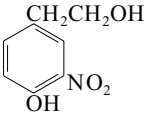
$C_8H_7NO_5$ 197.147
Prod. by *Streptomyces hygroscopicus* and the marine-derived *Flavobacterium* sp. T436. Metab. of *Pyricularia oryzae*. Isol. from mustard seeds. Shows antibacterial activity. Yellow cryst. (EtOH).
Mp 145-146°.

Me ester: [61873-93-6]
$C_9H_9NO_5$ 211.174
Prod. by *Flavobacterium* sp. T436. Cryst. (EtOAc/petrol).
Mp 69°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 171B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1038B (*nmr*)
Hugel, H.M. *et al., Synth. Commun.*, 1985, **15**, 1075 (*synth*)
Weinstock, J. *et al., J. Med. Chem.*, 1987, **30**, 1166 (*synth*)
Zhang, H. *et al., Kangshengsu*, 1990, **15**, 321; *CA*, **114**, 203220 (*isol*)
Sviridov, S.I. *et al., Khim. Prir. Soedin.*, 1990, 811 (*isol*)
Zhang, H. *et al., CA*, 1991, **115**, 131568 (*isol*)
Tesaki, S. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 998-1000 (*activity*)
Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

2-(4-Hydroxy-3-nitrophenyl)ethanol H-803

4-Hydroxy-3-nitrobenzeneethanol. 4-Hydroxy-3-nitrophenethyl alcohol. 3-Nitrotyrosol



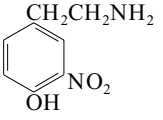
$C_8H_9NO_4$ 183.163
Metab. of *Pyricularia oryzae*. Isol. from the marine-derived *Flavobacterium* sp. T436. Phytotoxin. Yellow microcryst.
Mp 65° (56°). λ_{max} 214 (ϵ 16900); 276 (ϵ 6600); 358 (ϵ 3150) (MeOH) (Berdy).

*1-*O*-Octadecanoyl: 2-(4-Hydroxy-3-nitrophenyl)ethyl stearate*
$C_{26}H_{43}NO_5$ 449.629
Constit. of the roots of *Bignonia unguis-cati*.
Mp 97°. λ_{max} 258 (sh) (log ϵ 4.04); 270 (log ϵ 4.06) (MeOH).

Woodburn, H.M. *et al., J.A.C.S.*, 1950, **72**, 1361 (*synth*)
Sviridov, S.I. *et al., Khim. Prir. Soedin.*, 1990, **26**, 811; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 691 (*isol*)
Dinda, B. *et al., Indian J. Chem., Sect. B*, 2003, **42**, 1514-1518 (*synth, stearate*)
Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

2-(4-Hydroxy-3-nitrophenyl)ethylamine H-804

4-(2-Aminoethyl)-2-nitrophenol, 9CI. 4-Hydroxy-2-nitrophenethylamine. 3-Nitrotyramine
[49607-15-0]



$C_8H_{10}N_2O_3$ 182.179
Isol. from the cactus *Cereus validus*. Yellow orange prisms.
Mp 217° dec.

Hydrochloride: [63195-80-2]
Yellow-brown plates (EtOH). Mp 214-215°.

Nitrate: [63195-79-9]
Mp 214-216° dec.

N-*Ac:* N-*(4-Hydroxy-3-nitrophenylethyl)acetamide*
$C_{10}H_{12}N_2O_4$ 224.216
Metab. of *Pyricularia oryzae*. Isol. from the marine-derived *Flavobacterium* sp. T436. Yellow needles (C_6H_6/hexane).
Mp 95-98°.

Me ether: 2-(4-Methoxy-2-nitrophenyl)ethylamine
$C_9H_{12}N_2O_3$ 196.205
Oil.

Me ether, hydrochloride:
Yellow needles (MeOH). Mp 231-232°.

N-*(2-Methylpropanoyl):* **N-*(2-Methylpropionyl)-3-nitrotyramine***
[173791-66-7]
$C_{12}H_{16}N_2O_4$ 252.269
Isol. from a facultatively anaerobic, halophilic bacterium sediment from the Great Salt Plains, Oklahoma. Shows cytotoxicity against murine leukaemia P-388. Fine needles (CH_2Cl_2).
Mp 99-100°. λ_{max} 274 (ϵ 8860); 357 (ϵ 3350) (MeOH) (Berdy).

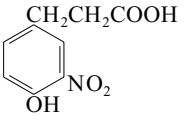
N-*(3-Methylbutanoyl):* **N-*(3-Methylbutanoyl)-3-nitrotyramine***
[173791-67-8]
$C_{13}H_{18}N_2O_4$ 266.296
Isol. from a facultatively anaerobic halophilic bacterium from sediment from the Great Salt Plains, Oklahoma. Fine needles (CH_2Cl_2).
Mp 88-89°.

Waser, E. *et al., Helv. Chim. Acta*, 1923, **6**, 55 (*synth*)
Callow, R.K. *et al., J.C.S.*, 1929, 1453 (*Me ether*)
Neme, G. *et al., Phytochemistry*, 1977, **16**, 277 (*isol*)

Sviridov, S.I. *et al., Khim. Prir. Soedin.*, 1990, **26**, 811; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 691 (*isol, deriv*)
Fu, X. *et al., J. Nat. Prod.*, 1995, **58**, 1950 (*N-2-Methylpropionyl, N-3-Methylbutanoyl*)
Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*N-Ac, marine, isol*)

3-(4-Hydroxy-3-nitrophenyl)propanoic acid H-805

4-Hydroxy-3-nitrobenzenepropanoic acid, 9CI. 4-Hydroxy-3-nitrohydrocinnamic acid, 8CI. 3-Nitrophloretic acid. T0007B$_2$. Antibiotic T0007B$_2$
[38196-09-7]



$C_9H_9NO_5$ 211.174
Prod. by *Streptomyces hygroscopicus* and the marine-derived *Flavobacterium* sp. T436. Cryst. (EtOH aq.).
Mp 95-96°. λ_{max} 218 (MeOH) (Berdy). λ_{max} 236 (MeOH-NaOH) (Berdy).

Me ester:
$C_{10}H_{11}NO_5$ 225.201
Yellow needles (EtOH aq.). Mp 64°.

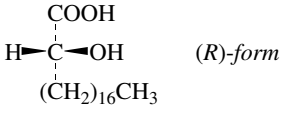
Et ester:
$C_{11}H_{13}NO_5$ 239.227
Yellow needles (EtOH aq.). Mp 38°.

Me ether: 3-(4-Methoxy-3-nitrophenyl)propanoic acid
$C_{10}H_{11}NO_5$ 225.201
Pale yellow needles (CCl_4). Mp 128-130.5°.

Callow, R.K. *et al., J.C.S.*, 1929, 1444 (*synth*)
Wright, J.B. *et al., J. Het. Chem.*, 1972, **9**, 681 (*synth*)
Zhang, H. *et al., Kangshengsu*, 1990, **15**, 321; *CA*, **114**, 203220 (*isol*)
Zhang, H. *et al., CA*, 1991, **115**, 131568 (*isol*)
Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

2-Hydroxynonadecanoic acid H-806

[93361-63-8]



(*R*)-*form*

$C_{19}H_{38}O_3$ 314.507

(*R*)-*form*

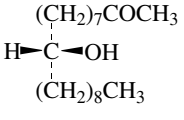
Me ether: 2-Methoxynonadecanoic acid
[88416-42-6]
$C_{20}H_{40}O_3$ 328.534
Constit. of the sponge *Higginsia tethyoides.*

(ξ)-*form*

Constit. of the sponge *Smenospongia auria*.

Ayanoglu, E. *et al., Lipids*, 1983, **18**, 830-836 (*Me ether*)
Carballeira, N.M. *et al., Lipids*, 1992, **27**, 681-685 (*isol*)

10-Hydroxy-2-nonadecanone H-807



$C_{19}H_{38}O_2$ 298.508

(*R*)-*form*

O-*[6-Deoxy-α-D-glucopyranosyl-(1→2)-[6-deoxy-β-D-talopyranosyl-(1→6)]-4-*O*-acetyl-3-*O*-butanoyl-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:* ***Caminoside A***
$C_{49}H_{86}O_{22}$ 1027.205
Isol. from the marine sponge *Caminus sphaeroconia*. Antibacterial agent. Glass. $[\alpha]_D^{25}$ -26 (c, 0.09 in MeOH).

O-*[6-Deoxy-α-D-glucopyranosyl-(1→2)-[6-deoxy-β-D-talopyranosyl-(1→6)]-3,4-di-*O*-butanoyl-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:* ***Caminoside B***
$C_{51}H_{90}O_{22}$ 1055.259
Isol. from *Caminus sphaeroconia*. Glass. $[\alpha]_D^{25}$ -22 (c, 0.17 in MeOH).

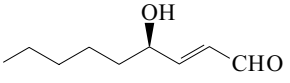
O-*[3-*O*-Butanoyl-6-deoxy-α-D-glucopyranosyl-(1→2)-[6-deoxy-β-D-talopyranosyl-(1→6)]-4-*O*-acetyl-3-*O*-butanoyl-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:* ***Caminoside C***
$C_{53}H_{92}O_{23}$ 1097.296
Isol. from *Caminus sphaeroconia*. Glass. $[\alpha]_D^{25}$ -9 (c, 0.006 in MeOH).

O-*[3-*O*-Butanoyl-6-deoxy-α-D-glucopyranosyl-(1→2)-[6-deoxy-β-D-talopyranosyl-(1→6)]-3,4-di-*O*-butanoyl-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:* ***Caminoside D***
$C_{55}H_{96}O_{23}$ 1125.35
Isol. from *Caminus sphaeroconia*. Glass. $[\alpha]_D^{25}$ -54 (c, 0.19 in MeOH).

MacMillan, J.B. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 5946-5951 (*cd, abs config*)
Sun, J.S. *et al., Synlett*, 2005, 437-440 (*Caminoside A, synth*)
Linington, R.G. *et al., J. Nat. Prod.*, 2006, **69**, 173-177 (*isol, pmr, cmr*)

4-Hydroxy-2-nonenal H-808

[29343-52-0]
[75899-68-2]



(2*E*,4*R*)–*form*

$C_9H_{16}O_2$ 156.224
Constit. of beef and pork. Lipid peroxidation product. Cytotoxic.

(2*E*,4*R*)-*form* [119008-08-1]
$[\alpha]_D^{25}$ -46 (c, 0.45 in $CHCl_3$) (95% op).

(2*E*,4*S*)-*form* [119008-09-2]
$[\alpha]_D^{25}$ +47.7 (c, 0.69 in $CHCl_3$) (95% op).

Ac:
$C_{11}H_{18}O_3$ 198.261
Oil. $[\alpha]_D^{25}$ +12.7 ($CHCl_3$).

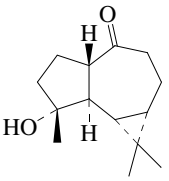
Di-Et acetal: 1,1-Diethoxy-2-nonen-4-ol
[158930-55-3]
$C_{13}H_{26}O_3$ 230.347
$[\alpha]_D^{22}$ +11.3 (c, 0.36 in CH_2Cl_2).

(±)-(*E*)-*form* [128946-65-6]
[18286-49-2]
Constit. of the red alga *Liagora farinosa*.
Oil. Sol. $CHCl_3$, hexane; poorly sol. H_2O. $Bp_{0.4}$ 84-87°. λ_{max} 217 (ε 12000) (MeOH) (Berdy). λ_{max} 225 (ε 11000) (MeOH) (Berdy).

[123620-46-2, 156619-59-9, 156619-64-6]

Esterbauer, H. *et al., Monatsh. Chem.*, 1967, **98**, 1884; 1994 (*synth*)
Paul, V.J. *et al., Tet. Lett.*, 1980, **21**, 3327 (*isol*)
Ball, J.R. *et al., J. Biol. Phys.*, 1986, **14**, 127 (*conformn*)
Gree, R. *et al., Tet. Lett.*, 1986, **27**, 4983 (*synth*)
De Montarby, L. *et al., Bull. Soc. Chim. Fr.*, 1989, 419 (*synth, pmr, cmr*)
Gardner, H.W. *et al., Lipids*, 1992, **27**, 686 (*synth*)
Yu, L. *et al., Chem. Comm.*, 1993, 232 (*synth*)
Allevi, P. *et al., J.O.C.*, 1993, **58**, 5000 (*isol, ms*)
Bringmann, G. *et al., Tetrahedron*, 1994, **50**, 10245 (*synth*)
Allevi, P. *et al., Tetrahedron: Asymmetry*, 1994, **5**, 13 (*synth*)
Sakai, T. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1379 (*occur*)
Matsushita, Y. *et al., Tet. Lett.*, 1995, **36**, 1879 (*synth*)
Chandra, A. *et al., Lipids*, 1997, **32**, 779-782 (*synth*)

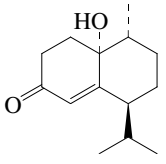
4-Hydroxy-14-nor-10-aromadendranone H-809



$C_{14}H_{22}O_2$ 222.327

(1β,4α,5α,6β,7β)-*form* [77346-92-0]
Constit. of *Clavularia koellikeri*.
Oil. $[\alpha]_D^{25}$ -21.3 (c, 0.13 in $CHCl_3$).
Iguchi, K. *et al., J. Nat. Prod.*, 2004, **67**, 577-583 (*isol, pmr, cmr*)

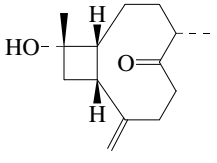
1-Hydroxy-15-nor-5-cadinen-4-one H-810



$C_{14}H_{22}O_2$ 222.327

(1α,7β,10α)-*form* [865723-20-2]
Constit. of *Dictyopteris divaricata*.
Amorph. solid. $[\alpha]_D^{20}$ -28 (c, 0.3 in MeOH).
Song, F. *et al., J. Nat. Prod.*, 2005, **68**, 1309-1313 (*Dictyopteris divaricata constit*)

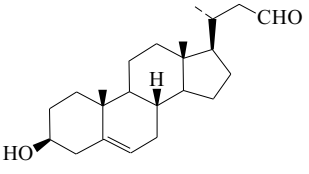
11-Hydroxy-13-nor-3(15)-caryophyllen-6-one H-811



$C_{14}H_{22}O_2$ 222.327

(2β,7α,11α)-*form*
Nanonorcaryophyllene B
[681145-44-8]
Constit. of *Sinularia nanolobata*.
Oil. $[\alpha]_D^{25}$ -7.6 (c, 0.92 in $CHCl_3$).
Ahmed, A.F. *et al., J. Nat. Prod.*, 2004, **67**, 592-597 (*isol, pmr, cmr*)

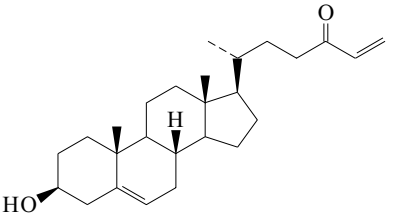
3-Hydroxy-24-norchol-5-en-23-al, 9CI H-812



$C_{23}H_{36}O_2$ 344.536

3β-*form* [51231-27-7]
Constit. of a sponge, *Hyrtios* sp.
23-Carboxylic acid: 3-Hydroxy-24-norchol-5-en-23-oic acid
[19408-50-5]
Constit. of a *Euryspongia* sp.
Cryst. (Me_2CO).
Mp 244.5-245°. $[\alpha]_D^{16}$ -41.2 (c, 0.741 in EtOH). $[\alpha]_{365}^{25}$ -105 (c, 0.75 in $CHCl_3$).
23-Carboxylic acid, Me ester: [69454-96-2]
$C_{24}H_{38}O_3$ 374.562
Mp 143-145°. $[\alpha]_D^{16}$ -42.5 (c, 0.873 in $CHCl_3$).
23-Carboxylic acid, Ac: [34751-25-2]
$C_{25}H_{38}O_4$ 402.573
Cryst. (Me_2CO/petrol). Mp 197.5-198.5°. $[\alpha]_D^{25}$ -42 (c, 1.14 in $CHCl_3$).
23-Carboxylic acid, Ac, Me ester: [33168-65-9]
$C_{26}H_{40}O_4$ 416.6
Long needles (MeOH). Mp 132.8-133.4°. $[\alpha]_D^{22}$ -46.7 (c, 2 in $CHCl_3$).
Plattner, P.A. *et al., Helv. Chim. Acta*, 1943, **26**, 1241 (*carboxylic acid, synth*)
Ryer, A.I. *et al., J.A.C.S.*, 1952, **74**, 41 (*carboxylic acid, synth*)
Dygos, J.H. *et al., J.O.C.*, 1979, **44**, 1590 (*carboxylic acid, synth*)
Koch, P. *et al., Helv. Chim. Acta*, 1983, **66**, 2431 (*isol*)
Seldes, A.M. *et al., Magn. Reson. Chem.*, 1986, **24**, 239 (*cmr*)
Mandeau, A. *et al., Steroids*, 2005, **70**, 873-878 (*Euryspongia constit*)

3-Hydroxy-27-norcholesta-5,25-dien-24-one H-813

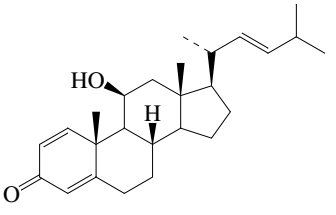


$C_{26}H_{40}O_2$ 384.601

3β-*form*
Metab. of *Eisenia bicyclis*.
Ac: [132278-41-2]
Cryst. (MeOH). Mp 151-152°. $[\alpha]_D$ -31 (c, 1.08 in $CHCl_3$).
Kurata, K. *et al., Phytochemistry*, 1990, **29**, 3678 (*isol, pmr, cmr*)

11-Hydroxy-24-norcholesta-1,4,22-trien-3-one H-814

11-Hydroxy-26,27-dinorergosta-1,4,22-trien-3-one

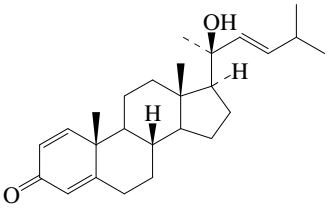


$C_{26}H_{38}O_2$ 382.585

(11β,22*E*)-*form* [862286-72-4]
Constit. of *Anthomastus bathyproctus*.
Amorph. powder. $[\alpha]_D^{25}$ +4 (c, 0.08 in $CHCl_3$).
Mellado, G.G. *et al., J. Nat. Prod.*, 2005, **68**, 1111-1115

20-Hydroxy-24-norcholesta-1,4,22-trien-3-one H-815

20-Hydroxy-26,27-dinorergosta-1,4,22-trien-3-one

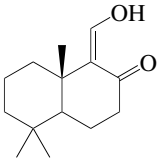


$C_{26}H_{38}O_2$ 382.585

(20*S*,22*E*)-*form* [862286-73-5]
Constit. of *Anthomastus bathyproctus*.
Amorph. powder. $[\alpha]_D^{25}$ +11.1 (c, 0.09 in $CHCl_3$). λ_{max} 245 (log ϵ 4.19) (MeOH).
Mellado, G.G. *et al., J. Nat. Prod.*, 2005, **68**, 1111-1115

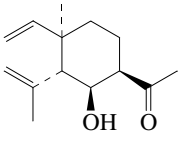
11-Hydroxy-12-nor-9(11)-drimen-8-one H-816

[198423-24-4]



$C_{14}H_{22}O_2$ 222.327
Enolised β-ketoaldehyde. Constit. of a *Dysidea* sp. Solid.
Mp 79-80°. $[\alpha]_D^{25}$ +9.6 (c, 0.1 in MeOH). λ_{max} 294 (log ϵ 3.34) (MeOH).
Paul, V.J. *et al., J. Nat. Prod.*, 1997, **60**, 1115-1120 (*isol, pmr, cmr*)

6-Hydroxy-13-nor-1,3-elemadien-11-one H-817

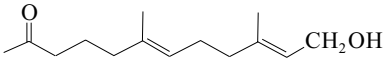


$C_{14}H_{22}O_2$ 222.327

(5β,6β,10α)-*form*
*6-O-(4-Hydroxy-4-methyl-2*E*-pentenoyl):* [865668-55-9]
$C_{20}H_{30}O_4$ 334.455
Constit. of a *Eunicea* sp. Oil. $[\alpha]_D^{25}$ +12.3 (c, 1 in $CHCl_3$). λ_{max} 206 (ϵ 13400) (MeOH).
Garzón, S.P. *et al., J. Nat. Prod.*, 2005, **68**, 1354-1359 (*Eunicea constit*)

1-Hydroxy-13-nor-2,6-farnesadien-11-one H-818

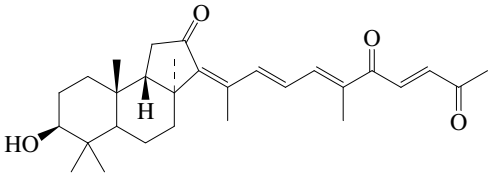
12-Hydroxy-6,10-dimethyl-6,10-dodecadien-2-one



$C_{14}H_{24}O_2$ 224.342

(2*E*,6*E*)-*form*
Oxocrinol
[60346-03-4]
Constit. of *Cystoseira crinita*.
Oil.
Fattorusso, E. *et al., Tet. Lett.*, 1976, 937 (*struct*)
Kato, T. *et al., Chem. Lett.*, 1977, **8**, 100g (*synth*)
Kad, G.L. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 832 (*synth, pmr*)

3-Hydroxy-27-nor-13,15,17(20),23-isomalabaricatetraene-12,22,25-trione H-819



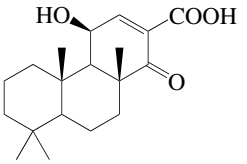
$C_{29}H_{40}O_4$ 452.633

(3β,13*Z*,15*E*,17(20)*E*,23*E*)-*form*
3-Ac: ***Geoditin B***
[386274-86-8]
$C_{31}H_{42}O_5$ 494.67
Constit. of *Geodia japonica*. Yellow cryst.
Mp 144-145°. $[\alpha]_D^{25}$ -271.6 (c, 0.014 in $CHCl_3$). λ_{max} 293 (log ϵ 1.53); 351 (log ϵ 1.59) (MeOH).
3-Ketone: 27-Nor-13,15,17(20),23-isomalabaricatetraene-3,12,22,25-tetrone. ***Geoditin A***
[386274-85-7]
$C_{29}H_{38}O_4$ 450.617
Constit. of *Geodia japonica*. Yellow cryst.
Mp 127-128°. $[\alpha]_D^{25}$ -138.9 (c, 0.011 in MeOH). λ_{max} 293 (log ϵ 2.4); 357 (log ϵ 3.26) (MeOH).

(3β,13*E*,17(20)*E*,23*Z*)-*form*
3-Ketone: ***13*E*-Isogeoditin A***
[823815-01-6]
$C_{29}H_{38}O_4$ 450.617
Constit. of *Rhabdastrella* aff. *distincta*. Yellow oil. $[\alpha]_D^{25}$ -5.9 (c, 0.15 in Me_2CO).

(3β,13*Z*,17(20)*E*,23*Z*)-*form*
3-Ac: ***Isogeoditin B***
[823815-02-7]
$C_{31}H_{42}O_5$ 494.67
Constit. of *Rhabdastrella* aff. *distincta*. Yellow oil. $[\alpha]_D^{25}$ -74.6 (c, 0.05 in Me_2CO).
3-Ketone: ***Isogeoditin A***
[823815-00-5]
$C_{29}H_{38}O_4$ 450.617
Constit. of *Rhabdastrella* aff. *distincta*. Yellow oil. $[\alpha]_D^{25}$ +68.7 (c, 0.34 in MeOH).
Zhang, W.-H. *et al., J. Nat. Prod.*, 2001, **64**, 1489-1492 (*isol, pmr, cmr*)
Lv, F. *et al., J. Nat. Prod.*, 2004, **67**, 2033-2036 (*Isogeoditins*)

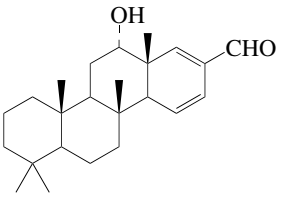
11-Hydroxy-15-nor-14-oxo-12-isocopalen-16-oic acid H-820



$C_{19}H_{28}O_4$ 320.428

11β-*form*
Ac, Me ester: ***Aplypallidenone***
[200497-04-7]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Aplysilla pallida*. Cryst. (cyclohexane).
Mp 99-101°. $[\alpha]_D$ +135. λ_{max} 211 (ϵ 9640); 336 (ϵ 60) (cyclohexane).
12α,13α-Epoxide, Ac, Me ester: ***Aplypallidoxone***
[200497-08-1]
$C_{22}H_{32}O_6$ 392.491
Constit. of *Aplysilla pallida*. Cryst. (cyclohexane).
Mp 143-144°. $[\alpha]_D$ -32. λ_{max} 299 (ϵ 43) (cyclohexane).
12α,13α-Epoxide, 11-ketone, Me ester: ***Aplypallidione***
[200497-12-7]
$C_{20}H_{28}O_5$ 348.438
Constit. of *Aplysilla pallida*. Needles (CH_2Cl_2/petrol). λ_{max} 294 (ϵ 58) (cyclohexane).
Hambley, T.W. *et al., Aust. J. Chem.*, 1997, **50**, 903-909 (*isol, pmr, cmr, cryst struct*)

12-Hydroxy-25-nor-15,17-scalaradien-24-al H-821

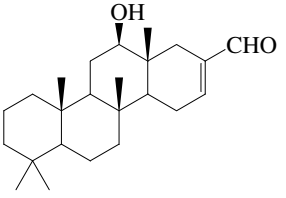


$C_{24}H_{36}O_2$ 356.547

12α-*form*

Ac: ***Norscalaral C***
[186803-32-7]
$C_{26}H_{38}O_3$ 398.584
Constit. of *Cacospongia scalaris*. Amorph. powder. $[\alpha]_D$ +22.3 (c, 0.2 in $CHCl_3$). λ_{max} 290 (ϵ 5317) (MeOH).
Rueda, A. *et al., J.O.C.*, 1997, **62**, 1481-1485 (*isol, pmr, cmr*)

12-Hydroxy-25-nor-16-scalaren-24-al H-822

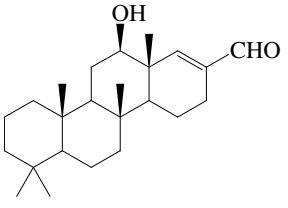


$C_{24}H_{38}O_2$ 358.563

12β-*form*
De-O-acetylhyrtial
[131711-36-9]
Constit. of *Hyrtios erecta* and *Collospongia auris*.

Ac: ***Hyrtial***
[97889-56-0]
$C_{26}H_{40}O_3$ 400.6
Constit. of *Hyrtios erecta*. Shows antinflammatory activity.
Crews, P. *et al., Experientia*, 1985, **41**, 690 (*Hyrtial*)
Bergquist, P.R. *et al., Biochem. Syst. Ecol.*, 1990, **18**, 349-357 (*Collospongia auris constit*)
Miyaoka, H. *et al., J. Nat. Prod.*, 2000, **63**, 1369-1372 (*Hyrtios erectus constit*)

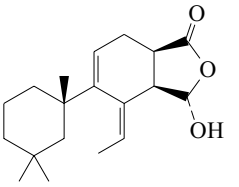
12-Hydroxy-25-nor-17-scalaren-24-al H-823



$C_{24}H_{38}O_2$ 358.563

12β-*form* [301842-58-0]
Constit. of *Hyrtios erecta*.
Amorph. solid. $[\alpha]_D^{25}$ +22.3 (c, 0.44 in $CHCl_3$). λ_{max} 234 (log ϵ 4) (MeOH).
Miyaoka, H. *et al., J. Nat. Prod.*, 2000, **63**, 1369-1372 (*isol, pmr, cmr*)

15-Hydroxy-17-nor-5,6-seco-7,9(11)-spongiadien-16,15-olide H-824



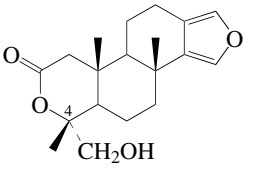
$C_{19}H_{28}O_3$ 304.428

15α-*form*

Ac: ***Aplytandiene 2***
[117823-34-4]
$C_{21}H_{30}O_4$ 346.466
Constit. of *Spongionella gracilis* and *Aplysilla tango*. Cryst. (MeCN aq.), prisms ($CHCl_3$).
Mp 102-103° (99-102°). $[\alpha]_D$ -103 (c, 0.46 in $CHCl_3$). $[\alpha]_D$ -85 (c, 0.2 in $CHCl_3$).
Mayol, L. *et al., Gazz. Chim. Ital.*, 1988, **118**, 559 (*isol, pmr, cmr*)
Poiner, P. *et al., Aust. J. Chem.*, 1990, **43**, 1713 (*isol, pmr, cmr*)

18-Hydroxy-3-nor-2,3-seco-13(16),14-spongiadien-2,4-olide H-825

[207924-39-8]

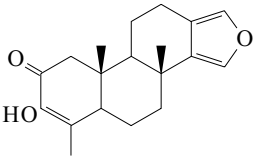


$C_{19}H_{26}O_4$ 318.412
Constit. of *Spongia matamata*. Powder. $[\alpha]_D$ +12.8 (c, 0.2 in $CHCl_3$).

4-Epimer: ***19-Hydroxy-3-nor-2,3-seco-13(16),14-spongiadien-2,4-olide***
[207924-40-1]
$C_{19}H_{26}O_4$ 318.412
Constit. of *Spongia matamata*. Powder. $[\alpha]_D$ +15.2 (c, 0.27 in $CHCl_3$).
Li, C.-J. *et al., J. Nat. Prod.*, 1998, **61**, 546-547 (*isol, pmr, cmr*)

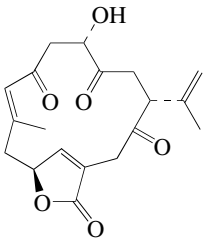
3-Hydroxy-19-nor-3,13(16),14-spongiatrien-2-one H-826

Spongiadiosphenol
[130611-12-0]



$C_{19}H_{24}O_3$ 300.397
Constit. of a *Spongia* sp. Cryst. ($CHCl_3$).
Mp 145-147°. $[\alpha]_D$ +3 (c, 0.1 in $CHCl_3$).
Gunasekera, S.P. *et al., J.O.C.*, 1991, **56**, 1256 (*isol, pmr, cmr*)
Sakamoto, T. *et al., Tetrahedron*, 1995, **51**, 5771 (*synth*)

4-Hydroxy-16-nor-3,6,14-trioxo-7,11,15-cembratrien-19,10-olide H-827

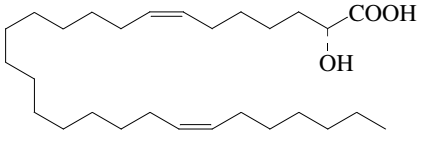


$C_{19}H_{22}O_6$ 346.379

(1*R,4*S**,7*E*,10*S**)-*form***

Et ether: ***Gorgiacerolide***
[203575-51-3]
$C_{21}H_{26}O_6$ 374.433
Constit. of *Pseudopterogorgia acerosa*. Oil. $[\alpha]_D^{25}$ +15 (c, 1.2 in $CHCl_3$). λ_{max} 248 (ϵ 2500) ($CHCl_3$).
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1998, **61**, 401-404 (*isol, pmr, cmr*)

2-Hydroxy-7,21-octacosadienoic acid H-828

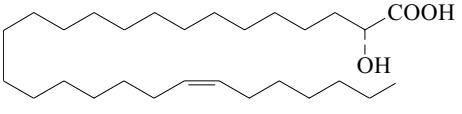


$C_{28}H_{52}O_3$ 436.717

(2*R*,7*Z*,21*Z*)-*form*

Me ether: 2-Methoxy-7,21-octacosadienoic acid
[88416-41-5]
$C_{29}H_{54}O_3$ 450.744
Constit. of the sponge *Higginsia tethyoides.*
Ayanoglu, E. *et al., Lipids*, 1983, **18**, 830-836 (*isol*)

2-Hydroxy-21-octacosenoic acid H-829

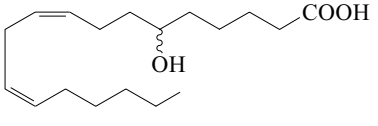


$C_{28}H_{54}O_3$ 438.733

(2*R*,21*Z*)-*form*

Me ether: 2-Methoxy-21-octacosenoic acid
[86304-15-6]
$C_{29}H_{56}O_3$ 452.76
Constit. of the phospholipids of the sponge *Higginsia tethyoides.*
Ayanoglu, E. *et al., Tet. Lett.*, 1983, **24**, 1111-1114 (*isol, struct*)

6-Hydroxy-9,12-octadecadienoic acid H-830



$C_{18}H_{32}O_3$ 296.449

(9*Z*,12*Z*)-*form*

6-Hydroxylinoleic acid
6-Ac: ***6-Acetoxylinoleic acid***
[137052-51-8]
$C_{20}H_{34}O_4$ 338.486
Isol. from the marine alga *Spatoglossum pacificum*. Pollen growth inhibitor. $[\alpha]_D^{23}$ -1.04 (c, 0.5 in $CHCl_3$). C-6 config. not determined.
Tazaki, H. *et al., Agric. Biol. Chem.*, 1991, **55**, 2149 (*isol*)

7-Hydroxy-9,12-octadecadien-5-ynoic acid H-831

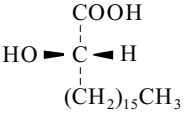
$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CHCH_2CH(OH)C{\equiv}C(CH_2)_3COOH$

$C_{18}H_{28}O_3$ 292.417

(9*Z*,12*Z*)-(+)-*form* [76152-34-6]
Constit. of the red marine alga *Liagora farinosa*.
$[\alpha]_D$ +6.8 (c, 1.5 in $CHCl_3$).
Paul, V.J. *et al., Tet. Lett.*, 1980, **21**, 3327 (*isol, pmr, cmr*)

2-Hydroxyoctadecanoic acid, 9CI H-832

2-Hydroxystearic acid
[629-22-1]



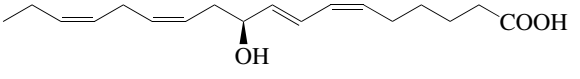
(S)–form

$C_{18}H_{36}O_3$ 300.481
Occurs in Actinomycete bacteria and the sphingolipids of the influenza virus. Has mycobactericidal activity.

(ξ)-*form*

Constit. of the sponge *Suberites massa*.
Me ether: 2-Methoxyoctadecanoic acid
$C_{19}H_{38}O_3$ 314.507
Isol. from the sponge *Callyspongia fallax*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*Callyspongia fallax constit*)

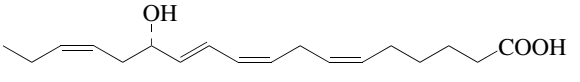
10-Hydroxy-6,8,12,15-octadecatetraenoic acid H-833



$C_{18}H_{28}O_3$ 292.417

(6*Z*,8*E*,10*S*,12*Z*,15*Z*)-*form* [135378-21-1]
[135378-19-7]
Isol. from the red alga *Gracilariopsis lemaneiformis.*
Jiang, Z.D. *et al., Phytochemistry*, 1991, **30**, 1187-1190

13-Hydroxy-6,9,11,15-octadecatetraenoic acid H-834

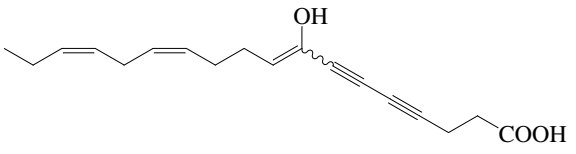


$C_{18}H_{28}O_3$ 292.417

(6*Z*,9*Z*,11*E*,13*S*,15*Z*)-*form* [200357-12-6]
Constit. of the alga *Laminaria saccharina*.
Rorrer, G.L. *et al., Phytochemistry*, 1997, **46**, 871-877 (*isol*)

8-Hydroxy-8,12,15-octadecatriene-4,6-diynoic acid H-835

8-Oxo-12,15-octadecadiene-4,6-diynoic acid



$C_{18}H_{22}O_3$ 286.37

Enol.

(8ξ,12*Z*,15*Z*)-*form*

8-Ac, 2ξ,3-dihydroxypropyl ester: ***Peyssonenyne A***

$C_{23}H_{30}O_6$ 402.486

Constit. of the red alga *Peyssonnelia caulifera*. DNA methyltransferase inhibitor. Oil. λ_{max} 208 (log ϵ 3.25); 215 (log ϵ 3.36); 240 (log ϵ 2.83); 253 (log ϵ 2.81); 267 (log ϵ 2.87); 282 (log ϵ 2.78) (MeOH).

8-Isomer, 8-Ac, 2ξ,3-dihydroxypropyl ester: ***Peyssonenyne B***

$C_{23}H_{30}O_6$ 402.486

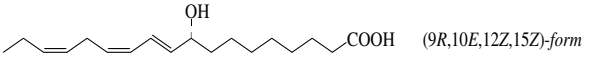
Constit. of *Peyssonnelia caulifera*. DNA methyltransferase inhibitor. Oil. λ_{max} 215 (log ϵ 2.28); 239 (log ϵ 2.01); 253 (log ϵ 2.04); 267 (log ϵ 2.08); 283 (log ϵ 2.05) (MeOH).

McPhail, K.L. *et al., J. Nat. Prod.*, 2004, **67**, 1010-1013 (*isol, pmr, cmr*)

9-Hydroxy-10,12,15-octadecatrienoic acid H-836

[21402-68-6]

[51197-09-2, 166735-07-5]



(9*R*,10*E*,12*Z*,15*Z*)-*form*

$C_{18}H_{30}O_3$ 294.433

(9*R*,10*E*,12*Z*,15*Z*)-*form* [133397-71-4]

Isol. from the cyanobacterium *Anabaena flos-aquae* NIES 74, *Hydra vulgaris* and *Ehretia dicksonii*. Antiinflammatory agent.

9-Ketone: 9-Oxo-10,12,15-octadecatrienoic acid

[125559-74-2]

$C_{18}H_{28}O_3$ 292.417

Constit. of *Glechoma hederacea* and from *Hydra vulgaris*.

(9*S*,10*E*,12*Z*,15*Z*)-*form* [89886-42-0]

Constit. of *Artocarpus communis* (breadfruit), *Conyza welwitschii*, *Dunaliella acidophila*, *Glechoma hederacea* and *Pistia stratiotes*. ACE inhibitor. Phytoalexin in rice plant. $[\alpha]_D$ +5.3 (c, 0.5 in $CHCl_3$). λ_{max} 236 (EtOH).

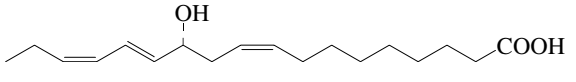
(9*RS*,10*E*,12*Z*,15*Z*)-*form* [115511-52-9]

[115476-07-8] Antiinflammatory agent. Oil (as Me ester).

Rao, A.V. *et al., Tetrahedron*, 1987, **43**, 4385-4394 (*synth*)
Pollio, A. *et al., Biochim. Biophys. Acta*, 1988, **963**, 53-60 (*isol*)
Kuehn, H. *et al., Eur. J. Biochem.*, 1989, **186**, 155-162 (*isol*)
Zdero, C. *et al., Phytochemistry*, 1990, **29**, 2247-2252 (*isol*)
Aliotta, G. *et al., J. Chem. Ecol.*, 1991, **17**, 2223-2234 (*isol*)
Kato, T. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 373-375 (*synth*)
Murakami, N. *et al., Lipids*, 1992, **27**, 776-778 (*Anabaena flos-aquae constit*)
Hamberg, M. *et al., J.C.S. Perkin 1*, 1993, 3065-3072 (*synth*)
Gianfrani, C. *et al., Experientia*, 1995, **51**, 48-56 (*isol*)
McLean, S. *et al., Magn. Reson. Chem.*, 1996, **34**, 719-722 (*isol, pmr, cmr*)
Dong, M. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 882-886 (*isol, activity*)

12-Hydroxy-9,13,15-octadecatrienoic acid H-837

[81325-64-6, 133397-70-3, 161169-50-2, 167936-49-4]



$C_{18}H_{30}O_3$ 294.433

(9*Z*,12*R*,13*E*,15*Z*)-*form* [118711-41-4]

Isol. from *Dunaliella acidophila* and *Croton cortesianus*. C-12 config. not determined for *Croton* sp. isolate.

12-Ketone: 12-Oxo-9,13,15-octadecatrienoic acid

[94451-45-3]

$C_{18}H_{28}O_3$ 292.417

Constit. of the seed oil of *Galeopsis bifida*. Stereochem. not determined.

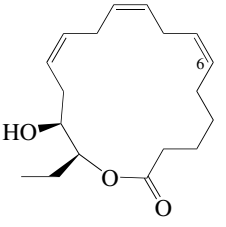
[65179-52-4, 65179-53-5]

Gusakova, S.D. *et al., Khim. Prir. Soedin.*, 1984, **20**, 286-291; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 266-270 (*12-oxo acid*)
Pollio, A. *et al., Biochim. Biophys. Acta*, 1988, **963**, 53-60 (*isol*)
Aliotta, G. *et al., J. Chem. Ecol.*, 1991, **17**, 2223-2234 (*isol*)
Laneuville, O. *et al., J. Biol. Chem.*, 1995, **270**, 19330-19336 (*synth*)

15-Hydroxy-6,9,12-octadecatrien-16-olide H-838

Aplyolide C

[192935-69-6]



$C_{18}H_{28}O_3$ 292.417

Isol. from the marine mollusc *Aplysia depilans*. Ichthyotoxin. Oil. $[\alpha]_D^{25}$ -26.7 (c, 0.7 in $CHCl_3$).

6,7-Dihydro: 15-Hydroxy-9,12-octadecadien-16-olide. ***Aplyolide B***

[192935-68-5]

$C_{18}H_{30}O_3$ 294.433

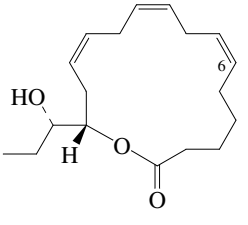
Isol. from *Aplysia depilans*. Ichthyotoxin. Oil. $[\alpha]_D^{25}$ -42.8 (c, 0.2 in $CHCl_3$).

Spinella, A. *et al., J.O.C.*, 1997, **62**, 5471-5475 (*isol, ir, pmr, cmr, ms*)
Spinella, A. *et al., Tet. Lett.*, 2002, **43**, 1681-1683 (*Aplyolide B, synth*)

16-Hydroxy-6,9,12-octadecatrien-15-olide H-839

16-(1-Hydroxypropyl)oxacyclohexadeca-7,10,13-trien-2-one, 9CI.
Aplyolide E

[192935-72-1]



$C_{18}H_{28}O_3$ 292.417

Isol. from the marine mollusc *Aplysia depilans*. Ichthyotoxin. Oil. $[\alpha]_D^{25}$ +46.3 (c, 0.3 in $CHCl_3$).

6,7-Dihydro: 16-Hydroxy-9,12-octadecadien-15-olide. ***Aplyolide D***

[192935-71-0]

$C_{18}H_{30}O_3$ 294.433

Isol. from *Aplysia depilans*. Ichthyotoxin. Oil. $[\alpha]_D^{25}$ +28 (c, 0.1 in $CHCl_3$).

Spinella, A. *et al., J.O.C.*, 1997, **62**, 5471-5475 (*isol, ir, pmr, cmr, ms*)
Spinella, A. *et al., Tet. Lett.*, 2002, **43**, 1681-1683 (*Aplyolide D, synth*)

2-Hydroxy-6,12,15-octadecatrien-8-ynoic acid H-840

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH_2C{\equiv}CCH{=}CHCH_2CH_2CH_2CH(OH)COOH$

$C_{18}H_{26}O_3$ 290.402

(2ξ,6*E*,12*Z*,15*E*)-*form*

Me ether: 2-Methoxy-6,12,15-octadecatrien-8-ynoic acid
[809279-54-7]
$C_{19}H_{28}O_3$ 304.428
Constit. of the sponge *Cinachyrella australiensis.*
Li, L. *et al., CA*, 2005, **142**, 52432n (*isol*)

2-Hydroxy-6-octadecenoic acid H-841

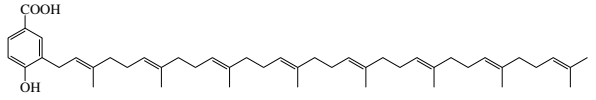
$H_3C(CH_2)_{10}CH{=}CH(CH_2)_3CH(OH)COOH$
$C_{18}H_{34}O_3$ 298.465

(2ξ,6*Z*)-*form*

Me ether: 2-Methoxy-6-octadecenoic acid
$C_{19}H_{36}O_3$ 312.492
Isol. from *Spheciospongia cuspidifera*.
Carballeira, N.M. *et al., Lipids*, 2002, **37**, 305-308 (*isol, ms*)

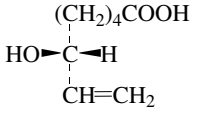
4-Hydroxy-3-octaprenylbenzoic acid H-842

[24869-95-2]



$C_{47}H_{70}O_3$ 683.068
Constit. of an *Ircinia* sp.
Erdogan, I. *et al., Nat. Prod. Sci.*, 1999, **5**, 177-180; *CA*, **132**, 234468 (*isol, pmr, cmr*)

6-Hydroxy-7-octenoic acid H-843

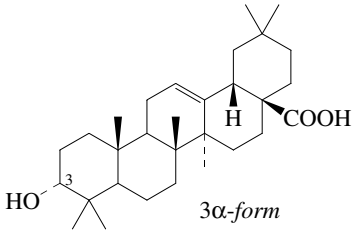


$C_8H_{14}O_3$ 158.197

(*R*)-*form*

$[\alpha]_D^{25}$ -28.5 (MeOH).
O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:* ***Ilicifolioside C***
$C_{25}H_{42}O_{17}$ 614.597
Constit. of the aerial parts of *Acanthus ilicifolius.* Amorph. powder. $[\alpha]_D^{25}$ -48 (c, 0.6 in MeOH).
Wu, J. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1201-1203 (*isol, pmr, cmr*)

3-Hydroxy-12-oleanen-28-oic acid H-844



$C_{30}H_{48}O_3$ 456.707
Many glycosides of Oleanolic acid are known. See also Oleanolic acid 3-glycosides and Oleanolic acid bisdesmosides.

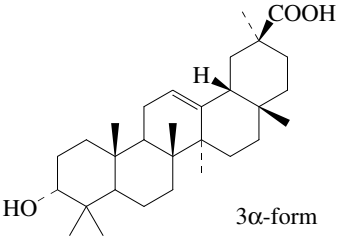
3β-*form*

Oleanolic acid. *Oleanol. Caryophyllin. Swertiaic acid. Sugarbeet acid. Guagenin. Momorgenin. Taraligenin. Panaxsapogenin. Araligenin. Taragenin. Viscic acid†. Mistletoe sapogenin. Oleanic acid. Astrantiagenin C. Giganteumgenin C. Virgaureagenin B. Gledigenin 1*
[508-02-1]
Occurs as glycosides in mistletoe, cloves (*Syzygium aromaticum*), sugar beet (*Beta vulgaris*), olive leaves, etc. Very widely distributed aglycone. Isol. from a Black Sea alga, family Cladophoraceae and from *Ulva fasciata*. Shows antiinflammatory activity, inhibitor of type I allergic reactions. Anti-HIV principle. Active against gram-positive bacteria. Shows ichthyotoxic activity and antiulcer props.
Cryst. (EtOH).
Mp 306-308°. $[\alpha]_D^{12}$ +79.5 ($CHCl_3$). Log P 8.59 (uncertain value) (calc).
▶ RK0177965

[39316-91-1, 70620-39-2]

Bischoff, B. *et al., Helv. Chim. Acta*, 1949, **32**, 1911-1921 (*struct, ir*)
Savoir, R. *et al., Bull. Soc. Chim. Belg.*, 1967, **76**, 335-367 (*pmr*)
Renwick, J.D. *et al., J.C.S.(C)*, 1969, 2544-2549 (*cd, ord*)
Tori, K. *et al., Tet. Lett.*, 1974, 4227-4230 (*cmr*)
Seo, S. *et al., Chem. Comm.*, 1975, 270-271 (*biosynth, cmr*)
Roques, R. *et al., Acta Cryst. B*, 1978, **34**, 2367-2370 (*cryst struct, Ac*)
Seo, S. *et al., Chem. Comm.*, 1986, 1141-1143 (*biosynth*)
Hadjieva, P. *et al., Z. Naturforsch., C*, 1987, **42**, 1019-1022 (*isol, alga*)
Maillard, M. *et al., Phytochemistry*, 1992, **31**, 1321-1323 (*Oleanolic acid, cmr*)
Konoike, T. *et al., Tetrahedron*, 1999, **55**, 14901-14914 (*synth*)

3-Hydroxy-12-oleanen-30-oic acid H-845



$C_{30}H_{48}O_3$ 456.707

3α-*form*

20-Epikatonic acid
[525598-55-4]
Constit. of *Bocconia arborea*.
Cryst.
Mp 271-272°.

3β-*form*

11-Deoxoglycyrrhetinic acid. *Betuloleanolic acid. Anaphalisoleanenoic acid*
[564-16-9]
Isol. from roots of *Glycyrrhiza glabra* (licorice) and *Anaphalis araneosa*.
Cryst. (AcOH).
Mp 105-107° Mp 330°. $[\alpha]_D$ +148 (c, 0.473 in $CHCl_3$). $[\alpha]_D^{18}$ +3.3 (c, 0.03 in MeOH). Unexplained major difference in phys. props. of the isolates.

3-O-[β-D-Glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]: ***Licoricesaponin B2***. *Deoxoglycyrrhizin*
[118536-86-0]
$C_{42}H_{64}O_{15}$ 808.959
Isol. from roots of *Glycyrrhiza uralensis* (Chinese licorice).
Monohydrate.
Mp 209-210°. $[\alpha]_D^{19}$ +54 (MeOH).

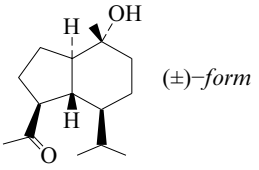
3-Ac: ***Betuloleanolic acid acetate***
[53402-18-9]
$C_{32}H_{50}O_4$ 498.745
Constit. of stem bark of *Betula pendula* and present in the hexacoral *Echinopora lamellosa*. Cryst. (EtOH).
Mp 280-281°. $[\alpha]_D^{25}$ +18. λ_{max} 209 (log ϵ 6.2) (MeOH).

3-Ketone: ***3-Oxo-12-oleanen-30-oic acid***
$C_{30}H_{46}O_3$ 454.692
Constit. of *Dillenia papuana*. Needles (MeOH).
Mp 270-272°. $[\alpha]_D^{22}$ +110 (c, 0.06 in $CHCl_3$).

Canonica, L. *et al., Gazz. Chim. Ital.*, 1966, **96**, 833 (*isol, struct*)
Chakrabarti, P. *et al., J. Indian Chem. Soc.*, 1969, **46**, 626 (*synth*)
Sanduja, R. *et al., J. Het. Chem.*, 1984, **21**, 845-848 (*Ac, isol, Echinopora*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3710 (*Licoricesaponin B2*)
Nick, A. *et al., Phytochemistry*, 1995, **40**, 1691 (*isol, pmr, cmr*)
Pellegata, R. *et al., Org. Prep. Proced. Int.*, 1999, **31**, 181-187 (*synth*)
Sharma, S.K. *et al., Indian J. Chem., Sect. B*, 2003, **42**, 2858-2862 (*Anaphalisoleanenoic acid*)
Chávez, M.I. *et al., Magn. Reson. Chem.*, 2003, **41**, 143-144 (*3α-form, pmr, cmr*)
Mukhtar, H.M. *et al., Pharmazie*, 2003, **58**, 671-673 (*Betuloleanolic acid acetate*)

10-Hydroxy-4-oplopanone H-846

Oplopanone



(±)–*form*

$C_{15}H_{26}O_2$ 238.369

Cadinane numbering system.

(+)-*form*

Constit. of soft coral *Nephthea* sp.
Needles (petrol).
Mp 83-84°. $[\alpha]_D^{22}$ +19 (c, 0.8 in dioxan).

(-)-*form* [1911-78-0]

Constit. of *Oplopanax japonicus* and *Alisma orientalis.*
Cryst. (Et_2O/petrol).
Mp 96-97°. $[\alpha]_D^{25}$ -20 (c, 0.6 in dioxan).

(ξ)-*form*

Orientalol F

[462106-99-6]

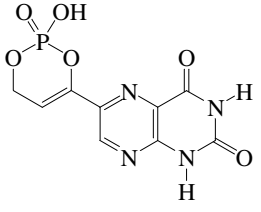
Constit. of *Alisma orientalis.*

Ac: Oplopanyl acetate
$C_{17}H_{28}O_3$ 280.406
Isol. from *Chamaecyparis pisifera*.

Takeda, K. *et al., Tetrahedron, Suppl.*, 1966, **7**, 219 (*isol, ir, pmr, ord, struct*)
Caine, D. *et al., J.O.C.*, 1973, **38**, 3663 (*synth*)
Wratten, S.J. *et al., J.O.C.*, 1977, **42**, 3343 (*isol*)
Taber, D.F. *et al., J.O.C.*, 1978, **43**, 4925 (*synth*)
Koster, F.-H. *et al., Tet. Lett.*, 1981, **22**, 3937 (*synth*)
Piers, E. *et al., J.O.C.*, 1990, **55**, 2380 (*synth*)
De Bruyn, A. *et al., Magn. Reson. Chem.*, 1990, **28**, 1030 (*acetate*)
San Feliciano, A. *et al., J. Nat. Prod.*, 1995, **58**, 1059 (*pmr, cmr*)
Su, W.-C. *et al., Phytochemistry*, 1995, **39**, 603 (*cmr*)
peng, G. *et al., Tianran Chanwu Yanjiu Yu Kaifa*, 2001, **13**, 9-11; *CA*, **138**, 21864t (*isol, pmr, cmr*)
Chen, D. *et al., Fenxi Huaxue*, 2002, **30**, 809-811; *CA*, **137**, 260032f (*Orientalol F*)

6-(2-Hydroxy-2-oxido-4*H*-1,3,2-dioxaphosphorin-6-yl)-2,4(1*H*,3*H*)-pteridinedione, 9CI H-847

[149230-97-7]



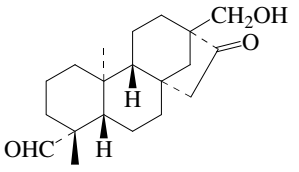
$C_9H_7N_4O_6P$ 298.151
Isol. from the marine polychaete *Odontosyllis undecimdonta*. Pale yellow cryst.
Mp 225-235° dec.

N^3-*Me:* [149230-96-6]
$C_{10}H_9N_4O_6P$ 312.178
Isol. from *Odontosyllis undecimdonta*. Pale yellow needles (MeOH aq.).
Mp 230-235° dec.

N^1,N^3-*Di-Me:* [149230-95-5]
$C_{11}H_{11}N_4O_6P$ 326.205
Isol. from *Odontosyllis undecimdonta*. Pale yellow prisms (MeOH aq.).
Mp 220-227° dec.

Inou, S. *et al., Heterocycles*, 1993, **35**, 147-150 (*isol, pmr, cmr, P-31 nmr*)

17-Hydroxy-16-oxo-19-beyeranal H-848



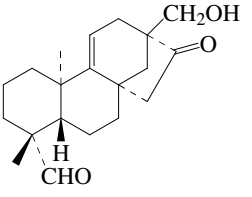
$C_{20}H_{30}O_3$ 318.455

(ent)-form [765315-63-7]

Constit. of *Bruguiera gymnorrhiza*.
Amorph. solid. $[\alpha]_D^{20}$ -35 (c, 0.3 in $CHCl_3$).

Han, L. *et al., J. Nat. Prod.*, 2004, **67**, 1620-1623 (*isol, pmr, cmr*)

17-Hydroxy-16-oxo-9(11)-beyeren-19-al H-849



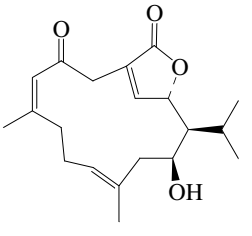
$C_{20}H_{28}O_3$ 316.439

ent-form [873222-59-4]

Constit. of *Bruguiera sexangula* var. *rhynchopetala*.
Amorph. powder. $[\alpha]_D^{20}$ -77.4 (c, 0.14 in $CHCl_3$).

Bao, S. *et al., Helv. Chim. Acta*, 2005, **88**, 2757-2763 (*Bruguiera sexangula constit*)

14-Hydroxy-6-oxo-3,7,11-cembratrien-18,2-olide H-850



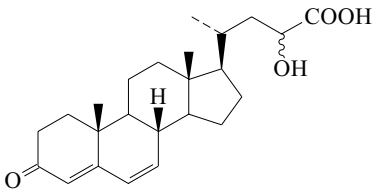
$C_{20}H_{28}O_4$ 332.439

(1*S*,2*S*,7*Z*,11*E*,14*S*)-*form*

Ac: ***Sarcophytonolide D***
[862248-74-6]
$C_{22}H_{30}O_5$ 374.476
Constit. of a *Sarcophyton* sp. Oil. $[\alpha]_D^{20}$ -17 (c, 0.17 in $CHCl_3$). λ_{max} 231 (log ϵ 2.25) (MeOH).

Jia, R. *et al., Helv. Chim. Acta*, 2005, **88**, 1028-1033 (*Sarcophytonolide D*)

23-Hydroxy-3-oxochola-4,6-dien-24-oic acid H-851



$C_{24}H_{34}O_4$ 386.53

(23ξ)-*form*

Constit. of *Deltocyathus magnificus*.

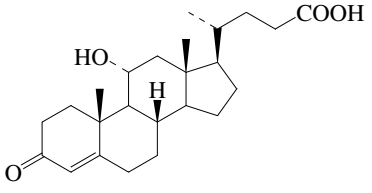
Me ester: [180603-64-9]
$[\alpha]_D^{20}$ -5.5 (c, 0.1 in EtOH).

6,7-Dihydro: ***23-Hydroxy-3-oxochol-4-en-24-oic acid***
$C_{24}H_{36}O_4$ 388.546
Constit. of *Deltocyathus magnificus*.

6,7-Dihydro, Me ester: [180603-67-2]
$[\alpha]_D^{20}$ +33.8 (c, 0.08 in EtOH).

Guirriero, A. *et al., Helv. Chim. Acta*, 1996, **79**, 982-988 (*isol, pmr, cmr*)

11-Hydroxy-3-oxochol-4-en-24-oic acid H-852

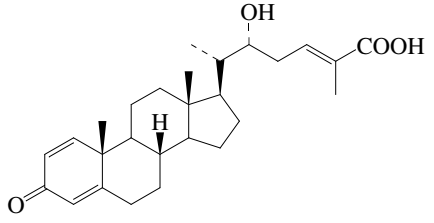


$C_{24}H_{36}O_4$ 388.546

11α-*form*

11-Ac: [832723-73-6]
$C_{26}H_{38}O_5$ 430.583
Constit. of an *Eleutherobia* sp. Glass. $[\alpha]_D^{20}$ +63.9 (c, 0.072 in EtOH). λ_{max} 258 (log ϵ 2.95); 304 (log ϵ 2.02) ($CHCl_3$).
Lievens, S.C. *et al., J. Nat. Prod.*, 2004, **67**, 2130-2132 (*isol, pmr, cmr*)

22-Hydroxy-3-oxocholesta-1,4,24-trien-26-oic acid H-853



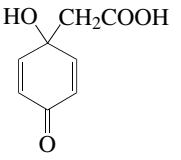
$C_{27}H_{38}O_4$ 426.595

(22*R*,24*E*)-*form*

22-Ac, Me ester: [862286-70-2]
$C_{30}H_{42}O_5$ 482.659
Constit. of *Anthomastus bathyproctus*. Amorph. powder. $[\alpha]_D^{25}$ -4.9 (c, 0.08 in $CHCl_3$). λ_{max} 221 (log ϵ 4.25); 238 (log ϵ 4.19) (MeOH).
Mellado, G.G. *et al., J. Nat. Prod.*, 2005, **68**, 1111-1115

1-Hydroxy-4-oxo-2,5-cyclohexadiene-1-acetic acid H-854

[55604-87-0]



$C_8H_8O_4$ 168.149
Constit. of *Ajuga parviflora*, *Pseudogynoxys cunninghammii*, *Jacaranda caucana* and the marine alga *Delesseria sanguinea*. Larvicide, leishmanicidal agent. Cryst. (EtOAc). Sol. Et_2O, MeOH; poorly sol. H_2O.
Mp 103-104°. Log P -0.69 (calc). λ_{max} 224 (log ϵ 5.8) (MeOH).

Me ester: ***Jacaranone***
[60263-07-2]
$C_9H_{10}O_4$ 182.176
Constit. of *Ajuga parviflora*, *Cineraria* spp., *Jacaranda* spp., *Pseudogynoxys* spp. and *Senecio* spp. Also isol. from marine alga *Delesseria sanguinea*. Cytotoxic agent. Metamorphosis inducer for *Pecten* larvae. Cryst. ($CHCl_3$/hexane).
Mp 80-81° (76-77°). λ_{max} 227 (ϵ 12500) (EtOH).

Et ester: [60263-06-1]
$C_{10}H_{12}O_4$ 196.202
Constit. of *Ajuga parviflora*, *Emilia* sp., *Jacaranda* and *Senecio* spp. Cytotoxic agent. Cryst. ($CHCl_3$/hexane).
Mp 72-74°.

Amide: 1-Hydroxy-4-oxo-2,5-cyclohexadiene-1-acetamide. 4-(Carbamoylmethyl)-4-hydroxy-2,5-cyclohexadien-1-one. Verongiaquinol
[86254-99-1]
$C_8H_9NO_3$ 167.164
Parent compd. unknown.

Ac, Me ester: [60508-82-9]
$C_{11}H_{12}O_5$ 224.213
Constit. of *Ajuga parviflora*. Oil.

Ac, Et ester: [100118-30-7]
$C_{12}H_{14}O_5$ 238.24
Constit. of *Ajuga parviflora*. Needles.
Mp 69-70°. λ_{max} 201; 235 (MeOH).

Di-Me acetal, amide: 1-Hydroxy-4,4-dimethoxy-2,5-cyclohexadiene-1-acetamide
$C_{10}H_{15}NO_4$ 213.233
Isol. from *Verongia aerophoba*. Cryst.
Mp 187-189°.

Di-Et acetal, amide: 4,4-Diethoxy-1-hydroxy-2,5-cyclohexadiene-1-acetamide
[253308-66-6]
$C_{12}H_{19}NO_4$ 241.286
Isol. from the sponge *Verongia aerophoba*. Cryst.
Mp 183-187°.

Et-Me acetal, amide: 4-Ethoxy-1-hydroxy-4-methoxy-2,5-cyclohexadiene-1-acetamide
$C_{11}H_{17}NO_4$ 227.26
Isol. from *Verongia aerophoba*. Cryst.
Mp 183-184°.

2,3,5,6-Tetrahydro, Me ester: 4-Hydroxy-4-(methoxycarbonylmethyl)cyclohexanone
[81053-14-7]
$C_9H_{14}O_4$ 186.207
Constit. of *Senecio clevelandii*. Oil.

3-Bromo, amide: ***3-Bromoverongiaquinol***
[137006-40-7]
$C_8H_8BrNO_3$ 246.06
Isol. from the marine sponge *Verongia cavernicola* and from *Suberea creba*. Sticky semi-solid. Sol. MeOH, C_6H_6; poorly sol. H_2O. Racemic. λ_{max} 235 (ϵ 5500) (MeOH) (Berdy).

3-Bromo, 5-chloro, amide: ***3-Bromo-5-chloroverongiaquinol***
[98349-14-5]
$C_8H_7BrClNO_3$ 280.505
Isol. from *Verongia cavernicola*. Cryst.
Mp 175-177°. Racemic.

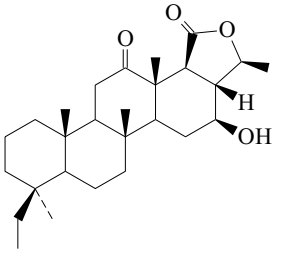
3,5-Dibromo, Et ester: [24744-57-8]
$C_{10}H_{10}Br_2O_4$ 353.995
Isol. from the mollusc *Tylodina fungina*. Needles (hexane/CH_2Cl_2).
Mp 127-127.5° (121°). λ_{max} 257 (ϵ 9596) (MeOH).

3,5-Dibromo, amide: ***3,5-Dibromoverongiaquinol***
[16628-93-6]
$C_8H_7Br_2NO_3$ 324.956
Isol. from *Verongia cauliformis* (*Aplysina cauliformis*). Shows antibiotic props. Needles (Et_2O/Me_2CO).
Mp 195-196°. λ_{max} 200 (sh) (ϵ) (MeOH/NaOH) (Derep). λ_{max} 257 (ϵ 8300) (MeOH) (Derep).

3,5-Dichloro, amide: ***Dichloroverongiaquinol***
[88290-16-8]
$C_8H_7Cl_2NO_3$ 236.054
Isol. from the Mediterranean sponges *Aplysina cavernicola* and *Aplysina fistularis*. Inhibitor of gram-positive and gram-negative bacteria. Cryst.
Mp 162-163°.

Sharma, G.M. *et al., J. Antibiot., Ser. A*, 1967, **20**, 200 (*isol*)
Sharma, G.M. *et al., Tet. Lett.*, 1967, 4147 (*synth*)
Saito, I. *et al., J.A.C.S.*, 1975, **97**, 5272-5277 (*synth, uv, ir, pmr*)
Bohlmann, F. *et al., Chem. Ber.*, 1976, **109**, 2014-2020 (*Jacaranone, Et ester*)
Ogura, M. *et al., J. Nat. Prod.*, 1976, **39**, 255-257; 1977, **40**, 157-168 (*Jacaranone*)
Evans, D.A. *et al., J.O.C.*, 1977, **42**, 350-352 (*3,5-dibromo amide*)
Parker, K.A. *et al., J.O.C.*, 1979, **44**, 3964-3966 (*Jacaranone, synth*)
Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 2425-2427 (*isol, ir, pmr, ms*)
D'Ambrosio, M. *et al., Experientia*, 1983, **39**, 1091-1092 (*Dichloroverongiaquinol, isol, uv, ir, pmr, ms, synth*)
Fischer, A. *et al., Tet. Lett.*, 1983, **24**, 131-134 (*3,5-dibromo amide, synth*)
D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1984, **67**, 1484-1492 (*3-Bromoverongiaquinol*)
Goo, Y.M. *et al., Arch. Pharmacal Res.*, 1985, **8**, 21-30 (*Dichloroverongiaquinol*)
Yvin, J.C. *et al., J. Nat. Prod.*, 1985, **48**, 814-816 (*Me ester, isol, synth*)
Jakupovic, J. *et al., Fitoterapia*, 1987, **58**, 187 (*isol*)
Araki, S. *et al., J.C.S. Perkin 1*, 1991, 499-500 (*Jacaranone, Et ester, synth*)
Bicchierini, N. *et al., Tet. Lett.*, 1991, **32**, 4039-4040 (*bromoamide, dibromoamide, chlorobromoamide*)
Muhammad, P. *et al., Fitoterapia*, 1999, **70**, 229-232 (*Ac Me ester, Ac Et ester*)
Aydogmuş, Z. *et al., Turk. J. Chem.*, 1999, **23**, 339-344 (*di-Et acetal amid, di-Me acetal amide, Et-Me acetal amide*)
Akhbar, E. *et al., Z. Naturforsch., B*, 2001, **56**, 842-846 (*isol, pmr, cmr*)

16-Hydroxy-12-oxo-20,24-dimethyl-25,24-scalaranolide H-855



$C_{27}H_{42}O_4$ 430.626

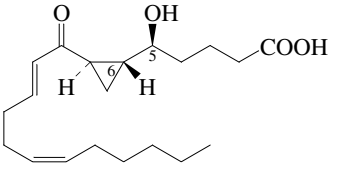
(16β,24β)-*form*
Phyllofolactone A
[134985-07-2]
Constit. of *Phyllospongia foliascens*.
Needles (Me_2CO).
Mp 332-334°. $[\alpha]_D^{20}$ +78.4 (c, 0.051 in $CHCl_3$).

Ac: ***Acetylphyllofolactone A***. *Acetoxyphyllofolactone A (incorr.)*
$C_{29}H_{44}O_5$ 472.664
Isol. from sponge *Phyllospongia foliascens*.

Zeng, L. *et al., J. Nat. Prod.*, 1991, **54**, 421 (*isol, pmr, cmr*)
Fu, X. *et al., Gaodeng Xuexiao Huaxue Xuebao*, 1992, **13**, 628-629 (*Acetylphyllofolactone A*)

δ-Hydroxy-2-(1-oxo-2,6-dodecadienyl)cyclopropanepentanoic acid H-856

5-Hydroxy-6,7-methylene-8-oxo-9,13-nonadecadienoic acid
[121072-76-2]

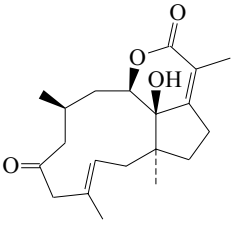


$C_{20}H_{32}O_4$ 336.47

(5*S*,6*R*,7*R*,9*E*,13*Z*)-*form* [148218-34-2]
[165038-19-7]
Metab. of in the soft coral *Plexaura homomalla*.

White, J.D. *et al., J.A.C.S.*, 1995, **117**, 6224-6233 (*synth, config*)

11-Hydroxy-6-oxo-3,12(18)-dolabelladien-19,10-olide H-857



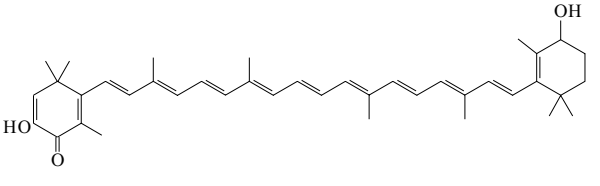
$C_{20}H_{28}O_4$ 332.439

(3*E*,10β,11β)-*form*
Clavirolide A
Constit. of *Clavularia viridis*.
Cryst.
Mp 188-190°. $[\alpha]_D$ -328.8 (c, 0.22 in $CHCl_3$). λ_{max} 202 (ϵ 9000); 226 (ϵ 23000) (MeOH) (Derep).

Su, J. *et al., J.O.C.*, 1991, **56**, 2337 (*isol, pmr, cmr*)

4′-Hydroxy-3-oxoechinenone H-858

4-Hydroxy-3′,4′-dioxo-β-carotene. 2,3-Didehydro-3,4′-dihydroxy-β,β-caroten-4-one
[58720-56-2]



$C_{40}H_{52}O_3$ 580.849
Isol. from nitrogen deficient strains of *Protosiphon botryoides*; synthesised sequentially from Echinenone, E-2. Needles (C_6H_6/EtOH).
Mp 149-150°. λ_{max} 476-480 ($CHCl_3$); 484 nm (C_6H_6).

Kleinig, H. *et al., Z. Naturforsch., B*, 1969, **24**, 927 (*isol*)
Cooper, R.D.G. *et al., J.C.S. Perkin 1*, 1975, 2195 (*synth*)

11-Hydroxy-16-oxo-5,8,12,14,17-eicosapentaenoic acid, 9CI H-859

$H_3CCH_2CH{=}CHCOCH{=}CHCH{=}CHCH(OH)CH_2CH{=}CHCH_2CH{=}CH(CH_2)_3COOH$

$C_{20}H_{28}O_4$ 332.439

(5Z,8Z,12E,14E,17E)-form

Ptilodene

[115330-89-7]

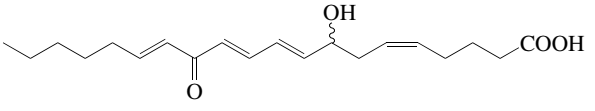
Isol. from red marine alga *Ptilota filicina*. Shows antibacterial activity. Inhibits human *S*-lipoxygenase.

Unstable. λ_{max} 224 (ϵ 8450); 275 (ϵ 6800) (MeOH) (Derep). λ_{max} 224 (ϵ 6800); 275 (ϵ 8450) (MeOH) (Berdy).

[115330-88-6]

Gerwick, W.H. *et al., Tet. Lett.*, 1988, 1505 (*isol, pmr, ms, uv, cmr*)

8-Hydroxy-13-oxo-5,9,11,14-eicosatetraenoic acid H-860



$C_{20}H_{30}O_4$ 334.455

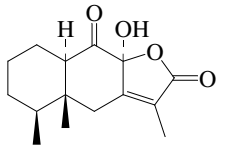
(5Z,8ξ,9E,11E,14E)-form

[132679-89-1]

Isol. from the algae *Lithothamnion* spp. (as Et ester).

Guerriero, A. *et al., Helv. Chim. Acta*, 1990, **73**, 2183-2189 (*isol, uv, pmr*)

8-Hydroxy-9-oxo-7(11)-eremophilen-12,8-olide H-861



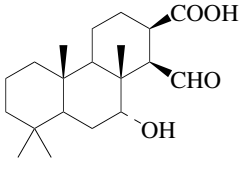
$C_{15}H_{20}O_4$ 264.321

8α-OH-form [392717-70-3]

Metab. of the marine fungus *Hypoxylon oceanicum*.

Li, H.-J. *et al., Zhongshan Daxue Xuebao Ziran Kexueban*, 2001, **40**, 70-72; *CA*, **136**, 131298c (*isol, pmr, cmr*)

7-Hydroxy-15-oxo-16-isocopalanoic acid H-862



$C_{20}H_{32}O_4$ 336.47

7α-form

Ac, Me ester: ***Aplyroseol 13***

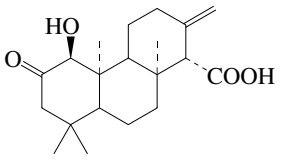
[200437-62-3]

$C_{23}H_{36}O_5$ 392.534

Constit. of *Aplysilla rosea*. Glass.

Taylor, W.C. *et al., Aust. J. Chem.*, 1997, **50**, 895-902 (*isol, pmr, cmr*)

1-Hydroxy-2-oxo-13(16)-isocopalen-15-oic acid H-863



$C_{20}H_{30}O_4$ 334.455

(ent-1α)-form

Mycgranol

[849334-80-1]

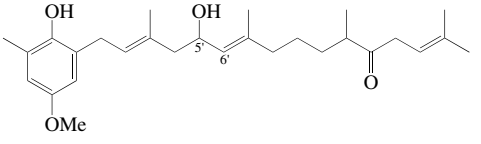
Constit. of *Mycale* aff. *graveleyi*.

Oil. $[\alpha]_D$ +2.5 (c, 2.5 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 2005, **68**, 280-281 (*isol, pmr, cmr*)

5′-Hydroxy-12′-oxoisohalidrol H-864

5′-Hydroxy-12′-oxohalidrol (incorr.)



(6′E)-form

$C_{28}H_{42}O_4$ 442.637

(6′E)-form

Constit. of the brown alga *Halidrys siliquosa*.

Oil. $[\alpha]_D^{20}$ +2.3 (c, 8.9 in MeOH).

5′-Ketone: 5′,12-Dioxoisohalidrol

[80756-05-4]

$C_{28}H_{40}O_4$ 440.622

From *Halidrys siliquosa*. Oil. $[\alpha]_D^{20}$ -1.24 (c, 11.3 in MeOH).

(6′Z)-form

5′-Ketone: 5′,12′-Dioxohalidrol

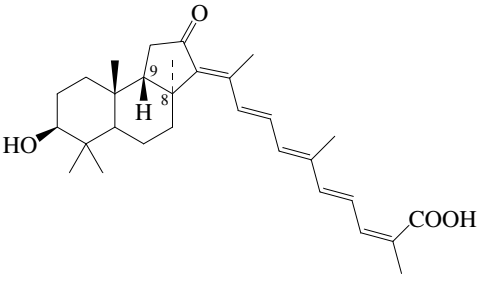
[80756-04-3]

$C_{28}H_{40}O_4$ 440.622

From *Halidrys siliquosa*. Oil. $[\alpha]_D^{20}$ -10.7 (c, 15 in MeOH).

Higgs, M.D. *et al., Tetrahedron*, 1981, **37**, 3209-3213

3-Hydroxy-12-oxo-13,15,17(20),22,24-isomalabaricapentaen-26-oic acid H-865



(3β,8α,9β,13*E*,15*E*,17(20)*E*,22*E*,24*Z*)-*form*

$C_{30}H_{42}O_4$ 466.659

(3β,8α,9β,13E,15E,17(20)E,22E,24Z)-form

Ac: ***Stellettin H***

[405202-89-3]

$C_{32}H_{44}O_5$ 508.697

Constit. of *Rhabdastrella globostellata*. Orange-yellow glass. $[\alpha]_D$ -83 (c, 0.19 in $CHCl_3$). λ_{max} 234 (log ϵ 3.46); 294 (log ϵ 3.62); 392 (log ϵ 4.03); 410 (log ϵ 3.99) (MeOH).

3-Ketone: ***Stellettin F****. Rhabdastrellic acid A*
[184885-90-3]
$C_{30}H_{40}O_4$ 464.644
Constit. of a *Stelletta* sp. and *Rhabdastrella globostellata*. Yellow cryst. (C_6H_6/Me_2CO). $[\alpha]_D$ -61.6 (c, 0.6 in Me_2CO). Props. refer to Rhabdastrellic acid A. Stellettin F was characterised as the Me ester. λ_{max} 396 (ϵ 87400); 410 (ϵ 85200) (Me_2CO) (Me ester).

(3β,8α,9β,13*Z*,15*E*,17(20)*E*,22*E*,24*E*)-*form*

Ac: ***Stellettin I***
[405202-90-6]
$C_{32}H_{44}O_5$ 508.697
Constit. of *Rhabdastrella globostellata*. Yellow oil. $[\alpha]_D$ -31 (c, 0.22 in $CHCl_3$). λ_{max} 234 (log ϵ 3.28); 294 (log ϵ 3.46); 394 (log ϵ 3.91); 410 (log ϵ 3.88) (MeOH).

3-Ketone: ***Stellettin E***
[184885-89-0]
$C_{30}H_{40}O_4$ 464.644
Constit. of a *Stelletta* sp. Yellow solid (as Me ester). $[\alpha]_D$ +36 (c, 0.05 in $CHCl_3$) (Me ester). λ_{max} 294 (log ϵ 4.08); 395 (log ϵ 4.56); 410 (log ϵ 4.52) (EtOH) (Me ester).

(3β,8α,9β,13*Z*,15*E*,17(20)*E*,22*E*,24*Z*)-*form*

Ac: ***3β-Acetoxy-12-oxo-8,9-bisepi-13,15,17(20),22,24-malabaricapentaen-26-oic acid****. 3-Acetoxy-12-oxo-13,15,17(20),22,24-isomalabaricapentaen-26-oic acid*
[84025-32-1]
$C_{32}H_{44}O_5$ 508.697
Constit. of sponge *Jaspis stellifera*. Bright yellow foam (as Me ester). $[\alpha]_D^{20}$ -135.7 (c, 1.0 in $CHCl_3$) (Me ester).

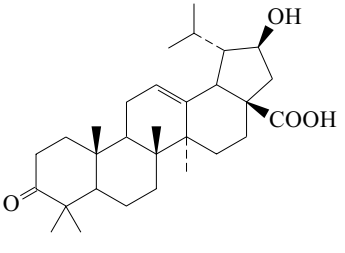
3-Ketone: 3,12-Dioxo-13,15,17(20),22,24-isomalabaricapentaen-26-oic acid. ***Stellettin G***
[184885-92-5]
$C_{30}H_{40}O_4$ 464.644
From *Jaspis stellifera* and a *Stelletta* sp.
$[\alpha]_D^{20}$ +31 (c, 1.0 in $CHCl_3$) (as Me ester). λ_{max} 294 (log ϵ 3.81); 395 (log ϵ 4.55); 415 (log ϵ 4.53) (EtOH) (as Me ester). λ_{max} 396 (ϵ 29200); 417 (ϵ 23750) (EtOH) (Berdy).

3-Ketone, 22-hydroxy, lactone: See 3,12-Dioxo-13,15,17(20),22,24-isomalabaricapentaen-26,22-olide, D-1056

[83972-25-2]

Ravi, B.N. *et al., J.O.C.*, 1981, **46**, 1998 (*isol*)
McCabe, T. *et al., Tet. Lett.*, 1982, **23**, 3307 (*struct*)
McCormick, J.L. *et al., J. Nat. Prod.*, 1996, **59**, 1047-1050 (*Stellettins*)
Rao, Z. *et al., J. Nat. Prod.*, 1997, **60**, 1163-1164 (*Rhabdastrellic acid A*)
Deng, S. *et al., Zhongguo Haiyang Yaowu*, 1999, **18**, 1-3; *CA*, **133**, 86885s (*isol, pmr, cmr*)
Tasdemir, D. *et al., J. Nat. Prod.*, 2002, **65**, 210-214 (*Stellettins H, I*)

21-Hydroxy-3-oxo-12-lupen-28-oic acid H-866

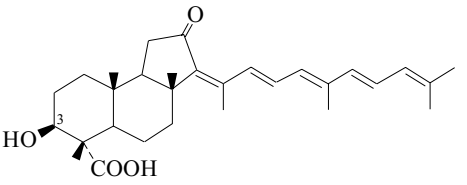


$C_{30}H_{46}O_4$ 470.691

21β-*form*

28→21 Lactone: 3-Oxo-12-lupen-28,21-olide
$C_{30}H_{44}O_3$ 452.676
Constit. of *Hemidesmus indicus*.
Gupta, M.M. *et al., Phytochemistry*, 1992, **31**, 4036 (*isol, pmr*)

3-Hydroxy-12-oxo-13,15,17(20),22,24-malabaricapentaen-28-oic acid H-867



$C_{30}H_{42}O_4$ 466.659

(3β,13*Z*,15*E*,17(20)*E*,22*E*)-*form*
Constit. of *Jaspis stellifera*.
Yellow foam (as Me ester). $[\alpha]_D^{20}$ +22.8 (c, 0.5 in $CHCl_3$) (Me ester). λ_{max} 280 (ϵ 15000); 402 (ϵ 45000) (MeOH) (Derep).

3-Ac:
$C_{32}H_{44}O_5$ 508.697
Constit. of *Jaspis stellifera*. λ_{max} 403 (ϵ 43200) (MeOH) (Derep).

Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 39

11-Hydroxy-12-oxo-6,9,15-octadecatrienoic acid H-868

$H_3CCH_2CH{=}CHCH_2CH_2COCH(OH)CH{=}CHCH_2CH{=}CH(CH_2)_4COOH$

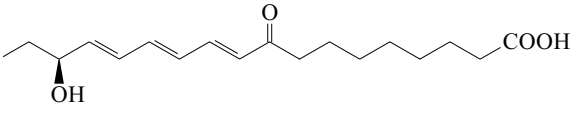
$C_{18}H_{28}O_4$ 308.417

(6*Z*,9*Z*,11ξ,15*Z*)-*form*

Lactone: 12-(1-Oxo-4-heptenyl)oxacyclododeca-7,10-dien-2-one. 12-(4-Heptenoyl)oxacyclododeca-7,10-dien-2-one
$C_{18}H_{26}O_3$ 290.402
Isol. from the brown alga *Eisenia bicyclis*. Oil. $[\alpha]_D^{20}$ +12 (c, 0.08 in $CHCl_3$). Oxylipin.

Kousaka, K. *et al., J. Nat. Prod.*, 2003, **66**, 1318-1323 (*isol, pmr, cmr*)

16-Hydroxy-9-oxo-10,12,14-octadecatrienoic acid H-869



$C_{18}H_{28}O_4$ 308.417

(10*E*,12*E*,14*E*,16*S*)-*form*
Corchorifatty acid B
Constit. of *Corchorus olitorius* (Jew's mallow). Powder. $[\alpha]_D^{28}$ +17.3 (c, 0.2 in Me_2CO). λ_{max} 309 (log ϵ 4.3) (MeOH).

Me ester: [147383-00-4]
$C_{19}H_{30}O_4$ 322.444
Isol. from the green alga *Acrosiphonia coalita*. Oil. $[\alpha]_D^{25}$ +19 (c, 0.25 in Me_2CO).

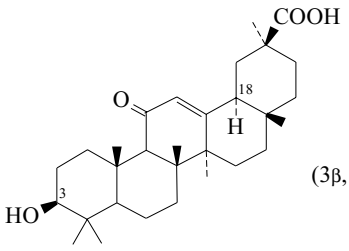
(10*E*,12*Z*,14*E*,16*S*)-*form*
Corchorifatty acid D
Constit. of *Corchorus olitorius* (Jew's mallow). Powder. $[\alpha]_D^{26}$ +19.7 (c, 0.04 in Me_2CO). λ_{max} 311 (log ϵ 4.3) (MeOH).

(10*E*,12*Z*,14*E*,16*RS*)-*form*

Me ester: [147292-99-7]
Isol. from *Acrosiphonia coalita*, poss. in enantiomeric form. Oil.

Bernart, M.W. *et al., Phytochemistry*, 1993, **56**, 245 (*isol, struct*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1008-1014 (*isol, uv, ir, pmr, cmr, ms*)

3-Hydroxy-11-oxo-12-oleanen-30-oic acid H-870



(3β,18α)–*form*

$C_{30}H_{46}O_4$ 470.691
Log P 6.25 (calc).

▶ RK0180000

(3β,18β)-*form*

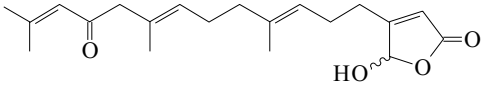
Glycyrrhetic acid. *α-Glycyrrhetinic acid. Enoxolone, BAN, INN. Biogastrone acid. Biosone. Glycyrrhetin. Glycyrrhetinic acid. Rhetinic acid. Uralenic acid*
[471-53-4]
Isol. from hexacoral *Echinopora lamellosa*. Aglycone from licorice (*Glycyrrhiza glabra*) and some other plants. Antibacterial, antitussive agent. Used in treatment of noninfective inflammatory disorders (skin, mouth, etc.). Cryst. (MeOH).
Mp 300-304°. $[\alpha]_D$ +161 ($CHCl_3$). Log P 6.25 (calc). Sweet taste.
▶ LD_{50} (mus, ivn) 56 mg/kg, inhibits 11β-hydroxysteroid dehydrogenase.

3-Ac: ***Acetylenoxolone***. *Acetoxolone*
[6277-14-1]
$C_{32}H_{48}O_5$ 512.728
Isol. from *Echinopora lamellosa*. Antiulcer agent.
Mp 245°. Log P 7.19 (uncertain value) (calc).
▶ RK0177570

Sanduja, R. *et al., J. Het. Chem.*, 1984, **21**, 845-848 (*isol, Echinopora*)

20-Hydroxy-13-oxo-2,6,10,14-phytatetraen-1,20-olide H-871

*5-Hydroxy-4-(4,8,12-trimethyl-10-oxo-3,7,11-tridecatrienyl)-2(5*H*)-furanone*



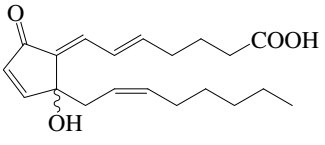
$C_{20}H_{28}O_4$ 332.439

(6*E*,10*E*,20ξ)-*form*

Metab. of *Bifurcaria bifurcata*.

Hougaard, L. *et al., Phytochemistry*, 1991, **30**, 3049 (*isol, pmr, cmr*)

12-Hydroxy-9-oxo-5,7,10,14-prostatetraenoic acid H-872



(5*E*,7*E*,12ξ,14*Z*)-*form*

$C_{20}H_{28}O_4$ 332.439

Abs. stereochem. not clear. Shown by Shen *et. al.* with the 12*S*-config. shown, but this does not appear to have been proved.

(5*E*,7*E*,12ξ,14*Z*)-*form*

Me ester: [461045-33-0]
$C_{21}H_{30}O_4$ 346.466
Isol. from *Clavularia viridis*. Pale yellow oil. $[\alpha]_D^{25}$ +54 (c, 0.8 in CH_2Cl_2).

Ac, Me ester: ***Claviridenone E***
[475111-75-2]
[461045-37-4]
$C_{23}H_{32}O_5$ 388.503
Isol. from the soft coral *Clavularia viridis*. Cytotoxic. Oil. $[\alpha]_D^{25}$ +8.6 (c, 0.3 in $CHCl_3$). λ_{max} 226 (log ϵ 3.88); 290 (log ϵ 4.04) (MeOH).

(5*E*,7*Z*,12ξ,14*Z*)-*form*

Me ester: [681138-11-4]
$C_{21}H_{30}O_4$ 346.466
Isol. from *Clavularia viridis*. Pale yellow oil. $[\alpha]_D^{25}$ +15 (c, 0.8 in CH_2Cl_2).

Ac, Me ester: ***Claviridenone G***
[475111-77-4]
$C_{23}H_{32}O_5$ 388.503
Isol. from *Clavularia viridis*. Cytotoxic. Oil. $[\alpha]_D^{25}$ +5.4 (c, 0.1 in $CHCl_3$). λ_{max} 223 (log ϵ 3.89); 286 (log ϵ 4.06) (MeOH).

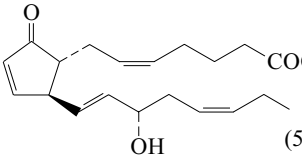
(5*Z*,7*E*,12ξ,14*Z*)-*form*

Me ester: [461045-34-1]
$C_{21}H_{30}O_4$ 346.466
Isol. from *Clavularia viridis*. Pale yellow oil. $[\alpha]_D^{25}$ +24 (c, 0.4 in CH_2Cl_2).

Ac, Me ester: ***Claviridenone F***
[475111-76-3]
[461045-36-3]
$C_{23}H_{32}O_5$ 388.503
Isol. from *Clavularia viridis*. Cytotoxic. Amorph. solid. $[\alpha]_D^{25}$ +6.7 (c, 0.3 in $CHCl_3$). λ_{max} 224 (log ϵ 3.89); 288 (log ϵ 4.06) (MeOH).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1535-1539 (*isol, pmr, cmr, ms*)
Shen, Y.-C. *et al., J. Nat. Prod.*, 2004, **67**, 542-546 (*isol, cd, pmr, cmr, ms*)

15-Hydroxy-9-oxo-5,10,13,17-prostatetraenoic acid H-873



(5*Z*,13*E*,15*S*,17*Z*)–*form*

$C_{20}H_{28}O_4$ 332.439

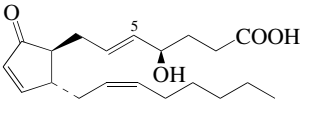
(5*Z*,13*E*,15*S*,17*Z*)-*form*

Prostaglandin A_3
[36614-31-0]
Isol. from seminal fluid of sheep. λ_{max} 220 (ϵ 9600) (no solvent reported).

1,15-Lactone: [133206-39-0]
$C_{20}H_{26}O_3$ 314.424
Isol. from the nudibranch *Tethys fimbria*.

Ger. Pat., 1973, 2 314 519; *CA*, **80**, 595645 (*isom*)
Schevchenko, V.P. *et al., J. Labelled Compd. Radiopharm.*, 1989, **27**, 1177-1193 (*synth*)
Cimino, G. *et al., Experientia*, 1991, **47**, 56-60 (*lactone, isol*)

4-Hydroxy-9-oxo-5,10,14-prostatrien-1-oic acid H-874



(4*R*,5*E*,8*S*,12*R*,14*Z*)-*form*

$C_{20}H_{30}O_4$ 334.455

(4*R*,5*E*,8*S*,12*R*,14*Z*)-*form*

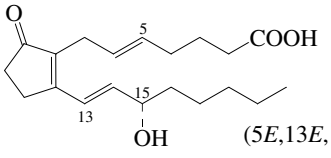
γ-Lactone: ***Preclavulone lactone II***
[185139-32-6]
$C_{20}H_{28}O_3$ 316.439
Isol. from the Okinawan soft coral *Clavularia viridis*. Biosynth. intermed. of Clavulones, C-701. $[\alpha]_D^{25}$ -110.

(4*R*,5*Z*,8*S*,12*R*,14*Z*)-*form*

γ-Lactone: ***Preclavulone lactone I***
[185139-31-5]
$C_{20}H_{28}O_3$ 316.439
Isol. from *Clavularia viridis*. Biosynth. intermediate of Clavulones, C-701. $[\alpha]_D^{25}$ -168.
Iwashima, M. *et al., Tet. Lett.*, 1997, **38**, 8319-8322 (*isol, synth, pmr, cmr, abs config*)

15-Hydroxy-9-oxo-5,8(12),13-prostatrienoic acid, 9CI H-875

7-[2-(3-Hydroxy-1-octenyl)-5-oxo-1-cyclopenten-1-yl]-5-heptenoic acid, 8CI



(5*E*,13*E*,15*S*)-*form*

$C_{20}H_{30}O_4$ 334.455

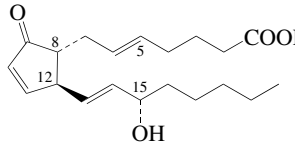
(5*E*,13*E*,15*S*)-*form*

Ac, Me ester:
$C_{23}H_{34}O_5$ 390.519
Isol. from *Plexaura nina*. Yellowish oil. $[\alpha]_D^{20}$ -21.8 ($CHCl_3$). λ_{max} 253 (ϵ 1620) (hexane).

(5*Z*,13*E*,15*S*)-*form*

Prostaglandin B_2. *PGB_2*
[13367-85-6]
Occurs in human seminal plasma. Most abundant prostaglandin released from osteoblasts. Also occurs in marine organisms such as *Haliotis ovina*, *Crenomytilus grayanus*, *Mytilus edulis*, *Modiolus difficilis*, *Stichopus japonicus*, *Distolasterias nippon*, *Halocynthia aurantium*, *Seriola quinqueradiata* and *Sarcophyton crassocaule*. Inhibits uterine motility (*in vitro*). Cryst. $[\alpha]_D^{25}$ +16.3 (c, 0.024 in $CHCl_3$).
Me ester: [55760-05-9]
$C_{21}H_{32}O_4$ 348.481
Constit. of *Sarcophyton crassocaule*. Light brown liq. $[\alpha]_D^{25}$ +17.8 (c, 0.02 in $CHCl_3$).
Ac, Me ester: Isol. from the coral *Plexaura nina*.
Yellowish oil. $[\alpha]_D^{20}$ -25.5 ($CHCl_3$). λ_{max} 253 (ϵ 1630) (hexane).
Hamberg, M. *et al., Prostaglandins, Proc. Nobel Symp., 2nd., 1966*, 1967, 63 (*occur*)
Ger. Pat., 1970, 2 011 969; *CA*, **74**, 87486n (*synth*)
Middleditch, B.S. *et al., Lipids*, 1973, **8**, 267-270 (*ms*)
Feyen, J.H.M. *et al., Prostaglandins*, 1984, **28**, 769-781 (*isol*)
Karotchenko, O.D. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1999, **35**, 612-615 (*occur, marine*)
Ammanamanchi, S.R. *et al., J. Nat. Prod.*, 2000, **63**, 112-118 (*Sarcophyton crassocaule constits*)
Agalias, A. *et al., Z. Naturforsch., C*, 2000, **55**, 425-430 (*Ac, Me ester*)

15-Hydroxy-9-oxo-5,10,13-prostatrien-1-oic acid, 9CI H-876



(5*E*,8*R*,12*S*,13*E*,15*S*)-*form*

$C_{20}H_{30}O_4$ 334.455Log P 2.73 (calc).

(5*E*,8*R*,12*S*,13*E*,15*S*)-*form*

(5E)-Prostaglandin A_2
Constit. of *Plexaura homomalla*.
Pale yellow oil. $[\alpha]_D$ +128 ($CHCl_3$). $[\alpha]_D$ +137 ($CHCl_3$).

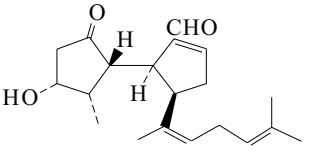
(5*Z*,8*R*,12*S*,13*E*,15*R*)-*form*

15-Epiprostaglandin A_2
Constit. of *Plexaura homomalla*. Antiinflammatory agent.

(5*Z*,8*R*,12*S*,13*E*,15*S*)-*form*

15α-(5Z,13E)-form. Prostaglandin A_2. PGA_2
[13345-50-1]
Constit. of the gorgonian *Plexaura homomalla* and human seminal plasma. More pharmacologically active than the 15*R*-form. Oil. $[\alpha]_D^{20}$ +140 (c, 1.15 in $CHCl_3$). Different chemotypes of the gorgonian *P. homomalla* produce either the 15*S*- or 15*R*-epimers.
▶ Exp. reprod. and teratogenic effects (low doses). LD_{50} (mus, ipr) 93 mg/kg. UK8050000
Me ester: [31753-19-2]
Pale yellow oil. $[\alpha]_D$ +148.
1,15-Lactone: [62443-66-7]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Tethys fimbria*.
Ac: [36323-03-2]
$[\alpha]_D$ +102.
13,14-Dihydro, 15-ketone: 9,15-Dioxo-5,10-prostadienoic acid
[74872-89-2]
$C_{20}H_{30}O_4$ 334.455
Metab. of prostaglandin biosynth. Viscous oil.
Hamberg, M. *et al., J. Biol. Chem.*, 1966, **241**, 257-263 (*isol*)
Weinheimer, A.J. *et al., Tet. Lett.*, 1969, 5185-5188 (*Plexaura homomalla constits, isol, struct*)
Schneider, W.P. *et al., J.A.C.S.*, 1972, **94**, 2122-2123 (*Plexaura homomalla constit*)
Bundy, G.L. *et al., J.A.C.S.*, 1972, **94**, 2124 (*isol, uv*)
Corey, E.J. *et al., J.A.C.S.*, 1973, **95**, 6831-6832; 6832-6833 (*synth*)
Lukacs, G. *et al., Tet. Lett.*, 1973, 515-518 (*cmr*)
Stork, G. *et al., J.A.C.S.*, 1976, **98**, 1583-1584 (*synth, uv*)
Hansen, H.S. *et al., Prostaglandins Ser.*, 1976, **12**, 647-679 (*rev*)
Uekama, K. *et al., Chem. Lett.*, 1977, 1389-1392 (*cd*)
Schneider, W.P. *et al., J.A.C.S.*, 1977, **99**, 1222-1232 (*isol, ir, uv, ms*)
Buendia, J. *et al., Bull. Soc. Chim. Fr.*, 1978, 140-143 (*synth, uv, ir, pmr, ms*)
Greene, A.E. *et al., J.O.C.*, 1978, **43**, 4377-4379 (*Plexaura homomalla constits*)
Finch, M.A.W. *et al., Chem. Comm.*, 1979, 677-678 (*synth*)
Peskar, B.M. *et al., FEBS Lett.*, 1980, **115**, 123-126 (*biochem*)
Greene, A.E. *et al., J.O.C.*, 1982, **47**, 2553-2564 (*synth*)
Newton, R.F. *et al., J.C.S. Perkin 1*, 1983, 683-685 (*synth*)
Suemune, H. *et al., Chem. Pharm. Bull.*, 1988, **36**, 15-21 (*synth*)
Cimino, G. *et al., Experientia*, 1991, **47**, 56-60 (*1,15-lactone, isol*)
Rodríguez, A.D. *et al., Tetrahedron*, 1995, **51**, 4571-4618 (*rev, occur, marine*)
Nicolaou, K.C. *et al., Classics in Total Synthesis, Targets, Strategies, Methods*, VCH, 1996, 137 (*bibl, synth*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1411
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, MCA025

2-Hydroxy-10-oxo-4,10-seco-4,13(15),17-spatatrien-12-al H-877

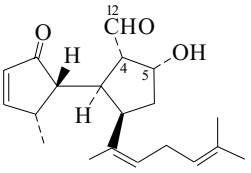


$C_{20}H_{28}O_3$ 316.439

(2*R*,13(15)*Z*)-*form*

Ac: 2-Acetoxy-10-oxo-4,10-seco-4,13(15),17-spatatrien-12-al
$C_{22}H_{30}O_4$ 358.477
Constit. of *Dilophus marginatus*. Oil. $[\alpha]_D^{20}$ +155 (c, 1.6 in CCl_4).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 129

5-Hydroxy-10-oxo-4,10-seco-2,13(15),17-spatatrien-12-al H-878



(4*S*,5*R*,13(15)*Z*)*–form*

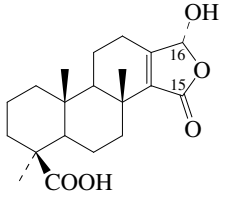
$C_{20}H_{28}O_3$ 316.439

(4*S*,5*R*,13(15)*Z*)-*form* [81623-60-1]
Constit. of *Dilophus marginatus*.
Foam. $[\alpha]_D^{20}$ +45 (c, 1.1 in $CHCl_3$).
Ac:
$C_{22}H_{30}O_4$ 358.477
Constit. of *Dilophus marginatus*. Oil. $[\alpha]_D^{22}$ +22 (c, 1.12 in CCl_4).

(4*S*,5*S*,13(15)*Z*)-*form* [81575-03-3]
Constit. of *Dilophus marginatus*.
Oil. $[\alpha]_D^{20}$ +15 (c, 1.2 in $CHCl_3$).

(4ξ,5ξ,13(15)*Z*)-*form*
12-Alcohol, 5-Ac: ***5-Acetoxy-12-hydroxy-4,10-seco-2,13(15),17-spatatrien-10-one***
$C_{22}H_{32}O_4$ 360.492
Isol. from *Dilophus marginatus*. Oil. $[\alpha]_D^{20}$ +25 (c, 1.2 in $CHCl_3$).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 129

16-Hydroxy-15-oxo-13-spongien-19-oic acid H-879



16α-*form*

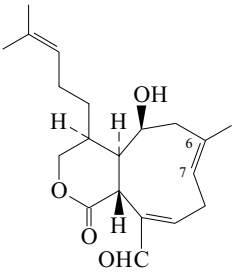
$C_{20}H_{28}O_5$ 348.438

16α-*form*
Me ether: 16-Methoxy-15-oxo-13-spongien-19-oic acid
[220304-52-9]
$C_{21}H_{30}O_5$ 362.465
Constit. of *Spongia matamata*. Powder. $[\alpha]_D$ -92.6 (c, 0.11 in $CHCl_3$/MeOH). λ_{max} 222 (MeOH).
16-Ketone (lactone), 15ξ-alcohol: 15-Hydroxy-16-oxo-13-spongien-19-oic acid. ***Spongiabutenolide A***
[247115-26-0]
$C_{20}H_{28}O_5$ 348.438
Constit. of *Coscinoderma mathewsi* and a *Spongia* sp. Amorph. solid. $[\alpha]_D$ -46 (c, 0.12 in $CHCl_3$/MeOH). $[\alpha]_D$ +28.7 (c, 7.1 in MeOH). Two isolates having different opt. rotns.; could be 15-epimers. The +ve opt. rotn. refers to Spongiabutenolide A. λ_{max} 215 (ϵ 9330) (MeOH).
16-Ketone (lactone), 15α-alcohol, Me ether: 15-Methoxy-16-oxo-13-spongien-19-oic acid
[220304-53-0]
$C_{21}H_{30}O_5$ 362.465
Constit. of *Spongia matamata*. Powder. $[\alpha]_D$ +45 (c, 0.225 in $CHCl_3$/MeOH). λ_{max} 222 (MeOH).
16-Ketone(lactone), 15ξ-alcohol(lactol), 19-alcohol: 15,19-Dihydroxy-13-spongien-16-one. ***Spongiabutenolide C***
[247115-28-2]
Constit. of a *Spongia* sp.
Solid.
15-Deoxo, 16-ketone (lactone): 16-Oxo-13-spongien-19-oic acid
[220304-56-3]
$C_{20}H_{28}O_4$ 332.439
Constit. of *Spongia matamata*. Cryst.
Mp 273-275°. $[\alpha]_D$ -379 (c, 0.63 in $CHCl_3$/MeOH). λ_{max} 220 (ϵ 13240) (MeOH).
16-Deoxy: ***15-Oxo-13-spongien-19-oic acid***
[220304-55-2]
$C_{20}H_{28}O_4$ 332.439
Constit. of *Spongia matamata*. Cryst.
Mp 280-282°. $[\alpha]_D$ -290 (c, 1 in $CHCl_3$/MeOH). λ_{max} 220 (ϵ 12800) (MeOH).

16β-*form*
Me ether: [220304-51-8]
Constit. of *Spongia matamata*.
Powder. $[\alpha]_D$ +62.5 (c, 0.16 in $CHCl_3$/MeOH). λ_{max} 220 (ϵ 3500) (MeOH).

16ξ-*form*
Spongiabutenolide B
[247115-27-1]
Constit. of a *Spongia* sp.
Solid. $[\alpha]_D$ +27.1 (c, 3.4 in MeOH). λ_{max} 209 (ϵ 8480) (MeOH).
19-Alcohol: 16,19-Dihydroxy-13-spongien-15-one. ***Spongiabutenolide D***
[247115-29-3]
$C_{20}H_{30}O_4$ 334.455
Constit. of a *Spongia* sp. Solid.
Li, C.J. *et al., J. Nat. Prod.*, 1999, **62**, 287-290 (*Spongia matamata constits*)
Mitchell, S.S. *et al., Tetrahedron*, 1999, **55**, 10887-10892 (*Spongiabutenolides*)
Hyosu, M. *et al., J. Nat. Prod.*, 2000, **63**, 422-423 (*Coscinoderma mathewsi constit*)

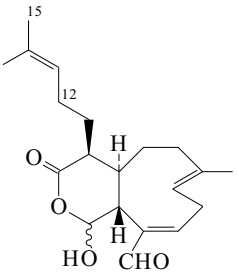
4-Hydroxy-19-oxo-1(9),6,13-xenicatrien-18,17-olide H-880



$C_{20}H_{28}O_4$ 332.439

(1(9)*E*,4*S*,6*E*,10*S*) [133585-89-4]
Constit. of *Dictyota divaricata*.
Oil. $[\alpha]_D^{25}$ -151.3 (c, 0.3 in $CHCl_3$). λ_{max} 228 (ϵ 7750) (MeOH) (Berdy).
6R,7R-Epoxide: ***6,7-Epoxy-4-hydroxy-19-oxo-1(9),13-xenicadien-18,17-olide***
[133607-86-0]
$C_{20}H_{28}O_5$ 348.438
Constit. of *Dictyota divaricata*. Oil. $[\alpha]_D^{25}$ -178.3 (c, 0.06 in $CHCl_3$).
König, G.M. *et al., Tetrahedron*, 1991, **47**, 1399-1410 (*Dictyota divaricata constits*)

18-Hydroxy-19-oxo-1(9),6,13-xenicatrien-17,18-olide H-881



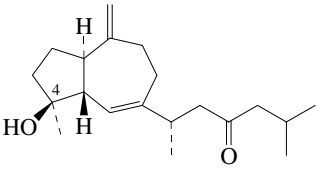
$C_{20}H_{28}O_4$ 332.439

Ac: ***18-Acetoxy-19-oxo-1(9),6,13-xenicatrien-17,18-olide***
$C_{22}H_{30}O_5$ 374.476
Constit. of *Dictyota prolificans*. Gum. $[\alpha]_D^{20}$ -299 (c, 1 in $CHCl_3$).

12,15-Didehydro, Ac: ***18-Acetoxy-19-oxo-1(9)*****E,*****6E,12E,14-xenicatetraen-17,18-olide***
$C_{22}H_{28}O_5$ 372.46
Constit. of *Dictyota prolificans*. Foam. $[\alpha]_D^{20}$ -224 (c, 1 in $CHCl_3$).

Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 121

4-Hydroxy-6,10(18)-pachydictyadien-13-one H-882



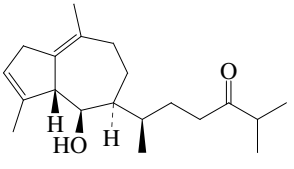
(1α,4β,5β,11α)-*form*

(1α,4β,5β,11α)-*form*
Xeniolone
[96603-00-8]
Constit. of coral *Xenia* sp.
Oil. $[\alpha]_D$ -20 ($CHCl_3$).

(1β,4α,5α,11α)-*form*
Isoxeniolone
[96603-01-9]
Constit. of *Xenia* sp.
Oil. $[\alpha]_D$ +31 ($CHCl_3$).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1309-1312 (*struct, abs config*)

6-Hydroxy-1(10),3-pachydictyadien-14-one H-883

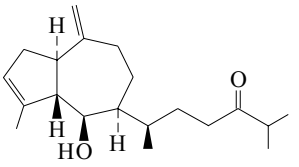


$C_{20}H_{32}O_2$ 304.472

(5β,6β,11*R*)-*form*
Acutilol B
[182284-98-6]
Constit. of *Dictyota acutiloba*.
Oil. $[\alpha]_D^{25}$ -28 (c, 0.08 in $CHCl_3$).

Hardt, I.H. *et al., Phytochemistry*, 1996, **43**, 71-73 (*isol, pmr, cmr*)

6-Hydroxy-3,10(18)-pachydictyadien-14-one H-884



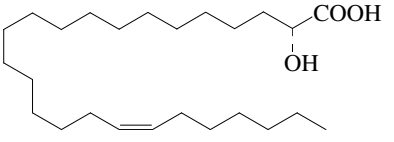
$C_{20}H_{32}O_2$ 304.472

6β-*form*
Dictyone
[84164-88-5]
Constit. of brown alga *Dictyota dichotoma*.
Oil. $[\alpha]_D^{28}$ +48.5 (c, 1.15 in $CHCl_3$).

Ac: ***Dictyone acetate***
[604806-42-0]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Cystoseira myrica* and *Dictyota dichotoma*. Oil.

Enoki, N. *et al., Chem. Lett.*, 1982, 1837
Gedara, S.R. *et al., Z. Naturforsch., C*, 2003, **58**, 17-22 (*Ac*)
Ayyad, S.-E. *et al., Z. Naturforsch., C*, 2003, **58**, 33-38 (*Ac*)

2-Hydroxy-18-pentacosenoic acid H-885



$C_{25}H_{48}O_3$ 396.652

(2*R*,18*Z*)-*form*
Me ether: 2-Methoxy-18-pentacosenoic acid
[88426-44-2]
$C_{26}H_{50}O_3$ 410.679
Constit. of the sponge *Higginsia tethyoides*.

Ayanoglu, E. *et al., Lipids*, 1983, **18**, 830-836 (*isol*)

4-Hydroxy-5,7-pentadecadiyn-2-one H-886

Montiporyne I
$H_3C(CH_2)_6C{\equiv}CC{\equiv}CCH(OH)CH_2COCH_3$
$C_{15}H_{22}O_2$ 234.338

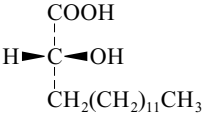
(ξ)-*form*
Isol. from the coral *Montipora* sp.
Light yellow oil. λ_{max} 256 (ϵ 691); 291 (ϵ 1116); 308 (ϵ 1068) (MeOH).

14,15-Didehydro: 4-Hydroxy-14-pentadecene-5,7-diyn-2-one. ***Montiporyne J***
$C_{15}H_{20}O_2$ 232.322
Isol. from *Montipora* sp. Light yellow oil.

Alam, N. *et al., J. Nat. Prod.*, 2001, **64**, 1059-1063

2-Hydroxypentadecanoic acid, 9CI H-887

[2507-54-2]



(*R*)–*form*

$C_{15}H_{30}O_3$ 258.4

(ξ)-*form*
Constit. of a *Pseudosuberites* sp.

Me ether: 2-Methoxypentadecanoic acid
$C_{16}H_{32}O_3$ 272.427
Isol. from the sponge *Callyspongia fallax*.

Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*Me ether*)

9-Hydroxypentadecanoic acid H-888

$H_3C(CH_2)_5CH(OH)(CH_2)_7COOH$
$C_{15}H_{30}O_3$ 258.4

Me ether: 9-Methoxypentadecanoic acid
$C_{16}H_{32}O_3$ 272.427
Constit. of the red alga *Schizymenia dubyi*.

Barnathan, G. *et al., Phytochemistry*, 1998, **47**, 761-765 (*isol, ms*)
Carballeira, N.M. *et al., Chem. Phys. Lipids*, 2003, **124**, 63-67 (*synth*)

2-Hydroxy-6-pentadecenoic acid H-889

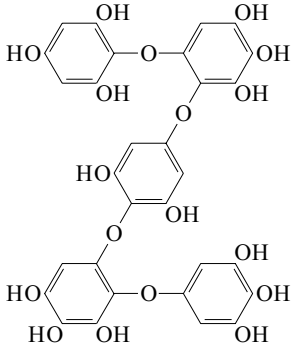
$H_3C(CH_2)_7CH{=}CH(CH_2)_3CH(OH)COOH$
$C_{15}H_{28}O_3$ 256.384

(2ξ,6*Z*)-*form*
Me ether: 2-Methoxy-6-pentadecenoic acid
$C_{16}H_{30}O_3$ 270.411
Isol. from the sponge *Callyspongia fallax*.

Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623,

Hydroxypentafuhalol A H-890

[137809-92-8]

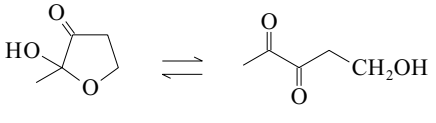


$C_{30}H_{22}O_{18}$ 670.493
Constit. of *Carpophyllum maschalocarpum*, *Carpophyllum angustifolium* and *Sargassum spinuligerum*.

Glombitza, K.-W. *et al., Phytochemistry*, 1991, **30**, 2741-2745; 1995, **38**, 975-985 (*isol, pmr*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

5-Hydroxy-2,3-pentanedione H-891

*4,5-Dihydro-2-hydroxy-2-methyl-3(2*H*)-furanone.* ***Laurencione***
[142937-56-2]
[148159-54-0]



$C_5H_8O_3$ 116.116
Equilib. mixt. (87:13) of the cyclic hemiacetal and open-chain forms. Constit. of *Laurencia spectabilis*. Light green oil.

Bernart, M.W. *et al., Phytochemistry*, 1992, **31**, 1273-1276 (*isol, pmr, cmr*)
De Kimpe, N. *et al., J.O.C.*, 1995, **60**, 5262 (*synth*)
De Kimpe, N. *et al., Synthesis*, 1996, 1131-1134 (*synth*)
Wolf, E. *et al., Can. J. Chem.*, 1997, **75**, 942-948 (*synth, pmr, cmr*)
Aelterman, W. *et al., J. Nat. Prod.*, 1997, **60**, 385-386 (*synth*)
Putra, S.R. *et al., Tet. Lett.*, 1998, **39**, 6185-6188 (*biosynth*)

3-Hydroxypentanoic acid, 9CI H-892

3-Hydroxyvaleric acid
[10237-77-1]

$C_5H_{10}O_3$ 118.132

(*R*)-*form* [53538-53-7]
Constit. of the sponge *Carteriospongia* sp.
Oil. Insol. CS_2, petrol.
Mp 30-31°. $Bp_{0.08}$ 89-90°. $[\alpha]_D^{25}$ -37.6 (c, 1.25 in $CHCl_3$).

Me ester: [60793-22-8]
$C_6H_{12}O_3$ 132.159
d_4^{23} 1.03. Bp_{20} 84°. $[\alpha]_D^{23}$ -18.8 (neat).

Et ester: [73143-60-9]
$C_7H_{14}O_3$ 146.186
Oil. $[\alpha]_D^{20}$ -15.6 (Et_2O).

Nitrile:
C_5H_9NO 99.132
Oil. Bp_{18} 110-112°. $[\alpha]_D^{20}$ +10 (Et_2O).

(*S*)-*form* [79516-59-9]
$[\alpha]_D^{23}$ +2.3.

Me ester: [42558-50-9] Bp_{17} 81°. $[\alpha]_D^{20}$ +18.6 (neat).

(±)-*form* [42482-20-2]
Mp 43-44°.

Et ester: [54074-85-0] Bp_{10} 83-85°.

Amide: [155053-71-7]
$C_5H_{11}NO_2$ 117.147
Mp 53-53.5°.

Levene, P.A. *et al., J. Biol. Chem.*, 1928, **76**, 415 (*synth*)
Adickes, F. *et al., Annalen*, 1943, **555**, 41 (*synth*)
Serck-Hanssen, K. *et al., Ark. Kemi*, 1956, **10**, 135 (*abs config*)
Vinital, L. *et al., Helv. Chim. Acta*, 1974, **57**, 1713 (*pmr*)
Seebach, D. *et al., Annalen*, 1976, 1357-1369 (*R-form, Me ester*)
Seebach, D. *et al., Tet. Lett.*, 1984, **25**, 2747 (*deriv, synth, pmr*)
Mori, K. *et al., Tetrahedron*, 1985, **41**, 919 (*deriv, synth*)
Mohr, P. *et al., Helv. Chim. Acta*, 1987, **70**, 142 (*synth, ir, pmr, ester*)
Zimmerman, J. *et al., Helv. Chim. Acta*, 1987, **70**, 1104 (*synth, ir, pmr, cmr, ms*)
Koenig, G.M. *et al., Planta Med.*, 1999, **65**, 679-680 (*isol*)
Hann, E.C. *et al., Adv. Synth. Catal.*, 2003, **345**, 775-782 (*synth, pmr, cmr, ms, amide*)

43-Hydroxy-2,44-pentatetracontapentaenediynoic acid H-893

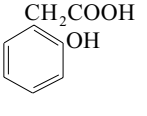
$C_{45}H_{72}O_3$ 661.062

Me ester: ***Petroformyne B***
[128646-24-2]
$C_{46}H_{74}O_8$ 755.086
Constit. of the sponge *Petrosia ficiformis*. Toxic to brine shrimp. Posn. of ethylenic groups not determined. λ_{max} 245 (ε 4500) (MeOH) (Berdy).

Cimino, G. *et al., J. Nat. Prod.*, 1990, **53**, 345-353 (*isol*)

2-Hydroxyphenylacetic acid H-894

2-Hydroxybenzeneacetic acid, 9CI. o-*Hydroxy-α-toluic acid*
[614-75-5]



$C_8H_8O_3$ 152.149
Isol. from leaves of *Astilbe* spp. Prod. by some microorganisms. Needles (Et_2O), prisms ($CHCl_3$).
Mp 147-149°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 151D; 152B; 430B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1004A; 1005B; 1488C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1320A (*ir*)
Pschorr, R. *et al., Annalen*, 1910, **373**, 76 (*synth*)
Kindl, H. *et al., Nature (London)*, 1962, **194**, 579 (*isol*)
Shapiro, B.L. *et al., J. Phys. Chem. Ref. Data*, 1977, **6**, 919 (*nmr*)
Maissant, J.M. *et al., J. Mol. Catal.*, 1980, **9**, 237 (*synth*)
Wahlund, K.G. *et al., J. Liq. Chromatogr.*, 1981, **4**, 309 (*chromatog*)

4-Hydroxyphenylacetic acid H-895

4-Hydroxybenzeneacetic acid, 9CI. p-*Hydroxy-α-toluic acid*
[156-38-7]
$C_8H_8O_3$ 152.149
Constit. of sweet clover (*Melilotus officinalis*) and also from seeds of *Taraxacum officinale* yeast, wool and other biol. sources. Needles (H_2O). Sol. EtOH, Et_2O, hot H_2O.
Mp 148-150°. pK_a 4.59 (10% EtOH aq.).

▶ AI2680000

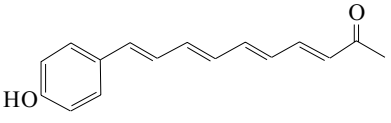
Amide: p-*Hydroxyphenylacetamide*
[17194-82-0]
$C_8H_9NO_2$ 151.165
Isol. from the sponge *Suberites tylobtusa*. Prod. by *Cytophaga marinoflava* sp. AM13.1. Antitumour agent. Leaflets (H_2O). Mp 175°.

▶ AC3851500

Li, S. *et al., CA*, 1984, **100**, 117826y (*amide, nitrile*)
Strauss, C.R. *et al., Org. Prep. Proced. Int.*, 1995, **27**, 552-555 (*amides*)
Kumar, A. *et al., Synth. Commun.*, 1997, **27**, 1133-1141 (*synth, amide*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*Cytophaga, amide*)

10-(4-Hydroxyphenyl)-3,5,7,9-decatetraen-2-one H-896

4-(9-Oxo-1,3,5,7-decatetraenyl)phenol



$C_{16}H_{16}O_2$ 240.301

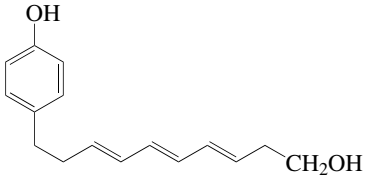
(all-E)-form
Navenone C
[62695-69-6]
Pheromone from *Navanax inermis*. Not obt. pure. λ_{max} 412 (ε 11400) (MeOH) (Berdy). λ_{max} 432 (ε 12500) (MeOH-NaOH) (Berdy).

Ac: [62695-72-1]
Cryst. (C_6H_6). Mp 135-137°.

Sleeper, H.L. *et al., J.A.C.S.*, 1977, **99**, 2367-2368 (*isol*)
Soullez, D. *et al., Nat. Prod. Lett.*, 1994, **4**, 203 (*synth*)

10-(4-Hydroxyphenyl)-3,5,7-decatrien-1-ol H-897

4-(10-Hydroxy-3,5,7-decatrienyl)phenol



$C_{16}H_{20}O_2$ 244.333

(all-E)-form

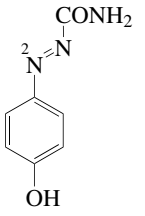
1-Ac: 4-(10-Acetoxy-3,5,7-decatrienyl)phenol
[206666-56-0]
$C_{18}H_{22}O_3$ 286.37
Alarm pheromone of marine mollusc *Haminoea callidegenita*.

Di-Ac: 1-Acetoxy-4-(10-acetoxy-3,5,7-decatrienyl)benzene
[206666-55-9]
$C_{20}H_{24}O_4$ 328.407
Alarm pheromone of *Haminoea callidegenita*.

Spinella, A. *et al., Tet. Lett.*, 1998, **39**, 2005-2008 (*isol, pmr, cmr*)
Izzo, I. *et al., Tet. Lett.*, 2000, **41**, 3975-3978 (*synth*)

2-(4-Hydroxyphenyl)diazenecarboxamide, 9CI H-898

4-Hydroxyphenyl-1-azoformamide



$C_7H_7N_3O_2$ 165.151

(E)-form [193888-34-5]
Isol. from *Calvatia craniformis*. Yellow needles. Mp 177-179°. λ_{max} 242 (log ε 4.12); 342 (log ε 4.27) (MeOH).

N^2-*Oxide: 4-Hydroxyphenyl-1*-ONN-*azoxyformamide*
[193888-36-7]
$C_7H_7N_3O_3$ 181.151
Isol. from *Calvatia craniformis*. Yellow needles. Mp 156-158°. λ_{max} 227 (log ε 4.19); 302 (log ε 4.25) (MeOH).

4′-Me ether: 2-(4-Methoxyphenyl)diazenecarboxamide, 9CI. 4-Methoxyphenyl-1-azoformamide. ***Antibiotic FL 142IIB****. FL 142IIB*
[193888-35-6]
[87699-29-4]
$C_8H_9N_3O_2$ 179.178
Isol. from *Calvatia craniformis* and *Lycoperdon pyriforme*. Antiparasitic, nematocide. Orange needles. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 156-158°. λ_{max} 238 (log ε 4.13); 334 (log ε 4.24) (MeOH).

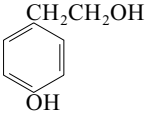
4′-Me ether, N^2*-oxide: 4-Methoxyphenyl-1*-ONN-*azoxyformamide.* ***Antibiotic FL 142IIA****. FL 142IIA*
[193888-37-8]
[87699-28-3]
$C_8H_9N_3O_3$ 195.177
Isol. from *Calvatia craniformis* and *Lycoperdon pyriforme*. Antiparasitic, nematocide. Yellow needles. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 196-198°. λ_{max} 227 (log ε 4.27); 298 (log ε 4.33) (MeOH).

3′,5′-Dichloro, Me-ether, N^2*-oxide: 3,5-Dichloro-4-methoxyphenyl-1*-ONN-*azoxyformamide*
[229334-15-0]
$C_8H_7Cl_2N_3O_3$ 264.067
Isol. from *Lycoperdon pyriforme*. Cytotoxic.

Okuda, T. *et al., CA*, 1983, **99**, 191453b (*isol*)
Takaishi, Y. *et al., Phytochemistry*, 1997, **45**, 997-1001 (*isol, uv, ir, pmr, cmr, ms*)
Köpcke, B. *et al., Nat. Prod. Lett.*, 1999, **13**, 41-46 (*Dichloromethoxyphenylazoxyformamide*)

2-(4-Hydroxyphenyl)ethanol H-899

4-Hydroxybenzeneethanol, 9CI. p-*Hydroxyphenethyl alcohol. Salidrosol. Tyrosol*
[501-94-0]



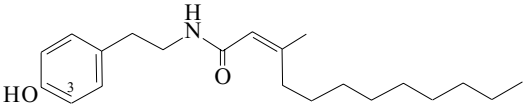
$C_8H_{10}O_2$ 138.166
Prod. by several *Ceratocystis* spp. Isol. from leaves of *Ligustrum ovalifolium* and bark of *Fraxinus excelsior*. Prod. by *Gibberella*

fujikuroi and by the marine strain *Bacillus subtilis* KMM3427 associated with sea sponge *Verongia* sp. Also isol. from peanuts. Needles ($CHCl_3$). Sol. H_2O, EtOH, Et_2O, Me_2CO; spar. sol. petrol. Mp 85-86°.

Ivanova, E.P. *et al., CA*, 2001, **134**, 190470 (*marine isolate*)

N-[2-(4-Hydroxyphenyl)ethyl]-3-methyl-2-dodecenamide, 9CI H-900

3-Methyl-2-dodecenoic acid p-*hydroxyphenethylamide*



(Z)–*form*

$C_{21}H_{33}NO_2$ 331.497

(*E*)-*form* [75513-93-8] Synthetic.
Pale yellow oil which rapidly darkens and slowly solidifies on prolonged storage.

(*Z*)-*form* [75513-94-9]
Isol. from the soft coral *Sinularia flexibilis*. Shows antiinflammatory, cytotoxic and cardiotoxic activities. Sol. MeOH, CH_2Cl_2; poorly sol. H_2O. Mp 70-72°. λ_{max} 278 (ϵ 2860) (MeOH) (Derep).

Me ether, 3-hydroxy: **N-*[2-(3-Hydroxy-4-methoxyphenyl)ethyl]-3-methyl-2-dodecenamide, 9CI***
[75513-96-1]
$C_{22}H_{35}NO_3$ 361.523
Isol. from *Sinularia flexibilis*. Shows antiinflammatory and cardiotoxic props. Oil which slowly solidifies. Sol. MeOH, CH_2Cl_2; poorly sol. H_2O. λ_{max} 280 (ϵ 3400); 287 (sh) (MeOH) (Derep).

3-Methoxy: **N-*[2-(4-Hydroxy-3-methoxyphenyl)ethyl]-3-methyl-2-dodecenamide, 9CI***
[75513-95-0]
$C_{22}H_{35}NO_3$ 361.523
Isol. from *Sinularia flexibilis*. Shows antiinflammatory and cardiotoxic props. Oil which slowly solidifies. Sol. MeOH, CH_2Cl_2; poorly sol. H_2O. λ_{max} 280 (ϵ 3400); 287 (sh) (MeOH) (Derep).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1980, **33**, 1799 (*isol, uv, ir, pmr, cmr, ms, struct, synth*)
Sheu, J.-H. *et al., J. Chin. Chem. Soc. (Taipei)*, 1999, **46**, 253-257 (*isol, activity*)

3-Hydroxy-7-phenyl-4,6-heptadienoic acid H-901

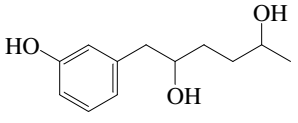
PhCH=CHCH=CHCH(OH)CH_2COOH

$C_{13}H_{14}O_3$ 218.252

(+)-(*E,E*)-*form* [156699-88-6]
Isol. from the ascidian *Didemnum granulatum*.
Unstable yellow-brown solid. $[\alpha]_D$ +5 (c, 0.5 in MeOH).
Isaacs, S. *et al., J. Nat. Prod.*, 1994, **57**, 648-649 (*isol, pmr, cmr*)

1-(3-Hydroxyphenyl)-2,5-hexanediol H-902

3-(2,5-Dihydroxyhexyl)phenol
[862694-07-3]

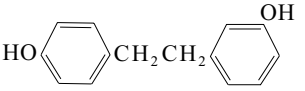


$C_{12}H_{18}O_3$ 210.272
Constit. of the stems of the mangrove *Bruguiera gymnorrhiza*. Amorph. solid. $[\alpha]_D$ -5.7 (c, 0.4 in MeOH). λ_{max} 275 (log ϵ 3.17) (MeOH). λ_{max} 290 (log ϵ 3.34) (MeOH/NaOH). λ_{max} 275 (log ϵ 3.06) (MeOH/HCl).

Han, L. *et al., Planta Med.*, 2005, **71**, 160-164 (*isol, uv, pmr, cmr*)

1-(3-Hydroxyphenyl)-2-(4-hydroxyphenyl)ethane H-903

3-[2-(4-Hydroxyphenyl)ethyl]phenol, 9CI. 3,4′-Dihydroxybibenzyl. 3,4′-Ethylenebisphenol. ***Lunularin***
[37116-80-6]



$C_{14}H_{14}O_2$ 214.263
Isol. from *Marchantia polymorpha*, *Morus laevigata*, liverwort *Lunularia cruciata*, *Ulva lactuca* and green alga *Chlorella* sp. Needles (C_6H_6). Mp 108.5-109°.

Di-Ac:
Prisms (MeOH). Mp 67-68°.

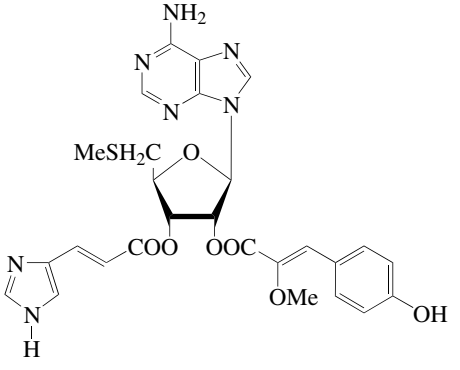
3-Me ether: 4-[2-(3-Methoxyphenyl)ethyl]phenol. 4′-Hydroxy-3-methoxybibenzyl
[59586-27-5]
$C_{15}H_{16}O_2$ 228.29
Constit. of *Frullania* spp., *Plagiochila stephensoniana* and *Radula frondescens*. Shows antibacterial and antifungal activities. Oil.

4′-Me ether: 1-(3-Hydroxyphenyl)-2-(4-methoxyphenyl)ethane. 3-Hydroxy-4′-methoxybibenzyl
[65819-30-9]
$C_{15}H_{16}O_2$ 228.29
Constit. of *Frullania davurica*. Mp 67-68°.

Di-Me ether: 1-(3-Methoxyphenyl)-2-(4-methoxyphenyl)ethane. 3,4′-Dimethoxybibenzyl
[52528-97-9]
$C_{16}H_{18}O_2$ 242.317
Constit. of *Frullania* spp., *Plagiochila* sp. and *Radula* sp. Platelets (petrol). Mp 33-34.5°.

Pryce, R.J. *et al., Phytochemistry*, 1972, **11**, 1355 (*biosynth*)
Hopkins, B.J. *et al., J.C.S. Perkin 1*, 1974, 32 (*isol, synth*)
Deshpande, V.H. *et al., Indian J. Chem.*, 1975, **13**, 453 (*isol*)
Huneck, S. *et al., Tetrahedron*, 1976, **32**, 109 (*synth*)
Gorham, J. *et al., Phytochemistry*, 1977, **16**, 249 (*isol*)
Asakawa, Y. *et al., Phytochemistry*, 1981, **20**, 2187; 1982, **21**, 2481; 2663; 1987, **26**, 1023; 1117; 1988, **27**, 1797 (*derivs*)
Lorimer, S.D. *et al., J. Nat. Prod.*, 1993, **56**, 1444 (*4-Hydroxy-3′-methoxybibenzyl*)
Bracher, F. *et al., Nat. Prod. Lett.*, 2000, **14**, 305-310 (*synth*)

2′-*O*-[3-(4-Hydroxyphenyl)-2-methoxypropenoyl]-3′-*O*-[3-(1*H*-imidazol-4-yl)propenoyl]-*S*-methyl-5′-thioadenosine H-904



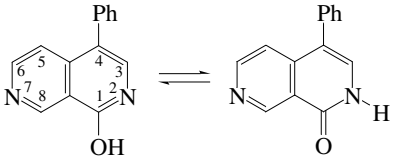
$C_{27}H_{27}N_7O_7S$ 593.619
Isol. from the ascidian *Atriolum robustum*. Amorph. solid. $[\alpha]_D^{24}$ -115 (c, 0.18 in MeOH). λ_{max} 293 (ϵ 44800) (MeOH).

S-*Oxide:*
$C_{27}H_{27}N_7O_8S$ 609.618
Isol. from *Atriolum robustum*. Amorph. solid. $[\alpha]_D^{24}$ -124.1 (c, 0.08 in MeOH). λ_{max} 288 (ϵ 44000) (MeOH).

Kehraus, S. *et al., J. Med. Chem.*, 2004, **47**, 2243-2255 (*isol, pmr, cmr, ms*)

1-Hydroxy-4-phenyl-2,7-naphthyridine H-905

4-Phenyl-2,7-naphthyridin-1(2H)-one, 9CI. ***Lophocladine A***



$C_{14}H_{10}N_2O$ 222.246

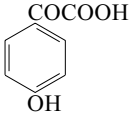
Alkaloid from *Lophocladia* sp. Displays affinity for NMDA receptors. δ-Opioid receptor antagonist. Needles (DMSO). Mp 211-213°. λ_{max} 224 (log ϵ 4.06); 250 (log ϵ 4.03); 314 (log ϵ 3.88) (MeOH).

Gross, H. *et al., J. Nat. Prod.*, 2006, **69**, 640-644 (*isol, pmr, cmr, ms*)

2-(4-Hydroxyphenyl)-2-oxoacetic acid H-906

4-Hydroxy-α-oxobenzeneacetic acid, 9CI. p-*Hydroxyphenylglyoxylic acid, 8CI. 4-Hydroxybenzoylformic acid.* ***Pisolithin A***

[15573-67-8]



$C_8H_6O_4$ 166.133

Metab. of the fungus *Pisolithus tinctorius*. Needles (Et_2O/C_6H_6/petrol). Mp 177.5-178°. λ_{max} 206; 226; 296 (HCl) (Berdy). λ_{max} 240; 334 (NaOH) (Berdy).

Oxime:
$C_8H_7NO_4$ 181.148
Mp 145-146°.

Me ester: [38250-16-7]
$C_9H_8O_4$ 180.16
Oil.

Et ester: [70080-54-5]
$C_{10}H_{10}O_4$ 194.187
Mp *ca.* 60°.

Me ether: 4-Methoxy-α-oxobenzeneacetic acid. Anisoylformic acid
[7099-91-4]
$C_9H_8O_4$ 180.16
Needles (C_6H_6). Mp 93°.

Me ether, oxime:
$C_9H_9NO_4$ 195.174
Mp 145-146°.

Me ether, Me ester: Methyl 2-(4-methoxyphenyl)-2-oxoacetate. Methyl anisoylformate. Methyl (4-methoxyphenyl)glyoxylate
[32766-61-3]
$C_{10}H_{10}O_4$ 194.187
Isol. from *Polycarpa aurata*. Amorph. solid.
Mp 55°. λ_{max} 226 (ϵ 10860); 294 (ϵ 19520) (EtOH).

Me ether, butyl ester: Butyl 2-(4-methoxyphenyl)-2-oxoacetate. Butyl anisoylformate
$C_{13}H_{16}O_4$ 236.267
Isol. from the ascidian *Polycarpa aurata*. Oil. λ_{max} 225 (ϵ 5020); 292 (ϵ 7284) (MeOH).

Me ether, amide:
$C_9H_9NO_3$ 179.175
Needles (C_6H_6). Mp 151-152°.

*Me ether, methylamide: 2-(4-Methoxyphenyl)-*N*-methyl-2-oxoacetamide*
$C_{10}H_{11}NO_3$ 193.202
Isol. from the ascidian *Polycarpa aurata*. Oil. λ_{max} 225 (ϵ 8738); 293 (ϵ 1675) (EtOH).

Me ether, nitrile:
$C_9H_7NO_2$ 161.16
Mp 63-64°.

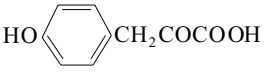
[54537-30-3]

Mauthner, F. *et al., Ber.*, 1909, **42**, 188
Vorländer, D. *et al., Ber.*, 1911, **44**, 2455
Sprenger, R.D. *et al., J.A.C.S.*, 1950, **72**, 2874
Rai, M. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 169 (*synth*)
Barnish, I.T. *et al., J. Med. Chem.*, 1981, **24**, 399 (*synth*)
Matsuki, Y. *et al., Chem. Pharm. Bull.*, 1982, **30**, 196 (*synth*)
Tsantrizos, Y.S. *et al., Phytochemistry*, 1991, **30**, 1113 (*isol*)
Abas, S.A. *et al., J.O.C.*, 1996, **61**, 2709-2712 (*Me ether Me ester*)
Wessels, M. *et al., J. Nat. Prod.*, 2001, **64**, 1556-1558 (*Me ether derivs*)
Chen, Y.T. *et al., J. Med. Chem.*, 2002, **45**, 3946-3952 (*synth, Me ester, pmr, cmr*)

3-(4-Hydroxyphenyl)-2-oxopropanoic acid H-907

2-Hydroxy-3-(4-hydroxyphenyl)-2-propenoic acid. 4-Hydroxy-α-oxobenzenepropanoic acid. 4-Hydroxyphenylpyruvic acid

[156-39-8]



$C_9H_8O_4$ 180.16

Exhibits keto-enol tautom. Enol form predominates. Constit. of *Erythraea centaurium* (preferred genus name *Centaurium*), *Euphrasia rostkoviana*, *Lysimachia nummularia*, *Phlox* spp. and *Thuja plicata*. Prod. by *Aerobacter aerogenes*. Isol. from the red alga *Ceratodictyon spongiosum* and its sponge symbiont *Haliclona cymaeformis*. Biosynthetic intermed. for aromatic compds. Enzyme substrate. Cryst. (H_2O).
Mp 220° dec. (212-214°). Rapidly oxidised in alkaline soln.

4-Sulfate: 4-Sulfooxyphenylpyruvic acid
$C_9H_8O_7S$ 260.224
Constit. of the alga *Ceratodictyon spongiosum* and its sponge symbiont *Haliclona cymaeformis*. Amorph. solid. λ_{max} 208 (log ϵ 3.6); 220 (log ϵ 3.6); 298 (log ϵ 3.8) (MeOH).

Oxime: 4-Hydroxy-α-(hydroxyimino)benzenepropanoic acid, 9CI
[56401-28-6]
$C_9H_9NO_4$ 195.174
Dehydroaminoacid from the sponge *Hymeniacidon sanguinea*. Cryst.
Mp 168-169°.

Phenylhydrazone: Mp 161-162°.

Me ester:
[214534-53-9, 214534-54-0]
$C_{10}H_{10}O_4$ 194.187
Constit. of the green alga *Caulerpa taxifolia*. Isol. as a mixt. of *E*/*Z*-enol isomers (*Z*-predominant).

Me ester, oxime:
Cryst. ($CHCl_3$). Mp 135.5-137°.

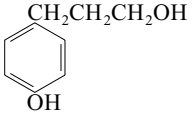
4-Me ether: 4-Methoxy-α-oxobenzenepropanoic acid. 4-Methoxyphenylpyruvic acid
[28030-16-2]
$C_{10}H_{10}O_4$ 194.187
Mp 194° dec. (190° dec.).

[114-75-0, 10589-28-3, 126585-59-9]

Gaudruy, R. *et al., Can. J. Chem.*, 1951, **29**, 427 (*synth*)
Org. Synth., 1963, **43**, 49
Brandner, G. *et al., Acta Chem. Scand.*, 1964, **18**, 574 (*isol*)
Org. Synth., Coll. Vol., 5, 1973, 627 (*synth, bibl*)
Cimino, G. *et al., Experientia*, 1975, **31**, 756 (*isol, struct, uv, pmr*)
Forrester, A.R. *et al., J.C.S. Perkin 1*, 1975, 2340 (*synth*)
Moeller, B.L. *et al., Acta Chem. Scand., Ser. B*, 1977, **31**, 343 (*synth, pmr*)
Moeller, B.L. *et al., CA*, 1980, **93**, 65114e (*ms*)
Klein, C. *et al., Annalen*, 1983, 1638 (*synth*)
Luczak, S. *et al., Acta Pol. Pharm.*, 1989, **46**, 381 (*isol*)
Hanai, K. *et al., J. Phys. Chem.*, 1989, **93**, 6013 (*ir, Raman, tautom*)
Simchen, G. *et al., Synthesis*, 1989, 945 (*deriv*)
Mancini, I. *et al., Helv. Chim. Acta*, 1998, **81**, 1681-1691 (*Me ester*)
Bugni, T.S. *et al., Phytochemistry*, 2002, **60**, 361-363 (*isol, pmr, cmr, 4-sulfate*)

3-(4-Hydroxyphenyl)-1-propanol H-908

4-Hydroxybenzenepropanol, 9CI. 4-γ-Hydroxypropylphenol. 4-(3-Hydroxypropyl)phenol. Dihydro-p-*coumaroyl alcohol*
[10210-17-0]



$C_9H_{12}O_2$ 152.193
Constit. of *Fucus vesiculosus*, *Pinus sylvestris* (Scotch pine), *Taxus baccata* and *Zanthoxylum cuspidatum*. Cryst. (Et_2O/petrol).
Mp 55°.

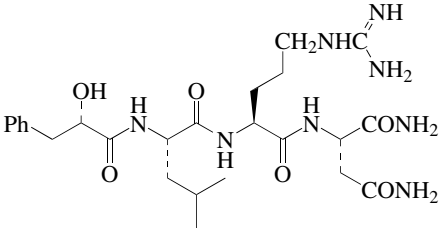
1-[3-(3,4-Dihydroxyphenyl)propanoyl]:
$C_{18}H_{20}O_5$ 316.353
Constit. of the stems of the mangrove *Lumnitzera racemosa*.
Needles (MeOH).
Mp 185°.

[125092-37-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1167A; 1167B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 409B; 409C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1086B; 1086C (*ir*)
v. Braun, J. *et al., Ber.*, 1912, **45**, 2504-2522 (*synth*)
Perold, G.W. *et al., J.C.S. Perkin 1*, 1972, 2450-2457 (*synth*)
Henley-Smith, P. *et al., J.C.S. Perkin 1*, 1980, 614-622 (*synth*)
Hori, M. *et al., J.O.C.*, 1998, **63**, 889-894 (*synth, pmr*)
Anjaneyulu, A.S.R. *et al., ARKIVOC*, 2003, **iii**, 25-30 (*3,4-dihydroxyphenylpropanoate*)

N-(2-Hydroxy-3-phenylpropanoyl)leucylarginylaspartamide H-909

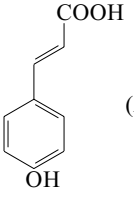
3-Phenyllactoylleucylarginylaspartamide. ***Antho-RN amide***
[129536-35-2]



$C_{25}H_{40}N_8O_6$ 548.641
Neuropeptide. Isol. from the sea anemone *Anthopleura elegantissima*. Neurotransmitter. Muscle excitatory agent.
Grimmelikhuijzen, C.J.P. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1990, **87**, 5410-5414 (*isol, struct*)

3-(4-Hydroxyphenyl)-2-propenoic acid, 9CI H-910

p-*Hydroxycinnamic acid, 8CI*. p-*Hydroxyphenylacrylic acid.* **p-*Coumaric acid***. *Naringenic acid. Naringeninic acid.* p-*Cumaric acid*
[7400-08-0]



(*E*)–*form*

$C_9H_8O_3$ 164.16
▶ LD_{50} (mus, ipr) 657 mg/kg. Exp. reprod. effects. GD9094000

(*E*)-*form* [501-98-4]
Widespread in plants, e.g. peel of black cherry (*Prunus serotina*), lentil seeds and from red clover (*Trifolium pratense*) and *Daviesia latifolia*. Occurs as many glycosides. Found by Bate-Smith in 48% of investigated dicotyledonous and 55% of monocotyledonous spp. Shows cytostatic activity. Immunoactive agent, inhibitor of stilbene oxidase. Cryst. + $1H_2O$ (cold H_2O), anhyd. cryst. (hot H_2O). Sol. Et_2O, hot EtOH; spar. sol. C_6H_6; insol. petrol.
Mp 210-213°. pK_{a1} 4.64; pK_{a2} 9.45 (25°). $SOCl_2$-activated polycondensation gives the homopolyester with an all-*trans* struct. Polyesters with other hydroxy acids are also known. λ_{max} 225; 290; 310 (MeOH) (Berdy). λ_{max} 223 (ε 14450); 286 (ε 19000) (EtOH) (Berdy).
▶ GD9095000

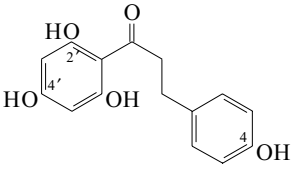
O-*Sulfate:* p-*Coumaric acid sulfate*
$C_9H_8O_6S$ 244.225
Constit. of *Zostera marina*. Marine antifouling agent.

[830-09-1, 1929-30-2, 2979-06-8, 3943-97-3, 7139-64-2, 13080-39-2, 14364-05-7, 117405-48-8, 117405-49-9, 155339-66-5, 155339-67-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 180C; 181A; 440D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1051C; 1506A (*nmr*)
Zincke, T. *et al., Annalen*, 1902, **322**, 224 (*isol*)
Ogawa, S. *et al., Bull. Chem. Soc. Jpn.*, 1927, **2**, 25 (*isol*)
Dippy, F.J.F. *et al., J.C.S.*, 1938, 357 (*synth*)
Bate-Smith, E.C. *et al., Sci. Proc. R. Dublin Soc.*, 1956, **27**, 165 (*occur*)
Bloomfield, J.J. *et al., J.O.C.*, 1961, **26**, 2991 (*synth, uv*)
U.S. Pat., 1963, 3 094 471; *CA*, **60**, 16556 (*isom*)
Cohen, M.D. *et al., J.C.S.*, 1964, 2000 (*cryst struct, deriv*)
Utsumi, H. *et al., Bull. Chem. Soc. Jpn.*, 1967, **40**, 426 (*cryst struct*)
Aulin-Erdtman, G. *et al., Acta Chem. Scand.*, 1968, **22**, 1187 (*props, uv*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, nos. 951; 953; 955 (*occur*)
Quick, J. *et al., Chem. Comm.*, 1978, 355 (*synth, isom, nmr, deriv*)
Coutrot, P. *et al., Synthesis*, 1978, 128 (*synth*)
Todd, J.S. *et al., Phytochemistry*, 1993, **34**, 401 (*sulfate*)

3-(4-Hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)-1-propanone H-911

2′,4,4′,6′-Tetrahydroxydihydrochalcone. ***Phloretin***. *Asebogenol. Dihydronarigenin. Phloretol*
[60-82-2]



$C_{15}H_{14}O_5$ 274.273
Chalcone numbering shown. Found in free state in *Helichrysum splendidum*, *Pyrus malus* and *Kalmia latifolia*. Shows antioxidant activity. Bactericidal. Inhibitor of topoisomerase II. Needles (EtOH aq.). Sol. MeOH, Me_2CO, bases; poorly sol. H_2O, Et_2O, $CHCl_3$, C_6H_6. Mp *ca.* 262-264° dec. Log P 2.07 (calc).

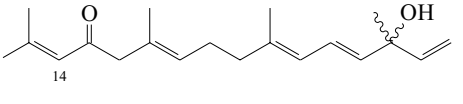
4′,6′-Di-Ac, 2′-O-β-D-glucopyranoside: ***Zosterin***
[145039-89-0]
$C_{25}H_{28}O_{12}$ 520.489
Isol. from the marine alga *Zostera* sp.

[7061-54-3]

Yang, Z. *et al., CA*, 1993, **118**, 18925v (*Zosterin*)

3-Hydroxy-1,4,6,10,14-phytapentaen-13-one H-912

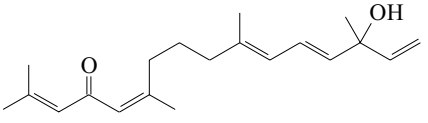
14-Hydroxy-2,6,10,14-tetramethyl-2,6,10,12,15-hexadecapentaen-4-one



$C_{20}H_{30}O_2$ 302.456

(3ξ,4*E*,6*E*,10*E*)-*form*
Styxenol A
[144101-92-8]
Constit. of *Myrmekioderma styx*.
$[\alpha]_D^{25}$ +13.4 (c, 0.091 in hexane). $[\alpha]_D$ +15.1 (CH_2Cl_2).
14,15-Dihydro: ***3-Hydroxy-1,4,6,10-phytatetraen-13-one***
[144101-94-0]
$C_{20}H_{32}O_2$ 304.472
Isol. from *Myrmekioderma styx*. $[\alpha]_D^{25}$ +12.3 (c, 0.013 in hexane). λ_{max} 241 (ϵ 21529) (EtOH) (Berdy).
Albrizio, S. *et al., J. Nat. Prod.*, 1992, **55**, 1287 (*isol, pmr, cmr*)
Sennett, S.H. *et al., J. Nat. Prod.*, 1992, **55**, 1421 (*isol, pmr, cmr*)

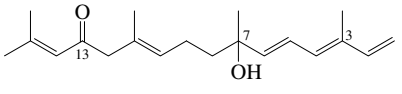
3-Hydroxy-1,4,6,11,14-phytapentaen-13-one H-913
14-Hydroxy-2,6,10,14-tetramethyl-2,5,10,12,15-hexadecapentaen-4-one



$C_{20}H_{30}O_2$ 302.456

(6*E*,6*E*,11*Z*)-*form* [144101-93-9]
Constit. of *Myrmekioderma styx*. $[\alpha]_D^{25}$ +14.2 (c, 0.007 in hexane). λ_{max} 243 (ϵ 27170) (EtOH) (Berdy).
Albrizio, S. *et al., J. Nat. Prod.*, 1992, **55**, 1287 (*isol, pmr, cmr*)

7-Hydroxy-1,3,5,10,14-phytapentaen-13-one H-914
10-Hydroxy-2,6,10,14-tetramethyl-2,6,11,13,15-hexadecapentaen-4-one, 9CI



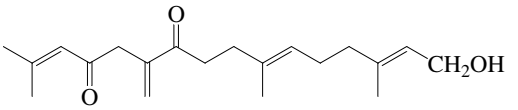
(3*E*,5*E*,10*E*)-*form*

$C_{20}H_{30}O_2$ 302.456

(3*E*,5*E*,10*E*)-*form* [68582-63-8]
Constit. of *Didiscus* sp. Oil. $[\alpha]_D^{20}$ 0.
Et ether: 7-Ethoxy-1,3,5,10,14-phytapentaen-13-one
[68582-64-9]
$C_{22}H_{34}O_2$ 330.509
Constit. of *Didiscus* sp. Oil.
13-Deoxo, Et ether: 7-Ethoxy-1,3,5,10,14-phytapentaene. 7-Ethoxy-3,7,11,15-tetramethyl-1,3,5,10,14-hexadecapentaene
[68582-65-0]
$C_{22}H_{34}O$ 314.51
Constit. of *Didiscus* sp. Oil.

(3*Z*,5*E*,10*E*)-*form* [68602-58-4]
Constit. of *Didiscus* sp.
Oil.
Et ether: [68629-49-2]
Constit. of *Didiscus* sp.
Oil.
13-Deoxy, Et ether: [68582-66-1]
Constit. of *Didiscus* sp.
Oil.
Ravi, B.N. *et al., J.O.C.*, 1979, **44**, 968

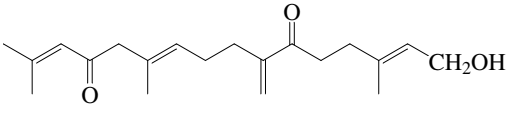
1-Hydroxy-2,6,11(18),14-phytatetraene-10,13-dione H-915
16-Hydroxy-2,10,14-trimethyl-6-methylene-2,10,14-hexadecatriene-4,7-dione



$C_{20}H_{30}O_3$ 318.455

(2*E*,6*E*)-*form* [260437-93-2]
Constit. of *Bifurcaria bifurcata*.
Ac: [260437-95-4]
Oil. λ_{max} 245 (ϵ 14000) ($CHCl_3$).
Culioli, G. *et al., Phytochemistry*, 1999, **52**, 1447-1454 (*isol, pmr, cmr*)

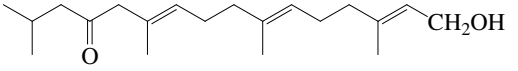
1-Hydroxy-2,7(19),10,14-phytatetraene-6,13-dione H-916
16-Hydroxy-2,6,14-trimethyl-10-methylene-2,6,14-hexadecatriene-4,11-dione



$C_{20}H_{30}O_3$ 318.455

(2*E*,10*E*)-*form* [79404-58-3]
Constit. of *Bifurcaria bifurcata*.
Culioli, G. *et al., Biochem. Syst. Ecol.*, 2000, **28**, 185-187 (*isol*)

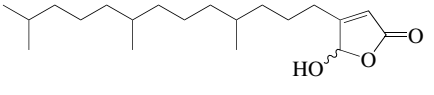
1-Hydroxy-2,6,10-phytatrien-13-one H-917
16-Hydroxy-2,6,10,14-tetramethyl-6,10,14-hexadecatrien-4-one



$C_{20}H_{34}O_2$ 306.487

(2*E*,6*E*,10*E*)-*form* [260437-92-1]
Constit. of *Bifurcaria bifurcata*.
Oil.
Culioli, G. *et al., Phytochemistry*, 1999, **52**, 1447-1454 (*isol, pmr, cmr*)

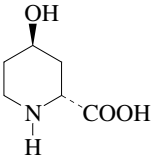
20-Hydroxy-2-phyten-1,20-olide H-918
Cacospongionolide C
[169217-40-7]



$C_{20}H_{36}O_3$ 324.503
Constit. of *Fasciospongia cavernosa*. Toxic to brine shrimp. Oil.
$[\alpha]_D$ -18 (c, 0.32 in $CHCl_3$). λ_{max} 220 (MeOH) (Berdy).
De Rosa, S. *et al., Tetrahedron*, 1995, **51**, 10731-10736 (*isol, pmr, cmr*)

4-Hydroxy-2-piperidinecarboxylic acid, 9CI H-919

4-Hydroxypipecolic acid. ***Pegaline***
[14228-16-1]



(2*R*,4*R*)-*form*

$C_6H_{11}NO_3$ 145.158

(2*R*,4*R*)-*form*
D-trans-*form*
[189385-64-6]
Gum. $[\alpha]_D^{20}$ +12.6 (c, 0.8 in H_2O).

(2*R*,4*S*)-*form*
D-cis-*form*
[175671-49-5]
Gum. $[\alpha]_D^{20}$ +19.3 (c, 0.7 in H_2O).

(2*S*,4*R*)-*form*
L-cis-*form*
Isol. from leaves of *Calliandra pittieri* and *Strophanthus scandeus.*
Cryst. + 1 or $2H_2O$ (EtOH aq.).
Mp 265° dec. $[\alpha]_D^{25}$ -23.5 (c, 1 in H_2O) (99.8% ee).

Me ester:
$C_7H_{13}NO_3$ 159.185
Beige solid (as hydrochloride). Mp 172.5-174.5° dec. (hydrochloride). $[\alpha]_D^{25}$ +9.9 (c, 1.01 in MeOH) (95.8% ee).

tert-*Butylamide:*
$C_{10}H_{20}N_2O_2$ 200.28
Solid. Mp 165.5-168°. $[\alpha]_D^{25}$ -18.5 (c, 1.02 in MeOH).

N-*Benzoyl:*
$C_{13}H_{15}NO_4$ 249.266
Mp 104° Mp 191° (dimorph.).

N-*(2,4-Dinitrophenyl):*
Yellow prisms (EtOH aq.). Mp 134°.

(2*S*,4*S*)-*form*
L-trans-*form*
[4382-31-4]
Isol. from heartwood, sapwood and leaves of *Acacia* spp. and *Armeria* spp. (Leguminosae, Plumbaginaceae).
Prisms (EtOH aq.).
Mp 294° dec. $[\alpha]_D^{20}$ -13 (c, 1 in H_2O). $[\alpha]_D^{20}$ -2.7 (c, 1 in 5*M* HCl).

Hydrochloride:
Cryst. (EtOH aq.). Mp 161-163°.

4-Sulfo: ***4-Hydroxypipecolic acid 4-sulfate***
[99694-77-6]
$C_6H_{11}NO_6S$ 225.222
Isol. from seeds of *Peltophorum africanum, Peltophorum adnatum, Peltophorum dubium, Peltophorum ferrugineum, Peltophorum inerme, Peltophorum pterocarpum* and *Peltophorum tonkinense.*
Also isol. from various sponges. Glutamate receptor agonist.
Cryst. + $1H_2O$ (H_2O).
Mp 248° dec. $[\alpha]_D^{20}$ +6.5 (H_2O).

N-*Benzoyl:*
$C_{13}H_{15}NO_4$ 249.266
Needles (EtOH aq.). Mp 174°. $[\alpha]_D^{15}$ -54 (c, 1 in EtOH).

N-*Me:* ***Ovalin***
[73710-91-5]
$C_7H_{13}NO_3$ 159.185
Obt. from seeds of *Millettia ovalifolia* (Leguminosae).
Mp 280-281°.

N-*(2,4-Dinitrophenyl):*
Orange prisms (EtOH aq.). Mp 183°.

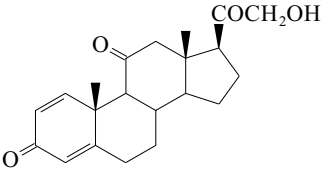
Me ether: 4-Methoxy-2-piperidinecarboxylic acid. ***4-Methoxypipecolic acid***
[135607-86-2]
$C_7H_{13}NO_3$ 159.185
Isol. from *Inga paterno* and other *Inga* spp. (Leguminosae).

(2*RS*,4*RS*)-*form*
(±)-trans-*form*
[143616-98-2]
Mp 161-163° (as hydrochloride). CAS no. refers to hydrochloride.

Clark-Lewis, J.W. *et al., J.C.S.*, 1961, 189 (*isol, struct*)
Shooley, J.N. *et al., Acta Chem. Scand.*, 1962, **16**, 2547 (*pmr, conformn*)
Witkop, B. *et al., J.A.C.S.*, 1964, **86**, 1844 (*synth*)
Murakoshi, I. *et al., Yakugaku Zasshi*, 1969, **89**, 1723 (*isol, struct*)
Gupta, R.K. *et al., Phytochemistry*, 1979, **18**, 2021 (*deriv*)
Callens, R.E.A. *et al., Bull. Soc. Chim. Belg.*, 1982, **91**, 713 (*synth*)
Evans, S.V. *et al., Phytochemistry*, 1985, **24**, 2593-2596 (*4-sulfate*)
Morton, T.C. *et al., Phytochemistry*, 1991, **30**, 2397 (*4-methoxypipecolic acid*)
Pellicciari, R. *et al., Med. Chem. Res.*, 1992, **2**, 491 (*synth, sulfate*)
Gillard, J. *et al., J.O.C.*, 1996, **61**, 2226 (*2S,4R-form, synth, ir, pmr, cmr, bibl*)
Di Nardo, C. *et al., J.O.C.*, 1999, **64**, 6119-6125 (*synth*)
Haddad, M. *et al., Tetrahedron: Asymmetry*, 1999, 4231-4237 (*2S,4R-form, synth, pmr, cmr*)
Davis, F.A. *et al., Synthesis*, 2000, 2106-2112 (*isomers, synth*)
Brooks, C.A. *et al., Tet. Lett.*, 2000, **41**, 3551-3553 (*synth*)
Agami, C. *et al., Eur. J. Org. Chem.*, 2001, 2385-2389 (*2S,4R-form, synth, pmr, cmr*)
Lloyd, R.C. *et al., Org. Process Res. Dev.*, 2002, **66**, 762-766 (*isomers, synth, pmr, cmr*)
Sakai, R. *et al., J. Nat. Prod.*, 2003, **66**, 784-787 (*4-sulfate, isol, pmr, cmr, activity*)

21-Hydroxypregna-1,4-diene-3,11,20-trione H-920

[67067-81-6]



$C_{21}H_{26}O_4$ 342.434
Isol. from bile of *Raja* sp. (skate). Cryst.
Mp 220-220° dec.

Truscott, S. *et al., Steroids*, 1978, **31**, 573

11-Hydroxypregna-4,20-dien-3-one H-921

$C_{21}H_{30}O_2$ 314.467

11α-*form* [70165-45-6]
Cryst. (MeOH aq.). Mp 156-158°. $[\alpha]_D$ +59 ($CHCl_3$).

Ac: 11α-Acetoxypregna-4,20-dien-3-one
[70165-44-5]
$C_{23}H_{32}O_3$ 356.504
Constit. of *Eunicella cavolini*. Oil. $[\alpha]_D$ +30 ($CHCl_3$).

Cimino, G. *et al., Experientia*, 1979, **35**, 298

3-Hydroxypregnan-20-one, 9CI H-922

[4406-35-3]

$C_{21}H_{34}O_2$ 318.498
λ_{max} 262 (ε 4626); 269 (ε 4064); 303 (ε 8853) (EtOH) (Berdy).

(3β,5α)-*form* [516-55-2]
Isol. from Black Sea sponges *Haliclona* spp.
Cryst. (Me_2CO/hexane) or needles (C_6H_6).
Mp 194.5°. $[\alpha]_D^{30}$ +87 (c, 1 in $CHCl_3$).

▶ TU4383200

[1491-77-6, 4469-03-8, 21788-58-9, 26961-00-2, 58701-70-5]

Jones, R.N. *et al., J.A.C.S.*, 1958, **80**, 6121 (*ir*)
Friedland, S.S. *et al., Anal. Chem.*, 1959, **31**, 169 (*ms*)
Rubin, M.B. *et al., J.O.C.*, 1964, **29**, 1932 (*synth*)
Mitsuhashi, H. *et al., Steroids*, 1964, **4**, 483 (*synth*)
Bach, G. *et al., Can. J. Chem.*, 1968, **46**, 733 (*synth, ir*)
Crabbé, P. *et al., J.O.C.*, 1972, **37**, 4003; 1973, **38**, 1478 (*synth, ir, 3β5α-form*)
Leibfritz, D. *et al., J.A.C.S.*, 1973, **95**, 4996 (*cmr*)
Kim, D.J. *et al., Can. J. Chem.*, 1976, **54**, 3776 (*cmr*)
Cheng, M.T. *et al., J.A.C.S.*, 1983, **105**, 1510 (*ms*)
Elenkov, I. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1999, **123**, 357-360 (*isol*)

12-Hydroxypregna-2,7,16-trien-20-one H-923

$C_{21}H_{28}O_2$ 312.451

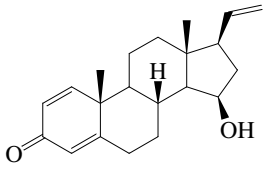
(5α,12β)-*form*
Agnatasterone A
[114318-21-7]
Constit. of *Axinella agnata*.
Cryst. (hexane).
Mp 123-124°. $[\alpha]_D^{20}$ +63.5 (c, 0.6 in $CHCl_3$).
Guella, G. *et al., Helv. Chim. Acta*, 1988, **71**, 62 (*isol, pmr, cmr*)

12-Hydroxypregna-3,7,16-trien-20-one H-924

$C_{21}H_{28}O_2$ 312.451

(5α,12β)-*form*
Agnatasterone B
[114318-22-8]
Constit. of *Axinella agnata*.
Cryst. (hexane).
Mp 104-105°. $[\alpha]_D^{20}$ +17.6 (c, 0.45 in $CHCl_3$).
Guella, G. *et al., Helv. Chim. Acta*, 1988, **71**, 62 (*isol, pmr, cmr*)

15-Hydroxypregna-1,4,20-trien-3-one H-925



$C_{21}H_{28}O_2$ 312.451

15β-*form*
Ac: [790699-24-0]
$C_{23}H_{30}O_3$ 354.488
Constit. of a *Carijoa* sp. Oil. $[\alpha]_D$ -44.7 (c, 0.9 in $CHCl_3$). λ_{max} 243 (ε 10420) (MeOH).
Ciavatta, M.L. *et al., Tet. Lett.*, 2004, **45**, 7745-7748 (*isol, pmr, cmr*)

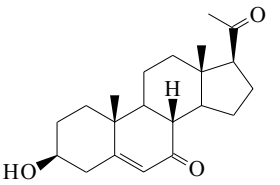
18-Hydroxypregna-1,4,20-trien-3-one H-926

[74055-43-9]

$C_{21}H_{28}O_2$ 312.451
Constit. of *Telesto riisei*. Oil.

Ac: 18-Acetoxypregna-1,4,20-trien-3-one
[74055-42-8]
$C_{23}H_{30}O_3$ 354.488
Constit. of *Telesto riisei* and a *Carijoa* sp. Oil. $[\alpha]_D$ +32.9 (c, 0.7 in $CHCl_3$). λ_{max} 243 (ε 10800) (MeOH).
Ross, R.A. *et al., Tet. Lett.*, 1979, 4701
Ciavatta, M.L. *et al., Tet. Lett.*, 2004, **45**, 7745-7748 (*Carijoa constit*)

3-Hydroxypregn-5-ene-7,20-dione, 9CI H-927

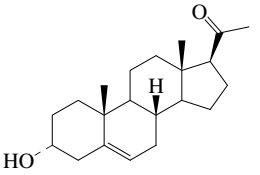


$C_{21}H_{30}O_3$ 330.466

3β-*form* [33530-84-6]
Constit. of *Stelodoryx chlorophylla*.
Mp 209-210°. $[\alpha]_D$ -45.8 (c, 0.4 in $CHCl_3$).
▶ TU5072000
Ac:
$C_{23}H_{32}O_4$ 372.503
Mp 152.5°. $[\alpha]_D^{20}$ -74.6 (c, 1.2 in $CHCl_3$).

(3β,17α)-*form* [16649-41-5]
Cryst. (MeOH). Mp 182-183°. $[\alpha]_D^{25}$ -191 (c, l in $CHCl_3$).
Ac: [16649-44-8]
Cryst. (EtOAc/hexane). Mp 217-218°.
Schenck, G.O. *et al., Annalen*, 1958, **618**, 202 (*synth, uv*)
Rubin, M.B. *et al., J.O.C.*, 1968, **33**, 2794 (*synth, uv, ir*)
De Riccardis, F. *et al., J. Nat. Prod.*, 1993, **56**, 282 (*isol, pmr, cmr, ms*)

3-Hydroxypregn-5-en-20-one H-928



(3α)-*form*

$C_{21}H_{32}O_2$ 316.483
Log P 4.03 (uncertain value) (calc).

3α-*form* [19037-28-6]
Cryst. (2,3,3-trimethylpentane). Mp 156-157°.
Ac: Mp 146-148°.
Discontinued**3β-*form***
Pregnenolone, INN. *Arthenolone. Bina-Skin. Enelone. Natolone. Pregnetan. Pregneton. Pregnolon. Prenolon. Regnosone. Sharmone. Skinostelon*
[145-13-1]
Intermed. in the biosynth. of adrenal cortical steroids and also of cardenolides. Isol. from several plant and animal spp., e.g. *Dictamnus dasycarpus*, *Damiriana hawaiiana*. Occurs in the sponge *Haliclona rubens* and the soft corals *Lobophytum* sp. and *Sarcophyton crassocaule*. Glucocorticoid used to treat rheumatoid arthritis. Cryst. (hexane/Et_2O).
Mp 192-194°. $[\alpha]_D$ +28 (EtOH).
▶ TU5560700
3-O-*Sulfate:* [1247-64-9]
[1986-28-3]
$C_{21}H_{32}O_5S$ 396.547
Constituent of human urine. Cryst. (as K or NH_4 salt).
Mp 210-212° (K salt). $[\alpha]_D^{25}$ +24.
Ac: ***Pregnenolone acetate***. *Antofin. Pregno-Pan. Previsone*
[1778-02-5]
$C_{23}H_{34}O_3$ 358.52
Glucocorticoid. Cryst. (MeOH). Mp 149-151° (145-145.5°). $[\alpha]_D$ +22 (EtOH). $[\alpha]_D^{21}$ +20.6 (c, 1.24 in EtOH). Log P 4.97 (uncertain value) (calc).
3-Carboxypropanoyl: ***Pregnenolone succinate, USAN***. *Panzalone. Formula 405*
[4598-67-8]
$C_{25}H_{36}O_5$ 416.556Log P 4.71 (uncertain value) (calc).

Me ether: 3β-Methoxypregn-5-en-20-one
[511-26-2]
$C_{22}H_{34}O_2$ 330.509
Cryst. (MeOH aq.). Mp 124-125°.

(3β,13α)-*form*
Ac: [34000-01-6]
Needles (Me_2CO/hexane). Mp 87-89°. $[\alpha]_D^{18}$ -45.5 (c, 0.09 in $CHCl_3$).

(3β,13α,17α)-*form*
Ac: [33999-94-9]
Needles (Me_2CO/hexane). Mp 116-117°. $[\alpha]_D^{10}$ -115 (c, 0.10 in $CHCl_3$).

(3β,17α)-*form* [566-63-2]
Cryst. (Me_2CO/hexane). Mp 173-174°. $[\alpha]_D^{18}$ -138 (c, 2.2 in $CHCl_3$). $[\alpha]_D^{20}$ -140.5 (EtOH).
Ac: [3915-73-9]
$C_{23}H_{34}O_3$ 358.52
Cryst. (EtOH). Mp 171°. $[\alpha]_D^{30}$ -120 (c, 1 in $CHCl_3$).
Me ether:
Cryst. (MeOH). Mp 131-132°. $[\alpha]_D^{26}$ -154 ($CHCl_3$).

[1778-02-5, 2122-98-7, 6192-84-3, 33999-97-2, 60562-58-5, 60562-60-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1051D; 1061C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 577B; 601A (*nmr*)
Butenandt, A. *et al., Ber.*, 1937, **70**, 96; 1939, **72**, 1112 (*synth, 3β,17α-form*)
Wettstein, A. *et al., Helv. Chim. Acta*, 1940, **23**, 1373 (*synth*)
Marker, R.E. *et al., J.A.C.S.*, 1940, **62**, 3349 (*synth*)
Cremlyn, R.J.W. *et al., J.C.S.*, 1953, 1847 (*synth, 3β,17α-form*)
Weinman, J. *et al., Steroids*, 1965, **6**, 683 (*synth, ir*)
U.S. Pat., 1965, 3 197 367; *CA*, **63**, 8136c (*succinate*)
Caspi, E. *et al., Experientia*, 1966, **22**, 506 (*biosynth*)
Joseph, J.P. *et al., Steroids*, 1966, **7**, 577-587 (*3-sulfates*)
Sucrow, W. *et al., Chem. Ber.*, 1967, **100**, 259 (*synth, 3β-form*)
Van Lier, J.E. *et al., J.O.C.*, 1970, **35**, 2627 (*synth, ir, 3β-form*)
Nambara, T. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1937 (*deriv*)
Jankowski, K. *et al., Steroids*, 1972, **19**, 189 (*pmr*)
Naqvi, S.H.M. *et al., Steroids*, 1973, **22**, 285 (*ms*)
Danishefsky, S. *et al., J.O.C.*, 1975, **40**, 1989 (*synth*)
Ballantine, J.A. *et al., Tet. Lett.*, 1977, 1547-1550 (*Pregnenolone, isol, Haliclona*)
Bordner, J. *et al., Cryst. Struct. Commun.*, 1978, **7**, 513 (*cryst struct*)
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476 (*isol, Damiriana*)
Terada, S. *et al., Tet. Lett.*, 1978, 1995 (*cmr*)
Brunke, E.J. *et al., Tetrahedron*, 1979, **35**, 781 (*pmr, 3α-form*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 13163
Maitra, U. *et al., Tet. Lett.*, 1986, **27**, 3087
Kirk, D.N. *et al., J.C.S. Perkin 2*, 1990, 1567 (*pmr*)
Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1992, **31**, 708-710 (*Pregnenolone, isol*)
Takeuchi, N. *et al., Chem. Pharm. Bull.*, 1993, **41**, 923-925 (*isol, pmr*)
Szendi, Z. *et al., Steroids*, 1995, **60**, 442 (*pmr, cmr*)
Ammanamanchi, S.R. *et al., J. Nat. Prod.*, 2000, **63**, 112-118 (*Pregnenolone, isol*)
Bernès, S. *et al., Acta Cryst. E*, 2003, **59**, o1372-o1375 (*cryst struct*)

20-Hydroxypregn-1-en-3-one H-929

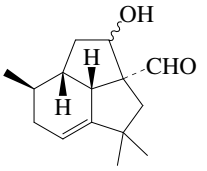
$C_{21}H_{32}O_2$ 316.483

(5α,20*R*)-*form*
5α,20β-form
Ac:
$C_{23}H_{34}O_3$ 358.52
Needles (MeOH). Mp 180-183°. $[\alpha]_D^{21}$ +75 (c, 1.034 in $CHCl_3$).

(5α,20*S*)-*form*
Ac: [813436-41-8]
Constit. of a *Scleronephthya* sp.
Cryst.
Mp 179-182°. $[\alpha]_D$ +76 (c, 0.42 in $CHCl_3$).

Schütt, W. *et al., Helv. Chim. Acta*, 1958, **41**, 1751 (*synth*)
Yan, X.-H. *et al., Youji Huaxue*, 2004, **24**, 1233-1238; *CA*, **142**, 71702 (*isol, pmr, cmr*)

15-Hydroxy-4-probotryen-14-al H-930

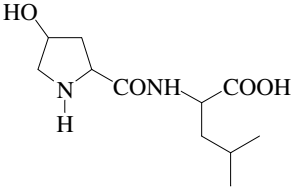


$C_{15}H_{22}O_2$ 234.338

15ξ-*form* [850715-12-7]
Metab. of a *Geniculosporium* sp. isol. from a *Polysiphonia* sp.
Gum. $[\alpha]_D^{25}$ +11.7 (c, 0.06 in CH_2Cl_2).
Krohn, K. *et al., J. Nat. Prod.*, 2005, **68**, 400-405 (*isol, pmr, cmr*)

N-(4-Hydroxyprolyl)leucine H-931

[804551-64-2]

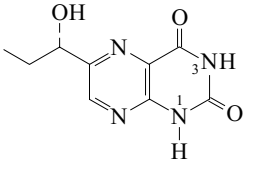


$C_{11}H_{20}N_2O_4$ 244.29
Prod. by a marine-derived *Streptomyces acrimycini*. CAS no. not found CA 140-141.

Hernandez, I.L.C. *et al., J. Braz. Chem. Soc.*, 2004, **15**, 441-444 (*isol, pmr, cmr*)

6-(1-Hydroxypropyl)lumazine H-932

*6-(1-Hydroxypropyl)-2,4(1*H*,3*H*)-pteridinedione, 9CI*



(*S*)–*form*

$C_9H_{10}N_4O_3$ 222.203

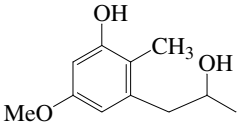
(*S*)-*form*
1-Me: 6-(1-Hydroxypropyl)-1-methyllumazine. ***Leucettidine***
[79121-29-2]
$C_{10}H_{12}N_4O_3$ 236.23
Isol. from the calcareous sponge *Leucetta microraphis*. Sol. MeOH. $[\alpha]_D^{21}$ -35.9 (c, 1.26 in MeOH). Struct. revised in 1988. λ_{max} 237 (ε 13200); 248 (sh) (ε 12000); 334 (ε 7080) (MeOH) (Derep). λ_{max} 218 (ε 10400); 245 (ε 19500); 288 (ε 2900); 343 (ε 8320) (MeOH/NaOH) (Derep).
3-Me: ***6-(1-Hydroxypropyl)-3-methyllumazine***
[155758-91-1]
$C_{10}H_{12}N_4O_3$ 236.23
Isol. from the marine polychaete *Odontosyllis undecimdonta*.
$[\alpha]_D^{25}$ -76 (c, 0.938 in MeOH) (synthetic).
1,3-Di-Me: ***6-(1-Hydroxypropyl)-1,3-dimethyllumazine***
[155758-92-2]
$C_{11}H_{14}N_4O_3$ 250.257
From *Odontosyllis undecimdonta*.
Mp 173-174° (synthetic). $[\alpha]_D$ -59.6 (c, 1.079 in MeOH) (synthetic).

(±)-*form*
Cryst.
1-Me: Mp 195°.

Cardellina, J.H. *et al., J.O.C.*, 1981, **46**, 4782-4784 (*Leucettidine, isol, uv, ir, pmr, ms*)
Pfleiderer, W. *et al., Tetrahedron*, 1988, **44**, 3373-3378 (*struct, synth, uv, pmr*)
Tanino, H. *et al., Heterocycles*, 1994, **38**, 971-974 (*Odontosyllis undecimdonta constits*)

3-(2-Hydroxypropyl)-5-methoxy-2-methylphenol H-933

3-Hydroxy-5-methoxy-α,2-dimethylbenzeneethanol, 9CI. ***Deoxyanserinone B***

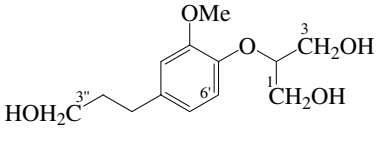


$C_{11}H_{16}O_3$ 196.246
Prod. by a mixture of strains of the marine *Penicillium corylophilum*. Not obt. pure.

Gautschi, J.T. *et al., J. Nat. Prod.*, 2004, **67**, 362-367 (*isol, pmr, cmr*)

2-[4-(3-Hydroxypropyl)-2-methoxyphenoxy]-1,3-propanediol H-934

[71046-09-8]



$C_{13}H_{20}O_5$ 256.298
Constit. of *Vitis vinifera* cv. Gewurztraminer and the bark of *Illicium difengpi*. Amorph. powder.

1-O-*β*-D-*Xylopyranoside:*
$C_{18}H_{28}O_9$ 388.414
Constit. of Scotch pine (*Pinus sylvestris*) bark. Famine food. $[\alpha]_D$ -39.1 (c, 0.7 in MeOH). λ_{max} 224; 277 (MeOH).

3″-α-L-*Rhamnopyranoside:* ***Ampelopsisrhamnoside***
[138614-65-0]
$C_{19}H_{30}O_9$ 402.441
Constit. of *Ampelopsis brevipedunculata*. Oil. $[\alpha]_D$ -18.1 (c, 0.04 in MeOH).

1-O-*β*-D-*Glucopyranoside:* [68340-35-2]
$C_{19}H_{30}O_{10}$ 418.44
Constit. of *Larix leptolepis* and in Riesling wine.

1-O-*[4-Hydroxybenzoyl-(→6)-β-D-glucopyranoside]:* [145630-97-3]
$C_{26}H_{34}O_{12}$ 538.547
Constit. of the bark of *Illicium difengpi*. Syrup. $[\alpha]_D^{20}$ -20.2 (c, 1.3 in MeOH).

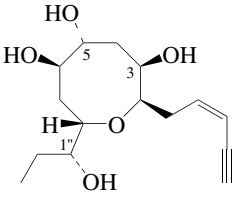
1-O-*[4-Hydroxy-3-methoxybenzoyl-(→6)-β-D-glucopyranoside]:*
$C_{27}H_{36}O_{13}$ 568.574
Constit. of the bark of *Illicium difengpi*. Syrup. $[\alpha]_D^{13}$ -18.4 (c, 0.2 in MeOH).

6′-Methoxy, 1-O-*β*-D-*glucopyranoside:* [291772-97-9]
$C_{20}H_{32}O_{11}$ 448.466
Constit. of the leaves of *Heritiera littoralis*.

Sakakibara, A. *et al., Holzforschung*, 1987, **41**, 1 (*glucoside, isol*)
Inuda, A. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2437 (*Ampelopsisrhamnoside*)
Kouno, I. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2461-2464 (*isol, pmr, cmr*)
Marinos, V.A. *et al., Phytochemistry*, 1992, **31**, 4307-4312 (*glucoside*)
Kouno, I. *et al., Phytochemistry*, 1993, **32**, 1573-1577 (*isol*)
Pan, H. *et al., Phytochemistry*, 1996, **42**, 1185-1189 (*xyloside*)
Baltenweck-Guyot, R. *et al., J. Agric. Food Chem.*, 2000, **48**, 6178-6182 (*isol, pmr, cmr, ms*)
Takeda, Y. *et al., Nat. Med. (Tokyo)*, 2000, **54**, 22-25 (*6′-methoxy 1-glucoside*)

8-(1-Hydroxypropyl)-2-(2-penten-4-ynyl)-3,5,6-oxocanetriol H-935

4,10-Epoxy-12-pentadecen-14-yne-3,6,7,9-tetrol



(1"*R*,2*R*,2'*Z*,3*R*,5*R*,6*R*,8*S*)-*form*

$C_{15}H_{24}O_5$ 284.352
Parent compd. not known.

(1″*R*,2*R*,2′*Z*,3*R*,5*R*,6*R*,8*S*)-*form*

1″,3,5-Tri-Ac: 3,7,9-Triacetoxy-4,10-epoxy-12-pentadecen-14-yn-6-ol
[157580-64-8]
$C_{21}H_{30}O_8$ 410.463
Constit. of the red alga *Laurencia* sp. cf. *Laurencia gracilis*. Cryst. Mp 132-133°. $[\alpha]_D^{25}$ +45 (c, 0.04 in $CHCl_3$).

1″,3,6-Tri-Ac: 3,6,9-Triacetoxy-4,10-epoxy-12-pentadecen-14-yn-7-ol
[157580-65-9]
$C_{21}H_{30}O_8$ 410.463
Constit. of *Laurencia* sp. cf. *Laurencia gracilis*. Oil. $[\alpha]_D^{25}$ +21 (c, 0.3 in $CHCl_3$).

Tetra-Ac: [157580-66-0]
Powder. $[\alpha]_D^{25}$ +40.3 (c, 0.4 in $CHCl_3$).

5-Deoxy, 5-chloro, tri-Ac: 7,10,13-Triacetoxy-9-chloro-6,12-epoxy-3-pentadecen-1-yne
[157580-63-7]
$C_{21}H_{29}ClO_7$ 428.909
Constit. of *Laurencia* sp. cf. *Laurencia gracilis*. Cryst. Mp 126.5-127.5°. $[\alpha]_D^{25}$ +21.1 (c, 0.2 in $CHCl_3$).

(1″ξ,2ξ,2′ξ,3ξ,5ξ,6ξ,8ξ)-*form*

1″-Ac: ***Doliculol A***
[149732-39-8]
$C_{17}H_{26}O_6$ 326.389
Isol. from the sea hare *Dolabella auricularia*. Oil. $[\alpha]_D^{26}$ +37 (c, 0.78 in $CHCl_3$). λ_{max} 223 (ϵ 10700) (MeOH) (Derep).

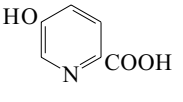
1″,3-Di-Ac: ***Doliculol B***
[149732-40-1]
$C_{19}H_{28}O_7$ 368.426
Isol. from *Dolabella auricularia*. Oil. $[\alpha]_D^{25}$ +40 (c, 0.9 in $CHCl_3$). λ_{max} 223 (ϵ 10700) (MeOH) (Derep).

Tetra-Ac:
Needles (EtOAc/hexane). Mp 154-155°. $[\alpha]_D^{20}$ +58 (c, 0.13 in $CHCl_3$).

Ojika, M. *et al., Tet. Lett.*, 1993, **34**, 3461-3462 (*Doliculols A,B*)
König, G.M. *et al., J. Nat. Prod.*, 1994, **57**, 477 (*Laurencia constitis*)

5-Hydroxy-2-pyridinecarboxylic acid, 9CI H-936

5-Hydroxypicolinic acid
[15069-92-8]



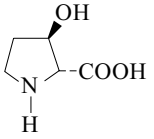
$C_6H_5NO_3$ 139.11
Detected in culture filtrate of *Nocardia* sp. Isol. from marine macrophytes. Cryst. + $1H_2O$ (H_2O) or powder. Mp 269-271° (258°). λ_{max} 250; 283 (EtOH) (Berdy). λ_{max} 252 (EtOH-HCl) (Berdy). λ_{max} 273; 303 (EtOH-NaOH) (Berdy).

Duesel, B.F. *et al., J.A.C.S.*, 1949, **71**, 1866 (*synth*)
Paulsen, H. *et al., Chem. Ber.*, 1973, **106**, 1525 (*synth*)
Entsch, B. *et al., J. Biol. Chem.*, 1976, **251**, 2550 (*biochem*)

Grachev, V.T. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1977, 2273 (*uv, ir*)
Lezina, V.P. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1980, 98; 1981, 2218 (*pmr*)
Oehlke, J. *et al., Pharmazie*, 1983, **38**, 591; 624 (*synth, derivs, ms, uv, pmr*)
Makar'eva, T.N. *et al., Khim. Prir. Soedin.*, 1989, 140-141; *Chem. Nat. Compd. (Engl. Transl.)*, 1989, **25**, 125-126 (*isol*)

3-Hydroxy-2-pyrrolidinecarboxylic acid H-937

3-Hydroxyproline, 9CI



(2*R*,3*R*)–*form*

$C_5H_9NO_3$ 131.131

(2*R*,3*R*)-*form*
D-trans-*form*
[119677-21-3]
Powder (EtOH aq.). Mp 229-236° dec. $[\alpha]_D^{20}$ +18.4 (c, 1.2 in H_2O).

(2*R*,3*S*)-*form*
D-cis-*form*
[118492-86-7]
Cryst. (H_2O). Mp 240-255° dec. $[\alpha]_D$ +85.2 (c, 1.25 in H_2O) (93% ee).

(2*S*,3*R*)-*form*
L-cis-*form*
[567-35-1]
Constit. of the antibiotic Telomycin. Cryst. (EtOH aq.). Mp 245-255° dec. $[\alpha]_D^{20}$ -91.5 (c, 0.61 in H_2O). $[\alpha]_D$ -54.3 (c, 0.50 in 1*M* HCl).

N-*Me:*
$C_6H_{11}NO_3$ 145.158
Isol. from an Australian sponge *Dendrilla* sp. Pale yellow oil. $[\alpha]_D$ -15.3 (c, 0.65 in H_2O). λ_{max} 266 (ϵ 1600) (EtOH).

Me ether: 3-Methoxy-2-pyrrolidinecarboxylic acid
$C_6H_{11}NO_3$ 145.158
Mp 212-214°. $[\alpha]_D^{25}$ -110.8 (c, 1 in H_2O). $[\alpha]_D$ -65.7 (c, 1 in 5*M* HCl).

(2*S*,3*S*)-*form*
L-trans-*form*
[4298-08-2]
Constit. of collagen and the antibiotic Telomycin.
Cryst. (EtOH aq.). Mp 230-236° (dec.) (232°). $[\alpha]_D^{20}$ -23.3 (c, 0.92 in H_2O).

Et ester:
$C_7H_{13}NO_3$ 159.185
Mp 125-130° (as hydrochloride).

N-*Me: 3-Hydroxy-1-methyl-2-pyrrolidinecarboxylic acid. 3-Hydroxy-1-methylproline*
Isol. from *Tamarix ramosissima*.
Cryst. (as hydrochloride). Abs. config. apparently not detd., probably as given here.

Me ether:
Cryst. (EtOH). Mp 216.5-219°. $[\alpha]_D^{25}$ -25.3 (c, 1 in H_2O). $[\alpha]_D$ +7.8 (c, 1 in 5*M* HCl).

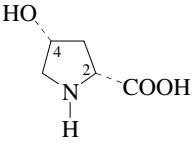
(2*RS*,3*SR*)-*form*
(±)-cis-*form*
[4298-05-9]
Mp 225-235° dec.

(2*RS*,3*RS*)-*form*
(±)-trans-*form*
Mp 224-230° dec.

Sheehan, J.C. *et al., J.A.C.S.*, 1962, **84**, 3980; 1963, **85**, 3863 (*synth*)
Irreverre, F. *et al., J.A.C.S.*, 1963, **85**, 2832 (*synth*)
Gallina, C. *et al., Org. Magn. Reson.*, 1972, **4**, 31 (*pmr*)
Szymanovicz, G. *et al., Biochimie*, 1978, **60**, 499 (*synth*)
Häusler, J. *et al., Annalen*, 1981, 1073 (*synth*)
Cooper, J. *et al., Chem. Comm.*, 1988, 509 (*synth*)
Thaning, M. *et al., Acta Chem. Scand.*, 1989, **43**, 290 (*synth*)
Roemmele, R.C. *et al., J.O.C.*, 1989, **54**, 1866 (*synth*)
Hughes, P. *et al., J.O.C.*, 1989, **54**, 3260 (*synth*)
Cooper, J. *et al., J.C.S. Perkin 1*, 1993, 1313 (*synth, ir, pmr, cmr, ms*)
Jones, G.P. *et al., Acta Cryst. C*, 1995, **51**, 287 (*cryst struct, N-Me*)
Mulzer, J. *et al., J.O.C.*, 1996, **61**, 566 (*synth, pmr, cmr, ir, ms*)
Capon, R.J. *et al., Aust. J. Chem.*, 1998, **51**, 169-170 (*isol, N-Me*)
Durand, J.-O. *et al., Tet. Lett.*, 1998, **39**, 5743-5746 (*synth*)
Lee, J.H. *et al., Tetrahedron*, 2001, **57**, 1071-1076 (*2R,3S-form, 2S,3S-form*)
El-Ashry, E.H. *et al., Carbohydr. Res.*, 2003, **338**, 2265-2290 (*rev, synth*)
Huang, P.-Q. *et al., Synth. Commun.*, 2004, **34**, 1377-1382 (*2S,3S-form, synth, ir, pmr, cmr*)

4-Hydroxy-2-pyrrolidinecarboxylic acid H-938

4-Hydroxyproline. Oxyproline



(2*R,4R*)-*form*

$C_5H_9NO_3$ 131.131

(2*R*,4*R*)-*form*
D-allo-*form*. D-cis-*form*
[2584-71-6]
Mp 237-241°. $[\alpha]_D^{25}$ +58.6 (c, 0.65 in H_2O). Insipid taste.

(2*R*,4*S*)-*form*
D-trans-*form*
[3398-22-9]
Mp 274°. $[\alpha]_D^{21}$ +75.2 (H_2O). Insipid taste.

(2*S*,4*R*)-*form*
L-trans-*form*
[51-35-4]
Constit. of proteins. Chiral building block.
Mp 274°. $[\alpha]_D^{26}$ -74.6. pK_{a1} 1.92; pK_{a2} 9.73 (25°). Sweet taste.

N-*Me:* N-*Methyl*-trans-*4-hydroxy*-L-*proline*. ***4-Hydroxyhygrinic acid***. *Aceprolinum*. *Joint*. *Problaston*. *Thioprol*
[4252-82-8]
$C_6H_{11}NO_3$ 145.158
Constit. of *Copaifera* spp., *Croton gubougia*, *Dalbergia sympathetica*, *Erythroxylum argentinum*, *Toddalia aculeata* and *Afrormosia elata* (preferred genus name *Pericopsis*). Also from the red alga *Chondria coerulescens* and other red algae. Cryst. (MeOH).
Mp 238-240° dec. $[\alpha]_D$ -86.6 (c, 1.5 in H_2O). Isolate from *Dalbergia sympathetica* originally thought to be a 2-piperidone but struct. was corrected by Winkler, *et al* in 2006.

N-*Me; hydrochloride:* Mp 181-183°. $[\alpha]_D$ -55 (c, 2.3 in MeOH).

(2*S*,4*S*)-*form*
L-allo-*form*. L-cis-*form*
[618-27-9]
Occurs in toxic peptides of the death cap mushroom (*Amanita phalloides*).
Mp 238-241°. $[\alpha]_D^{25}$ -57.7 (c, 0.65 in H_2O). Sweet taste.

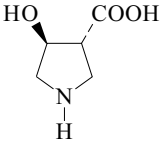
(2*RS*,4*RS*)-*form*
DL-allo-*form*. (±)-cis-*form*
[49761-17-3]
Mp 238°.

(2*RS*,4*SR*)-*form*
(±)-trans-*form*
[618-28-0]
Cryst. (EtOH aq.). Mp 247°.

[67463-44-9, 89771-43-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 583D; 584A; 584B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 887B; 887C (*nmr*)
Abraham, R.J. *et al., J.C.S.*, 1964, 3739 (*pmr*)
Koetzle, T.F. *et al., Acta Cryst. B*, 1973, **29**, 231 (*cryst struct*)
Shamala, N. *et al., Acta Cryst. B*, 1976, **32**, 3267 (*cryst struct*)
Ramaswamy, S.G. *et al., J.O.C.*, 1977, **42**, 3440 (*synth*)
Hara, J. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 3871 (*synth*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 13051
De Martino, G. *et al., J. Het. Chem.*, 1990, **27**, 507 (*synth*)
Puripattanavong, J. *et al., Planta Med.*, 2000, **66**, 740-745 (*isol, N-Me*)
Kimura, R. *et al., Bull. Chem. Soc. Jpn.*, 2002, **75**, 2517-2525 (*2S,4S-form, synth, ir, pmr*)
Croce, P.D. *et al., Tetrahedron: Asymmetry*, 2002, **13**, 197-201 (*2R,4R-form, synth, pmr, cmr*)
Schuch, C.M. *et al., Tetrahedron: Asymmetry*, 2002, **13**, 1973-1980 (*2R,4S-form, synth*)
El-Ashry, E.H. *et al., Carbohydr. Res.*, 2003, **338**, 2265-2290 (*rev, synth*)
Winkler, T. *et al., Magn. Reson. Chem.*, 2006, **44**, 571-572 (*N-Me, pmr, cmr*)
Jain, S.C. *et al., Phytochemistry*, 2006, **67**, 1005-1010 (*N-Me, pmr, cmr, cryst struct*)

4-Hydroxy-3-pyrrolidinecarboxylic acid H-939

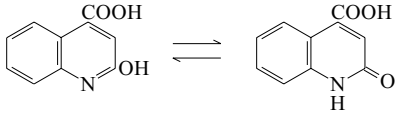


$C_5H_9NO_3$ 131.131

(3R*,4S*)-form
(+)-trans-*form*
N,N-*Di-Me, betaine: 4-Hydroxy*-N,N-*dimethyl-3-pyrrolidinecarboxylate*
[117845-15-5]
$C_7H_{13}NO_3$ 159.185
Isol. from the Mediterranean red alga *Grateloupia proteus*. Off-white hygroscopic powder. $[\alpha]_D^{25}$ +14.42 (c, 0.34 in H_2O).
Sciuto, S. *et al., J. Nat. Prod.*, 1988, **51**, 1017 (*isol, pmr, cmr, ms, struct*)

2-Hydroxy-4-quinolinecarboxylic acid H-940

*1,2-Dihydro-2-oxo-4-quinolinecarboxylic acid. 2(1*H*)-Quinolinone-4-carboxylic acid. 2-Hydroxycinchoninic acid. Carbostyril-4-carboxylic acid*
[84906-81-0]



$C_{10}H_7NO_3$ 189.17
NH-form is major tautomer. Isol. from poppy straw (*Papaver somniferum*). Needles (H_2O). Mp 343° (anhyd.) Mp 310° (monohydrate).

Me ester:
$C_{11}H_9NO_3$ 203.197
Prod. by a marine bacterium strain He159b. Needles (H_2O). Mp 248-251°.

*Et ester: **4-Ethoxycarbonyl-2-(1H)-quinolinone***
[5466-27-3]
$C_{12}H_{11}NO_3$ 217.224
Alkaloid from the fruit of *Brucea javanica* and *Parthenocissus tricuspidata*. Needles (EtOH aq.).
Mp 207-210°.

NH-form [15733-89-8]
N-*Me:*
$C_{11}H_9NO_3$ 203.197
Mp 244°.

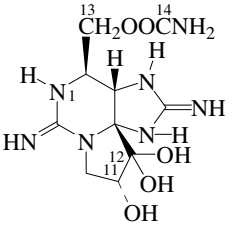
OH-form
Me ether: 2-Methoxy-4-quinolinecarboxylic acid
[10222-62-5]
$C_{11}H_9NO_3$ 203.197
Cryst. (MeOH). Mp 175°.

Et ether: 2-Ethoxy-4-quinolinecarboxylic acid
$C_{12}H_{11}NO_3$ 217.224
Needles (H_2O). Mp 145-146°.

Et ether, Et ester:
$C_{14}H_{15}NO_3$ 245.277
Needles. Mp 86°.

Wojahn, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1931, **269**, 422 (*synth*)
Sugasawa, S. *et al., Yakugaku Zasshi*, 1937, **57**, 296 (*synth*)
Schmid, H. *et al., Helv. Chim. Acta*, 1945, **28**, 722 (*isol*)
Org. Synth., Coll. Vol., 3, 1955, 456 (*synth*)
Kadaba, P.K. *et al., Synthesis*, 1972, 628 (*deriv*)
Sawayama, T. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2305 (*synth*)
Wang, Y.Z. *et al., Yaoxue Xuebao*, 1982, **17**, 466; *CA*, **97**, 107056 (*isol, deriv*)
Mirek, J. *et al., Z. Naturforsch., A*, 1982, **37**, 1276 (*tautom, uv*)
Yu, Y.N. *et al., Yaoxue Xuebao*, 1990, **25**, 382; *CA*, **113**, 227957 (*isol, deriv*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*Me ester, marine, isol*)

11-Hydroxysaxitoxin H-941



11α-*form*

$C_{10}H_{17}N_7O_5$ 315.288

11α-*form* [78780-57-1]
Isol. from *Gonyaulax tamarensis*.
11-O-*Sulfate: **Gonyautoxin II**. GTX2*
[60508-89-6]
$C_{10}H_{17}N_7O_8S$ 395.352
From *Gonyaulax* and *Protogonyaulax* spp. and present in other marine organisms. Neurotoxin. Sol. H_2O.
▶ Toxic.

11-O-*Sulfate,* N^{14}*-sulfonic acid: **Protogonyautoxin I**. Toxin C_1. Toxin PX_1*
[80173-30-4]
$C_{10}H_{17}N_7O_{11}S_2$ 475.417
From *Gonyaulax* and *Protogonyaulax* spp. Neurotoxin. Prisms + H_2O (MeOH aq.).
▶ Toxic.

*Decarbamoyl: **Decarbamoyl-11α-hydroxysaxitoxin***
$C_9H_{16}N_6O_4$ 272.263
Isol. from shellfish. No CAS no. 8-14 CI.

Decarbamoyl, 11-O-*sulfate: **Decarbamoylgonyautoxin II***
[86996-87-4]
$C_9H_{16}N_6O_7S$ 352.327
Isol. from various shellfish.

Decarbamoyl, O^{13}*-Ac, 11*-O-*sulfate: **13-Acetyldecarbamoylgonyautoxin II**. LWTX3*
[200816-97-3]
$C_{11}H_{18}N_6O_8S$ 394.365
Isol. from *Lyngbya wollei*.

Decarbamoyl, 13-O-*(4-hydroxybenzoyl), 11*-O-*sulfate: **GC 1***
[603125-80-0]
$C_{16}H_{20}N_6O_9S$ 472.435
Isol. from *Gymnodinium catenatum*.

De(carbamoyloxy), 11-O-*sulfate:* ***Decarbamoyloxygonyautoxin II***
[186249-38-7]
$C_9H_{16}N_6O_6S$ 336.328
Isol. from *Alexandrium* sp.

N^1-*Hydroxy:* ***11α-Hydroxyneosaxitoxin***
$C_{10}H_{17}N_7O_6$ 331.288
Isol. from shellfish. No CAS no found 8-14CI.

N^1-*Hydroxy, 11*-O-*sulfate:* ***Gonyautoxin I***. *GTX1*
[60748-39-2]
$C_{10}H_{17}N_7O_9S$ 411.352
Prod. by *Gonyaulax* and *Protogonyaulax* spp. and isol. from shellfish and other marine organisms. Neurotoxin, causal agent, with Saxitoxin, of shellfish poisoning. Sol. H_2O. The Gonyautoxins, esp. the *N*-sulfates, show reduced toxicity compared with Saxitoxin.
▶ Toxic.

N^1-*Hydroxy, 11*-O-*sulfate,* N^{14}-*sulfonic acid:* ***Protogonyautoxin 3***. *Toxin C_3. Toxin PX_3*
[89614-45-9]
$C_{10}H_{17}N_7O_{12}S_2$ 491.416
From *Gonyaulax* and *Protogonyaulax* spp. Neurotoxin.
▶ Toxic.

N^1-*Hydroxy, decarbamoyl:* ***Decarbamoyl-11α-hydroxyneosaxitoxin***
$C_9H_{16}N_6O_5$ 288.263
No CAS no. found 8-14CI.

N^1-*Hydroxy, decarbamoyl, 11*-O-*sulfate:* ***Decarbamoylgonyautoxin I***
[122075-86-9]
$C_9H_{16}N_6O_8S$ 368.327
Isol. from *Gymnodinium catenatum* and *Alexandrium* sp.

11β-*form* [99685-70-8]

11-O-*Sulfate:* ***Gonyautoxin III***. *GTX3*
[60537-65-7]
$C_{10}H_{17}N_7O_8S$ 395.352
From *Gonyaulax* and *Protogonyaulax* spp. and other marine organisms. Neurotoxin. Sol. H_2O.
▶ Toxic.

11-O-*Sulfate,* N^{14}-*sulfonic acid:* ***Gonyautoxin VIII***. *GTX8*. *Protogonyautoxin 2*. *Toxin C_2*. *Toxin PX_2*
[80226-62-6]
$C_{10}H_{17}N_7O_{11}S_2$ 475.417
From *Gonyaulax* and *Protogonyaulax* spp. Neurotoxin. Large cryst. + H_2O (H_2O).
▶ Toxic. UU6858700

Decarbamoyl: ***Decarbamoyl-11β-hydroxysaxitoxin***
$C_9H_{16}N_6O_4$ 272.263
Isol. from shellfish. No CAS no found 8-14CI.

Decarbamoyl, 11-O-*sulfate:* ***Decarbamoylgonyautoxin III***
[87038-53-7]
$C_9H_{16}N_6O_7S$ 352.327
Isol. from various shellfish.

Decarbamoyl, O^{13}-*Ac, 11*-O-*sulfate:* ***13-Acetyldecarbamoylgonyautoxin III***. *LWTX2*
[200816-96-2]
$C_{11}H_{18}N_6O_8S$ 394.365
Isol. from *Lyngbya wollei*.

Decarbamoyl, 13-O-*(4-hydroxybenzoyl), 11*-O-*sulfate:* ***GC 2***
[603125-81-1]
$C_{16}H_{20}N_6O_9S$ 472.435
Isol. from *Gymnodinium catenatum*.

De(carbamoyloxy), 11-O-*sulfate:* ***Decarbamoylgonyautoxin III***
[155666-11-8]
$C_9H_{16}N_6O_6S$ 336.328
Isol. from *Gymnodinium catenatum* and *Alexandrium* sp.

N^1-*Hydroxy:* ***11β-Hydroxyneosaxitoxin***
$C_{10}H_{17}N_7O_6$ 331.288
Isol. from shellfish. No CAS no found 8-14CI.

N^1-*Hydroxy, 11*-O-*sulfate:* ***Gonyautoxin IV***. *GTX4*
[64296-26-0]
$C_{10}H_{17}N_7O_9S$ 411.352
From *Gonyaulax* and *Protogonyaulax* spp. and other marine organisms. Neurotoxin. Sol. H_2O.
▶ Toxic.

N^1-*Hydroxy, 11*-O-*sulfate,* N^{14}-*sulfonic acid:* ***Protogonyautoxin 4***. *Toxin C_4. Toxin PX_4*
[89674-98-6]
$C_{10}H_{17}N_7O_{12}S_2$ 491.416
From *Gonyaulax* and *Protogonyaulax* spp. Neurotoxin.
▶ Toxic.

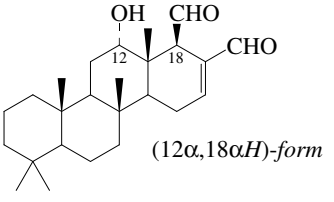
N^1-*Hydroxy, decarbamoyl:* ***Decarbamoyl-11β-hydroxyneosaxitoxin***
$C_9H_{16}N_6O_5$ 288.263
Isol. from shellfish.

N^1-*Hydroxy, decarbamoyl, 11*-O-*sulfate:* ***Decarbamoylgonyautoxin IV***
[122169-51-1]
$C_9H_{16}N_6O_8S$ 368.327
Isol. from *Gymnodinium catenatum* and *Alexandrium* sp.

12-Deoxy, decarbamoyl, O^{13}-*Ac, 11*-O-*sulfate: LWTX1*
[200816-95-1]
$C_{11}H_{18}N_6O_7S$ 378.365
Isol. from *Lyngbya wollei*.

Onoue, Y. *et al., J. Agric. Food Chem.*, 1983, **31**, 420-430 (*props*)
Oshima, Y. *et al., Agric. Biol. Chem.*, 1984, **48**, 1707-1711 (*chromatog, bibl*)
Maruyama, J. *et al., Agric. Biol. Chem.*, 1984, **48**, 2783-2788 (*ms*)
Hall, S. *et al., Tet. Lett.*, 1984, **25**, 3537-3538 (*Toxins C3, C4*)
Shimizu, Y. *et al., Tetrahedron*, 1984, **40**, 539-544 (*props*)
Anderson, D.M. *et al., Toxicon*, 1989, **27**, 665-674 (*Decarbamoylgonyautoxins*)
Hall, S. *et al., ACS Symp. Ser.*, 1990, 418 (*book*)
Gallacher, S. *et al., Appl. Environ. Microbiol.*, 1997, **63**, 239-245 (*Decarbamoyloxygonyautoxins*)
Onodera, H. *et al., Nat. Toxins*, 1997, **5**, 146-151 (*LWTX toxins*)
Food Sci. Technol., *Seafood and Freshwater Toxins*, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*revs*)
Negri, A. *et al., Chem. Res. Toxicol.*, 2003, **16**, 1029-1033 (*GC1, GC2*)
Ciminiello, P. *et al., Eur. J. Org. Chem.*, 2004, 2533-2551 (*rev*)
Llewellyn, L.E. *et al., Nat. Prod. Rep.*, 2006, **23**, 200-222 (*rev*)

12-Hydroxy-16-scalarene-24,25-dial H-942



(12α,18α*H*)-*form*

$C_{25}H_{38}O_3$ 386.573

(12α,18α*H*)-*form*

Desacetylscalaradial
[77282-60-1]
Constit. of *Cacospongia mollior*. Shows *in vitro* cytotoxicity vs. L-1210 cells. Cryst. (EtOH).
Mp 200-203°. $[\alpha]_D^{25}$ -19 (c, 0.7 in $CHCl_3$). λ_{max} 230 (ϵ 12500) (EtOH) (Derep).

Ac: ***Scalaradial***
[53527-28-9]
$C_{27}H_{40}O_4$ 428.611
Isol. from *Cacospongia mollior*, *Cacospongia scalaris*, *Spongia nitens* and *Hyrtios erecta*. Phospholipase A_2 inhibitor; antiinflammatory and ichthyotoxic agent. Cryst. (EtOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 111-113°. $[\alpha]_D$ +47.5 (c, 0.9 in MeOH). λ_{max} 229 (ϵ 11700) (MeOH) (Derep).

25-Alcohol, 12-Ac: 12-Acetoxy-25-hydroxy-16-scalaren-24-al. ***19-Dihydroscalaradial***
[186383-07-3]
$C_{27}H_{42}O_4$ 430.626
Constit. of *Cacospongia scalaris*. Amorph. powder. $[\alpha]_D$ +50.5 (c, 0.4 in $CHCl_3$). λ_{max} 230 (ϵ 2184) (MeOH).

12 Ketone: ***12-Oxo-16-scalarene-24,25-dial***
[823804-84-8]
$C_{25}H_{36}O_3$ 384.558
Constit. of *Glossodoris rufomarginata*. Oil. $[\alpha]_D$ -118.2 (c, 0.1 in $CHCl_3$).

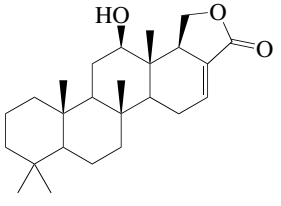
(12α,18β*H*)-*form*
Ac: ***18-Episcalaradial***
[186382-49-0]
$C_{27}H_{40}O_4$ 428.611
Constit. of *Cacospongia scalaris*. Amorph. powder. $[\alpha]_D$ -37.9 (c, 0.8 in $CHCl_3$). λ_{max} 226 (ϵ 6236) (MeOH).
12-Ketone: ***12-Deacetyl-18-epi-12-oxoscalaradial***
[104900-66-5]
$C_{25}H_{36}O_3$ 384.558
Constit. of *Chromodoris youngbleuthi* and *Spongia oceania*. Cryst. Mp 179-182°. $[\alpha]_D$ +120 (c, 0.25 in CH_2Cl_2).

(12β,18α*H*)-*form*
12-Deacetyl-12-episcalaradial
[104900-65-4]
Constit. of nudibranch *Chromodoris youngbleuthi* and of *Collospongia auris*.
Cryst.
Mp 201-203°. $[\alpha]_D$ +38.1 (c, 0.21 in CH_2Cl_2). λ_{max} 230 (EtOH).
Ac: ***12-Episcalaradial***
[72300-72-2]
Isol. from the marine sponges *Spongia nitens*, *Spongia agaricina* and *Cacospongia* sp., and *Hyrtios erecta*. Bee venom inhibitor.
Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 188-190°. $[\alpha]_D$ +36.5 ($CHCl_3$). λ_{max} 230 (ϵ 12500) (EtOH) (Derep). λ_{max} 229 (ϵ 11700) (MeOH) (Berdy).

(12β,18β*H*)-*form*
12-Deacetyl-12,18-diepiscalaradial
[75266-25-0]
Constit. of *Spongia idia*. Molluscicide, ichthyotoxin, phospholipase A2 inibitor, antiinflammatory. Cryst.
Mp 216-218°. $[\alpha]_D$ -129 (c, 1.2 in $CHCl_3$). λ_{max} 230 (ϵ 12500) (MeOH).
Ac: [72300-73-3]
Constit. of *Spongia nitens*, *Cacospongia* sp. and *Hyrtios erecta*.
Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 210-213°. $[\alpha]_D$ -149 ($CHCl_3$). λ_{max} 228 (ϵ 10700) (MeOH).

Cimino, G. *et al., Experientia*, 1974, **30**, 846-847; 1979, **35**, 1277-1279 (*isol, ir, pmr, cmr*)
Walker, R.P. *et al., J.O.C.*, 1980, **45**, 4976-4979 (*12-Deacetyl-12,18-diepiscalaradial*)
Yasuda, F. *et al., Experientia*, 1981, **37**, 110 (*biochem*)
Crews, P. *et al., J. Nat. Prod.*, 1986, **49**, 1041 (*isol*)
Terem, B. *et al., Tetrahedron*, 1986, **42**, 4409-4412 (*isol*)
Potts, B.C.M. *et al., J.A.C.S.*, 1992, **114**, 5093-5100 (*Scalaradial, isol, activity*)
De Rosa, S. *et al., J. Nat. Prod.*, 1994, **57**, 256 (*isol, pmr, cmr, cryst struct*)
Puliti, R. *et al., Acta Cryst. C*, 1995, **51**, 1703 (*cryst struct*)
Rueda, A. *et al., J.O.C.*, 1997, **62**, 1481 (*19-Dihydroscalaradial, 18-Episcalaradial*)
Gavagnin, M. *et al., J. Nat. Prod.*, 2004, **67**, 2104-2107 (*Glossodoris rufomarginata constit*)

12-Hydroxy-16-scalaren-24,25-olide H-943

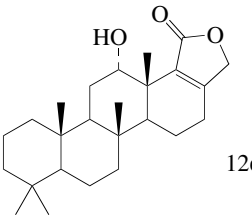


$C_{25}H_{38}O_3$ 386.573
λ_{max} (MeOH).

12β-*form*
12-O-Deacetyl-17-deoxyscalarin
[40772-12-1]
Constit. of *Heteronema erecta* and *Hyrtios erecta*. Shows moderate inhibition against P388 cell line. Oil or needles (MeOH). 3Mp 274-275°. $[\alpha]_D$ -22.4 (c, 1 in $CHCl_3$). $[\alpha]_D^{25}$ -2 (c, 0.15 in MeOH). λ_{max} 221 (ϵ 9500) (MeOH). λ_{max} 222 (log ϵ 3.95) (MeOH).

Venkateswarlu, Y. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 563-564 (*isol, pmr, cmr*)
Pettit, G.R. *et al., Coll. Czech. Chem. Comm.*, 1998, **63**, 1671-1677 (*isol, pmr, cmr, cryst struct*)

12-Hydroxy-17-scalaren-25,24-olide H-944



12α-*form*

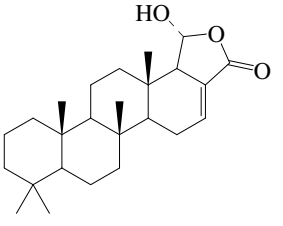
$C_{25}H_{38}O_3$ 386.573

12α-*form*
Ac: ***12-Epiacetylscalarolide***
$C_{27}H_{40}O_4$ 428.611
Constit. of *Cacospongia scalaris*. Amorph. powder. $[\alpha]_D$ +47.8 (c, 0.9 in $CHCl_3$). λ_{max} 216 (ϵ 4871) (MeOH).

12β-*form*
Scalarolide
[75266-23-8]
Constit. of *Spongia idia*.
Cryst.
Mp 300° dec. $[\alpha]_D$ +24.9 (c, 1.4 in $CHCl_3$). λ_{max} 219 (ϵ 24500) (MeOH) (Derep).

Walker, R.P. *et al., J.O.C.*, 1980, **45**, 4976 (*isol, struct*)
Ragoussis, V. *et al., J.C.S. Perkin 1*, 1990, 2545 (*synth*)
Rueda, A. *et al., J.O.C.*, 1997, **62**, 1481 (*12-Epiacetylscalarolide*)
Cambie, R.C. *et al., Acta Cryst. C*, 1999, **55**, 112-114 (*Scalarolide, cryst struct*)

25-Hydroxy-16-scalaren-24,25-olide H-945



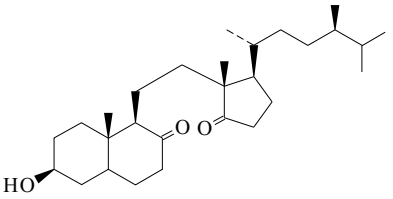
$C_{25}H_{38}O_3$ 386.573

25α-*form*
Ac: [798557-98-9]
$C_{27}H_{40}O_4$ 428.611
Constit. of a *Brachiaster* sp. Amorph. solid. $[\alpha]_D$ -24.3 (c, 0.014 in MeOH). λ_{max} 227 (log ϵ 3.78) (MeOH).

Wonganuchitmeta, S.-N. *et al., J. Nat. Prod.*, 2004, **67**, 1767-1770 (*Brachiaster constit*)

3-Hydroxy-8,14-secoergostane-8,14-dione H-946

3-Hydroxy-24-methyl-8,14-secocholestane-8,14-dione



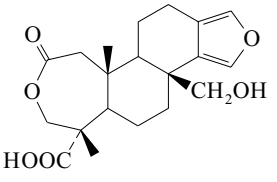
$C_{28}H_{48}O_3$ 432.685

(3β,24*R*)-*form*

Me ether: 3-Methoxy-8,14-secoergostane-8,14-dione. ***Jereisterol B***
[135474-10-1]
$C_{29}H_{50}O_3$ 446.712
Constit. of *Jereicopsis graphidiophora*.
D'Auria, M.V. *et al., Tet. Lett.*, 1991, **32**, 2149-2152 (*isol, pmr*)

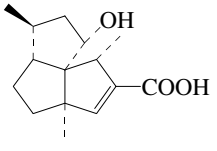
17-Hydroxy-2,3-seco-13(16),14-spongiadien-2,3-olid-18-oic acid H-947

17-Hydroxy-4-epispongialactone A
[130574-80-0]



$C_{20}H_{26}O_6$ 362.422
Constit. of a *Spongia* sp.
Gunasekera, S.P. *et al., J.O.C.*, 1991, **56**, 1250 (*isol, pmr, cmr*)

11-Hydroxy-5-silphiperfolen-13-oic acid H-948



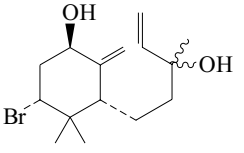
$C_{15}H_{22}O_3$ 250.337
Some authors use alternative numbering system.

11α-*form*

2-Hydroxysubergorgic acid
[118000-35-4]
Constit. of *Subergorgia suberosa*.
Cryst.
Mp 146°. $[\alpha]_D^{20}$ -95 (c, 1 in MeOH). λ_{max} 225 (MeOH).
Me ester: [209673-66-5]
$C_{16}H_{24}O_3$ 264.364
Constit. of *Subergorgia suberosa*. Oil. $[\alpha]_D^{20}$ -49.4 (c, 0.85 in MeOH). λ_{max} 225 (MeOH).
Ac: [443999-12-0]
$C_{17}H_{24}O_4$ 292.374
Constit. of *Subergorgia suberosa*. Oil. $[\alpha]_D^{31}$ -40 (c, 0.21 in $CHCl_3$).
Ac, Me ester: [209673-67-6]
$C_{18}H_{26}O_4$ 306.401
Constit. of *Subergorgia suberosa*. Oil. $[\alpha]_D^{20}$ -81.6 (c, 1 in MeOH).
11-Ketone: 11-Oxo-5-silphiperfolen-13-oic acid. ***Subergorgic acid***
[97718-45-1]
[84607-62-5]
$C_{15}H_{20}O_3$ 248.321
Constit. of coral *Subergorgia suberosa* and from *Isis hippuris.*
Shows cardiotoxic props. Neuromuscular transmission inhibitor.
Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 179-180° Mp 200-202°. $[\alpha]_D^{20}$ -128 (c, 1 in MeOH). λ_{max} 225 (MeOH). λ_{max} 225 (MeOH) (Berdy). λ_{max} 219 (ϵ 9000) (EtOH) (Berdy).
▶ LD_{50} (mus, ivn) 22.8 mg/kg.
11-Ketone, Me ester: ***Methyl subergorgate***
[97649-27-9]
$C_{16}H_{22}O_3$ 262.348
Constit. of *Subergorgia suberosa*. Oil. $[\alpha]_D^{20}$ -112 (c, 1 in MeOH). λ_{max} 224 (MeOH).
Wu, Z. *et al., CA*, 1983, **98**, 68827d (*Subergorgic acid, isol*)
Groweiss, A. *et al., Tet. Lett.*, 1985, **26**, 2379 (*Subergorgic acid, cryst struct*)
Iwata, C. *et al., J.O.C.*, 1988, **53**, 1623 (*synth*)
Wender, P.A. *et al., Tet. Lett.*, 1990, **31**, 5429 (*synth*)
Paquette, L.A. *et al., J.A.C.S.*, 1993, **115**, 49 (*synth*)
Parameswaran, P.S. *et al., J. Nat. Prod.*, 1998, **61**, 832-834; 1074 (*Me ester, ketone Me ester, isol, pmr, cmr*)
Wang, G.-H. *et al., J. Nat. Prod.*, 2002, **65**, 1033-1036 (*Ac*)

4-Hydroxy-β-snyderol H-949

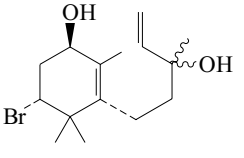
8-Hydroxy-β-snyderol
[134788-17-3]



$C_{15}H_{25}BrO_2$ 317.265
Constit. of *Laurencia caespitosa*. Oil. $[\alpha]_D$ +8.7 (c, 0.172 in $CHCl_3$).
Norte, M. *et al., Can. J. Chem.*, 1991, **69**, 518 (*isol, pmr, cmr*)

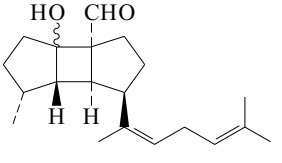
4-Hydroxy-γ-snyderol H-950

8-Hydroxy-γ-snyderol
[134788-18-4]



$C_{15}H_{25}BrO_2$ 317.265
Constit. of *Laurencia caespitosa*. Oil. $[\alpha]_D$ +16.8 (c, 0.136 in $CHCl_3$).
Norte, M. *et al., Can. J. Chem.*, 1991, **69**, 518 (*isol, pmr, cmr*)

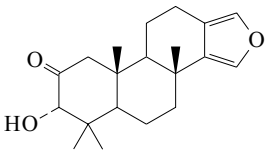
10-Hydroxy-13(15),17-spatadien-12-al H-951



$C_{20}H_{30}O_2$ 302.456

(10ξ,13(15)*Z*)-*form* [81575-12-4]
Isol. from *Dilophus marginatus.*
Yellow oil. $[\alpha]_D^{20}$ +59 (c, 1.5 in $CHCl_3$).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 129

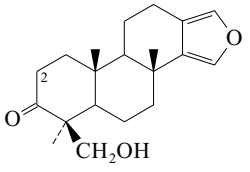
3-Hydroxy-13(16),14-spongiadien-2-one H-952



$C_{20}H_{28}O_3$ 316.439

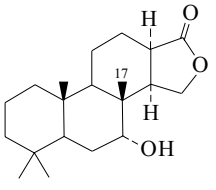
3α-*form* [157799-15-0]
Constit. of a *Spongia* sp.
Solid.
Searle, P.A. *et al., Tetrahedron*, 1994, **50**, 9893 (*isol, pmr, cmr*)

19-Hydroxy-13(16),14-spongiadien-3-one H-953



$C_{20}H_{28}O_3$ 316.439
Constit. of *Hyatella intestinalis*. Cryst. (Me_2CO/hexane).
Mp 143-144°. $[\alpha]_D^{21}$ +18.8 (c, 0.6 in $CHCl_3$).
Cambie, R.C. *et al., J. Nat. Prod.*, 1988, **51**, 293,

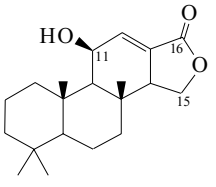
7-Hydroxy-16-spongianone H-954



$C_{20}H_{32}O_3$ 320.471

7α-*form* [178180-02-4]
Constit. of *Chromodoris obsoleta*.
Plates (MeOH).
Mp 260-263°. $[\alpha]_D^{28}$ +30.3 (c, 0.22 in $CHCl_3$).
Ac: 7α-Acetoxy-16-spongianone. ***Aplyroseol 7***
[106009-80-7]
$C_{22}H_{34}O_4$ 362.508
Constit. of *Dendrilla rosea*, *Chromodoris inopinata*, *Chelonaplysilla violacea*, *Chromodoris obsoleta*, *Dictyodendrilla cavernosa* and *Aplysilla rosea*. Oil.
Karuso, P. *et al., Aust. J. Chem.*, 1986, **39**, 1629-1641; 1643-1653 (*isol, Ac, pmr, cmr*)
De Silva, E.D. *et al., J. Nat. Prod.*, 1991, **54**, 993-997 (*Ac, isol*)
Bergquist, P.R. *et al., Advanced Inorganic Chemistry*, 1993, **46**, 622-632 (*Ac, isol*)
Miyamoto, T. *et al., Tetrahedron*, 1996, **52**, 8187-8198 (*isol, pmr, cmr, cryst struct*)

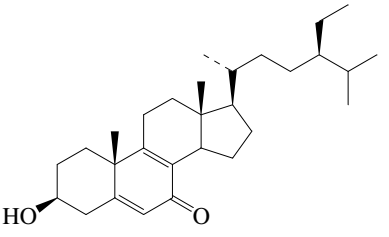
11-Hydroxy-12-spongien-16-one H-955



$C_{20}H_{30}O_3$ 318.455

11β-*form*
Constit. of *Spongia officinalis*.
Cryst.
Mp 199-200°. $[\alpha]_D$ +74.6 (c, 1.22 in $CHCl_3$).
Ac: 11β-Acetoxy-12-spongien-16-one
$C_{22}H_{32}O_4$ 360.492
Constit. of *Spongia officinalis*. Cryst.
Mp 195-197°. $[\alpha]_D$ +184.1 (c, 1.09 in $CHCl_3$).
Gonzalez, A.G. *et al., Tetrahedron*, 1985, **40**, 4109

3-Hydroxystigmasta-5,8-dien-7-one H-956



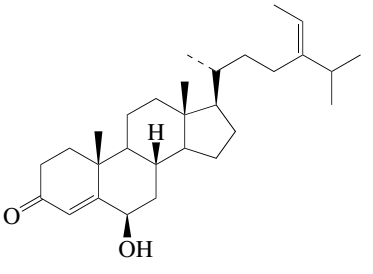
$C_{29}H_{46}O_2$ 426.681

(3β,24*R*)-*form* [459832-67-8]
Constit. of *Polymastia tenax*.
Amorph. solid. $[\alpha]_D^{25}$ +9.1 (c, 0.05 in CH_2Cl_2).
Santafé, G. *et al., J. Nat. Prod.*, 2002, **65**, 1161-1164 (*isol, pmr, cmr*)

6-Hydroxystigmasta-4,24-dien-3-one, 9CI H-957
6-Hydroxy-24-ethylcholesta-4,24-dien-3-one
$C_{29}H_{46}O_2$ 426.681

6β-*form* [134887-27-7]
Constit. of a *Stelletta* sp.
Oil. $[\alpha]_D^{20}$ +17.1 (c, 0.26 in $CHCl_3$). Genus name incorr. given as Stelleta.
6-Ketone: ***Stigmasta-4,24-diene-3,6-dione, 9CI***. *24-Ethylcholesta-4,24-diene-3,6-dione*
[134887-26-6]
$C_{29}H_{44}O_2$ 424.665
Constit. of a *Stelletta* sp. Oil. $[\alpha]_D^{20}$ -18.8 ($CHCl_3$).
[134887-31-3]
Guerriero, A. *et al., Helv. Chim. Acta*, 1991, **74**, 487-494 (*isol, pmr, cmr*)

6-Hydroxystigmasta-4,24(28)-dien-3-one H-958
24-Ethylidene-6-hydroxycholest-4-en-3-one

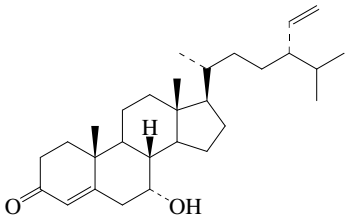


$C_{29}H_{46}O_2$ 426.681

(6β,24(28)*E*)-*form* [219832-37-8]
Constit. of *Turbinaria conoides*.
Powder.
Mp 171.5-173°. $[\alpha]_D^{28}$ +25 (c, 0.09 in $CHCl_3$). λ_{max} 239 (log ε 4.03) (EtOH).
6-Ketone: ***Stigmasta-4,24(28)-diene-3,6-dione***. *24-Ethylidenecholest-4-ene-3,6-dione*
[219832-35-6]
$C_{29}H_{44}O_2$ 424.665

Constit. of *Turbinaria conoides*. Cryst.
Mp 134-136°. $[\alpha]_D^{28}$ -39 (c, 0.24 in $CHCl_3$). λ_{max} 251 (log ϵ 3.83) (EtOH).
Sheu, J.-H. *et al., J. Nat. Prod.*, 1999, **62**, 224-227 (*isol, pmr, cmr*)

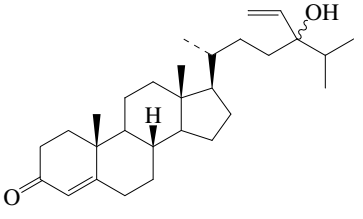
7-Hydroxystigmasta-4,25-dien-3-one H-959



$C_{29}H_{46}O_2$ 426.681

(7α,24*S*)-*form*
7-O-*β*-D-*Fucopyranoside:* ***Iyengaroside A***
[494862-72-5]
$C_{35}H_{56}O_6$ 572.824
Constit. of *Codium iyengarii*. Powder. $[\alpha]_D$ -13.5 (c, 1.155 in $CHCl_3$). λ_{max} 240 (log ϵ 4.1) ($CHCl_3$).
Ali, M.S. *et al., Nat. Prod. Lett.*, 2002, **16**, 407-413 (*isol, pmr, cmr*)

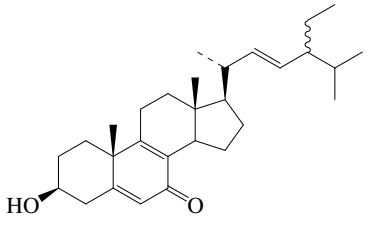
24-Hydroxystigmasta-4,28-dien-3-one H-960



$C_{29}H_{46}O_2$ 426.681

(24ξ)-*form*
Saringosterone
[634202-10-1]
Constit. of *Sargassum asperifolium*.
Oil.
Ayyad, S.-E.N. *et al., Z. Naturforsch., C*, 2003, **58**, 333-336 (*isol, pmr, cmr*)

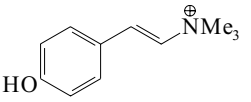
3-Hydroxystigmasta-5,8,22-trien-7-one H-961
24-Ethyl-3-hydroxycholesta-5,8,22-trien-7-one



$C_{29}H_{44}O_2$ 424.665

(3β,22*E*,24ξ)-*form* [121714-76-9]
Isol. from Mediterranean sponge *Clathrina clathrus*. λ_{max} 245 (ϵ 14000) (no solvent reported).
Aiello, A. *et al., Steroids*, 1988, **52**, 533-542 (*isol, pmr, ms, struct*)

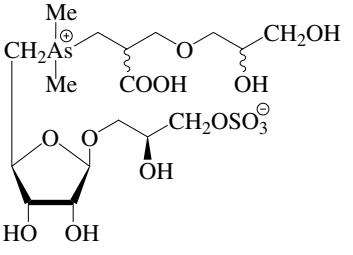
(4-Hydroxystyryl)trimethylammonium(1+) H-962
2-(4-Hydroxyphenyl)-N,N,N-*trimethylethenaminium, 9CI*



$C_{11}H_{16}NO^{\oplus}$ 178.253

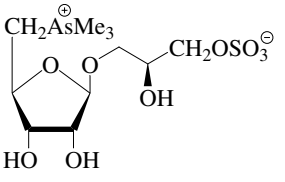
(*E*)-*form* [162827-15-8]
Metab. of the Palauan sponge *Axinyssa aplysinoides*.
Highly hygroscopic solid (as chloride). CAS No. refers to chloride.
Compagnone, R.S. *et al., J. Nat. Prod.*, 1995, **58**, 145 (*isol, uv, ir, pmr, cmr, struct*)

2-Hydroxy-3-(sulfooxy)propyl 5-[[2-carboxy-3-(2,3-dihydrooxypropoxy)propyl]dimethylarsonio]-5-deoxy-β-D-ribofuranoside inner salt, 9CI H-963
[138348-44-4]



$C_{17}H_{33}AsO_{14}S$ 568.427
Isol. from *Sargassum lacerifolium*.
Francesconi, K.A. *et al., J.C.S. Perkin 1*, 1991, 2707-2716; 1992, 1349-1357 (*isol, cryst struct*)

2-Hydroxy-3-(sulfooxy)propyl-5-deoxy-5-(trimethylarsonio)-β-D-ribofuranoside, 9CI H-964

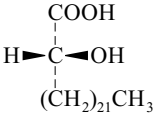


(2'*R*-β-D)-*form*

$C_{11}H_{23}AsO_9S$ 406.285

(2'*R*-β-D)-*form* [138382-73-7]
Constit. of the kidney of the giant clam *Tridacna maxima*. Also from *Chaetoceros gracilis* and *Sargassum thunbergii*.
Solid.
[115299-23-5]
Shibata, Y. *et al., Agric. Biol. Chem.*, 1988, **52**, 1087-1089 (*isol, struct*)
Edmonds, J.S. *et al., Nat. Prod. Rep.*, 1993, **10**, 421-428 (*rev*)

2-Hydroxytetracosanoic acid H-965
Cerebronic acid. *α-Hydroxylignoceric acid. Phrenosic acid. Phrenosinic acid*
[544-57-0]



(*R*)–*form*

$C_{24}H_{48}O_3$ 384.641

(*R*)-*form* [26632-11-1]
Constit. of various glycosphingolipids derived from various origins such as brain, wheat, corn, other plant spp., lichens and sponges. Isol. from *Penicillium* cultures, *Polyporus umbellatus* and *Aspergillus flavus*.
Cryst. ($CHCl_3$); plates (Me_2CO).
Mp 104.5-105.5° (99.5-100°). $[\alpha]_D^{25}$ +3.4 (c, 1.6 in Py). This is the predominant nat. prod. but the *S*-enantiomer may also occur.

Me ester:
$C_{25}H_{50}O_3$ 398.668
Mp 64-65°. $[\alpha]_D$ -3.25 (c, 0.92 in $CHCl_3$).

Ac: [127061-75-0]
$C_{26}H_{50}O_4$ 426.679
Cryst. (petrol or MeCN). Mp 81.5-82.5°. $[\alpha]_D^{20}$ +8.46 (c, 1.01 in $CHCl_3$).

Me ether: ***2-Methoxytetracosanoic acid***
[88416-38-0]
$C_{25}H_{50}O_3$ 398.668
Constit. of the sponge *Higginsia tethyoides*.

(*S*)-*form* [54563-87-0]
Cryst.

(±)-*form* [139237-67-5]
Cryst. (C_6H_6). Mp 99.5-100° (94-95°).

(ξ)-*form*
Constit. of various sponges incl. *Aplysina archeri*, *Callyspongia fallax* and *Pseudosuberites* sp.

[2433-95-6, 54563-85-8, 54563-86-9, 54563-88-1, 73580-21-9, 132842-33-2, 139237-68-6]

Ashton, R. *et al., J.C.S.*, 1936, 283 (*synth*)
Muller, A. *et al., Ber.*, 1939, **72B**, 615 (*synth*)
Yoshioka, I. *et al., Yakugaku Zasshi*, 1964, **84**, 742 (*isol, deriv*)
Vacheron, H.J. *et al., Phytochemistry*, 1968, **7**, 1645 (*isol*)
Hoshi, M. *et al., J. Biol. Chem.*, 1973, **248**, 4123 (*pharmacol*)
Tatsumi, K. *et al., Arch. Biochem. Biophys.*, 1974, **165**, 656 (*abs config*)
Ayanoglu, E. *et al., Lipids*, 1983, **18**, 830-836 (*Me ether*)
Florentina, N. *et al., Chem. Phys. Lipids*, 1984, **34**, 257 (*synth*)
Koike, K. *et al., Carbohydr. Res.*, 1987, **162**, 237 (*synth*)
Sugiyama, S. *et al., Annalen*, 1990, 1063 (*synth*)
Yamagata, K. *et al., J.C.S. Perkin 1*, 1990, 3355 (*synth*)
Sugai, T. *et al., Tet. Lett.*, 1991, **32**, 7063 (*synth, bibl*)
Barnathan, G. *et al., J. Nat. Prod.*, 1993, **56**, 2104-2113 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*isol*)

3-Hydroxytetracosanoic acid H-966

[91297-89-1]
$H_3C(CH_2)_{20}CH(OH)CH_2COOH$
$C_{24}H_{48}O_3$ 384.641
Constit. of the bark and latex of *Parahancornia arnapa*. Also found in marine sediments.

Me ether: 3-Methoxytetracosanoic acid
$C_{25}H_{50}O_3$ 398.668
Isol. from conidia of *Blumeria graminis* f. sp. *tritici*.

Sobrinho, D.C. *et al., J. Braz. Chem. Soc.*, 1991, **2**, 15 (*isol*)
Muchembled, J. *et al., Phytochemistry*, 2005, **66**, 793-796 (*Me ether*)

2-Hydroxy-21-tetracosene-3,12,14,16,23-pentaynoic acid H-967

Aikupikanyne F
$HC{\equiv}CCH{=}CH(CH_2)_3C{\equiv}CC{\equiv}CC{\equiv}C(CH_2)_7C{\equiv}CCH(OH)COOH$
$C_{24}H_{26}O_3$ 362.468

(2ξ,21*Z*)-*form*
Isol. from a *Callyspongia* sp.
Unstable yellowish oil.

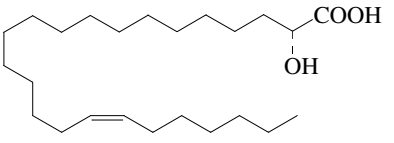
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2000, **63**, 1406-1410

2-Hydroxy-15-tetracosenoic acid H-968

[95746-76-2]
$H_3C(CH_2)_7CH{=}CH(CH_2)_{12}CH(OH)COOH$
$C_{24}H_{46}O_3$ 382.626

(*Z*)-*form* [73572-07-3]
Constit. of the sea urchin *Tripneustes esculentus*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1994, **57**, 614 (*isol, ms*)

2-Hydroxy-17-tetracosenoic acid H-969

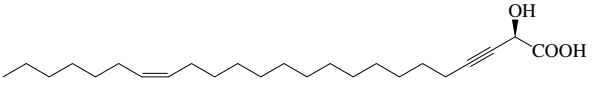


$C_{24}H_{46}O_3$ 382.626

(2*R*,17*Z*)-*form*
Me ether: 2-Methoxy-17-tetracosenoic acid
[88416-37-9]
$C_{25}H_{48}O_3$ 396.652
Constit. of the sponge *Higginsia tethyoides*.
Ayanoglu, E. *et al., Lipids*, 1983, **18**, 830-836 (*isol*)

2-Hydroxy-17-tetracosen-3-ynoic acid H-970

Callysponginol



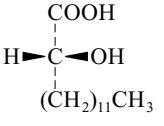
$C_{24}H_{42}O_3$ 378.594

(2*R*,17*Z*)-*form*
2-O-*Sulfate:* ***Callysponginol sulfate A***
$C_{24}H_{42}O_6S$ 458.658
Isol. from the sponge *Callyspongia truncata*. Membrane type 1 matrix metalloproteinase inhibitor. Powder. $[\alpha]_D^{24}$ -0.2 (c, 0.1 in MeOH).

Fujita, M. *et al., J. Nat. Prod.*, 2003, **66**, 569-571 (*isol, pmr, cmr*)

2-Hydroxytetradecanoic acid H-971

2-Hydroxymyristic acid
[2507-55-3]



(R)–form

$C_{14}H_{28}O_3$ 244.373

(*R*)-*form* [26632-17-7]
Present in wool wax and in brain cerebrosides.
Mp 88.2-88.5°. $[\alpha]_D$ -3.1 ($CHCl_3$).

Me ester:
$C_{15}H_{30}O_3$ 258.4
Mp 34.8-35°. Bp_1 133.5-136.5°.

(*S*)-*form* [67253-09-2]
Occurs in *Salmonella* lipopolysaccharides.

(±)-*form* [37639-48-8]
Occurs in Actinomycetales bacteria.
Mp 81-82°.

4-Nitrobenzyl ester: Mp 67-68°.

Amide:
$C_{14}H_{29}NO_2$ 243.389
Mp 150°.

Nitrile:
$C_{14}H_{27}NO$ 225.373
Cryst. (petrol). Mp 44.5°.

(ξ)-*form*
Constit. of *Pseudosuberites* sp. and *Suberites massa*.

Me ether: 2-Methoxytetradecanoic acid
$C_{15}H_{30}O_3$ 258.4
Isol. from the sponge *Callyspongia fallax*. Antifungal agent.

Horn, D.H.S. *et al., J.C.S.*, 1954, 177
Annett, R.L. *et al., Anal. Biochem.*, 1972, **47**, 638 (*resoln*)
Sokolov, V.P. *et al., Zh. Obshch. Khim.*, 1972, **42**, 2119 (*ir*)
Konen, D.A. *et al., J.O.C.*, 1975, **40**, 3253 (*synth*)
Dahlen, B. *et al., Acta Cryst. B*, 1976, **32**, 2059 (*cryst struct*)
Bryn, K. *et al., Eur. J. Biochem.*, 1978, **86**, 311
Barnathan, G. *et al., J. Nat. Prod.*, 1993, **56**, 2104-2113 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*Me ether, isol*)
Carballeira, N.M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 2004, **337**, 152-155 (*Me ether, synth, pmr, cmr, ms*)

14-Hydroxy-5,8,11,13-tetradecatetraenoic acid H-972

$HOCH{=}CHCH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_3COOH$

$C_{14}H_{20}O_3$ 236.31

(5*Z*,8*Z*,11*Z*,13*E*)-*form*

1,3-Hexadienyl ether(Z,Z-): 14-(1,3-Hexadienyloxy)-5,8,11,13-tetradecatetraenoic acid
[151675-36-4]
$C_{20}H_{28}O_3$ 316.439
Constit. of the brown alga *Laminaria* sp. Isol. as Me ester to which registry number refers.

Proteau, P.J. *et al., Lipids*, 1993, **28**, 783-787 (*isol*)

2-Hydroxy-6-tetradecenoic acid H-973

$H_3C(CH_2)_6CH{=}CH(CH_2)_3CH(OH)COOH$

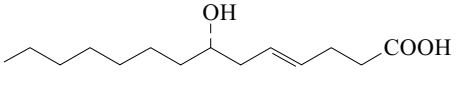
$C_{14}H_{26}O_3$ 242.358

(2ξ,6*Z*)-*form*

Me ether: 2-Methoxy-6-tetradecenoic acid
$C_{15}H_{28}O_3$ 256.384
Isol. from *Callyspongia fallax*.

Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623

7-Hydroxy-4-tetradecenoic acid H-974



$C_{14}H_{26}O_3$ 242.358

(4*E*,7*S*)-*form* [70607-98-6]
Cryst. (pentane). Mp 41-42.5°. $[\alpha]_D^{24}$ +2.5 (c, 2 in $CHCl_3$).

Me ether: 7-Methoxy-4-tetradecenoic acid, 9CI. ***Lyngbic acid***
[70607-97-5]
$C_{15}H_{28}O_3$ 256.384
Constit. of the cyanobacterium *Lyngbya majuscula*. Oil. $Bp_{0.005}$ 120-130°. $[\alpha]_D^{23}$ -14.1 (c, 0.34 in $CHCl_3$). $[\alpha]_D^{20}$ -11.3 (c, 5 in $CHCl_3$).

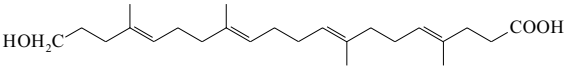
Me ether, Et ester: [70608-01-4]
$C_{17}H_{32}O_3$ 284.438
Oil. $[\alpha]_D^{26}$ -9 (c, 7.3 in $CHCl_3$).

[70608-02-5]

Cardellina, J.H. *et al., Phytochemistry*, 1978, **17**, 2091-2095 (*isol, synth, ir, pmr, cmr, ms*)
Gerwick, W.H. *et al., Phytochemistry*, 1987, **26**, 1701-1704 (*isol*)
Fryhle, C.B. *et al., Tet. Lett.*, 1992, **33**, 2327 (*synth*)
Müller, C. *et al., Annalen*, 1995, 673 (*synth*)
Orjala, J. *et al., J. Nat. Prod.*, 1995, **58**, 764-768 (*isol*)
Sankaranarayanan, S. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 2639-2643 (*synth*)
Virolleaud, M.-A. *et al., Tet. Lett.*, 2006, **47**, 5127-5130 (*synth*)

20-Hydroxy-4,8,13,17-tetramethyl-4,8,12,16-eicosatetraenoic acid H-975

[158964-70-6]

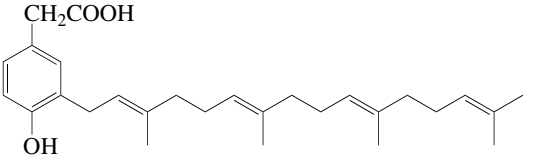


$C_{24}H_{40}O_3$ 376.578
Constit. of the brown alga *Turbinaria ornata*. Gastropod antifeedant.

Sawai, Y. *et al., Fish. Sci.*, 1994, **60**, 199 (*isol*)

4-Hydroxy-3-(3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)benzeneacetic acid H-976

(4-Hydroxy-3-tetraprenylphenyl)acetic acid



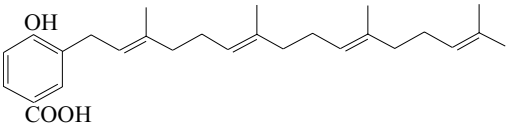
$C_{28}H_{40}O_3$ 424.622

(*all-E*)-*form* [179822-85-6]
Constit. of the sponge *Ircinia muscarum*.
Oil. λ_{max} 279 (ε 1064) (MeOH).

Baz, J.P. *et al., J. Nat. Prod.*, 1996, **59**, 960-961 (*isol, uv, ir, pmr, cmr*)

4-Hydroxy-3-(3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)benzoic acid H-977

3-Geranylgeranyl-4-hydroxybenzoic acid
[39703-10-1]

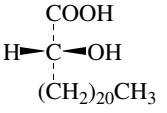


$C_{27}H_{38}O_3$ 410.595
Constit. of *Ircinia spinosula* and *Piper saltuum*. Analgesic. Muscle relaxant. Viscous yellow oil.

Cimino, G. *et al., Experientia*, 1972, **28**, 1401
Maxwell, A. *et al., J. Nat. Prod.*, 1989, **52**, 614 (*isol, uv, ir, pmr, cmr, ms*)

2-Hydroxytricosanoic acid, 9CI H-978

[2718-37-8]



(*R*)-*form*

$C_{23}H_{46}O_3$ 370.615

(*R*)-*form* [26632-12-2]
Present in cerebrosides of the brain.

Me ether: ***2-Methoxytricosanoic acid***
[88416-36-8]
$C_{24}H_{48}O_3$ 384.641
Constit. of the sponge *Higginsia tethyoides*.

(ξ)-*form*

Constit. of various sponges incl. *Amphimedon compressa*, *Callyspongia fallax* and *Suberites massa*.

Downing, D.T. *et al., Aust. J. Chem.*, 1961, **14**, 150 (*isol*)
Ayanoglu, E. *et al., Lipids*, 1983, **18**, 830-836 (*Me ether*)
Barnathan, G. *et al., J. Nat. Prod.*, 1993, **56**, 2104-2113 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*isol*)

15-Hydroxytricosanoic acid H-979

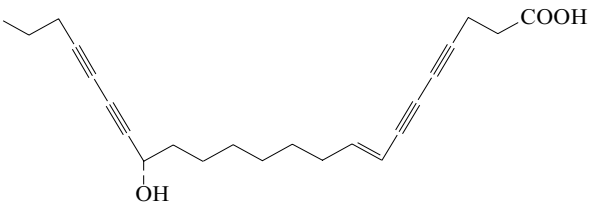
$H_3C(CH_2)_7CH(OH)(CH_2)_{13}COOH$

$C_{23}H_{46}O_3$ 370.615

Me ether: 15-Methoxytricosanoic acid
$C_{24}H_{48}O_3$ 384.641
Constit. of the red alga *Schizymenia dubyi*.

Barnathan, G. *et al., Phytochemistry*, 1998, **47**, 761-765 (*isol, ms*)

16-Hydroxy-8-tricosene-4,6,17,19-tetraynoic acid H-980



$C_{23}H_{28}O_3$ 352.472

(8*E*,16*S*)-*form*

Carduusyne E
[158182-79-7]
Constit. of the marine sponge *Phakellia carduus.*
Oil (as Et ester). $[\alpha]_D$ +7.7 (c, 2.5 in $CHCl_3$) (Et ester). Contains 17% (16*R*)-isomer. λ_{max} 213 (ϵ 18300); 230 (ϵ 3200); 241 (ϵ 6500); 254 (ϵ 12700); 268 (ϵ 17500); 284 (ϵ 14200) (MeOH) (as Et ester).

Me ether: ***Carduusyne C***
[158182-77-5]
$C_{24}H_{30}O_3$ 366.499
Constit. of *Phakellia carduus.* Oil (as Et ester). $[\alpha]_D$ -16.4 (c, 0.58 in $CHCl_3$) (Et ester). Contains 17% (16*R*)-isomer. λ_{max} 213 (ϵ 17900); 230 (ϵ 3100); 242 (ϵ 6600); 254 (ϵ 17800); 268 (ϵ 17500); 284 (ϵ 14300) (MeOH) (as Et ester).

Barrow, R.A. *et al., Aust. J. Chem.*, 1994, **47**, 1901-1918 (*isol, uv, ir, pmr, cmr*)

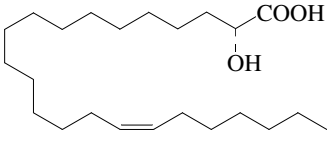
2-Hydroxy-14-tricosenoic acid H-981

$H_3C(CH_2)_7CH{=}CH(CH_2)_{11}CH(OH)COOH$

$C_{23}H_{44}O_3$ 368.599

(Z)-form [156576-71-5]
Constit. of the sea urchin *Tripneustes esculentus.*
Carballeira, N.M. *et al., J. Nat. Prod.*, 1994, **57**, 614

2-Hydroxy-16-tricosenoic acid H-982



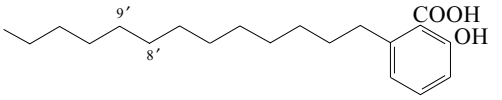
$C_{23}H_{44}O_3$ 368.599

(2*R*,16*Z*)-*form*

Me ether: 2-Methoxy-16-tricosenoic acid
[88416-44-8]
$C_{24}H_{46}O_3$ 382.626
Constit. of the sponge *Higginsia tethyoides.*
Ayanoglu, E. *et al., Lipids*, 1983, **18**, 830-836 (*isol*)

2-Hydroxy-6-tridecylbenzoic acid, 9CI H-983

6-Tridecylsalicylic acid
[20261-38-5]



$C_{20}H_{32}O_3$ 320.471
Isol. from *Ginkgo biloba* (ginkgo), *Pistacia vera* and the brown alga *Caulocystis cephalornithos.* Shows antiinflammatory activity. Plates (hexane). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O.
Mp 85-86° (73-74°). Log P 8.48 (uncertain value) (calc). λ_{max} 244; 308 (MeOH) (Berdy).

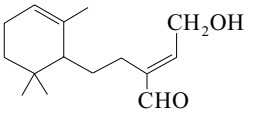
▶ DH2944000

8′,9′-Didehydro (Z-): 2-Hydroxy-6-(8-tridecenyl)benzoic acid. 6-(8-Tridecenyl)salicylic acid
[88640-88-4]
$C_{20}H_{30}O_3$ 318.455
Isol. from *Pistacia vera*.

Durrani, A.A. *et al., J.C.S. Perkin 1*, 1979, 2069 (*synth*)
Buckle, P.J. *et al., Agents Actions*, 1980, **10**, 361 (*pharmacol*)
Kazlauskas, R. *et al., Aust. J. Chem.*, 1980, **33**, 2097 (*isol, pmr, cmr, ir, ms*)
Yalponi, M. *et al., Phytochemistry*, 1983, **22**, 2263 (*isol, deriv*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3016 (*isol, ms, ir, pmr*)
Zehnter, R. *et al., Annalen*, 1995, 2209 (*synth, ir, pmr, cmr*)

4-Hydroxy-2-[2-(2,6,6-trimethyl-2-cyclohexen-1-yl)ethyl]-2-buten-1-al H-984

3-Formyl-5-(2,6,6-trimethyl-2-cyclohexenyl)-2-penten-1-ol

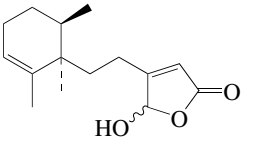


$C_{15}H_{24}O_2$ 236.353

Ac:
$C_{17}H_{26}O_3$ 278.391
Constit. of *Caulerpa flexilis.* Oil. $Bp_{0.8}$ 160°. $[\alpha]_D$ -59 (c, 12 in MeOH).

Capon, R.J. *et al., Aust. J. Chem.*, 1981, **34**, 1775

5-Hydroxy-4-[2-(1,2,6-trimethyl-2-cyclohexen-1-yl)ethyl]-2(5*H*)-furanone H-985

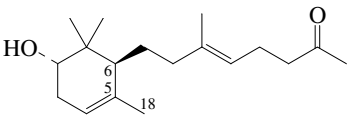


$C_{15}H_{22}O_3$ 250.337

Me ether: [216868-54-1]
$C_{16}H_{24}O_3$ 264.364
Constit. of *Dysidea fragilis.* Oil. $[\alpha]_D$ -17.9 (c, 0.5 in $CHCl_3$). Related to 2-Oxomicrocionin 2-lactone, O-160.

Venkateswarlu, Y. *et al., Nat. Prod. Sci.*, 1998, **4**, 158-160; *CA*, **130**, 35836g (*isol, pmr, cmr*)

8-(5-Hydroxy-2,6,6-trimethyl-2-cyclohexenyl)-6-methyl-5-octen-2-one H-986



$C_{18}H_{30}O_2$ 278.434
Carotene numbering shown.

(2S,6S,9E)-form [81374-00-7]
Constit. of *Cystophora moniliformis*.
Oil. $[\alpha]_D^{21}$ -10.9 (c, 1.1 in CH_2Cl_2).

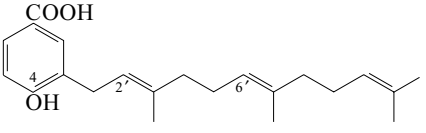
Δ^5-Isomer: ***8-(5-Hydroxy-2,6,6-trimethyl-1-cyclohexenyl)-6-methyl-5-octen-2-one***
[81374-01-8]
$C_{18}H_{30}O_2$ 278.434
Isol. from *Cystophora moniliformis*. Oil. $[\alpha]_D^{22}$ +0.5 (c, 2.2 in CH_2Cl_2).

$\Delta^{5,18}$-Isomer: ***8-(2,2-Dimethyl-3-hydroxy-5-methylenecyclohexyl)-6-methyl-5-octen-2-one***
[81373-99-1]
$C_{18}H_{30}O_2$ 278.434
Isol. from *Cystophora moniliformis*. Oil. $[\alpha]_D^{22}$ -8.6 (c, 1 in CH_2Cl_2).

Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 171-182 (*Cystophora moniliformis constits*)

4-Hydroxy-3-(3,7,11-trimethyl-2,6,10-dodecatrienyl)benzoic acid, 9CI H-987

3-Farnesyl-4-hydroxybenzoic acid
[53696-64-3]



$C_{22}H_{30}O_3$ 342.477
Isol. from *Dictyopteris divaricata*, *Perithalia caudata*, *Phacelia* spp. and *Piper* spp. Oil.

4-Me ether: 3-Farnesyl-4-methoxybenzoic acid
[114567-40-7]
$C_{23}H_{32}O_3$ 356.504
Isol. from *Piper marginatum*. Amorph.
Mp 56-57°.

6′,7′-Dihydro, 6′,7′-dihydroxy: 3-(6,7-Dihydroxy-3,7,11-trimethyl-2,10-dodecadienyl)-4-hydroxybenzoic acid. ***Kuhistanol B***
[266352-37-8]
$C_{22}H_{32}O_5$ 376.492
Constit. of the roots of *Ferula kuhistanica*. Amorph. powder. λ_{max} 208 (log ϵ 4); 258 (log ϵ 4) (MeOH).

10′,11′-Dihydro, 10′,11′-dihydroxy: 3-(10,11-Dihydroxy-3,7,11-trimethyl-2,6-dodecadienyl)-4-hydroxybenzoic acid. ***Kuhistanol A***
[266352-36-7]
$C_{22}H_{32}O_5$ 376.492
Constit. of the roots of *Ferula kuhistanica*. Amorph. powder. $[\alpha]_D^{25}$ +1.6 (c, 1 in MeOH). λ_{max} 214 (log ϵ 4.3); 259 (log ϵ 4.1) (MeOH).

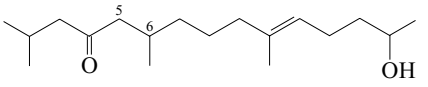
5-Chloro, amide: 3-Chloro-5-farnesyl-4-hydroxybenzamide
[352459-34-8]
$C_{22}H_{30}ClNO_2$ 375.937
Isol. from an unidentified South African soil fungus. Antibacterial agent.
Mp 47-49°. λ_{max} 233 (ϵ 5850); 257 (ϵ 7790); 274 (ϵ 45270); 429 (ϵ 600) (CH_2Cl_2).

[104777-73-3, 114567-37-2]

Reynolds, G.W. *et al., Planta Med.*, 1985, **40**, 394 (*pmr, cmr*)
Reynolds, G.W. *et al., Phytochemistry*, 1986, **25**, 1617 (*isol*)
Maxwell, A. *et al., J. Nat. Prod.*, 1988, **51**, 370 (*isol, deriv*)
Segawa, M. *et al., Phytochemistry*, 1990, **29**, 973 (*isol*)
Rochfort, S.J. *et al., J. Nat. Prod.*, 1994, **57**, 849 (*isol, pmr, cmr*)
Chen, B. *et al., J. Nat. Prod.*, 2000, **63**, 362-365 (*Kuhistanols*)
Krohn, K. *et al., Nat. Prod. Lett.*, 2001, **15**, 9-12 (*Chlorofarnesylhydroxybenzamide*)

14-Hydroxy-2,6,10-trimethyl-10-pentadecen-4-one H-988

[71801-99-5]



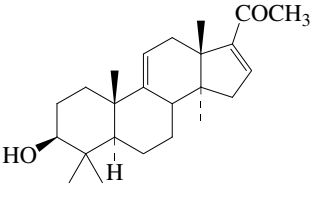
$C_{18}H_{34}O_2$ 282.465
Constit. of *Sargassum micracanthum*.

5,6-Didehydro: 14-Hydroxy-2,6,10-trimethyl-5,10-pentadecadien-4-one, 9CI
[71801-98-4]
$C_{18}H_{32}O_2$ 280.45
Constit. of *Sargassum micracanthum*.
$[\alpha]_D$ -3.2 ($CHCl_3$).

[73542-72-0, 73542-73-1]

Kusumi, T. *et al., Chem. Lett.*, 1979, 1181 (*isol, ir, pmr, ms*)

3-Hydroxy-4,4,14-trimethylpregna-9(11),16-dien-20-one H-989

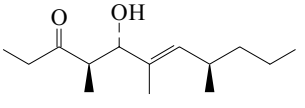


$C_{24}H_{36}O_2$ 356.547

(3β,5α)-form
Kurilogenin
[90139-20-1]
Isol. from the holothurian *Duasmodactyla kurilensis*.
Cryst. (MeOH aq.).
Mp 152-154°. $[\alpha]_D^{20}$ +79.3 (c, 2.2 in $CHCl_3$).

Kalinovskii, A.I. *et al., Khim. Prir. Soedin.*, 1983, **19**, 724-727; *Chem. Nat. Compd. (Engl. Transl.)*, 1983, **19**, 688-691

5-Hydroxy-4,6,8-trimethyl-6-undecen-3-one H-990



$C_{14}H_{26}O_2$ 226.358

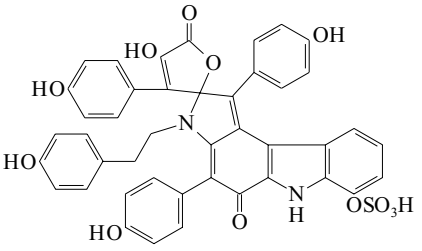
(4R,5S,8R)-form

Propanoyl: 4,6,8-Trimethyl-5-(propanoyloxy)-6-undecen-3-one
[91466-59-0]
$C_{17}H_{30}O_3$ 282.422
Isol. from the mollusc *Siphonaria australis*.
$[\alpha]_D$ -19.4 ($CHCl_3$).

Hochlowski, J.E. *et al., J.O.C.*, 1984, **49**, 3838-3840 (*isol*)
Sundram, U.N. *et al., Tet. Lett.*, 1992, **33**, 437-440 (*synth, abs config*)

4-Hydroxy-1′,3,4′-tris(4-hydroxyphenyl)-3′-[2-(4-hydroxyphenyl)ethyl]-7′-(sulfooxy)spiro[furan-2(5*H*),2′(3′*H*)-pyrrolo[2,3-*c*]carbazole]-5,5′(6′*H*)-dione, 9CI H-991

[149444-91-7]



$C_{43}H_{30}N_2O_{12}S$ 798.782

Isol. from the marine sponge *Dictyodendrilla* sp. Potent aldose reductase inhibitor. Purple solid (as Na salt).

Mp 300° (Na salt). Opt. inactive (racemic). λ_{max} 229 (ϵ 40800); 289 (ϵ 20900); 324 (ϵ 19800); 391 (ϵ 9700); 475 (ϵ 1200) (EtOH) (Derep).

[149444-90-6]

Sato, A. *et al., J.O.C.*, 1993, **58**, 7632 (*isol, uv, ir, pmr, cmr, struct*)

41-Hydroxy-2,42-tritetracontapentaenediynoic acid H-992

$C_{43}H_{68}O_3$ 633.008

Me ester: ***Petroformyne A***

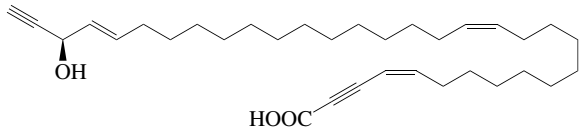
[128646-22-0]

$C_{44}H_{70}O_3$ 647.035

Constit. of the sponge *Petrosia ficiformis*. Posns. of ethylenic groups not determined. λ_{max} 248 (ϵ 8400) (MeOH) (Berdy).

Cimino, G. *et al., J. Nat. Prod.*, 1990, **53**, 345

31-Hydroxy-4,15,29-tritriacontatriene-2,32-diynoic acid H-993



$C_{33}H_{52}O_3$ 496.772

(4*Z*,15*Z*,29*E*,31*R*)-*form*

Triangulynic acid

[182314-15-4]

Isol. from the sponge *Pellina triangulata*. Cytotoxic agent. Oil. $[\alpha]_D$ -12.9 (c, 1.2 in $CHCl_3$). λ_{max} 203 (log ϵ 4); 241 (log ϵ 4); 247 (log ϵ 4) (MeOH).

Dai, J.-R. *et al., J. Nat. Prod.*, 1996, **59**, 860-865 (*isol, uv, ir, pmr, cmr, ms*)

31-Hydroxy-4,18,29-tritriacontatriene-2,32-diynoic acid H-994

HC≡CCH(OH)CH=CH$(CH_2)_9$CH=CH$(CH_2)_{12}$CH=CHC≡CCOOH

$C_{33}H_{52}O_3$ 496.772

(-)-(4*Z*,18*Z*,29*E*)-*form*

Pellynic acid

[186248-08-8]

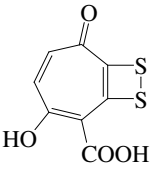
Isol. from the sponge *Pellina triangulata*.

Gum. $[\alpha]_D$ -10.5 (c, 0.3 in $CHCl_3$/MeOH).

Fu, X. *et al., Tetrahedron*, 1997, **53**, 799 (*isol, ir, pmr, cmr, ms*)

Hydroxytropodithietic acid H-995

*4-Hydroxy-7-oxo-7*H*-3-cycloheptadithietecarboxylic acid*



$C_8H_4O_4S_2$ 228.249

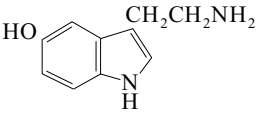
Prod. by the marine-derived *Ruegeria* sp. strain T5. Pale yellow solid. λ_{max} 237; 268; 355; 399 (no solent reported).

Liang, L. *et al., Dissertation*, Univ. of Göttingen, 2003, (*isol, uv, pmr, cmr, ms, cryst struct*)

5-Hydroxytryptamine H-996

*3-(2-Aminoethyl)-1*H*-indol-5-ol, 9CI. 3-(2-Aminoethyl)-5-hydroxyindole. Anthemovister. Enteramine. Hippophaine.* ***Serotonin****. Thrombocytin. Thrombotonin. 5HT. 5-HT*

[50-67-9]



$C_{10}H_{12}N_2O$ 176.218

Found in blood and other tissues. Widespread alkaloid from terrestrial and marine organisms, e.g. *Mucuna pruriens*, bananas (*Musa* sp.) and other fruits, basidiomycete *Panaeolus campanulatus*, cotton (*Gossypium hirsutum*) and other plants. Also from the sea anemone *Calliactis parasitica*, *Hippophae rhaminoides*, *Panaeolus* sp., *Pentacta crassa*, *Thelenota ananas*, *Octopus vulgaris*, *Eledone moschata*, *Corallistes undulatus*, *Physalia* sp., *Hydra littoralis* , *Sycon ciliatum* and arthropod venoms and constit. of toad venom (*Bufo* spp.). Vasoconstrictor, hypotensive agent, neurotransmitter. Plays a major role in regulating behaviour such as aggression, depression, psychosis. pK_{a1} 1; pK_{a2} 4.52; pK_{a3} 15 (20°). Log P 0.61 (calc). Echinoderm name given apparently incorrectly as Pentacter crasa.

▶ LD_{50} (mus, orl) 60 mg/kg. Exp. reprod. and teratogenic effects. NM2450000

Creatinine sulfate complex: Antemovis

[971-74-4]

[61-47-2]

Found in mammalian sera. Potent vasoconstrictor. Plates +1H_2O. Mp 214-216° dec. (monohydrate).

▶ NM2550000

O-*Sulfate:* [16310-20-6]

$C_{10}H_{12}N_2O_4S$ 256.282

Metab. of 5-hydroxytryptamine excreted in mammalian urine. Cryst. (H_2O).

Mp 192-194°.

N^b-*Ac:* [1210-83-9]

$C_{12}H_{14}N_2O_2$ 218.255

Metab. of 5-hydroxytryptamine. Enzyme inhibitor. Melanophore which produces night coloration in fish.

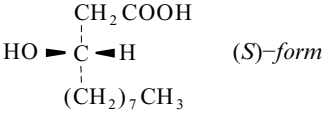
Mp 120-122°.

Hamlin, K.E. *et al., J.A.C.S.*, 1951, **73**, 5007-5008 (*synth, uv*)
Speeter, H.E. *et al., J.A.C.S.*, 1951, **73**, 5514-5515 (*synth*)
Asero, B. *et al., Annalen*, 1952, **576**, 69-74 (*synth, uv*)
Bowden, K. *et al., Nature (London)*, 1954, **174**, 925-926 (*isol*)
Abramovitch, R.A. *et al., Chem. Ind. (London)*, 1955, 1255 (*synth*)
Mathias, A.P. *et al., Nature (London)*, 1957, **180**, 658-659 (*isol, occur*)
Thewalt, U. *et al., Acta Cryst. B*, 1972, **28**, 82-92 (*cryst struct*)
Couch, M.W. *et al., Anal. Biochem.*, 1972, **50**, 612-622 (*ms*)
Biagini, S. *et al., J.C.S. Faraday 2*, 1983, **79**, 491-496 (*pmr, cmr*)
Borgulya, J. *et al., Synthesis*, 1983, 29-30 (*O-sulfate*)
Falcon, J. *et al., Ann. Endocrinol.*, 1986, **47**, 65-66 (N^b-*Ac, activity*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1411
Somei, M. *et al., Heterocycles*, 1997, **46**, 91-94 (*synth*)
Zaunreiter, M. *et al., NeuroReport*, 1998, **9**, 1475-1479; *CA*, **129**, 173288 (*N^b-Ac, activity*)
Neuropsychopharmacology, Special Supplement Issue, Serotonin 50th Anniversary, 1999, **21**, 2S-115S (***rev***)
Somei, M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 87-96 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, (*AJX500, AJX750*)

3-Hydroxyundecanoic acid, 9CI H-997

[40165-88-6]



(*S*)–*form*

$C_{11}H_{22}O_3$ 202.293

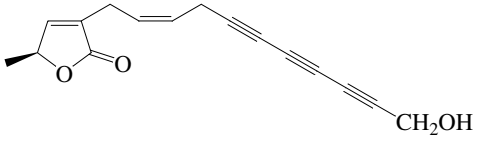
(S)-form [66997-62-4]
Mp 64-65°. $[\alpha]_D^{18}$ +17.1 (c, 2.1 in $CHCl_3$).

(±)-form
Occurs in *Pseudomonas maltophilia*.
Cryst. (petrol).
Mp 73-73.5°.

(ξ)-form
O-*[α-L-Rhamnopyranosyl-(1→3)-3-hydroxyundecanoyl]*: ***Pyolipic acid***
[637780-11-1]
$C_{28}H_{52}O_9$ 532.713
Prod. by *Pseudomonas aeruginosa* and the marine-derived *Pseudomonas* sp. strain NUDMB50-11.

Skogh, M. *et al., Acta Chem. Scand.*, 1952, **6**, 809 (*synth*)
Itoh, S. *et al., J. Antibiot.*, 1971, **24**, 855-859 (*Pyolipic acid*)
Moss, C.W. *et al., J. Bacteriol.*, 1973, **114**, 1018 (*ms, ir*)
Tahara, S. *et al., Agric. Biol. Chem.*, 1978, **42**, 879 (*synth*)
Burgess, J.G. *et al., Biofouling*, Suppl., 2003, **19**, 197-205 (*Pyolipic acid*)

3-(11-Hydroxy-2-undecene-5,7,9-triynyl)-5-methyl-2(5*H*)-furanone H-998



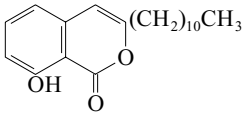
$C_{16}H_{14}O_3$ 254.285

(S,Z)-form
Isol. from *Sarcophyton tracheliophorum*.
Pale brown oil. $[\alpha]_D$ +39.5 (c, 0.14 in EtOH). λ_{max} 313 (log ϵ 4.12) (EtOH).

Rezanka, T. *et al., Tetrahedron*, 2001, **57**, 8743-8749

8-Hydroxy-3-undecyl-1*H*-2-benzopyran-1-one H-999

8-Hydroxy-3-undecylisocoumarin
[132185-29-6]

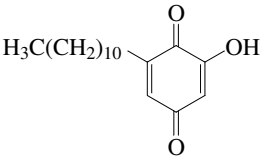


$C_{20}H_{28}O_3$ 316.439
Isol. from the brown alga *Caulocystis cephalornithos*.

Amico, V. *et al., J. Nat. Prod.*, 1990, **53**, 1379 (*isol*)

2-Hydroxy-6-undecyl-1,4-benzoquinone H-1000

2-Hydroxy-6-undecyl-2,5-cyclohexadiene-1,4-dione, 9CI. 2-Deoxyembelin

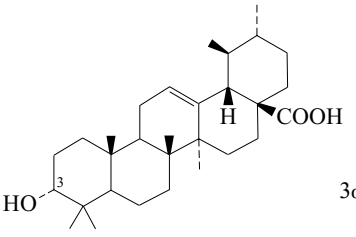


$C_{17}H_{26}O_3$ 278.391

Me ether: 2-Methoxy-6-undecyl-1,4-benzoquinone. ***2-Deoxy-5-O-methylembelin***
[95168-94-8]
$C_{18}H_{28}O_3$ 292.417
Constit. of the mangrove plant *Aegiceras corniculatum*.
Mp 72°.

König, W.A. *et al., Z. Naturforsch., B*, 1993, **48**, 387-393 (*synth, pmr, ms*)
Xu, M. *et al., J. Nat. Prod.*, 2004, **67**, 762-766 (*isol*)

3-Hydroxy-12-ursen-28-oic acid H-1001



3α–*form*

$C_{30}H_{48}O_3$ 456.707

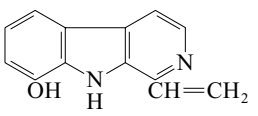
3β-form
Ursolic acid. *Micromerol. Formosolic acid. Forucosolic acid. Bungeolic acid. Prunol. Urson. Malol*
[77-52-1]
Identity of Formosolic (?Forucosolic) acid not clear from abstract. Constit. of *Rhododendron* spp. and *Epigaea asiatica*, also found in wax of apples, pears and other fruits. V. widely distributed in plants. Isol from a Black Sea alga, family Cladophoraceae. Diuretic. Antineoplastic agent. Possesses antiulcer and angiogenesis inhibiting props. Shows anti-HIV activity. Inhibits skin tumourigenesis. Inhibits protein kinase C. HIV-1 protease inhibitor. Cryst. (Et_2O).
Mp 291°. $[\alpha]_D$ +66 (EtOH). Log P 8.59 (uncertain value) (calc). A compd. claimed to be an unidentified stereoisomer of ursolic acid was isol. from a Black Sea bryozoan *Conopeum seuratum* but the exp. evidence was not conclusive.

[74984-66-0, 117804-17-8, 117804-18-9, 117804-25-8]

Ruzicka, L. *et al., Helv. Chim. Acta*, 1945, **28**, 199 (*struct*)
Huneck, S. *et al., J. Prakt. Chem.*, 1968, **38**, 233 (*ms*)
Seo, S. *et al., Chem. Comm.*, 1975, 270; 954 (*biosynth, pmr*)
Seo, S. *et al., Tet. Lett.*, 1975, 7 (*cmr*)
Romeo, G. *et al., Org. Magn. Reson.*, 1977, **9**, 29 (*pmr*)
Johns, S.R. *et al., Aust. J. Chem.*, 1983, **36**, 2537 (*cmr*)
Tomita, Y. *et al., Chem. Comm.*, 1985, 1087 (*biosynth*)
Seo, S. *et al., Chem. Comm.*, 1986, 1141 (*biosynth*)
Hadjieva, P. *et al., Z. Naturforsch., C*, 1987, **42**, 1019-1022 (*isol, alga, bryozoan*)
Simon, A. *et al., Acta Cryst. C*, 1992, **48**, 726 (*cryst struct*)
Tomita, Y. *et al., Phytochemistry*, 1994, **35**, 121 (*biosynth*)
Alves, J.S. *et al., Magn. Reson. Chem.*, 2000, **38**, 201-206 (*pmr, cmr*)

8-Hydroxy-1-vinyl-β-carboline H-1002

*1-Ethenyl-9*H*-pyrido[3,4-*b*]indol-8-ol, 9CI*
[138683-69-9]

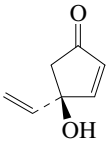


$C_{13}H_{10}N_2O$ 210.235
Alkaloid from the marine bryozoans *Cribricellina cribraria* and *Catenicella cribraria*. Exhibits cytotoxicity. Yellow oil. Pmr data revised in 1993. λ_{max} 240 (ϵ 11700); 262 (ϵ 11500); 287 (ϵ 10800); 386 (ϵ 6610) (MeOH/NaOH) (Derep). λ_{max} 230 (ϵ 11500); 244 (ϵ 12300); 296 (ϵ 9330); 369 (ϵ 8510) (MeOH) (Derep). λ_{max} 240 (ϵ 11750); 262 (ϵ 11450); 287 (ϵ 10715); 386 (ϵ 6600) (EtOH) (Berdy).

Prinsep, M.R. *et al., J. Nat. Prod.*, 1991, **54**, 1068 (*isol, uv, ir, pmr, cmr, struct*)
Beutler, J.A. *et al., J. Nat. Prod.*, 1993, **56**, 1825 (*isol, pmr*)

4-Hydroxy-4-vinyl-2-cyclopenten-1-one H-1003

4-Ethenyl-4-hydroxy-2-cyclopenten-1-one, 9CI

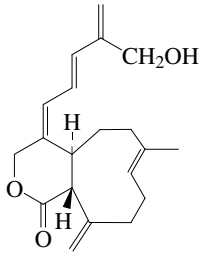


$C_7H_8O_2$ 124.139

(*R*)-*form*
Trichodenone A
[203243-21-4]
Prod. by a strain of *Trichoderma harzianum* from the sponge *Halichondria okadai*. Cytotoxic agent. Oil. Sol. MeOH, EtOAc, hexane, Me_2CO, $CHCl_3$, DMSO; poorly sol. H_2O. $[\alpha]_D^{28}$ +56.3 (c, 0.7 in $CHCl_3$) (natural). $[\alpha]_D$ +141.6 (c, 0.9 in $CHCl_3$) (synthetic). The nat. prod. is prob. a partial racemate. λ_{max} 223 (log ϵ 3.74) (EtOH).

Amagata, T. *et al., J. Antibiot.*, 1998, **51**, 33-40 (*isol, uv, ir, cd, pmr, cmr*)
Usami, Y. *et al., Synlett*, 1999, 723-724 (*synth, abs config*)

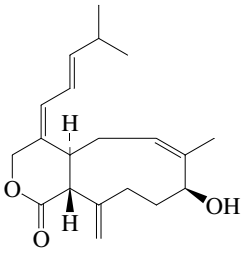
15-Hydroxy-1(19),6,10,12,14(16)-xenicapentaen-18,17-olide H-1004



$C_{20}H_{26}O_3$ 314.424

(6*E*,10*E*,12*E*)-*form*
Xeniaol
[251343-61-0]
Constit. of a *Xenia* sp.
Oil. $[\alpha]_D^{26}$ -3.9 (c, 3.9 in $CHCl_3$). λ_{max} 275 (ϵ 15700) (EtOH).
Miyaoka, H. *et al., Tetrahedron*, 1999, **55**, 12977-12982 (*isol, pmr, cmr*)

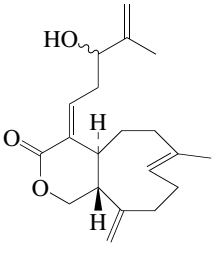
7-Hydroxy-1(19),5,10,12-xenicatetraen-18,17-olide H-1005



$C_{20}H_{28}O_3$ 316.439

(5*Z*,7β,10*E*,12*E*)-*form*
Florlide H
[267417-31-2]
Constit. of *Xenia florida*.
Oil. $[\alpha]_D$ +305 (c. 0.06 in MeOH). λ_{max} 246 (log ϵ 4.16) (MeOH).
Iwagawa, T. *et al., J. Nat. Prod.*, 2000, **63**, 468-472 (*isol, pmr, cmr*)

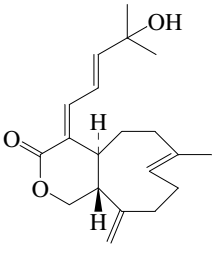
13-Hydroxy-1(19),6,10,14-xenicatetraen-17,18-olide H-1006



$C_{20}H_{28}O_3$ 316.439

Ac: ***Xeniolide C***
[195259-82-6]
$C_{22}H_{30}O_4$ 358.477
Constit. of *Eleutherobia aurea*. Oil. $[\alpha]_D^{21}$ +96.4 (c, 1.17 in $CHCl_3$).
Hooper, G.J. *et al., J. Nat. Prod.*, 1997, **60**, 889-893 (*isol, pmr, cmr*)

14-Hydroxy-1(19),6,10,12-xenicatetraen-17,18-olide H-1007



(6*E*,10*E*,12*E*)-*form*

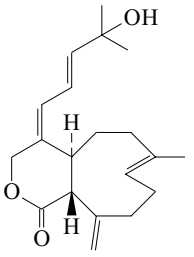
$C_{20}H_{28}O_3$ 316.439

(6*E*,10*E*,12*E*)-*form*
8-Deoxyxeniolide A. *9-Deoxyxeniolide A*
[181306-74-1]
Constit. of a *Xenia* sp.

(6*E*,10*Z*,12*E*)-*form* [866228-93-5]
Constit. of *Xenia blumi*.
Oil. $[\alpha]_D^{25}$ +36 (c, 0.6 in $CHCl_3$). λ_{max} 265 (log ϵ 4.1) (MeOH).
Vervoort, H.C. *et al., Nat. Prod. Lett.*, 1995, **6**, 49-55 (*8-Deoxyxeniolide A*)
El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 1336-1340 (*Xenia blumi constit*)

14-Hydroxy-1(19),6,10,12-xenicatetraen-18,17-olide H-1008

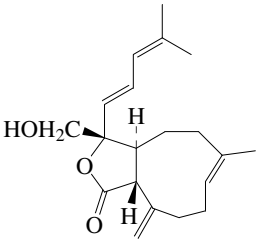
8-Deoxyxeniolide B. *9-Deoxyxeniolide B*
[181306-75-2]



$C_{20}H_{28}O_3$ 316.439
Constit. of a *Xenia* sp.

18β-Alcohol (lactol): 17,18-Epoxy-1(19),6,10,12-xenicatetraene-14,18-diol. ***9-Deoxyxenialactol C***
[479067-63-5]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Xenia umbellata*. Amorph. solid. $[\alpha]_D^{25}$ -18.8 (c, 0.52 in $CHCl_3$). λ_{max} 221 (log ϵ 3.79) (MeOH).
Vervoort, H.C. *et al., Nat. Prod. Lett.*, 1995, **6**, 49 (*isol, pmr, cmr*)
Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1882-1885 (*9-Deoxyxenialactol C*)

17-Hydroxy-1(19),6,11,13-xenicatetraen-18,10-olide H-1009

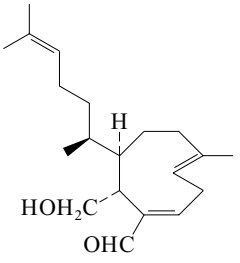


$C_{20}H_{28}O_3$ 316.439

(6*E*,10α,11*E*)-*form*
Xeniolactone C
[861676-59-7]
Constit. of *Xenia florida*.
Amorph. powder. $[\alpha]_D^{25}$ -60 (c, 0.1 in CH_2Cl_2). λ_{max} 228 (MeOH).
Shen, Y.-C. *et al., Tet. Lett.*, 2005, **46**, 4793-4796 (*Xeniolactone C*)

18-Hydroxy-1(9),6,13-xenicatrien-19-al H-1010

Dictyolal

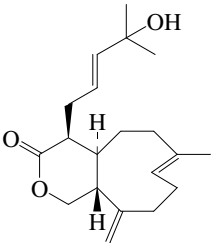


$C_{20}H_{32}O_2$ 304.472

Ac: ***Acetyldictyolal***
$C_{22}H_{34}O_3$ 346.509
Constit. of marine algae *Dictyota dichotoma* and *Pachydictyon coriaceum*. Oil. $[\alpha]_D^{19}$ -104 (c, 0.5 in $CHCl_3$).

18-Aldehyde: 1(9),6,13-Xenicatriene-18,19-dial. ***Dictyodial A***
[70552-61-3]
$C_{20}H_{30}O_2$ 302.456
Isol. from *Dictyota crenulata*, *Dictyota flabellata* and *Aplysia depilans*. HIV reverse transcriptase (HIV-rt) inhibitor. Algicide. Oil. Sol. MeOH, hexane. $[\alpha]_D^{25}$ -95 (c, 1.2 in $CHCl_3$). λ_{max} 232 (ϵ 7300) (EtOH) (Berdy).
Finer, J. *et al., J.O.C.*, 1979, **44**, 2044-2047 (*isol, cryst struct*)
Ishitsuka, M. *et al., Chem. Lett.*, 1982, 1517 (*isol*)
Enoki, N. *et al., Chem. Lett.*, 1982, 1749 (*isol*)
Kirkup, M.P. *et al., Phytochemistry*, 1983, **22**, 2539 (*isol*)
Nagaoka, H. *et al., Tet. Lett.*, 1988, **29**, 5945 (*abs config*)

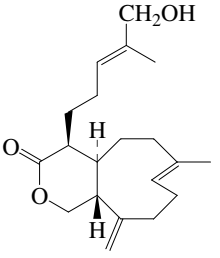
14-Hydroxy-1(19),6,12-xenicatrien-17,18-olide H-1011



$C_{20}H_{30}O_3$ 318.455

(6*E*,10α*H*,12*E*)-*form*
Acalycixeniolide J
[340156-18-5]
Constit. of *Acalycigorgia inermis*.
Amorph. solid.
Mp 93-95°. $[\alpha]_D^{25}$ +49.4 (c, 0.14 in MeOH).
Rho, J.-R. *et al., J. Nat. Prod.*, 2001, **64**, 540-543 (*isol, pmr, cmr*)

15-Hydroxy-1(19),6,13-xenicatrien-17,18-olide H-1012



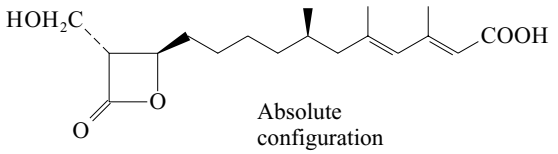
$C_{20}H_{30}O_3$ 318.455

(6*E*,10α*H*,13*E*)-*form*
Acalycixeniolide I
[340156-17-4]
Constit. of *Acalycigorgia inermis*.
Amorph. solid.
Mp 95-98°. $[\alpha]_D$ +103.9 (c, 0.35 in MeOH).
Rho, J.-R. *et al., J. Nat. Prod.*, 2001, **64**, 540-543 (*isol, pmr, cmr*)

Hymeglusin H-1013

11-[3-(Hydroxymethyl)-4-oxo-2-oxetanyl]-3,5,7-trimethyl-2,4-undecadienoic acid, 9CI. 12-Hydroxy-13-(hydroxymethyl)-3,5,7-trimethyl-2,4-tetradecadiene-1,14-dioic acid (12→14)-lactone. 1233A. F 244. L 659699. Antibiotic 1233A. Antibiotic F 244. Antibiotic L 659699

[29066-42-0]



$C_{18}H_{28}O_5$ 324.416

Metab. of a *Cephalosporium* sp., *Scopulariopsis* sp. and *Fusarium* sp. Active against gram-positive bacteria. Specific inhibitor of Cholesterol biosynth. and HMG-CoA synthetase in animal cells. Prisms (Et_2O/petrol).

Mp 76-77°. $[\alpha]_D$ +28.6 (c, 0.26 in $CHCl_3$). λ_{max} 267 (ϵ 12200) (MeOH) (Derep).

▶ YQ1170000

Ac:

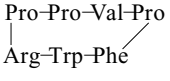
Solid (MeOH aq.). Mp 59.5-61°.

[112924-46-6]

Aldridge, D.C. *et al., J.C.S.(C)*, 1971, 3888 (*struct, ir, uv, ms, nmr, isol*)
Omura, S. *et al., J. Antibiot.*, 1987, **40**, 1356; 1988, **41**, 247 (*isol, props*)
Greenspan, M.D. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1987, **84**, 7488 (*isol*)
Chiang, Y.-C. *et al., J.O.C.*, 1988, **53**, 4599; 1989, **54**, 5708 (*abs config, synth, bibl*)
Mori, K. *et al., Annalen*, 1991, 1057 (*synth, bibl*)
Koseki, K. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1728 (*struct*)
Kumagai, H. *et al., J. Antibiot.*, 1992, **45**, 563 (*biosynth*)
Sunazuka, T. *et al., J. Antibiot.*, 1992, **45**, 1139 (*synth, bibl*)
Wovkulich, P.M. *et al., J.O.C.*, 1993, **58**, 832 (*synth, bibl*)
Wattanasin, S. *et al., J.O.C.*, 1993, **58**, 1610 (*synth, bibl*)
Saepudin, E. *et al., Can. J. Chem.*, 1995, **73**, 1 (*biosynth*)
Dymock, B.W. *et al., Synthesis*, 1998, 1655-1661 (*synth, ir, uv, pmr, cmr*)
Bates, R.W. *et al., J.C.S. Perkin 1*, 1999, 1917-1925 (*synth*)
Höller, U. *et al., Mycol. Res.*, 2000, **104**, 1354-1365 (*isol, pmr, cmr*)
Tomoda, H. *et al., Biochim. Biophys. Acta*, 2004, **1636**, 22-28 (*activity*)

Hymenamide A H-1014

[148472-99-5]



$C_{46}H_{61}N_{11}O_7$ 880.057

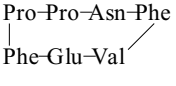
Isol. from the marine sponge *Hymeniacidon* sp. Amorph. solid. Sol. MeOH, butanol.

Mp 126-128°. $[\alpha]_D^{20}$ -46 (c, 0.53 in MeOH). λ_{max} 280 (ϵ 2100) (MeOH) (Berdy).

Kobayashi, J. *et al., Tetrahedron*, 1993, **49**, 2391 (*isol*)

Hymenamide B H-1015

[148473-00-1]



$C_{42}H_{54}N_8O_{10}$ 830.936

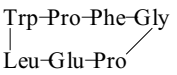
Isol. from the marine sponge *Hymeniacidon* sp. Amorph. solid. Sol. MeOH, butanol.

Mp 157-158°. $[\alpha]_D^{20}$ -30 (c, 1.2 in MeOH). λ_{max} 210 (ϵ 14000); 280 (ϵ 400) (MeOH) (Berdy).

Kobayashi, J. *et al., Tetrahedron*, 1993, **49**, 2391 (*isol*)

Hymenamide C H-1016

[151606-41-6]



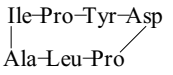
$C_{43}H_{54}N_8O_9$ 826.948

Isol. from the marine sponge *Hymeniacidon* sp. Immunomodulator. Amorph. solid. $[\alpha]_D^{17}$ -138 (c, 0.41 in MeOH). λ_{max} 282 (ϵ 3200); 291 (ϵ 2700) (MeOH) (Berdy).

Tsuda, M. *et al., Tetrahedron*, 1993, **49**, 6785-6796 (*isol, pmr, cmr*)
Napolitano, A. *et al., Tetrahedron*, 2001, **57**, 6249-6255 (*synth, pmr, cmr*)

Hymenamide D H-1017

[151606-42-7]



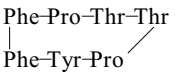
$C_{38}H_{55}N_7O_{10}$ 769.893

Isol. from the marine sponge *Hymeniacidon* sp. Amorph. solid. $[\alpha]_D^{17}$ -70.8 (c, 0.15 in MeOH). λ_{max} 279 (ϵ 1400) (MeOH) (Berdy).

Tsuda, M. *et al., Tetrahedron*, 1993, **49**, 6785 (*isol*)

Hymenamide E H-1018

[151606-43-8]



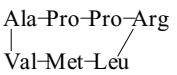
$C_{45}H_{55}N_7O_{10}$ 853.97

Isol. from the marine sponge *Hymeniacidon* sp. Amorph. solid. $[\alpha]_D^{20}$ -108 (c, 0.94 in MeOH). λ_{max} 279 (ϵ 1700) (MeOH) (Berdy).

Tsuda, M. *et al., Tetrahedron*, 1993, **49**, 6785 (*isol*)

Hymenamide F H-1019

[176678-83-4]



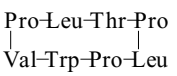
$C_{35}H_{60}N_{10}O_7S$ 764.988

Cyclic peptide. Isol. from the sponge *Hymeniacidon* sp. Amorph. solid (as *S*-oxide). $[\alpha]_D^{20}$ -25 (0.2 in MeOH) (*S*-oxide).

Kobayashi, J. *et al., Tetrahedron*, 1996, **52**, 6355-6360 (*isol, pmr, cmr, struct*)

Hymenamide H H-1020

[156281-00-4]



$C_{47}H_{69}N_9O_9$ 904.117

Isol. from the marine sponge *Hymeniacidon* sp. Amorph. solid. Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. $[\alpha]_D^{20}$ -88 (c, 1.02 in MeOH). λ_{max} 226 (sh); 279 (MeOH). λ_{max} 279 (ϵ 1400) (MeOH) (Berdy).

Tsuda, M. *et al., Tetrahedron*, 1994, **50**, 4667 (*isol, uv, ir, pmr, cmr*)

Hymenamide J H-1021

[156281-01-5]

Pro–Tyr–Asp–Phe
| |
Tyr–Val–Lys–Trp

$C_{58}H_{70}N_{10}O_{12}$ 1099.251

Isol. from the marine sponge *Hymeniacidon* sp. Amorph. solid. $[\alpha]_D^{20}$ -69 (c, 0.17 in MeOH). λ_{max} 222 (ϵ 38000); 280 (ϵ 7000) (MeOH).

Tsuda, M. *et al., Tetrahedron*, 1994, **50**, 4667 (*isol, uv, ir, pmr, cmr*)

Hymenamide K H-1022

[156281-03-7]

Pro–Tyr–Asp–Phe
| |
Val–Ala–Lys–Trp

$C_{52}H_{66}N_{10}O_{11}$ 1007.154

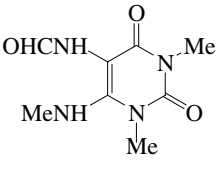
Isol. from the marine sponge *Hymeniacidon* sp. Amorph. solid. Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. $[\alpha]_D^{20}$ -36 (c, 0.45 in MeOH). λ_{max} 221 (ϵ 25000); 280 (ϵ 5000) (MeOH). λ_{max} 221 (ϵ 25000); 280 (ϵ 5000) (MeOH) (Berdy).

Tsuda, M. *et al., Tetrahedron*, 1994, **50**, 4667 (*isol, uv, ir, pmr, cmr*)

Hymeniacidine H-1023

5-(Formylamino)-6-(methylamino)-2,4-pyrimidinedione. 5-(Formylamino)-6-(methylamino)uracil. N-*Methyl*-N-*[1,2,3,4-tetrahydro-1,3-dimethyl-6-(methylamino)-2,4-dioxo-5-pyrimidinyl]formamide, 9CI*

[104509-28-6]



$C_8H_{12}N_4O_3$ 212.208

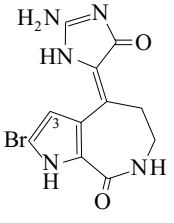
Seco-xanthine formamide. Alkaloid from the sponge *Hymeniacidon* sp. Viscous pale yellow oil (natural). Cryst. (EtOAc) (synthetic).
Mp 158-159° (synthetic). Exists as two formamide rotamers. λ_{max} 271 (ϵ 11400) (MeOH).

Capon, R.J. *et al., J. Nat. Prod.*, 2002, **65**, 368-370 (*isol, synth, pmr, cmr, ms*)

Hymenialdisine H-1024

4-(2-Amino-4-oxo-2-imidazolidin-5-ylidene)-2-bromo-4,5,6,7-tetrahydropyrrolo[2,3-c]azepin-8-one

[82005-12-7]



$C_{11}H_{10}BrN_5O_2$ 324.136

Isol. from the Okinawan marine sponge *Hymeniacidon aldis*, the Red Sea sponge *Acanthella aurantiaca* and the sponges *Axinella verrucosa* and *Axinella carteri*. Exhibits potent cytotoxicity against murine P388 lymphocytic leukaemia cells. Shows insecticidal activity. Inhibits interleukin-1 stimulated rheumatoid synovial fibroblasts. Antiinflammatory agent. Yellow needles + 1MeOH (MeOH aq.) or yellow amorph. solid. Sol. DMSO, insol. most solvs.
Mp 160-164° dec. λ_{max} 229 (ϵ 11900); 270 (ϵ 11700); 346 (ϵ 15900) (MeOH) (Derep).

*(*E*)-Isomer:* ***(10E)-Hymenialdisine***
$C_{11}H_{10}BrN_5O_2$ 324.136
Isol. from the marine sponge *Stylotella aurantium*.

Debromo: ***Debromohymenialdisine***
[75593-17-8]
$C_{11}H_{11}N_5O_2$ 245.24
Isol. from the Great Barrier Reef sponge *Phakellia flabellata, Hymeniacidon aldis*, and from an unidentified sponge from Korolevu, Fiji. Exhibits potent cytotoxicity against murine P388 lymphocytic leukaemia cells. Also shows insecticidal activity. Cryst. + $2H_2O$ (H_2O).
Mp 220-225° dec. λ_{max} 224 (ϵ 8600); 252 (ϵ 6300); 338 (ϵ 15900) (HCl salt) (Derep). λ_{max} 228 (ϵ); 272 (ϵ); 365 (ϵ) (5% NaOH) (Derep). λ_{max} 228 (ϵ 11700); 262 (ϵ 10000); 346 (ϵ 18000) (MeOH) (Derep).

Debromo; hydrochloride: Mp 230-235° dec.

*Debromo, (*E*)-isomer:* ***(10E)-Debromohymenialdisine***
$C_{11}H_{11}N_5O_2$ 245.24
Isol. from the marine sponge *Stylotella aurantium*.

3-Bromo: ***3-Bromohymenialdisine***
[175421-15-5]
$C_{11}H_9Br_2N_5O_2$ 403.032
From *Axinella carteri*. Cytotoxic agent. λ_{max} 269; 332 (MeOH) (Berdy).

*3-Bromo, (*E*)-isomer:* ***Spongiacidin A***
$C_{11}H_9Br_2N_5O_2$ 403.032
Isol. from a *Hymeniacidon* sp. and *Stylissa carteri*. Enzyme inhibitor. Amorph. solid. λ_{max} 206 (ϵ 10000); 270 (ϵ 7000); 332 (ϵ 7000) (MeOH).

*3-Bromo, 2-debromo, (*E*)-isomer:* ***Spongiacidin B***
$C_{11}H_{10}BrN_5O_2$ 324.136
Isol. from a *Hymeniacidon* sp. Enzyme inhibitor. Amorph. solid. λ_{max} 204 (ϵ 10000); 272 (ϵ 10000); 331 (ϵ 9000) (MeOH).

Sharma, G.M. *et al., Chem. Comm.*, 1980, 435 (*deriv*)
Mattia, C.A. *et al., Acta Cryst. B*, 1982, **38**, 2513 (*cryst struct*)
Cimino, G. *et al., Tet. Lett.*, 1982, **23**, 767 (*isol, uv, pmr, cmr, cryst struct*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2321 (*isol, uv, ir, cmr, ms, cryst struct, deriv*)
Schmitz, F.J. *et al., J. Nat. Prod.*, 1985, **48**, 47 (*isol, uv, ir, pmr, ms*)
Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1985, **21**, 578; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 547 (*isol, deriv*)
Annoura, H. *et al., Tet. Lett.*, 1995, **36**, 413 (*synth, Hymenialdisine, Debromohymenialdisine*)
Supriyono, A. *et al., Z. Naturforsch., C*, 1995, **50**, 669 (*3-Bromohymenialdisine*)
Williams, D.H. *et al., Nat. Prod. Lett.*, 1996, **9**, 57 (*10E-Hymenialdisine, 10E-Debromohymenialdisine*)
Roshak, A. *et al., J. Pharmacol. Exp. Ther.*, 1997, **283**, 955-961 (*pharmacol*)
Xu, Y. *et al., J.O.C.*, 1997, **62**, 456 (*synth, Hymenialdisine, Debromohymenialdisine*)
Inaba, K. *et al., J. Nat. Prod.*, 1998, **61**, 693-695 (*Spongiacidins*)
Barrios Sosa, A.C. *et al., J.O.C.*, 2000, **65**, 610-611 (*Debromohymenialdisine, synth*)
Papeo, G. *et al., Org. Lett.*, 2005, **7**, 5641-5644 (*synth*)

Hymenistatin 1 H-1025

[129536-23-8]

Ile–^{2}Ile–Pro–Pro
| |
Leu–Pro–Val–Tyr

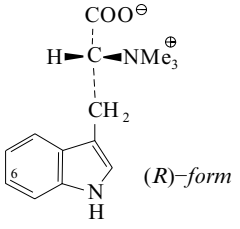
$C_{47}H_{72}N_8O_9$ 893.134

Cyclic peptide. Isol. from the sponge *Hymeniacidon* sp. and *Axinella carteri*. Cytotoxic agent. Amorph. solid.
Mp 180-182°. $[\alpha]_D$ -8.6 (c, 1 in $CHCl_3$). λ_{max} 222 (ϵ 6610); 278 (ϵ 1450) (MeOH) (Derep).

2-L-Leucine analogue: ***Axinastatin 5***. *Hymenamide G*
[156281-02-6]
$C_{47}H_{72}N_8O_9$ 893.134
Isol. from the sponge *Axinella* cf. *carteri* and *Hymeniacidon* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{17}$ -127 (c, 0.97 in MeOH).
Pettit, G.R. *et al., Can. J. Chem.*, 1990, **68**, 708 (*isol, ms*)
Konat, R.K. *et al., Helv. Chim. Acta*, 1993, **76**, 1649 (*synth, pmr, cmr, conformn*)
Pettit, G.R. *et al., Bioorg. Med. Chem. Lett.*, 1994, **4**, 2935-2940 (*Axinastatin 5*)
Tsuda, M. *et al., Tetrahedron*, 1994, **50**, 4667 (*Hymenamide G, isol, uv, ir, pmr, cmr*)

Hypaphorine H-1026

α-Carboxy-N,N,N-*trimethyl-1*H-*indole-3-ethanaminium hydroxide inner salt, 9CI. Trimethyltryptophan betaine. 1-Trimethylammonio-3-(3-indolyl)propionate. Tryptophan betaine. Glyyunnanenine. Lenticine*



(*R*)–*form*

$C_{14}H_{18}N_2O_2$ 246.308

(R)-form
D-form
6-Bromo: ***6-Bromohypaphorine***
[158250-30-7]
$C_{14}H_{17}BrN_2O_2$ 325.205
Isol. from the Okinawan marine sponge *Aplysina* sp. Yellow needles.
Mp 275° dec. $[\alpha]_D^{19}$ -27 (c, 0.80 in MeOH/CF_3COOH 8:1). λ_{max} 227 (ϵ 36000); 285 (ϵ 9300); 293 (ϵ 8000) (MeOH) (Berdy).

(S)-form
L-form
[487-58-1]
Present in seeds of the genus *Erythrina* (Leguminosae), from *Abrus precatorius* and seedlings of lentil (*Lens culinaris*). Feeding deterrent for a seed-eating rodent (*Lionys salvini*).
Cryst. (H_2O or dil. acid). V. sol. H_2O, EtOH, insol. most other solvs.
Mp 255°. $[\alpha]_D^{25}$ +133.6 (H_2O).
▶ Convulsive poison.
5-Bromo: ***5-Bromohypaphorine***
$C_{14}H_{17}BrN_2O_2$ 325.205
Isol. from the sponge *Thorectandra* sp. Yellow solid. $[\alpha]_D^{25}$ +46.3 (c, 0.5 in MeOH).
6-Bromo: [64364-14-3]
$C_{14}H_{17}BrN_2O_2$ 325.204
Metab. of the sponge *Pachymatisma johnstoni*. Rods.
Mp 275-280° dec. $[\alpha]_D^{15}$ +58 (MeOH/CF_3COOH 8:1).
5-Iodo, 7-chloro: ***Plakohypaphorine F***
$C_{14}H_{16}ClIN_2O_2$ 406.65
Isol. from *Plakortis simplex*. Pale yellow solid. $[\alpha]_D^{25}$ +26.7 (c, 1.5 in MeOH/TFA). λ_{max} 226 (ϵ 17200); 286 (ϵ 3740) (MeOH).
7-Iodo: ***Plakohypaphorine A***
[502686-54-6]
$C_{14}H_{17}IN_2O_2$ 372.205
Isol. from the sponge *Plakortis simplex*. Pale yellow solid. $[\alpha]_D^{25}$ +17.3 (c, 1.5 in MeOH/CF_3COOH). λ_{max} 224 (ϵ 17210); 286 (ϵ 3740) (MeOH).
5,6-Diiodo: ***Plakohypaphorine D***
$C_{14}H_{16}I_2N_2O_2$ 498.102
Isol. from *Plakortis simplex*. Pale yellow solid. $[\alpha]_D^{25}$ +27.1 (c, 2 in MeOH/TFA). λ_{max} 224 (ϵ 17200); 288 (ϵ 3700) (MeOH).
5,7-Diiodo: ***Plakohypaphorine C***
[502686-56-8]
$C_{14}H_{16}I_2N_2O_2$ 498.102
Isol. from the sponge *Plakortis simplex*. Yellow solid. $[\alpha]_D^{25}$ +29.1 (c, 1 in MeOH/CF_3COOH). λ_{max} 231 (ϵ 8190); 284 (ϵ 1210) (MeOH).
6,7-Diiodo: ***Plakohypaphorine B***
[502686-55-7]
$C_{14}H_{16}I_2N_2O_2$ 498.102
Isol. from the sponge *Plakortis simplex*. Yellow solid. $[\alpha]_D^{25}$ +30.4 (c, 1.2 in MeOH/CF_3COOH). λ_{max} 236 (ϵ 18600); 290 (ϵ 3690) (MeOH).
5,6,7-Triiodo: ***Plakohypaphorine E***
$C_{14}H_{15}I_3N_2O_2$ 623.998
Isol. from *Plakortis simplex*. Pale yellow solid. $[\alpha]_D^{25}$ +31.2 (c, 4 in MeOH/TFA). λ_{max} 224 (ϵ 17210); 288 (ϵ 3740) (MeOH).

(±)-form [64363-86-6]
Mp 253-255°.
Van Romburgh, P. *et al., J.C.S.*, 1911, **99**, 2068-2071 (*struct, synth*)
Cahill, W.M. *et al., J. Biol. Chem.*, 1938, **126**, 29-36 (*synth*)
Folkers, K. *et al., J.A.C.S.*, 1940, **62**, 436-441 (*isol*)
Hofinger, M. *et al., Phytochemistry*, 1975, **14**, 475-477 (*isol, biosynth*)
Raverty, W.D. *et al., J.C.S. Perkin 1*, 1977, 1204-1211 (*6-Bromohypaphorine, synth, isol*)
Kondo, K. *et al., J. Nat. Prod.*, 1994, **57**, 1008-1011 (*isol, uv, ir, pmr, cmr, struct, 6-Bromohypaphorine*)
Hu, J.-F. *et al., CA*, 1996, **124**, 50632g (*Glyyunnanenine*)
Campagnuolo, C. *et al., Eur. J. Org. Chem.*, 2003, 284-287; 2004, 3227-3232 (*Plakohypaphorines*)
Segraves, N.L. *et al., J. Nat. Prod.*, 2005, **68**, 1484-1488 (*5-Bromohypaphorine*)

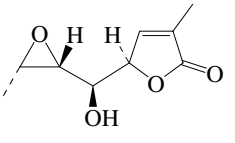
Hypnin A H-1027

Polypeptide with 3 isoforms (A1, A3, A3); Hypnin A1 contains 90 amino acid residues with 4 disulfide bonds. Isol. from the red alga *Hypnea japonica*. Haemagglutinin.

[280587-90-8, 280587-91-9]

Hori, K. *et al., Biochim. Biophys. Acta*, 1986, **873**, 228-236; 2000, **1474**, 226-236 (*isol, struct*)

Hypoxylactone H-1028

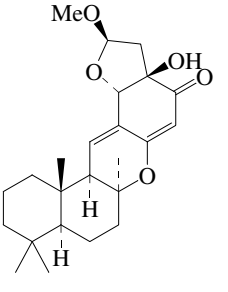


$C_9H_{12}O_4$ 184.191
Prod. by *Hypoxylon croceum*. Oil. $[\alpha]_D$ +153 (c, 0.7 in $CHCl_3$).

Daferner, M. *et al., Z. Naturforsch., C*, 1999, **54**, 474-480

Hyrtenone H-1029

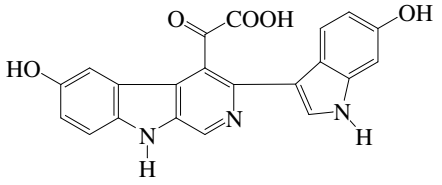
[503138-07-6]



$C_{24}H_{34}O_5$ 402.53
Constit. of a *Hyrtios* sp. sponge. Cryst. (MeOH).
Mp 104-105°. $[\alpha]_D^{28}$ -119.4 (c, 0.06 in $CHCl_3$). λ_{max} 302 (log ϵ 4.39) (MeOH).

Amagata, T. *et al., J. Nat. Prod.*, 2003, **66**, 230-235 (*isol, pmr, cmr, cryst struct*)

Hyrtioerectine A H-1030

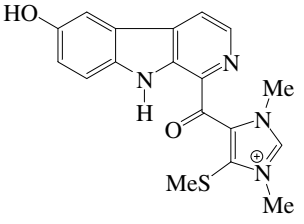


$C_{21}H_{13}N_3O_5$ 387.351
Alkaloid from the sponge *Hyrtios erectus*. Amorph. yellow solid. λ_{max} 387 (log ϵ 4.05) (MeOH).

Youssef, D.T.A. *et al., J. Nat. Prod.*, 2005, **68**, 1416-1419 (*isol, pmr, cmr*)

Hyrtiomanzamine H-1031

[177988-05-5]



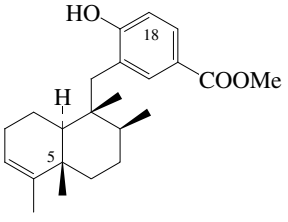
$C_{18}H_{17}N_4O_2S^{\oplus}$ 353.424
Related to Dragmacidonamine A, D-1250. Counterion not specified. Charge is delocalised. Alkaloid from the marine sponge *Hyrtios erecta*. Shows immunosuppressive activity. Orange glassy solid. λ_{max} 394 (MeOH) (Berdy).

Deoxo: ***Gesashidine A***
$C_{18}H_{19}N_4OS^{\oplus}$ 339.44
Alkaloid from an unidentified sponge of the family Thorectidae. Amorph. yellow solid. λ_{max} 212 (ϵ 25000); 246 (ϵ 7300); 289 (ϵ 4400); 297 (ϵ 5600); 364 (ϵ 1400) (MeOH).

Bourguet-Kondracki, M.L. *et al., Tet. Lett.*, 1996, **37**, 3457-3460 (*isol, pmr, cmr*)
Iinuma, Y. *et al., J. Nat. Prod.*, 2005, **68**, 1109-1110 (*Gesashidine A*)

Hyrtiophenol H-1032

[267650-81-7]



$C_{23}H_{32}O_3$ 356.504
Constit. of *Hyrtios* spp. and *Petrosaspongia metachromia*. Amorph. solid. $[\alpha]_D^{23}$ -15.2 (c, 0.125 in $CHCl_3$). λ_{max} 215 (ϵ 12990); 262 (ϵ 9250) (MeOH).

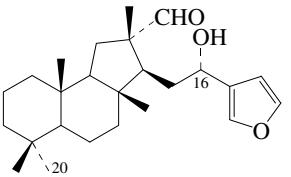
18-Hydroxy: ***18-Hydroxyhyrtiophenol***
[267650-84-0]
$C_{23}H_{32}O_4$ 372.503
Constit. of *Petrosaspongia metachromia* and *Hyrtios* spp. Amorph. solid. $[\alpha]_D^{23}$ -37.5 (c, 0.008 in $CHCl_3$). λ_{max} 220 (ϵ 12500); 269 (ϵ 5510); 305 (sh) (ϵ 2580) (MeOH).

5-Epimer: ***5-Epihyrtiophenol***
[267650-82-8]
$C_{23}H_{32}O_3$ 356.504
Constit. of *Hyrtios* spp. Amorph. solid. λ_{max} 216 (ϵ 15075); 262 (ϵ 9945) (MeOH).

5-Epimer, 18-hydroxy: ***18-Hydroxy-5-epihyrtiophenol***
[267650-83-9]
$C_{23}H_{32}O_4$ 372.503
Constit. of *Hyrtios* spp. Amorph. solid. λ_{max} 221 (ϵ 17440); 269 (ϵ 7460); 305 (sh) (ϵ 3341) (MeOH).

Salmoun, M. *et al., J. Nat. Prod.*, 2000, **63**, 452-456 (*isol, pmr, cmr*)
Kwak, J.H. *et al., J. Nat. Prod.*, 2000, **63**, 1153-1156 (*isol, pmr, cmr*)

Hyrtiosal H-1033



(-)-*form*

$C_{25}H_{38}O_3$ 386.573

(-)-*form* [138355-07-4]
Constit. of *Hyrtios erecta*. Platelet aggregation inhibitor, Ngf synthesis stimulator. Cryst.
Mp 119-121°. $[\alpha]_D$ -73.8 (c, 0.42 in $CHCl_3$).

(+)-*form*

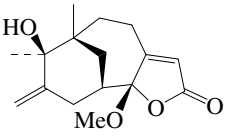
20-Oxo: ***(+)-20-Formylhyrtiosal***
[705279-70-5]
$C_{25}H_{36}O_4$ 400.557
Constit. of *Hyrtios erectus*. Amorph. solid. $[\alpha]_D^{25}$ +60 (c, 0.245 in MeOH).

20-Oxo, 16-Ac: [705279-71-6]
$C_{27}H_{38}O_5$ 442.594
Constit. of *Hyrtios erectus*. Oil. $[\alpha]_D^{25}$ +65 (c, 0.2 in MeOH).

Iguchi, K. *et al., J.O.C.*, 1992, **57**, 522-524 (*Hyrtiosal*)
Lunardi, I. *et al., Tet. Lett.*, 2002, **43**, 3609-3611 (*synth*)
Qiu, Y. *et al., J. Nat. Prod.*, 2004, **67**, 921-924 (*20-oxo derivs*)

Hyrtiosenolide A H-1034

[777858-97-6]

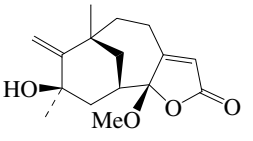


$C_{16}H_{22}O_4$ 278.347
Constit. of a *Hyrtios* sp. Solid. $[\alpha]_D$ -57.2 (c, 0.1 in MeOH aq.). λ_{max} 205 (log ϵ 3.47) (MeOH).

Youssef, D.T.A. *et al., J. Nat. Prod.*, 2004, **67**, 1736-1739 (*isol, pmr, cmr*)

Hyrtiosenolide B H-1035

[777858-98-7]

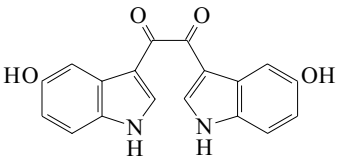


$C_{16}H_{22}O_4$ 278.347
Constit. of a *Hyrtios* sp. Solid. $[\alpha]_D$ -132.4 (c, 0.16 in MeOH aq.). λ_{max} 207 (log ϵ 3.48) (MeOH).

Youssef, D.T.A. *et al., J. Nat. Prod.*, 2004, **67**, 1736-1739 (*isol, pmr, cmr*)

Hyrtiosin B† H-1036

*Bis(5-hydroxy-1*H*-indol-3-yl)ethanedione, 9CI*
[132922-99-7]



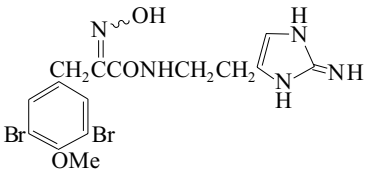
$C_{18}H_{12}N_2O_4$ 320.304
Alkaloid from the marine sponge *Hyrtios erecta*. Pale green solid. Mp >400°. λ_{max} 212 (ϵ 30000); 255 (ϵ 12800); 290 (ϵ 12100); 332 (ϵ 11000) (MeOH) (Berdy).

*Dideoxy: Di-1*H*-indol-3-ylethanedione, 9CI. Di-3-indolylglyoxal*
[65610-87-9]
$C_{18}H_{12}N_2O_2$ 288.305
Alkaloid from the sponge *Smenospongia* sp. Yellow cryst. (Me_2CO aq.).
Mp 279-280°. λ_{max} 247 (log ϵ 4.28); 266 (log ϵ 4.27); 326 (log ϵ 4.27) (no solvent reported).

Bergman, J. *et al., Tetrahedron*, 1990, **46**, 6061-6066 (*Bisindolylethanedione, synth*)
Kobayashi, J. *et al., Tetrahedron*, 1990, **46**, 7699-7702 (*isol, uv, ir, pmr, cmr, ms, struct*)
Bergman, J. *et al., Synthesis*, 1999, 580-585 (*synth, ir, pmr, cmr*)
McKay, M.J. *et al., J. Nat. Prod.*, 2002, **65**, 595-597 (*Bisindolylethanedione*)
Krasyushkin, M.M. *et al., Zh. Org. Khim.*, 2005, **41**, 895-902; *Russ. J. Org. Chem. (Engl. Transl.)*, 2005, **41**, 875-883 (*dideoxy, synth*)

Ianthelline I-1

[105596-36-9]

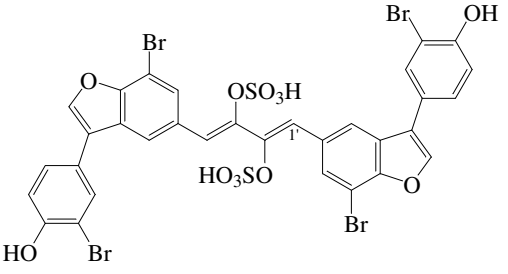


$C_{15}H_{17}Br_2N_5O_3$ 475.139

Amino acid-derived antibiotic. Isol. from the sponge *Ianthella ardis* and *Pseudoceratina crassa*. Shows antibacterial and antifungal props. Pale yellow powder.
Mp 113-115°.

Litaudon, M. *et al., Tet. Lett.*, 1986, **27**, 4455 (*isol, ir, pmr, cmr, ms, struct*)

Iantheran A I-2

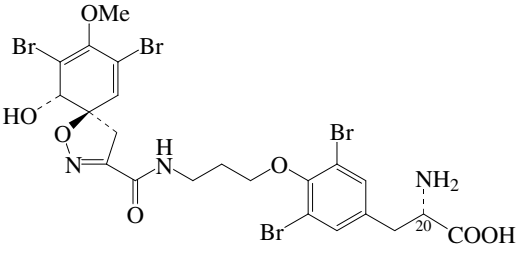


$C_{32}H_{18}Br_4O_{12}S_2$ 978.235
Isol. from a marine sponge *Ianthella* sp. Na/K ATP-ase inhibitor. Pale yellow cryst. (as di-Na salt).
Mp 172-173° (dec.) (di-Na salt). λ_{max} 325 (ϵ 36700); 337 (ϵ 39700); 352 (ϵ 27000) (MeOH) (Berdy).

(1′Z)-Isomer: ***Iantheran B***
$C_{32}H_{18}Br_4O_{12}S_2$ 978.235
Isol. from *Ianthella* sp. ATPase inhibitor. Pale yellow cryst. (MeOH aq.) (as di-Na salt).
Mp 155-156° dec. (di-Na salt). λ_{max} 215 (ϵ 62500); 242 (ϵ 44900); 279 (sh) (ϵ 28900); 321 (ϵ 25300); 331 (sh) (ϵ 25000); 355 (sh) (ϵ 12900) (MeOH (di-Na salt)).

Okamoto, Y. *et al., Tet. Lett.*, 1999, **40**, 507-510 (*isol, pmr, cmr, ms*)
Okamoto, Y. *et al., Bioorg. Med. Chem.*, 2001, **9**, 179-183 (*isol, pmr, cmr, activity*)

Ianthesine B I-3



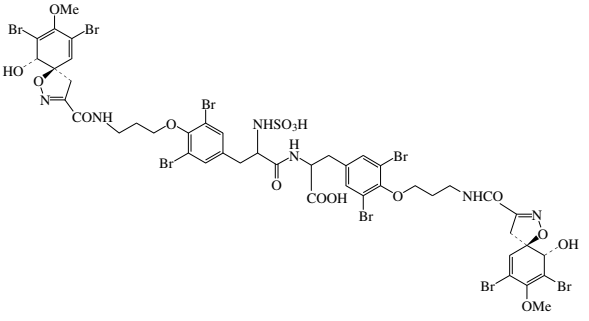
$C_{22}H_{23}Br_4N_3O_7$ 761.056
Alkaloid from the marine sponge *Ianthella* sp. Cryst. (MeOH aq.).
Mp 154-157°. $[\alpha]_D^{22}$ -97 (c, 0.58 in MeOH). λ_{max} 207 (ϵ 45400); 283 (ϵ 7300) (MeOH).

20-Epimer, N^{20}*-di-Me:* ***Ianthesine A***
$C_{24}H_{27}Br_4N_3O_7$ 789.109
Alkaloid from *Ianthella* sp. Cryst. (MeOH aq.).
Mp 154-156°. $[\alpha]_D^{22}$ -118 (c, 1 in MeOH). λ_{max} 210 (ϵ 29500); 283 (ϵ 7390) (MeOH).

N^{20}*-Sulfo:* ***Ianthesine D***
$C_{22}H_{23}Br_4N_3O_{10}S$ 841.12
Alkaloid from *Ianthella* sp. Powder (as Na salt).
Mp 190° dec. (Na salt). $[\alpha]_D^{25}$ -69 (c, 0.19 in MeOH) (Na salt).
C-20 config. not determined. λ_{max} 206 (ϵ 53200); 220 (sh) (ϵ 25000); 282 (ϵ 6760) (MeOH) (Na salt).

Okamoto, Y. *et al., Tetrahedron*, 2000, **56**, 5813-5818

Ianthesine C I-4

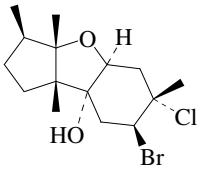


$C_{44}H_{44}Br_8N_6O_{16}S$ 1584.16
Alkaloid from the marine sponge *Ianthella* sp. Yellow powder (DMSO aq.) (as Na salt).
Mp 200° dec. (Na salt). $[\alpha]_D^{26}$ -93 (c, 0.86 in DMSO) (Na salt).
λ_{max} 231 (ϵ 26900); 283 (ϵ 11900) (MeOH/DMSO) (Na salt).

Okamoto, Y. *et al., Tetrahedron*, 2000, **56**, 5813-5818

Ibhayinol I-5

[251455-24-0]

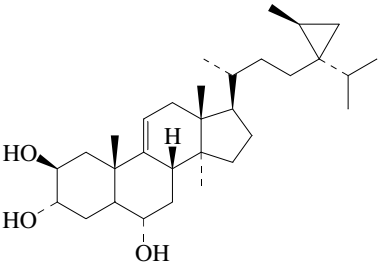


$C_{15}H_{24}BrClO_2$ 351.71

Struct. revised in 2002. Constit. of *Aplysia dactylomela*. Amorph. powder. $[\alpha]_D^{22}$ +8.8 (c, 0.57 in $CHCl_3$).

McPhail, K.L. *et al., J. Nat. Prod.*, 1999, **62**, 1618-1623 (*isol, pmr, cmr*)
Copley, R.C.B. *et al., J. Nat. Prod.*, 2002, **65**, 580-582 (*cryst struct, abs config*)

Ibisterol I-6



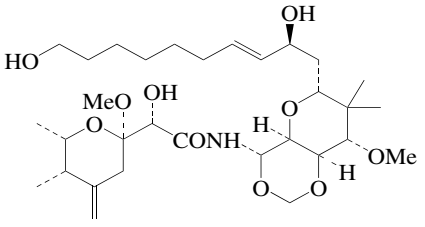
$C_{31}H_{52}O_3$ 472.75
Shows anti-HIV activity. Sol. MeOH.

Tri-O-*sulfate:* ***Ibisterol sulfate***
[148101-50-2]
$C_{31}H_{52}O_{12}S_3$ 712.943
Constit. of a *Topsentia* sp.

McKee, T.C. *et al., Tet. Lett.*, 1993, **34**, 389 (*isol, pmr, cmr*)
McKee, T.C. *et al., J. Med. Chem.*, 1994, **37**, 793-797 (*activity*)

Icadamide B I-7

[173792-59-1]



$C_{31}H_{53}NO_{10}$ 599.76

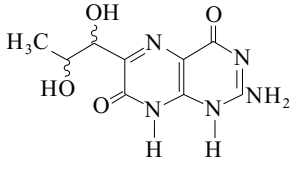
Related to Onnamide B, O-108 and Theopederin B, T-298. Isol. from the sponge *Leiosella* sp. Cytotoxic agent. Oil. $[\alpha]_D$ +96 (c, 0.9 in MeOH).

U.S. Pat., 1995, 5 476 953; *CA*, **124**, 165232u

Ichthyopterin I-8

*2-Amino-6-(1,2-dihydroxypropyl)-4,7(1*H*,8*H*)-pteridinedione, 9CI. 6-(1,2-Dihydroxypropyl)isoxanthopterin. 7-Hydroxybiopterin. 2-Amino-4,7-dihydroxy-6-(1,2-dihydroxypropyl)pteridine*

[490-58-4]



$C_9H_{11}N_5O_4$ 253.217

Pigment present in the scales of various fish (e.g. *Cyprinus carpio*). Also isol. from scorpion flies (*Panorpa japonica*). Stereochem. not determined.

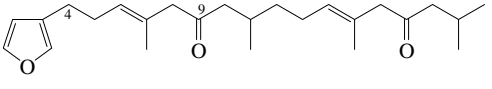
Mono-Ac: [18503-57-6]
Cryst. (EtOH). Mp 143-153°.

N,O,O-*Tri-Ac:* [18503-60-1]
Cryst. (EtOH). Mp 188-196° dec.

Tschesche, R. *et al., Chem. Ber.*, 1958, **91**, 2081 (*synth*)
Hüttel, R. *et al., Chem. Ber.*, 1960, **93**, 2439
Ohta, K. *et al., J. Biochem. (Tokyo)*, 1968, **63**, 127 (*esters*)
Nakagoshi, M. *et al., Experientia*, 1983, **39**, 742 (*isol, bibl*)

Idiadione I-9

[75266-24-9]



$C_{25}H_{38}O_3$ 386.573

Constit. of *Spongia idia* and *Cadlina luteoarginata*. Toxic to several predatory marine organisms (sea star, abalone larvae, brine shrimp). Ichthyotoxic, algicide and molluscicide. Oil. Sol. MeOH, hexane. $[\alpha]_D$ -6.6 (c, 2.6 in $CHCl_3$). λ_{max} 211 (ϵ 27300) (MeOH) (Derep).

4S-*Hydroxy, 9-deoxo, 10,11-didehydro:* ***4-Hydroxy-9-deoxoidiadione***
[782491-81-0]
$C_{25}H_{38}O_3$ 386.573
Constit. of a *Smenospongia* sp. Amorph. solid. $[\alpha]_D^{25}$ -5.5 (c, 0.29 in MeOH).

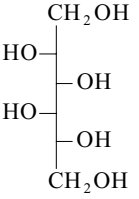
4S-*Acetoxy, 9-deoxo, 10,11-didehydro:* ***4-Acetoxy-9-deoxoidiadione***
[782491-82-1]
$C_{27}H_{40}O_4$ 428.611
Constit. of a *Smenospongia* sp. Amorph. solid. $[\alpha]_D^{25}$ -19.2 (c, 0.34 in MeOH).

Walker, R.P. *et al., J.O.C.*, 1980, **45**, 4976
Thompson, L.E. *et al., Tetrahedron*, 1982, **38**, 1865 (*isol*)
Noda, Y. *et al., Heterocycles*, 2001, **55**, 1839-1841 (*synth*)
Rho, J.-R. *et al., J. Nat. Prod.*, 2004, **67**, 1748-1751 (*Smenospongia constits*)

Iditol, 9CI, 8CI I-10

Sorbieritol. ido-*Hexitol*

[24557-79-7]



D–*form*

$C_6H_{14}O_6$ 182.173

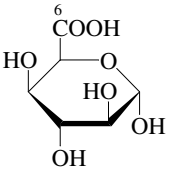
D-*form* [25878-23-3]
Isol. from *Stypopodium schimperi*.
Mp 73-74°. $[\alpha]_D^{20}$ +3.5 (H_2O).

[45007-61-2]

Sampli, P. *et al., Nat. Prod. Lett.*, 2000, **14**, 365-372 (D-*form, isol*)

Iduronic acid I-11

[3402-98-0]



α-D-Pyranose-*form*

$C_6H_{10}O_7$ 194.141

L-*form* [2073-35-0]
Constit. of heparin, dermatan sulfate and the type-specific polysaccharide of *Clostridium perfringens*. Also a component of Protuberic acid. Constit. of dermatan from *Ascidia nigra*.
Cryst. (MeOH/EtOAc).
Mp 131-132°. $[\alpha]_D^{22}$ +37 → +33 (c, 3.0 in H_2O).

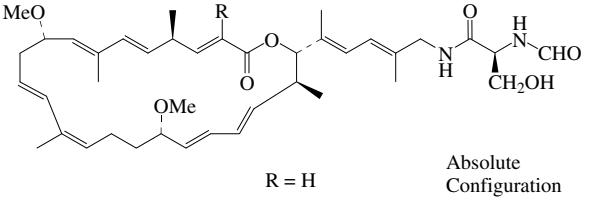
2-Sulfate: [89846-17-3]
[69098-37-9 (α-pyranose)]
$C_6H_{10}O_{10}S$ 274.205
Constit. of dermatans from *Ascidia nigra*, porcine intestines and heparin.

[32449-81-3]

Pavao, M.S.G. *et al., J. Biol. Chem.*, 1995, **270**, 31027-31036 (α-L-*pyr 2-sulfate, occur*)

Iejimalide A I-12

[117582-91-9]



R = H

Absolute Configuration

$C_{40}H_{58}N_2O_7$ 678.907

Isol. from the tunicate *Eudistoma* cf. *rigida* and a *Cystodytes* sp. Antileukaemic agent. Non-cryst. solid. Sol. MeOH, toluene, C_6H_6; poorly sol. H_2O.

Mp 71-73°. $[\alpha]_D^{23}$ -36.4 (c, 0.17 in $CHCl_3$). λ_{max} 231 (ϵ 26000) (MeOH) (Berdy).

O-*Sulfate:* ***Iejimalide C***
[133613-80-6]
$C_{40}H_{58}N_2O_{10}S$ 758.972
Isol. from *Eudistoma* cf. *rigida* (as Na salt) and a *Cystodytes* sp. Antileukaemic agent. $[\alpha]_D^{20}$ -56 (c, 0.13 in MeOH). λ_{max} 231 (ϵ 28000) (MeOH) (Berdy).

Kobayashi, J. *et al., J.O.C.*, 1988, **53**, 6147-6150 (*isol, pmr, cmr*)
Kikuchi, Y. *et al., Tet. Lett.*, 1991, **32**, 797-798 (*Iejimalide C*)
Nozawa, K. *et al., Bioorg. Med. Chem.*, 2006, **14**, 1063-1067 (*abs config*)

Iejimalide B I-13

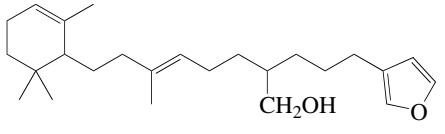
[117582-92-0]
As Iejimalide A, I-12 with
R = $-CH_3$
$C_{41}H_{60}N_2O_7$ 692.934
Isol. from the tunicate *Eudistoma* cf. *rigida*. Antileukaemic agent. Non-cryst. solid. Sol. MeOH, toluene, C_6H_6; poorly sol. H_2O. Mp 69-71°. $[\alpha]_D^{23}$ -17.6 (c, 0.17 in $CHCl_3$). λ_{max} 235 (ϵ 27000) (MeOH) (Berdy).

O-*Sulfate:* ***Iejimalide D***
[133613-81-7]
$C_{41}H_{60}N_2O_{10}S$ 772.998
Isol. from *Eudistoma* cf. *rigida* (as Na salt). Antileukaemic agent. λ_{max} 241 (ϵ 29000) (MeOH) (Berdy).

Kobayashi, J. *et al., J.O.C.*, 1988, **53**, 6147-6150 (*isol, pmr, cmr*)
Kikuchi, Y. *et al., Tet. Lett.*, 1991, **32**, 797-798 (*Iejimalide D*)
Nozawa, K. *et al., Bioorg. Med. Chem.*, 2006, **14**, 1063-1067 (*abs config*)

Igernellin I-14

[181363-78-0]

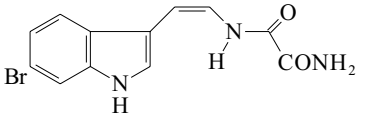


$C_{25}H_{40}O_2$ 372.59
Constit. of an *Igernella* sp. Oil. λ_{max} 227 (CH_2Cl_2). λ_{max} 227 (MeOH) (Berdy).

Liu, G. *et al., Nat. Prod. Lett.*, 1995, **7**, 297 (*isol, pmr, cmr*)

Igzamide I-15

[149355-80-6]

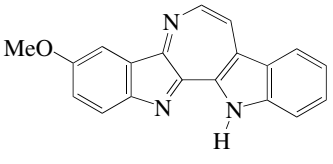


$C_{12}H_{10}BrN_3O_2$ 308.134
Alkaloid from the northeastern Pacific sponge *Plocamissa igzo*. Yellow solid. Genus name given as Plocamissma, which appears to be an error. λ_{max} 228 (ϵ 12800); 294 (ϵ 4900) (MeOH) (Berdy).

Dumdei, E. *et al., J. Nat. Prod.*, 1993, **56**, 792-794 (*isol, uv, ir, pmr, cmr, ms, struct*)

Iheyamine A I-16

[221160-80-1]

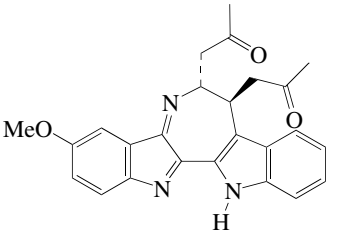


$C_{19}H_{13}N_3O$ 299.331
Alkaloid from an ascidian *Polycitorella* sp. Cytotoxic agent. Amorph. purple solid (as trifluoroacetate). λ_{max} 284 (ϵ 16000); 325 (sh) (ϵ 33000); 341 (ϵ 36000); 360 (sh) (ϵ 30000); 388 (ϵ 19000); 499 (ϵ 5200) (MeOH) (as trifluoroacetate salt). λ_{max} 287; 346; 395; 515 (MeOH) (Berdy). λ_{max} 348 (ϵ 42000); 480 (ϵ 4400) (MeOH/NaOH) (Berdy).

Sasaki, T. *et al., Tet. Lett.*, 1999, **40**, 303-306 (*isol, uv, ir, pmr, cmr*)

Iheyamine B I-17

[221160-84-5]



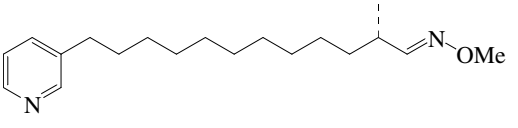
Relative Configuration

$C_{25}H_{23}N_3O_3$ 413.475
Alkaloid from an ascidian *Polycitorella* sp. Cytotoxic agent. Amorph. purple solid. $[\alpha]_D^{25}$ -16 (c, 0.0002 in $CHCl_3$). λ_{max} 276 (sh) (ϵ 18000); 300 (ϵ 36000); 307 (ϵ 36000); 330 (sh) (ϵ 14000); 526 (ϵ 7400) ($CHCl_3$). λ_{max} 284 (ϵ 16000); 341 (ϵ 36000); 388 (ϵ 19000); 499 (ϵ 5200) (MeOH) (Berdy).

Sasaki, T. *et al., Tet. Lett.*, 1999, **40**, 303-306 (*isol, uv, ir, pmr, cmr*)

Ikimine A I-18

α-Methyl-3-pyridinedodecanal O*-methyloxime, 9CI*
[131479-30-6]



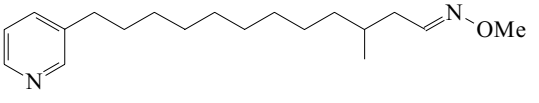
$C_{19}H_{32}N_2O$ 304.475
Alkaloid from the Okinawan sponge *Niphates* sp. and another sponge. Cytotoxic agent. Shows antibacterial and antifungal activity. Oil. Occurs as a partial racemate of the *E*-form with the *S*-enantiomer, illus., predominating. The *Z*-isomer, also isol., is prob. an artifact. λ_{max} 260 (ϵ 2090); 265 (ϵ 7760); 272 (ϵ 1660) (MeOH) (Derep). λ_{max} 260 (ϵ 2090); 263 (ϵ 3300); 265 (ϵ 8912); 272 (ϵ 1660) (MeOH) (Berdy).

[131564-74-4]

Carroll, A.R. *et al., Tetrahedron*, 1990, **46**, 6637 (*isol, uv, ir, pmr, cmr, ms, struct, activity*)
Kobayashi, J. *et al., J.C.S. Perkin 1*, 1992, 1291 (*isol, uv, ir, pmr, cmr, ms*)
Bracher, F. *et al., Nat. Prod. Lett.*, 1994, **4**, 223 (*synth*)
Nicholas, G.M. *et al., Tetrahedron*, 2000, **56**, 2921-2927 (*isol, abs config*)

Ikimine B I-19

β-Methyl-3-pyridinedodecanal O*-methyloxime, 9CI*
[131479-31-7]



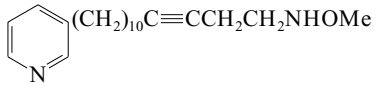
$C_{19}H_{32}N_2O$ 304.475
The struct. illus. has been shown to be in doubt (2004). Alkaloid from an unidentified sponge. Cytotoxic. Oil. The *syn*-isomer, also isol., is prob. an artifact. λ_{max} 260 (ϵ 2090); 265 (ϵ 7760); 272 (ϵ 1660) (MeOH) (Derep). λ_{max} 260 (ϵ 1995); 264 (ϵ 10964); 274 (ϵ 1348) (MeOH) (Berdy).

[131564-75-5]

Carroll, A.R. *et al., Tetrahedron*, 1990, **46**, 6637-6644 (*isol, uv, ir, pmr, cmr, ms, struct*)
Romeril, S.P. *et al., Tet. Lett.*, 2004, **45**, 3273-3277 (*struct*)

Ikimine D **I-20**

N-*Methoxy-14-(3-pyridinyl)-3-tetradecyn-1-amine, 9CI*
[131479-33-9]

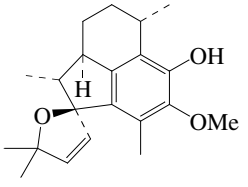


$C_{20}H_{32}N_2O$ 316.486
Alkaloid from an unidentified sponge. Cytotoxic. Oil. λ_{max} 260 (ϵ 2000); 265 (ϵ 6610); 270 (ϵ 2880) (MeOH) (Derep).

Carroll, A.R. *et al., Tetrahedron*, 1990, **46**, 6637 (*isol, uv, ir, pmr, cmr, ms, struct*)

Ileabethin **I-21**

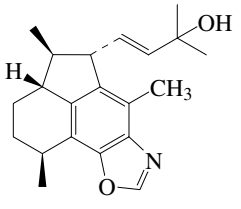
[467434-70-4]



$C_{21}H_{28}O_3$ 328.45
Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{25}$ +12.7 (c, 1.1 in $CHCl_3$).

Rodríguez, A.D. *et al., Tet. Lett.*, 2002, **43**, 5601-5604 (*isol, pmr, cmr*)

Ileabethoxazole **I-22**



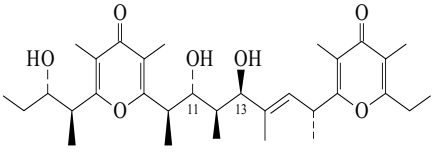
Relative Configuration

$C_{21}H_{27}NO_2$ 325.45
Alkaloid from *Pseudopterogorgia elisabethae*. Antimycobacterial agent. Pale yellow oil. $[\alpha]_D^{20}$ +6.8 (c, 1 in $CHCl_3$). λ_{max} 225 (ϵ 22200); 277 (ϵ 2300); 288 (ϵ 1800) (MeOH).

Rodriguez, I.I. *et al., Tet. Lett.*, 2006, **47**, 3229-3232 (*isol, pmr, cmr*)

Ilikonapyrone **I-23**

[88130-78-3]



$C_{32}H_{48}O_7$ 544.727
Defence allomone of the mollusc *Onchidium verruculatum*. Cryst. Mp 96-98°. $[\alpha]_D$ -16 (c, 1.5 in CH_2Cl_2). Related to Onchitriol I, O-103. λ_{max} 260 (ϵ 12700) (MeOH) (Derep).

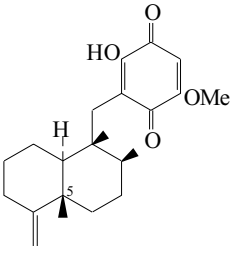
11,13-Dipropanoyl: [88130-79-4]
$C_{38}H_{56}O_9$ 656.855

From *Onchidium verruculatum*. Probable defence allomone, antifeedant. Sol. Me_2CO, $CHCl_3$; poorly sol. H_2O. λ_{max} 260 (MeOH) (Berdy).

Ireland, C.M. *et al., J.O.C.*, 1984, **49**, 559-561 (*isol*)
Arimoto, H. *et al., Tet. Lett.*, 1993, **34**, 5781-5784 (*abs config*)

Ilimaquinone **I-24**

[71678-03-0]



Absolute configuration

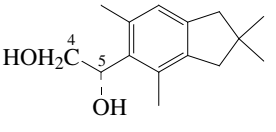
$C_{22}H_{30}O_4$ 358.477
Isol. from various sponges *Hippospongia metachromia*, *Smenospongia* spp., *Polyfibrospongia australis*, *Hyatella* spp., *Dactylospongia elegans*, *Petrosaspongia metachromia*. Shows antistaphylococcal activity. HIV reverse transcriptase inhibitor, shows anti-HIV activity. Induces the vesiculation of Golgi membranes. Cryst. (hexane). Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 113-114°. $[\alpha]_D^{23}$ -23.2 (c, 1.12 in $CHCl_3$). Log P 5.78 (calc). λ_{max} 214 (ϵ 10500); 286 (ϵ 13200); 435 (ϵ 537) (MeOH) (Derep). λ_{max} 204 (ϵ 10200); 285 (ϵ 16300); 425 (ϵ 790) (MeOH/HCl) (Berdy). λ_{max} 287 (ϵ 16200); 420 (ϵ 575) ($CHCl_3$) (Berdy).

O-*De-Me:* ***Smenoquinone***
[121994-50-1]
$C_{21}H_{28}O_4$ 344.45
Constit. of *Smenospongia* sp. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 350°. λ_{max} 214 (ϵ 10500); 286 (ϵ 13200); 435 (ϵ 537) (MeOH) (Derep). λ_{max} 214; 286 (EtOH) (Berdy).

5-Epimer: ***5-Epiilimaquinone***
[96806-31-4]
$C_{22}H_{30}O_4$ 358.477
Constit. of a *Fenestraspongia* sp., *Dactylospongia elegans* and *Hyrtios* sp. Toxic against *Artemia* larvae. $[\alpha]_D$ +29.8 (c, 0.4 in $CHCl_3$). λ_{max} 214 (ϵ 10500); 286 (ϵ 13200); 435 (ϵ 537) (MeOH) (Derep).

Luibrand, R.T. *et al., Tetrahedron*, 1979, **35**, 609 (*isol*)
Carté, B. *et al., J.O.C.*, 1985, **50**, 2785 (*Epiilimaquinone*)
Capon, R.J. *et al., J.O.C.*, 1987, **52**, 5059 (*abs config*)
Kondracki, M.-L. *et al., Tetrahedron*, 1989, **45**, 1995 (*Smenoquinone*)
Loya, S. *et al., Antimicrob. Agents Chemother.*, 1990, **34**, 2009 (*anti-HIV activitiy*)
Rodríguez, J. *et al., Tetrahedron*, 1992, **48**, 6667-6680 (*Epiilimaquinone*)
Takizawa, P.A. *et al., Cell (Cambridge, Mass.)*, 1993, **73**, 1079 (*Ilimaquinone, pharmacol*)
Acharya, U. *et al., J. Cell Biol.*, 1995, **129**, 577 (*Ilimaquinone, pharmacol*)
Bruner, S.D. *et al., J.O.C.*, 1995, **60**, 1114 (*synth*)
Poigny, S. *et al., J.O.C.*, 1998, **63**, 5890-5894 (*synth*)
Popov, A.M. *et al., Pharm. Chem. J. (Engl. Transl.)*, 1999, **33**, 71; *CA*, 2000, **132**, 61495f (*activity*)
Salmoun, M. *et al., J. Nat. Prod.*, 2000, **63**, 452 (*isol, activity*)
Ling, T. *et al., J.A.C.S.*, 2002, **124**, 12261-12267 (*synth*)
Ling, T. *et al., Org. Lett.*, 2002, **4**, 819-822 (*Ilimaquinone, synth*)

2,6,8-Illudalatriene-4,5-diol **I-25**

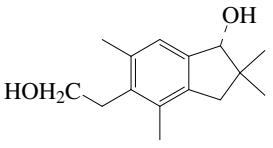


$C_{15}H_{22}O_2$ 234.338

(S)-form

4-Nitrate ester: ***Alcyopterosin F***
[288851-32-1]
$C_{15}H_{21}NO_4$ 279.335
Constit. of *Alcyonium paessleri*. Oil. $[\alpha]_D^{25}$ -29.13 (c, 0.23 in $CHCl_3$). λ_{max} 220 (log ϵ 3.29); 234 (log ϵ 3.88); 274 (log ϵ 3.3); 282 (log ϵ 3.28) (CH_2Cl_2).
Palermo, J.A. *et al., J.O.C.*, 2000, **65**, 4482-4486 (*isol, pmr, cmr*)

2,6,8-Illudalatriene-4,10-diol I-26



$C_{15}H_{22}O_2$ 234.338

(R)-form

4-Nitrate ester: ***Alcyopterosin H***
[288851-34-3]
$C_{15}H_{21}NO_4$ 279.335
Constit. of *Alcyonium paessleri*. Oil. $[\alpha]_D^{25}$ -13.9 (c, 1.05 in $CHCl_3$). λ_{max} 232 (log ϵ 3.46); 272 (log ϵ 2.89); 306 (log ϵ 3.33) (CH_2Cl_2).

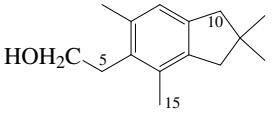
10-Ketone: 4-Hydroxy-2,6,8-illudalatrien-10-one. ***Alcyopterosin N***
[223545-13-9]
$C_{15}H_{20}O_2$ 232.322
Constit. of *Alcyonium paessleri*. Cryst. (MeOH).
Mp 103-104°. λ_{max} 226 (log ϵ 3.72); 230 (log ϵ 3.58); 260 (log ϵ 4.18); 306 (log ϵ 3.52) (CH_2Cl_2).

10-Ketone, 4-nitrate ester: ***Alcyopterosin C***
[288851-29-6]
$C_{15}H_{19}NO_4$ 277.319
Constit. of *Alcyonium paessleri*. Cryst. (MeOH).
Mp 83-84°. λ_{max} 228 (log ϵ 3.68); 256 (log ϵ 4.22); 306 (log ϵ 3.54) (CH_2Cl_2).

15-Hydroxy, 10-ketone: 4,15-Dihydroxy-2,6,8-illudalatrien-10-one
$C_{15}H_{20}O_3$ 248.321

15-Hydroxy, 10-ketone, 4-nitrate ester: ***Alcyopterosin J***
[288851-36-5]
$C_{15}H_{19}NO_5$ 293.319
Constit. of *Alcyonium paessleri*. Cryst. (MeOH).
Mp 118-121°. λ_{max} 230 (log ϵ 3.87); 252 (log ϵ 4.21); 306 (log ϵ 3.67) (CH_2Cl_2).
Palermo, J.A. *et al., J.O.C.*, 2000, **65**, 4482-4486 (*isol, pmr, cmr*)
Nakao, Y. *et al., J.A.C.S.*, 2004, **126**, 15650-15661 (*synth*)

2,6,8-Illudalatrien-4-ol I-27



$C_{15}H_{22}O$ 218.338

Nitrate ester: ***Alcyopterosin B***
[288851-28-5]
$C_{15}H_{21}NO_3$ 263.336
Constit. of *Alcyonium paessleri*. Oil. λ_{max} 234 (log ϵ 3.49); 274 (log ϵ 2.99); 283 (log ϵ 3.02) (CH_2Cl_2).

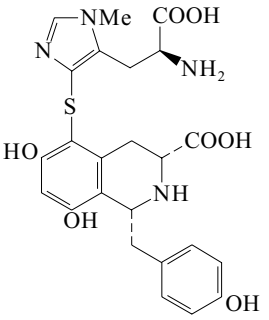
15-Hydroxy: 2,6,8-Illudalatriene-4,15-diol. ***Alcyopterosin O***
[288851-40-1]
$C_{15}H_{22}O_2$ 234.338
Constit. of *Alcyonium paessleri*. Oil. λ_{max} 212 (log ϵ 4.01); 233 (log ϵ 3.89); 282 (log ϵ 3.28) (CH_2Cl_2).

15-Hydroxy, 4-nitrate ester: ***Alcyopterosin G***
[288851-33-2]
$C_{15}H_{21}NO_4$ 279.335
Constit. of *Alcyonium paessleri*. Oil. λ_{max} 212 (log ϵ 4.07); 232 (log ϵ 3.89); 286 (log ϵ 3.24) (CH_2Cl_2).

15-Hydroxy, 4-Ac:
$C_{17}H_{24}O_3$ 276.375
Metab. of *Clitocybe rivulosa*. Wax.
Palermo, J.A. *et al., J.O.C.*, 2000, **65**, 4482-4486 (*isol, pmr, cmr*)
Schlegel, B. *et al., Pharmazie*, 2002, **57**, 778-779 (*Clitocybe rivulosa metab*)

Imbricatine† I-28

[105372-70-1]



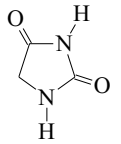
Absolute configuration

$C_{24}H_{26}N_4O_7S$ 514.558
Alkaloid from the starfish *Dermasterias imbricata*. Amorph. solid. First example of a benzyltetrahydroisoquinoline alkaloid from a marine organism, and apparently the first example from a non-plant source.

Pathirana, C. *et al., J.A.C.S.*, 1986, **108**, 8288-8289 (*pmr, cmr, struct*)
Burgoyne, D.L. *et al., Can. J. Chem.*, 1991, **69**, 20-27 (*abs config*)
Ohba, M. *et al., Tetrahedron*, 1999, **55**, 4999-5016 (*deriv, synth*)

2,4-Imidazolidinedione, 9CI I-29

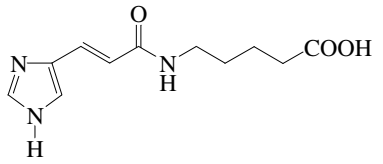
Hydantoin. Diketotetrahydroglyoxaline. Glycollylurea. 2,4-Dioxoimidazolidine. 2,4(5)-Dihydroxyimidazole
[461-72-3]



$C_3H_4N_2O_2$ 100.077
Present in tobacco smoke. Needles (MeOH). Spar. sol. H_2O, sol. alkalis. Mp 217-220°. pK_{a1} 8.93 (25°).
► Exp. teratogen. MT8210000

3-Me: 3-Methyl-2,4-imidazolidinedione. 3-Methylhydantoin
[6843-45-4]
$C_4H_6N_2O_2$ 114.104
Isol. from an endophytic mangrove fungus No. 1839. Prisms (H_2O). Sol. H_2O.
Mp 155-157°. Sublimes.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 807C; 807D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1315A; 1315B (*nmr*)
Anschütz, R. *et al., Annalen*, 1889, **254**, 258 (*synth*)
Thielemann, H. *et al., Z. Chem.*, 1978, **18**, 174 (*synth*)
Yu, F.-L. *et al., Acta Cryst. C*, 2004, **60**, o714-o717 (*cryst struct*)
Chen, G. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2006, **42**, 138-141 (*3-Me, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HGO600; NKJ000

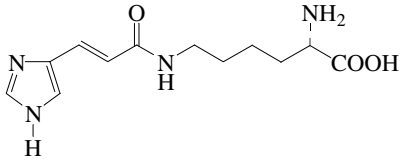
5-[[3-(1*H*-Imidazol-4-yl)propenoyl]amino]pentanoic acid I-30



$C_{11}H_{15}N_3O_3$ 237.258

(*E*)-*form*
Isol. from the ascidian *Atriolum robustum*.
Amorph. solid. λ_{max} 277 (ϵ 39500) (H_2O).
Kehraus, S. *et al., J. Med. Chem.*, 2004, **47**, 2243-2255 (*isol, pmr, cmr*)

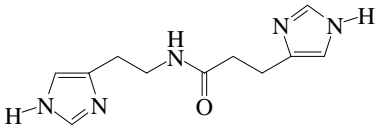
N^6-[3-(1*H*-Imidazol-4-yl)propenoyl]lysine I-31
*2-Amino-6-[[3-(1*H*-imidazol-4-yl)-2-propenoyl]amino]hexanoic acid*



$C_{12}H_{18}N_4O_3$ 266.299

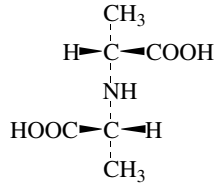
(*S,E*)-*form*
Isol. from the ascidian *Atriolum robustum*.
Amorph. solid. $[\alpha]_D^{25}$ -9 (c, 1.7 in H_2O). λ_{max} 280 (ϵ 25500) (H_2O).
Kehraus, S. *et al., J. Med. Chem.*, 2004, **47**, 2243-2255 (*isol, pmr, cmr*)

N^{α}-[3-(1*H*-Imidazol-4-yl)propenyl]histamine I-32
*3-(1*H*-Imidazol-4-yl)-N-[2-(1*H*-imidazol-4-yl)ethyl]propanamide*
[50767-80-1]



$C_{11}H_{15}N_5O$ 233.272
Isol. from the Philippine gastropod *Drupa concatenata*. Cryst. (MeOH).
Mp 163-164°.
Roseghini, M. *et al., Experientia*, 1973, **29**, 940-941 (*isol*)
Baures, P.W. *et al., Molecules*, 2002, **7**, 813-816 (*synth, pmr, cmr*)

2,2′-Iminobispropanoic acid I-33
N-(1-Carboxyethyl)alanine, 9CI. 2,2′-Iminodipropionic acid, 8CI. Diethylamine-1,1′-dicarboxylic acid. 1,1′-Dicarboxydiethylamine. Alanopine
[73890-66-1]



(*R,R*)-*form*

$C_6H_{11}NO_4$ 161.157

(*R,R*)-*form* [66642-87-3]
Constit. of *Patinopecten yessoensis*, lugworm *Arenicola marina*, oyster *Crassostrea gigas*, *Tapes japonica* and many other marine organisms.
Cryst. (EtOH aq.).
Mp 242° (synthetic).

(*S,S*)-*form*
L-form
[92283-80-2]
Mp 247°. $[\alpha]_D^{14}$ +12.1.

Di-Et ester: [84028-99-9]
$C_{10}H_{19}NO_4$ 217.264
Light yellow liq. $[\alpha]_D^{21}$ -59.54 (c, 1.295 in MeOH).

N-*Hydroxy:* N-*(1-Carboxyethyl)*-N-*hydroxyalanine, 9CI.* N-*Hydroxy-2,2′-iminodipropanoic acid*
[50825-12-2]
$C_6H_{11}NO_5$ 177.157
Prod. by *Armillaria* sp. and *Amanita muscaria*. Chelating agent.
Hygroscopic cryst. (EtOH aq.). V. sol. H_2O.
Mp 145-146° dec.

(*RS,RS*)-*form*
(±)-form
[19149-54-3]
Found in the squid, *Todarodes pacificus*.
Needles (H_2O).
Mp 254-255° Mp 234-235° dec.

Di-Me ester:
$C_8H_{15}NO_4$ 189.211
Bp_{30} 122-124°.

Di-Et ester:
Bp_{15} 123-124°.

Monoamide:
$C_6H_{12}N_2O_3$ 160.172
Mp 232° (210°).

Diamide: 2,2′-Iminobispropanamide
$C_6H_{13}N_3O_2$ 159.188
Mp 127°.

Dinitrile: 2,2′-Iminobispropanenitrile, 9CI. 1,1′-Dicyanodiethylamine
[2869-25-2]
$C_6H_9N_3$ 123.157
Mp 68°.

▶ UG2965000

Imide: 3,5-Dimethyl-2,6-piperazinedione
$C_6H_{10}N_2O_2$ 142.157
Mp 186°.

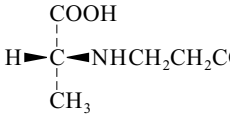
(*RS,SR*)-*form*
meso-*form*
[65621-33-2]
Isol. from lugworm *Arenicola marina*, *Tapes japonica*, and from scallops (*Patinopecten yessoensis*) and squids (possibly *Todarodes pacificus*) and many other marine organisms.
Needles.
Mp 232-233°.

[101541-15-5, 103954-11-6]

Karrer, P. *et al., Helv. Chim. Acta*, 1942, **25**, 595-599 (*synth, S,S-form, R,R-form, meso-form*)
Bayer, E. *et al., Z. Naturforsch., B*, 1972, **27**, 207 (*N-hydroxy*)
Bejaud, M. *et al., Tet. Lett.*, 1975, 2985-2986 (*synth*)
Sato, M. *et al., Nippon Suisan Gakkaishi*, 1977, **43**, 1441-1443; 1978, **44**, 247-250; 1979, **45**, 635-638; 1982, **48**, 1411-1414; *CA*, **88**, 84761; **89**, 39648; **91**, 71955; **98**, 86545 (*isol, rev*)
Fields, J.H.A. *et al., Arch. Biochem. Biophys.*, 1980, **201**, 110-114 (*isol, Crassostrea*)
Felcman, J. *et al., Inorg. Chim. Acta*, 1984, **93**, 101-108 (*N-hydroxy*)
Garrigues, B. *et al., Tetrahedron*, 1984, **40**, 1151-1156 (*synth*)
Siegmund, B. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **82**, 337-345 (*isol, Arenicola*)
Kneifel, H. *et al., J.A.C.S.*, 1986, **108**, 3075-3077 (*N-hydroxy*)
Insaf, S.S. *et al., Tetrahedron*, 2000, **56**, 2359-2367 (*S,S-form, di-Et ester, synth, pmr, cmr*)

2,3′-Iminobispropanoic acid I-34

N-*2-(Carboxyethyl)-α-alanine, 9CI. 2,3′-Iminodipropionic acid, 8CI. Alanine*-N-*propionic acid. β-Alanopine*



(*R*)–*form*

$C_6H_{11}NO_4$ 161.157

(*R*)-*form* [2254-38-8]
Constit. of the muscle of the mollusc *Scapharca broughtonii*. Opine.

(*S*)-*form* [7671-31-0]
Cryst. (hot H_2O). Prac. insol. EtOH, Et_2O. Mp 220-221°. $[\alpha]_D^{20}$ +3.2 (c, 2.47 in H_2O). $[\alpha]_D^{22}$ +6 (c, 3.43 in H_2O).

(±)-*form* [91548-47-9]
Cryst. (Me_2CO aq.). Mp 200-202° dec.

Di-Et ester:
$C_{10}H_{19}NO_4$ 217.264
Bp 245° sl. dec. $Bp_{1.5}$ 89-91° (lit. gives a pressure range).
n_D^{25} 1.4325.

Di-Et ester, hydrochloride: Mp 74-76°.

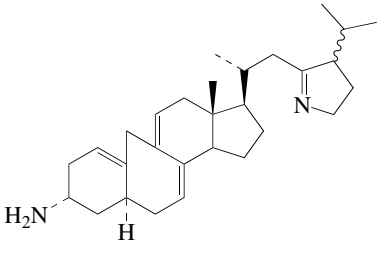
Di-Et ester, N-*Ac:*
$C_{12}H_{21}NO_5$ 259.302
Bp 315° Bp 170-175° $Bp_{1.5}$ 142-145° (lit. gives a pressure range).

Di-Et ester, N-*benzoyl:*
$C_{17}H_{23}NO_5$ 321.372
$Bp_{1.5}$ 167-168° (lit. gives a pressure range).

[2254-38-8]

McKinney, L.L. *et al., J.A.C.S.*, 1952, **74**, 1942; 5183 (*synth*)
Battersby, A.R. *et al., J.C.S.*, 1960, 1214 (*synth*)
Trojanek, J. *et al., Chem. Ind. (London)*, 1965, 1261 (*synth*)
Okamoto, K. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 3134 (*synth, resoln*)
Wasserman, H.H. *et al., J.O.C.*, 1975, **40**, 1505 (*ester*)
Kawashiro, K. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 1097 (*synth, ms, pmr*)
Sato, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1987, **88**, 803 (*isol*)

23,29-Imino-*B*(9*a*)-homo-19-norstigmasta-1(10),7,9(11),23(*N*)-tetraen-3-amine I-35



$C_{29}H_{44}N_2$ 420.68

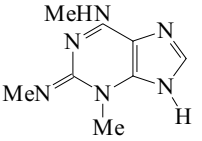
(3α,5α,24ξ)-*form* [215245-26-4]
Alkaloid from the marine sponge *Corticium* sp.
$[\alpha]_D$ -50 (c, 0.01 in $CHCl_3$). λ_{max} 207 (log ε 3.62); 248 (log ε 3.72) (MeOH).

9,11-Dihydro: ***23,29-Imino-B(9a)-homo-19-norstigmasta-1(10),7,23(N)-trien-3-amine***
[215245-28-6]
$C_{29}H_{46}N_2$ 422.696
Alkaloid from *Corticium* sp.
$[\alpha]_D$ -8.1 (c, 0.01 in $CHCl_3$). λ_{max} 210 (log ε 3.74); 240 (log ε 3.5) (MeOH).

De Marino, S. *et al., Tet. Lett.*, 1998, **39**, 7611-7614 (*isol, uv, pmr, cmr*)

2-Iminomethyl-3-methyl-6-methylamino-9*H*-purine I-36

*3,7-Dihydro-*N*,3-dimethyl-2-(methylimino)-2*H*-purin-6-amine, 9CI*
[112058-06-7]

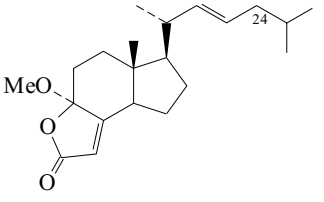


$C_8H_{12}N_6$ 192.223
Isol. from the sea-anemone *Sagartia troglodytes*. Phytotoxic agent.
Cryst. (MeOH).
Mp 226-227°. λ_{max} 288 (ε 14000) (MeOH) (Berdy).

De Rosa, S. *et al., J. Nat. Prod.*, 1987, **50**, 876 (*isol, uv, pmr, ms, cryst struct*)

Incisterol I-37

[125974-95-0]



$C_{21}H_{32}O_3$ 332.482
Constit. of the sponge *Dictyonella incisa*.

O-*De-Me:* ***Demethylincisterol A1***
[849752-85-8]
$C_{20}H_{30}O_3$ 318.455
Constit. of a *Homaxinella* sp. Oil. λ_{max} 220 (log ε 3.98) (MeOH).

*24*R-*Methyl,* O-*de-Me:* ***Demethylincisterol A3***
[166318-86-1]
$C_{21}H_{32}O_3$ 332.482
Constit. of a *Homaxinella* sp. Oil. $[\alpha]_D^{21}$ +74 (c, 0.1 in MeOH).

*24*S-*Methyl,* O-*de-Me:* ***Demethylincisterol A2***
[849752-86-9]
$C_{21}H_{32}O_3$ 332.482
Constit. of a *Homaxinella* sp. Oil. $[\alpha]_D^{21}$ +28 (c, 0.08 in MeOH).

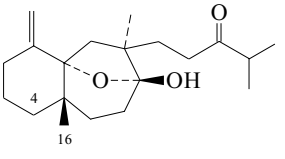
*24*R-*Ethyl:* ***17*R-Ethylincisterol***
[125974-97-2]
$C_{23}H_{36}O_3$ 360.536
Constit. of *Dictyonella incisa*.

*24*R-*Ethyl,* O-*de-Me:* ***Demethylincisterol A4***
[849752-87-0]
$C_{22}H_{34}O_3$ 346.509
Constit. of a *Homaxinella* sp. Oil.

Ciminiello, P. *et al., J.A.C.S.*, 1990, **112**, 3505 (*isol, pmr, cmr*)
De Riccardis, F. *et al., Tet. Lett.*, 1995, **36**, 4303 (*synth*)
Mansoor, T.A. *et al., J. Nat. Prod.*, 2005, **68**, 331-336 (*Homaxinella constits*)

Indicol† I-38

[128700-85-6]



$C_{20}H_{32}O_3$ 320.471
Constit. of *Dictyota indica*. Viscous oil. $[\alpha]_D$ -44 (c, 0.426 in $CHCl_3$).

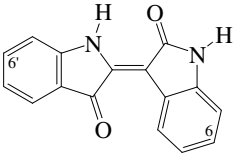
4α,16-Dihydroxy: ***Indicarol***
[128700-81-2]
$[\alpha]_D$ -46.42 (c, 0.28 in $CHCl_3$).

4α-Hydroxy, 16-acetoxy: ***Indicarol acetate***
[128700-80-1]
$C_{22}H_{34}O_6$ 394.507
Constit. of *Dictyota indica*. Viscous oil. $[\alpha]_D$ -36.9 (c, 0.676 in $CHCl_3$).

Bano, S. *et al., J. Nat. Prod.*, 1990, **53**, 492 (*isol, pmr, cmr*)

Indirubin I-39

*3-(1,3-Dihydro-3-oxo-2*H*-indol-2-ylidene)-1,3-dihydro-2*H*-indol-2-one, 9CI. Δ$^{2,3'}$-Biindoline-2′,3-dione. Couroupitine B. Indigo red. C.I. 75790*
[479-41-4]



$C_{16}H_{10}N_2O_2$ 262.267
Alkaloid from *Indigofera* spp. as minor constit. of indigo. Isol. from the molluscs *Hexaplex trunculus* and *Murex brandaris* (as component of Tyrian purple). Constit. of *Couroupita guianensis*, root of *Isatis indigotica*, *Isatis tinctoria*, *Polygonum tinctorium* and *Baphicacanthus cusia*. Isol. from the fungal pigment of a *Schizophyllum commune* mutant. Inhibitor of Lewis lung carcinoma and Walker 256 carcinosarcoma in mice. Red cryst. Sol. EtOH, AcOH; poorly sol. H_2O, hexane.
Mp >400° subl. λ_{max} 522; 561 (xylene). λ_{max} 207; 239; 290; 360; 540 (MeOH) (Berdy).

▶ DU2995000

1,1′-Di-Ac: Mp 192-193°.

Oxime: [160807-49-8]
$C_{16}H_{11}N_3O_2$ 277.282
Glycogen synthase kinase (GSK-3) inhibitor. Deep red cryst. Mp 246°.

6-Bromo: ***6-Bromoindirubin***
[200273-66-1]
$C_{16}H_9BrN_2O_2$ 341.163
Isol. from the mollusc *Hexaplex trunculus*. Selective inhibitor of GSK-3.

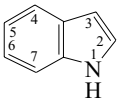
6′-Bromo: [200273-67-2]
$C_{16}H_9BrN_2O_2$ 341.163
Isol. from the mollusc *Hexaplex trunculus*.

6,6′-Dibromo: [171565-08-5]
$C_{16}H_8Br_2N_2O_2$ 420.059
Isol. from the molluscs *Hexaplex trunculus* and *Nucella lapillus*. λ_{max} 305 (log ϵ 4.43); 350 (sh); 367 (log ϵ 3.94); 387 (sh); 525 (sh); 552 (log ϵ 4.07) ($CHCl_3$). λ_{max} 305 (log ϵ 4.28); 371 (log ϵ 3.73); 552 (log ϵ 3.89) (CCl_4).

De Diesbach, H. *et al., Helv. Chim. Acta*, 1945, **28**, 690-700 (*synth*)
v. Eller-Pandraud, H. *et al., Bull. Soc. Chim. Fr.*, 1958, 712-714 (*cryst struct*)
Epstein, E. *et al., CA*, 1966, **66**, 102443 (*isol*)
Plieninger, D.W. *et al., Chem. Ber.*, 1966, **99**, 3063-3069 (*synth*)
Sen, A.K. *et al., Tet. Lett.*, 1974, 609-610 (*isol*)
Bergmann, J. *et al., Tet. Lett.*, 1977, 2625-2626 (*struct*)
Bergmann, J. *et al., Tetrahedron*, 1985, **41**, 2879-2891 (*isol, struct, props*)
Shen, Y. *et al., Yaoxue Tongbao*, 1985, **19**, 601-602; *CA*, **102**, 10071 (*isol*)
Ji, X. *et al., Yaoxue Xuebao*, 1985, **20**, 137-139; *CA*, **103**, 98313 (*activity*)
Zhang, S. *et al., Yaoxue Xuebao*, 1985, **20**, 301-305; *CA*, **103**, 92918 (*detn*)
Clark, R.J.H. *et al., J. Soc. Dyers Colour.*, 1997, **113**, 316-321 (*Bromoindirubins*)
Leclerc, S. *et al., J. Biol. Chem.*, 2001, **276**, 251-260 (*oxime, pharmacol, synth, pmr, cmr*)
Cooksey, C.J. *et al., Molecules*, 2001, **6**, 736-769 (*6,6′-Dibromoindirubin, rev*)
Maugard, T. *et al., Phytochemistry*, 2001, **58**, 897-904 (*isol, uv*)
Meijer, L. *et al., Chem. Biol.*, 2003, **10**, 1255-1266 (*Bromoindirubins*)
Mak, N.K. *et al., Biochem. Pharmacol.*, 2004, **67**, 167-174 (*oxime, pharmacol*)
Xie, Y. *et al., Neurosci. Lett.*, 2004, **367**, 355-359 (*oxime, pharmacol*)

Indole, 9CI, 8CI I-40

1-Benzazole. 2,3-Benzopyrrole. 1-Azaindene. Ketole (obsol.). FEMA 2593
[120-72-9]



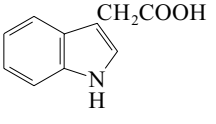
C_8H_7N 117.15
Constit. of coal tar. Constit. of several flower oils, esp. of *Jasminum* and *Citrus* spp. (Oleaceae, Rutaceae). A prod. of bacterial dec. of proteins, ubiquitous in faeces. Constit. of anal gland secretion of aardwolf *Proteles cristatus*. Prod. by marine bacterium strain Ta-6 from *Tapes philippinarum* and by a range of microorganisms isol. from fish and shellfish. Perfumery and flavouring ingredient. Used as 0.5% EtOH soln. for photometric detn. of $NO_2^{\ominus}$. λ_{max} 530 nm (ϵ 9500, 2.5-5*M* HCl). Cryst. (H_2O). Sol. EtOH, MeOH, Et_2O; poorly sol. H_2O.
Mp 52°. Bp 253-254° Bp_5 122.5-124°. pK_{a1} -2.4; pK_{a2} 16.97 (25°,NH, KOH aq.). λ_{max} 216; 270; 278; 281; 295 (MeOH) (Berdy).

▶ LD_{50} (rat, orl) 1000 mg/kg. NL2450000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 653A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 121A; 153B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1497A (*ir*)
Stowe, B.B. *et al., Prog. Chem. Org. Nat. Prod.*, 1959, **17**, 250-297 (*occur*)
Gray, A.P. *et al., J.O.C.*, 1960, **25**, 1939-1943 (*N-Et*)
Sawicki, E. *et al., Talanta*, 1963, **10**, 641-655 (*use*)
Jennings, A.L. *et al., J.O.C.*, 1964, **29**, 2065-2066 (*ms*)
Black, P.J. *et al., Aust. J. Chem.*, 1965, **18**, 353-361 (*pmr*)
Chignell, D.A. *et al., J. Phys. Chem.*, 1968, **72**, 2934-2941 (*uv*)
Bravo, P. *et al., Gazz. Chim. Ital.*, 1970, **100**, 652-664 (*synth*)
Parker, R.G. *et al., J.O.C.*, 1970, **35**, 996-999 (*cmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 925 (*rev, tox*)
Lieto, J. *et al., Bull. Soc. Chim. Fr.*, 1976, 1246-1250 (*synth*)
Nakazuki, M. *et al., J.O.C.*, 1976, **41**, 1877 (*synth*)
Ito, Y. *et al., J.A.C.S.*, 1977, **99**, 3532-3534 (*synth*)
Rahim, S.A. *et al., Microchem. J.*, 1983, **28**, 479-484 (*use*)
Apps, P.J. *et al., J. Chem. Ecol.*, 1989, **15**, 1681-1688 (*occur*)
Takao, T. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1780-1783 (*isol, occur*)
Hodson, H.F. *et al., Tetrahedron*, 1994, **50**, 1899-1906 (*N-tosyl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, ICM000

1*H*-Indole-3-acetic acid, 9CI I-41

3-Indolylacetic acid. Heteroauxin. Rhizopin. IAA. Rhizipon A
[87-51-4]



$C_{10}H_9NO_2$ 175.187
Isol. from the marine alga *Undaria pinnatifida*. Widely distributed in higher plants, also in bacteria, algae, yeasts and fungi. Plant growth hormone (auxin). Involved in root development. Phytotoxic agent. Cryst. ($CHCl_3$). Sol. EtOH, Me_2CO; fairly sol. H_2O, $CHCl_3$.
Mp 164-165°. pK_{a1} 4.36; pK_{a2} 16.9 (NH). λ_{max} 229 (ϵ 10400); 273 (ϵ 9900); 278 (ϵ 10000); 289 (ϵ 8700) (MeOH) (Berdy).

▶ Exp. reprod. and teratogenic effects. NL3150000

*Amide: 1*H*-Indole-3-acetamide*
[879-37-8]
$C_{10}H_{10}N_2O$ 174.202
Isol. from etiolated seedlings of the black gram (*Phaseolus*

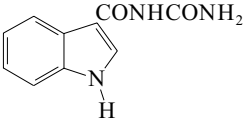
mungo). Also from the sponges *Dysidea etheria* and *Ulosa ruetzleri*. Plant growth regulator.
Mp 150-151°.

[2338-19-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 667C; 675D; 676D; 678C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 138B; 149A; 154A; 159A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1503C (*ir*)
Stowe, B.B. *et al., Prog. Chem. Org. Nat. Prod.*, 1959, **17**, 248 (*bibl*)
Isogai, Y. *et al., Chem. Pharm. Bull.*, 1963, **11**, 1217 (*isol, amide*)
Abe, H. *et al., Agric. Biol. Chem.*, 1972, **36**, 2259 (*isol, uv, ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, nos. 2514; 2515 (*bibl*)
Chandrasekhar, K. *et al., Acta Cryst. B*, 1982, **38**, 2534 (*cryst struct*)
Vekrel, J. *et al., Spectrochim. Acta A*, 1983, **39**, 887 (*ir, pmr, ms*)
Cardellina, J.H. *et al., J. Nat. Prod.*, 1986, **49**, 1065-1067 (*isol, amide*)
Pfeiffer, D. *et al., Cryst. Res. Technol.*, 1987, **22**, KI (*cryst struct*)
Morales-Rios, M.S. *et al., Magn. Reson. Chem.*, 1987, **25**, 377 (*cmr*)
Pesticide Manual, 9th edn., 1991, No. 7260
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A232
Nagarathnam, D. *et al., J. Het. Chem.*, 1992, **29**, 953 (*synth*)
Fukuyama, T. *et al., J.A.C.S.*, 1994, **116**, 3127 (*synth*)
Faul, M. *et al., J.O.C.*, 1998, **63**, 6053-6058 (*N-Me, amide, synth, pmr, cmr, uv, ir*)
Shimada, A. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 187 (*isol, activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ICN000; ICW000

N-(1*H*-Indole-3-carbonyl)urea I-42

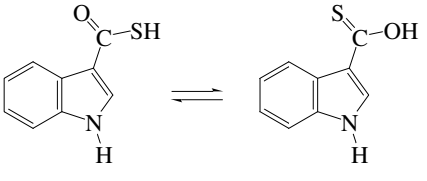
N-*(Aminocarbonyl)-1*H-*indole-3-carboxamide, 9CI*
[159308-53-9]



$C_{10}H_9N_3O_2$ 203.2
Metab. from the sponge *Zyzza massalis*.

Mancini, I. *et al., Helv. Chim. Acta*, 1994, **77**, 1886-1894 (*isol, uv, pmr, cmr, ms, struct*)

1*H*-Indole-3-carbothioic acid, 9CI I-43



C_9H_7NOS 177.226

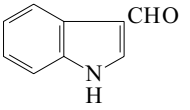
SH-form

Me ester: S-*Methyl 1*H-*indole-3-carbothioate. Methyl 1*H-*indolethiolcarboxylate*
[54584-28-0]
$C_{10}H_9NOS$ 191.253
Isol. from the marine-derived *Oceanibulbus indolifex* Hel 45.
Cryst. (C_6H_6/petrol).
Mp 164-166°.

Barbero, M. *et al., Synthesis*, 1988, 300-302 (*synth, pmr, cmr*)
Wagner-Döbler, I. *et al., Int. J. Syst. Evolut. Microbiol.*, 2004, **54**, 1177-1184 (*isol*)

1*H*-Indole-3-carboxaldehyde, 9CI I-44

Indole-3-aldehyde. 3-Formylindole
[487-89-8]



C_9H_7NO 145.16
Alkaloid from the stem bark of *Murraya exotica* and from the red alga *Botryocladia leptopoda*. Also found in barley and tomato seedlings, cotton, *Pseudomonas syringae, Rhizobium* sp. and the coral *Tubastrea coccinea*.
Mp 180° Mp 197-199°. pK_{a2} 12.36 (25°,NH).

▶ NL5993600

Oxime: [2592-05-4]
$C_9H_8N_2O$ 160.175
Mp 197-198°.

Phenylhydrazone: [16578-92-0]
Mp 198°.

2,4-Dinitrophenylhydrazone: [40941-43-3]
Red cryst. (dioxan). Mp 300°.

Semicarbazone: Mp 265-270° dec.

Anil:
$C_{15}H_{12}N_2$ 220.273
Mp 240-246° dec.

N-*Ac:* [22948-94-3]
$C_{11}H_9NO_2$ 187.198
Mp 159-162°.

N-tert-*Butyloxycarbonyl:* [57476-50-3]
$C_{14}H_{15}NO_3$ 245.277
Solid (EtOAc/hexane). Mp 124° (117-118°).

N-*Benzenesulfonyl:* [80360-20-9]
$C_{15}H_{11}NO_3S$ 285.323
Cryst. (EtOH). Mp 157.5-158.5°.

N-*Me: 1-Methyl-1*H-*indole-3-carboxaldehyde*
[19012-03-4]
$C_{10}H_9NO$ 159.187
Cryst. Mp 67° (65-68°).

N-*Me, oxime:* [24666-30-6]
$C_{10}H_{10}N_2O$ 174.202
Solid. Mp 144-146°.

N-*Benzyl:* [10511-51-0]
$C_{16}H_{13}NO$ 235.285
Cryst. Mp 108-109° (102-104°).

N-*Hydroxy: 1-Hydroxy-1*H-*indole-3-carboxaldehyde, 9CI*
[67282-51-3]
$C_9H_7NO_2$ 161.16
Cryst. (EtOAc/hexane). Mp 145-152°.

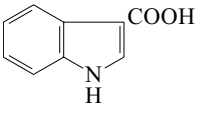
N-*Methoxy:* ***1-Methoxy-1*H-*indole-3-carboxaldehyde, 9CI***.
1-Methoxy-3-formylindole
[67282-55-7]
$C_{10}H_9NO_2$ 175.187
Stress metab. from the Japanese radish Daikon (*Raphanus sativus* var. *hortensis*) inoculated with *Pseudomonas cichorii*. Prisms + $^1/_2H_2O$ (Et_2O/hexane).
Mp 50-51°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 666B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 136A; 136B; 153C (*nmr*)
Org. Synth., Coll. Vol., 4, 1963, 539 (*synth*)
Jackson, A.H. *et al., J.C.S.*, 1964, 5510-5517 (*synth*)
Bestmann, H.J. *et al., Annalen*, 1968, **718**, 24 (*synth*)
Hart, J.C. *et al., Can. J. Chem.*, 1970, **48**, 177 (*synth*)
Chowdhury, B.K. *et al., Phytochemistry*, 1971, **10**, 481 (*isol, ir, pmr, ms*)
Schneider, E.A. *et al., J. Exp. Bot.*, 1972, **23**, 152 (*occur*)
Fetizon, M. *et al., J. Het. Chem.*, 1976, **13**, 525 (*deriv, synth*)
Wratten, S.J. *et al., Antimicrob. Agents Chemother.*, 1977, **11**, 411 (*isol*)
Oikawa, Y. *et al., J.O.C.*, 1977, **42**, 1213 (*synth*)
Acheson, R.M. *et al., J.C.S. Perkin 1*, 1978, 1117-1125 (*N-methoxy*)

Jo, S. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 2120 (*synth*)
Lahoti, R.J. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 1007 (*synth*)
Komiyama, M. *et al., Makromol. Chem. Rapid Commun.*, 1981, **2**, 757 (*synth*)
Badenoch-Jones, J. *et al., Biomed. Mass Spectrom.*, 1982, **9**, 429 (*isol, ms*)
Okuda, R.K. *et al., Pure Appl. Chem.*, 1982, **54**, 1907 (*isol*)
Moody, C.J. *et al., J.C.S. Perkin 1*, 1984, 2903 (*synth*)
Golubev, S.N. *et al., Zh. Strukt. Khim.*, 1984, **25**, 145; *CA*, **101**, 141424 (*cryst struct*)
Pindur, U. *et al., Annalen*, 1986, 1621 (*synth, ir, pmr, ms*)
Somei, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 677 (*N-methoxy, synth*)
Bano, S. *et al., J. Nat. Prod.*, 1986, **49**, 549 (*isol*)
Evidente, A. *et al., J. Nat. Prod.*, 1986, **49**, 938 (*isol*)
Kawasaki, T. *et al., Heterocycles*, 1991, **32**, 221-227 (*N-hydroxy*)
Amat, M. *et al., J.O.C.*, 1994, **59**, 10 (*synth*)
Monde, K. *et al., Heterocycles*, 1997, **44**, 157-163 (*N-hydroxy*)
Tholander, J. *et al., Tetrahedron*, 1999, **55**, 6243-6260 (*N-benzenesulfonyl*)
Oliveira, D.de.J. *et al., Synth. Commun.*, 2000, **30**, 2143-2159 (*N-tert-butyloxycarbonyl*)
Sugimoto, O. *et al., Helv. Chim. Acta*, 2001, **84**, 1112-1118 (*synth, pmr*)
Everett, S.A. *et al., J.C.S. Perkin 2*, 2001, 1989-1997 (*oximes, synth, pmr*)
Kimura, R. *et al., Bull. Chem. Soc. Jpn.*, 2002, **75**, 2517-2525 (*N-tert-butyloxycarbonyl*)

1*H*-Indole-3-carboxylic acid **I-45**

Indole-β-carboxylic acid
[771-50-6]



$C_9H_7NO_2$ 161.16
Present in plants, e.g. apple (*Pyrus malus*), garden pea (*Pisum sativum*), *Brassica* spp, and the marine algae *Undaria pinnatifida* and *Botryocladia leptopoda*.
Mp 210-218° (198-200°). pK_{a1} 3.87; pK_{a2} 15.59 (25°,NH).
λ_{max} 270; 280; 288 (EtOH).

α-L-Rhamnopyranosyl ester: [309297-78-7]
$C_{15}H_{17}NO_6$ 307.302
Prod. by *Streptomyces* sp. GT 61150. Light yellow powder ($CHCl_3$/MeOH).
Mp 132-133°. $[\alpha]_D^{25}$ -36.8 (c, 0.1 in MeOH). λ_{max} 211 (log ϵ 3.45); 227 (sh) (log ϵ 1.56); 284 (log ϵ 0.97) (MeOH).

Me ester: [942-24-5]
$C_{10}H_9NO_2$ 175.187
Isol. from the red alga *Botryocladia leptopoda*. Phytotoxin.
Mp 147-148° (140°). Probably an artifact.

Et ester: [776-41-0]
$C_{11}H_{11}NO_2$ 189.213
Mp 122-124°.

Amide: ***1*H-Indole-3-carboxamide, 9CI***
[1670-85-5]
$C_9H_8N_2O$ 160.175
Isol. from the sponge *Zyzza massalis*. Solid (EtOAc/hexane).
Mp 201-203°.

*Nitrile: 1*H-*Indole-3-carbonitrile, 9CI. 3-Cyanoindole*
[5457-28-3]
$C_9H_6N_2$ 142.16
Alkaloid from a facultatively anaerobic, halophilic bacterium.
Mp 178°.

N-*Ac, nitrile:*
$C_{11}H_8N_2O$ 184.197
Mp 202°.

N-*Ethoxycarbonyl, Et ester: Diethyl 1*H-*indole-1,3-dicarboxylate*
[13328-43-3]
$C_{14}H_{15}NO_4$ 261.277
Cryst. (EtOH). Mp 102-104°.

N-*Me:* [32387-21-6]
$C_{10}H_9NO_2$ 175.187
Cryst. (2-propanol) or plates (Me_2CO aq.). Mp 212° (200-201° dec.). λ_{max} 215; 243 (sh); 286; 298 (sh) (MeOH).

N-*Me, Et ester:* [56559-60-5]
$C_{12}H_{13}NO_2$ 203.24
Mp 69.7-70.2°.

N-*Me, amide:* [118959-44-7]
$C_{10}H_{10}N_2O$ 174.202
Solid. Mp 176-177°.

N-*Me, nitrile: 3-Cyano-1-methyl-1*H-*indole*
[24662-37-1]
$C_{10}H_8N_2$ 156.187
Cryst. (Et_2O/hexane). Mp 60-61°.

N-*(1,1-Dimethyl-2-propenyl), Me ester:* [306776-02-3]
$C_{15}H_{17}NO_2$ 243.305
Alkaloid from the fungus *Aporpium caryae*. Antifungal agent. Oil.
λ_{max} 240 (log ϵ 3.05); 244 (log ϵ 3.05); 288 (log ϵ 3.03) (CH_2Cl_2).

N-*(2,3-Dihydroxy-1,1-dimethylpropyl)(*S-*), Me ester:* [306776-03-4]
$C_{15}H_{19}NO_4$ 277.319
Alkaloid from the fungus *Aporpium caryae*. Oil. $[\alpha]_D$ -11.8 (c, 0.21 in CH_2Cl_2). λ_{max} 242 (log ϵ 3.05); 248 (log ϵ 3.05); 284 (log ϵ 3.03) (CH_2Cl_2).

N-*Benzyl:* [27018-76-4]
$C_{16}H_{13}NO_2$ 251.284
Cryst. (EtOAc/hexane). Mp 194-196° Mp 198-204°.

N-*Hydroxy: 1-Hydroxy-1*H-*indole-3-carboxylic acid, 9CI*
[18377-48-5]
$C_9H_7NO_3$ 177.159
Pale orange solid. Mp 135-137° dec.

N-*Hydroxy, amide:* [69111-90-6]
$C_9H_8N_2O_2$ 176.174
Green-brown rods (H_2O). Mp 181-182° dec.

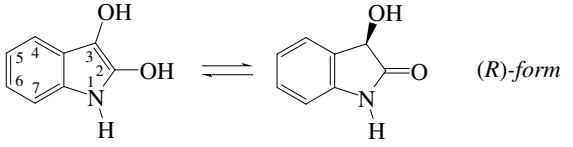
N-*Hydroxy, nitrile: 1*H-*Indole-3-carbonitrile* N-*oxide*
[69111-88-2]
$C_9H_6N_2O$ 158.159
Cryst. (C_6H_6/hexane). Mp 127-128°.

N-*Methoxy, Me ester:* ***Methyl 1-methoxy-1*H-*indole-3-carboxylate***
[18377-50-9]
$C_{11}H_{11}NO_3$ 205.213
Prod. by Japanese horseradish (*Wasabia japonica*). Phytoalexin. Antifungal agent. Prisms ($CHCl_3$).
Mp 45-46° (40-41°) Mp 40-41°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 138A; 158B (*nmr*)
Whalley, W.B. *et al., J.C.S.*, 1954, 1651-1653 (*N-Me, synth*)
Millich, F. *et al., J.O.C.*, 1958, **23**, 1096-1102 (*N-Me, synth*)
Hart, G. *et al., J.O.C.*, 1962, **27**, 2940-2942 (*N-Me, synth*)
Kasparek, S. *et al., Can. J. Chem.*, 1966, **40**, 2805-2811 (*synth*)
Glombitza, K.W. *et al., Planta*, 1966, **69**, 135-149 (*biosynth*)
Katner, A.S. *et al., Org. Prep. Proced. Int.*, 1970, **2**, 297-303 (*synth*)
Aldridge, D.C. *et al., J.C.S.(C)*, 1971, 1623-1627 (*isol*)
Abe, H. *et al., Agric. Biol. Chem.*, 1972, **36**, 2259-2260 (*isol, uv, ms*)
Acheson, R.M. *et al., J.C.S. Perkin 1*, 1978, 1117-1125 (*N-hydroxy*)
Mehta, G. *et al., Synthesis*, 1978, 374-376 (*synth, amide, nitrile*)
Acheson, R.M. *et al., J. Chem. Res., Synop.*, 1984, 101; *J. Chem. Res., Miniprint*, 1984, 1301-1319 (*N-hydroxy, N-methoxy Me ester, synth*)
Plate, R. *et al., Tetrahedron*, 1986, **42**, 6511-6518 (*N-Me, uv*)
Bano, S. *et al., Planta Med.*, 1987, **53**, 117-118 (*isol, uv, pmr, cmr, ms, esters*)
Baiocchi, L. *et al., J. Het. Chem.*, 1988, **25**, 1905-1909 (*synth, N-Me, N-benzyl*)
Swain, C.J. *et al., J. Med. Chem.*, 1992, **35**, 1019-1031 (*N-Me, nitrile*)
Buttery, C.D. *et al., J.C.S. Perkin 1*, 1993, 1425-1431 (*N-Me, synth, ir, pmr*)
Mancini, I. *et al., Helv. Chim. Acta*, 1994, **77**, 1886-1894 (*amide, isol*)
Vorbrüggen, H. *et al., Tetrahedron*, 1994, **50**, 6549-6558 (*nitrile*)
Fu, X. *et al., J. Nat. Prod.*, 1995, **58**, 1950-1954 (*isol, nitrile*)
Prashad, M. *et al., Synth. Commun.*, 1995, **25**, 95-100 (*Me ester, synth*)
Pedras, M.S.C. *et al., Phytochemistry*, 1998, **49**, 1959-1965 (*1-methoxy Me ester*)
Hu, J.-F. *et al., J. Antibiot.*, 2000, **53**, 944-953 (*rhamnosyl ester*)
Levy, L.M. *et al., Phytochemistry*, 2000, **54**, 941-943 (*N-1,1-dimethylpropyl derivs*)
SomeiM *et al., Heterocycles*, 2001, **54**, 425-432 (*1-methoxy Me ester synth*)
Everett, S.A. *et al., J.C.S. Perkin 2*, 2001, 1989-1997 (*N-Me amide*)
Sala, G.D. *et al., Tet. Lett.*, 2002, **43**, 8839-8841 (*N-1,1-dimethylpropyl derivs, synth*)

1*H*-Indole-2,3-diol I-46

*1,3-Dihydro-3-hydroxy-2*H-*indol-2-one, 9CI. Dioxindole.* o-*Aminomandelic lactam. 3-Hydroxyoxindole. 2,3-Dihydroxyindole*
[61-71-2]
[5638-85-7]



(*R*)-*form*

$C_8H_7NO_2$ 149.149

Oxindole form predominates. Prod. by a marine bacterial strain isol. from gills of *Sphyraena japonica* and prod. by a range of microorganisms present in fish and shellfish. Prod. of metab. of Indole, I-40 by microorganisms. Antioxidant. Cryst. (H_2O or EtOH).
Mp 167-168°.

▶ NM3289460

Hydrochloride: Mp 156°.

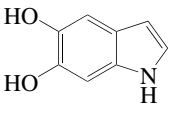
Oxindole-form, (*R*-) [124508-45-8]
Prisms (H_2O). Mp 167-168°. $[\alpha]_D^{25}$ +7 (c, 1 in MeOH). $[\alpha]_D^{20}$ +34 (c, 2.1 in Me_2CO). $[\alpha]_D^{25}$ +42.5 (c, 1 in EtOH) (98% ee).

Oxindole-form, (±) [71711-19-8]

Ziegler, E. *et al., Monatsh. Chem.*, 1963, **94**, 453-459 (*synth*)
Fujioka, M. *et al., Biochim. Biophys. Acta*, 1965, **158**, 70-78 (*isol*)
Tallec, A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1971, **273**, 1378-1381 (*synth*)

1*H*-Indole-5,6-diol, 9CI I-47

5,6-Dihydroxyindole. Dopamine lutine
[3131-52-0]



$C_8H_7NO_2$ 149.149
Alkaloid from the leaves of *Rhaphidophora korthalsii* and *Epipremnum pinnatum*. Cytotoxic agent. Intermed. in the tyrosinase-catalysed biosynth. pathway from tyrosine to melanin. Needles (C_6H_6/petrol). Sol. hot H_2O; insol. petrol.
Mp 140° dec. Unstable on storage, undergoes spont. oxidn. and condensation to melanin.

▶ Toxic.

N,O^6-*Disulfo:* ***Ancorinolate B***
$C_8H_7NO_8S_2$ 309.277
Alkaloid from the sponge *Ancorina* sp. Powder (as di-Na salt). λ_{max} 222 (log ϵ 4.08); 265 (log ϵ 3.61); 296 (log ϵ 3.39) (MeOH) (di-Na salt).

O,O-*Di-Ac:* [15069-79-1]
$C_{12}H_{11}NO_4$ 233.223
Prisms (C_6H_6/petrol). Mp 138-139°.

N-*Me:* [4821-00-5]
$C_9H_9NO_2$ 163.176
Cryst. (petrol). Mp 134°.

N-*Me, di*-O-*Ac:* [13988-19-7]
$C_{13}H_{13}NO_4$ 247.25
Mp 109-110° (101°).

O^5-*Me: 5-Methoxy-1*H-*indol-6-ol. 6-Hydroxy-5-methoxyindole*
[2380-82-7]
$C_9H_9NO_2$ 163.176
Mp 110-112°.

O^6-*Me: 6-Methoxy-1*H-*indol-5-ol. 5-Hydroxy-6-methoxyindole*
[2380-83-8]
$C_9H_9NO_2$ 163.176
Mp 113°.

Di-Me ether: 5,6-Dimethoxyindole
[14430-23-0]
$C_{10}H_{11}NO_2$ 177.202
Leaflets (EtOH/petrol), rods (C_6H_6), needles (EtOH aq.). Mp 154-155°. Bp_8 198°. Darkens rapidly.

Di-Me ether, N-*Ac:*
$C_{12}H_{13}NO_3$ 219.24
Yellow-brown leaflets (petrol). Mp 150-152°.

Di-Me ether, N-*Me:* [80639-40-3]
$C_{11}H_{13}NO_2$ 191.229
Needles (heptane). Mp 134-136°.

*Methylene ether: 5*H-*1,3-Dioxolo[4,5-f]indole, 9CI. 5,6-Methylenedioxyindole*
[267-48-1]
$C_9H_7NO_2$ 161.16
Cryst. Mp 110-111°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 128C (*nmr*)
Raper, H.S. *et al., Biochem. J.*, 1927, **21**, 89-96 (*di-Me ether*)
Oxford, A.E. *et al., J.C.S.*, 1927, 417-422 (*di-Me ether*)
Beer, R.J.S. *et al., J.C.S.*, 1948, 2223-2226 (*synth, di-Me ether*)
Harley-Mason, J. *et al., J.C.S.*, 1950, 1276-1282; 1953, 200-203 (*synth, N-Me*)
Heacock, P.A. *et al., J.A.C.S.*, 1963, **85**, 1825-1831 (*synth*)
Grotjahn, D.B. *et al., J. Het. Chem.*, 1983, **20**, 1031-1036 (*methylene ether, synth*)
Murphy, B.P. *et al., J.O.C.*, 1985, **50**, 2790 (*synth, uv, pmr, cmr, ir*)
Corradini, M.G. *et al., Tetrahedron*, 1986, **42**, 2083 (*deriv, synth, props*)
Rogers, C.B. *et al., J. Het. Chem.*, 1987, **24**, 941 (*derivs*)
Carpenter, J.F. *et al., J.O.C.*, 1993, **58**, 1607 (*deriv, synth, pmr, cmr*)
Wong, K.T. *et al., Nat. Prod. Lett.*, 1996, **9**, 137-140 (*isol, ir, pmr, cmr, ms*)
Meragelman, K.M. *et al., J.O.C.*, 2002, **67**, 6671-6677 (*Ancorinolate B*)

1*H*-Indole-6,7-diol, 9CI I-48

6,7-Dihydroxyindole

$C_8H_7NO_2$ 149.149
Poss. marine alkaloid from several *Agelas* spp. Identified on the basis of colour reacns. only; struct. of the alkaloid requires reinvestigation. Could be the isomer 4,6-Dihydroxyindole.

*6-Me ether: 7-Hydroxy-6-methoxyindole. 6-Methoxy-1*H-*indol-7-ol*
$C_9H_9NO_2$ 163.176
Mp 89°.

*7-Me ether: 6-Hydroxy-7-methoxyindole. 7-Methoxy-1*H-*indol-6-ol*
$C_9H_9NO_2$ 163.176
Mp 85-86°.

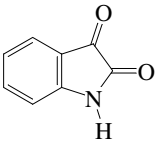
7-Me ether, Ac:
$C_{11}H_{11}NO_3$ 205.213
Mp 81°.

*Di-Me ether: 6,7-Dimethoxy-1*H-*indole*
[31165-13-6]
$C_{10}H_{11}NO_2$ 177.202
Mp 101-103°.

Beer, R.J.S. *et al., J.C.S.*, 1951, 2029 (*synth*)
Stempien, M.F. *et al., Am. Zool.*, 1966, **6**, 363 (*isol*)
Magnus, P. *et al., Tetrahedron*, 2002, **58**, 3423-3443 (*di-Me ether*)

1*H*-Indole-2,3-dione, 9CI I-49

2,3-Indolinedione. ***Isatin***
[91-56-5]



$C_8H_5NO_2$ 147.133
Isol. from the fungal pigment of a mutant of *Schizophyllum commune*. Prod. by *Alteromonas* sp.I2 and a marine *Halomonas* sp. RK377. Also prod. by an *Alteromonas* sp. commensal in shrimp embryos *Palaemon macrodactylus*. Intermed. for indigoid dyestuffs. Used as 0.2% MeOH soln. for photometric detn. of thiophene, proline, hydroxyproline. Chromatog. spray for amino

acids. Shows antifungal activity in the marine environment.
Orange cryst. Spar. sol. H_2O.
Mp 203.5° dec. Sublimes.

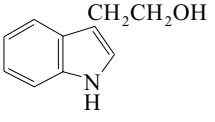
▶ Exp. reprod. effects. NL7873000

[73859-64-0, 73859-66-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 393D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1438B (*nmr*)
Hantzsch, A. *et al., Ber.*, 1921, **54**, 1242 (*synth*)
Org. Synth., 1925, **5**, 71
Epstein, E. *et al., CA*, 1966, **66**, 102443 (*isol*)
Maquestiau, A. *et al., Org. Mass Spectrom.*, 1974, **9**, 149 (*ms*)
Popp, F.D. *et al., Adv. Heterocycl. Chem.*, 1975, **18**, 1 (*rev*)
Gassmann, P.G. *et al., J.O.C.*, 1977, **42**, 1344 (*synth*)
Winkler, T. *et al., Org. Magn. Reson.*, 1979, **12**, 101 (*cmr*)
Peet, N.P. *et al., Org. Mass Spectrom.*, 1984, **19**, 171 (*ms*)
Hewawasam, P. *et al., Tet. Lett.*, 1994, **35**, 7303 (*synth, bibl*)
Da Silva, J.F.M. *et al., J. Braz. Chem. Soc.*, 2001, **12**, 273-324 (*rev, synth, pharmacol*)
Gribble, G.W. *et al., Org. Prep. Proced. Int.*, 2001, **33**, 615-619 (*synth, pmr, cmr*)
Smith, K. *et al., Synthesis*, 2003, 2047-2051 (*synth, ir, pmr, cmr, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ICR000

1*H*-Indole-3-ethanol, 9CI I-50

3-(2-Hydroxyethyl)indole. 2-(3-Indolyl)ethanol. ***Tryptophol***
[526-55-6]



$C_{10}H_{11}NO$ 161.203
Isol. from tryptophan fermentations, plant seedlings and *Candida* spp., *Aspergillus niger*, *Agrobacterium tumefaciens*, *Ceratocystis* spp. and *Rhizobium* spp. Also isol. from the sponge *Ircinia spinulosa*. Plant auxin. Active against gram-positive bacteria and *Candida albicans*. Associated with fungal diseases of trees. Prisms (C_6H_6/petrol); plates (Et_2O/petrol). Sol. most org. solvs.; spar. sol. H_2O, petrol.
Mp 59°. Bp_2 174°. Red. soln. in warm conc. H_2SO_4.

▶ LD_{50} (mus, ipr) 351 mg/kg. KL3685000

Picrate:
Red needles (H_2O). Mp 100-101°.

O-*Ac:* [13137-14-9]
$C_{12}H_{13}NO_2$ 203.24
Oil.

N-*Benzoyl:*
$C_{17}H_{15}NO_2$ 265.311
Yellow prisms and plates (petrol). Mp 76°.

O-*β*-D-*Galactopyranoside: Tryptophol galactoside*
[95088-52-1]
$C_{16}H_{21}NO_6$ 323.345
Isol. from *Euglena gracilis*.

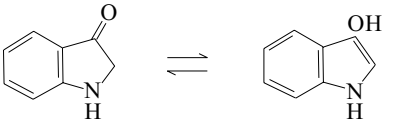
O-*β*-D-*Glucopyranoside: Tryptophol glucoside*
[40883-44-1]
$C_{16}H_{21}NO_6$ 323.345
Isol. from numerous plant and algae. Plant growth promotor.

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [149817-65-2]
$C_{21}H_{29}NO_{10}$ 455.461
Isol. from *Lycium chinense* (Chinese boxthorn). Pale yellow powder. $[\alpha]_D^{20}$ -32.7 (c, 0.4 in MeOH).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 659B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 130A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1502A (*ir*)
Ehrlich, F. *et al., Ber.*, 1912, **45**, 884
Jackson, R.W. *et al., J. Biol. Chem.*, 1930, **88**, 659
Oddo, B. *et al., Gazz. Chim. Ital.*, 1937, **69**, 10
Snyder, H.R. *et al., J.A.C.S.*, 1948, **70**, 3770
Fish, M.S. *et al., J.A.C.S.*, 1959, **78**, 3668
Nogrady, T. *et al., Can. J. Chem.*, 1964, **42**, 485
Narayanan, T.K. *et al., Antimicrob. Agents Chemother.*, 1976, **9**, 375 (*isol, props*)
Magnus, V. *et al., Carbohydr. Res.*, 1979, **76**, 261 (*synth, glucoside*)
Lacan, G. *et al., Plant Physiol.*, 1984, **76**, 889; 1985, **78**, 447 (*glucoside, galactoside*)
Ayer, W.A. *et al., Can. J. Chem.*, 1986, **64**, 904 (*isol*)
Yahara, S. *et al., Chem. Pharm. Bull.*, 1993, **41**, 703 (*xylosylglucoside*)
Novák, L. *et al., Annalen*, 1995, 1877 (*Ac*)
Böhlendorf, B. *et al., Annalen*, 1996, 49 (*isol, ir, pmr, cmr, ms*)
Erdogan, I. *et al., Biochem. Syst. Ecol.*, 2000, **28**, 793-794 (*isol, sponge*)
Garcez, W.S. *et al., J. Braz. Chem. Soc.*, 2005, **16**, 1382-1386 (*glucoside, isol, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ICS000

1*H*-Indol-3-ol, 9CI I-51

*1,2-Dihydro-3*H*-indol-3-one, 9CI. Indoxyl. Dihydro-3-oxoindole. 3-Hydroxyindole. Pseudoindoxyl*



oxo–form *OH–form*

C_8H_7NO 133.149
OH-form prob. favoured for parent. Unstable yellow solid. Mp 85°. Readily oxidised in air, especially in alkaline soln. to Indigotin.

N-*Ac:* [33025-60-4]
$C_{10}H_9NO_2$ 175.187
Needles (H_2O). Mp 139° (135°). Shown by ir studies to exist in soln. as oxo-form.

OH-form [480-93-3]

O-*Sulfate:*
$C_8H_7NO_4S$ 213.214
Isol. from *Murex trunculus*.

O-*β*-D-*Glucopyranoside:* ***Indican***. *Plant indican*. *Uroxanthin*
[487-60-5]
$C_{14}H_{17}NO_6$ 295.291
Occurs in *Polygonum tinctorium, Isatis tinctoria*, *Celosia argentea* and *Indigofera* spp. Biosynth. precursor to Indigotin. Shows growth inhibitory activity on the germination of lettuce. Cryst. + $3H_2O$ (H_2O).
Mp 57-58° (hydrate) Mp 180° (anhyd.). $[\alpha]_D^{15}$ -66.2 (H_2O).

O-*β*-D-ribo-*Hexopyranos-3-uloside:* ***Isatan B***
[20307-14-6]
$C_{14}H_{15}NO_6$ 293.276
Constit. of *Isatis tinctoria*. Precursor of Indigotin. Beige amorph. powder. $[\alpha]_D^{20}$ -14 (c, 1 in MeOH). Readily undergoes hydrol. Occurs as hydrate in aq. solns. λ_{max} 223 (ϵ 32200); 281 (ϵ 5700) (MeOH).

O-*(6*-O-*Malonyl-β*-D-ribo-*hexopyranos-3-uloside):* ***Isatan A***
$C_{17}H_{17}NO_9$ 379.323
Constit. of *Isatis tinctoria*. Precursor of Indigotin. Beige amorph. powder. $[\alpha]_D^{20}$ -10.5 (c, 1 in MeOH). Readily undergoes hydrol. Occurs as hydrate in aq. solns. λ_{max} 212 (log ϵ 2.03); 251 (log ϵ 3.51); 280 (log ϵ 4.61) (MeOH).

O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: 3-Indolyl gentiobioside.* ***Glucoindican***
$C_{20}H_{27}NO_{11}$ 457.433
Constit. of *Calanthe discolor* and *Calanthe liukiuensis*. Powder. $[\alpha]_D^{25}$ +164 (MeOH). λ_{max} 224 (log ϵ 5.4); 282 (log ϵ 4.7) (no solvent reported).

O-*Ac: 3-Acetoxy-1*H*-indole*
[608-08-2]
$C_{10}H_9NO_2$ 175.187
Alkaloid from *Strychnos cathayensis*. Cryst. (H_2O).
Mp 127.5°.

▶ LD_{50} (mus, ipr) 600 mg/kg. AI3325000

1,3-Di-Ac: [16800-67-2]
$C_{12}H_{11}NO_3$ 217.224
Cryst. (H_2O). Mp 82°.

1-Benzoyl, 3-Ac: [90539-82-5]
$C_{17}H_{13}NO_3$ 279.295
Cryst. (EtOH). Mp 87°.

3-Benzoyl, 1-Ac: [110912-16-8]
$C_{17}H_{13}NO_3$ 279.295
Cryst. (2-propanol). Mp 158-160°.

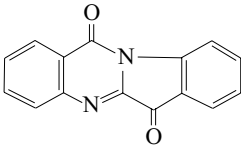
1-Me, 3-Ac: [3260-63-7]
$C_{11}H_{11}NO_2$ 189.213
Cryst. (EtOH aq.). Mp 56.5°.

[487-94-5, 3260-61-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 675B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 148B (*nmr*)
Spencer, G. *et al., J. Soc. Chem. Ind., London*, 1931, **50**, 63T (*N-Ac, 3-O-Ac, synth*)
Robertson, A. *et al., J.C.S.*, 1933, 30 (*Indican*)
Holt, S.J. *et al., J.C.S.*, 1958, 1217 (*N-Ac, conformn, ir*)
Kirby, G.W. *et al., Chem. Comm.*, 1965, 381 (*synth*)
Raileanu, D. *et al., Rev. Roum. Chim.*, 1967, **12**, 105; *CA*, **68**, 21775 (*N-Ac, di-Ac, synth*)
Baker, J.T. *et al., Tet. Lett.*, 1968, 43; 1976, 1233-1234 (*sulfate*)
Fouquet, H. *et al., Angew. Chem., Int. Ed.*, 1971, **10**, 816-817 (*sulfate, isol*)
Rodd's Chem. Carbon Compd. (2nd edn.), 1973, **4A**, 454 (*rev*)
Strobel, J. *et al., Biochem. Physiol. Pflanz.*, 1989, **184**, 321 (*occur*)
Traldi, P. *et al., Rapid Commun. Mass Spectrom.*, 1990, **4**, 335 (*ms*)
Xia, Z.-Q. *et al., Phytochemistry*, 1992, **31**, 2695 (*Indican, Isatan B, biosynth, cmr*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 886-888 (*Glucoindican*)
Sawabe, A. *et al., Stud. Plant Sci.*, 1999, **6**, 290-296 (*Indican, isol, activity*)
Cheng, M.-J. *et al., J. Chin. Chem. Soc. (Taipei)*, 2001, **48**, 235-239 (*3-Acetoxyindole, isol*)
Cooksey, C.J. *et al., Molecules*, 2001, **6**, 736-769 (*sulfate, rev*)
Oberthür, C. *et al., Chem. Biodiversity*, 2004, **1**, 174-182 (*Isatans A,B*)

Indolo[2,1-*b*]quinazoline-6,12-dione, 9CI I-52

*6,12-Dihydro-6,12-dioxoindolo[2,1-*b*]quinazoline.* ***Tryptanthrine.*** *Couroupitine A*
[13220-57-0]

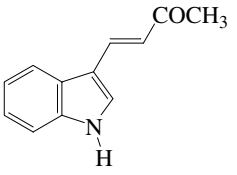


$C_{15}H_8N_2O_2$ 248.24
Isol. from the yeast *Candida lipolytica* grown in the presence of L-tryptophan. Also from *Couroupita guianensis* (Lecythidaceae), *Isatis indigotica* and *Polygonum tiucforum*. Prod. by *Cytophaga marinoflava* sp. AM13.1. Antifungal and antimicrobial agent showing specific activity against dermatophytes. Active against *Helicobacter pylori*. Yellow needles. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, bases, acids.
Mp 266-267°. Subl. *in vacuo*. Couroupitine A was initially assigned an incorr. struct. λ_{max} 248; 252; 277; 311; 328; 387 (MeOH) (Berdy). λ_{max} 254 (ε 34800); 280 (ε 7000); 340 (ε 7200); 405 (ε 6600) (EtOH) (Berdy).

Brufani, M. *et al., Experientia*, 1971, **27**, 1249 (*cryst struct, pmr, ms*)
Fedeli, W. *et al., J.C.S. Perkin 2*, 1974, 1621 (*cryst struct*)
Bergman, J. *et al., Tet. Lett.*, 1977, 2625 (*struct, synth*)
Karpf, H. *et al., Tet. Lett.*, 1978, 3007 (*synth, ir, uv, ms*)
Honda, G. *et al., Planta Med.*, 1979, **37**, 172 (*props*)
Mitscher, L.A. *et al., Heterocycles*, 1981, **15**, 1017 (*synth*)
Capuano, L. *et al., Chem. Ber.*, 1983, **116**, 741 (*synth*)
Eguchi, S. *et al., Heterocycles*, 1992, **33**, 153 (*synth*)
Cornforth, J. *et al., J.C.S. Perkin 1*, 1996, 2787 (*synth*)
Hashimoto, T. *et al., Nat. Med. (Tokyo)*, 1999, **53**, 27 (*isol, activity*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*Cytophaga, isol, pmr, cmr*)

4-(1*H*-Indol-3-yl)-3-buten-2-one, 9CI I-53

[31951-75-4]



$C_{12}H_{11}NO$ 185.225

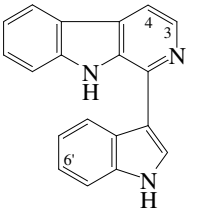
(E)-form [57598-80-8]
Alkaloid from the sponge *Tedania ignis*.
Cryst. (petrol or C_6H_6).
Mp 145-146°. Possible artifact. λ_{max} 223 (ε 19000); 276 (ε 9400); 353 (ε 17800) (no solvent reported).

*6-Bromo: 4-(6-Bromo-1*H*-indol-3-yl)-3-buten-2-one*
[654649-67-9]
$C_{12}H_{10}BrNO$ 264.121
Alkaloid from the sponge *Iotrochota birotulata*. Powder.
Mp 145-148°. λ_{max} 270; 290; 340 (MeOH).

Nonnenmacher, A. *et al., Annalen*, 1983, 2135-2140 (*synth, pmr*)
Dillman, R.L. *et al., J. Nat. Prod.*, 1991, **54**, 1056-1061 (*isol*)
Li, L. *et al., Pharmazie*, 2003, **58**, 680-681 (*6-bromo*)

1-(3-Indolyl)-β-carboline I-54

*1-(1*H*-Indol-3-yl)-9*H*-pyrido[3,4-*b*]indole, 9CI.* ***Eudistomin U***
[155885-64-6]



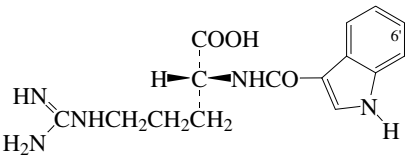
$C_{19}H_{13}N_3$ 283.332
Alkaloid from the Caribbean ascidian *Lissoclinum fragile*. Exhibits antibacterial activity. DNA binder. Yellow foam. Sol. MeOH. λ_{max} 220 (ε 8000); 240 (ε 3500); 252 (ε 10500); 270 (ε 7700); 340 (ε 9020); 380 (ε 13000); 470 (ε 5120) (MeOH) (Berdy).

3,4-Dihydro: ***3,4-Dihydroeudistomin U.*** *Isoeudistomin U. Eudisin B*
[155885-65-7]
$C_{19}H_{15}N_3$ 285.348
From *Lissoclinum fragile* and a *Eudistoma* sp. Exhibits antibacterial activity. Yellow foam. Originally assigned an α-carboline struct. by Badre *et al* (1994). The name Isoeudistomin U is now misleading. λ_{max} 208 (ε 27500); 248 (ε 11200); 274 (ε 6100); 282 (ε 6100); 330 (ε 9560); 397 (ε 9530) (MeOH). λ_{max} 210 (ε 60000); 243 (sh); 314 (ε 9340) (MeOH).

3,4-Dihydro, 6′-bromo: ***19-Bromo-3,4-dihydroeudistomin U.*** *19-Bromoisoeudistomin U (incorr.). Eudisin A*
[186820-55-3]
$C_{19}H_{14}BrN_3$ 364.244
Alkaloid from a *Eudistoma* sp. tunicate. Antitumour agent. Yellow-green powder. λ_{max} 220 (ε 56600); 290 (ε 17500); 325 (ε 20700); 396 (ε 10400) (MeOH). λ_{max} 206 (ε 70000); 245 (sh); 292 (ε 7040); 315 (ε 9020) (MeOH). λ_{max} 206 (ε 70000); 292 (ε 7040); 315 (ε 9020) (MeOH-NAOH) (Berdy).

Badre, A. *et al., J. Nat. Prod.*, 1994, **57**, 528-533 (*isol, uv, ir, pmr, cmr, ms, struct*)
Massiot, G. *et al., J. Nat. Prod.*, 1995, **58**, 1636-1639 (*Isoeudistomin U*)
Molina, P. *et al., Tet. Lett.*, 1995, **36**, 3581-3582 (*synth*)
Rocca, P. *et al., Tet. Lett.*, 1995, **36**, 7085-7088 (*synth*)
Kang, H. *et al., Nat. Prod. Lett.*, 1996, **9**, 7-12 (*Isoeudistomin U, 19-Bromoisoeudistomin U*)

N^{α}-(1*H*-Indol-3-ylcarbonyl)arginine I-55



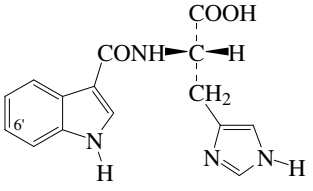
(*R*)-*form*

$C_{15}H_{19}N_5O_3$ 317.347

(*R*)-*form* [178495-40-4]
Isol. from the ascidian *Leptoclinides dubius*. Sol. MeOH, butanol. $[\alpha]_D^{20}$ -133.3 (c, 0.1 in MeOH). λ_{max} 214 (log ε 3.65); 246 (log ε 3.13); 282 (log ε 3.11); 286 (log ε 3.1) (MeOH).

(*S*)-*form*
6′-Bromo: N^{α}-*(6-Bromo-1*H*-indol-3-ylcarbonyl)arginine*
[178495-41-5]
$C_{15}H_{18}BrN_5O_3$ 396.243
Isol. from *Leptoclinides dubius*. Sol. MeOH, butanol. $[\alpha]_D^{20}$ +3.6 (c, 0.5 in MeOH). λ_{max} 222 (log ε 3.78); 250 (log ε 3.43); 280 (log ε 3.18) (MeOH).
Garcia, A. *et al., J. Nat. Prod.*, 1996, **59**, 782-785 (*isol*)

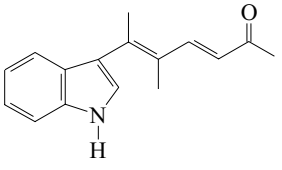
N^{α}-(1*H*-Indol-3-ylcarbonyl)histidine I-56



$C_{15}H_{14}N_4O_3$ 298.301

(*S*)-*form*
6′-Bromo: N^{α}-*(6-Bromo-1*H*-indol-3-ylcarbonyl)histidine*
[178495-42-6]
$C_{15}H_{13}BrN_4O_3$ 377.197
Isol. from the ascidian *Leptoclinides dubius*. Sol. MeOH, butanol. $[\alpha]_D^{20}$ +26.6 (c, 0.5 in MeOH). λ_{max} 222 (log ε 3.53); 250 (log ε 3.17); 282 (log ε 2.92) (MeOH).
Garcia, A. *et al., J. Nat. Prod.*, 1996, **59**, 782-785 (*isol*)

6-(1*H*-Indol-3-yl)-5-methyl-3,5-heptadien-2-one, 9CI I-57

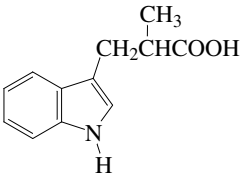


$C_{16}H_{17}NO$ 239.316

(3*E*,5*E*)-*form* [136685-36-4]
Isol. from the sponge *Tedania ignis*. Phytotoxic agent. λ_{max} 224 (ε 12300); 290 (ε 8300) (EtOH) (Berdy).
Dillman, R.L. *et al., J. Nat. Prod.*, 1991, **54**, 1056 (*isol, uv, ir, pmr, ms, cmr, struct*)

3-(1*H*-Indol-3-yl)-2-methylpropanoic acid I-58

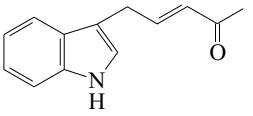
*α-Methyl-1*H*-indole-3-propanoic acid, 9CI.* ***Rhizophorine***
[15142-91-3]
[69088-73-9]



$C_{12}H_{13}NO_2$ 203.24

(ξ)-*form* [61755-28-0]
Constit. of *Rhizophora mucronata*. Plant growth inhibitor. Off-white needles (H_2O).
Mp 129-130°.
Et ester: [57901-11-8]
$C_{14}H_{17}NO_2$ 231.294
$Bp_{0.75}$ 165°.
Johnson, H.E. *et al., J.O.C.*, 1963, **28**, 2030-2032 (*synth*)
Saha, P.K. *et al., Plant Biochem. J.*, 1978, **5**, 65-68 (*isol*)

5-(1*H*-Indol-3-yl)-3-penten-2-one, 9CI I-59

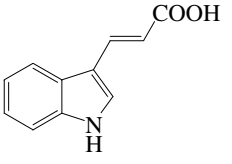


$C_{13}H_{13}NO$ 199.252

(*E*)-*form* [136685-35-3]
Isol. from the sponge *Tedania ignis*. Possibly an artifact.
Dillman, R.L. *et al., J. Nat. Prod.*, 1991, **54**, 1056 (*isol, uv, ir, pmr, ms, cmr, struct*)

3-(1*H*-Indol-3-yl)-2-propenoic acid I-60

*1*H*-Indole-3-propenoic acid. 3-(3-Indolyl)acrylic acid*
[1204-06-4]



(*E*)-*form*

$C_{11}H_9NO_2$ 187.198
Major auxin from roots of *Lens culinaris* (lentil) (Leguminosae).
▶ Exp. carcinogenic data. NL3680000

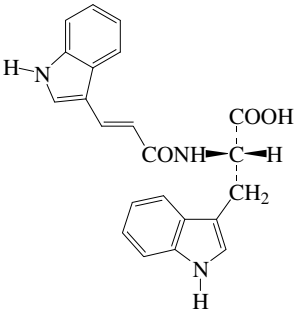
(*E*)-*form* [29953-71-7]
Alkaloid from the red alga *Chondria* sp.
Red-brown cryst. (H_2O or AcOH).
Mp 195-196°.
Me ester:
$C_{12}H_{11}NO_2$ 201.224
Cryst. (C_6H_6). Mp 153-154°.
Me ester, N-*Ac:*
$C_{14}H_{13}NO_3$ 243.262
Cryst. (C_6H_6). Mp 179-180°.
*Amide: 3-(1*H*-Indol-3-yl)-2-propenamide.* ***3-(3-Indolyl)acrylamide***
$C_{11}H_{10}N_2O$ 186.213
Alkaloid from *Chondria atropurpurea*. Anthelminthic agent.
Amber cryst. (Me_2CO).
Mp 212.8-214.2°. λ_{max} 226 (log ε 1.49); 275 (log ε 1.25); 322 (log ε 1.55) (MeOH). λ_{max} 226; 275; 322 (MeOH) (Berdy).
Amide, N^b*-formyl:* N-*Formyl-3-(1*H*-indol-3-yl)-2-propenamide, 9CI.* **N-*Formyl-3-indoleacrylamide***
[142677-08-5]
$C_{12}H_{10}N_2O_2$ 214.223
From *Chondria* sp. Oil.

Nitrile: [85452-78-4]
$C_{11}H_8N_2$ 168.198
Beige solid. Mp 143-144°.

*7′-Hydroxy: 3-(7-Hydroxy-1*H*-indol-3-yl)-2-propenoic acid, 9CI.* ***7-Hydroxy-3-indoleacrylic acid***
[142677-11-0]
$C_{11}H_9NO_3$ 203.197
From *Chondria* sp.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 668B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 139B (*nmr*)
Furst, A. *et al., Arch. Biochem. Biophys.*, 1951, **31**, 190 (*synth*)
Inhoffen, H.H. *et al., Annalen*, 1963, **668**, 104-121 (*Me ester*)
Rappe, C. *et al., Acta Chem. Scand.*, 1964, **18**, 818 (*config*)
Hofinger, M. *et al., Phytochemistry*, 1970, **9**, 1757 (*isol*)
Palermo, J.A. *et al., Tet. Lett.*, 1992, **33**, 3097 (*Chondria derivs, isol*)
Davyt, D. *et al., J. Nat. Prod.*, 1998, **61**, 1560-1563 (*isol, amide*)
Slätt, J. *et al., J. Het. Chem.*, 2005, **42**, 141-145 (*nitrile*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ICO000

N^a-[3-(1*H*-Indol-3-yl)propenoyl]tryptophan I-61

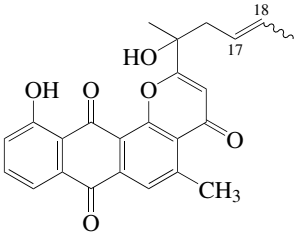


$C_{22}H_{19}N_3O_3$ 373.41
Deriv. of 3-(1*H*-Indol-3-yl)-2-propenoic acid, I-60.

(S,E)-form
L-trans-*form*
Et ester: [142677-12-1]
$C_{24}H_{23}N_3O_3$ 401.464
Minor constit. of a red alga *Chondria* sp. Prob. artifact.
Palermo, J.A. *et al., Tet. Lett.*, 1992, **33**, 3097-3100 (*Et ester, isol*)

β-Indomycinone I-62

*11-Hydroxy-2-(1-hydroxy-1-methyl-3-pentenyl)-5-methyl-4*H*-anthra[1,2-*b*]pyran-4,7,12-trione, 9CI*
[152987-14-9]

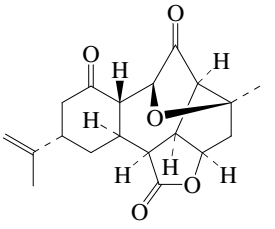


$C_{24}H_{20}O_6$ 404.418
Prod. by a *Streptomyces* sp. Yellow solid.
Mp 178°. λ_{max} 239; 240; 267 (sh); 410 (sh); 416 (EtOH). λ_{max} 239; 267; 416 (MeOH) (Berdy).

17,18-Dihydro, 18-hydroxy: ***δ-Indomycinone***
[199169-59-0]
$C_{24}H_{22}O_7$ 422.434
Prod. by a marine *Streptomyces* sp. Antioxidant. Yellow solid.
Mp 181°. λ_{max} 220; 260; 416 (MeOH).
Schumacher, R.W. *et al., J. Nat. Prod.*, 1995, **58**, 613 (*isol, uv, ir, pmr, cmr*)
Biabani, M.A.F. *et al., J. Antibiot.*, 1997, **50**, 874-877 (*isol, uv, ir, pmr, cmr*)

Ineleganolide I-63

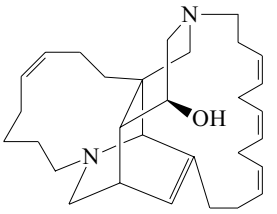
[247086-97-1]



$C_{19}H_{22}O_5$ 330.38
Constit. of *Sinularia inelegans.* Cryst.
Mp 190-192°. $[\alpha]_D^{25}$ +26.4 (c, 0.05 in $CHCl_3$).
Duh, C.-Y. *et al., Tet. Lett.*, 1999, **40**, 6033-6035 (*isol, pmr, cmr, cryst struct*)

Ingamine A I-64

[156310-17-7]

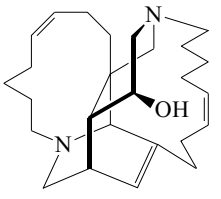


$C_{30}H_{44}N_2O$ 448.69
Alkaloid from the marine sponge *Xestospongia ingens.* Exhibits *in vitro* cytotoxicity against murine leukaemia P388 cells. Glass. Sol. MeOH, EtOAc. $[\alpha]_D$ +131 (c, 0.18 in MeOH).

Deoxy: ***Ingamine B***
[156310-18-8]
$C_{30}H_{44}N_2$ 432.691
From *Xestospongia ingens.* Exhibits *in vitro* cytotoxicity against murine leukaemia P388 cells. Glass. Sol. MeOH, EtOAc. $[\alpha]_D$ +108 (c, 0.5 in MeOH).
Kong, F. *et al., Tetrahedron*, 1994, **50**, 6137; 1995, **51**, 2895 (*isol, ir, pmr, cmr, ms, struct, abs config*)

Ingenamine I-65

[155210-52-9]



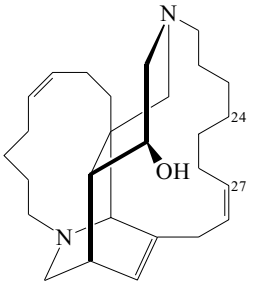
$C_{26}H_{40}N_2O$ 396.615
Alkaloid from the Papua New Guinea *Xestospongia ingens.* Cytotoxic. Amorph. solid. Sol. MeOH, EtOAc. $[\alpha]_D$ +62 (c, 0.14 in MeOH).

Deoxy: ***Keramaphidin B***
[157536-35-1]
$C_{26}H_{40}N_2$ 380.615
Alkaloid from *Xestospongia ingens* and from the Okinawan marine sponge *Amphimedon* sp. Exhibits cytotoxicity against P388 murine leukaemia and KB human epidermoid carcinoma cells. Poss. biogenetic precursor of manzamine alkaloids (e.g. Manzamine A, M-95). Amorph. solid. $[\alpha]_D$ +29.8 (c, 1.1 in MeOH). The isolate (Mp 131-132°) from *Amphimedon* sp. is racemic.
Kong, F. *et al., Tet. Lett.*, 1994, **35**, 1643 (*isol, pmr, cmr, struct*)

Kobayashi, J. *et al., Tet. Lett.*, 1994, **35**, 4383 (*Keramaphidin B*)
Kong, F. *et al., Tetrahedron*, 1995, **51**, 2895 (*abs config*)
Tsuda, M. *et al., Heterocycles*, 1997, **46**, 765-795 (*rev*)
Matzanke, N. *et al., Org. Prep. Proced. Int.*, 1998, **30**, 3-51 (*rev, Keramaphidin B*)

Ingenamine B I-66

[164081-00-9]



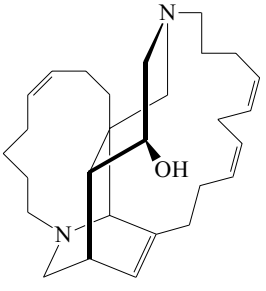
$C_{27}H_{42}N_2O$ 410.642
Minor alkaloid from the Papua New Guinea sponge *Xestospongia ingens.* Powder. $[\alpha]_D$ +22.4 (c, 0.25 in MeOH).

27,28-Dihydro, 24,25-didehydro(Z-), Ac: ***Ingenamine C acetate***
[164081-02-1]
$C_{29}H_{44}N_2O_2$ 452.679
Minor alkaloid from *Xestospongia ingens.* Glass. $[\alpha]_D$ +41.6 (c, 0.09 in MeOH).

Kong, F. *et al., Tetrahedron*, 1995, **51**, 2895 (*isol, pmr, cmr, ms, struct*)

Ingenamine D I-67

[164081-03-2]

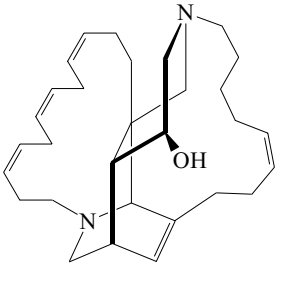


$C_{28}H_{42}N_2O$ 422.653
Minor alkaloid from the Papua New Guinea sponge *Xestospongia ingens.* Glass.

Kong, F. *et al., Tetrahedron*, 1995, **51**, 2895 (*isol, pmr, cmr, ms, struct*)

Ingenamine E I-68

[164081-04-3]

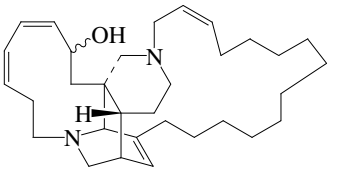


$C_{30}H_{44}N_2O$ 448.69
Minor alkaloid from the Papua New Guinea sponge *Xestospongia ingens.* Glass. $[\alpha]_D$ -23.8 (c, 0.062 in MeOH).

Deoxy: ***Ingenamine F***
[164122-97-8]
$C_{30}H_{44}N_2$ 432.691
Minor alkaloid from *Xestospongia ingens.* Glass. $[\alpha]_D$ -64.3 (c, 0.062 in MeOH).

Kong, F. *et al., Tetrahedron*, 1995, **51**, 2895 (*isol, pmr, cmr, ms, struct*)

Ingenamine G I-69



Probable Absolute Configuration

$C_{32}H_{50}N_2O$ 478.76
Alkaloid from the Brazilian sponge *Pachychalina* sp. Cytotoxic. Glassy solid. $[\alpha]_D^{29}$ -59.2 (c, 0.05 in MeOH). λ_{max} 230 (ϵ 2500); 283 (ϵ 625) (MeOH).

De Oliveira, J.H.H.L. *et al., J. Nat. Prod.*, 2004, **67**, 1685-1689 (*isol, pmr, cmr*)

Mytilus Inhibitory peptides I-70

Asp-Ser-Pro-Leu-Phe-Val-NH_2
Struct. of MIP-3 shown. Isol. from the anterior byssus retractor muscle of the edible mussel *Mytilus edulis.* Muscle contraction inhibitors. See also Glycylalanylprolylmethionylphenylalanyl-valinamide, G-129.

MIP-3
DSPLFV amide
[132738-55-7]
$C_{32}H_{49}N_7O_9$ 675.781

MIP-4
YAPRFV amide
[139332-83-5]
$C_{37}H_{54}N_{10}O_7$ 750.896

MIP-5
ASHIPRFV amide
[139332-84-6]
$C_{43}H_{68}N_{14}O_9$ 925.099

MIP-6
RAPLFI amide
[151808-92-3]
$C_{35}H_{58}N_{10}O_6$ 714.907

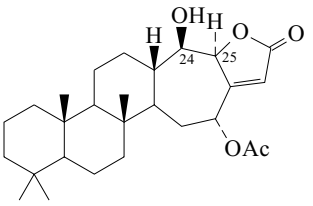
MIP-7
RSPMFV amide
[151808-93-4]
$C_{33}H_{54}N_{10}O_7S$ 734.918

MIP-RP
MIP-related peptide. MRYFV amide
[151808-94-5]
$C_{34}H_{51}N_9O_6S$ 713.9

Fujisawa, Y. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1991, **100**, 525-531; 1993, **106**, 261-267 (*isol*)

Inorolide A I-71

[145038-58-0]



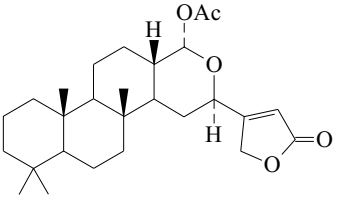
$C_{27}H_{40}O_5$ 444.61
Constit. of *Chromodoris inornata*. Cytotoxic agent. Cryst. (EtOH).
Mp 118-120°. $[\alpha]_D$ -26.7 (c, 0.3 in $CHCl_3$). λ_{max} 217 (ϵ 10000) (MeOH) (Derep).

24-Deoxy, 24,25-didehydro: ***Inorolide B***
[145038-57-9]
$C_{27}H_{38}O_4$ 426.595
Isol. from *Chromodoris inornata*. Needles.
Mp 84-85°. $[\alpha]_D$ +52 (c, 0.8 in $CHCl_3$). λ_{max} 217 (ϵ 10000) (MeOH) (Derep).

Miyamoto, T. *et al., Tet. Lett.*, 1992, **33**, 5811-5814 (*isol, pmr, cmr, cryst struct*)
Miyamoto, T. *et al., Tetrahedron*, 1999, **55**, 9133-9142 (*pmr, cmr*)

Inorolide C I-72

[145038-56-8]

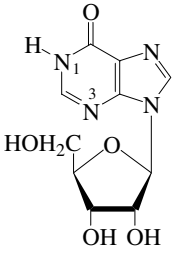


$C_{27}H_{40}O_5$ 444.61
Constit. of *Chromodoris inornata*. Cytotoxic agent. Rods (MeOH).
Mp 181-183°. $[\alpha]_D$ -43.9 (c, 0.4 in $CHCl_3$). λ_{max} 217 (ϵ 10000) (MeOH) (Derep).

Miyamoto, T. *et al., Tet. Lett.*, 1992, **33**, 5811-5814 (*isol, pmr, cmr, cryst struct*)
Miyamoto, T. *et al., Tetrahedron*, 1999, **55**, 9133-9142 (*pmr, cmr*)

Inosine, 9CI, INN, JAN I-73

*1,9-Dihydro-9-β-D-ribofuranosyl-6*H*-purin-6-one, 9CI. 9-β-D-Ribofuranosylhypoxanthine, 8CI. Hypoxanthine riboside. Hypoxanthosine. Aminosin†. Carnine. Delimmun. Inosie. Oxiamine. Trophicardyl*
[58-63-9]



1*H-form*

$C_{10}H_{12}N_4O_5$ 268.229
Present in meat extracts and sugar beet. Also prod. by microorganisms, e.g. *Bacillus subtilis, Escherichia coli, Saccharomyces cerevisiae, Fusarium* spp. A minor constit. of *t*-RNA's. Activates cellular functions. Cardiotonic. Suggested to be capable of forming base pairs with Adenine, A-103, Cytosine or Uracil thus contributing to genetic code degeneracy by causing stable mispairings. Used to treat cardiac disorders. Egg-release pheromone of *Nereis succinea*.
Mp 215° dec. $[\alpha]_D^{18}$ -49.2 (c, 0.9 in H_2O). pK_{a1} 1.5; pK_{a2} 8.85; pK_{a3} 12.5 (25°). Log P -3.76 (calc). λ_{max} 249 (ϵ 12200) (H_2O) (pH 6).

▶ Probable mutagen. Exp. reprod. effects (very high dose) LD_{50} (mus, ivn) 3000 mg/kg. NM7460000

3′-O-α-D-Glucopyranosyl: ***3′-O-α-D-Glucopyranosylinosine***
$C_{16}H_{22}N_4O_{10}$ 430.371
Isol. from the crustacean *Ligia exotica*. Amorph. solid. $[\alpha]_D^{20}$ +38 (c, 0.34 in H_2O). λ_{max} 248 (ϵ 8400) (H_2O).

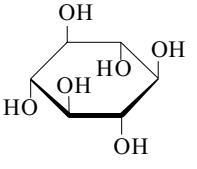
2′-Me: ***2′-O-Methylinosine***
[3881-21-8]
$C_{11}H_{14}N_4O_5$ 282.255
Isol. from the starfish *Asterias rollestoni.*
Mp 153-156°.

[35908-31-7]

Kim, S.H. *et al., J. Nat. Prod.*, 2000, **63**, 1188-1191 (*3′-α-D-glucosyl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IDE000

scyllo-Inositol I-74

(1α,2β,3α,4β,5α,6β)-Cyclohexanehexol. Scyllitol. 1,3,5/2,4,6-Inositol. Quercin. Scylloinositol. Cocositol
[488-59-5]



$C_6H_{12}O_6$ 180.157
Occurs in animals, notably plagiostomous fish, plants such as flowering dogwood; detected in insects and mammalian urine.
Mp 350-354°. Opt. inactive (*meso*-).

*Hexa-Ac: 1,2,3,4,5,6-Hexa-*O*-acetyl-*scyllo*-inositol*
[20108-52-5]
$C_{18}H_{24}O_{12}$ 432.38
Mp 300-301°.

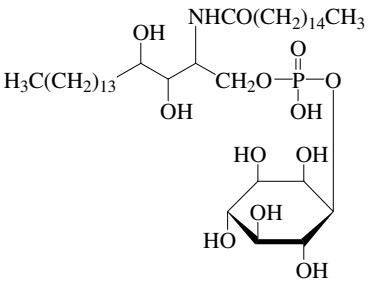
*Mono-Me ether: 1-*O*-Methyl-*scyllo*-inositol*
[23887-12-9]
$C_7H_{14}O_6$ 194.184
Cryst. (EtOH aq.). Mp 239-242°.

*Hexa-Me ether: 1,2,3,4,5,6-Hexa-*O*-methyl-*scyllo*-inositol*
[148906-41-6]
$C_{12}H_{24}O_6$ 264.318
Cryst. (petrol). V. sol. all common solvs. Mp 114-115°.

[41546-32-1]

Anderson, R.C. *et al., J.A.C.S.*, 1948, **70**, 2931-2935 (*synth*)
Anderson, L. *et al., Arch. Biochem. Biophys.*, 1958, **78**, 518-531 (*mono-Me ether*)
Kindl, H. *et al., Prog. Chem. Org. Nat. Prod.*, 1966, **24**, 149 (*rev*)
Lichtenthaler, F.W. *et al., Carbohydr. Res.*, 1968, **7**, 121-137 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 290 (*occur*)
Angyal, S.J. *et al., Carbohydr. Res.*, 1982, **100**, 43-54 (*cmr*)
Kohne, B. *et al., Annalen*, 1985, 866-868 (*synth*)
Anderson, J.E. *et al., Carbohydr. Res.*, 1995, **272**, 141-148 (*synth, cryst struct, hexa-Me ether*)
Salazar-Pereda, V. *et al., J. Carbohydr. Chem.*, 1997, **16**, 1479-1507 (*cryst struct, cmr, conformn*)
Husson, C. *et al., Carbohydr. Res.*, 1998, **307**, 163-165 (*synth*)
Takahashi, H. *et al., Tet. Lett.*, 1998, **39**, 9707-9710 (*synth*)
Chung, S.K. *et al., Bioorg. Med. Chem.*, 1999, **7**, 2577-2589 (*synth, pmr*)
Sarmah, M.P. *et al., Carbohydr. Res.*, 2003, **338**, 999-1001 (*synth*)
Podeschwa, M. *et al., Eur. J. Org. Chem.*, 2003, 1958-1972 (*synth*)

Gracilaria verrucosa Inositol cerebroside I-75

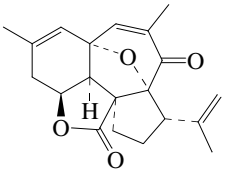


$C_{40}H_{80}NO_{12}P$ 798.045
Isol. from the red alga *Gracilaria verrucosa*.

Khotimchenko, S.V. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2004, **30**, 168-171 (*isol*)

Intricarene I-76

[852468-89-4]

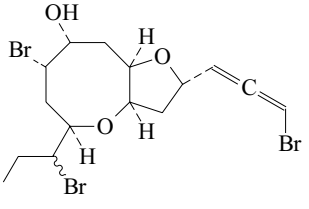


$C_{20}H_{22}O_4$ 326.391
Constit. of *Pseudopterogorgia kallos*. Cryst. $[\alpha]_D^{20}$ +50 (c, 0.7 in $CHCl_3$). λ_{max} 245 (ϵ 6200) (MeOH).

Marrero, J. *et al., Org. Lett.*, 2005, **7**, 1877-1880 (*Intricarene, cryst struct*)
Tang, B. *et al., Tet. Lett.*, 2006, **47**, 6401-6404 (*synth*)

Intricata bromoallene I-77

[123297-18-7]

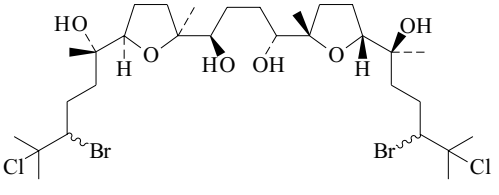


$C_{15}H_{21}Br_3O_3$ 489.041
Constit. of *Laurencia intricata*. Oil. $[\alpha]_D^{21}$ +95.8 (c, 0.6 in $CHCl_3$).

Suzuki, M. *et al., Phytochemistry*, 1989, **28**, 2145 (*isol, pmr, cmr*)

Intricatetraol I-78

[150527-31-4]



$C_{30}H_{54}Br_2Cl_2O_6$ 741.466
Metab. of *Laurencia intricata*. Cytotoxic. Cryst. (MeOH).
Mp 109-111°. $[\alpha]_D^{20}$ +53 (c, 0.625 in $CHCl_3$).

Suzuki, M. *et al., Phytochemistry*, 1993, **33**, 651-656 (*isol, pmr, cmr, ms*)
Morimoto, Y. *et al., Org. Biomol. Chem.*, 2006, **4**, 3220-3222 (*config*)

Iodoacetic acid, 9CI, 8CI I-79

[64-69-7]
ICH_2COOH
$C_2H_3IO_2$ 185.949
Constit. of the red alga *Asparagopsis taxiformis*. Used as a chromatographic derivatisation reagent for the *S*-carboxymethylation of cystine and cysteine in peptides. Plates (petrol). V. sol. Et_2O; sol. H_2O, EtOH.
Mp 82-83°. pK_a 3.18 (25°, H_2O).
▶ Corrosive and irritating to eyes, skin and mucous membranes.
LD_{50} (mus, orl) 83 mg/kg. AI3500000

Me ester: Methyl iodoacetate
[5199-50-8]
$C_3H_5IO_2$ 199.976
Liq. Bp 169-171°.

Et ester: Ethyl iodoacetate. KSK
[623-48-3]
$C_4H_7IO_2$ 214.003
War gas, tear gas. Oil. Bp 178-180° Bp_{16} 73°.
▶ Highly lachrymatory and irritant. AI3575000

Chloride: Iodoacetyl chloride
[38020-81-4]
C_2H_2ClIO 204.394
Yellow-brown oil. d^{25} 2.25. Bp_{15} 49-52°.

Amide: Iodoacetamide, 9CI
[144-48-9]
C_2H_4INO 184.964
Constit. of *Asparagopsis taxiformis*. Reagent for cleavage of methionine containing peptides. Flaky cryst. (H_2O).
Mp 95°.
▶ LD_{50} (mus, orl) 74 mg/kg. AC4200000

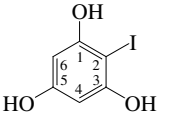
Nitrile: Iodoacetonitrile. Cyanoiodomethane
[624-75-9]
C_2H_2IN 166.949
Oil. Bp_{12} 76-77°.

Anhydride: [54907-61-8]
$C_4H_4I_2O_3$ 353.883
Cryst. (EtOH aq.). V. sol. $CHCl_3$, EtOAc, Et_2O; less sol. H_2O, EtOH. Mp 46°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 509C; 651C; 751B; 848D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 791B; 1010A; 1172A; 1366B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 701A; 807C (*ir*)
v. Braun, J. *et al., Ber.*, 1908, **41**, 2130 (*synth, nitrile, amide*)
Abderhalden, E. *et al., Ber.*, 1908, **41**, 2852 (*synth*)
Jacobs, W.A. *et al., J.A.C.S.*, 1919, **41**, 2090 (*amide*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 504 (*amide, use*)
Paraskewas, S. *et al., Synthesis*, 1974, 574 (*amide*)
Moodie, I.M. *et al., J. Chromatogr.*, 1976, **124**, 315 (*use*)
Woolard, F.X. *et al., Tetrahedron*, 1976, **32**, 2843-2846 (*amide, isol*)
Karpitskaya, L.G. *et al., Zh. Org. Khim.*, 1976, **12**, 462 (*synth*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617-620 (*isol*)
Dillon, K.B. *et al., J. Magn. Reson.*, 1980, **39**, 499 (*pmr*)
Lorenzi-Riatsch, A. *et al., Helv. Chim. Acta*, 1981, **64**, 1563 (*ms*)
Cooper, J.D.H. *et al., J. Chromatogr.*, 1982, **227**, 158 (*use*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2822-2824 (*nitrile, use*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 730
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ELQ000; IDW000; IDZ000

2-Iodo-1,3,5-benzenetriol, 9CI I-80

2-Iodophloroglucinol
[134810-54-1]



$C_6H_5IO_3$ 252.008

Isol. from the brown alga *Eisenia arborea* (as tri-Ac) and from *Cystophora retroflexa* and *Carpophyllum angustifolium*. Light yellow cryst. ($MeNO_2$).
Mp 162-164° dec.

3,5-Di-Me ether: 2-Iodo-3,5-dimethoxyphenol
$C_8H_9IO_3$ 280.062
Cryst. Mp 73°.

Tri-Me ether: 2-Iodo-1,3,5-trimethoxybenzene
[2510-49-8]
$C_9H_{11}IO_3$ 294.089
Cryst. (CH_2Cl_2/MeOH). Mp 122-123°.

[96820-11-0]

Glombitza, K.-W. *et al., Phytochemistry*, 1985, **24**, 543-551 (*isol*)
Thomsen, I. *et al., Acta Chem. Scand.*, 1991, **45**, 539-542 (*synth*)
Orito, K. *et al., Synthesis*, 1995, 1273 (*tri-Me ether*)
Vasil'ev, A.A. *et al., J.O.C.*, 1998, **63**, 3911-3917 (*di-Me ether, tri-Me ether, synth, pmr, cmr*)
Sailler, B. *et al., Nat. Toxins*, 1999, **7**, 57-62 (*isol*)

1-Iodobutane, 9CI I-81

Butyl iodide
[542-69-8]
$H_3CCH_2CH_2CH_2I$
C_4H_9I 184.02
Isol. from several marine algae. Used to esterify fatty acids for gc anal. Liq. d_4^{20} 1.62.
Fp -103. Bp 130.4-131°.
▶ Flammable, fl. p. 36°. LD_{50} (rat, ipr) 692 mg/kg. Exp. neoplastic agent. EK4400000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 57A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 84A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 84C (*ir*)
Adams, R. *et al., J.A.C.S.*, 1919, **41**, 789 (*synth*)
Org. Synth., 1971, **51**, 44 (*synth*)
Boschi, R.A. *et al., Mol. Phys.*, 1972, **24**, 289 (*uv*)
Greeley, R.H. *et al., J. Chromatogr.*, 1974, **88**, 229 (*use*)
Ikuta, S. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 66 (*ms*)
Miyano, S. *et al., Nippon Kagaku Kaishi*, 1977, 138 (*synth*)
Eweiss, N.F. *et al., Synthesis*, 1977, 634 (*synth*)
Hsiu, S.L. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2091 (*cmr, pmr*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BRQ250

Iodoethane, 9CI, 8CI I-82

Ethyl iodide
[75-03-6]
H_3CCH_2I
C_2H_5I 155.966
Isol. from several marine algae. Used to esterify fatty acids for gc anal. Heavy, refractive liq. with ethereal odour, turns red in light. Misc. org. solvs.; v. spar. sol. H_2O (gradual dec.). d^{15} 1.95.
Fp -108. Bp 72.3°. Light sensitive. Silver leaf retards dec.
▶ Eye, skin and mucous membrane irritant. High vapour conc. narcotic. LD_{50} (rat, ipr) 330 mg/kg. KI4750000

[6485-58-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 55C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 82A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 83A (*ir*)
Hunt, B.A. *et al., J.C.S.*, 1920, **117**, 1592 (*synth*)
Hirao, N. *et al., Nippon Kagaku Kaishi*, 1931, **52**, 269 (*synth*)
Boschi, R.A. *et al., Mol. Phys.*, 1972, **24**, 289 (*uv*)
Greeley, R.H. *et al., J. Chromatogr.*, 1974, **88**, 229 (*use*)
Ikuta, S. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 66 (*ms*)
Jung, M.E. *et al., J.O.C.*, 1977, **42**, 3761 (*synth*)
Jung, M.E. *et al., Tet. Lett.*, 1977, 2659 (*synth*)
Ejchart, A. *et al., Org. Magn. Reson.*, 1980, **13**, 368 (*cmr*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2471-2473 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 733
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ELP500

2-Iodoethanol, 9CI, 8CI I-83

Ethylene iodohydrin. 2-Iodoethyl alcohol. 1-Hydroxy-2-iodoethane
[624-76-0]
ICH_2CH_2OH
C_2H_5IO 171.965
Isol. from red alga *Asparagopsis taxiformis*. Liq. d^{20} 2.91. Bp 176-177° Bp_{12} 65-67°.
▶ KL3820000

Ac: [627-10-1]
$C_4H_7IO_2$ 214.003
Liq. with burning taste. d^{20} 2.44. Bp_{43} 95-96°.

4-Nitrobenzoyl:
Cryst. Mp 68-69°.

Me ether: 1-Iodo-2-methoxyethane
[4296-15-5]
C_3H_7IO 185.992
Narcotic, sweet-smelling oil with burning, sweet taste. d_4^{15} 1.83. Bp_{50} 137.8°.

Et ether: See 1-Ethoxy-2-iodoethane in *The Combined Chemical Dictionary.*

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 268A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 180C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 252A (*ir*)
Laughton, P.M. *et al., Can. J. Chem.*, 1961, **39**, 2155 (*synth*)
Cornforth, J.W. *et al., J.C.S.(C)*, 1970, 846 (*synth*)
Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*isol, ms, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IEL000

3-Iodohexadecanoic acid I-84

3-Iodopalmitic acid
$H_3C(CH_2)_{12}CHICH_2COOH$
$C_{16}H_{31}IO_2$ 382.324

(±)-form
Mp 50.5°.

(ξ)-form
Me ester: [62885-99-8]
$C_{17}H_{33}IO_2$ 396.351
Constit. of the marine alga *Centroceras clavulatum*.
Robinet, M. *et al., Bull. Soc. Chim. Belg.*, 1931, **40**, 710
Takahashi, A. *et al., CA*, 1976, **86**, 185945 (*Me ester*)

Iodomethane, 9CI, 8CI I-85

Methyl iodide
[74-88-4]
H_3CI
CH_3I 141.939
Isol. from marine algae and giant kelp. Methylating agent. Soil fumigant. Liq. with pleasant odour. Spar. sol. H_2O. d_4^{20} 2.28.
Fp -66.5. Bp 42.5°. n_D^{20} 1.5317. Darkens on exp. to light.
▶ Eye and skin irritant. High vapour conc. narcotic. Lower conc. cause other adverse CNS effects. LD_{50} (mus, ipr) 172 mg/kg. Exp. neoplastic agent. PA9450000

Hydrate: Mp -4°.

[865-50-9, 2722-33-0, 4227-95-6, 16170-82-4, 54245-42-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 55A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 81A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 82A (*ir*)
Timmermans, J. *et al., J. Chem. Phys.*, 1934, **31**, 85 (*synth*)
Vogel, A.I. *et al., J.C.S.*, 1943, 636 (*synth, props*)
Org. Synth., Coll. Vol., 2, 1943, 399; 404 (*synth*)
Von Buenau, G. *et al., Ber. Bunsen-Ges. Phys. Chem.*, 1969, **73**, 473 (*ms*)
Kawaguchi, T. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 53 (*cryst struct*)
Stahl-Larivière, H. *et al., Org. Magn. Reson.*, 1974, **6**, 170 (*pmr*)
Olah, G.A. *et al., J.A.C.S.*, 1975, **97**, 680 (*cmr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 342 (*use*)
IARC Monog., 1986, **41**, 213; *Suppl.* 7, 66 (*rev, tox*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2828-2832 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1-423 (*rev, occur*)

Zheng, W. *et al., J. Agric. Food Chem.*, 2003, **51**, 673-679 (*use, props*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 3446
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0425
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 735
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MKW200

(Iodomethyl)trimethylammonium(1+) I-86

1-Iodo-N,N,N-*trimethylmethanaminium, 9CI*
[39895-69-7]
$Me_3N^{\oplus}CH_2I$
$C_4H_{11}IN^{\oplus}$ 200.042
Isol. from the Japanese gastropod *Turbo marmorata*.

Chloride: [65603-17-0]
$C_4H_{11}ClIN$ 235.495
Counterion for natural product.

Iodide: [39741-91-8]
$C_4H_{11}I_2N$ 326.947
Cryst. (1,2-ethanediol). Mp 192° dec.(approx.) Mp 240° dec.(approx.) (double Mp).

Schreiber, J. *et al., Angew. Chem., Int. Ed.*, 1971, **10**, 330-331 (*synth*)
Laber, R.A. *et al., Spectrochim. Acta A*, 1977, **33**, 1079-1081 (*ir, Raman*)
Kotaki, Y. *et al., CA*, 1978, **88**, 100056h (*isol*)
Wittmann, H. *et al., Monatsh. Chem.*, 1982, **113**, 1451-1458 (*synth, pmr*)
Almarzoqi, B. *et al., Tetrahedron*, 1986, **42**, 601-607 (*synth*)

1-Iodopentane, 9CI, 8CI I-87

n-*Amyl iodide*
[628-17-1]
$H_3C(CH_2)_3CH_2I$
$C_5H_{11}I$ 198.046
Isol. from a marine alga. d_4^{20} 1.52. Bp_{20} 62°.
▶ Flammable, fl. p. 47°. LD_{50} (rat, ipr) 948 mg/kg. SA2975600

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 85B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 58A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 85C (*ir*)
Lieben, *et al., Annalen*, 1871, **159**, 74 (*synth*)
Marker, A. *et al., Chem. Comm.*, 1972, 724 (*cmr*)
Boschi, R.A. *et al., Mol. Phys.*, 1972, **24**, 289 (*uv*)
Schrumpf, G. *et al., Chem. Ber.*, 1973, **106**, 266 (*pmr*)
Houriet, R. *et al., Helv. Chim. Acta*, 1976, **59**, 119 (*ms*)
Miyano, S. *et al., Nippon Kagaku Kaishi*, 1977, 138; *CA*, **86**, 139323 (*synth*)
Brunet, J.J. *et al., Tet. Lett.*, 1985, **26**, 5445 (*synth*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)

1-Iodopropane, 9CI, 8CI I-88

Propyl iodide
[107-08-4]
$H_3CCH_2CH_2I$
C_3H_7I 169.993
Isol. from a marine alga. Used to prepare propyl derivs. for gc. studies. Colourless or sl. yellow liq. Prac. insol. H_2O, misc. EtOH, Et_2O. d_4^{20} 1.75.
Fp -101.3 Mp 0° -98.7°. Bp 102.5°.
▶ Flammable, fl. p. 50 (mus, ipr) 297 mg/kg. Exp. neoplastic agent. TZ4100000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 56B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 83A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 83D (*ir*)
Adams, R. *et al., J.A.C.S.*, 1919, **41**, 789 (*synth*)
Hirao, N. *et al., Nippon Kagaku Kaishi*, 1931, **52**, 269 (*synth*)
Boschi, R.A. *et al., Mol. Phys.*, 1972, **24**, 289 (*uv*)
Houriet, R. *et al., Helv. Chim. Acta*, 1976, **59**, 119 (*ms*)
Arbin, A. *et al., J. Chromatogr.*, 1977, **144**, 85 (*use*)
Gusev, Yu. *et al., Zh. Obshch. Khim.*, 1977, **47**, 45 (*synth*)
Hsiu, S.L. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2091 (*cmr, pmr*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PNO750

2-Iodopropane, 9CI, 8CI I-89

Isopropyl iodide
[75-30-9]
$H_3CCHICH_3$
C_3H_7I 169.993
Isol. from a marine alga. Liq. Prac. insol. H_2O, misc. EtOH, C_6H_6, $CHCl_3$, Et_2O. d_4^{20} 1.7. Readily discolours in light and air.
▶ Highly flammable, fl. p. 21/43°. LD_{50} (mus, ipr) 1300 mg/kg. Exp. neoplastic agent. TZ4200000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 66A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 96C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 94B (*ir*)
Récsei, A. *et al., Biochem. Z.*, 1927, **190**, 57 (*synth*)
Feshchenko, N.G. *et al., Zh. Obshch. Khim.*, 1970, **40**, 770 (*synth*)
Gross, M.L. *et al., J.A.C.S.*, 1971, **93**, 253 (*ms*)
Marker, A. *et al., Chem. Comm.*, 1972, 724 (*cmr*)
Boschi, R.A. *et al., Mol. Phys.*, 1972, **24**, 735 (*uv*)
Jung, M.E. *et al., J.O.C.*, 1977, **42**, 3761 (*synth*)
Gusev, Yu. *et al., Zh. Obshch. Khim.*, 1977, **47**, 45 (*synth*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2842-2843 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IPS000

1-Iodo-2-propanone, 9CI, 8CI I-90

Iodoacetone
[3019-04-3]
H_3CCOCH_2I
C_3H_5IO 183.976
Isol. from the alga *Asparagopsis taxiformis*. Chemical warfare agent, used during 1st World War. Yellow liq. d^{25} 2.17. Bp_{11} 58.4°.
▶ Highly irritant and lachrymatory.

Oxime:
C_3H_6INO 198.991
Prisms (petrol). Mp 64.5°.

Scholl, R. *et al., Ber.*, 1896, **29**, 1550 (*synth*)
Rây, P.C. *et al., Nature (London)*, 1933, **132**, 749 (*synth*)
Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*isol*)
Guerrero, S.A. *et al., J.C.S. Perkin 2*, 1983, 1053 (*ir, uv*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 745

3-Iodo-2-propenoic acid, 9CI I-91

3-Iodoacrylic acid, 8CI
[71815-44-6]
IHC═CHCOOH
$C_3H_3IO_2$ 197.96
Minor component of the aq. extract of Hawaiian red alga *Asparagopsis taxiformis*.

(E)-form [6372-02-7]
Cryst. Mp 144-147°. pK_a 5.59 (25°, 80% 2-methoxyethanol aq.).

Me ester: [6213-88-3]
$C_4H_5IO_2$ 211.987
Liq. $Bp_{18.200001}$ 61°.

Et ester: [31930-37-7]
$C_5H_7IO_2$ 226.014
Liq. d_4^{22} 1.74. Bp_{10} 74-75°. n_D^{22} 1.5260.

(Z)-form [6214-35-3]
Sl. yellow solid. Mp 67-68° (63-65°). pK_a 5.85 (25°, 80% 2-methoxyethanol aq.).

Me ester: [6214-23-9]
Liq. (sl. yellow). $Bp_{12.2}$ 62-63°.

Et ester: [31930-36-6]
Liq. d_4^{22} 1.77. Bp_{10} 83-84°. n_D^{22} 1.5300.

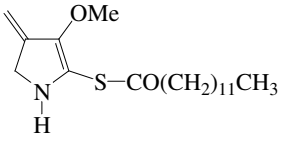
Amide: [137627-61-3]
C_3H_4INO 196.975
Solid. Mp 98-102°.

Stolz, F. *et al., Ber.*, 1886, **19**, 536-545 (*synth*)
Biougne, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1971, **272**, 858-861 (*Et ester, synth, pmr, ir*)

Brouwer, H. *et al., Can. J. Chem.*, 1972, **50**, 601-611 (*cmr, pmr*)
Bowden, K. *et al., J.C.S. Perkin 2*, 1972, 206-209 (*pKa*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617-620 (*isol, glc, synth*)
Jung, M.E. *et al., Tet. Lett.*, 1983, **24**, 3973-3974 (*Z-form, synth, pmr*)
Moss, R.A. *et al., J.A.C.S.*, 1989, **111**, 6729-6734 (*Z-form, synth, pmr, ir, glc*)
Ma, S. *et al., J.O.C.*, 1992, **57**, 709-713 (*Z-form, synth, pmr, ir, ms*)
Piers, E. *et al., Can. J. Chem.*, 1994, **72**, 1816-1819 (*Z-form, Me ester, synth*)
Abarbri, M. *et al., Synthesis*, 1996, 82-86 (*synth, ir, pmr, cmr, ms*)
Kotora, M. *et al., Synthesis*, 1997, 121-128 (*Z-form, synth, pmr, cmr, ir*)
Jung, M.E. *et al., J.O.C.*, 1998, **63**, 2968-2974 (*E-form, synth, Et ester, pmr*)
Org. Synth., Coll. Vol., 9, 1998, 510-515 (*E-form, Et ester, synth, ir, pmr, cmr*)
Takeuchi, R. *et al., J.O.C.*, 2000, **65**, 1558-1561 (*synth, Et ester, pmr, cmr*)
Suh, Y.-G. *et al., J.O.C.*, 2002, **67**, 4127-4137 (*Z-form, synth, pmr*)
Org. Synth., 2003, **80**, 129-132 (*E-form, synth, pmr, cmr*)

Ircinamine I-92

*1-[(4,5-Dihydro-3-methoxy-4-methylene-1*H*-pyrrol-2-yl)thio]-1-tridecanone*
[437980-03-5]

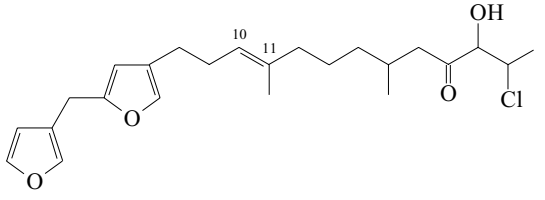


$C_{19}H_{33}NO_2S$ 339.541
Alkaloid from the sponge *Ircinia* sp. Cytotoxic. Amorph. solid. λ_{max} 242 (ϵ 1270) (MeOH).

Kuramoto, M. *et al., Chem. Lett.*, 2002, 464-465 (*isol, pmr, cmr, ms*)

Ircinia chlorohydrin 1 I-93

[133056-62-9]



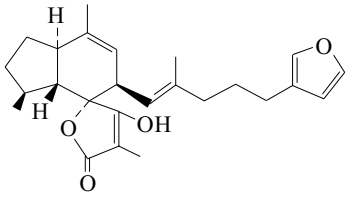
$C_{24}H_{33}ClO_4$ 420.975
Compd. not named in the paper. Constit. of *Ircinia oros.* Toxic to brine shrimp. $[\alpha]_D^{25}$ +34 (c, 1.3 in $CHCl_3$).

*Δ^{11}-Isomer (*Z*-):* ***Ircinia chlorohydrin 2***
[133056-63-0]
$C_{24}H_{33}ClO_4$ 420.975
Constit. of *Ircinia oros.* Toxic to brine shrimp. $[\alpha]_D^{25}$ +40 (c, 0.7 in $CHCl_3$). Not named in the paper.

De Giulio, A. *et al., J. Nat. Prod.*, 1990, **53**, 1503 (*isol, pmr, cmr*)

Ircinianin I-94

[63555-48-6]



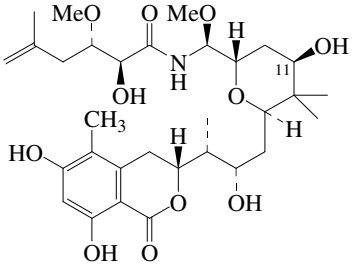
$C_{25}H_{32}O_4$ 396.525
Constit. of *Ircinia* spp. Cryst. (Me_2CO/toluene).
Mp 165-167°. $[\alpha]_D^{25}$ -232 (c, 0.5 in $CHCl_3$). λ_{max} 264 (ϵ 18200) (EtOH/NaOH) (Derep). λ_{max} 208 (ϵ 22900); 238 (sh) (ϵ 11000); 268 (sh) (ϵ 2000) (EtOH) (Derep).

Sulfate:
$C_{25}H_{32}O_7S$ 476.59
Constit. of *Ircinia wistarii*. Light yellow gum.
Mp 138-140° (dec.). $[\alpha]_D^{20}$ -160 (c, 0.02 in MeOH).

Hofheinz, W. *et al., Helv. Chim. Acta*, 1977, **60**, 1367 (*isol, struct*)
Takeda, K. *et al., Tet. Lett.*, 1986, **27**, 3903 (*synth*)
Coll, J.C. *et al., J. Nat. Prod.*, 1997, **60**, 1178-1179 (*isol, pmr, cmr, sulfate*)
Uenishi, J. *et al., J.O.C.*, 1997, **62**, 1691 (*synth*)

Irciniastatin A I-95

Psymberin



Absolute Configuration

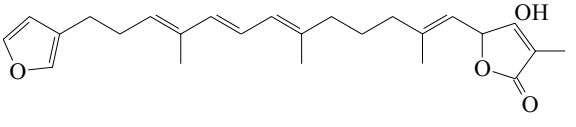
$C_{31}H_{47}NO_{11}$ 609.712
Isol. from the sponges *Ircinia ramosa* and *Psammocinia* sp. Cytotoxic. Amorph. powder. $[\alpha]_D$ +29 (c, 0.02 in MeOH). λ_{max} 215; 230 (sh); 270; 310 (MeOH aq.).

11-Ketone: ***Irciniastatin B***
$C_{31}H_{45}NO_{11}$ 607.697
Isol. from *Ircinia ramosa*. Cytotoxic. Amorph. powder. $[\alpha]_D$ -4.7 (c, 0.15 in MeOH). λ_{max} 215; 230 (sh); 270; 310 (MeOH).

Pettit, G.R. *et al., J. Med. Chem.*, 2004, **47**, 1149-1152 (*isol, pmr, cmr*)
Cichewitz, R.H. *et al., Org. Lett.*, 2004, **6**, 1951-1954 (*Psymberin*)
Jiang, X. *et al., J.A.C.S.*, 2005, **127**, 11254-11255 (*synth, abs config*)
Kiren, S. *et al., Org. Lett.*, 2005, **7**, 2905-2908 (*pmr, cmr, config*)

Ircinic acid I-96

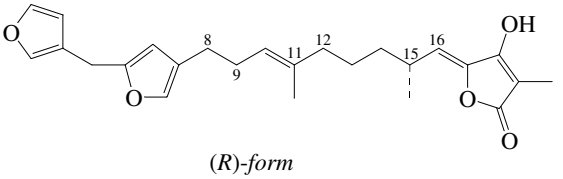
[106534-60-5]



$C_{25}H_{32}O_4$ 396.525
Constit. of an *Ircinia* sp. Oil.

Manes, L.V. *et al., J. Nat. Prod.*, 1986, **49**, 787

Ircinin 1 I-97



(*R*)-*form*

$C_{25}H_{30}O_5$ 410.509

(R)-form
Constit. of a *Sarcotragus* sp.
Oil. $[\alpha]_D^{25}$ +32.3 (c, 0.05 in MeOH).

*Δ^{11}-Isomer (*Z*-):* ***15R-Ircin 2***
$C_{25}H_{30}O_5$ 410.509
Constit. of a *Sarcotragus* sp. Oil. $[\alpha]_D^{25}$ +34.8 (c, 0.06 in MeOH).

*16*E*-Isomer:* ***Sarcotin D***
[369367-33-9]
$C_{25}H_{30}O_5$ 410.509

Constit. of a *Sarcotragus* sp. Oil. $[\alpha]_D^{25}$ +36.1 (c, 0.05 in MeOH).

*16*E-*Isomer, Δ^{11}-isomer(Z-):* ***Sarcotin E***

[369367-34-0]

$C_{25}H_{30}O_5$ 410.509

Constit. of a *Sarcotragus* sp. Oil. $[\alpha]_D^{25}$ +41.6 (c, 0.06 in MeOH).

(*S*)-*form* [35731-89-6]

Constit. of marine sponge *Ircinia oros*. Shows antibacterial props. Oil. Sol. MeOH. $[\alpha]_D^{19.5}$ -34.12 (MeOH). λ_{max} 248 (ϵ 10500); 310 (ϵ 7500) (MeOH/NaOH) (Derep). λ_{max} 260 (ϵ 12500) (MeOH) (Derep). λ_{max} 264 (ϵ 11800) (EtOH) (Berdy).

O-*Sulfate:* [183593-70-6]

$C_{25}H_{30}O_8S$ 490.573

Constit. of *Ircinia* spp. Ichthyotoxin. Toxic to brine shrimp. Amorph. powder. $[\alpha]_D$ +9.5 ($CHCl_3$). λ_{max} 272 (ϵ 18000) (MeOH).

8,9-Didehydro: ***8,9-Dehydroircinin 1***

[94935-99-6]

$C_{25}H_{28}O_5$ 408.493

Constit. of marine sponge *Cacospongia scalaris*. Inhibits division of fertilised starfish eggs. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ +94.2 (as acetate). λ_{max} 234 (ϵ); 312 (ϵ) (EtOH/NaOH) (Derep). λ_{max} 234 (ϵ 36000); 265 (sh) (ϵ 22000) (EtOH) (Derep).

Δ^{11}-Isomer(Z-): ***Ircinin 2***

[35761-52-5]

$C_{25}H_{30}O_5$ 410.509

From *Ircinia* spp. Toxic to brine shrimp. Oil. $[\alpha]_D^{19.5}$ -40.2 (MeOH). λ_{max} 248 (ϵ 10500); 310 (ϵ 7500) (MeOH/NaOH) (Derep). λ_{max} 260 (ϵ 12500) (MeOH) (Derep). λ_{max} 266 (ϵ 11500) (EtOH) (Berdy).

Δ^{11}-Isomer(Z-), O-*sulfate:* [183593-71-7]

$C_{25}H_{30}O_8S$ 490.573

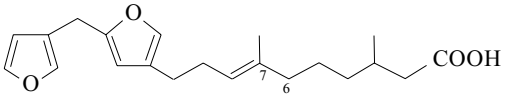
Constit. of *Ircinia* spp. Ichthyotoxin. Toxic to brine shrimp. Amorph. powder. $[\alpha]_D$ +9.5 ($CHCl_3$). λ_{max} 272 (ϵ 18000) (MeOH).

Cimino, G. *et al., Tetrahedron*, 1972, **28**, 333 (*isol*)
Fusetani, N. *et al., Tet. Lett.*, 1984, **15**, 4941 (*8,9-Dehydroircinin 1*)
Manes, L.V. *et al., J. Nat. Prod.*, 1986, **49**, 787 (*isol, struct*)
Capon, R.J. *et al., Nat. Prod. Lett.*, 1994, **4**, 51 (*abs config*)
De Rosa, S. *et al., Nat. Prod. Lett.*, 1996, **8**, 245-251 (*sulfates*)
Liu, Y. *et al., J. Nat. Prod.*, 2001, **64**, 1301-1304 (*Sarcotins D,E, Ircinins 1,2*)

Ircinin 3 I-98

10-[5-(β-Furanylmethyl)-3-furanyl]-3,7-dimethyl-7-decenoic acid

[41060-08-6]



$C_{21}H_{28}O_4$ 344.45

Isol. from the marine sponge *Ircinia oros*.

Me ester:

Oil. $[\alpha]_D$ +2.1 (c, 1.0 in $CHCl_3$).

Δ^6-Isomer (Z-): ***Ircinin 4***

[41060-09-7]

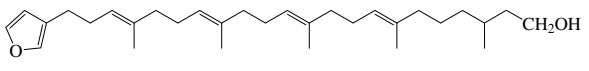
$C_{21}H_{28}O_4$ 344.45

From *Ircinia oros*.

Cimino, G. *et al., Tetrahedron*, 1972, **28**, 5983

Ircinol I-99

22-(3-Furanyl)-3,7,11,15,19-pentamethyl-7,11,15,19-docosatetraen-1-ol, 9CI



$C_{31}H_{50}O_2$ 454.735

Sulfate: ***Ircinol sulfate***

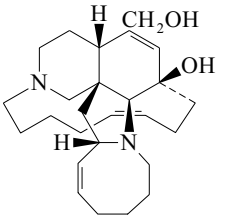
[170312-93-3]

$C_{31}H_{50}O_5S$ 534.799

Isol. from *Ircinia* sp. Registry number refers to Na salt.

Bifulco, G. *et al., J. Nat. Prod.*, 1995, **58**, 1444-1449 (*isol, cmr*)

Ircinol A I-100



$C_{26}H_{40}N_2O_2$ 412.614

The enantiomer of Ircinol A itself so far characterised has the opposite abs. config. to other Manzamine alkaloids, but Ircinal A belonged to the 'normal' series.

(+)-*form*

Aldehyde: ***Ircinal A***

[139975-55-6]

$C_{26}H_{38}N_2O_2$ 410.598

Alkaloid from the Okinawan marine sponge *Ircinia* sp. and *Amphimedon* sp. Exhibits cytotoxicity against L1210 murine leukaemia cells and KB human epidermoid carcinoma cells. Plausible biogenetic precursor of manzamine alkaloids.

Mp 70°. $[\alpha]_D^{25}$ +48 (c, 2.9 in $CHCl_3$). λ_{max} 231 (ϵ 8500) (MeOH) (Derep).

12-Deoxy, 12,28-epoxide, 1-aldehyde: ***12,28-Oxaircinal A***

$C_{26}H_{36}N_2O_2$ 408.583

Alkaloid fron an *Acanthostrongylophora* sp. Yellow powder. $[\alpha]_D^{25}$ +56.6 (c, 0.06 in $CHCl_3$). λ_{max} 208 (log ϵ 3.63); 268 (log ϵ 3.78) (MeOH).

(-)-*form* [157000-77-6]

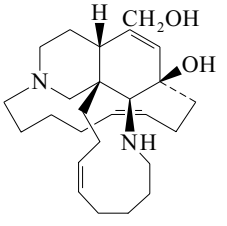
Alkaloid from the Okinawan marine sponge *Amphimedon* sp. Cytotoxic. Endothelin converting enzyme inhibitor. Amorph. solid.

Mp 83-85°. $[\alpha]_D^{18}$ -19 (c, 0.54 in MeOH).

Kondo, K. *et al., J.O.C.*, 1992, **57**, 2480 (*Ircinal A*)
Tsuda, M. *et al., Tetrahedron*, 1994, **50**, 7957 (*isol, ir, pmr, cmr, ms, struct*)
Tsuda, M. *et al., Heterocycles*, 1997, **46**, 765-794 (*rev*)
Winkler, J.D. *et al., J.A.C.S.*, 1998, **120**, 6425-6426 (*synth*)
Martin, S.F. *et al., J.A.C.S.*, 1999, **121**, 866-867 (*Ircinal A, synth*)
Rao, K.V. *et al., J. Nat. Prod.*, 2006, **69**, 1034-1040 (*12,28-Oxaircinal A*)

Ircinol B I-101

[157000-78-7]



$C_{26}H_{42}N_2O_2$ 414.63

Alkaloid from the Okinawan marine sponge *Amphimedon* sp. Cytotoxic, endothelin converting enzyme inhibitor. Amorph. solid.

Mp 78-79°. $[\alpha]_D^{18}$ -2.8 (c, 0.12 in MeOH). Possesses opposite config. to Manzamine alkaloids.

Enantiomer, 1-aldehyde: ***Ircinal B***

[139975-56-7]

$C_{26}H_{40}N_2O_2$ 412.614

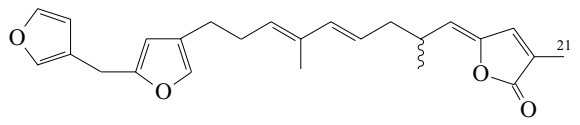
Alkaloid from the Okinawan marine sponge *Ircinia* sp. and *Amphimedon* sp. Exhibits cytotoxicity against L1210 murine leukaemia cells and KB human epidermoid carcinoma cells. Plausible biogenetic precursor of manzamine alkaloids.

Mp 95°. $[\alpha]_D^{25}$ +18 (c, 1.1 in $CHCl_3$). λ_{max} 224 (ϵ 12000) (MeOH) (Derep).

Kondo, K. *et al., J.O.C.*, 1992, **57**, 2480 (*Ircinal B*)
Tsuda, M. *et al., Tetrahedron*, 1994, **50**, 7957 (*isol, ir, pmr, cmr, ms struct*)
Tsuda, M. *et al., Heterocycles*, 1997, **46**, 765-794 (*rev*)

Ircinolide I-102

[62008-11-1]

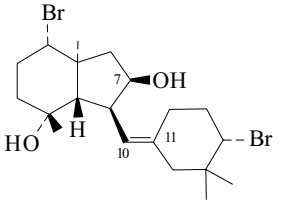


$C_{25}H_{28}O_4$ 392.494
Constit. of *Thorecta marginalis*. Oil.

21-Hydroxy: ***21-Hydroxyircinolide***
[62008-02-0]
$C_{25}H_{28}O_5$ 408.493
Constit. of *Thorecta marginalis*. Oil.
Kazlauskas, R. *et al., Tet. Lett.*, 1976, 2635 (*isol, struct*)

Iriediol I-103

[55708-74-2]



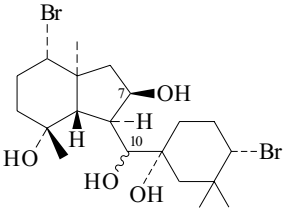
$C_{20}H_{32}Br_2O_2$ 464.28
Constit. of *Laurencia irieii*. Cryst. ($CHCl_3$).
Mp 103-105°. $[\alpha]_D^{23}$ -183 (c, 0.25 in $CHCl_3$).

7-Deoxy: ***Irieol***
[67506-11-0]
$C_{20}H_{32}Br_2O$ 448.28
Isol. from *Laurencia irieii*. Oil. $[\alpha]_D^{23}$ -23.1 (c, 1.34 in $CHCl_3$).

7-Deoxy, 10β,11β-epoxide: ***Irieol A***
[58844-61-4]
$C_{20}H_{32}Br_2O_2$ 464.28
Isol. from *Laurencia irieii*. Cryst. ($CHCl_3$).
Mp 142-144°. $[\alpha]_D^{25}$ 0 (c, 1.73 in $CHCl_3$).
Howard, B. *et al., Tet. Lett.*, 1975, 3983 (*isol, cryst struct*)
Howard, B. *et al., J.O.C.*, 1978, **43**, 4401 (*isol, abs config*)

Irieol F I-104

[67506-16-5]



$C_{20}H_{34}Br_2O_4$ 498.294
Constit. of *Laurencia irieii*. Cryst.
Mp 147-148°. $[\alpha]_D^{25}$ -27 (c, 3.38 in $CHCl_3$).

7-Ac: ***Irieol D***
[67506-14-3]
$C_{22}H_{36}Br_2O_5$ 540.331
Constit. of *Laurencia irieii*. Amorph. solid. $[\alpha]_D^{25}$ -30 (c, 4.02 in $CHCl_3$).

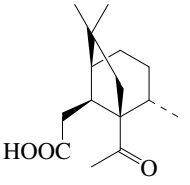
10-Ac: ***Irieol G***
[67506-17-6]
$C_{22}H_{36}Br_2O_5$ 540.331
From *Laurencia irieii*. Amorph. solid.

7-Deoxy: ***Irieol E***
$C_{20}H_{34}Br_2O_3$ 482.295
From *Laurencia irieii*. Amorph. solid. $[\alpha]_D^{25}$ -30.4 (c, 3.22 in $CHCl_3$).

10-Deoxy: ***Irieol B***
[67506-18-7]
$C_{20}H_{34}Br_2O_3$ 482.295
Constit. of *Laurencia irieii*. Amorph. solid.
Howard, B.M. *et al., J.O.C.*, 1978, **43**, 4401

Isishippuric acid A I-105

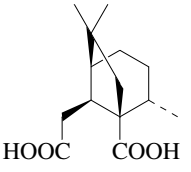
[761439-89-8]



$C_{15}H_{24}O_3$ 252.353
Constit. of *Isis hippuris*. Oil. $[\alpha]_D^{25}$ -107 (c, 1 in $CHCl_3$).
Sheu, J.-H. *et al., Tet. Lett.*, 2004, **45**, 6413-6416 (*Isishippuric acid A*)

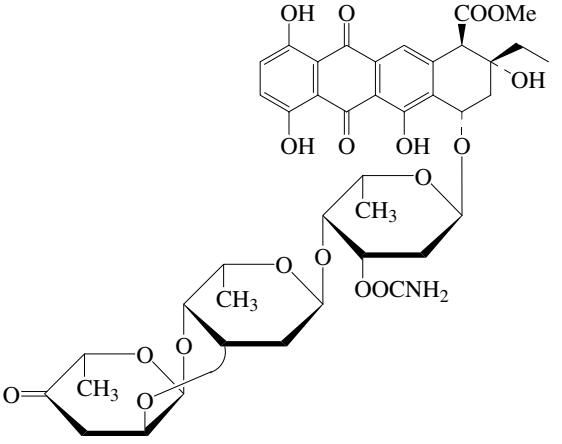
Isishippuric acid B I-106

[761439-91-2]



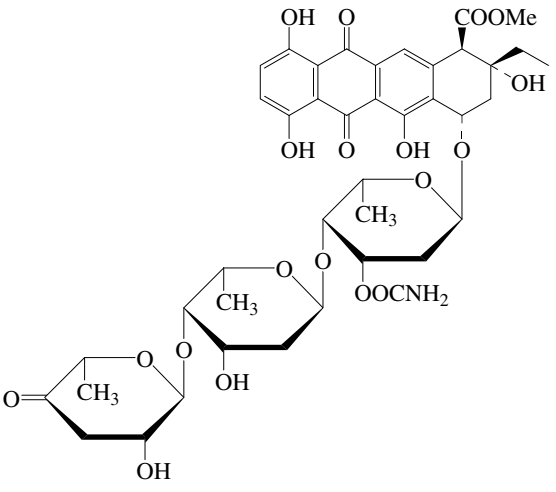
$C_{14}H_{22}O_4$ 254.325
Constit. of *Isis hippuris*. Powder.
Mp>300°. $[\alpha]_D^{25}$ -115 (c, 1 in $CHCl_3$).
Sheu, J.-H. *et al., Tet. Lett.*, 2004, **45**, 6413-6416

Islamomycin A I-107



$C_{41}H_{47}NO_{18}$ 841.818
Anthracycline antibiotic. Prod. by the marine *Streptomyces* sp. B8904. Dark red powder.
Shaaban, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*isol, pmr, cmr, ms*)

Islamomycin B I-108



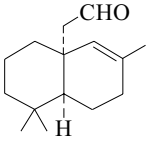
$C_{41}H_{49}NO_{19}$ 859.833

Anthracycline antibiotic. Prod. by the marine *Streptomyces* sp. B8904. Dark red powder.

Shaaban, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*isol, pmr, cmr, ms*)

Isoacanthodoral I-109

*1,3,4,7,8,8*a*-Hexahydro-1,1,6-trimethyl-4*a*(2*H*)-naphthaleneacetaldehyde, 9CI*
[90839-03-5]



$C_{15}H_{24}O$ 220.354

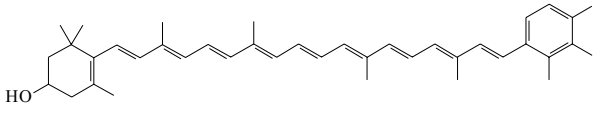
Constit. of *Acanthodoris nanaimoensis*.

4-Bromophenylurethane:
Oil. $[\alpha]_D$ -39 (hexane).

Ayer, S.W. *et al., J.O.C.*, 1984, **49**, 2653 (*cryst struct*)
Liu, H.-J. *et al., Can. J. Chem.*, 1994, **72**, 7416 (*synth*)
Graziani, E.I. *et al., J.A.C.S.*, 1996, **118**, 4701 (*biosynth*)

Isoagelaxanthin A I-110

β,χ-Caroten-3-ol
[83572-78-5]



$C_{40}H_{52}O$ 548.85

Constit. of *Acanthella vulgata*.

Mp 176-177°.

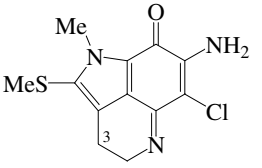
Me ether: ***Aaptopurpurin****. 3-Methoxy-β,χ-carotene*
[100288-41-3]
$C_{41}H_{54}O$ 562.877

Isol. from *Aaptos aaptos*. Cryst. (petrol).

Shimada, A. *et al., Tet. Lett.*, 1981, **22**, 773 (*synth*)
Tanaka, Y. *et al., Nippon Suisan Gakkaishi*, 1982, **48**, 1169; 1985, **51**, 1743 (*isol, ms, pmr*)

Isobatzelline A I-111

*7-Amino-6-chloro-3,4-dihydro-1-methyl-2-(methylthio)pyrrolo[4,3,2-*de*]quinolin-8(1*H*)-one, 9CI*
[133401-01-1]



$C_{12}H_{12}ClN_3OS$ 281.765

Alkaloid from the marine sponge *Batzella* sp. Exhibits cytotoxic and moderate antifungal activities. Brown solid. λ_{max} 262 (ϵ 15500); 342 (ϵ 9000); 430 (ϵ 3100) (MeOH) (Derep).

3,4-Didehydro: ***Isobatzelline D***
[133401-04-4]
$C_{12}H_{10}ClN_3OS$ 279.749

From *Batzella* sp. Exhibits cytotoxic and moderate antifungal activities. Red-brown solid. λ_{max} 239 (ϵ 33900); 263 (ϵ 25000); 439 (ϵ 25200) (MeOH) (Derep).

Dechloro: ***Isobatzelline B***
[133401-02-2]
$C_{12}H_{13}N_3OS$ 247.32

From *Batzella* sp. Exhibits cytotoxic and moderate antifungal activities. Red-brown solid. λ_{max} 264 (ϵ 14200); 362 (ϵ 7000); 402 (ϵ 5000) (MeOH) (Derep).

De(methylthio): ***Isobatzelline C***
[133401-03-3]
$C_{11}H_{10}ClN_3O$ 235.672

From *Batzella* sp., *Zyzzya massalis* and *Zyzzya fuliginosa*. Exhibits cytotoxic and moderate antifungal activities. Green-brown or red solid. λ_{max} 244 (ϵ 9700); 344 (ϵ 5900); 394 (ϵ 2600) (MeOH) (Derep). λ_{max} 224 (log ϵ 3.72); 341 (log ϵ 2.26); 422 (log ϵ 3.43) (MeOH).

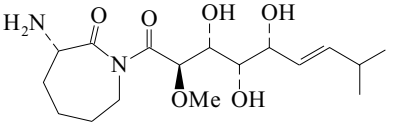
De(methylthio), 3,4-didehydro: ***Isobatzelline E***
[437980-21-7]
$C_{11}H_8ClN_3O$ 233.656

Isol. from *Zyzzya fuliginosa* and *Zyzzya massalis*. Orange solid. λ_{max} 224 (ϵ 21500); 290 (ϵ 4800); 422 (ϵ 13400) (MeOH).

Sun, H.H. *et al., J.O.C.*, 1990, **55**, 4964-4966 (*isol, uv, ir, pmr, ms, struct, cmr*)
Tao, X.L. *et al., Tetrahedron*, 1994, **50**, 2017 (*Isobatzelline C, synth*)
Yamada, F. *et al., Heterocycles*, 1995, **41**, 1905-1908 (*Isobatzelline C, synth*)
Roberts, D. *et al., J.O.C.*, 1997, **62**, 568 (*Isobatzelline C, synth*)
Alvarez, M. *et al., Tet. Lett.*, 1998, **39**, 679-680 (*Isobatzelline B, synth*)
Alvarez, M. *et al., Eur. J. Org. Chem.*, 1999, 1173-1183 (*synth*)
Chang, L.C. *et al., J. Nat. Prod.*, 2002, **65**, 775-778 (*Isobatzellines C,E*)
Dijoux, M.-G. *et al., Bioorg. Med. Chem.*, 2005, **13**, 6035-6044 (*Isobatzellines C,E*)

Isobengamide E I-112

[118477-05-7]



Absolute configuration

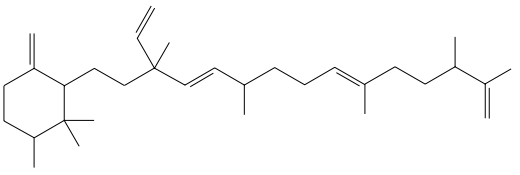
$C_{17}H_{30}N_2O_6$ 358.434

Metab. of an undescribed Fijian marine sponge (Jaspidae). Anthelmintic. Nematocide. Oil. $[\alpha]_D^{20}$ +17.1 (c, 0.052 in MeOH).

Adamczeski, M. *et al., J.A.C.S.*, 1989, **111**, 647 (*isol, ir, pmr, cmr, ms, struct*)
Adamczeski, M. *et al., J.O.C.*, 1990, **55**, 240 (*abs config*)

Isobraunicene I-113

[117021-05-3]

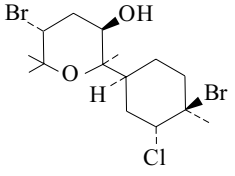


$C_{32}H_{54}$ 438.779
Metab. of *Botryococcus braunii*.

Huang, Z. *et al., J.O.C.*, 1988, **53**, 5390 (*isol, pmr, ms*)

Isocaespitol I-114

[53915-39-2]



$C_{15}H_{25}Br_2ClO_2$ 432.622
Constit. of *Laurencia caespitosa*. Cryst. (hexane). Poorly sol. hexane.
Mp 92-93°. $[\alpha]_D$ -15.

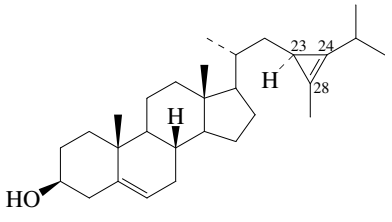
Deoxy: ***8-Deoxyisocaespitol***
[74323-44-7]
$C_{15}H_{25}Br_2ClO$ 416.623
Constit. of *Laurencia caespitosa*. Cryst.
Mp 95-96°. $[\alpha]_D$ -27.

[74364-62-8]

González, A.G. *et al., Tetrahedron*, 1975, **31**, 2449 (*isol, struct*)
González, A. *et al., Tet. Lett.*, 1976, 2279; 1979, 2719; 1980, 187 (*synth, isol, cmr*)
Chang, M. *et al., Phytochemistry*, 1989, **28**, 1417 (*abs config*)

Isocalysterol I-115

[83511-84-6]



Absolute Configuration

$C_{29}H_{46}O$ 410.682
Constit. of sponge *Calyx nicaeensis* and *Calyx podatypa*. Cryst. (Et_2O/MeOH).
Mp 115-116°. $[\alpha]_D^{20}$ -47.3 (c, 4 in $CHCl_3$).

5β,6-Dihydro: ***Isocalystanol***
[123158-94-1]
$C_{29}H_{48}O$ 412.698
Isol. from *Calyx nicaeensis*, prob. as a prod. of endobacterial metab.

*$\Delta^{23(28)}$-Isomer(24α*H*): 24*H*-Isocalysterol*
[84582-62-7]
$C_{29}H_{46}O$ 410.682
Isol. from the sponge *Calyx nicaeensis*.

*$\Delta^{23(28)}$-Isomer(24α*H*), 5α,6-dihydro: (24*S*)-24*H*-5α-Isocalystanol*
[116972-92-0]
$C_{29}H_{48}O$ 412.698
Isol. from *Calyx podatypa*.

*3-Epimer, 5β,6-dihydro: 5β-23*H*-Isocalystan-3α-ol*
[123158-92-9]
$C_{29}H_{48}O$ 412.698
Minor sterol from *Calyx nicaeensis*, prob. as endobacterial metab.

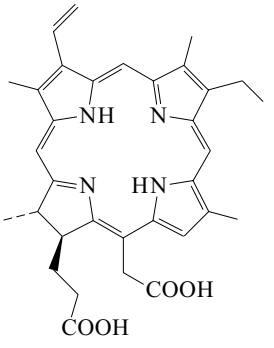
*23-Epimer: (23*S*)-23*H*-Isocalysterol*
[85798-19-2]
$C_{29}H_{46}O$ 410.682
Isol. from sponge *Calyx podatypa*.
Mp 112-113°.

*23-Epimer, 5α,6-dihydro: (23*S*)-23*H*-5α-Isocalystanol*
[116972-93-1]
$C_{29}H_{48}O$ 412.698
Isol. from sponge *Calyx podatypa*.

Li, L.N. *et al., J.A.C.S.*, 1982, **104**, 6726-6732 (*struct*)
Itoh, T. *et al., J.O.C.*, 1983, **48**, 890-892 (*24H-Isocalysterol*)
Margot, C. *et al., Chem. Comm.*, 1987, 1441-1442 (*24H-Isocalysterol*)
Doss, G.A. *et al., J.A.C.S.*, 1988, **110**, 8124-8128 (*23S-23H-Isocalysterol, 23S-23H-5α-Isocalystanol, 24S-24H-5α-Isocalystanol*)
Ha, T.B.T. *et al., Steroids*, 1989, **53**, 487-499 (*dihydro*)
Wicha, J. *et al., J.A.C.S.*, 1995, **117**, 1849-1850 (*synth, bibl*)
Kurek-Tyrlik, A. *et al., Eur. J. Org. Chem.*, 2000, 1027-1036 (*synth*)

Isochlorin e_4 I-116

[74578-42-0]

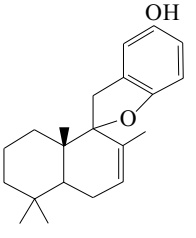


$C_{33}H_{36}N_4O_4$ 552.672
Isol. from the red alga *Dasya pedicellata*. Blue-green pigment.

Frankmolle, W.P. *et al., Phytochemistry*, 1994, **36**, 361 (*isol, bibl*)

Isochromazonarol I-117

[57291-89-1]

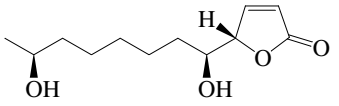


$C_{21}H_{28}O_2$ 312.451
Constit. of *Dictyopteris undulata*. Gum. $[\alpha]_D^{25}$ +110 (c, 0.85 in $CHCl_3$).

Fenical, W. *et al., Experientia*, 1975, **31**, 1004

Isocladospolide B I-118

*5-(1,7-Dihydroxyoctyl)-2(5*H*)-furanone. NG 261*
[164521-26-0]



Absolute Configuration

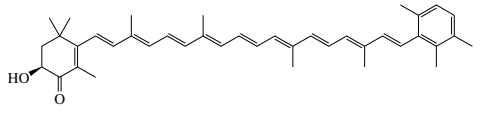
$C_{12}H_{20}O_4$ 228.288

Stereochem. revised in 2005. Isol. from fungal isolate I96S215 obtained from a marine sponge and from *Cladosporium cladosporioides* sp. TF-0380. Nerve growth factor agonist. Amorph. solid. $[\alpha]_D$ -90 (c, 0.23 in MeOH). λ_{max} 209 (ϵ 8600) (MeOH).

Japan. Pat., 1995, 95 70 101; *CA*, **123**, 40926w
Smith, C.J. *et al., J. Nat. Prod.*, 2000, **63**, 142-145 (*isol, pmr, cmr*)
Franck, X. *et al., Tet. Lett.*, 2001, **42**, 2801-2803 (*synth*)
Gesner, S. *et al., J. Nat. Prod.*, 2005, **68**, 1350-1353 (*abs config*)
Pandey, S.K. *et al., Tet. Lett.*, 2005, **46**, 6625-6627 (*synth*)
Sharma, G.V.M. *et al., Tet. Lett.*, 2006, **47**, 6531-6535; 6537-6540 (*synth, abs config*)

Isoclathriaxanthin I-119

3-Hydroxy-β,ϕ-caroten-4-one
[82438-78-6]



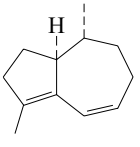
Absolute Configuration

$C_{40}H_{50}O_2$ 562.834
Constit. of *Agelas mauritiana* and *Tedania digitata*.

Tanaka, Y. *et al., Nippon Suisan Gakkaishi*, 1982, **48**, 531; *CA*, **97**, 52851a (*isol*)
Tanaka, Y. *et al., Fish. Sci.*, 2001, **67**, 378-379 (*isol, abs config*)

Isoclavukerin A I-120

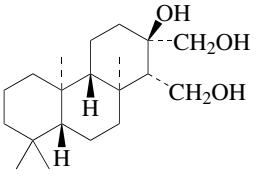
[140223-38-7]



$C_{12}H_{18}$ 162.274
Constit. of a *Clavularia* coral. Liq. Bp_{100} 80-90°. $[\alpha]_D^{25}$ -100 (c, 1 in $CHCl_3$). λ_{max} 246 (ϵ 10400) (MeOH) (Derep).

Kusumi, T. *et al., Tet. Lett.*, 1992, **33**, 2019 (*isol, pmr, cmr*)
Shimizu, I. *et al., Tet. Lett.*, 1994, **35**, 1905 (*synth*)
Trost, B.M. *et al., J.A.C.S.*, 1996, **118**, 10094 (*synth*)
Friese, J.C. *et al., Tet. Lett.*, 2002, **43**, 2683-2685 (*synth*)

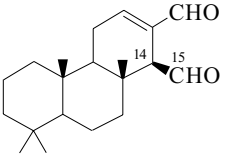
13,15,16-Isocopalanetriol I-121



$C_{20}H_{36}O_3$ 324.503

(ent*-13α*OH*,14α*H*)-*form
15,16-Di-Ac: ***Anisodorin 5***
[220866-43-3]
$C_{24}H_{40}O_5$ 408.577
Constit. of *Anisodoris fontaini*.
$[\alpha]_D$ -3.2 (c, 0.15 in $CHCl_3$).
Gavagnin, M. *et al., J. Nat. Prod.*, 1999, **62**, 269-274 (*isol, pmr, cmr*)
Ungur, N. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 1635-1636 (*abs config*)

12-Isocopalene-15,16-dial I-122



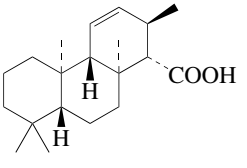
14α*H–form*

$C_{20}H_{30}O_2$ 302.456

(14α*H*)-form [84807-61-4]
Constit. of *Spongia officinalis.*
Cryst.
Mp 139-142° dec. $[\alpha]_D$ +48 (c, 1.5 in $CHCl_3$).
15-Alcohol: ***15-Hydroxy-12-isocopalen-16-al***
[157924-84-0]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Spongia zimocca*.
15-Alcohol, 15-Ac: 15-Acetoxy-12-isocopalen-16-al
[84807-63-6]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Spongia officinalis.*
$[\alpha]_D$ +4.2 (c, 3.2 in $CHCl_3$).

14β*H*-form [84807-62-5]
Constit. of *Spongia officinalis.*
Cryst.
Mp 115-118°. $[\alpha]_D$ +190 (c, 1.5 in $CHCl_3$).
Cimino, G. *et al., Tet. Lett.*, 1982, **23**, 4139-4142 (*isol, struct*)
Nakano, T. *et al., J. Chem. Res., Synop.*, 1984, 262-263 (*synth*)
Mischne, M.P. *et al., J.O.C.*, 1984, **44**, 2035-2037 (*synth*)
Zubía, E. *et al., J. Nat. Prod.*, 1994, **57**, 725-731 (*15-alcohol, isol, pmr, cmr*)
Pulita, R. *et al., Acta Cryst. C*, 1999, **55**, 2160-2163 (*cryst struct*)

11-Isocopalen-15-oic acid I-123

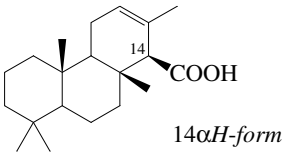


$C_{20}H_{32}O_2$ 304.472

(ent*-13β*H*)-*form
*(3-Acetoxy-2-hydroxypropyl) ester (*S-*):* ***Verrucosin 1***
[183388-19-4]
[183239-56-7 undefined side-chain config]
$C_{25}H_{40}O_5$ 420.588
Constit. of *Doris verrucosa*. Protein kinase C activator. Morphogenetic hydra tentacle regeneration agent. Tumour promoter. $[\alpha]_D$ -48.7 (c, 0.7 in $CHCl_3$).
(2-Acetoxy-3-hydroxypropyl) ester: ***Verrucosin 6***
[183388-18-3]
$C_{25}H_{40}O_5$ 420.588
Constit. of *Doris verrucosa*. Protein kinase C activator. Morphogenetic hydra tentacle regeneration agent. Tumour promoter. $[\alpha]_D$ -37 (c, 0.1 in $CHCl_3$).
Gavagnin, M. *et al., Tetrahedron*, 1997, **53**, 1491-1504 (*isol, pmr, cmr*)

12-Isocopalen-15-oic acid I-124

12-Isoagathen-15-oic acid. Isocopalic acid



14α*H-form*

$C_{20}H_{32}O_2$ 304.472

14α*H-form* [91200-12-3]
[276864-71-2]
Cryst. (petrol). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 177-178°. $[\alpha]_D$ -9.1 (c, 0.3 in $CHCl_3$).

2S,3-Dihydroxypropyl ester: [89210-13-9]
$C_{23}H_{38}O_4$ 378.551
Constit. of nudibranchs *Archidoris montereyensis*, *Archidoris tuberculata* and *Archidoris odhneri*. Fish antifeedant. Cryst. (Et_2O/hexane).
Mp 125-126°. $[\alpha]_D$ -12.5 (c, 0.4 in $CHCl_3$).

(2-Acetoxy-3-hydroxypropyl) ester: [97530-69-3]
$C_{25}H_{40}O_5$ 420.588
Constit. of *Archidoris montereyensis*, *Archidoris carvi* and *Archidoris tuberculata*. Ichthyotoxic. Oil. $[\alpha]_D$ -33 (c, 0.83 in $CHCl_3$).

(3-Acetoxy-2-hydroxypropyl) ester: [97530-68-2]
$C_{25}H_{40}O_5$ 420.588
Constit. of *Archidoris montereyensis*, *Archidoris carvi* and *Archidoris tuberculata*. Ichthyotoxic. Cryst. (Et_2O/hexane).
Mp 117-119°. $[\alpha]_D$ -53.7 (c, 0.13 in $CHCl_3$).

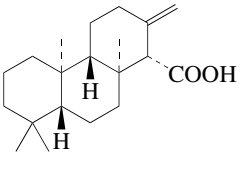
(*ent*-14α*H*)-*form*

(2-Acetoxy-3-hydroxypropyl) ester: [150176-67-3]
Constit. of *Archidoris carvi*.
$[\alpha]_D$ +66.9 (c, 0.07 in $CHCl_3$).

(3-Acetoxy-2-hydroxypropyl) ester: [150200-40-1]
Constit. of *Archidoris carvi* and *Doris verrucosa*.
$[\alpha]_D$ +21.9 (c, 0.22 in $CHCl_3$).

Gustafson, K. *et al., Tet. Lett.*, 1984, **25**, 11-14 (*14αH-form 2S,3-dihydroxypropyl ester, cryst struct*)
Gustafson, K. *et al., Tetrahedron*, 1985, **41**, 1101-1108 (*14αH-form, isol, ir, pmr, cmr, ms, ent-14αH-form esters*)
Zubía, E. *et al., Experientia*, 1993, **49**, 268-271 (*ent-14αH-form, isol, pmr, cmr, ms, ir, cd, esters*)
Urones, J.G. *et al., Nat. Prod. Lett.*, 1994, **5**, 217 (*synth*)
Ungur, N. *et al., Tet. Lett.*, 1996, **37**, 3549-3552 (*14αH-form, synth*)
Gavagnin, M. *et al., Tetrahedron*, 1997, **53**, 1491-1504 (*isol, Doris*)
Ungur, N. *et al., Tetrahedron*, 2000, **56**, 2503-2512 (*14αH-form esters*)

13(16)-Isocopalen-15-oic acid I-125



$C_{20}H_{32}O_2$ 304.472

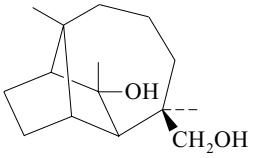
(*ent*-14α*H*)-*form* [220862-73-7]
Cryst. (Et_2O/petrol). Mp 222-223°.

2-Acetoxy-3-hydroxypropyl ester: ***Anisodorin 2***
[220866-40-0]
$C_{25}H_{40}O_5$ 420.588
Constit. of *Anisodoris fontaini*.
$[\alpha]_D$ -92.9 (c, 0.1 in $CHCl_3$).

3-Acetoxy-2-hydroxypropyl ester: ***Anisodorin 1***
[220866-39-7]
$C_{25}H_{40}O_5$ 420.588
Constit. of *Anisodoris fontaini*.
$[\alpha]_D$ +2.1 (c, 0.14 in $CHCl_3$).
Gavagnin, M. *et al., J. Nat. Prod.*, 1999, **62**, 269-274 (*isol, pmr, cmr, synth*)

Isoculmorin I-126

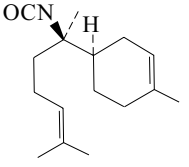
[174846-64-1]



$C_{15}H_{26}O_2$ 238.369
Constit. of *Kallichroma tethys*. Needles (MeOH).
Mp 165-167°. $[\alpha]_D^{25}$ +156 (c, 0.2 in MeOH).
Alam, M. *et al., J. Nat. Prod.*, 1996, **59**, 454-456 (*isol, pmr, cmr, cryst struct*)

7-Isocyanato-2,10-bisaboladiene I-127

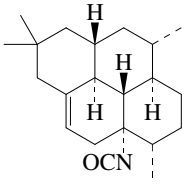
7-Isocyanato-7,8-dihydro-α-bisabolene



$C_{16}H_{25}NO$ 247.38

(6*R*,7*R*)-*form* [105281-35-4]
Constit. of a *Ciocalypta* sp.
Oil. $[\alpha]_D^{25}$ -24.3 (c, 0.094 in hexane). λ_{max} 205 (ϵ 5000); 248 (ϵ 500) (hexane) (Derep).
Gulavita, N.K. *et al., J.O.C.*, 1986, **51**, 5136 (*isol, cryst struct*)

8-Isocyanato-10-cycloamphilectene I-128



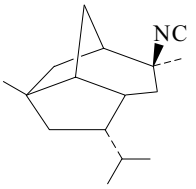
$C_{21}H_{31}NO$ 313.482

8α-*form* [697299-20-0]
Constit. of a *Stylissa* sp.
Oil. $[\alpha]_D^{26}$ -20.1 (c, 2 in $CHCl_3$).

8-Isothiocyanate: ***8-Isothiocyanato-10-cycloamphilectene***
[697299-21-1]
$C_{21}H_{31}NS$ 329.549
Constit. of a *Stylissa* sp. Powder.
Mp 73-75°. $[\alpha]_D^{22}$ -46.9 (c, 0.3 in $CHCl_3$). Has -NCS in place of -NCO.
Mitome, H. *et al., J. Nat. Prod.*, 2004, **67**, 833-837 (*isol, pmr, cmr, cryst struct*)

Isocyanoallopupukeanane I-129

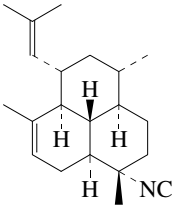
[138949-83-4]



$C_{16}H_{25}N$ 231.38
Constit. of *Phyllidia pustulosa*. Gum. $[\alpha]_D$ +16.2 (c, 0.075 in $CHCl_3$).

Fusetani, N. *et al., Tet. Lett.*, 1991, **32**, 7291 (*isol, pmr, cmr*)
Ho, T.-L. *et al., Org. Lett.*, 1999, **1**, 1051-1052 (*synth*)
Srikrishna, A. *et al., Tet. Lett.*, 2006, **47**, 367-370 (*synth*)

7-Isocyano-10,14-amphilectadiene I-130



(1α,7α)-*form*

$C_{21}H_{31}N$ 297.483

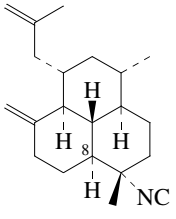
(1α,7α)-*form* [175861-84-4]
Constit. of *Cymbastela hooperi*.
Oil. $[\alpha]_D$ -3.7 (c, 0.38 ini $CHCl_3$). Genus name given as Cymbastella.

(1β,7α)-*form* [697299-17-5]
Constit. of a *Stylissa* sp.
Oil. $[\alpha]_D^{24}$ -19.1 (c, 1.52 in $CHCl_3$).

König, G.K. *et al., J.O.C.*, 1996, **61**, 3259-3267 (*Cymbastela hooperi constit*)
Mitome, H. *et al., J. Nat. Prod.*, 2004, **67**, 833-837 (*Stylissa constit*)

7-Isocyano-11(20),15-amphilectadiene I-131

[176019-13-9]

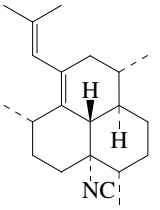


$C_{21}H_{31}N$ 297.483
Struct. revised in 1996. Constit. of *Adocia* spp. and *Cymbastela hooperi*. Cryst. (hexane).
Mp 148-149°. $[\alpha]_D^{25}$ +14 (c, 0.84 in $CHCl_3$).

8-Epimer: [251108-43-7]
$C_{21}H_{31}N$ 297.483
Constit. of a *Cribrochalina* sp. Solid. $[\alpha]_D$ +65 (c, 1.2 in $CHCl_3$). Struct. revised in 2005.

Kazlauskas, R. *et al., Tet. Lett.*, 1980, **21**, 315-318 (*isol*)
Koenig, G.K. *et al., J.O.C.*, 1996, **61**, 3259-3267 (*isol, pmr, cmr, cryst struct*)
Ciavatta, M.L. *et al., Tetrahedron*, 1999, **55**, 12629-12636 (*8-epimer*)
Ciavatta, M.L. *et al., Tetrahedron*, 2005, **61**, 8049-8053 (*Cribrochalina constit, struct*)

8-Isocyano-1(12),14-amphilectadiene I-132



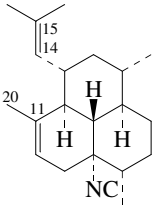
$C_{21}H_{31}N$ 297.483

8α-*form* [697299-19-7]
Constit. of a *Stylissa* sp.
Powder.
Mp 58-60°. $[\alpha]_D^{24}$ +239.6 (c, 3 in $CHCl_3$).

Mitome, H. *et al., J. Nat. Prod.*, 2004, **67**, 833-837 (*isol, pmr, cmr*)

8-Isocyano-10,14-amphilectadiene I-133

[108695-81-4]



Absolute Configuration

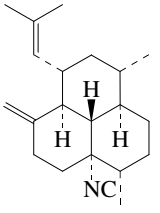
$C_{21}H_{31}N$ 297.483
Constit. of a *Halichondria* sp. Oil. $[\alpha]_D$ -79.8 (c, 2 in $CHCl_3$). Abs. config. revised in 2005.

$\Delta^{11(20)}$-Isomer, 14,15-dihydro, 15-isocyano: ***8,15-Diisocyano-11(20)-amphilectene***
[70206-86-9]
[251108-41-5]
$C_{22}H_{32}N_2$ 324.508
Isol. from the marine sponge *Hymeniacidon amphilecta* and a *Cribrochalina* sp. Active against gram-positive bacteria and yeasts. Cryst. (hexane).
Mp 105-106°. $[\alpha]_D$ -56 (c, 1 in $CHCl_3$).

$\Delta^{11(20)}$-Isomer, 14,15-dihydro, 15-isothiocyano: ***8-Isocyano-15-isothiocyano-11(20)-amphilectene***
[863684-41-7]
$C_{22}H_{32}N_2S$ 356.574
Constit. of a *Cribrochalina* sp. Oil. $[\alpha]_D$ -52 (c, 0.1 in $CHCl_3$).

Wratten, S.J. *et al., Tet. Lett.*, 1978, 4345-4348 (*isol, ir, pmr, cmr, struct, derivs*)
Molinski, T.F. *et al., J.O.C.*, 1987, **52**, 3334-3337 (*isol, struct*)
Piers, E. *et al., Can. J. Chem.*, 1993, **71**, 1484 (*synth*)
Piers, E. *et al., Tetrahedron*, 1993, **49**, 5791 (*synth*)
Ciavatta, M.L. *et al., Tetrahedron*, 1999, **55**, 12629-12636; 2005, **61**, 8049-8053 (*pmr, cmr, abs config*)

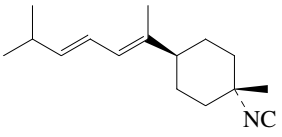
8-Isocyano-11(20),14-amphilectadiene I-134



$C_{21}H_{31}N$ 297.483

(1α,8α)-*form* [697299-18-6]
Constit. of a *Stylissa* sp.
Oil. $[\alpha]_D^{26}$ -34.1 (c, 0.4 in $CHCl_3$).
Mitome, H. *et al., J. Nat. Prod.*, 2004, **67**, 833-837 (*isol, pmr, cmr*)

3-Isocyano-7,9-bisaboladiene **I-135**
4-(1,5-Dimethyl-1,3-hexadienyl)-1-isocyano-1-methylcyclohexane, 9CI. 3-Isocyanotheonellin. ***Theonelline isocyanide***
[105281-40-1]

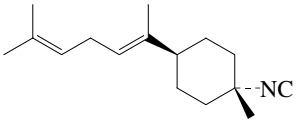


$C_{16}H_{25}N$ 231.38
Constit. of *Phyllidia pustulosa* and *Halichondria* cf. *lendenfeldi*. Oil. λ_{max} 203 (ϵ 6400); 232 (sh) (ϵ 1100); 239 (ϵ 11600) (MeOH) (Derep).

Isothiocyanate: ***Theonelline isothiocyanate***
[94663-94-2]
$C_{16}H_{25}NS$ 263.446
Constit. of the sponge *Theonella* cf. *swinhoei*. Shows antibacterial props. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Has -NCS relacing -NC. λ_{max} 238 (ϵ 30200) (MeOH) (Derep). λ_{max} 230 (MeOH) (Berdy).

Formamide: ***Theonelline formamide****. 3-Formamidotheonellin*
[94663-93-1]
$C_{16}H_{27}NO$ 249.395
Constit. of the sponge *Theonella* cf. *swinhoei* and *Axinyssa* sp. Oil. Sol. MeOH, $CHCl_3$, Me_2CO; poorly sol. H_2O. Has -NHCHO replacing -NC. λ_{max} 238 (ϵ 24000) (MeOH) (Derep). λ_{max} 238 (ϵ 24000) (MeOH) (Berdy).
Nakamura, H. *et al., Tet. Lett.*, 1984, **25**, 5401-5404 (*isothiocyanate, formamide*)
Gulavita, N.K. *et al., J.O.C.*, 1986, **51**, 5136
Kassühlke, K.E. *et al., J.O.C.*, 1991, **56**, 3747-3750 (*isol*)
Fusetani, N. *et al., Tet. Lett.*, 1991, **32**, 7291
Kitano, Y. *et al., J.C.S. Perkin 1*, 2002, 2251-2255 (*synth*)

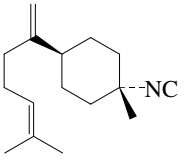
3-Isocyano-7,10-bisaboladiene **I-136**



$C_{16}H_{25}N$ 231.38

(3α,6α*H*,7*E*)-*form* [475282-77-0]
Constit. of an *Axinyssa* sponge.
Oil. $[\alpha]_D^{25}$ 0 (c, 0.75 in $CHCl_3$).
Iwashima, M. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1286-1289 (*isol, pmr, cmr*)

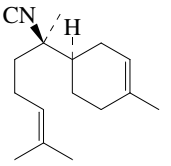
3-Isocyano-7(14),10-bisaboladiene **I-137**



$C_{16}H_{25}N$ 231.38

(3α,6α*H*)-*form* [786704-43-6]
Constit. of *Phyllidiella pustulosa*.
Oil.
Manzo, E. *et al., J. Nat. Prod.*, 2004, **67**, 1701-1704 (*isol, pmr, cmr*)

7-Isocyano-2,10-bisaboladiene **I-138**
7-Isocyano-7,8-dihydro-α-bisabolene



(6*R*,7*R*)-*form*

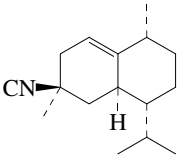
$C_{16}H_{25}N$ 231.38
λ_{max} 195 (ϵ 14500) (hexane) (Derep).

(6*R*,7*R*)-*form* [105281-36-5]
Constit. of a *Ciocalypta* sp.
Oil. $[\alpha]_D^{22}$ -49.9 (c, 0.033 in hexane).

(6*R*,7*S*)-*form*

Isothiocyanate: ***7-Isothiocyanato-2,10-bisaboladiene***
[105281-46-7]
$C_{16}H_{25}NS$ 263.446
Isol. from a *Halichondria* sp. and *Phyllidia pustulosa*. Oil. $[\alpha]_D^{20}$ +60.5 (c, 6.8 in $CHCl_3$). Has -NCS in place of -NC.
Sullivan, B.W. *et al., J.O.C.*, 1986, **51**, 5134-5136 (*isothiocyanate, isol, pmr, cmr*)
Gulavita, N.K. *et al., J.O.C.*, 1986, **51**, 5136 (*isocyanide*)
Kassühlke, K.E. *et al., J.O.C.*, 1991, **56**, 3747-3750 (*isothiocyanate, isol*)

4-Isocyano-1-cadinene **I-139**



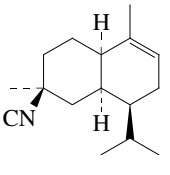
$C_{16}H_{23}N$ 229.364

(4β*NC*,6α,7α,10α)-*form* [162827-14-7]
[146307-03-1]
Constit. of *Axinyssa aplysinoides*.
Oil. $[\alpha]_D$ -75.1 (c, 0.6 in $CHCl_3$).

Isothiocyanate: 4-Isothiocyanato-1-cadinene. ***Halipanicine***
[134779-33-2]
$C_{16}H_{25}NS$ 263.446
Constit. of *Axinyssa aplysinoides* and *Halichondria panicea*. Oil. $[\alpha]_D^{23}$ -106.8 (c, 0.31 in CCl_4). Has -NCS replacing -NC. λ_{max} 202 (ϵ 14000); 250 (ϵ 1900) (hexane) (Berdy).

Formamide: ***4-Formamido-1-cadinene***
[162935-03-7]
[146307-02-0]
$C_{16}H_{27}NO$ 249.395
Constit. of *Axinyssa aplysinoides*. Oil. $[\alpha]_D$ -43.6 (c, 0.55 in $CHCl_3$). Has -NHCHO replacing -NC. λ_{max} 204 (ϵ 7790); 238 (ϵ 1375) (MeOH) (Berdy).
Nakamura, H. *et al., Agric. Biol. Chem.*, 1991, **55**, 581-583 (*Halipanicine*)
Nakamura, H. *et al., Tet. Lett.*, 1992, **33**, 8113-8116 (*Halipanicine, synth*)
Compagnone, R.S. *et al., J. Nat. Prod.*, 1995, **58**, 145-148 (*isocyanide, formamide*)
Ye, B. *et al., Tetrahedron*, 1996, **52**, 6361-6372 (*Halipanicine, synth*)

4-Isocyano-9-cadinene **I-140**



(1α,4β*NC*,6α,7β)-*form*

$C_{16}H_{25}N$ 231.38

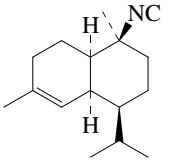
(1α,4β*NC*,6α,7β)-*form*

Isothiocyanate: ***4-Isothiocyanato-9-cadinene****. 4-Isothiocyanato-9-amorphene*
[133738-44-0]
$C_{16}H_{25}NS$ 263.446
Metab. of *Axinyssa fenestratus*. Anthelmintic. Oil. $[\alpha]_D$ +111.7 (c, 2.5 in $CHCl_3$). Has -NCS replacing -NC.

(1β,4α*NC*,6β,7α)-*form*

4-Isocyano-9-amorphene
[138949-84-5]
Constit. of *Phyllidia pustulosa*.
Oil. $[\alpha]_D$ -13.7 (c, 0.035 in $CHCl_3$).
Alvi, K.A. *et al., J. Nat. Prod.*, 1991, **54**, 71-78 (*isothiocyanate*)
Fusetani, N. *et al., Tet. Lett.*, 1991, **32**, 7291-7294 (*isol, pmr, cmr*)

10-Isocyano-4-cadinene I-141



(1α,6α,7β,10β)-*form*

$C_{16}H_{25}N$ 231.38

(1α,6α,7β,10β)-*form*

Isothiocyanate: (+)-10-Isothiocyanato-10-amorphene
[133813-24-8]
Metab. of *Axinyssa fenestratus* and *Phyllidia pustulosa*. Anthelmintic, antibarnacle agent (larval antisettlement agent and development inhibitor). Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D$ +100.45 (c, 5.47 in CCl_4). Has -NCS in place of -NC.

(1α,6β,7β,10α)-*form* [178963-63-8]
Constit. of *Phyllidia pustulosa*, *Phyllidia varicosa*, *Acanthella cavernosa* and *Phyllidiopsis krempfi*. Barnacle larval settlement and metamorphosis inhibitor. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{23}$ +63.6 (c, 0.6 in $CHCl_3$).

Isothiocyanate: ***10-Isothiocyanato-4-cadinene***
[286465-89-2]
$C_{16}H_{25}NS$ 263.446
Constit. of *Acanthella cavernosa*, *Phyllidiella pustulosa* and *Phakellia carduus*. Oil. $[\alpha]_D$ +3 (c, 0.0015 in CH_2Cl_2). $[\alpha]_D^{22}$ +75.3 (c, 0.16 in $CHCl_3$).

Formamide: ***10-Formamido-4-cadinene***
$C_{16}H_{27}NO$ 249.395
Constit. of *Acanthella cavernosa*.
$[\alpha]_D^{22}$ +8.3 (c, 0.001 in $CHCl_3$). Has -NHCHO replacing -NC.

(1α,6β,7β,10β)-*form*

Isothiocyanate: [697299-15-3]
Constit. of a *Stylissa* sp.
Powder.
Mp 54-56°. $[\alpha]_D^{26}$ +75.7 (c, 2.4 in $CHCl_3$). Has -NCS in place of -NC. λ_{max} 246 (ϵ 1085) (EtOH).

(1β,6α,7α,10β)-*form*

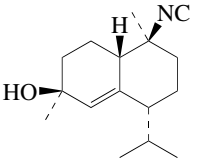
Formamide: [188987-59-9]
$C_{16}H_{27}NO$ 249.395
Isol. from *Acanthella cavernosa*. Antifouling agent. Has -NHCHO replacing -NC.

(1β,6β,7α,10α)-*form*

Isothiocyanate: (-)-10-Isothiocyanato-10-amorphene
[54537-22-3]
Metab. of a *Halichondria* sp.
Oil. $[\alpha]_D$ -63 (CCl_4).

(1β,6β,7β,10α)-*form* [145632-88-8]
Constit. of *Acanthella* cf. *cavernosa*.
$[\alpha]_D$ +101 (c, 0.52 in MeOH).
Burreson, B.J. *et al., Tetrahedron*, 1975, **31**, 2015-2018 (*(-)-10-Isothiocyanato-4-amorphene*)
Alvi, K.A. *et al., J. Nat. Prod.*, 1991, **54**, 71-78 (*(+)-10-Isothiocyanato-4-amorphene*)
Fusetani, N, *et al., Tet. Lett.*, 1992, **33**, 6823-6826 (*10-Isocyano-4-muurolene*)
Okino, T. *et al., Tetrahedron*, 1996, **52**, 9447-9454 (*Phyllidia constits*)
Clark, R.J. *et al., Tetrahedron*, 2000, **56**, 3071-3076 (*Acanthella cavernosa constits*)
Nogata, Y. *et al., Biofouling*, Suppl., 2003, **19**, 193-196 (*formamide*)
Wright, A.D. *et al., Comp. Biochem. Physiol., A: Comp. Physiol.*, 2003, **134**, 307-313 (*Phyllidiella pustulosa constits*)
Mitome, H. *et al., J. Nat. Prod.*, 2004, **67**, 833-837 (*Stylissa constit*)

10-Isocyano-5-cadinen-4-ol I-142

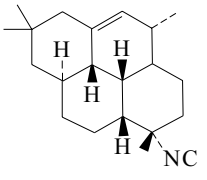


$C_{16}H_{25}NO$ 247.38

(1β,4β,7α,10β)-*form* [217481-02-2]
Constit. of *Phyllidia pustulosa* and *Axinyssa* sp. Antifouling agent. $[\alpha]_D$ +88.8 (c, 0.025 in $CHCl_3$).
Hirota, H. *et al., Tetrahedron*, 1998, **54**, 13971-13980 (*isol, pmr, cmr*)

7-Isocyano-1-cycloamphilectene I-143

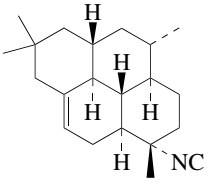
[108695-79-0]



$C_{21}H_{31}N$ 297.483
Constit. of a *Halichondria* sp. Needles (hexane).
Mp 182-183°. $[\alpha]_D$ -14 (c, 0.41 in $CHCl_3$).
Molinski, T.F. *et al., J.O.C.*, 1987, **52**, 3334 (*isol, cryst struct*)

7-Isocyano-10-cycloamphilectene I-144

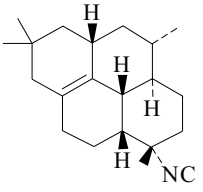
[175861-82-2]



$C_{21}H_{31}N$ 297.483
Constit. of *Cymbastela hooperi*. Shows antimalarial props. Cryst. (hexane).
Mp 134.4-135.3°. $[\alpha]_D^{25}$ +80.4 (c, 0.53 in $CHCl_3$). Genus name given as Cymbastella.
König, G.K. *et al., J.O.C.*, 1996, **61**, 3259-3267 (*isol, pmr, cmr*)

7-Isocyano-11-cycloamphilectene I-145

[108695-80-3]



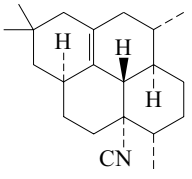
$C_{21}H_{31}N$ 297.483
Constit. of a *Halichondria* sp. and *Cymbastela hooperi*. Prisms (hexane).
Mp 134°. $[\alpha]_D^{25}$ +17 (c, 1.9 in $CHCl_3$).

7-Formamide: ***7-Formamido-11-cycloamphilectene***
[459412-05-6]
$C_{21}H_{33}NO$ 315.498
Constit. of an *Axinella* sponge. Cryst. $[\alpha]_D^{20}$ +36.8 (c, 0.4 in $CHCl_3$). Has -NHCHO replacing -NC.

Molinski, T.F. *et al., J.O.C.*, 1987, **52**, 3334 (*isol, cryst struct*)
Konig, G.K. *et al., J.O.C.*, 1996, **61**, 3529 (*isol, pmr, cmr*)
Ciasullo, L. *et al., J. Nat. Prod.*, 2002, **65**, 1210-1212 (*formamide, isol, cryst struct*)

8-Isocyano-1(12)-cycloamphilectene I-146

[108695-82-5]

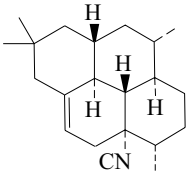


$C_{21}H_{31}N$ 297.483
Struct. revised in 1987. Constit. of *Adocia* spp. and a *Halichondria* sp. Gum. Poorly sol. hexane. $[\alpha]_D^{20}$ +39.6 (c, 0.6 in $CHCl_3$).

Kaslauskas, R. *et al., Tet. Lett.*, 1980, 315 (*isol*)
Molinski, T.F. *et al., J.O.C.*, 1987, **52**, 3334 (*isol, cryst struct*)

8-Isocyano-10-cycloamphilectene I-147

[74799-59-0]



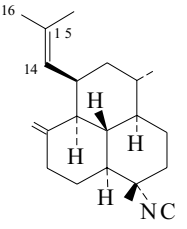
Relative configuration

$C_{21}H_{31}N$ 297.483
Constit. of *Adocia* spp. Cryst. Poorly sol. hexane.
Mp 88-89°. $[\alpha]_D^{20}$ -21.7 (c, 2.0 in $CHCl_3$).

Kaslauskas, R. *et al., Tet. Lett.*, 1980, 315 (*cryst struct*)

7-Isocyano-11(20),14-epiamphilectadiene I-148

[74799-60-3]



$C_{21}H_{31}N$ 297.483
Constit. of *Adocia* spp. and *Cymbastela hooperi*. Cryst.
Mp 113-115°. $[\alpha]_D^{20}$ +116.8 (c, 1.0 in $CHCl_3$).

14,15-Dihydro, 15-isocyano: ***7,15-Diisocyano-11(20)-epiamphilectene***
[74799-58-9]
$C_{22}H_{32}N_2$ 324.508
Constit. of *Adocia* spp. Oil. Poorly sol. hexane. $[\alpha]_D^{20}$ +3.6 (c, 1.6 in $CHCl_3$).

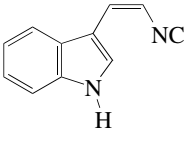
Δ^{11}-Isomer: ***7-Isocyano-11,14-epiamphilectadiene***
[175861-86-6]
$C_{21}H_{31}N$ 297.483
Isol. from *Cymbastela hooperi*. Antimalarial agent. Cryst. (hexane).
Mp 106.6-108.3°. $[\alpha]_D^{25}$ -55.9 (c, 0.9 in $CHCl_3$).

Δ^{15}-Isomer: ***7-Isocyano-11(20),15-epiamphilectadiene***
[74799-56-7]
$C_{21}H_{31}N$ 297.483
Constit. of *Adocia* spp. Poorly sol. hexane.

Kazlauskas, R. *et al., Tet. Lett.*, 1980, 315-318 (*Adocia constits, cryst struct*)
König, G.K. *et al., J.O.C.*, 1996, **61**, 3259-3267 (*Cymbastela hooperi constit*)

3-(2-Isocyanoethenyl)-1*H*-indole, 9CI I-149

2-(3-Indolyl)vinyl isocyanide. Indoleacryloisonitrile. B 371. Antibiotic B 371. SF 2636. Antibiotic SF 2636

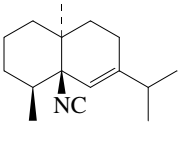


$C_{11}H_8N_2$ 168.198
The struct. given in the 1990 CAS abstract is prob. incorrect.

(Z)-form [61168-06-7]
Isol. from an unidentified *Pseudomonas* sp. and from the marine *Streptomyces* sp. SF2636. Shows antibiotic activity against *Staphylococcus* and other bacteria and yeasts. Probable biosynth. precursor to various cyanobacterial indole alkaloids. Extremely unstable, storeable only in soln. for a short period. λ_{max} 273 (sh) (ε); 279 (ε); 288 (ε) (MeOH/HCl) (Derep). λ_{max} 275 (sh) (ε); 313 (ε) (MeOH) (Derep).

Evans, J.R. *et al., J. Antibiot.*, 1976, **29**, 850-852 (*isol*)
Hoppe, I. *et al., Annalen*, 1984, 600-607 (*synth, ir, pmr, ms*)
Hatsu, M. *et al., CA*, 1990, **113**, 112056f (*isol*)
Stratmann, K. *et al., J.A.C.S.*, 1994, **116**, 9935-9942 (*biochem*)

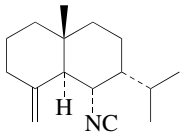
5-Isocyano-6-eudesmene I-150



$C_{16}H_{25}N$ 231.38

(4β,5β,10α)-*form* [786703-09-1]
Constit. of *Phyllidiella pustulosa*.
Oil. $[\alpha]_D$ +23 (c, 2 in $CHCl_3$).
Manzo, E. *et al., J. Nat. Prod.*, 2004, **67**, 1701-1704 (*isol, pmr, cmr*)

6-Isocyano-4(15)-eudesmene I-151



(5α,6α,7α,10β)-*form*

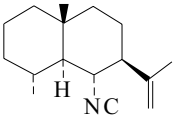
$C_{16}H_{25}N$ 231.38

(5α,6α,7α,10β)-*form* [91466-62-5]
Isol. from *Axinella cannabina*.
Oil. $[\alpha]_D$ +39.6 (c, 0.3 in $CHCl_3$).
Isothiocyanate: [91466-63-6]
$C_{16}H_{25}NS$ 263.446
Isol. from *Axinella cannabina*. Oil. $[\alpha]_D$ +41 (c, 0.35 in $CHCl_3$).
Formamide: [91466-64-7]
$C_{16}H_{27}NO$ 249.395
Isol. from *Axinella cannabina*. Oil. $[\alpha]_D$ +48.5 (c, 0.3 in $CHCl_3$).

(5α,6α,7β,10α)-*form*
Constit. of *Axinella cannabina* and *Acanthella acuta*.
Cryst. or oil.
Mp 78-79°. $[\alpha]_D$ +92.9 (c, 1.8 in $CHCl_3$). Incorr. config. assigned in CAS.
Isothiocyanate: ***6-Isothiocyanato-4(15)-eudesmene***
$C_{16}H_{25}NS$ 263.446
Constit. of *Acanthella acuta* and *Axinella cannabina*.
Mp 52-53°. $[\alpha]_D$ +88.4 (c, 1.0 in $CHCl_3$). Has -NCS replacing -NC. Incorr. config. assigned in CAS.
Formamide: ***6-Formamido-4(15)-eudesmene***
$C_{16}H_{27}NO$ 249.395
Constit. of *Axinella cannabina*. Oil. Has -NHCHO replacing -NC. Incorr. config. assigned in CAS.

(5α,6α,7β,10β)-*form*
Halichonadin C
[847605-78-1]
Constit. of a *Halichondria* sp.
Amorph. solid. $[\alpha]_D^{19}$ -130 (c, 1 in $CHCl_3$).
Isothiocyanate: ***Acanthene B***
$C_{16}H_{25}NS$ 263.446
Constit. of an *Acanthella* sp. Solid. $[\alpha]_D$ -34 (c, 0.18 in $CHCl_3$). Incorr. config. assigned in CAS.
Formamide: ***Acanthene C***
$C_{16}H_{27}NO$ 249.395
Constit. of *Cadlina luteomarginata* which feed on *Acanthella* sp.
Amorph. solid. Incorr. config. assigned in CAS.
Ciminiello, P. *et al., J.O.C.*, 1984, **49**, 3949-3951 (*5α,6α,7α,10β-form Axinella cannabina constits*)
Ciminiello, P. *et al., J. Nat. Prod.*, 1987, **50**, 217-220 (*5α,6α,7β,10α-form Axinella and Acanthella constits*)
Burgoyne, D.L. *et al., Tetrahedron*, 1993, **49**, 4503-4510 (*Acanthenes B,C*)
Ishiyama, H. *et al., Tetrahedron*, 2005, **61**, 1101-1105 (*Halichonadin C*)

6-Isocyano-11-eudesmene I-152

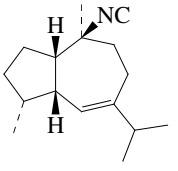


$C_{16}H_{25}N$ 231.38

(4α,5α,6α,10β)-*form*
Acanthellin 1
[54462-52-1]
Constit. of sponges *Acanthella acuta* and *Axinella cannabina*.
Oil. Sol. MeOH, Et_2O, CCl_4; poorly sol. H_2O. $[\alpha]_D$ -41.2 (c, 5 in $CHCl_3$).
Isothiocyanate: ***6-Isothiocyanato-11-eudesmene***
[91466-60-3]
$C_{16}H_{25}NS$ 263.446
Isol. from sponge *Axinella cannabina*.
$[\alpha]_D$ -24.4. Has -NCS in place of -NC.
Formamide: ***6-Formamido-11-eudesmene***
[91466-61-4]
$C_{16}H_{27}NO$ 249.395
Isol. from *Axinella cannabina*. Oil. $[\alpha]_D$ -24. Has -NHCHO in place of -NC.
Minale, L. *et al., Tetrahedron*, 1974, **30**, 1341
Ciminiello, P. *et al., J.O.C.*, 1984, **49**, 3949-3951 (*isol, isothiocyanate, formamide*)

10-Isocyano-6-guaiene I-153

6-Guaiene-10-isocyanate



(1β,4α,5β,10β)-*form*

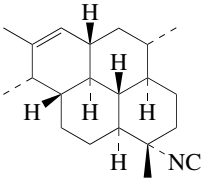
$C_{16}H_{25}N$ 231.38

(1β,4α,5β,10β)-*form* [114944-03-5]
Constit. of an unidentified sponge.
Cryst.
Mp 57-59°. $[\alpha]_D$ -60.1 (c, 0.4 in $CHCl_3$).
10-Isothiocyanate: ***10-Isothiocyanato-6-guaiene***
[120574-26-7]
$C_{16}H_{25}NS$ 263.446
Constit. of *Trachyopsis aplysinoides*. Oil. $[\alpha]_D$ -33.9 (c, 0.28 in $CHCl_3$). Has –NCS replacing –NC.

(1β,4β,5α,10β)-*form* [786704-42-5]
Constit. of *Phyllidiella pustulosa*.
Oil. $[\alpha]_D$ +28.6 (c, 0.06 in $CHCl_3$).
Tada, H. *et al., J.O.C.*, 1988, **53**, 3366-3368 (*isol, pmr, cryst struct*)
He, H. *et al., J.O.C.*, 1989, **54**, 2511-2514 (*isothiocyanate*)
Kikuchi, J. *et al., Chem. Lett.*, 1994, 1701 (*synth*)
Manzo, E. *et al., J. Nat. Prod.*, 2004, **67**, 1701-1704 (*Phyllidiella pustulosa constit*)

7-Isocyano-14-isocycloamphilectene I-154

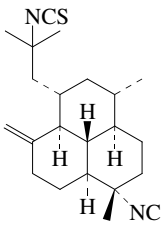
[175861-81-1]



$C_{21}H_{31}N$ 297.483
Constit. of *Cymbastela hooperi*. Shows antimalarial props. Cryst. (hexane).
Mp 124.3-125.6°. $[\alpha]_D^{25}$ +4.9 (c, 0.53 in $CHCl_3$). Genus name given as Cymbastella.
König, G.K. *et al., J.O.C.*, 1996, **61**, 3259-3267 (*isol, pmr, cmr*)

7-Isocyano-15-isothiocyanato-11(20)-amphilectene **I-155**

[175861-85-5]



Absolute Configuration

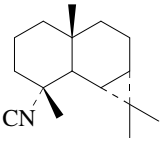
$C_{22}H_{32}N_2S$ 356.574
Constit. of *Cymbastela hooperi*. Cryst. (hexane).
Mp 102.8-103.7°. $[\alpha]_D^{25}$ +1.5 (c, 0.55 in $CHCl_3$). Genus name given as Cymbastella. λ_{max} 247 (ϵ 1520) (MeOH).

8-Epimer: [251108-42-6]
$C_{22}H_{32}N_2S$ 356.574
Constit. of a *Cribrochalina* sp. Solid. $[\alpha]_D$ +42.9 (c, 0.5 in $CHCl_3$). Struct. revised in 2005.

Koenig, G.K. *et al., J.O.C.*, 1996, **61**, 3259-3267 (*isol, pmr, cmr*)
Ciavatta, M.L. *et al., Tetrahedron*, 1999, **55**, 12629-12636; 2005, **61**, 8049-8053 (*8-epimer*)

4-Isocyanomaaliane **I-156**

[133109-45-2]

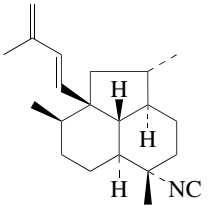


$C_{16}H_{25}N$ 231.38
Isol. from the mollusc *Cadlina luteomarginata*.
$[\alpha]_D$ +36 (c, 0.2 in $CHCl_3$).

Thompson, J.E. *et al., Tetrahedron*, 1982, **38**, 1865 (*isol, pmr, cmr, ms*)
Burgoyne, D.L. *et al., Tetrahedron*, 1993, **49**, 4503-4510 (*isol*)

7-Isocyano-1(14),15-neoamphilectadiene **I-157**

[175861-88-8]

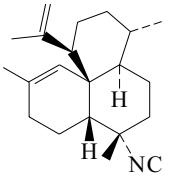


$C_{21}H_{31}N$ 297.483
Constit. of *Cymbastela hooperi*. Shows antimalarial props. Oil.
$[\alpha]_D^{25}$ +67 (c, 0.79 in $CHCl_3$). Genus name given as Cymbastella.
λ_{max} 230 (ϵ 7900) (MeOH).

König, G.K. *et al., J.O.C.*, 1996, **61**, 3259-3267 (*isol, pmr, cmr*)

7-Isocyano-11,15-neoamphilectadiene **I-158**

[141672-07-3]

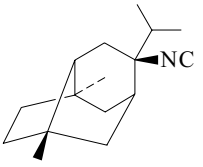


$C_{21}H_{31}N$ 297.483
Constit. of an Adocidae sponge. Cryst.
Mp 109-110°. $[\alpha]_D$ +31.8 (c, 2.3 in $CHCl_3$).

Sharma, H.A. *et al., Tet. Lett.*, 1992, **33**, 1593-1596 (*isol, pmr, cmr, cryst struct*)

9-Isocyanoneopupukeanane **I-159**

[119323-93-2]

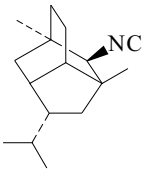


$C_{16}H_{25}N$ 231.38
Constit. of a *Ciocalypta* sp. Oil. $[\alpha]_D$ +33 (c, 1 in $CHCl_3$).

Karuso, P. *et al., J.O.C.*, 1989, **54**, 2092-2095; 2095-2097 (*isol, pmr, cmr, biosynth*)
Ho, T.-L. *et al., J.O.C.*, 1999, **64**, 8965-8967 (*synth*)
Krishna, A. *et al., Tetrahedron*, 2005, **61**, 8855-8859 (*synth*)

2-Isocyanopupukeanane **I-160**

[73069-50-8]



Absolute configuration

$C_{16}H_{25}N$ 231.38
Secreted by the nudibranch *Phyllidia varicosa* and from a sponge *Hymeniacidon* sp. Ichthyotoxin. Cryst. (MeOH aq.).
Mp 81-82°.

Isothiocyanate: ***2-Isothiocyanatopupukeanane***
[89398-13-0]
$C_{16}H_{25}NS$ 263.446
Constit. of *Phyllidia varicosa*. Has -NCS replacing -NC.

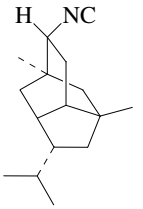
Formamide: ***2-Formamidopupukeanane***
[89398-14-1]
$C_{16}H_{27}NO$ 249.395
Constit. of *Phyllidia varicosa*. Has -NHCHO replacing -NC.

[72715-04-9, 72748-63-1]

Hagadone, M.R. *et al., Helv. Chim. Acta*, 1979, **62**, 2484-2494 (*cryst struct, abs config*)
Corey, E.J. *et al., Tet. Lett.*, 1979, **20**, 2745-2748 (*synth*)
Fráter, G. *et al., Helv. Chim. Acta*, 1984, **67**, 1702 (*synth*)
Hagadone, M.R. *et al., J.A.C.S.*, 1984, **106**, 2447-2448 (*isothiocyanate, formamide, biosynth*)
Kaliappan, K. *et al., Tet. Lett.*, 1997, **38**, 2185-2186 (*synth*)

9-Isocyanopupukeanane **I-161**

[57462-28-9]



Absolute Configuration

$C_{16}H_{25}N$ 231.38
Constit. of the secretions of molluscs *Phyllidia varicosa*, *Phyllidia bourguini*, *Phyllidia pustulosa* and isol. from sponges *Hymeniacidon*, *Ciocalypta* and *Axinyssa* sp. Ichthyotoxin; antimalarial agent. Oil. Sol. EtOH, CH_2Cl_2, $CHCl_3$, CCl_4; poorly sol. H_2O, hexane.

Isothiocyanate: ***9-Isothiocyanatopupukeanane***
[631914-44-8]
$C_{16}H_{25}NS$ 263.446
Isol. from an *Axinyssa aculeata* and *Phyllidia varicosa*.
$[\alpha]_D$ -68 (c, 0.35 in $CHCl_3$). Has -NCS replacing -NC.

9-Epimer: ***9-Epi-9-isocyanopupukeanane***
[131565-76-9]
$C_{16}H_{25}N$ 231.38
Constit. of *Phyllidia bourguini* and *Phyllidia pustulosa*. Shows ichthyotoxic and antifungal props. Oil. $[\alpha]_D$ +31 (c, 0.048 in $CHCl_3$).

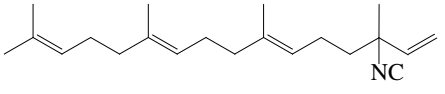
9-Epimer, isothiocyanate: [631914-45-9]
$C_{16}H_{25}NS$ 263.446
Constit. of *Phyllidia varicosa*, *Phyllidia pustulosa* and *Axinyssa aculeata*.

[70329-80-5]

Burreson, B.J. *et al., J.A.C.S.*, 1975, **97**, 4763-4764 (*isol*)
Hagadone, M.R. *et al., Helv. Chim. Acta*, 1979, **62**, 2484-2495 (*9-epimer, isothiocyanate*)
Corey, E.J. *et al., J.A.C.S.*, 1979, **101**, 1608-1609 (*synth*)
Yamamoto, H. *et al., J.A.C.S.*, 1979, **101**, 1609-1611 (*synth*)
Piers, E. *et al., Annalen*, 1982, 973-984 (*synth*)
Fusetani, N. *et al., Tet. Lett.*, 1990, **31**, 5623-5624; 1991, **32**, 7291-7294 (*isol, epimer*)
Simpson, J.S. *et al., Aust. J. Chem.*, 1997, **50**, 1123-1127 (*isothiocyanate*)
Simpson, J.S. *et al., Tet. Lett.*, 2001, **42**, 4267-4269 (*biosynth*)
Yasman, *et al., J. Nat. Prod.*, 2003, **66**, 1512-1514 (*isol, pmr, cmr*)

3-Isocyano-3,7,11,15-tetramethyl-1,6,10,14-hexadecatetraene, 9CI I-162

[55784-75-3]
[154614-35-4]



$C_{21}H_{33}N$ 299.498

(6*E*,10*E*)-(+)-*form*
Geranyllinaloyl isocyanide
[57766-63-9]
Isol. from *Halichondria* sp.
Oil. $[\alpha]_D$ +15 (c, 2.8 in CCl_4).

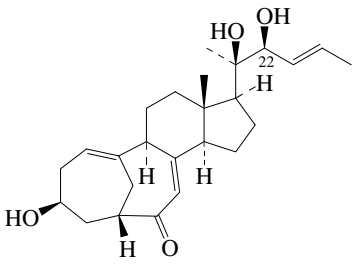
Isothiocyanate: Geranyllinaloyl isothiocyanate
$C_{21}H_{33}NS$ 331.564
Present in a *Halichondria* sp. sponge. Has -NCS in place of -NC.

Formamide: Geranyllinaloyl formamide
$C_{21}H_{35}NO$ 317.514
Present in a *Halichondria* sp. sponge. Has -NHCHO replacing -NC.

Burreson, B.J. *et al., Tetrahedron*, 1975, **31**, 2015-2018 (*isol, ir, pmr, cmr*)
Ichikawa, Y. *et al., J.C.S. Perkin 1*, 1993, 2429-2432 (*synth, ir, pmr, cmr*)

Isocyclocitrinol A I-163

[636599-88-7]



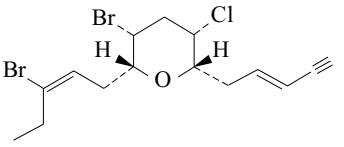
$C_{25}H_{36}O_4$ 400.557
Metab. of sponge-derived *Penicillium citrinum*.

22-Ac: ***22-Acetylisocyclocitrinol A***
[636596-94-6]
$C_{27}H_{38}O_5$ 442.594
Metab. of *Penicillium citrinum*.

Amagata, T. *et al., Org. Lett.*, 2003, **5**, 4393-4396 (*isol, pmr, cmr, cryst struct*)

Isodactylyne I-164

*3-Bromo-2-(3-bromo-2-pentenyl)-5-chlorotetrahydro-6-(2-penten-4-ynyl)-2*H*-pyran, 9CI. 9,13-Dibromo-7-chloro-6,10-epoxy-3,12-pentadecadien-1-yne*
[58001-90-4]

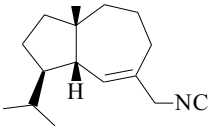


$C_{15}H_{19}Br_2ClO$ 410.575
Constit. of the sea hare *Aplysia dactylomela*. Shows antibiotic props. Oil. $[\alpha]_D^{24}$ -8.06 (c, 7.97 in $CHCl_3$). λ_{max} 223 (ϵ 12000) (isooctane) (Derep).

Vanderah, D.J. *et al., J.O.C.*, 1976, **41**, 3480 (*isol, ir, uv, ms, nmr, struct*)
Gao, L.-X. *et al., Heterocycles*, 1996, **42**, 745 (*synth, ir, pmr*)

6-Isodaucene 14-isonitrile I-165

[112767-02-9]



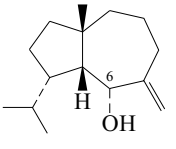
$C_{16}H_{25}N$ 231.38
Metab. of marine sponge *Acanthella acuta*. Oil. $[\alpha]_D$ +44 (c, 1.0 in $CHCl_3$).

Isothiocyanate: ***6-Isodaucene 14-isothiocyanate***
[112757-35-4]
$C_{16}H_{25}NS$ 263.446
Metab. of *Acanthella acuta*. Oil. $[\alpha]_D$ +36.2 (c, 0.2 in $CHCl_2$). Has -NCS replacing -NC.

Mayol, L. *et al., Tetrahedron*, 1987, **43**, 5381

7(14)-Isodaucen-6-ol I-166

Millecrol A
[154512-21-7]



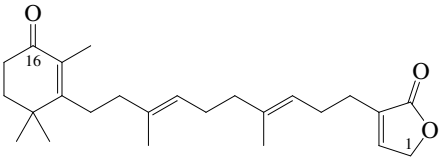
$C_{15}H_{26}O$ 222.37
Constit. of *Leminda millecra*. Oil.

6-Ketone: 7(14)-Isodaucen-6-one. ***Millecrone A***
[154512-19-3]
$C_{15}H_{24}O$ 220.354
Constit. of *Leminda millecra*. Oil. λ_{max} 223 (ϵ 3500) (MeOH) (Berdy).

Pika, J. *et al., Tetrahedron*, 1994, **50**, 3065-3070 (*isol, pmr, cmr*)

Isodehydroluffariellolide I-167

[132911-45-6]



$C_{25}H_{36}O_3$ 384.558

Constit. of *Fascaplysinopsis reticulata*. Oil. λ_{max} 249 (ϵ 28224); 334 (ϵ 5069); 406 (ϵ 1920) (MeOH).

16-Deoxo: ***3-[4,8-Dimethyl-10-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3,7-decadienyl]-2(5H)-furanone***

[283167-43-1]

$C_{25}H_{38}O_2$ 370.574

Constit. of *Hyrtios* cf. *erecta*. Yellow oil.

1-Ethoxy, 16-deoxo: [283167-44-2]

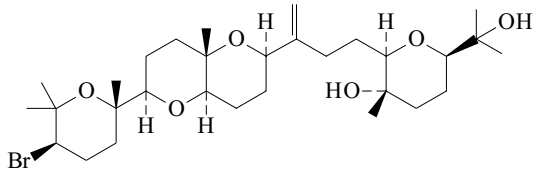
$C_{27}H_{42}O_3$ 414.627

Constit. of *Hyrtios* cf. *erecta*. Yellow oil.

Jimènez, C. *et al., J.O.C.*, 1991, **56**, 3403-3410 (*Isodehydroluffariellolide*)
Kirsch, G. *et al., J. Nat. Prod.*, 2000, **63**, 825-829 (*deoxo derivs*)

Isodehydrothyrsiferol I-168

[176447-96-4]



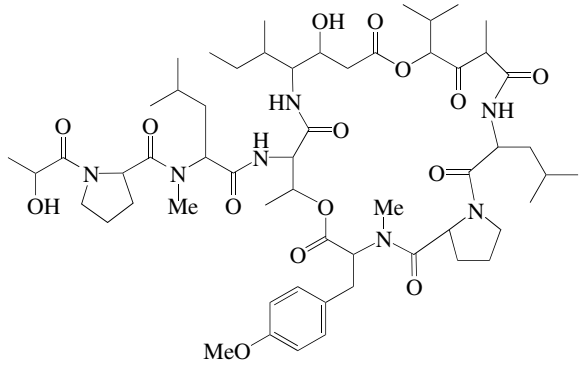
$C_{30}H_{51}BrO_6$ 587.633

Constit. of *Laurencia viridis*. Oil. $[\alpha]_D^{25}$ +6.5 (c, 0.23 in $CHCl_3$).

Norte, M. *et al., Tet. Lett.*, 1996, **37**, 2671 (*isol, pmr, cmr*)

Isodidemnin 1 I-169

[114607-50-0]



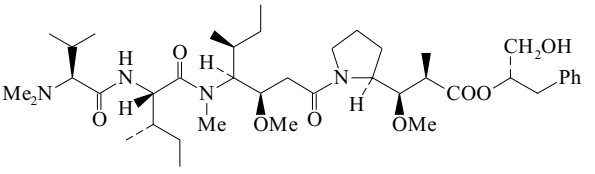
$C_{57}H_{89}N_7O_{15}$ 1112.368

Depsipeptide antibiotic. Isol. from the tunicate *Tridemnum cyanophorum*. Cytotoxic agent.
Mp 163-165°. $[\alpha]_D$ +93 ($CHCl_3$).

Guyot, M. *et al., C. R. Hebd. Seances Acad. Sci. Ser. 2*, 1987, **305**, 681-686 (*isol, pmr, ms*)

Isodolastatin H I-170

[173327-17-8]



$C_{41}H_{70}N_4O_8$ 747.026

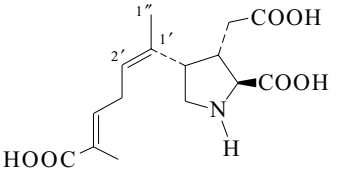
Peptide antibiotic. Isomer of Dolastatin H, D-1220. Isol. from the sea hare *Dolabella auricularia*. Cytotoxic agent. Powder.
$[\alpha]_D^{25}$ -47 (c, 0.04 in MeOH). λ_{max} 208 (ϵ 23000) (MeOH).

Sone, H. *et al., J.A.C.S.*, 1996, **118**, 1874 (*isol, uv, ir, pmr, cmr*)

Isodomoic acid A I-171

2-Carboxy-4-(5-carboxy-1-methyl-1,4-hexadienyl)-3-pyrrolidineacetic acid, 9CI

[101899-44-9]



$C_{15}H_{21}NO_6$ 311.334

Isol. from the red alga *Chondria armata* and the diatom *Nitzschia navis-varingica*. Anthelminthic; exhibits insecticidal activity. Sol. MeOH.
Mp 185-187° dec. $[\alpha]_D^{25}$ -70 (c, 0.1 in H_2O).

*1′*E*-Isomer:* ***Isodomoic acid B***

[101977-25-7]

$C_{15}H_{21}NO_6$ 311.334

Isol. from *Chondria armata* and *Nitzschia navis-varingica*. Anthelminthic; insecticide; vermifuge. Sol. H_2O, MeOH.
Mp 182-183° dec. $[\alpha]_D^{25}$ -8.1 (c, 0.14 in H_2O). λ_{max} 214 (ϵ 9850) (H_2O) (Berdy).

$\Delta^{1',1''}$-Isomer: ***Isodomoic acid C***

[101899-45-0]

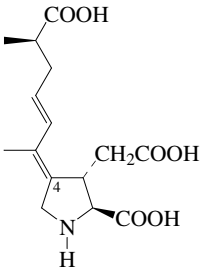
$C_{15}H_{21}NO_6$ 311.334

Isol. from *Chondria armata* and *Pseudo-nitzschia australis*. Insecticide. Sol. MeOH, H_2O.
Mp 257-260° dec. $[\alpha]_D^{25}$ -30 (c, 0.015 in H_2O). λ_{max} 213 (ϵ 5030) (MeOH) (Berdy).

Maeda, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4892 (*isol, uv, ir, pmr, cmr, ms*)
Holland, P.T. *et al., Chem. Res. Toxicol.*, 2005, **18**, 814-816 (*Isodomoic acid C, isol*)
Clayden, J. *et al., J.A.C.S.*, 2005, **127**, 2412-2413 (*Isodomoic acid C, synth*)
Clayden, J. *et al., Tetrahedron*, 2005, **61**, 5713-5724 (*rev*)
Kotaki, Y. *et al., Toxicon*, 2005, **46**, 946-953 (*isol*)

Isodomoic acid G I-172

2-Carboxy-4-(5-carboxy-1-methyl-2-hexenylidene)-3-pyrrolidineacetic acid
[188346-81-8]



Absolute Configuration

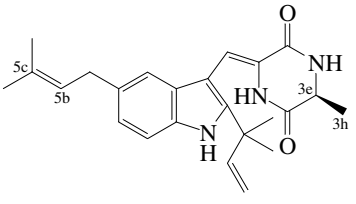
$C_{15}H_{21}NO_6$ 311.334
Isol. from the red alga *Chondria armata*.

4Z-Isomer: ***Isodomoic acid H***
[188346-82-9]
$C_{15}H_{21}NO_6$ 311.334
Isol. from *Chondria armata*.

Zaman, L. *et al., Toxicon*, 1997, **35**, 205-212 (*isol, pmr*)
Ni, Y. *et al., Org. Lett.*, 2003, **5**, 3771-3773 (*synth, abs config*)

Isoechinulin A I-173

*3-[[2-(1,1-Dimethyl-2-propenyl)-5-(3-methyl-2-butenyl)-1*H*-indol-3-yl]methylene]-6-methyl-2,5-piperazinedione, 9CI*
[60422-87-9]



$C_{24}H_{29}N_3O_2$ 391.512
Isol. from *Aspergillus ruber*. Mycotoxin.

*3*e,*3*h-*Didehydro:* ***Isoechinulin B***
[60422-88-0]
$C_{24}H_{27}N_3O_2$ 389.496
Isol. from *Aspergillus ruber*. Mycotoxin.

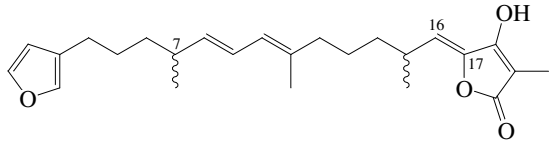
*5*b,*5*c-*Epoxide, 3*e,*3*h-*didehydro:* ***Isoechinulin C***
[60422-89-1]
$C_{24}H_{27}N_3O_3$ 405.496
Isol. from *Aspergillus ruber*.

*5*b,*5*c-*Dihydro, 5*bR,*5*c-*dihydroxy:* ***19,20-Dihydroxyisoechinulin A***
[744253-48-3]
$C_{24}H_{31}N_3O_4$ 425.527
Prod. by a marine *Aspergillus* sp. Oil. λ_{max} 209 (log ϵ 3.9); 226 (log ϵ 3.9); 289 (log ϵ 3.4); 340 (log ϵ 3.5) (MeOH).

Nagasawa, H. *et al., Tet. Lett.*, 1976, 1601-1604 (*isol, uv, ir, pmr, ms*)
Nagasawa, H. *et al., Agric. Biol. Chem.*, 1979, **43**, 1759-1763 (*cmr, struct*)
Li, Y. *et al., J. Antibiot.*, 2004, **57**, 337-340 (*Dihydroxyisoechinulin A*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 475; 476; 477

Isofasciculatin I-174

[94936-00-2]



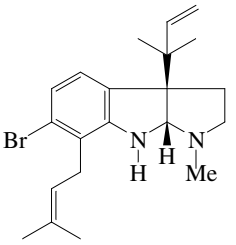
$C_{25}H_{34}O_4$ 398.541
Isol. from the sponge, *Cacospongia scalaris*. Inhibitor of fertilised starfish egg division. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ -34.7 (as acetate). λ_{max} 265 (EtOH) (Berdy).

*16,17ξ-Dihydro: 5-[13-(3-Furanyl)-2,6,10-trimethyl-6,8-tridecadienyl]-4-hydroxy-3-methyl-2(5*H*)-furanone*
[113994-72-2]
$C_{25}H_{36}O_4$ 400.557
Constit. of an *Ircinia* sp. Oil. Sol. MeOH, C_6H_6; poorly sol. hexane. $[\alpha]_D$ +41 (c, 3.7 in $CHCl_3$). Assigned 7*S*-config.

Fusetani, N. *et al., Tet. Lett.*, 1984, **25**, 4941-4942 (*Isofasciculatin*)
Capon, R.J. *et al., Aust. J. Chem.*, 1987, **40**, 1327-1330 (*Ircinia constit*)

Isoflustramine D I-175

[104387-14-6]



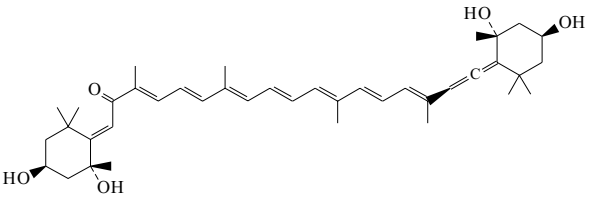
Relative Configuration

$C_{21}H_{29}BrN_2$ 389.377
Isol. as a 65:35 inseparable mixt. with Flustramine D, F-58. Metab. from the marine bryozoan *Flustra foliacea*.
$[\alpha]_D^{25}$ -14.6 (c, 0.07 in CH_2Cl_2). λ_{max} 240; 290 (MeOH) (Berdy).

Laycock, M.V. *et al., Can. J. Chem.*, 1986, **64**, 1312-1316 (*isol, uv, ir, pmr, ms, struct*)

Isofucoxanthinol I-176

6,6′,7,7′-Tetradehydro-4′,5,5′,6,7,8-hexahydro-3,3′,5,5′-tetrahydroxy-β,ϵ-caroten-8-one
[7176-05-8]



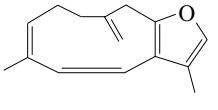
$C_{40}H_{56}O_5$ 616.879
Isol. from *Fucus vesiculosus*. Dark red needles (Me_2CO/petrol). Mp 207-209°. Poss. artifact; alkali rearrangement product of, 3′-Ac. λ_{max} 450 nm (Me_2CO).

3′-Ac: ***Isofucoxanthin***
[7218-76-0]
$C_{42}H_{58}O_6$ 658.917
Constit. of *Fucus vesiculosus* and *Styela clava*. Dark red needles (Me_2CO/petrol).
Mp 146-148°. Poss. artifact; known rearrangement product of Fucoxanthin (see Fucoxanthinol, F-116). λ_{max} 449 nm (Me_2CO).

Jensen, A. *et al., Acta Chem. Scand.*, 1966, **20**, 1728
Bonnett, R. *et al., J.C.S.(C)*, 1969, 429
Ookubo, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **81**, 137 (*occur*)
Haugan, J.A. *et al., Acta Chem. Scand.*, 1992, **46**, 614 (*props*)

Isofuranotriene I-177

8,12-Epoxy-3,5,7,10(14),11-germacrapentaene



$C_{15}H_{18}O$ 214.307

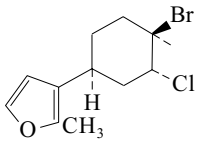
This struct. was prev. assigned to Furanotriene, F-140. Constit. of sea plume *Pseudopterogorgia americana*. Yellow oil.

Chan, W.R. *et al., Tetrahedron*, 1990, **46**, 1499-1502 (*isol, struct*)

Isofurocaespitane I-178

3-(4-Bromo-3-chloro-4-methylcyclohexyl)-2-methylfuran

[73436-45-0]



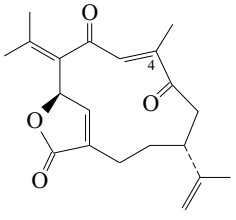
$C_{12}H_{16}BrClO$ 291.614

Constit. of *Laurencia caespitosa*. Oil. $[\alpha]_D$ -39.

González, A.G. *et al., Tet. Lett.*, 1979, 2719

Isogersemolide A I-179

[118025-69-7]



$C_{20}H_{24}O_4$ 328.407

Metab. of *Gersemia rubiformis*. Needles (MeOH).

Mp 121-124°. $[\alpha]_D^{25}$ -225 (c, 0.37 in CH_2Cl_2). λ_{max} 205 (ϵ 4700); 242 (sh) (ϵ) (MeOH) (Derep).

4Z-Isomer: ***Isogersemolide B***

[118101-23-8]

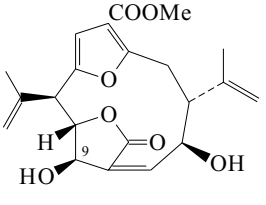
$C_{20}H_{24}O_4$ 328.407

Metab. of *Gersemia rubiformis*. Needles (Et_2O/MeOH). $[\alpha]_D^{25}$ -27 (C, 0.02 in CH_2Cl_2). λ_{max} 218 (ϵ 3050); 237 (sh) (ϵ) (MeOH) (Derep).

Williams, D.E. *et al., Can. J. Chem.*, 1988, **66**, 2928 (*isol, pmr, cmr*)

Isogorgiacerodiol I-180

[138828-01-0]



$C_{21}H_{24}O_7$ 388.416

Constit. of *Pseudopterogorgia acerosa*. Cryst.

Mp 174-176°. $[\alpha]_D$ -60.5 (c, 0.09 in $CHCl_3$).

9-Me ether: [83572-91-2]

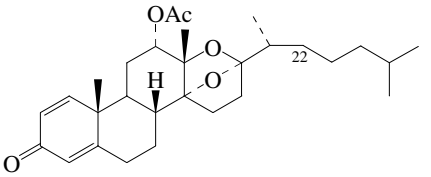
$C_{22}H_{26}O_7$ 402.443

Constit. of *Pseudopterogorgia acerosa*. Gum. $[\alpha]_D$ -116.6 (c, 0.53 in $CHCl_3$).

Tinto, W.F. *et al., Tetrahedron*, 1991, **47**, 8679 (*isol, pmr, cmr*)

Isogosterone A I-181

[194856-36-5]



$C_{29}H_{42}O_5$ 470.648

Constit. of a *Dendronephthya* sp.

$[\alpha]_D^{22}$ +28.3 (c, 0.145 in MeOH). λ_{max} 240 (ϵ 7200) (MeOH).

22ξ-Acetoxy: ***Isogosterone D***

[194856-42-3]

$C_{31}H_{44}O_7$ 528.684

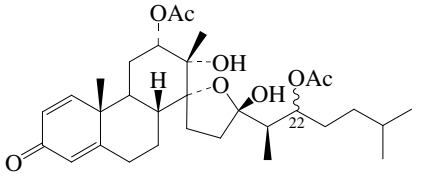
Constit. of a *Dendronephthya* sp.

$[\alpha]_D^{22}$ +34.3 (c, 0.21 in MeOH). λ_{max} 240 (ϵ 8100) (MeOH).

Tomono, Y. *et al., J.O.C.*, 1999, **64**, 2272-2275 (*isol, pmr, cmr*)

Isogosterone C I-182

[194856-40-1]



$C_{31}H_{46}O_8$ 546.7

Constit. of a *Dendronephthya* sp.

$[\alpha]_D^{22}$ +51.4 (c, 0.26 in MeOH). λ_{max} 241 (ϵ 6500) (MeOH).

22-De-Ac, 22-ketone: ***Isogosterone B***

[184173-52-2]

$C_{29}H_{42}O_7$ 502.647

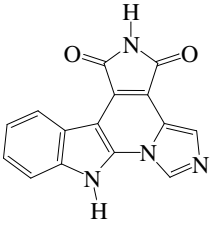
Constit. of a *Dendronephthya* sp.

$[\alpha]_D^{22}$ +60 (c, 0.135 in MeOH). λ_{max} 241 (ϵ 7500) (MeOH).

Tomono, Y. *et al., J.O.C.*, 1999, **64**, 2272-2275 (*isol, pmr, cmr*)

Isogranulatimide I-183

[219829-00-2]



$C_{15}H_8N_4O_2$ 276.254

Alkaloid from the ascidian *Didemnum granulatum*. G2 specific cell cycle checkpoint inhibitor. Deep purple cryst. (MeCN aq.) or amorph. red solid. λ_{max} 210 (ϵ 10230); 231 (ϵ 10650); 280 (ϵ 6550); 470 (ϵ 1880) (MeOH).

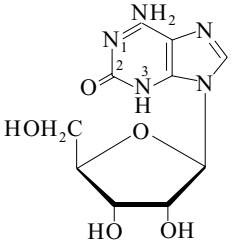
Berlinck, R.G.S. *et al., J.O.C.*, 1998, **63**, 9850-9856 (*isol, uv, ir, pmr, cmr, synth*)

Vervoort, H.C. *et al., J. Nat. Prod.*, 1999, **62**, 389-391 (*isol, uv, ir, pmr, cmr, ms*)

Piers, E. *et al., J.O.C.*, 2000, **65**, 530-535 (*synth*)

Isoguanosine I-184

*6-Amino-9-β-D-ribofuranosyl-9*H*-purin-2(1*H*)-one, 8CI. 9-β-D-Ribofuranosylisoguanine. Crotonoside. 2-Hydroxyadenosine*
[1818-71-9]



$C_{10}H_{13}N_5O_5$ 283.243
Occurs in the seeds of *Croton tiglium*. Also isol. from the nudibranch *Diaulula sandiegensis*. Incorporated into mammalian nucleic acids. Stimulates cyclic AMP incorporation into brain tissue, inhibitor of inosine monophosphate pyrophosphonylase and glutamic acid dehydrogenase. Cryst. (H_2O). Sol. H_2O. Mp 243-245° (237-252°) dec. $[\alpha]_D^{26}$ -71 (c, 1.1 in 0.1*M* NaOH). λ_{max} 235 (ϵ 6140); 283 (ϵ 12700) (0.05*N* HCl) (Derep). λ_{max} 251 (ϵ 6890); 285 (ϵ 10600) (0.05*N* NaOH) (Derep). λ_{max} 247 (ϵ 8930); 293 (ϵ 11100) (H_2O) (Derep).

*6*N-*Me:* [23605-76-7]
$C_{11}H_{15}N_5O_5$ 297.27
Mp 188-190° dec. $[\alpha]_D^{26}$ -63.1 (c, 0.9 in 0.1*M* NaOH).

*6*N-*Et:*
$C_{12}H_{17}N_5O_5$ 311.297
Mp 212° dec. $[\alpha]_D^{26}$ -68.2 (c, 0.97 in 0.1*M* NaOH).

*6*N-*Di-Me:* [24386-79-6]
$C_{12}H_{17}N_5O_5$ 311.297
Mp 184-186° (220°) dec. $[\alpha]_D^{26}$ -52 (c, 0.07 in 0.1*M* NaOH).

1-Me: See Doridosine, D-1235

3-Me: 3-Methylisoguanosine. 2,3-Dihydro-3-methyl-2-oxoadenosine
$C_{11}H_{15}N_5O_5$ 297.27
Needles + $1H_2O$ (H_2O). Mp 175-178° dec. $[\alpha]_D^{17}$ -44 (c, 0.129 in H_2O). pK_a 4.57 (25°).

O^2-*Me:* See 2-Methoxyadenosine, M-174

2′-Deoxy: 2′-Deoxyisoguanosine
[106449-56-3]
$C_{10}H_{13}N_5O_4$ 267.244
Cryst. (EtOH). Mp 230° dec.

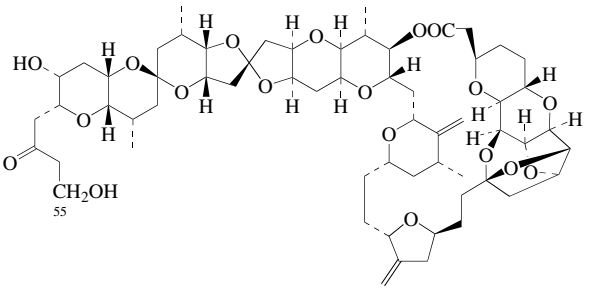
2′-Deoxy, 5′-triphosphate: [150668-64-7]
$C_{10}H_{16}N_5O_{13}P_3$ 507.184
λ_{max} 247; 292 (H_2O).

2′-Deoxy, 3′,5′-di-Ac: [173098-07-2]
$C_{14}H_{17}N_5O_6$ 351.318
Needles (EtOAc). Mp 235-237°.

Cherbuliez, E. *et al., Helv. Chim. Acta*, 1932, **15**, 464; 978 (*isol*)
Spies, J.R. *et al., J.A.C.S.*, 1939, **61**, 350 (*occur*)
Davoll, J. *et al., J.A.C.S.*, 1951, **73**, 3174 (*synth, isol*)
Yamazaki, A. *et al., Chem. Pharm. Bull.*, 1968, **16**, 2172 (*synth*)
South African Pat., 1968, (*Boehringer*)6 707 630; *CA*, **70**, 88212z (*6N-Me*)
Miura, K. *et al., Chem. Pharm. Bull.*, 1975, **23**, 2064 (*synth*)
Sepiol, J. *et al., Z. Naturforsch., C*, 1976, **37**, 361 (*uv*)
Fuhrmann, F.A. *et al., Science (Washington, D.C.)*, 1981, **212**, 557-558 (*isol*)
Nair, V. *et al., J.O.C.*, 1985, **50**, 406 (*synth, pmr*)
Itaya, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2971 (*3-Methylisoguanosine*)
Kazimierczuk, Z. *et al., Helv. Chim. Acta*, 1991, **74**, 1742 (*2′-Deoxyisoguanosine*)
Seela, F. *et al., Helv. Chim. Acta*, 1991, **74**, 1742-1748; 1994, **77**, 622-630; 1995, **78**, 1843-1854 (***synth, uv, pmr, cmr, 2′-Deoxyisoguanosine***)
Divakar, K.J. *et al., J.C.S. Perkin 1*, 1991, 771 (*synth, uv, pmr, cmr*)
Chern, J.-W. *et al., J.O.C.*, 1991, **56**, 4213 (*synth*)
De Napoli, L. *et al., J.C.S. Perkin 1*, 1995, 15 (***synth, bibl***)
Jurczyk, S.C. *et al., Helv. Chim. Acta*, 1999, **82**, 1005-1015 (*2′-Deoxyguanosine 5′-triphosphate*)

Isohomohalichondrin B I-185

[157078-48-3]



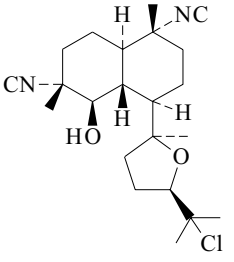
$C_{61}H_{86}O_{19}$ 1123.339
Polyether antibiotic. Isol. from the sponge *Lissodendoryx* sp. Antitumour agent. Amorph. powder. $[\alpha]_D$ -21.6 (c, 1 in MeOH).

55-Me ether: ***55-O-Methylisohomohalichondrin B***
$C_{62}H_{88}O_{19}$ 1137.366
Isol. from *Lissodendoryx* sp. Oil. C-55 is the carbon bearing the terminal primary OH group.

Litaudon, M. *et al., Tet. Lett.*, 1994, **35**, 9435 (*isol, ir, pmr, cmr, ms*)
Litaudon, M. *et al., J.O.C.*, 1997, **62**, 1868 (*Me ether*)

Isokalihinol B I-186

[126622-62-6]

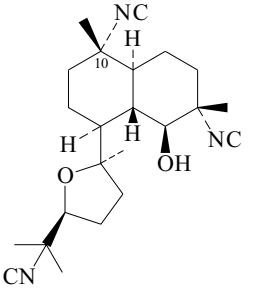


$C_{22}H_{33}ClN_2O_2$ 392.968
Metab. of sponge *Acanthella klethra* and *Acanthella cavernosa*. Cytotoxic and antifungal. $[\alpha]_D$ 0 ($CHCl_3$). $[\alpha]_D$ +56.7 (c, 0.03 in CH_2Cl_2).

Fusetani, N. *et al., Tet. Lett.*, 1990, **31**, 3599 (*isol, struct*)
Trimurtula, G. *et al., J. Nat. Prod.*, 1994, **57**, 501 (*isol, pmr, cmr*)

Isokalihinol F I-187

[117229-41-1]



$C_{23}H_{33}N_3O_2$ 383.533
Constit. of *Acanthella cavernosa*. Needles (Et_2O).
Mp 180-182°. $[\alpha]_D$ +13.6 (c, 0.018 in $CDCl_3$). Author misspelt sp. as *carvenosa*.

10-Epimer: ***10*-epi-*Isokalihinol F***. *10-Epiisokalihinol F*
$C_{23}H_{33}N_3O_2$ 383.533
Constit. of *Acanthella cavernosa*. Cryst. (CH_2Cl_2).
Mp 117°. $[\alpha]_D$ -21.2 (c, 0.41 in CH_2Cl_2).

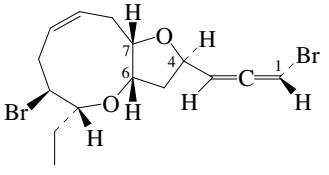
10-Isothiocyanate, 10-epimer: ***10*-epi-*Isokalihinol H***. *10-Epiisokalihinol H*
$C_{23}H_{33}N_3O_2S$ 415.599
Constit. of *Acanthella cavernosa*. Oil. $[\alpha]_D$ -32.1 (c, 0.17 in CH_2Cl_2). Has –NC replaced by –NCS at C-10.

8β-Hydroxy: ***8-Hydroxyisokalihinol F***
[286433-80-5]
$C_{23}H_{33}N_3O_3$ 399.532
Constit. of *Acanthella cavernosa*.
$[\alpha]_D$ +14 (c, 0.018 in CH_2Cl_2).

Omar, S. *et al., J.O.C.*, 1988, **53**, 5971-5972 (*isol, pmr, cmr*)
Trimurtula, G. *et al., J. Nat. Prod.*, 1994, **57**, 501 (*10-epi-Isokalihinol F, 10-epi-Isokalihinol H*)
Clark, R.J. *et al., Tetrahedron*, 2000, **56**, 3071-3076 (*8-Hydroxyisokalihinol F*)

Isolaurallene I-188

*6-Bromo-2-(3-bromo-1,2-propadienyl)-5-ethyl-2,3,3*a*,5,6,7,10,10*a*-octahydrofuro[3,2-*b*]oxonin, 9CI. 1,12-Dibromo-4,7:6,13-diepoxy-1,2,9-pentadecatriene*
[83140-64-1]



Absolute Configuration

$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of red alga *Laurencia nipponica*.
Mp 51-52°. $[\alpha]_D$ -113.9 (c, 1.00 in $CHCl_3$).

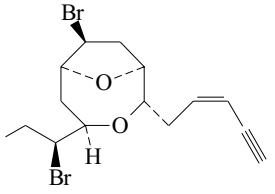
1,6,7-Triepimer: ***Itomanallene A***
$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of red alga *Laurencia intricata*. Oil. $[\alpha]_D^{23}$ +99 (c, 0.44 in $CHCl_3$). "1-Epimer" implies opposite chirality of the allene system.

1,4,6,7-Tetraepimer: ***Neolaurallene***
[91739-57-0]
$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of *Laurencia okamurai*. Cryst. (hexane). 88-89. $[\alpha]_D^{22}$ +180 (c, 0.62 in $CHCl_3$). "1-Epimer" implies the opposite chirality of the allene system.

Kurata, K. *et al., Chem. Lett.*, 1982, 1031-1034 (*Isolaurallene, isol, cryst struct*)
Suzuki, M. *et al., Chem. Lett.*, 1984, 1033-1034 (*Neolaurallene*)
Furusaki, A. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 803-809 (*Isolaurallene, Neolaurallene, cryst struct, abs config*)
Crimmins, M.T. *et al., J.A.C.S.*, 2001, **123**, 1533-1534 (*synth*)
Suzuki, M. *et al., Phytochemistry*, 2002, **60**, 861-867 (*Itomanallene A*)
Crimmins, M.T. *et al., Tetrahedron*, 2002, **58**, 1817-1834 (*synth*)

Isolaureatin I-189

7-Bromo-4-(1-bromopropyl)-2-(2-penten-4-ynyl)-3,9-dioxabicyclo[4.2.1]nonane, 9CI. 9,13-Dibromo-6,12;7,10-diepoxypentadec-3-en-1-yne
[19897-64-4]



Absolute configuration

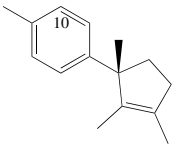
$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of *Laurencia nipponica*. Sol. MeOH, $CHCl_3$, C_6H_6, CCl_4; poorly sol. H_2O.
Mp 83-84°. $[\alpha]_D$ +40 (CCl_4). λ_{max} 223 (ϵ 12400) (EtOH).

E-*Isomer:* ***(3E)-Isolaureatin***
[112710-66-4]
$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D^{15}$ -8.73 (c, 1.11 in $CHCl_3$).

Irie, T. *et al., Tetrahedron*, 1970, **26**, 851-870 (*isol, ir, uv, pmr, ms, struct*)
Kurosawa, E. *et al., Tet. Lett.*, 1973, 3857 (*cryst struct*)
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 3791 (*isol*)

Isolaurene I-190

1-Methyl-4-(1,2,3-trimethyl-2-cyclopenten-1-yl)benzene, 9CI
[4608-39-3]



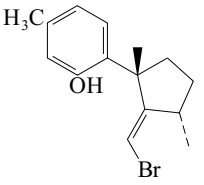
$C_{15}H_{20}$ 200.323
Constit. of *Laurencia glandulifera* and *Laurencia nipponica*. Oil. Bp_{21} 140-142°. $[\alpha]_D$ +108.7 (c, 1.4 in $CHCl_3$).

10-Hydroxy: ***10-Hydroxyisolaurene***
[862207-20-3]
$C_{15}H_{20}O$ 216.322
Constit. of *Laurencia okamurai*. Oil. $[\alpha]_D^{20}$ +25.4 (c, 0.34 in $CHCl_3$). λ_{max} 212 (log ϵ 4.31); 278 (log ϵ 3.63); 289 (log ϵ 3.48) (no solvent reported).

Irie, T. *et al., Tetrahedron*, 1969, **25**, 459 (*Isolaurene*)
Mao, S.-C. *et al., Helv. Chim. Acta*, 2005, **88**, 1034-1039 (*10-Hydroxyisolaurene*)

Isolaurenisol† I-191

[93236-38-5]



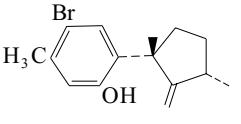
$C_{15}H_{19}BrO$ 295.218
Constit. of *Laurencia distichophylla* and *Aplysia dactylomela*. Oil. $[\alpha]_D^{25}$ -42 (c, 2.5 in $CHCl_3$). $[\alpha]_D^{20}$ +7 (c, 1.5 in $CHCl_3$). λ_{max} 205 (log ϵ 4.52); 275 (log ϵ 3.91) (MeOH) (Derep).

Ac: ***Isolaurenisol acetate***
$C_{17}H_{21}BrO_2$ 337.256
Constit. of *Aplysia dactylomela*. Glass. $[\alpha]_D^{20}$ -7 (c, 0.15 in MeOH). λ_{max} 205 (log ϵ 4.28); 273 (log ϵ 2.3) (MeOH).

Blunt, J.W. *et al., Phytochemistry*, 1984, **23**, 1951-1954 (*isol, uv, pmr, cmr*)
Appleton, D.R. *et al., Tetrahedron*, 2001, **57**, 10181-10189 (*isol, pmr, cmr*)

Isolaurinterol I-192

[29424-17-7]

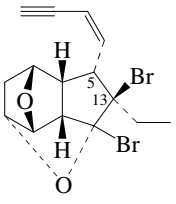


$C_{15}H_{19}BrO$ 295.218
Minor constit. of *Laurencia intermedia*. Oil. $Bp_{1.3}$ 144°. $[\alpha]_D$ -82 (c, 1.5 in $CHCl_3$). λ_{max} 240 (ϵ 30000) (EtOH) (Derep). λ_{max} 287 (ϵ 2300) (EtOH) (Berdy).

Ac:
Oil. $[\alpha]_D$ -70 (c, 1.42 in $CHCl_3$).
Irie, T. *et al., Tetrahedron*, 1970, **26**, 3271
Capon, R.J. *et al., J. Nat. Prod.*, 1988, **51**, 1302 (*isol, pmr, ir*)
Harrowven, D.C. *et al., Tet. Lett.*, 1999, **40**, 8271-8272 (*synth*)

Isomaneonene A I-193

[62583-57-7]



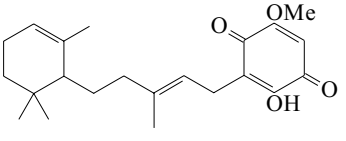
$C_{15}H_{16}Br_2O_2$ 388.098
Constit. of *Laurencia nidifica*. Yellow cryst.
Mp 114.5-115.5°. $[\alpha]_D^{21}$ +106 (c, 1.72 in $CHCl_3$).

5-Epimer: ***Lembyne B***
$C_{15}H_{16}Br_2O_2$ 388.098
Isol. from a *Laurencia* sp. Oil. $[\alpha]_D^{24}$ +157.1 (c, 0.1 in $CHCl_3$).

13-Epimer: ***Isomaneonene B***
[62623-94-3]
$C_{15}H_{16}Br_2O_2$ 388.098
Isol. from *Laurencia nidifica*. Cryst.
Mp 136.5-137°. $[\alpha]_D$ +87 (c, 0.83 in $CHCl_3$).
Waraszkiewicz, S.M. *et al., J.O.C.*, 1978, **43**, 3194-3204 (*Isomaneonenes*)
Vairappan, C.S. *et al., Phytochemistry*, 2001, **58**, 291-297 (*Lembyne B*)

Isometachromin I-194

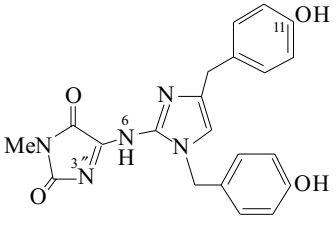
[145401-37-2]



$C_{22}H_{30}O_4$ 358.477
Constit. of a deep water sponge. Cytotoxic agent. Oil. $[\alpha]_D$ -9.6 (c, 0.08 in $CHCl_3$). λ_{max} 210 (ϵ 11500); 288 (ϵ 12500); 427 (ϵ 600) (MeOH) (Berdy).
McConnell, O.J. *et al., Experientia*, 1992, **48**, 891 (*isol, pmr, cmr*)

Isonaamidine A I-195

[110189-04-3]



$C_{21}H_{19}N_5O_4$ 405.412
Two tautomers of the –NH(6)C═N(3″) group are possible.
Alkaloid from the Red Sea sponge *Leucetta chagosensis* and from mollusc *Notodoris citrina*. λ_{max} 227 (ϵ 20000); 264 (ϵ 540); 358 (ϵ 6000); 366 (ϵ 6800); 380 (ϵ 590) (dioxan) (Derep).

O^{11}-Me: ***Isonaamidine B***
[121819-70-3]
$C_{22}H_{21}N_5O_4$ 419.439
Alkaloid from *Leucetta chagosensis*. Amorph. yellow solid (as Zn complex). Also isol. as the bimolecular Zn complex with Isonaamidine D. λ_{max} 226 (ϵ 19400); 276 (ϵ 4300); 374 (ϵ 8000) (MeOH) (Berdy). λ_{max} 228 (ϵ 22400); 278 (ϵ 3900); 368 (ϵ 8700); 380 (ϵ 8500) (MeOH) (as Zn complex).

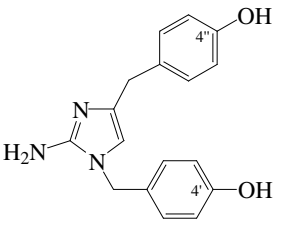
O^{11}-Me, $N^{1''}$-de-Me: ***Isonaamidine D***
$C_{21}H_{19}N_5O_4$ 405.412
Alkaloid from *Leucetta* cf. *chagoensis*. Amorph. yellow solid. λ_{max} 226 (ϵ 18900); 278 (ϵ 4000); 370 (ϵ 6600) (MeOH).

Di-Me ether: ***Isonaamidine C***
[146845-43-4]
$C_{23}H_{23}N_5O_4$ 433.466
Alkaloid from a *Leucetta* sp. and from *Notodoris gardineri*. Yellow solid (as Zn complex). Isol. as the Zn complex, to which the CAS no. refers. λ_{max} 263; 275; 367; 580 (MeOH) (Zn complex). λ_{max} 241 (ϵ 13100); 275 (ϵ 7400); 380 (ϵ 19100) ($CHCl_3$).

10-Methoxy, di-Me ether: ***Isonaamidine E***
$C_{24}H_{25}N_5O_5$ 463.492
Alkaloid from *Leucetta chagosensis*. Cytotoxic. Amorph. yellow solid. λ_{max} 237 (ϵ 23840); 279 (ϵ 5550); 383 (ϵ 11340) ($CHCl_3$).
Carmely, S. *et al., Tetrahedron*, 1989, **45**, 2193-2200 (*isol, uv, ir, pmr, cmr, ms, struct*)
Alvi, K.A. *et al., Tetrahedron*, 1993, **49**, 329 (*Isonaamidine C*)
Copp, B.R. *et al., J. Med. Chem.*, 1998, **41**, 3909-3911 (*Isonaamidine C*)
Fu, X. *et al., J. Nat. Prod.*, 1998, **61**, 384-386 (*Isonaamidine D complexes*)
Gross, H. *et al., J. Nat. Prod.*, 2002, **65**, 1190-1193 (*Isonaamidine E*)
Nakamura, S. *et al., Heterocycles*, 2003, **60**, 583-598 (*synth*)

Isonaamine A I-196

*4,4′-[(2-Amino-1*H*-imidazole-1,4-diyl)bis(methylene)]bisphenol, 9CI. 2-Amino-1,4-bis(*p*-hydroxybenzyl)imidazole*
[110189-02-1]

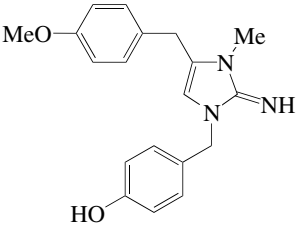


$C_{17}H_{17}N_3O_2$ 295.34
Alkaloid from the Red Sea sponge *Leucetta chagosensis* and the Indo-Pacific nudibranchs *Notodoris gardineri* and *Notodoris citrina*. Yellow powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 227; 265; 275; 294; 300 (MeOH) (Derep).

3″-Methoxy, 4′,4″-di-Me ether: ***Isonaamine C***
$C_{20}H_{23}N_3O_3$ 353.42
Alkaloid from the sponge *Leucetta chagosensis*. Cytotoxic. Amorph. yellow solid. λ_{max} 251 (ϵ 6080); 276 (ϵ 6450); 379 (ϵ 1210) ($CHCl_3$).
Carmely, S. *et al., Tetrahedron*, 1989, **45**, 2193 (*isol, ir, pmr, cmr, ms, struct*)
Alvi, K.A. *et al., J. Nat. Prod.*, 1991, **54**, 1509 (*isol, uv, pmr*)
Molina, P. *et al., J.O.C.*, 1999, **64**, 2540-2544 (*synth, pmr, cmr*)
Gross, H. *et al., J. Nat. Prod.*, 1998, **65**, 1190-1193 (*Isonaamine C*)

Isonaamine B I-197

[203116-58-9]



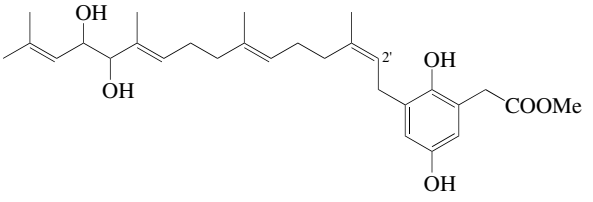
$C_{19}H_{21}N_3O_2$ 323.394

Alkaloid from the sponge *Leucetta* cf. *chagosensis*. Yellow glass. λ_{max} 226 (ϵ 19300); 276 (ϵ 5800); 308 (ϵ 3700) (MeOH).

Fu, X. *et al., J. Nat. Prod.*, 1998, **61**, 384-386 (*isol, uv, ir, pmr, cmr*)

Isonahocol D_1 I-198

[160335-94-4]

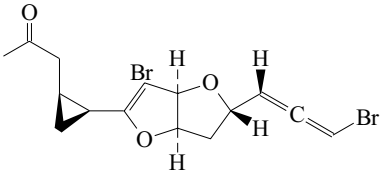


$C_{29}H_{42}O_6$ 486.647
Constit. of *Sargassum autumnale*. Oil. $[\alpha]_D^{25}$ +8.4 (c, 0.83 in EtOH). λ_{max} 210 (log ϵ 4.4); 293 (log ϵ 3.5) (EtOH).

*2′*E*-Isomer:* ***Isonahocol D_2***
[211557-67-4]
$C_{29}H_{42}O_6$ 486.647
Constit. of *Sargassum autumnale*. Oil. $[\alpha]_D^{25}$ +8.6 (c, 2.89 in EtOH). λ_{max} 205 (log ϵ 4.6); 294 (log ϵ 3.5) (EtOH).
Tsuchiya, N. *et al., Phytochemistry*, 1998, **48**, 1003-1011 (*isol, pmr, cmr*)

Isookamurallene I-199

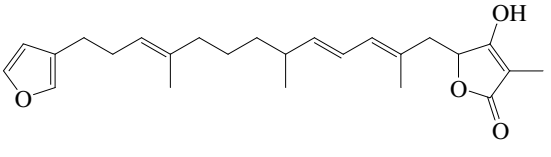
[81474-93-3]



$C_{15}H_{16}Br_2O_3$ 404.098
Constit. of *Laurencia okamurai*. Oil. $[\alpha]_D^{27}$ +130 (c, 1 in $CHCl_3$).

Suzuki, M. *et al., Chem. Lett.*, 1982, 289; 1992, 33 (*isol, abs config*)
Sukuki, M. *et al., Phytochemistry*, 1989, **28**, 2145 (*struct*)

Isopalinurin I-200

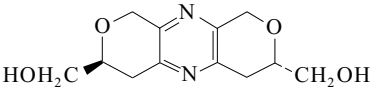


$C_{25}H_{34}O_4$ 398.541
Constit. of a *Dysidea* sp. Yellow oil. $[\alpha]_D$ +32.4 (c, 1.3 in $CHCl_3$). λ_{max} 292 (ϵ 6815) ($CHCl_3$).

Murray, L. *et al., Aust. J. Chem.*, 1993, **46**, 1291-1294 (*isol, pmr, cmr*)

Isopalythazine I-201

*4,6,7,9-Tetrahydro-1*H*,3*H*-dipyrano[3,4-*b*:4′,3′-*e*]pyrazine-3,7-dimethanol, 9CI*
[72681-95-9]

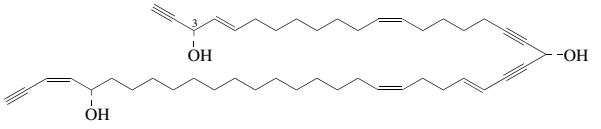


$C_{12}H_{16}N_2O_4$ 252.269
Isol. from the zoanthid *Palythoa tuberculosa*.
Mp 169-170° Mp 216-219°.

Uemura, D. *et al., Chem. Lett.*, 1979, 1481 (*isol, cmr, struct, synth*)
Jarglis, P. *et al., Angew. Chem., Int. Ed.*, 1982, **21**, 141

Isopetroformyne 1 I-202

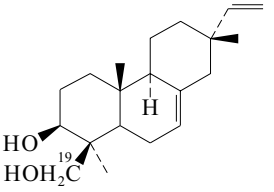
4,12,23,27,43-Hexatetracontapentaene-1,18,21,45-tetrayne-3,20,42-triol
[202982-24-9]



$C_{46}H_{68}O_3$ 669.041
Isol. from the sponge *Petrosia ficiformis*. Oil. $[\alpha]_D^{21}$ +2.5 (c, 0.2 in $CHCl_3$). λ_{max} 228 (ϵ 13090) (MeOH). λ_{max} 228 (ϵ 13088) (MeOH) (Berdy).

Guo, Y. *et al., J. Nat. Prod.*, 1998, **61**, 333-337 (*isol, uv, pmr, cmr*)

7,15-Isopimaradiene-3,19-diol I-203



$C_{20}H_{32}O_2$ 304.472

3β-*form*
Virescenol B
[22343-47-1]
Cryst. (Et_2O/petrol). Mp 146-147°. $[\alpha]_D$ -25 (c, 0.74 in $CHCl_3$).

19-O-*β*-D-*Altropyranoside:* ***Virescenoside B***
[28251-74-3]
$C_{26}H_{42}O_7$ 466.614
Metab. of *Oospora virescens* and from *Acremonium striatisporum* KMM 4401 isol. from the sea cucumber *Eupentacta fraudatrix*. Cytotoxic on sea urchin eggs and Ehrlich carcinoma cells. Amorph.
Mp 110°. $[\alpha]_D$ -32.3 (c, 1.05 in MeOH).

19-O-*β*-D-*Mannopyranoside:* ***Virescenoside Q***
[433334-40-8]
$C_{26}H_{42}O_7$ 466.614
Constit. of *Acremonium striatisporum* KMM 4401 isol. from the sea cucumber *Eupentacta fraudatrix*. Amorph. solid. $[\alpha]_D^{20}$ -20 (c, 0.45 in MeOH).

19-O-*β*-D-*Altropyranosiduronosyl:* ***Virescenoside G***
[34212-90-3]
$C_{26}H_{40}O_8$ 480.597
Metab. of *Oospora virescens*. Cryst. (EtOAc/MeOH). Sol. MeOH, $CHCl_3$.
Mp 192-194°. $[\alpha]_D$ -85 (c, 1.11 in MeOH).

19-O-*(4-Deoxy-β-*D*-*threo*-hex-4-enodialdopyranoside):* ***Virescenoside D***
[34212-92-5]
$C_{26}H_{38}O_6$ 446.583
Metab. of *Acremonium luzulae*. Solid ($CHCl_3$/hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -123.5 (c, 0.96 in MeOH). λ_{max} 258 (ϵ 6000) (EtOH) (Berdy).
▶ LD_{50} (mus, scu) 250 mg/kg.

19-O-*(4-Deoxy-β-*D*-*threo*-hex-4-enopyranoside):* ***Virescenoside H***
[34212-93-6]
$C_{26}H_{40}O_6$ 448.598
Metab. of *Acremonium luzulae*. Needles (EtOAc). Sol. MeOH, $CHCl_3$.
Mp 190-193°. $[\alpha]_D$ -149 (c, 0.72 in MeOH).

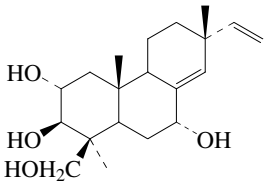
3-Ketone: 19-Hydroxy-7,15-isopimaradien-3-one. Virescenol C

[29478-42-0]
Cryst. (hexane). Mp 111-112°. $[\alpha]_D$ -78.4 (c, 0.96 in $CHCl_3$).

3-Ketone, 19-O-β-D-altropyranoside: ***Virescenoside C***
[29478-41-9]
$C_{26}H_{40}O_7$ 464.598
Metab. of *Oospora virescens* and from *Acremonium striatisporum* KMM 4401 isol. from the sea cucumber *Eupentacta fraudatrix*. Cytotoxic on sea urchin eggs and Ehrlich carcinoma cells. Cryst. (EtOAc). Sol. MeOH, $CHCl_3$; fairly sol. H_2O; poorly sol. hexane. Mp 160-162°. $[\alpha]_D$ -71.4 (c, 0.98 in MeOH).

Cagnoli-Bellavita, N. *et al., Gazz. Chim. Ital.*, 1969, **99**, 1354; 1977, **107**, 51 (*isol, struct*)
Polonsky, J. *et al., Bull. Soc. Chim. Fr.*, 1970, 1912 (*isol, struct*)
Cagnoli-Bellavita, N. *et al., Eur. J. Biochem.*, 1970, **15**, 356 (*isol, struct*)
Ceccherelli, P. *et al., Tetrahedron*, 1973, **29**, 449-454 (*Virescenoside G*)
Pellicciani, R. *et al., Ann. Chim. (Rome)*, 1975, **65**, 147 (*synth*)
Polonsky, J. *et al., Tet. Lett.*, 1975, 481 (*cmr, biosynth*)
Cagnoli-Bellavita, N. *et al., J.C.S. Perkin 1*, 1977, 351 (*Virescenoside D,L*)
Ceccherelli, P. *et al., J.O.C.*, 1977, **42**, 3438 (*synth*)
Bellavita, N. *et al., J.A.C.S.*, 1980, **102**, 17 (*nmr*)
Afiyatullov, S.S. *et al., J. Nat. Prod.*, 2000, **63**, 848-850; 2002, **65**, 641-644 (*Virescenosides B,C,Q, isol, activity*)

8(14),15-Isopimaradiene-2,3,7,19-tetrol I-204



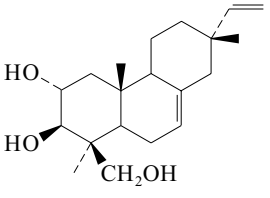
$C_{20}H_{32}O_4$ 336.47

(2α,3β,7α)-*form*

19-O-β-D-Altropyranoside: ***Virescenoside N***
[280144-92-5]
$C_{26}H_{42}O_9$ 498.612
Metab. of *Acremonium striatisporum* KMM 4401 isol. from the sea cucumber *Eupentacta fraudatrix*. Amorph. solid. $[\alpha]_D^{20}$ -18 (c, 0.25 in MeOH). Struct. revised in 2005.

Afiyatullov, S.Sh. *et al., J. Nat. Prod.*, 2000, **63**, 848-850; 2005, **68**, 1308 (*isol, pmr, cmr, struct*)

7,15-Isopimaradiene-2,3,19-triol I-205



$C_{20}H_{32}O_3$ 320.471

(2α,3β)-*form*

Virescenol A
[22343-46-0]
Cryst. Mp 149-150°. $[\alpha]_D$ -44 ($CHCl_3$).

19-O-β-D-Altropyranoside: ***Virescenoside A***
[28251-73-2]
$C_{26}H_{42}O_8$ 482.613
Metab. of *Acremonium luzulae* (*Oospora virescens*) and from *Acremonium striatisporum* KMM 4401 isol. from the sea cucumber *Eupentacta fraudatrix*. Cytotoxic to sea urchin eggs and Ehrlich carcinoma cells. Amorph. Sol. MeOH, EtOAc; fairly sol. H_2O; poorly sol. $CHCl_3$, hexane, Et_2O.
Mp 130°. $[\alpha]_D$ -42.7 (c 1.03 in MeOH).

19-β-D-Altropyranosiduronic acid: ***Virescenoside F***
[34212-88-9]
Metab. of *Acremonium luzulae* and *Oospora virescens*.
Cryst. (EtOAc/MeOH). Sol. MeOH, $CHCl_3$.
Mp 188-190°. $[\alpha]_D$ -82 (c, 1.13 in MeOH).

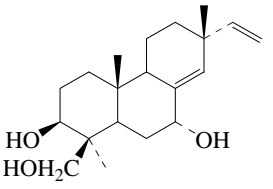
*19-O-β-D-*threo*-Hex-4-enodialdo-1,5-pyranoside:* ***Virescenoside E***
[34212-94-7]
$C_{26}H_{38}O_7$ 462.582
Isol. from *Acremonium luzulae*. Sol. MeOH, $CHCl_3$; poorly sol. hexane. $[\alpha]_D$ -113 (c, 0.97 in MeOH). λ_{max} 258 (ε 6000) (EtOH) (Berdy).
▶ LD_{50} (mus, scu) 250 mg/kg.

*19-O-β-D-*threo*-4-Deoxyhex-4-enopyranoside:* ***Virescenoside L***
[63758-60-1]
$C_{26}H_{40}O_7$ 464.598
Metab. of *Acremonium luzulae*. Microcryst. (EtOAc). $[\alpha]_D$ -154 (c, 0.57 in $CHCl_3$).

3-O-[α-D-Glucopyranosyl-(1→6)-β-D-altropyranoside]: ***Virescenoside R***
[724462-47-9]
$C_{32}H_{52}O_{13}$ 644.755
Prod. by *Acremonium striatisporum* KMM 4401 isol. from the sea cucumber *Eupentacta fraudatrix*. Amorph. solid. $[\alpha]_D^{20}$ +12 (c, 0.6 in MeOH).

Cagnoli-Bellavita, N. *et al., Gazz. Chim. Ital.*, 1969, **99**, 1354 (*isol*)
Polonsky, J. *et al., Bull. Soc. Chim. Fr.*, 1970, 1912 (*isol, struct*)
Ceccherelli, P. *et al., Tetrahedron*, 1973, **29**, 449-454 (*Virescenoside F*)
Polonsky, J. *et al., Tet. Lett.*, 1975, 481 (*cmr, biosynth*)
Ceccherelli, P. *et al., Gazz. Chim. Ital.*, 1977, **107**, 51-53 (*Virescenosides E and L*)
Bellavita, N. *et al., J.A.C.S.*, 1980, **102**, 17 (*nmr*)
Afiyatullov, S.S. *et al., J. Nat. Prod.*, 2000, **63**, 848-850 (*Virescenoside A, isol, activity*)
Afiyatullov, S.Sh. *et al., J. Nat. Prod.*, 2004, **67**, 1047-1051 (*Virescenoside R*)

8(14),15-Isopimaradiene-3,7,19-triol I-206



$C_{20}H_{32}O_3$ 320.471

(3β,7α)-*form*

19-O-β-D-Altropyranoside: ***Virescenoside O***
[433334-38-4]
$C_{26}H_{42}O_8$ 482.613
Constit. of *Acremonium striatisporum* KMM 4401 isol. from the sea cucumber *Eupentacta fraudatrix*. Amorph. solid. $[\alpha]_D^{20}$ -44 (c, 0.5 in MeOH).

3-Ketone: 7,19-Dihydroxy-8(14),15-isopimaradien-3-one
$C_{20}H_{30}O_3$ 318.455

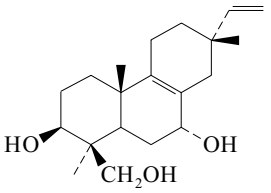
3-Ketone, 19-O-β-D-altropyranoside: ***Virescenoside S***
[724462-48-0]
$C_{26}H_{40}O_8$ 480.597
Constit. of *Acremonium striatisporum* KMM 4401 isol. from the sea cucumber *Eupentacta fraudatrix*. Amorph. solid. $[\alpha]_D^{20}$ -42.5 (c, 0.4 in MeOH).

3,7-Diketone: 19-Hydroxy-8(14),15-isopimaradien-3,7-dione

3,7-Diketone, 19-O-β-D-altropyranoside: ***Virescenoside U***
[724462-50-4]
$C_{26}H_{38}O_8$ 478.581
Constit. of *Acremonium striatisporum* KMM 4401 isol. from the sea cucumber *Eupentacta fraudatrix*. Amorph. solid. $[\alpha]_D^{20}$ -30 (c, 0.33 in MeOH). λ_{max} 247 (log ε 3.4) (MeOH).

Afiyatullov, S.Sh. *et al., J. Nat. Prod.*, 2002, **65**, 641-644; 2004, **67**, 1047-1051 (*isol*)

8,15-Isopimaradiene-3,7,19-triol I-207



$C_{20}H_{32}O_3$ 320.471

(3β,7α)-*form* [117255-00-2]
Constit. of *Juniperus thurifera*.

7-Ketone: 3,19-Dihydroxy-8,15-isopimaradien-7-one
[433264-62-1]
Amorph. solid. $[\alpha]_D^{20}$ +44 (c, 0.15 in MeOH). λ_{max} 253 (log ϵ 4.04) (MeOH).

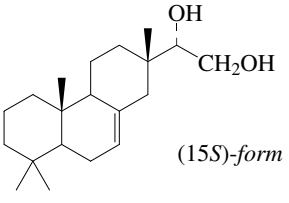
7-Ketone, 19-O-β-D-altropyranoside: ***Virescenoside P***
[433334-39-5]
$C_{26}H_{40}O_8$ 480.597
Constit. of *Acremonium striatisporum* KMM 4401 isol. from the sea cucumber *Eupentacta fraudatrix*. Amorph. solid. $[\alpha]_D^{20}$ +31 (c, 0.2 in MeOH). λ_{max} 248 (log ϵ 3.7) (MeOH).

3,7-Diketone: 19-Hydroxy-8,15-isopimaradiene-3,7-dione

3,7-Diketone, 19-O-β-D-altropyranoside: ***Virescenoside T***
[724462-49-1]
$C_{26}H_{38}O_8$ 478.581
Constit. of *Acremonium striatisporum* KMM 4401 isol. from the sea cucumber *Eupentacta fraudatrix*. Amorph. solid. $[\alpha]_D^{20}$ +23 (c, 0.48 in MeOH). λ_{max} 248 (log ϵ 3.7) (MeOH).

San Feliciano, A. *et al., Phytochemistry*, 1988, **27**, 2241-2248 (*isol, struct*)
Afiyatullov, S.Sh. *et al., J. Nat. Prod.*, 2002, **65**, 641-644 (*Virescenoside P*)
Afiyatullov, S.Sh. *et al., J. Nat. Prod.*, 2004, **67**, 1047-1051 (*Virescenoside T*)

7-Isopimarene-15,16-diol I-208



(15*S*)-*form*

$C_{20}H_{34}O_2$ 306.487

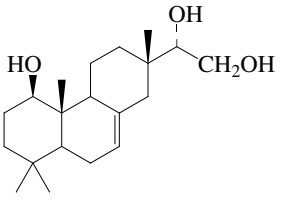
(15*S*)-*form* [238758-42-4]
Constit. of *Bruguiera gymnorhiza*.
Cryst.
Mp 150°. $[\alpha]_D^{30}$ +21 (c, 0.1 in $CHCl_3$). Error in struct. diag. in ref.

(15ξ)-*form*
Esquirolin B
Constit. of *Coleus esquirolii*.
Cryst.
Mp 95-96°. $[\alpha]_D^{27}$ -100 (c, 0.08 in $CHCl_3$).

15,16-O-Isopropylidene: ***Esquirolin C***
[136196-65-1]
$C_{23}H_{38}O_2$ 346.552
Constit. of *Coleus esquirolii*. Cryst.
Mp 63-65°. $[\alpha]_D^{26}$ +13.6 (c, 0.22 in $CHCl_3$).

Li, C.M. *et al., Chin. Chem. Lett.*, 1991, **2**, 223-226 (*Esquirolin C*)
Urones, J.G. *et al., Phytochemistry*, 1998, **48**, 1035-1038 (*Esquirolin B*)
Subrahmanyan, C. *et al., Phytochemistry*, 1999, **51**, 83-90 (*15S-form, isol, pmr, cmr*)

7-Isopimarene-1,15,16-triol I-209



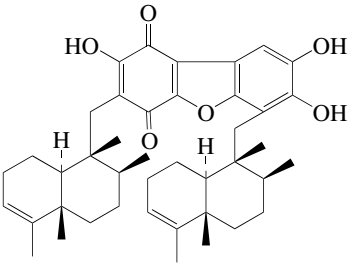
$C_{20}H_{34}O_3$ 322.487

(1β,15*S*)-*form*
Ceriopsin C
[478175-20-1]
Constit. of *Ceriops decandra*.
Oil. $[\alpha]_D^{25}$ +3 (c, 0.4 in $CHCl_3$).

Anjaneyulu, A.S.R. *et al., Phytochemistry*, 2002, **60**, 777-782 (*isol, pmr, cmr*)

Isopopopolohuanone E I-210

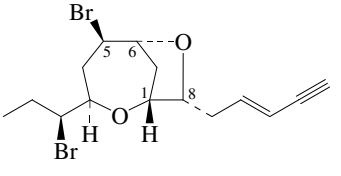
[193157-90-3]



$C_{42}H_{54}O_6$ 654.885
Not named in paper. Constit. of a *Dysidea* sp. Deep purple solid.
Stewart, M. *et al., Aust. J. Chem.*, 1997, **50**, 341-347 (*isol, pmr, cmr*)

Isoprelaurefucin I-211

5-Bromo-3-(1-bromopropyl)-8-(2-penten-4-ynyl)-2,7-dioxabicyclo[4.2.1]nonane, 9CI. 10,13-Dibromo-6,9:7,12-diepoxy-3-pentadecen-1-yne
[51918-97-9]



Absolute Configuration

$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of the seaweed *Laurencia nipponica* Yamada. Oil. $[\alpha]_D$ -54.4. λ_{max} 209 (ϵ 8700); 219 (ϵ 11800); 224 (ϵ 13200); 232 (sh) (ϵ 9800) (no solvent reported).

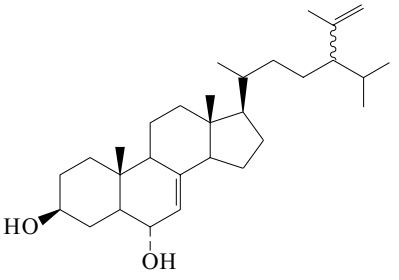
(Z)-Isomer: (3Z)-Isoprelaurefucin
$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of the seaweed *Laurencia nipponica* and *Laurencia subopposita*. Oil. $[\alpha]_D^{21}$ -75.5 (c, 1.41 in $CHCl_3$). λ_{max} 214 (sh) (ϵ 12800); 222 (ϵ 14600); 231 (ϵ 10900) (EtOH).

1,5,6,8-Tetraepimer:
$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D^{30}$ +32.9 (c, 2.1 in $CHCl_3$). (*E*)-Isomer of Neoisoprelaurefucin.

1,5,6,8-Tetraepimer, (Z)-isomer: ***Neoisoprelaurefucin***
[182697-63-8]
$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D^{23}$ +17.2 (c, 1.3 in $CHCl_3$).

Kurosawa, E. *et al., Tet. Lett.*, 1973, 4135-4138 (*isol, uv, ir, pmr, ms*)
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 2953-2955 (*abs config, bibl*)
Suzuki, M. *et al., Phytochemistry*, 1996, **43**, 121-124 (*Neoisoprelaurefucin*)
Lee, H. *et al., Tet. Lett.*, 2003, **44**, 6609-6612 (*Neoisoprlaurefucin, synth, abs config*)
Aydoğmuş, Z. *et al., Nat. Prod. Res.*, 2004, **18**, 43-49 (*Laurencia obtusa isomer*)
Lee, H. *et al., J.O.C.*, 2005, **70**, 8723-8729 (*synth*)

24-Isopropenylcholest-7-ene-3,6-diol I-212



$C_{30}H_{50}O_2$ 442.724

(3β,6α,24ξ)-*form*
Constit. of *Dysidea herbacea*.
Cryst. (MeOH).
Mp 198-199°.
Rambabu, M. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 1156

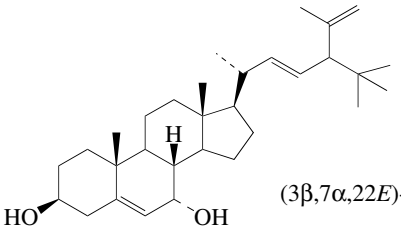
24-Isopropenylcholest-7-en-3-ol I-213

$C_{30}H_{50}O$ 426.724

(3β,24ξ)-*form*
Constit. of *Dysidea herbacea*.
Cryst. (MeOH).
Mp 149°.
Rambabu, M. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 1156

24-Isopropenyl-25-methylcholesta-5,22-diene-3,7-diol I-214

24-tert-*Butylcholesta-5,22,25-triene-3,7-diol. 28,28-Dimethylstigmasta-5,22,25-triene-3,7-diol*



(3β,7α,22*E*)-*form*

$C_{31}H_{50}O_2$ 454.735

(3β,7α,22*E*)-*form*
Topsentinol A
[197381-57-0]
Constit. of a *Topsentia* sp.
Needles.
Mp 189°. $[\alpha]_D^{26}$ -84 (c, 0.5 in $CHCl_3$).

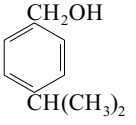
22,23-Dihydro: 24-Isopropenyl-25-methylcholest-5-ene-3,7-diol. 24-tert-*Butylcholesta-5,25-diene-3,7-diol. 28,28-Dimethylstigmasta-5,25-diene-3,7-diol.* ***Topsentinol C***
[197381-63-8]
$C_{31}H_{52}O_2$ 456.751
Constit. of a *Topsentia* sp. Needles.
Mp 223°. $[\alpha]_D^{28}$ -75 (c, 0.4 in $CHCl_3$).

(3β,7β,22*E*)-*form*
Topsentinol F
[197381-72-9]
Constit. of a *Topsentia* sp.
Amorph. solid. $[\alpha]_D^{25}$ -5.1 (c, 0.5 in $CHCl_3$).

22,23-Dihydro: ***Topsentinol H***
[197381-78-5]
$C_{31}H_{52}O_2$ 456.751
Constit. of a *Topsentia* sp.
Ishibashi, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1435-1438 (*isol, pmr, cmr*)

4-Isopropylbenzyl alcohol I-215

4-(1-Methylethyl)benzenemethanol, 9CI. p-*Cymen-7-ol, 8CI.* p-*Mentha-1,3,5-trien-7-ol.* ***Cuminyl alcohol****. Cumic alcohol. Cuminol. FEMA 2933*
[536-60-7]



$C_{10}H_{14}O$ 150.22
Isol. from oils of *Cuminum cyminum* (cumin), *Eucalyptus bakeri*, *Lavandula ver*a and *Ledum palustre*. Occurs in the bryozoan *Conopeum seratum*. Liq. with an intense caraway-like odour and an aromatic, burning taste. d^{20} 0.98. Bp 246° Bp_{20} 140°. n_D^{24} 1.5220.
▶ Skin irritant. LD_{50} (rat, orl) 1020 mg/kg. GZ7260000

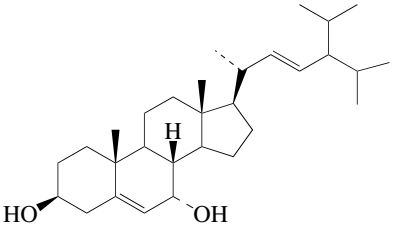
O-*[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranoside]:* ***Coleoside***
$C_{22}H_{34}O_{11}$ 474.504
Constit. of *Coleus forskohlii*. Yellow solid.

Ac: [59230-57-8]
$C_{12}H_{16}O_2$ 192.257
$Bp_{16.5}$ 136°.
▶ DA4977000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1133B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 349A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1057C (*ir*)
Bert, L. *et al., Bull. Soc. Chim. Fr.*, 1925, **37**, 1397; 1577
Palfray, L. *et al., C. R. Hebd. Seances Acad. Sci.*, 1936, **203**, 1523
Seidel, C.F. *et al., Helv. Chim. Acta*, 1944, **27**, 663 (*isol*)
v. Sydow, E. *et al., Acta Chem. Scand.*, 1963, **17**, 2504 (*ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 871 (*rev, tox*)
van Tamelen, E.E. *et al., J.A.C.S.*, 1974, **96**, 5290
Hadjieva, P. *et al., Z. Naturforsch., C*, 1987, **42**, 1019-1022 (*occur, bryozoan*)
Ahmed, B. *et al., Phytochemistry*, 1988, **27**, 3309
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 411
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1486-1487
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CQI250

24-Isopropylcholesta-5,22-diene-3,7-diol I-216

28-Methylstigmasta-5,22-diene-3,7-diol



(3β,7α,22*E*)-*form*

$C_{30}H_{50}O_2$ 442.724

(3β,7α,22*E*)-*form*
Topsentinol D
[197381-66-1]
Constit. of a *Topsentia* sp.
Needles.
Mp 216°. $[\alpha]_D^{28}$ -104 (c, 1 in $CHCl_3$).

22,23-Dihydro: 24-Isopropylcholest-5-ene-3,7-diol. 28-Methylstigmast-5-ene-3,7-diol. ***Topsentinol E***
[197381-69-4]
$C_{30}H_{52}O_2$ 444.74
Constit. of a *Topsentia* sp. Needles.
Mp 218°. $[\alpha]_D^{27}$ -72 (c, 0.5 in $CHCl_3$).

(3β,7α,22*Z*)-*form*
Topsentinol B
[197381-60-5]
Constit. of a *Topsentia* sp.
Needles.
Mp 216°. $[\alpha]_D^{27}$ -96 (c, 0.5 in $CHCl_3$).

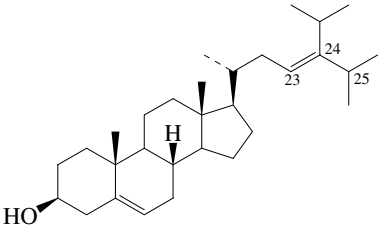
(3β,7β,22*E*)-*form*
Topsentinol I
[197381-81-0]
Constit. of a *Topsentia* sp.
Amorph. solid. $[\alpha]_D^{25}$ -19 (c, 1 in $CHCl_3$).

22,23-Dihydro: ***Topsentinol J***
[197381-83-2]
$C_{30}H_{52}O_2$ 444.74
Constit. of a *Topsentia* sp. Amorph. solid. $[\alpha]_D^{25}$ -6.7 (c, 1 in $CHCl_3$).

(3β,7β,22*Z*)-*form*
Topsentinol G
[197381-75-2]
Constit. of a *Topsentia* sp.
Ishibashi, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1435-1438 (*isol, pmr, cmr*)

24-Isopropyl-5,23-cholestadien-3-ol I-217

28-Methylstigmasta-5,23-dien-3-ol



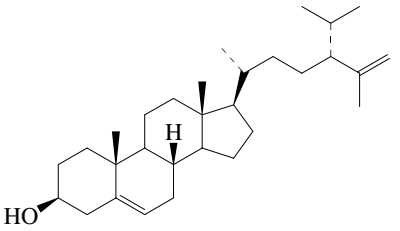
$C_{30}H_{50}O$ 426.724

3β-*form* [90195-40-7]
Component of the lipids of a marine unicellular green alga.

Δ^{24}-Isomer: ***24-Isopropyl-5,24-cholestadien-3-ol****. 28-Methylstigmasta-5,24-dien-3-ol*
[77643-24-4]
$C_{30}H_{50}O$ 426.724
Component of the lipids of a marine unicellular green alga.
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*isol, pmr*)

24-Isopropyl-5,25-cholestadien-3-ol I-218

28-Methylstigmasta-5,25-dien-3-ol



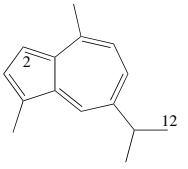
$C_{30}H_{50}O$ 426.724

(3β,24*R*)-*form* [71841-97-9]
Constit. of *Verongia cauliformis.*

(3β,24ξ)-*form* [75918-24-0]
Component of the lipids of a marine unicellular green alga, *Anoectochilus koshuensis* and of *Nervilia purpurea*.
Kikuchi, T. *et al., Helv. Chim. Acta*, 1979, **62**, 1310-1318 (*Nervilia purpurea constit*)
Kokke, W.C.M.C. *et al., Helv. Chim. Acta*, 1979, **62**, 1310-1318 (*Verongia cauliformis constit*)
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*marine alga constit*)
Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1985, **33**, 2235-2242 (*Nervilia purpurea constit*)
Ito, A. *et al., Phytochemistry*, 1994, **36**, 1465-1467 (*Anoectochilus kosunensis constit*)

7-Isopropyl-1,4-dimethylazulene I-219

1,4-Dimethyl-7-(1-methylethyl)azulene, 9CI. 1,3,5,7,9-Guaiapentaene. ***Guaiazulene****. S-Guaiazulene. Kessazulene. Azulon. Eucazulene. Azunol*
[489-84-9]



$C_{15}H_{18}$ 198.307
Obt. from essential oils, e.g. chamomile oil. Found also in marine red algae and the gorgonians *Euplexaura erecta* and *Alcyonium* sp. Antioxidant, inhibits lipid peroxidation. Antiinflammatory agent, also used to treat gastrointestinal disorders. Hepatoprotectant. Immunodepressant. Immunomodulatory and antiulcer agent.
Blue-violet plates (EtOH) or blue oil.
Mp 31.5°. Bp_{12} 167-168°. Log P 5.74 (calc). λ_{max} 286; 292; 350; 377; 600 ($CHCl_3$) (Berdy). λ_{max} 556; 581; 603; 632 (Et_2O).
▶ LD_{50} (rat, orl) 1550 mg/kg. CO4790000

1,3,5-Trinitrobenzene complex: [4968-29-0]
Black needles (EtOH). Mp 151-151.5°.

Picrate:
Black needles (EtOH). Mp 122-122.5°.

2-Chloro: 2-Chloro-1,3,5,7,9-guaiapentaene. 3-Chloro-7-isopropyl-1,4-dimethylazulene. ***3-Chloroguaiazulene***
[90052-60-1]
$C_{15}H_{17}Cl$ 232.752
Constit. of a gorgonian of the Paramuriceidae family. λ_{max} 246 (ϵ); 293 (ϵ); 307 (ϵ); 352 (ϵ); 369 (ϵ); 620 (ϵ) ($CHCl_3$) (Derep).

2-Bromo: 2-Bromo-1,3,5,7,9-guaiapentaene. 3-Bromo-7-isopropyl-1,4-dimethylazulene. ***3-Bromoguaiazulene***
[90052-61-2]
$C_{15}H_{17}Br$ 277.203
Constit. of a gorgonian of the Paramuriceidae family. Oil.

12-Bromo: 12-Bromo-1,3,5,7,9-guaiapentaene. 7-(2-Bromo-1-methylethyl)-1,4-dimethylazulene, 9CI. ***Ehuazulene***
[90052-62-3]

$C_{15}H_{17}Br$ 277.203

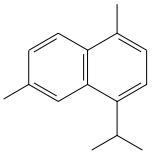
Constit. of a gorgonian of the Paramuriceidae family. Oil. $[\alpha]_D$ +2 (hexane). λ_{max} 245 (ϵ); 286 (ϵ); 293 (ϵ); 305 (sh) (ϵ); 352 (ϵ); 369 (ϵ); 608 (ϵ) ($CHCl_3$) (Derep).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 955D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 40B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 877B (*ir*)
Plattner, P.A. *et al., Helv. Chim. Acta*, 1949, **32**, 2137; 2452 (*synth*)
Šorm, F. *et al., Coll. Czech. Chem. Comm.*, 1951, **16**, 168; 626 (*isol, synth*)
Caujolle, F. *et al., Ann. Pharm. Fr.*, 1952, **10**, 412 (*pharmacol*)
Herz, A. *et al., Arzneim.-Forsch.*, 1953, **3**, 253 (*pharmacol*)
Jacob, T.M. *et al., Tetrahedron*, 1964, **20**, 2821 (*uv, synth*)
Llinas, J.R. *et al., Can. J. Chem.*, 1975, **53**, 2911 (*pmr, cmr*)
Hoffmann, W. *et al., Tet. Lett.*, 1975, 533 (*synth*)
Mukherjee, D. *et al., J.A.C.S.*, 1979, **101**, 251 (*synth*)
Fusetani, N. *et al., Experientia*, 1981, **37**, 680-681 (*isol*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1983, **36**, 211-214 (*isol, Alcyonium*)
Li, M.K.W. *et al., Tet. Lett.*, 1984, **25**, 587 (*derivs*)
Vidal-Ollivier, E. *et al., J. Chromatogr.*, 1989, **463**, 227 (*hplc*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1688
Kourounakis, A.P. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1997, **330**, 7 (*pharmacol*)
Carret, S. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 5130-5133 (*synth, ir, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DSJ800

4-Isopropyl-1,6-dimethylnaphthalene, 8CI I-220

1,6-Dimethyl-4-(1-methylethyl)naphthalene, 9CI. 1,3,5,7,9-Cadinapentaene. ***Cadalene***

[483-78-3]



$C_{15}H_{18}$ 198.307

Occurs in various plants, e.g. *Abies sibirica* resin and *Dictyopteris divaricata*. d_4^{19} 0.98. Bp_{720} 291-292° Bp_3 106°. n_D^{19} 1.5851.

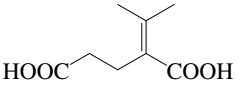
Picrate:

Orange needles (EtOH). Mp 115°.

Ruzicka, L. *et al., Helv. Chim. Acta*, 1922, **5**, 369 (*synth*)
Barnett, E. de B. *et al., J.C.S.*, 1933, 22 (*synth*)
Johnson, W.S. *et al., J.A.C.S.*, 1947, **69**, 792 (*synth*)
Nagasampagi, B.A. *et al., Tetrahedron*, 1966, **22**, 1949 (*uv, ir*)
Kohli, J.C. *et al., Experientia*, 1972, **28**, 131 (*synth*)
Takahashi, K. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2000 (*cmr*)
El-Seedi, H. *et al., Phytochemistry*, 1994, **35**, 1495-1497 (*isol, cmr*)

2-Isopropylidenepentanedioic acid I-221

2-(1-Methylethylidene)pentanedioic acid. 2-Isopropylideneglutaric acid



$C_8H_{12}O_4$ 172.18

Prod. by a marine-derived *Acremonium* sp. Cryst. (MeOH). Mp 131-132° (natural) Mp 163.5° (synthetic). $[\alpha]_D^{23}$ +4.4 (c, 0.8 in Me_2CO). Opt. rotation of natural isolate unaccounted for. λ_{max} 221 (log ϵ 3.8) (MeOH).

1-Me ester:

$C_9H_{14}O_4$ 186.207

Prod. by an *Acremonium* sp.

5-Me ester:

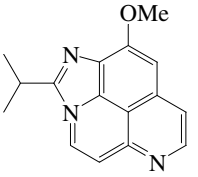
$C_9H_{14}O_4$ 186.207

Prod. by an *Acremonium* sp.

Puterbaugh, W.H. *et al., J.O.C.*, 1962, **27**, 4010-4015 (*synth*)
Fleury, J.P. *et al., Bull. Soc. Chim. Fr.*, 1963, 565-570 (*synth*)
Abdel-Lateff, A. *et al., J. Nat. Prod.*, 2002, **65**, 1605-1611 (*isol, pmr, cmr, cryst struct*)

2-Isopropyl-10-methoxybenzimidazo[6,7,1-*def*][1,6]-naphthyridine I-222

[597553-93-0]



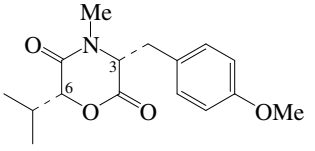
$C_{16}H_{15}N_3O$ 265.314

Alkaloid from a *Xestospongia* sp. Brown gum.

Calcul, L. *et al., Tetrahedron*, 2003, **59**, 6539-6544 (*isol, pmr, cmr*)

6-Isopropyl-3-(4-methoxybenzyl)-4-methyl-2,5-morpholinedione I-223

3-(4-Methoxyphenylmethyl)-4-methyl-6-(1-methylethyl)-2,5-morpholinedione, 9CI



$C_{16}H_{21}NO_4$ 291.346

(3*R,6*R**)-*form***

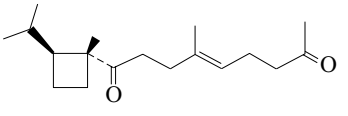
Isol. from the sea hare *Bursatella leachii*.

Amorph. solid. $[\alpha]_D^{20}$ -58.2 (c, 0.05 in MeOH). λ_{max} 223 (log ϵ 2.93); 250 (log ϵ 2.2); 273 (log ϵ 2.08); 281 (log ϵ 1.99) (MeOH).

Suntornchashwej, S. *et al., J. Nat. Prod.*, 2005, **68**, 951-955 (*isol, pmr, cmr*)

1-(2-Isopropyl-1-methylcyclobutyl)-4-methyl-4-nonene-1,8-dione I-224

[81374-03-0]



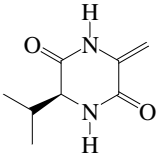
$C_{18}H_{30}O_2$ 278.434

Constit. of *Cystophora moniliformis*. Oil. $[\alpha]_D^{21}$ -7.4 (c, 1 in CH_2Cl_2).

Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 171

3-Isopropyl-6-methylene-2,5-piperazinedione, 8CI I-225

3-Methylene-6-(1-methylethyl)-2,5-piperazinedione, 9CI. Cyclo(dehydroalanylvalyl)



$C_8H_{12}N_2O_2$ 168.195

(*S*)-*form*

L-form

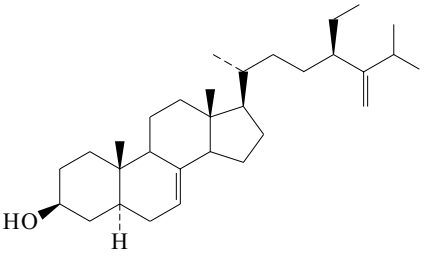
[25516-00-1]

Prod. by the marine bacterium *Vibrio parahaemolyticus*. No exptl. details given.

Izumiya, N. *et al., J.A.C.S.*, 1977, **99**, 8346-8348 (*synth*)
Bell, R. *et al., J. Nat. Prod.*, 1994, **57**, 1587-1590 (*isol*)

25-Isopropyl-27-norstigmasta-7,25-dien-3-ol I-226

25-(1-Methylethyl)-27-norstigmasta-7,25-dien-3-ol, 9CI. 26,26-Dimethylstigmasta-7,25(27)-dien-3-ol. 24-Ethyl-26,26-dimethyl-cholesta-7,25(27)-dien-3-ol



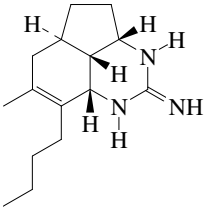
$C_{31}H_{52}O$ 440.751

(3β,5α)-*form*
Sutinasterol
[129620-23-1]
Constit. of a *Xestospongia* sp.
Cryst. (MeOH).
Mp 129-130°.

Kerr, R. *et al., J.O.C.*, 1991, **56**, 58-62 (*isol, pmr, cmr, cryst struct*)

Isoptilocaulin I-227

[78777-03-4]



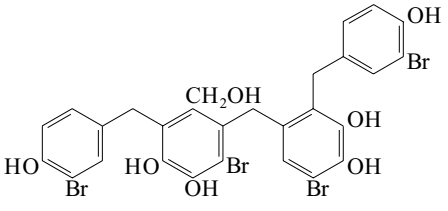
Absolute Configuration

$C_{15}H_{25}N_3$ 247.383
Constit. of the Caribbean sponge *Ptilocaulis* aff. *Ptilocaulis spiculifer*. Shows potent antitumour props. and activity against gram-positive bacteria. Poorly sol. hexane. λ_{max} 225 (ϵ 10000) (MeOH) (Derep).

Harbour, G.C. *et al., J.A.C.S.*, 1981, **103**, 5604 (*isol, pmr, cmr, ms, struct*)

Isorawsonol I-228

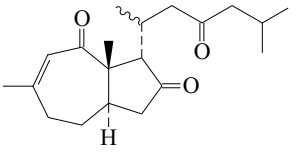
[158149-54-3]



$C_{28}H_{22}Br_4O_7$ 790.094
Constit. of the green alga *Avrainvillea rawsonii* (Halimedaceae). Inhibitor of inosine 5′-monophosphate dehydrogenase. Not an isomer of Rawsonol, R-11. λ_{max} 224 (ϵ 23000); 286 (ϵ 8900) (MeOH).

Chen, J.L. *et al., J. Nat. Prod.*, 1994, **57**, 947 (*isol, ms, pmr, cmr*)

Isoreiswigin I-229

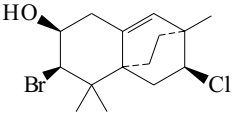


$C_{20}H_{30}O_3$ 318.455
Metab. of *Epipolasis reiswigi*. Oil. $[\alpha]_D^{25}$ +22 (c, 1.5 in $CHCl_3$). λ_{max} 240 (ϵ 2000) (heptane) (Derep).

Kashman, Y. *et al., J. Nat. Prod.*, 1991, **54**, 1430 (*isol, pmr, cmr*)

Isorhodolaureol I-230

[124596-91-4]

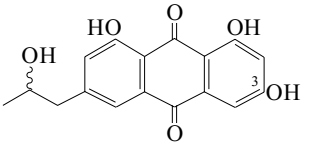


$C_{15}H_{22}BrClO$ 333.695
Metab. of *Laurencia majuscula*. Cryst.
Mp 120.5-122°. $[\alpha]_D$ +61 (c, 0.07 in $CHCl_3$).

Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1591 (*isol, pmr, cmr*)

Isorhodoptilometrin I-231

1,3,8-Trihydroxy-6-(2-hydroxypropyl)anthraquinone
[15979-75-6]



$C_{17}H_{14}O_6$ 314.294

Opt. active-*form* [97995-25-0]
Constit. of the crinoid *Ptilometra australis* and the starfish *Echinaster echinophorus*; also from *Lamprometra palmata gyges* and *Henricia leviuscula*.
Orange-red needles (MeOH). Spar. sol. org. solvs.
Mp 275-277°. Too insol. for optical rotation measurement.

Tetra-Ac:
Pale yellow needles (MeOH). Mp 161-162°. $[\alpha]_D$ -11 (c, 2.03 in $CHCl_3$).

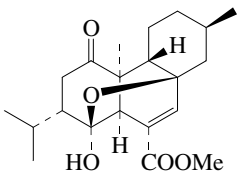
3-Me ether: ***Nalgiovensin***
[569-04-0]
$C_{18}H_{16}O_6$ 328.321
Produced by *Penicillium nalgiovensis*. Orange needles or plates.
Mp 199-200°. $[\alpha]_D^{20}$ +39.7 ($CHCl_3$).

(±)-*form*
Cryst. (MeOH). Mp 272-272.5°.

Birch, A.J. *et al., J.C.S.*, 1957, 2215-2217 (*Nalgiovensin*)
Powell, V.H. *et al., Aust. J. Chem.*, 1967, **20**, 541-553 (*uv*)
Banville, J. *et al., J.C.S. Perkin 1*, 1976, 613-619 (*synth*)
Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1977, **13**, 636-640; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 528-531 (*isol*)
Rideout, J.A. *et al., Aust. J. Chem.*, 1985, **38**, 793-808 (*isol*)
Ren, H. *et al., Arch. Pharmacal Res.*, 2006, **29**, 59-63 (*isol, pmr, cmr*)

Isosarcophytin I-232

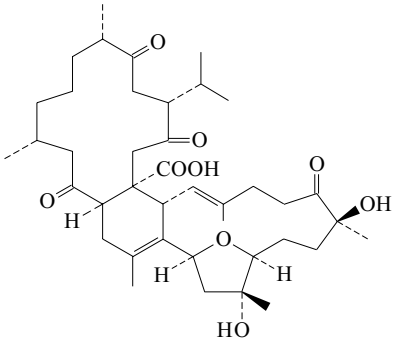
[259194-93-9]



$C_{21}H_{30}O_5$ 362.465
Constit. of *Sarcophyton elegans*. Needles (Me_2CO/hexane).
Mp 163-164°. $[\alpha]_D^{25}$ -61.2 (c, 0.25 in $CHCl_3$). λ_{max} 222 ($CHCl_3$).

Anjaneyulu, A.S.R. *et al., J. Indian Chem. Soc.*, 1999, **76**, 651-659 (*isol, pmr, cmr*)

Isosartortuic acid I-233



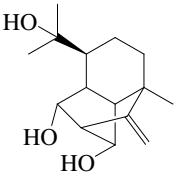
$C_{40}H_{60}O_9$ 684.909

Me ester: ***Methyl isosartortuate***
[100791-14-8]
$C_{41}H_{62}O_9$ 698.935
Constit. of *Sarcophyton tortuosum*. Cryst.
Mp 194-195°.

Jingyu, S. *et al., J.A.C.S.*, 1986, **108**, 177 (*isol, pmr, cmr, cryst struct*)

Isosativenetriol I-234

[405157-83-7]

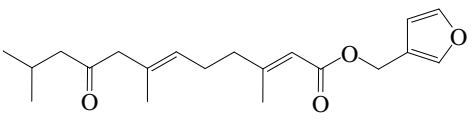


$C_{15}H_{24}O_3$ 252.353
Metab. of *Drechslera dematioidea*. Amorph. powder. $[\alpha]_D^{22}$ -2 (c, 0.1 in EtOH).

Osterhage, C. *et al., J. Nat. Prod.*, 2002, **65**, 306-313 (*isol, pmr, cmr*)

Isosecomarislin I-235

[78284-87-4]

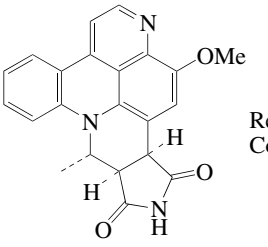


$C_{20}H_{28}O_4$ 332.439
Isol. from the nudibranch *Chromodoris marislae*. Oil.

Hochlowski, J.E. *et al., Tet. Lett.*, 1981, **22**, 271-274 (*isol, pmr*)

Isosegoline A I-236

[117694-97-0]



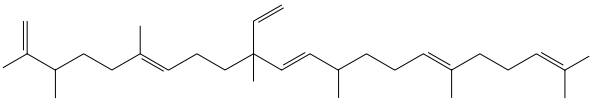
Relative Configuration

$C_{23}H_{19}N_3O_3$ 385.421
Alkaloid from the Red Sea tunicate *Eudistoma* sp.
$[\alpha]_D^{24}$ -660 (c, 0.001 in $CHCl_3$). λ_{max} 248 (ϵ 13400); 297 (ϵ 25000); 368 (ϵ 6100); 388 (ϵ 7700); 550 (ϵ 7800) (MeOH/HCl) (Derep). λ_{max} 242 (ϵ 13900); 274 (ϵ 19100); 330 (ϵ 9400); 360 (ϵ 2300); 386 (ϵ 3100); 470 (ϵ 3500) (MeOH) (Derep).

Rudi, A. *et al., J.O.C.*, 1989, **54**, 5331 (*isol, uv, ir, pmr, cmr, cd, struct*)

Isoshowacene I-237

10-Ethenyl-2,3,6,10,13,17,21-heptamethyl-1,6,11,16,20-docosapentaene, 9CI
[88361-08-4]

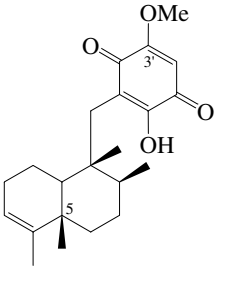


$C_{31}H_{52}$ 424.752
Constit. of *Botryococcus braunii* var. *shawa*. Related to the Botryococcenes.

Metzger, P. *et al., Tet. Lett.*, 1983, **24**, 4013 (*isol*)
Huang, Z. *et al., Phytochemistry*, 1989, **28**, 3043 (*isol, ms, pmr, cmr*)

Isospongiaquinone I-238

[69672-66-8]



$C_{22}H_{30}O_4$ 358.477
Constit. of *Stelospongia conulata*. Active against *Staphylococcus aureus*. Yellow cryst. (hexane).
Mp 135.5-136°. $[\alpha]_D^{20}$ +64.8 (c, 1 in $CHCl_3$). λ_{max} 218 (ϵ 23400); 243 (sh) (ϵ 12900); 289 (ϵ 74100); 525 (ϵ 4790) (EtOH/KOH) (Derep). λ_{max} 225 (ϵ 6610); 285 (ϵ 20400); 422 (ϵ 724) (EtOH) (Derep).

5-Epimer: ***5-Epiisospongiaquinone***
$C_{22}H_{30}O_4$ 358.477
Constit. of *Spongia hispida*. Yellow-orange oil. $[\alpha]_D^{20}$ -41.2 (c, 1.08 in $CHCl_3$). λ_{max} 205 (ϵ 12800); 285 (ϵ 2000) (EtOH).

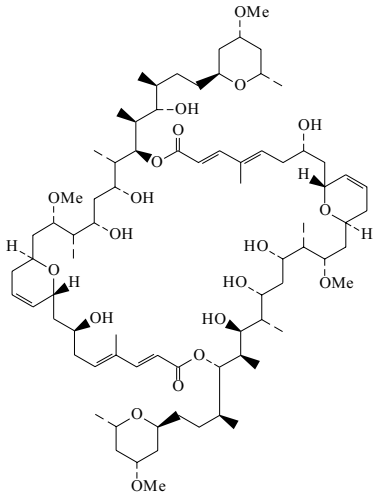
5-Epimer, 3′-O-de-Me, 3′-O-Et: ***5-Epihomoisospongiaquinone***
$C_{23}H_{32}O_4$ 372.503
Constit. of *Spongia hispida*. Yellow oil. $[\alpha]_D^{20}$ -28.8 (c, 0.17 in $CHCl_3$). Prob. artifact. λ_{max} 205 (ϵ 41000); 292 (ϵ 11300) (EtOH).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1978, **31**, 2685
Capon, R.J. *et al., J. Nat. Prod.*, 1990, **53**, 753 (*abs config*)

Urban, S. *et al., J. Nat. Prod.*, 1992, **55**, 1638-1642 (*isol, pmr, cmr*)
Popov, A.M. *et al., Pharm. Chem. J. (Engl. Transl.)*, 1999, **33**, 71-73; *CA*, 2000, **132**, 61495i (*isol, activity*)

Isoswinholide A I-239

[132923-57-0]

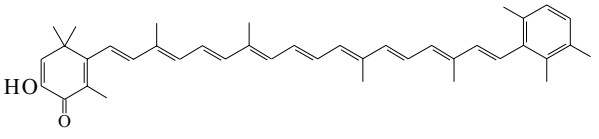


$C_{78}H_{132}O_{20}$ 1389.889
Constit. of the sponge *Theonella swinhoei*. Amorph. powder + $1H_2O$. $[\alpha]_D^{29}$ -42 (c, 0.51 in $CHCl_3$). Isomer of Swinholide A, S-548. λ_{max} 270 (ϵ 41400) (MeOH) (Derep). λ_{max} 269 (ϵ 38000) (MeOH) (Berdy).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2960 (*isol, pmr, cmr*)

Isotedanin I-240

2,3-Didehydro-3-hydroxy-β,ϕ-caroten-4-one
[74947-03-8]

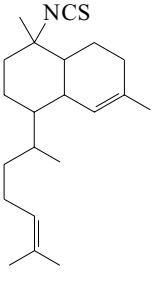


$C_{40}H_{48}O_2$ 560.818
Constit. of *Agelas mauritiana*. Purplish black needles. Mp 170-171°.

Yasuhara, M. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 1629 (*synth, uv, ir, pmr, ms*)
Tanaka, Y. *et al., Nippon Suisan Gakkaishi*, 1982, **48**, 531-533 (*occur*)

10-Isothiocyanato-4,15-bifloradiene I-241

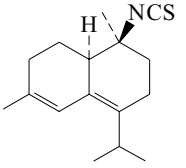
10-Isothiocyanato-1,14-bifloradiene
[141672-06-2]



$C_{21}H_{33}NS$ 331.564
Constit. of an Adocidae sponge and of *Cymbastela hooperi*. Oil. $[\alpha]_D$ +97 (c, 0.085 in $CHCl_3$). $[\alpha]_D^{25}$ +45 (c, 0.26 in $CHCl_3$).

Sharma, H.A. *et al., Tet. Lett.*, 1992, **33**, 1593 (*isol, pmr, cmr*)
Konig, G.M. *et al., J.O.C.*, 1996, **61**, 3529 (*isol, pmr, cmr*)

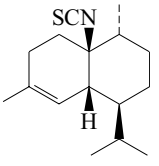
10-Isothiocyanato-4,6-cadinadiene I-242



$C_{16}H_{23}NS$ 261.43

(1α,10β)-*form*
10-Isothiocyanato-4,6-amorphadiene
[133738-45-1]
Metab. of *Axinyssa fenestratus*. Anthelmintic agent. Oil. $[\alpha]_D$ +74.4 (c, 9.8 in $CHCl_3$). λ_{max} 231 (ϵ 10700) (MeOH).
Alvi, K.A. *et al., J. Nat. Prod.*, 1991, **54**, 71-78 (*isol, pmr, cmr*)

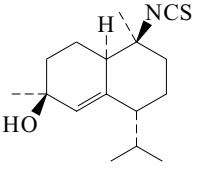
1-Isothiocyanato-4-cadinene I-243



$C_{16}H_{25}NS$ 263.446

(1β,6β,7β,10α)-*form*
1-Isothiocyanato-4-muurolene. 4-Muurolene-1-isothiocyanate
[117605-65-9]
Metab. of the sponge *Acanthella pulcherrima*.
Capon, R.J. *et al., Aust. J. Chem.*, 1988, **41**, 979-983

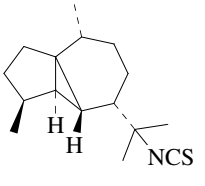
10-Isothiocyanato-5-cadinen-4-ol I-244



$C_{16}H_{25}NOS$ 279.446

(1α,4β,7α,10β)-*form*
10-Isothiocyanato-5-amorphen-4-ol
[133738-46-2]
Metab. of *Axinyssa fenestratus*. Anthelmintic agent. Oil.
Alvi, K.A. *et al., J. Nat. Prod.*, 1991, **54**, 71-78 (*isol, pmr, cmr*)

13-Isothiocyanatocubebane I-245



(5α,6β,7α,10α)-*form*

$C_{16}H_{25}NS$ 263.446

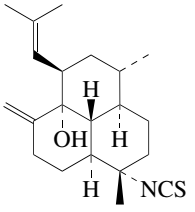
(5α,6β,7α,10α)-*form*
Constit. of *Axinyssa aplysinoides*.
Oil. $[\alpha]_D$ -19.9 (c, 1.1 in $CHCl_3$).

(5α,6β,7α,10β)-*form* [697299-16-4]
Constit. of a *Stylissa* sp.
Oil. $[\alpha]_D^{26}$ -15 (c, 1.2 in $CHCl_3$). λ_{max} 246 (ϵ 1339) (EtOH).
He, H.-Y. *et al., J.O.C.*, 1992, **57**, 3191 (*isol, pmr, cmr*)
Mitome, H. *et al., J. Nat. Prod.*, 2004, **67**, 833-837 (*Stylissa constit*)

12-Isothiocyanato-11-dodecenal **I-246**
SCNCH═CH$(CH_2)_9$CHO
$C_{13}H_{21}NOS$ 239.381

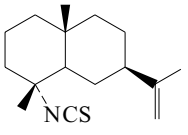
(*Z*)-*form* [111603-13-5]
Constit. of the marine sponge *Pseudaxinyssa* sp.
Karuso, P. *et al., Tet. Lett.*, 1987, **28**, 4633; 1988, **29**, 2506 (*isol*)

7-Isothiocyanato-11(20),14-epiamphilectadien-12-ol **I-247**
[175861-87-7]



$C_{21}H_{31}NOS$ 345.548
Constit. of *Cymbastela hooperi*. Shows antimalarial props.
$[\alpha]_D^{25}$ +78.4 (c, 0.56 in $CHCl_3$). Genus name given as Cymbastella.
λ_{max} 244 (ϵ 1530) (MeOH).
König, G.K. *et al., J.O.C.*, 1996, **61**, 3259-3267 (*isol, pmr, cmr*)

4-Isothiocyanato-11-eudesmene **I-248**



(4α,7α*H*)–*form*

$C_{16}H_{25}NS$ 263.446

(4α,7α*H*)-*form* [141696-05-1]
Constit. of *Acanthella klethra*.
Oil. $[\alpha]_D^{25}$ +180 (c, 0.025 in $CHCl_3$).

(4α,7β*H*)-*form* [141696-04-0]
Constit. of *Acanthella klethra*.
Cryst. (Et_2O).
Mp 62.3°. $[\alpha]_D^{25}$ +142.9 (c, 0.035 in $CHCl_3$).
König, G.M. *et al., J. Nat. Prod.*, 1992, **55**, 633-638 (*isol, pmr, cmr, cryst struct*)

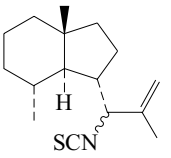
19-Isothiocyanato-18-nonadecenal **I-249**
SCNCH═CH$(CH_2)_{16}$CHO
$C_{20}H_{35}NOS$ 337.569

(*Z*)-*form* [111603-14-6]
Constit. of the marine sponge *Pseudaxinyssa* sp.
Karuso, P. *et al., Tet. Lett.*, 1987, **28**, 4633; 1988, **29**, 2506 (*isol*)

18-Isothiocyanato-17-octadecenal **I-250**
SCNCH═CH$(CH_2)_{15}$CHO
$C_{19}H_{33}NOS$ 323.542

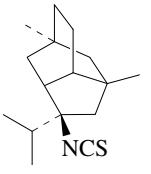
(*Z*)-*form* [111620-56-5]
Constit. of the marine sponge *Pseudaxinyssa* sp. λ_{max} 211 (ϵ 39400); 263 (sh) (ϵ 6400); 270 (ϵ 7200) (hexane). λ_{max} 211 (ϵ 39400); 270 (ϵ 7200) (hexane) (Berdy).
Karuso, P. *et al., Tet. Lett.*, 1987, **28**, 4633; 1988, **29**, 2506 (*isol, uv, ir, pmr, cmr*)

7-Isothiocyanato-11-oppositene **I-251**
10-Isothiocyanato-11-axene
[173692-42-7]



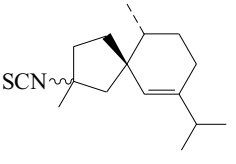
$C_{16}H_{25}NS$ 263.446
Constit. of *Acanthella cavernosa*.
$[\alpha]_D$ -52 (c, 0.1 in $CHCl_3$).
Hirota, H. *et al., Tetrahedron*, 1996, **52**, 2359 (*isol, pmr, cmr*)

5-Isothiocyanatopupukeanane **I-252**
[122762-78-1]



$C_{16}H_{25}NS$ 263.446
Constit. of an *Axinyssa* sp. Cryst. (hexane).
Mp 87-88°. $[\alpha]_D$ +33.5 (c, 7.6 in $CHCl_3$).
Marcus, A.H. *et al., J.O.C.*, 1989, **54**, 5184-5186 (*isol, pmr, cmr, cryst struct*)

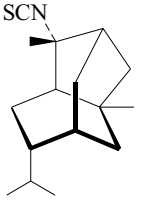
2-Isothiocyanato-6-spiroaxene **I-253**
2-Isothiocyanato-6-axene
[120475-54-9]



$C_{16}H_{25}NS$ 263.446
Constit. of *Trachyopsis aplysinoides*. Oil. $[\alpha]_D$ -13 (c, 0.25 in $CHCl_3$).

2-Formamide: 2-Formamido-6-spiroaxene. ***2-Formamido-6-axene***
[120475-57-2]
$C_{16}H_{27}NO$ 249.395
Constit. of *Trachyopsis aplysinoides*. Needles.
Mp 66-67°. $[\alpha]_D$ +14.8 (c, 1.5 in $CHCl_3$). Has –NHCHO replacing –NCS.
He, H. *et al., J.O.C.*, 1989, **54**, 2511 (*isol, pmr, cmr*)

2-Isothiocyanatotrachyopsane **I-254**
[120475-55-0]



$C_{16}H_{25}NS$ 263.446
Constit. of *Trachyopsis aplysinoides*. Needles.

Mp 52°. $[\alpha]_D$ +123.5 (c, 0.54 in $CHCl_3$). λ_{max} 244 (ϵ 1570) (MeOH) (Derep).

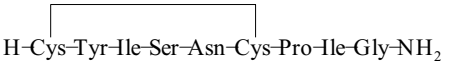
Isocyanide: ***2-Isocyanotrachyopsane***
[178888-21-6]
$C_{16}H_{25}N$ 231.38
Constit. of *Phyllidia varicosa* and *Phyllidia pustulosa*. Antifouling and antibarnacle agent. Larval settlement and metamorphosis inhibitor. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{23}$ +74.4 (c, 0.23 in $CHCl_3$). Has -NC replacing -NCS. λ_{max} 244 (ϵ 1570) (MeOH) (Derep).

Formamide: ***2-Formylaminotrachyopsane***
$C_{16}H_{27}NO$ 249.395
Constit. of *Axinyssa aplysinoides*. Cryst. $[\alpha]_D$ -67.5 (c, 0.56 in MeOH). Has -NHCHO replacing -NCS. λ_{max} 215; 354 (MeOH).

He, H. *et al., J.O.C.*, 1989, **54**, 2511-2514 (*isol, pmr, cmr, cryst struct*)
Okino, T. *et al., Tetrahedron*, 1996, **52**, 9447-9454 (*isocyanide*)
Patil, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 507-510 (*formamide, pmr, cmr, cryst struct*)

Isotocin I-255

4-L-Serine-8-L-isoleucineoxytocin, 9CI. Ichthyotocin
[550-21-0]

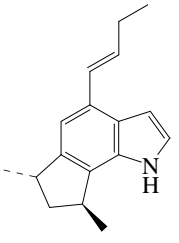


Oxytocin analogue. Isol. from various fish. Less biol. active than oxytocin. No phys. props. reported.

Acher, R. *et al., Biochim. Biophys. Acta*, 1962, **58**, 624 (*isol*)
Guttmann, S. *et al., Experientia*, 1962, **18**, 445 (*synth*)
Guttmann, S. *et al., Helv. Chim. Acta*, 1962, **45**, 2622 (*synth*)
Follett, B. *et al., J. Physiol. (London)*, 1964, **172**, 74 (*isol*)
Hruby, V.J. *et al., J.A.C.S.*, 1979, **101**, 202 (*cmr*)

Isotrikentrin B I-256

4-(1-Butenyl)-1,6,7,8-tetrahydro-6,8-dimethylcyclopent[g]indole, 9CI
[107368-94-5]
[152784-95-7]



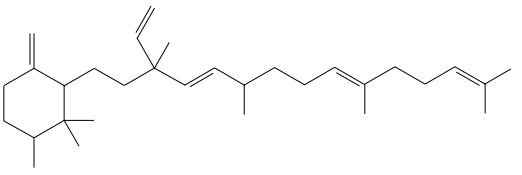
Absolute Configuration

$C_{17}H_{21}N$ 239.36
Inseparable mixt. with *cis*-Trikentrin B (ratio 2:3) (see Trikentrin B, T-697). Isol. from the marine sponge *Trikentrion flabelliforme*. Possesses antimicrobial activity. Unstable oil which darkens on storage. Sol. MeOH, $CHCl_3$. λ_{max} 240 (ϵ 44900); 298 (ϵ 12300) (MeOH).

Capon, R.J. *et al., Tetrahedron*, 1986, **42**, 6545-6550 (*isol, uv, ir, pmr, cmr, ms, struct*)
Muratake, H. *et al., Chem. Pharm. Bull.*, 1994, **42**, 854-864 (*abs config, synth*)

Isowolficene I-257

[117021-07-5]

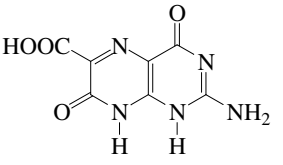


$C_{31}H_{52}$ 424.752
Metab. of *Botryococcus braunii*.

Huang, Z. *et al., J.O.C.*, 1988, **53**, 5390 (*isol, pmr, ms*)

Isoxanthopterincarboxylic acid I-258

2-Amino-1,4,7,8-tetrahydro-4,7-dioxo-6-pteridinecarboxylic acid, 9CI. 2-Amino-4,7-dihydroxy-6-pteridinecarboxylic acid, 8CI. Cyprino-Pourpre B
[3254-85-1]

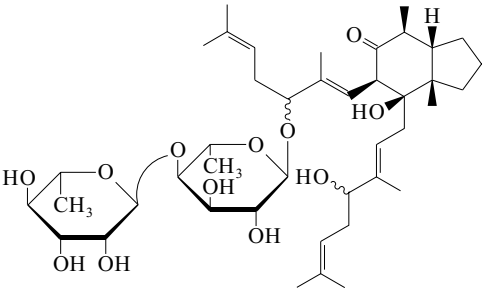


$C_7H_5N_5O_4$ 223.148
Isol. from the scales and skin of various fish. Cryst. Mp >360°. λ_{max} 224 (log ϵ 4.57); 259 (log ϵ 4); 282 (sh) (log ϵ 3.53); 347 (log ϵ 4.17) (0.1*M* NaOH).

Purrmann, R *et al., Annalen*, 1941, **548**, 284-292 (*synth*)
Matsuura, S *et al., J. Biochem. (Tokyo)*, 1955, **42**, 419-422 (*isol*)
Taylor, E.C. *et al., J.A.C.S.*, 1959, **81**, 2474-2479 (*synth*)
Taylor, E.C *et al., Tet. Lett.*, 1973, 2093-2095 (*synth*)

Isoxestovanin A I-259

[137415-08-8]

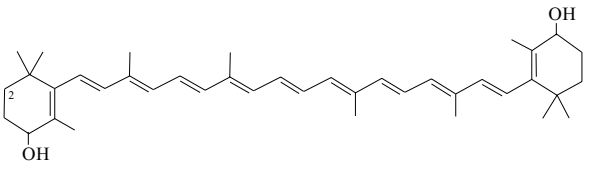


$C_{42}H_{68}O_{12}$ 764.992
Constit. of *Xestospongia vanilla*. Glass. $[\alpha]_D$ -4.4 (c, 0.16 in MeOH).

Morris, S.A. *et al., Can. J. Chem.*, 1991, **69**, 1352 (*isol, pmr, cmr*)

Isozeaxanthin I-260

β,β-Carotene-4,4′-diol. Aphanicol
[29065-03-0]



$C_{40}H_{56}O_2$ 568.881

Widespread in marine animals. Additive for salmon feed. Fine red needles (AcOH/petrol).
Mp 149-151°.

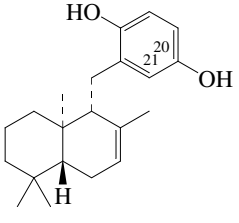
Diketone: ***Canthaxanthin***. *β,β-Carotene-4,4′-dione. Chlorellaxanthin. Aphanicin. Euglenanone. Carophyll red. E161g*
[514-78-3]
$C_{40}H_{52}O_2$ 564.85
Constit. of the edible mushroom *Cantharellus cinnabarinus*, sea trout, salmon and brine shrimp, *Corynebacterium michiganense* and the feathers and skin of flamingo *Phoeniconaias minor*. Also in green algae. Food colouring. Purple cryst. (C_6H_6/MeOH). Sol. $CHCl_3$, hexane; poorly sol. H_2O.
Mp 218°. Identity with Euglenanone is not certain. λ_{max} 470 (E1%/1cm 2250) (cyclohexane) (Berdy).

▶ FI0330000

Diketone, 2-hydroxy: ***2-Hydroxycanthaxanthin***. *2-Hydroxy-β,β-carotene-4,4′-dione*
[100485-10-7]
$C_{40}H_{52}O_3$ 580.849
Isol. from *Daphnia magna*. λ_{max} 470 (Me_2CO).

Isler, O. *et al., Helv. Chim. Acta*, 1956, **39**, 449 (*synth, ir*)
Warren, C.K. *et al., J.C.S.*, 1958, 3986 (*synth*)
Krinsky, N.I. *et al., Arch. Biochem. Biophys.*, 1960, **91**, 271 (*Euglenanone*)
Bodea, C. *et al., Annalen*, 1963, **666**, 189 (*ir*)
Di Accadia, F.D. *et al., Biochem. J.*, 1966, **101**, 735 (*Euglenanone*)
Hertzberg, S. *et al., Phytochemistry*, 1966, **5**, 565
Surmatis, J.D. *et al., Helv. Chim. Acta*, 1970, **53**, 974 (*synth*)
Kjoesen, H. *et al., Acta Chem. Scand.*, 1972, **26**, 2185 (*pmr*)
Gilchrist, B.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **54**, 343 (*biosynth*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97 (*cmr*)
Rosenberger, M. *et al., J.O.C.*, 1982, **47**, 2130 (*synth*)
Partali, V. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **82**, 767 (*2-Hydroxycanthaxanthin*)
Foss, P. *et al., Acta Chem. Scand., Ser. B*, 1986, **40**, 157 (*2-Hydroxycanthaxanthin*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 129; 380 (*bibl*)
Choi, S. *et al., J.O.C.*, 2005, **70**, 3328-3331 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CBE800

Isozonarol I-261



(+)-*form*

$C_{21}H_{30}O_2$ 314.467

The first-isolated enantiomer of Isozonarol (illus). belongs to the *ent*-series as generally understood. *ent*-Isozonarol, isol. more recently, belongs to the 'normal' series.

(+)-form [39707-55-6]
Constit. of *Dictyopteris zonarioides* and *Dictyopteris undulata*. Piscicide. Cryst. ($CHCl_3$). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O.
Mp 150-152°. $[\alpha]_D^{22}$ +28 (c, 1 in $CHCl_3$). λ_{max} 209 (ϵ 8210); 296 (ϵ 2700) (MeOH).

Quinone: ***Isozonarone***
[39707-59-0]
From *Dictyopteris undulata*. Ichthyotoxin. Piscicide. Yellow plates (MeOH).
Mp 111-112° Mp 130-132°. $[\alpha]_D$ +95.2 (MeOH). Poss. artifact.

ent-form
ent-*Isozonarol*
Constit. of *Dysidea* spp.
Yellow oil (as di-Ac). $[\alpha]_D^{25}$ -16.3 (c, 0.1 in $CHCl_3$) (di-Ac).

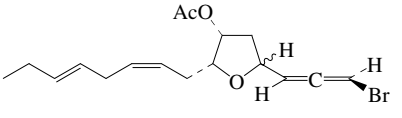
21-Hydroxy, 20-Ac: [852629-61-9]
$C_{23}H_{32}O_4$ 372.503
Constit. of *Dysidea* spp.
$[\alpha]_D^{19}$ -36.3 (c, 0.09 in $CHCl_3$) (-24). λ_{max} 284 (log ϵ 3.23) (MeOH).

21-Hydroxy, quinone: ***21-Hydroxy*-ent-*isozonarone***
[865357-53-5]
$C_{21}H_{28}O_3$ 328.45
Isol. from *Dysidea* cf. *cristagallii*. Yellow semicryst. solid. $[\alpha]_D^{19}$ -86 (c, 0.13 in $CHCl_3$). λ_{max} 254 (log ϵ 3.79); 409 (log ϵ 2.9) (MeOH).

[63813832 (±)-f-or-m]

Fenical, W. *et al., J.O.C.*, 1973, **38**, 2383-2387 (*ms, uv, ir*)
Welch, S.C. *et al., J.O.C.*, 1978, **43**, 1957-1961 (*synth, ir, uv, nmr*)
Ochi, M. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 629-630 (*isol*)
Schöder, J. *et al., Tet. Lett.*, 2000, **41**, 5469-5473 (*synth, pmr, cmr*)
Laube, T. *et al., Tetrahedron*, 2002, **58**, 4299-4309 (*synth*)
Perez-Garcia, E. *et al., J. Nat. Prod.*, 2005, **68**, 653-658 (*21-hydroxy-20-Ac*)
McNamara, C.E. *et al., J. Nat. Prod.*, 2005, **68**, 1431-1433 (*21-hydroxy, 21-hydroxy-20-Ac*)

Itomanallene B I-262

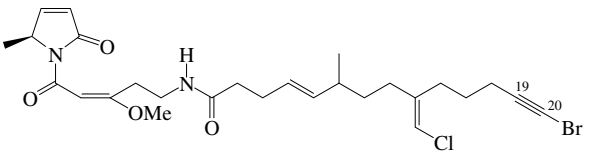


Relative Configuration

$C_{17}H_{23}BrO_3$ 355.271
Abs. config. of allene system is *S*- as shown. Constit. of *Laurencia intricata*. Oil. $[\alpha]_D^{23}$ +84 (c, 0.18 in $CHCl_3$).

Suzuki, M. *et al., Phytochemistry*, 2002, **60**, 861-867 (*isol, pmr, cmr, ms*)

Jamaicamide A J-1



$C_{27}H_{36}BrClN_2O_4$ 567.949
Isol. from *Lyngbya majuscula*. Neurotoxin. Pale yellow oil. $[\alpha]_D^{25}$ +44 (c, 1.5 in MeOH). λ_{max} 272 (log ϵ 3.9) (MeOH).

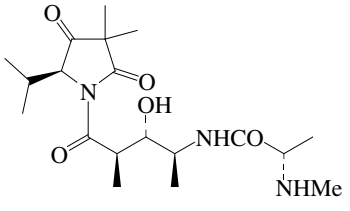
Debromo: ***Jamaicamide B***
$C_{27}H_{37}ClN_2O_4$ 489.053
Isol. from *Lyngbya majuscula*. Pale yellow oil. $[\alpha]_D^{25}$ +53 (c, 0.61 in MeOH). λ_{max} 272 (log ϵ 3.9) (MeOH).

Debromo, 19,20-dihydro: ***Jamaicamide C***
$C_{27}H_{39}ClN_2O_4$ 491.069
Isol. from *Lyngbya majuscula*. Pale yellow oil. $[\alpha]_D^{25}$ +49 (c, 0.39 in MeOH). λ_{max} 273 (log ϵ 3.8) (MeOH).

Edwards, D.J. *et al., Chem. Biol.*, 2004, **11**, 817-833 (*isol, biosynth, pmr, cmr*)

Janolusimide J-2

[103612-45-9]



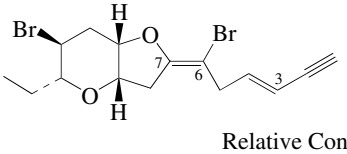
Absolute Configuration

$C_{19}H_{33}N_3O_5$ 383.487
Peptide toxin. Isol. from *Janolus cristatus*. Neurotoxin, atropine antagonist. Amorph. $[\alpha]_D^{25}$ -10.3 (c, 2.5 in $CHCl_3$).
▶ LD_{50} (mus, ipr) 5 mg/kg.

Sodano, G. *et al., Tet. Lett.*, 1986, **27**, 2505-2508 (*isol, struct, nmr*)
Giordano, A. *et al., Tet. Lett.*, 2000, **41**, 3979-3982 (*synth, abs config*)

Japonenyne A J-3

6,12-Dibromo-7,10:9,13-diepoxy-3-pentadecen-1-yne



Relative Configuration

$C_{15}H_{18}Br_2O_2$ 390.114
Constit. of the red alga *Laurencia japonensis*. Oil. $[\alpha]_D^{21}$ +40.2 (c, 1.39 in CH_2Cl_2).

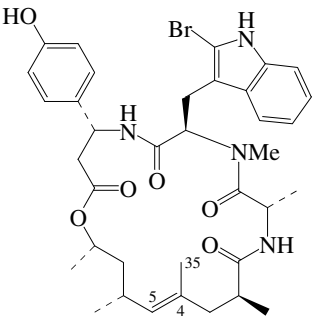
(3Z)-Isomer: ***Japonenyne B***
$C_{15}H_{18}Br_2O_2$ 390.114
Isol. from *Laurencia japonensis*. Oil. $[\alpha]_D^{21}$ +24.4 (c, 0.61 in CH_2Cl_2).

6,7-Dihydro, 7-methoxy: ***Japonenyne C***
$C_{16}H_{22}Br_2O_3$ 422.156
Isol. from *Laurencia japonensis*. Oil. $[\alpha]_D^{26}$ -35.5 (c, 0.06 in $CHCl_3$). Possible artifact. Stereochem. at C-6 and C-7 not determined.

Takahashi, Y. *et al., Phytochemistry*, 1999, **50**, 799-803 (*isol, ir, pmr, cmr, ms*)

Jaspamide J-4

Jasplakinolide
[102396-24-7]



$C_{36}H_{45}BrN_4O_6$ 709.679
Cyclodepsipeptide antibiotic. Isol. from the marine sponge *Jaspis* sp. F-actin inhibitor. Active against yeasts, nematodes and carcinoma. Possesses antifungal, anthelmintic and insecticidal props. $[\alpha]_D$ +35 (c, 3.62 in MeOH). λ_{max} 281 (ϵ 5400); 290 (ϵ 4100) (MeOH) (Derep).

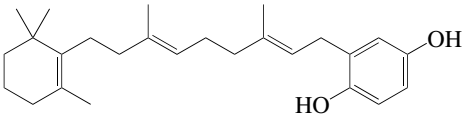
$\Delta^{4,35}$-Isomer, 5-oxo: ***Jaspamide B***
[219774-74-0]
$C_{36}H_{43}BrN_4O_7$ 723.662
Isol. from *Jaspis splendans*. Glass. $[\alpha]_D^{25}$ +11.4 (c, 0.0014 in $CHCl_3$). λ_{max} 232 (log ϵ 3.75); 278 (log ϵ 3.66) (MeOH).

$\Delta^{4,35}$-Isomer, 5ξ-hydroxy: ***Jaspamide C***
[219774-75-1]
$C_{36}H_{45}BrN_4O_7$ 725.678
Isol. from *Jaspis splendans*. Glass. $[\alpha]_D^{25}$ +25.4 (c, 0.0013 in $CHCl_3$). λ_{max} 220 (log ϵ 3.37); 276 (log ϵ 2.71) (MeOH).

Zabriskie, T.M. *et al., J.A.C.S.*, 1986, **108**, 3123 (*isol, ir, pmr, cmr, cryst struct*)
Crews, P. *et al., Tet. Lett.*, 1986, **27**, 2797 (*isol, uv, ir, pmr, cmr, ms, struct*)
Braekman, J.C. *et al., J. Nat. Prod.*, 1987, **50**, 994 (*isol, pmr, cmr, ir, uv, ms*)
Grieco, P.A. *et al., J.A.C.S.*, 1988, **110**, 1630 (*synth*)
Kato, S. *et al., Tet. Lett.*, 1988, **29**, 6465 (*synth*)
Inman, W. *et al., J.O.C.*, 1989, **54**, 2523 (*props, bibl*)
Konopelski, J.P. *et al., J.O.C.*, 1991, **56**, 1355 (*synth*)
Kang, S.K. *et al., Synlett*, 1991, 175 (*synth*)
Rao, A.V.R. *et al., Tet. Lett.*, 1993, **34**, 7085 (*synth*)
Hirai, Y. *et al., Heterocycles*, 1994, **39**, 603 (*synth*)
Imaeda, T. *et al., Tet. Lett.*, 1994, **35**, 591 (*synth*)
Ashworth, P. *et al., Synthesis*, 1995, 199 (*synth*)
Zampella, A. *et al., J. Nat. Prod.*, 1999, **62**, 332-334 (*Jaspamides B,C*)
Tabudravu, J.N. *et al., Org. Biomol. Chem.*, 2005, **3**, 745-749 (*conformn*)

Jaspaquinol J-5

[193074-50-9]

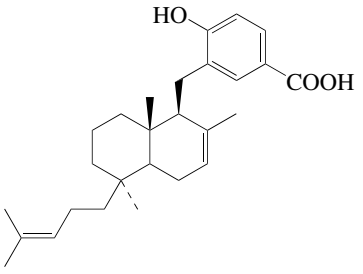


$C_{26}H_{38}O_2$ 382.585
Constit. of *Jaspis* cf. *johnstoni*. Yellow oil. λ_{max} 217; 290 (no solvent reported).

Murray, L.M. *et al., J.O.C.*, 1997, **62**, 5638-5641 (*isol, pmr, cmr*)

Jaspic acid J-6

[193074-49-6]

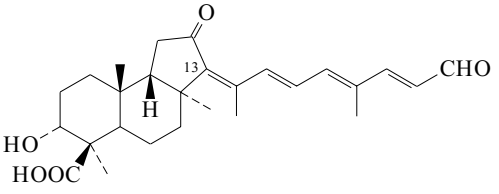


$C_{27}H_{38}O_3$ 410.595
Constit. of *Jaspis* cf. *johnstoni*. Yellow oil. $[\alpha]_D^{22}$ -22.9 (c, 0.8 in EtOH). λ_{max} 216; 258; 290 (no solvent reported).

Murray, L.M. *et al., J.O.C.*, 1997, **62**, 5638-5641 (*isol, pmr, cmr*)

Jaspiferal A J-7

[176181-86-5]



$C_{27}H_{36}O_5$ 440.578
Constit. of *Jaspis stellifera*. Oil (as Me ester). Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{22}$ -18.9 (c, 0.09 in C_6H_6) (Me ester). λ_{max} 273 (ϵ 10000); 374 (ϵ 41000); 392 (sh) (EtOH). λ_{max} 273 (ϵ 10000); 374 (ϵ 40000) (MeOH) (Berdy).

*13*E-*Isomer:* ***Jaspiferal B***
[176300-90-6]
$C_{27}H_{36}O_5$ 440.578
Constit. of *Jaspis stellifera*. Oil (as Me ester). Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{22}$ -123.7 (c, 0.07 in C_6H_6) (Me ester). λ_{max} 273 (ϵ 10000); 374 (ϵ 41000); 392 (sh) (EtOH). λ_{max} 273 (ϵ 10000); 374 (ϵ 40000) (MeOH) (Berdy).

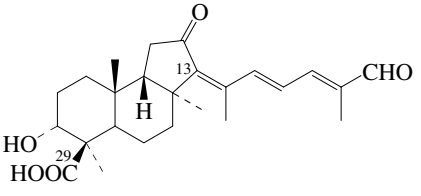
*13*E-*Isomer, 3-Ac:* ***3-Acetyljaspiferal B***
[282118-90-5]
$C_{29}H_{38}O_6$ 482.616
Constit. of a *Jaspis* sp.

*13*E-*Isomer, 3-Ac, Me ester:* [282118-85-8]
$C_{30}H_{40}O_6$ 496.642
Yellow amorph. solid. $[\alpha]_D^{25}$ -30.8 (c, 0.8 in $CHCl_3$). λ_{max} 268 (log ϵ 3.1); 363 (log ϵ 3.8); 385 (sh) (MeOH).

Kobayashi, J. *et al., Tetrahedron*, 1996, **52**, 5745 (*isol, pmr, cmr*)
Zampella, A. *et al., J. Nat. Prod.*, 2000, **63**, 943-946 (*3-Acetyljaspiferal B*)

Jaspiferal C J-8

[176181-87-6]



$C_{25}H_{34}O_5$ 414.541
Constit. of *Jaspis stellifera*. Cytotoxic to KB cells. Oil (as Me ester). Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{19}$ -24 (c, 0.14 in C_6H_6) (Me ester). λ_{max} 251 (ϵ 7800); 344 (ϵ 40000); 357 (sh) (MeOH).

29-Alcohol: ***Auroral 1***
[286437-74-9]
$C_{25}H_{36}O_4$ 400.557
Constit. of *Rhabdastrella globostellata*.

*13*E-*Isomer:* ***Jaspiferal D***
[176300-91-7]
$C_{25}H_{34}O_5$ 414.541
Constit. of *Jaspis stellifera*. Cytotoxic to KB cells. Oil (as Me ester). Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{19}$ -85 (c, 0.14 in C_6H_6) (Me ester). λ_{max} 251 (ϵ 7800); 344 (ϵ 40000); 357 (MeOH) (Berdy).

*13*E-*Isomer, 3-Ac:* ***3-Acetyljaspiferal D***
[282118-91-6]
$C_{27}H_{36}O_6$ 456.578
Constit. of a *Jaspis* sp.

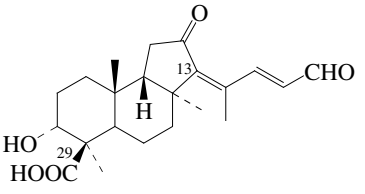
*13*E-*Isomer, 3-Ac, Me ester:* [282118-86-9]
$C_{28}H_{38}O_6$ 470.605
Yellow amorph. solid. $[\alpha]_D^{25}$ -198.4 (c, 1 in $CHCl_3$). λ_{max} 288 (log ϵ 3.1); 339 (log ϵ 3.8); 385 (sh) (MeOH).

*13*E-*Isomer, 29-alcohol:* ***Auroral 2***
[286437-75-0]
$C_{25}H_{36}O_4$ 400.557
Constit. of *Rhabdastrella globostellata*.

Kobayashi, J. *et al., Tetrahedron*, 1996, **52**, 5745-5750 (*Jaspis stellifera constits*)
Zampella, A. *et al., J. Nat. Prod.*, 2000, **63**, 943-946 (*3-Acetyljaspiferal D*)
Bourguet-Kondracki, M.-L. *et al., Tet. Lett.*, 2000, **41**, 3087-3090 (*Aurorals, activity*)

Jaspiferal E J-9

[176181-94-5]



$C_{22}H_{30}O_5$ 374.476
Constit. of *Jaspis stellifera*. Oil (as Me ester). Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{18}$ -51 (c, 0.18 in C_6H_6) (Me ester). λ_{max} 218 (ϵ 17800); 304 (ϵ 41300) (no solvent reported). λ_{max} 218 (ϵ 17800); 304 (ϵ 41300) (MeOH) (Berdy).

29-Alcohol: ***Auroral 3***
[286437-76-1]
$C_{22}H_{32}O_4$ 360.492
Constit. of *Rhabdastrella globostellata*.

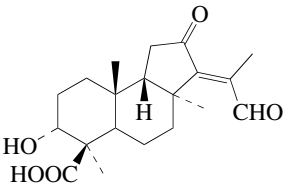
*13*E-*Isomer:* ***Jaspiferal F***
[176302-65-1]
$C_{22}H_{30}O_5$ 374.476
Constit. of *Jaspis stellifera*. Oil (as Me ester). Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{18}$ -116 (c, 0.12 in C_6H_6) (Me ester). λ_{max} 218 (ϵ 17800); 304 (ϵ 41300) (MeOH) (Berdy).

*13*E-*Isomer, 29-alcohol:* [286437-77-2]
$C_{22}H_{32}O_4$ 360.492
Constit. of *Rhabdastrella globostellata*.

Kobayashi, J. *et al., Tetrahedron*, 1996, **52**, 5745 (*isol, pmr, cmr*)
Bouguet-Kondracki, M.-L. *et al., Tet. Lett.*, 2000, **41**, 3087-3090 (*Aurorals*)

Jaspiferal G J-10

[176181-98-9]



$C_{20}H_{28}O_5$ 348.438
Constit. of *Jaspis stellifera*. Powder. Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 145-147°. $[\alpha]_D^{20}$ -54 (c, 0.3 in $CHCl_3$/MeOH). λ_{max} 202 (ϵ 7000); 266 (ϵ 14000) (MeOH).

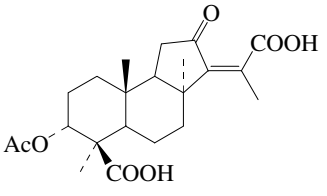
Ac: 3-Acetyljaspiferal G
[282118-92-7]
$C_{22}H_{30}O_6$ 390.475
Constit. of a *Jaspis* sp.

Ac, Me ester: [282118-87-0]
$C_{23}H_{32}O_6$ 404.502
Yellow amorph. solid. $[\alpha]_D^{25}$ -46.8 (c, 0.4 in $CHCl_3$). λ_{max} 207 (log ϵ 3.8); 260 (log ϵ 4) (MeOH).

Kobayashi, J. *et al., Tetrahedron*, 1996, **52**, 5745-5750 (*isol, pmr, cmr*)
Zampella, A. *et al., J. Nat. Prod.*, 2000, **63**, 943-946 (*Ac*)

Jaspiferoic acid A J-11

[282524-63-4]
[282118-88-1]

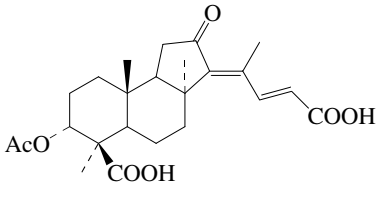


$C_{22}H_{30}O_7$ 406.475
Constit. of a *Jaspis* sp. Yellow amorph. solid (as di-Me ester). $[\alpha]_D^{25}$ -30.1 (c, 0.6 in $CHCl_3$) (di-Me ester). λ_{max} 208 (log ϵ 3.6); 240 (log ϵ 4.2) (MeOH) (di-Me ester).

Zampella, A. *et al., J. Nat. Prod.*, 2000, **63**, 943-946 (*isol, pmr, cmr*)

Jaspiferoic acid B J-12

[282524-64-5]
[282118-89-2]

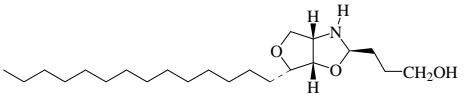


$C_{24}H_{32}O_7$ 432.513
Constit. of a *Jaspis* sp. Yellow amorph. solid (as di-Me ester). $[\alpha]_D^{25}$ -38.4 (c, 0.8 in $CHCl_3$) (di-Me ester). λ_{max} 215 (log ϵ 3.6); 304 (log ϵ 4.5) (di-Me ester).

Zampella, A. *et al., J. Nat. Prod.*, 2000, **63**, 943-946 (*isol, pmr, cmr*)

Jaspine A J-13

[501690-67-1]



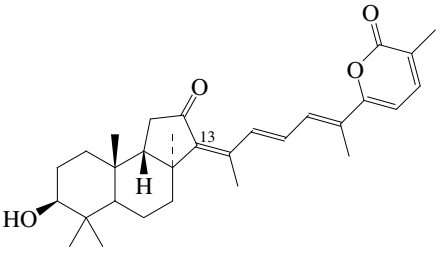
Absolute Configuration

$C_{22}H_{43}NO_3$ 369.587
Isol. from the sponge *Jaspis* sp. Cytotoxic. Amorph. powder. $[\alpha]_D^{20}$ +25 (c, 1 in $CHCl_3$).

Ledroit, V. *et al., Tet. Lett.*, 2003, **44**, 225-228 (*isol, pmr, cmr*)

Jaspolide A J-14

[890041-67-5]



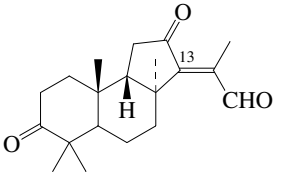
$C_{30}H_{40}O_4$ 464.644
Constit. of a *Jaspis* sponge. Yellow cryst.
Mp 260-263°. $[\alpha]_D^{25}$ -42.9 (c, 0.02 in Me_2CO).

*13*E-*Isomer:* ***Jaspolide B***
[890041-68-6]
$C_{30}H_{40}O_4$ 464.644
Constit. of a *Jaspis* sponge. Yellow cryst.
Mp 259-260°. $[\alpha]_D^{25}$ -86.7 (c, 0.03 in Me_2CO).

Tang, S. *et al., Chem. Pharm. Bull.*, 2006, **54**, 4-8 (*Jaspolides A and B*)

Jaspolide C J-15

[890041-69-7]



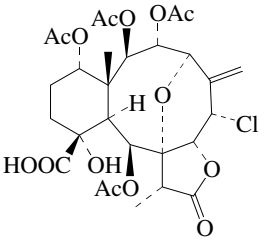
$C_{20}H_{28}O_3$ 316.439
Constit. of a *Jaspis* sponge. Oil. $[\alpha]_D^{25}$ -7.7 (c, 0.01 in Me_2CO).

13Z-Isomer: ***Jaspolide D***
[890041-70-0]
$C_{20}H_{28}O_3$ 316.439
Constit. of a *Jaspis* sponge. Oil. $[\alpha]_D^{25}$ -10.1 (c, 0.01 in Me_2CO).

Tang, S. *et al., Chem. Pharm. Bull.*, 2006, **54**, 4-8 (*Jaspolides C and D*)

Jaspolide E J-16

[890041-71-1]

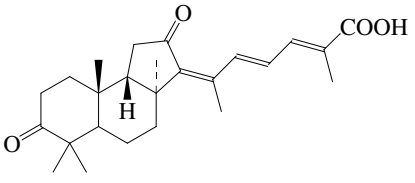


$C_{31}H_{42}O_5$ 494.67
Constit. of a *Jaspis* sponge. Yellow solid. $[\alpha]_D^{25}$ -8.6 (c, 0.2 in Me_2CO).

Tang, S. *et al., Chem. Pharm. Bull.*, 2006, **54**, 4-8 (*Jaspolide E*)

Jaspolide F J-17

[890041-72-2]

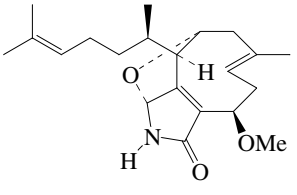


$C_{25}H_{34}O_4$ 398.541
Constit. of a *Jaspis* sponge. Pale yellow solid. $[\alpha]_D^{25}$ -14.9 (c, 0.01 in Me_2CO).

Tang, S. *et al., Chem. Pharm. Bull.*, 2006, **54**, 4-8 (*Jaspolide F*)

Joalin J-18

[150999-04-5]

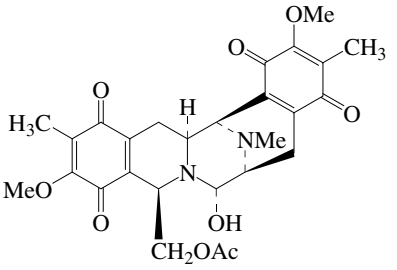


$C_{21}H_{31}NO_3$ 345.481
Constit. of a *Dictyota* sp. Semicryst. $[\alpha]_D^{29}$ -59 (c, 0.01 in $CHCl_3$). λ_{max} 205 (ϵ 12300); 245 (MeOH) (Berdy).

Guella, G. *et al., J.C.S. Perkin 1*, 1993, 1545 (*isol, pmr, cmr*)

Jorumycin J-19

[304852-37-7]



$C_{27}H_{30}N_2O_9$ 526.542

Related to Renieramycin A, R-17. Isol. from the marine nudibranch *Jorunna funebris*. Antitumour agent. Unstable pale yellow powder. $[\alpha]_D$ -57 (c, 0.05 in $CHCl_3$). λ_{max} 266 (ϵ 15000) (MeOH).

Fontana, A. *et al., Tetrahedron*, 2000, **56**, 7305-7308 (*isol*)
Saito, N. *et al., Tetrahedron*, 2004, **60**, 3873-3881 (*synth, pmr, cmr*)
Lane, J.W. *et al., J.A.C.S.*, 2005, **127**, 12684-12690 (*synth*)

Julianin S J-20

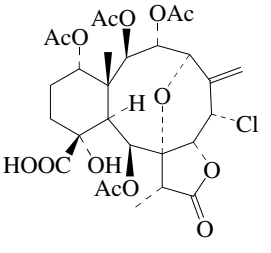
[125692-57-1]

Single chain protein. Isol. from the foetid secretion of the sea hare *Aplysia juliana*. Shows antimicrobial and antitumour activity. Toxic to crabs. Sol. H_2O. λ_{max} 280 (H_2O) (Berdy).

Kamiya, H. *et al., Toxicon*, 1989, **27**, 1269-1277 (*isol*)

Juncin N J-21

[656253-49-5]

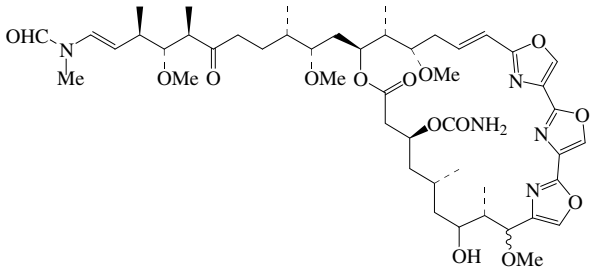


$C_{28}H_{35}ClO_{14}$ 631.029
Constit. of *Junceella juncea*. Powder (EtOAc).
Mp 214-216°. $[\alpha]_D^{25}$ +18 (c, 0.3 in $CHCl_3$).

Sung, P.-J. *et al., Heterocycles*, 2003, **61**, 587-592 (*isol, pmr, cmr, ms*)

Kabiramide C K-1

[100045-78-1]



$C_{48}H_{71}N_5O_{14}$ 942.114

Macrolide antibiotic. Related to Halichondramide, H-16. Isol. from the eggs of *Hexabranchus* sp. Shows antifungal props. Solid. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{23}$ +20 (c, 0.1 in $CHCl_3$). λ_{max} 245 (ϵ 26000) (MeOH) (Derep).

47-Hydroxy: ***Kabiramide A***
[101550-93-0]
$C_{48}H_{71}N_5O_{15}$ 958.113
Isol. from the eggs of *Hexabranchus* sp. Cytotoxic. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{23}$ +6 (c, 0.1 in $CHCl_3$). λ_{max} 245 (ϵ 26000) (MeOH) (Derep). λ_{max} 245; 345 (ϵ 25000) (MeOH) (Berdy).

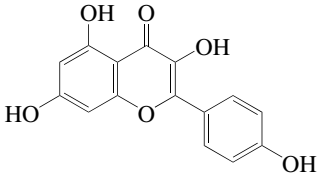
14-O-De-Me: ***Kabiramide B***
[101550-94-1]
$C_{47}H_{69}N_5O_{14}$ 928.087
Isol. from the eggs of *Hexabranchus* sp. Cytotoxic. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{23}$ +8 (c, 0.1 in $CHCl_3$). λ_{max} 245 (ϵ 26000) (MeOH) (Derep).

21-O-De(aminocarbonyl): ***Kabiramide D***
[101550-95-2]
$C_{47}H_{70}N_4O_{13}$ 899.089
Isol. from the eggs of *Hexabranchus* sp. Cytotoxic agent. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{23}$ -5 (c, 0.1 in $CHCl_3$). λ_{max} 245 (ϵ 26000) (MeOH) (Derep).

21-O-De(aminocarbonyl), 21-Ac: ***Kabiramide E***
[101550-96-3]
$C_{49}H_{72}N_4O_{14}$ 941.126
Isol. from the eggs of *Hexabranchus* sp. Cytotoxic agent. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{23}$ -20 (c, 0.1 in $CHCl_3$). λ_{max} 245 (ϵ 26000) (MeOH) (Derep).

Matsunaga, S. *et al., J.A.C.S.*, 1986, **108**, 847-849 (*isol, pmr, cmr*)
Matsunaga, S. *et al., J.O.C.*, 1989, **54**, 1360-1363 (*isol, pmr, cmr*)

Kaempferol 3-glycosides K-2



Glycosides of 3,4′,5,7-Tetrahydroxyflavone with glycosyl residue at O^3 only.

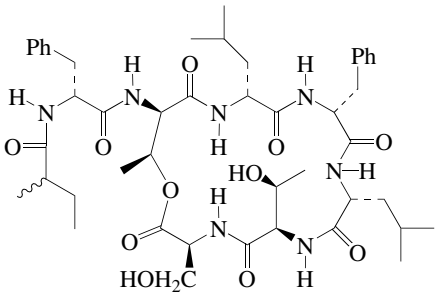
Monoglycosides

3-O-α-L-Fucopyranoside: Kaempferol 3-α-L-fucopyranoside. ***Acanthophorin A***
[200860-90-8]
$C_{21}H_{20}O_{10}$ 432.383
Isol. from the red alga *Acanthophora spicifera*. Amorph. yellow solid (MeOH/$CHCl_3$).
Mp 168-169°. $[\alpha]_D^{20}$ -161 (c, 0.02 in MeOH). λ_{max} 265 (log ϵ 4.13); 344 (log ϵ 3.75) (MeOH).

Zeng, L.-M. *et al., Chin. J. Chem.*, 2001, **19**, 1097-1100 (*Acanthophorin A*)

Kahalalide A K-3

[179733-11-0]



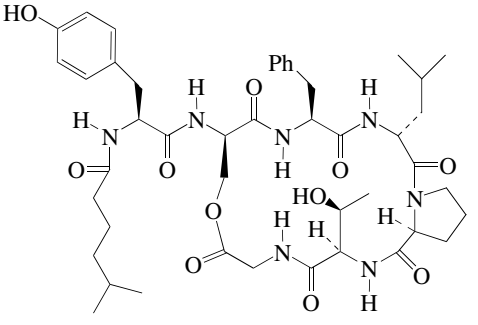
$C_{46}H_{67}N_7O_{11}$ 894.076

Depsipeptide. Isol. from the mollusc *Elysia rufescens* which feeds on the alga *Bryopsis* sp.
$[\alpha]_D$ -19 (c, 1 in MeOH). λ_{max} 204 (ϵ 33640) (MeOH).

Hamann, M.T. *et al., J.O.C.*, 1996, **61**, 6594-6600 (*isol, uv, ir, pmr, cmr*)
Bourel-Bonnet, L. *et al., J. Med. Chem.*, 2005, **48**, 1330-1335 (*synth*)

Kahalalide B K-4

[180714-95-8]



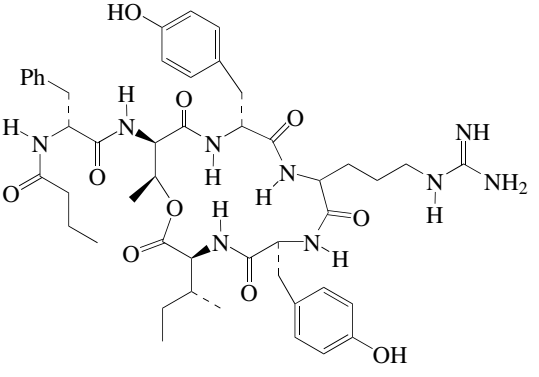
$C_{45}H_{63}N_7O_{11}$ 878.033

Depsipeptide. Isol. from the mollusc *Elysia rufescens* which feeds on the alga *Bryopsis* sp.
$[\alpha]_D$ +43 (c, 2.5 in MeOH). λ_{max} 204 (ϵ 51500); 226 (sh) (ϵ 21320); 274 (ϵ 17580) (MeOH).

Hamann, M.T. *et al., J.O.C.*, 1996, **61**, 6594-6600 (*isol, uv, ir, pmr, cmr*)
Lopez-Macia, A. *et al., Tet. Lett.*, 2000, **41**, 9765-9769 (*synth*)

Kahalalide C K-5

[180714-96-9]



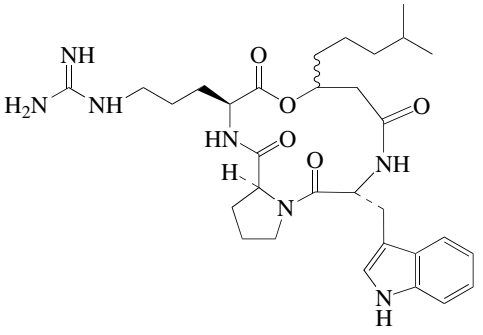
$C_{47}H_{63}N_9O_{10}$ 914.069

Isol. from the mollusc *Elysia rufescens* which feeds on the alga *Bryopsis* sp.
$[\alpha]_D$ +46 (c, 0.4 in MeOH). λ_{max} 202 (ϵ 16010); 224 (sh) (ϵ 1825) (MeOH).

Hamann, M.T. *et al., J.O.C.*, 1996, **61**, 6594-6600 (*isol, uv, ir, pmr, cmr*)

Kahalalide D K-6

[180714-97-0]



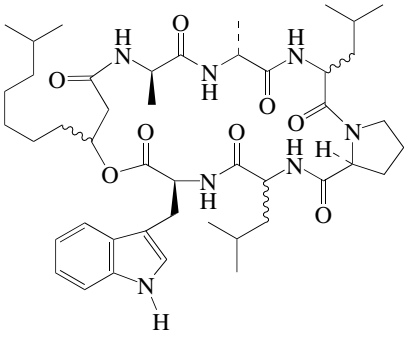
$C_{31}H_{45}N_7O_5$ 595.74

Depsipeptide. Isol. from the mollusc *Elysia rufescens* which feeds on the alga *Bryopsis* sp.
$[\alpha]_D$ +51 (c, 1 in MeOH). λ_{max} 206 (sh) (ϵ 16895); 220 (ϵ 18710); 282 (ϵ 3180) (MeOH).

Hamann, M.T. *et al., J.O.C.*, 1996, **61**, 6594-6600 (*isol, uv, ir, pmr, cmr*)

Kahalalide E K-7

[180714-98-1]



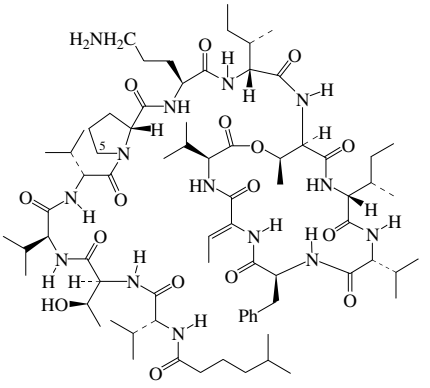
$C_{45}H_{69}N_7O_8$ 836.082

Depsipeptide. Isol. from the mollusc *Elysia rufescens* which feeds on an alga *Bryopsis* sp.
$[\alpha]_D$ +5 (c, 1 in MeOH). λ_{max} 204 (ϵ 23910); 222 (ϵ 24720); 272 (ϵ 15430) (MeOH).

Hamann, M.T. *et al., J.O.C.*, 1996, **61**, 6594-6600 (*isol, uv, ir, pmr, cmr*)

Kahalalide F K-8

[149204-42-2]



Absolute Configuration

$C_{75}H_{124}N_{14}O_{16}$ 1477.889

Depsipeptide antibiotic. Isol. from the mollusc *Elysia rufescens* and the alga *Bryopsis* sp. Cytotoxic and antifungal agent. Phase II clin. trial for the treatment of various tumours and for the treatment of severe psoriasis (2004). White powder. $[\alpha]_D$ -8 (c, 4.32 in MeOH). λ_{max} 204 (ϵ 89630) (MeOH) (Berdy).

Hamann, M.T. *et al., J.A.C.S.*, 1993, **115**, 5825-5826 (*isol, struct, pmr, cmr, props*)
Garcia-Rocha, M. *et al., Cancer Lett. (Shannon, Irel.)*, 1996, **99**, 43-50 (*pharmacol*)
Goetz, G. *et al., Tetrahedron*, 1999, **55**, 7739-7746 (*abs config*)
López-Macià, A. *et al., J.A.C.S.*, 2001, **123**, 11398-11401 (*synth, abs config*)
Bonnard, I. *et al., J. Nat. Prod.*, 2003, **66**, 1466-1470 (*abs config*)
Suarez, Y. *et al., Mol. Cancer Ther.*, 2003, **2**, 863-872 (*pharmacol*)
Gracia, C. *et al., J.O.C.*, 2006, **71**, 7196-7204 (*synth*)

Kahalalide G K-9

[180714-99-2]

$(H_3C)_2CH(CH_2)_3CO$ –Val—Thr—Val—Val—Pro—Orn—Ile—Thr—

Ile—Val—Phe—Dhb—Val—OH

Dhb = 2-amino-2-butenoic acid

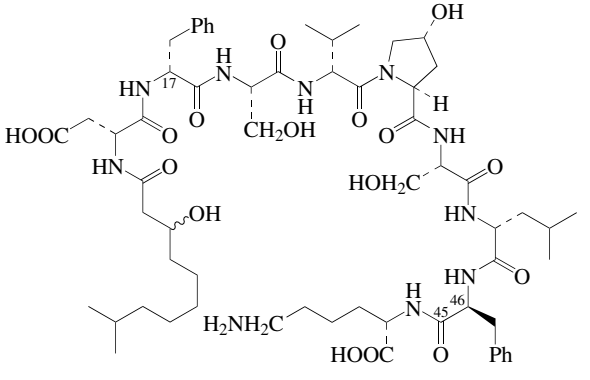
$C_{75}H_{126}N_{14}O_{17}$ 1495.904

Peptide antibiotic. Isol. from the green alga *Bryopsis* sp.
$[\alpha]_D$ +22.5 (c,1 in MeOH). λ_{max} 203 (ϵ 58300) (MeOH).

Scheuer, P.J. *et al., J. Nat. Prod.*, 1995, **58**, 340 (*rev*)
Hamann, M.T. *et al., J.O.C.*, 1996, **61**, 6594-6600 (*isol, uv, ir, pmr, cmr*)

Kahalalide J K-10

[190710-81-7]

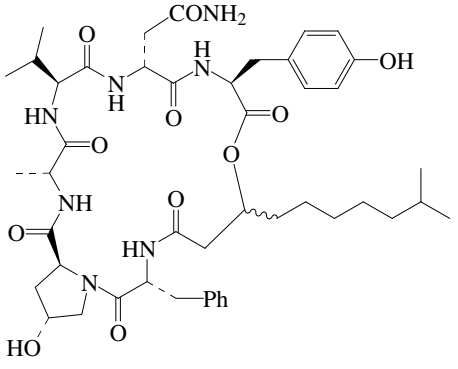


$C_{61}H_{94}N_{10}O_{17}$ 1239.47

Lipopeptide. Isol. from the mollusc *Elysia rufescens*. Amorph. solid. $[\alpha]_D^{20}$ +102.9 (c, 1.7 in MeOH). C-17 and C-46 configs. not confirmed. λ_{max} 208 (log ϵ 4.1); 282 (log ϵ 2.32) (MeOH).

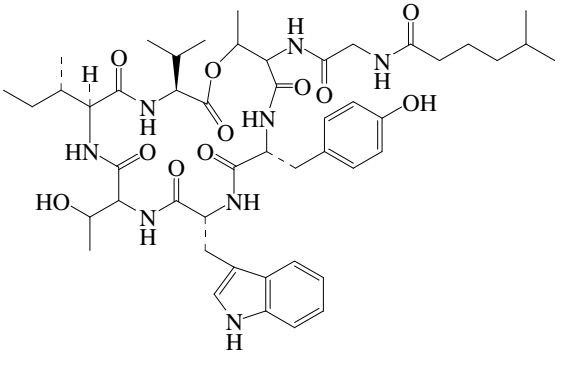
45-Delysyl: ***Kahalalide H***
[190710-80-6]
$C_{55}H_{82}N_8O_{16}$ 1111.297
Isol. from *Elysia rufescens*. Amorph. solid. $[\alpha]_D^{20}$ +38.8 (c, 4 in MeOH). λ_{max} 209 (log ϵ 4.43); 212 (log ϵ 4.41); 259 (log ϵ 2.65) (MeOH).
Goetz, G. *et al., J. Nat. Prod.*, 1997, **60**, 562-567 (*isol, uv, ir, pmr, cmr*)

Kahalalide K K-11



$C_{46}H_{65}N_7O_{11}$ 892.06
Depsipeptide. Isol. from a Hawaiian green alga, *Bryopsis* sp. $[\alpha]_D^{30}$ +36 (c, 2.5 in MeOH). λ_{max} 206 (log ϵ 4.38); 226 (log ϵ 4.06); 277 (log ϵ 3.26) (MeOH).
Kan, Y. *et al., J. Nat. Prod.*, 1999, **62**, 1169-1172 (*isol, uv, pmr, cmr*)

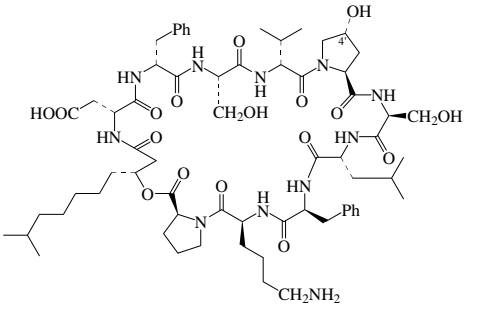
Kahalalide O K-12



$C_{48}H_{68}N_8O_{11}$ 933.112
Depsipeptide. Isol. from the mollusc *Elysia ornata* and its algal diet *Bryopsis* sp. Amorph. pale yellow solid. $[\alpha]_D^{28}$ -8 (c, 0.26 in MeOH). λ_{max} 221; 281 (MeOH).
Horgen, F.D. *et al., J. Nat. Prod.*, 2000, **63**, 152-154

Kahalalide P K-13

[878998-37-9]



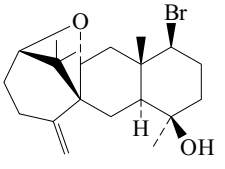
Absolute Configuration

$C_{66}H_{99}N_{11}O_{17}$ 1318.572
Isol. from a green alga *Bryopsis* sp. Powder. $[\alpha]_D^{25}$ +4.5 (c, 0.22 in MeOH).

4′-Deoxy: ***Kahalalide Q***
[878998-38-0]
$C_{66}H_{99}N_{11}O_{16}$ 1302.572
Isol. from a *Bryopsis* sp. Powder. $[\alpha]_D^{25}$ +10.5 (c, 0.03 in MeOH).
Dmitrenok, A. *et al., Tetrahedron*, 2006, **62**, 1301-1308 (*isol, pmr, cmr, ms*)

Kahukuene A K-14

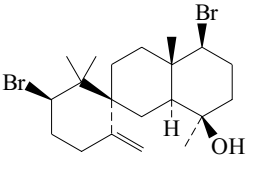
[146293-93-8]



$C_{20}H_{31}BrO_2$ 383.368
Constit. of *Laurencia majuscula*. Oil. $[\alpha]_D$ +25 (c, 1.12 in $CHCl_3$).
Brennan, M.R. *et al., J. Nat. Prod.*, 1993, **56**, 76 (*isol, pmr, cmr*)

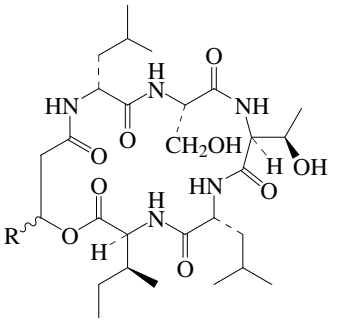
Kahukuene B K-15

[146293-94-9]



$C_{20}H_{32}Br_2O$ 448.28
Constit. of *Laurencia majuscula*. Oil. $[\alpha]_D$ +29 (c, 0.3 in $CHCl_3$).
Brennan, M.R. *et al., J. Nat. Prod.*, 1993, **56**, 76 (*isol, pmr, cmr*)

Kailuin K-16



Kailuin A R = $-(CH_2)_6CH_3$
B R = $-(CH_2)_8CH_3$
C R = $-(CH_2)_6CH(CH_3)_2$
D R = $-(CH_2)_3CH{=}CH(CH_2)_5CH_3$
E R = $-(CH_2)_{10}CH_3$

Lipodepsipeptide antibiotic complex. Prod. by a marine-derived gram-negative bacterium (BH-107). Exhibits mild cytotoxic activities.

Kailuin A [188051-15-2]
$C_{35}H_{63}N_5O_9$ 697.911
Oil. $[\alpha]_D$ +8.6 (c, 1 in MeOH).

Kailuin B [188051-16-3]
$C_{37}H_{67}N_5O_9$ 725.964
Oil. $[\alpha]_D$ +9.3 (c, 1 in MeOH).

Kailuin C [188051-17-4]
$C_{37}H_{67}N_5O_9$ 725.964
Oil. $[\alpha]_D$ +10 (c, 1 in MeOH).

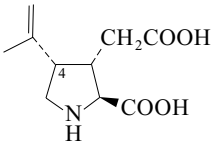
Kailuin D [188051-18-5]
$C_{39}H_{69}N_5O_9$ 752.002
Oil. $[\alpha]_D$ +9.5 (c, 1 in MeOH).

Kailuin E [291534-94-6]
$C_{39}H_{71}N_5O_9$ 754.018
Prod. by *Vibrio* sp. G1363. Algicide and surfactant.

Harrigan, G.G. *et al., Tetrahedron*, 1997, **53**, 1577 (*isol, ir, pmr, cmr*)
Japan. Pat., 2000, 245 497; *CA*, **133**, 221694w (*Kailuin E*)

Kainic acid, INN, JAN K-17

2-Carboxy-4-(1-methylethenyl)-3-pyrrolidineacetic acid, 9CI. 3-Carboxymethyl-4-isopropenylproline. α-Kaininic acid. Digenic acid. Digenin. α-Kainic acid
[487-79-6]



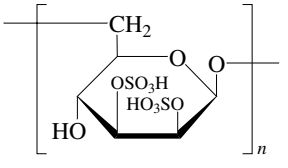
$C_{10}H_{15}NO_4$ 213.233
Constit. of red algae *Alsidium helminthochorton*, *Centroceras clavulatum* and *Digenea simplex*. Glutamate receptor agonist. Neurotoxin, formerly used as an anthelmintic agent. Cryst. + $1H_2O$ (EtOH aq.). Sol. H_2O.
Mp 253-254° dec. $[\alpha]_D^{24}$ -14.8 (c, 1 in H_2O). Log P -1.21 (calc).
▶ V. neurotoxic. UX9665250
Di-Me ester: [4071-37-8] Bp_4 145°. $[\alpha]_D^{20}$ +23.
N-*Ac:* [59845-92-0]
Mp 161-162°. $[\alpha]_D$ -53 (H_2O).
4-Epimer: ***α-Allokainic acid***. *α-Allokaininic acid*
[4071-39-0]
$C_{10}H_{15}NO_4$ 213.233
Constit. of *Digenea simplex*.
Mp 238-242° dec. $[\alpha]_D^{20}$ +7.7 (c, 1.3 in H_2O).

[58002-62-3, 92180-28-4, 92180-29-5]

Watase, H. *et al., Bull. Chem. Soc. Jpn.*, 1957, **30**, 889 (*cryst struct*)
Nitta, I. *et al., Nature (London)*, 1958, **181**, 761 (*struct*)
Impellizzeri, G. *et al., Phytochemistry*, 1975, **14**, 1549-1557 (*algae, isol*)
Kainic Acid Tool Neurobiol., (eds. McGeer, E.G. *et al*), Raven Press, 1978, (*book*)
Oppolzer, W. *et al., Tet. Lett.*, 1978, 3397-3400 (*α-Allokainic acid, synth*)
Oppolzer, W. *et al., Helv. Chim. Acta*, 1979, **62**, 2282 (*synth, bibl*)
Nadler, J.V. *et al., Life Sci.*, 1979, **24**, 289 (*rev, props*)
Kraus, G.A. *et al., Tet. Lett.*, 1983, **24**, 3427-3430 (*α-Allokainic acid, synth*)
DeShong, P. *et al., Tet. Lett.*, 1986, **27**, 3979-3982 (*α-Allokainic acid, synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 785
Yoo, S.-E. *et al., J.O.C.*, 1994, **59**, 6968-6972 (*synth*)
Agami, C. *et al., J.O.C.*, 1994, **59**, 7937-7940 (*synth*)
Parsons, A.F. *et al., Tetrahedron*, 1996, **52**, 4149-4174 (*rev*)
Todeschi, N. *et al., Bioorg. Med. Chem.*, 1997, **5**, 1943-1957 (*pmr, conformn*)
Bachi, M.D. *et al., Pure Appl. Chem.*, 1998, **70**, 259-262 (*rev, synth*)
Rubio, A. *et al., Tet. Lett.*, 1998, **39**, 2171-2174 (*synth*)
Chevliakov, M.V. *et al., J.A.C.S.*, 1999, **121**, 11139-11143 (*synth*)
Campbell, A.D. *et al., J.C.S. Perkin 1*, 2000, 3194-3204 (*synth*)
Miyata, O. *et al., Tetrahedron*, 2000, **56**, 6199-6207 (*synth, bibl*)
Anderson, J.C. *et al., J.O.C.*, 2003, **68**, 6160-6163 (*synth*)
Trost, B.M. *et al., Org. Lett.*, 2003, **5**, 1467-1470 (*synth*)
Cook, G.R. *et al., Org. Lett.*, 2004, **6**, 2481-2484 (*synth*)
Martinez, M.M. *et al., Eur. J. Org. Chem.*, 2005, 1427-1443 (*synth*)
Scott, M.E. *et al., Org. Lett.*, 2005, **7**, 3045-3047 (*synth*)
Morita, Y. *et al., Org. Lett.*, 2005, **7**, 4337-4340 (*synth*)
Pandey, S.K. *et al., TOrg. Lett.*, 2006, **8**, 5665-5668 (*synth*)

Kakelokelose K-18

[175069-04-2]



$C_6H_{10}O_{11}S_2$ 322.27
Sulfated mannose polysaccharide. Isol. from the Pacific tunicate *Didemnum molle*. Shows anti-HIV activity. Solid (as Na salt). $[\alpha]_D$ -76.4 (H_2O).

Riccio, R. *et al., Tet. Lett.*, 1996, **37**, 1979-1982 (*isol, pmr, cmr*)

Kalicludines K-19

Peptides containing 58-59 amino acid residues and 3 intramol. disulfide bonds. Isol. from the sea anemone *Anemonia sulcata*. K channel blocking toxin. Trypsin inhibitor.

Kallicludine 1
AsKC 1
[171758-79-5]
Contains 58 amino acid residues.

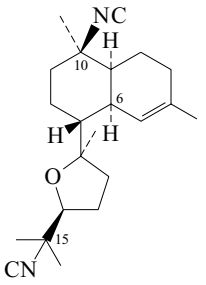
Kallicludine 2
AsKC 2
[171758-80-8]
Contains 58 amino acid residues.

Kallicludine 3
AsKC 3
[171758-81-9]
Contains 59 amino acid residues.

Schweitz, H. *et al., J. Biol. Chem.*, 1995, **270**, 25121-25126 (*isol, struct*)

Kalihinene K-20

[126622-61-5]



$C_{22}H_{32}N_2O$ 340.508
Metab. of sponges *Acanthella klethra* and *Acanthella cavernosa*. Cytotoxic and antifungal. Inhibitor of bacterial folate biosynth. Cryst. (EtOH). $[\alpha]_D^{25}$ +16 (c, 0.13 in $CHCl_3$). λ_{max} 208 (log ϵ 4.67); 238 (sh) (log ϵ 4.17) (MeOH).

10-Formamide: ***10-Formamidokalihinene***
$C_{22}H_{34}N_2O_2$ 358.523
Constit. of *Acanthella cavernosa*. Has -NHCHO replacing -NC at carbon 10.

15-Formamide: ***15-Formamidokalihinene***
$C_{22}H_{34}N_2O_2$ 358.523
Constit. of *Acanthella cavernosa*. Has -NHCHO replacing -NC at carbon 15.

10,15-Bis-formamide: ***10,15-Bisformamidokalihinene***
$C_{22}H_{36}N_2O_3$ 376.538
Constit. of *Acanthella cavernosa*. Has -NHCHO replacing both -NC groups.

6α-Hydroxy: ***6-Hydroxykalihinene***
$C_{22}H_{32}N_2O_2$ 356.507
Constit. of *Acanthella cavernosa*. Needles (EtOH).

6α-Hydroxy, 10-formamide: ***6-Hydroxy-10-formamidokalihinene***
$C_{22}H_{34}N_2O_3$ 374.522
Constit. of *Acanthella cavernosa*. Has -NHCHO replacing -NC at carbon 10.

6α-Hydroxy, 15-formamide: ***6-Hydroxy-15-formamidokalihinene***
$C_{22}H_{34}N_2O_3$ 374.522
Constit. of *Acanthella cavernosa*. Has -NHCHO replacing -NC at carbon 15.

6α-Hydroxy, 10-formamide, 15-thiocyanate: ***6-Hydroxy-10-formamido-15-thiocyanokalihinene***
$C_{22}H_{34}N_2O_3S$ 406.588
Constit. of *Acanthella cavernosa*. Has -NCHO replacing -NC at carbon 10 and -NCS replacing -NC at carbon 15.

1-Epimer: ***1*-epi-*Kalihinene***. *1-Epikalihinene*
[158249-46-8]
$C_{22}H_{32}N_2O$ 340.508
Constit. of *Acanthella cavernosa*. Oil. $[\alpha]_D$ +71.5 (c, 0.431 in CH_2Cl_2).

1-Epimer, 15-isothiocyanate: ***15-Isothiocyanato-1*-epi-*kalihinene***. *15-Isothiocyanato-1-epikalihinene*
[157521-09-0]
$C_{22}H_{32}N_2OS$ 372.574
Constit. of *Acanthella cavernosa*. Oil. $[\alpha]_D$ -149 (c, 0.132 in CH_2Cl_2).

1,10-Diepimer: ***1,10*-diepi-*Kalihinene***. *1,10-Diepikalihinene*
[158249-47-9]
$C_{22}H_{32}N_2O$ 340.508
Constit. of *Acanthella cavernosa*. Oil. $[\alpha]_D$ -66.2 (c, 0.47 in CH_2Cl_2).

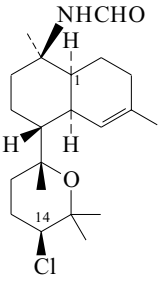
6,7-Diepimer: ***Kalihinene A***
$C_{22}H_{32}N_2O$ 340.508
Constit. of *Acanthella cavernosa*. Gummy solid. $[\alpha]_D$ -57.5 (c, 0.44 in CH_2Cl_2).

6,7,10-Triepimer: ***Kalihinene B***
$C_{22}H_{32}N_2O$ 340.508
Constit. of *Acanthella cavernosa*. Gummy solid. $[\alpha]_D$ 0 (c, 0.39 in CH_2Cl_2).

Fusetani, N. *et al., Tet. Lett.*, 1990, **31**, 3599 (*isol, cryst struct*)
Braekman, J.C. *et al., Bull. Soc. Chim. Belg.*, 1994, **103**, 187-191 (*Kalihinenes A and B*)
Trimurtula, G. *et al., J. Nat. Prod.*, 1994, **57**, 501-506 (*isol, pmr, cmr*)
Rodríguez, J. *et al., Tetrahedron*, 1994, **50**, 11079 (*isol, pmr, cmr, cryst struct*)
Bugni, T.S. *et al., Tetrahedron*, 2004, **60**, 6981-6988 (*isol, pmr, cmr*)

Kalihinene X K-21

[171370-56-2]



$C_{21}H_{34}ClNO_2$ 367.958
Constit. of *Acanthella cavernosa*. Antifouling agent. Larval settlement and metamorphosis inhibitor. $[\alpha]_D^{23}$ +26.7 (c, 0.3 in $CHCl_3$).

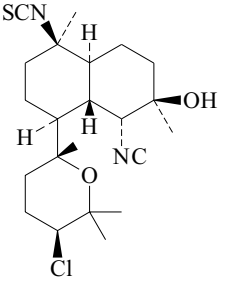
1-Epimer: ***Kalihinene Y***
[171485-62-4]
$C_{21}H_{34}ClNO_2$ 367.958
Constit. of *Acanthella cavernosa*. Antifouling agent. Larval settlement and metamorphosis inhibitor. $[\alpha]_D^{23}$ +11 (c, 0.01 in $CHCl_3$).

1,14-Diepimer: ***Kalihinene Z***
[171485-63-5]
$C_{21}H_{34}ClNO_2$ 367.958
Constit. of *Acanthella cavernosa*. Antifouling agent. Larval settlement and metamorphosis inhibitor. $[\alpha]_D^{23}$ +11.7 (c, 0.035 in $CHCl_3$).

Okino, T. *et al., Tet. Lett.*, 1995, **36**, 8637 (*isol, pmr, cmr*)
Miyaoka, H. *et al., Tet. Lett.*, 2002, **43**, 2227-2230 (*synth*)

Kalihinol X K-22

[109979-17-1]



$C_{22}H_{33}ClN_2O_2S$ 425.034
Metab. of *Acanthella* spp. Inhibitor of bacterial folate biosynth. Needles (hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 199-200°. $[\alpha]_D^{25}$ -30 (c, 0.09 in $CHCl_3$). λ_{max} 204 (log ϵ 4.41); 244 (log ϵ 4.12) (MeOH).

5-Formamide: ***Kalihinol J***
[133738-47-3]
$C_{22}H_{35}ClN_2O_3S$ 443.049
Metab. of *Acanthella carvenosa*. Anthelmintic agent. $[\alpha]_D^{25}$ +24 (c, 0.03 in $CHCl_3$). Has -NHCHO replacing -NC. λ_{max} 204 (log ϵ 4.36); 242 (log ϵ 3.47) (MeOH).

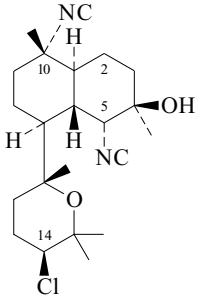
5-Isothiocyanate: ***Kalihinol I***
[133738-48-4]
$C_{22}H_{33}ClN_2O_2S_2$ 457.1
Metab. of *Acanthella carvenosa*. Anthelmintic agent. Needles (Et_2O).
Mp 180°. Has -NCS replacing -NC. λ_{max} 245 (E1%/1cm 673) (MeOH) (Berdy).

5-Isothiocyanate, 10-epimer: ***10-Epikalihinol I***
[217452-05-6]
$C_{22}H_{33}ClN_2O_2S_2$ 457.1
Constit. of *Acanthella* sp. Antimalarial agent. Cryst.
Mp 209-210°. $[\alpha]_D$ -52.4 (c, 0.3 in $CHCl_3$). λ_{max} 246 (ϵ 1161) (MeOH).

Chang, C.W.J. *et al., J.A.C.S.*, 1987, **109**, 6119 (*isol, pmr, cmr*)
Alvi, K.A. *et al., J. Nat. Prod.*, 1991, **54**, 71 (*isol, pmr, cmr*)
Miyaoka, H. *et al., Tetrahedron*, 1998, **54**, 13467-13474 (*10-Epikalihinol I*)
Miyaoka, H. *et al., Tennen Yuki Kagobutsu Toronkai Koen Yoshishu*, 2000, **42**, 685-690; *CA*, 2001, **134**, 340569 (*10-Epiklihinol I*)
Bugni, T.S. *et al., Tetrahedron*, 2004, **60**, 6981-6988 (*isol, pmr, cmr*)

Kalihinol A K-23

[91294-83-6]



$C_{22}H_{33}ClN_2O_2$ 392.968
Metab. of *Acanthella* spp. Active against *Bacillus subtilis*, *Staphylococcus aureus* and *Candida albicans*. Plates (hexane). Sol. MeOH, CCl_4, $CHCl_3$; poorly sol. H_2O.
Mp 233°. $[\alpha]_D$ +16 (c, 1 in $CHCl_3$).

2-Epimer: ***Kalihinol Z***
[110043-50-0]
$C_{22}H_{33}ClN_2O_2$ 392.968
Metab. of *Acanthella* spp. Plates (hexane/Me_2CO). Sol. $CHCl_3$, MeOH; poorly sol. H_2O.
Mp 228-230°. $[\alpha]_D$ -10 (c, 1 in $CHCl_3$).

14-Epimer: ***Kalihinol E***
[93528-15-5]
$C_{22}H_{33}ClN_2O_2$ 392.968
Metab. of *Acanthella* spp. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

10-Formamide: ***10-Formamidokalihinol A***
[173692-43-8]
$C_{22}H_{35}ClN_2O_3$ 410.983
Constit. of *Acanthella cavernosa*.
$[\alpha]_D$ +11 (c, 0.15 in $CHCl_3$). Has –NHCHO replacing –NC.

10-Formamide, 14-epimer: ***10-Formamidokalihinol E***
[173832-17-2]
$C_{22}H_{35}ClN_2O_3$ 410.983
Constit. of *Acanthella cavernosa*.
$[\alpha]_D$ -2.8 (c, 0.15 in $CHCl_3$). Has –NHCHO replacing –NC.

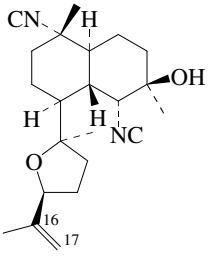
10-Formamide, 5-isocyanate: ***10-Formamido-5-isocyanatokalihinol A***
[173692-44-9]
$C_{22}H_{35}ClN_2O_4$ 426.982
Constit. of *Acanthella cavernosa*.
$[\alpha]_D$ -25 (c, 0.02 in $CHCl_3$). Has –NCHO replacing –NC at C-10 and –NCO replacing –NC at C-5.

10-Formamide, 5-isothiocyanate: ***10-Formamido-5-isothiocyanatokalihinol A***
[173692-45-0]
$C_{22}H_{35}ClN_2O_3S$ 443.049
Constit. of *Acanthella cavernosa*.
$[\alpha]_D$ +24 (c, 0.5 in $CHCl_3$). Has –NCS replacing –NC at C-5.

Chang, C.W.J. *et al., J.A.C.S.*, 1984, **106**, 4644-4646; 1987, **109**, 6119-6123 (*Kalihinols A,E, isol, cryst struct, abs config*)
Hirota, H. *et al., Tetrahedron*, 1996, **52**, 2359 (*isol, pmr, cmr*)
Shimomura, M. *et al., Tet. Lett.*, 1999, **40**, 8015-8017 (*synth, abs config*)

Kalihinol C K-24

[93426-93-8]



$C_{22}H_{32}N_2O_2$ 356.507
Metab. of *Acanthella* spp. Oil. $[\alpha]_D$ +6 (c, 1 in $CHCl_3$).

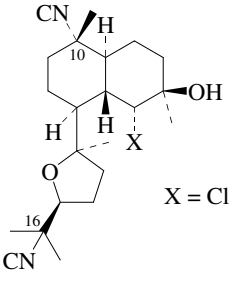
16,17-Dihydro, 16-chloro: ***Kalihinol B***
[93426-92-7]
$C_{22}H_{33}ClN_2O_2$ 392.968
Metab. of *Acanthella* spp. Oil. $[\alpha]_D$ +10 (c, 1 in $CHCl_3$).

10-Isothiocyanate: ***10-Isothiocyanatokalikinol C***
[216973-07-8]
$C_{22}H_{32}N_2O_2S$ 388.573
Constit. of *Phakellia pulcherrima*.
$[\alpha]_D^{20}$ -11 (c, 0.06 in $CHCl_3$).

Chang, C.W.J. *et al., J.A.C.S.*, 1987, **109**, 6119 (*isol, pmr, cmr*)
Wolf, D. *et al., J. Nat. Prod.*, 1998, **61**, 1524-1527 (*10-Isothiocyanatokalikinol C*)
White, R.D. *et al., Org. Lett.*, 2004, **6**, 1123-1126 (*synth*)

Kalihinol D K-25

[112406-52-7]



$C_{22}H_{33}ClN_2O_2$ 392.968
Metab. of *Acanthella* spp. Plates (heptane/Me_2CO). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 183-184°. $[\alpha]_D$ +8 (c, 1.5 in $CHCl_3$). λ_{max} 246 (hexane) (Berdy).

Chang, C.W.J. *et al., J.A.C.S.*, 1987, **109**, 6119 (*isol, pmr, cmr*)

Kalihinol F K-26

[93426-91-6]
As Kalihinol D, K-25 with
X = NC
$C_{23}H_{33}N_3O_2$ 383.533
Metab. of *Acanthella* spp. Topoisomerase I inhibitor. Cryst. (hexane/Me_2CO). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 176-178°. $[\alpha]_D$ +8 (c, 1 in $CHCl_3$). λ_{max} 204 (log ϵ 4.3); 236 (sh) (log ϵ 3.56) (MeOH).

10-Isothiocyanate: ***Kalihinol H***
[109979-16-0]
$C_{23}H_{33}N_3O_2S$ 415.599
Metab. of *Acanthella* spp. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +98 (c, 1 in $CHCl_3$). Has -NC replaced by -NCS at C-10.

16-Isothiocyanate: ***Kalihinol G***
[109979-15-9]
$C_{23}H_{33}N_3O_2S$ 415.599
Metab. of *Acanthella* spp. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -12 (c, 1 in $CHCl_3$). Has -NC replaced by -NCS at C-16.

10,16-Diisothiocyanate: ***10-Isocyanatokalihinol G***
[216973-05-6]
$C_{23}H_{33}N_3O_2S_2$ 447.665
Constit. of *Phakellia pulcherrima*.
$[\alpha]_D^{20}$ -26 (c, 0.38 in $CHCl_3$). Has -NC replaced by -NCS at C-10 and C-16.

5,10,16-Triisothiocyanate: ***5,10-Diisothiocyanatokalihinol G****. 5,10-Bisisothiocyanatokalihinol G*
$C_{23}H_{33}N_3O_2S_3$ 479.731
Constit. of *Acanthella* sp. Oil. $[\alpha]_D$ -62.7 (c, 0.8 in $CHCl_3$). Has -NC replaced by -NCS at C-5, C-10 and C-16. λ_{max} 246 (ϵ 1660) (MeOH).

10-Formamide: ***10-Formamidokalihinol F***
[749867-22-9]
$C_{23}H_{35}N_3O_3$ 401.548
Constit. of *Acanthella cavernosa*.
$[\alpha]_D^{25}$ +22 (c, 0.03 in $CHCl_3$). Has -NC replaced by -NHCHO at C-10. λ_{max} 204 (log ϵ 4.34) (MeOH).

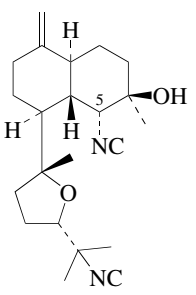
16-Formamide: ***16-Formamidokalihinol F****. 15-Formamidokalihinol F*
[749867-23-0]
$C_{23}H_{35}N_3O_3$ 401.548
Constit. of *Acanthella cavernosa*.
$[\alpha]_D^{25}$ +9 (c, 0.1 in $CHCl_3$). λ_{max} 206 (log ϵ 4.56) (MeOH).

10-Epimer, 10-isothiocyanate: ***10-Epikalihinol H***
$C_{23}H_{33}N_3O_2S$ 415.599
Constit. of *Phakellia pulcherrima*.
$[\alpha]_D^{20}$ -30 (c, 0.18 in $CHCl_3$). Has -NC replaced by -NCS at C-10 (10-epimer).

Patra, A. *et al., J.A.C.S.*, 1984, **106**, 7981 (*cryst struct*)
Chang, C.W.J. *et al., J.A.C.S.*, 1987, **109**, 6119 (*isol, pmr, cmr*)
Wolf, D. *et al., J. Nat. Prod.*, 1998, **61**, 1524-1527 (*10-Isothiocyanatokalihinol G, 10-Epikalihinol H*)
Miyaoka, H. *et al., Tetrahedron*, 1998, **54**, 13467-13474 (*5,10-Diisothiocyanatokalihinol G*)
Ohta, E. *et al., Biosci., Biotechnol., Biochem.*, 2003, **67**, 2365-2372 (*activity*)
Bugni, T.S. *et al., Tetrahedron*, 2004, **60**, 6981-6988 (*Formamidokalihinol F derivs*)

Kalihinol K K-27

[216973-03-4]

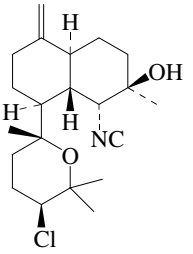


$C_{22}H_{32}N_2O_2$ 356.507
Constit. of *Phakellia pulcherrima*.
$[\alpha]_D^{20}$ -9 (c, 0.7 in $CHCl_3$).

5-Isothiocyanate: ***Kalihinol L***
[216973-04-5]
$C_{22}H_{32}N_2O_2S$ 388.573
Constit. of *Phakellia pulcherrima*.
$[\alpha]_D^{20}$ -5 (c, 0.19 in. $CHCl_3$). Has -NC replaced by -NCS at C-5.
Wolf, D. *et al., J. Nat. Prod.*, 1998, **61**, 1524-1527 (*isol, pmr, cmr*)

Kalihinol Y K-28

[109979-18-2]



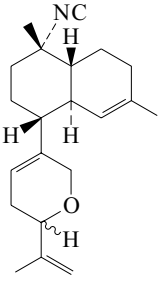
$C_{21}H_{32}ClNO_2$ 365.942
Metab. of *Acanthella* spp. Inhibitor of bacterial folate biosynth. Needles (hexane/EtOAc). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 176-179°. $[\alpha]_D$ -34 (c, 1 in $CHCl_3$). λ_{max} 204 (log ϵ 4.47); 238 (sh) (log ϵ 3.64) (MeOH).

Δ^9-Isomer: ***Δ^9-Kalihinol Y***
[216973-02-3]
$C_{21}H_{32}ClNO_2$ 365.942
Constit. of *Acanthella* sp. and *Phakellia pulcherrima*. Antimalarial agent. Needles.
Mp 188-190°. $[\alpha]_D$ +38.4 (c, 0.24 in $CHCl_3$). $[\alpha]_D^{20}$ +9 (c, 0.05 in $CHCl_3$).

Chang, C.W.J. *et al., J.A.C.S.*, 1987, **109**, 6119 (*isol, pmr, cmr*)
Wolf, D. *et al., J. Nat. Prod.*, 1998, **61**, 1524-1527 (*Δ^9-Kalihinol Y*)
Miyaoka, H. *et al., Tetrahedron*, 1998, **54**, 13467-13474 (*Δ^9-Kalihinol*)
Bugni, T.S. *et al., Tetrahedron*, 2004, **60**, 6981-6988 (*isol, pmr, cmr*)

Kalihipyran K-29

[157622-52-1]

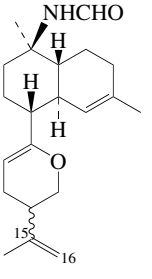


$C_{21}H_{29}NO$ 311.466
Constit. of *Acanthella cavernosa*. Oil. $[\alpha]_D$ +104.1 (c, 0.29 in CH_2Cl_2).

Trimurtulu, G. *et al., J. Nat. Prod.*, 1994, **57**, 501 (*isol, pmr, cmr*)

Kalihipyran A K-30

[184430-00-0]



$C_{21}H_{31}NO_2$ 329.481

Constit. of *Acanthella cavernosa*. Antifouling agent. Oil. $[\alpha]_D^{23}$ +38.6 (c, 0.08 in $CHCl_3$).

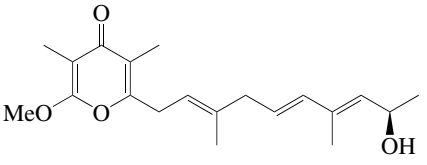
15-Chloro, 15,16-dihydro: ***Kalihipyran B***
[184430-01-1]
$C_{21}H_{32}ClNO_2$ 365.942
Constit. of *Acanthella cavernosa*. Antifouling agent. Oil. $[\alpha]_D^{23}$ +73.4 (c, 0.035 in $CHCl_3$).
Okino, T. *et al., J. Nat. Prod.*, 1996, **59**, 1081-1083 (*isol, pmr, cmr*)

Kaliseptine K-31

[171758-82-0]
Peptide containing 36 amino acid residues and 3 intramol. disulfide bonds. Isol. from the sea anemone *Anemonia sulcata*. $K^{\oplus}$-channel-blocking toxin.
Schweitz, H. *et al., J. Biol. Chem.*, 1995, **270**, 25121-25126 (*isol*)

Kalkipyrone K-32

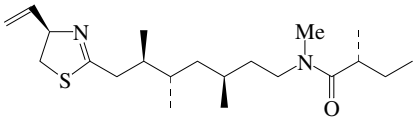
[205813-99-6]



$C_{20}H_{28}O_4$ 332.439
Similar to Actinopyrones. Isol. from an assemblage of the cyanobacteria *Lyngbya majuscula* and *Tolypothrix* spp. Oil. $[\alpha]_D$ +8.2 (c, 0.2 in $CHCl_3$). λ_{max} 204 (log ϵ 4.3); 238 (log ϵ 4.5) (EtOH). λ_{max} 238 (ϵ 33000) (MeOH) (Berdy). λ_{max} 204 (ϵ 19950); 238 (ϵ 31600) (EtOH) (Berdy).
Graber, M.A. *et al., J. Nat. Prod.*, 1998, **61**, 677-680 (*isol, uv, ir, pmr, cmr, ms*)

Kalkitoxin K-33

[247184-89-0]

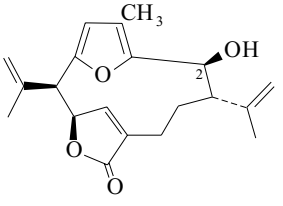


Absolute Configuration

$C_{21}H_{38}N_2OS$ 366.61
Isol. from *Lyngbya majuscula*. Neurotoxin and ichthyotoxin. Cytotoxic.
Berman, F.W. *et al., Toxicon*, 1999, **37**, 1645-1648 (*isol, activity*)
Wu, M. *et al., J.A.C.S.*, 2000, **122**, 12041-12042 (*synth, struct*)
White, J.D. *et al., Org. Biomol. Chem.*, 2004, **2**, 2092-2012 (*synth*)
Yokokawa, F. *et al., Tetrahedron*, 2004, **60**, 6859-6880 (*synth, abs config*)

Kallolide A K-34

[99528-59-3]



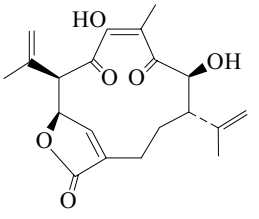
$C_{20}H_{24}O_4$ 328.407
Constit. of *Pseudopterogorgia kallos*. Has strong antiinflammatory props. that exceed the potency of indomethacin. Amorph. solid. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ +145 (c, 0.67 in $CHCl_3$). λ_{max} 218 (ϵ 13000) (MeOH) (Derep).

Ac: ***Kallolide A acetate***
[99457-89-3]
$C_{22}H_{26}O_5$ 370.444
From *Pseudopterogorgia kallos*. Cryst. (Et_2O).
Mp 198-199.5°. $[\alpha]_D^{20}$ +55 (c, 0.65 in $CHCl_3$).

2-Deoxy: ***Kallolide B***
[99457-90-6]
$C_{20}H_{24}O_3$ 312.408
From *Pseudopterogorgia kallos*. Oil. $[\alpha]_D^{20}$ +123 (c, 0.81 in $CHCl_3$). λ_{max} 218 (ϵ 13000) (MeOH) (Derep).
Look, S.A. *et al., J.O.C.*, 1985, **50**, 5741
Marshall, J.A. *et al., J.O.C.*, 1995, **60**, 796; 1996, **61**, 5729; 1998, **63**, 5962-5970 (*synth*)
Rodriguez, A.D. *et al., J.O.C.*, 1998, **63**, 4425 (*isol, activity*)

Kallolide C K-35

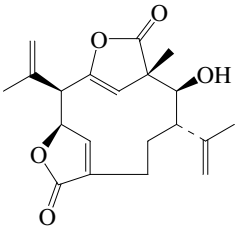
[99457-91-7]



$C_{20}H_{24}O_6$ 360.406
Constit. of *Pseudopterogorgia kallos*. Amorph. solid. $[\alpha]_D^{20}$ -14 (c, 0.91 in $CHCl_3$). λ_{max} 286 (ϵ 4030) (MeOH) (Derep).
Look, S.A. *et al., J.O.C.*, 1985, **50**, 5741

Kallosin A K-36

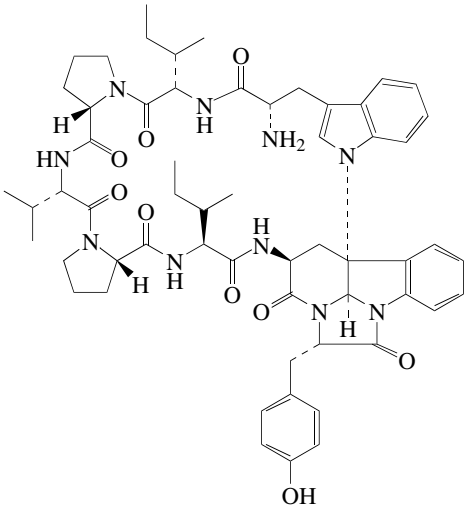
[549502-97-8]



$C_{20}H_{24}O_5$ 344.407
Constit. of *Pseudopterogorgia kallos*. Cryst. $[\alpha]_D^{20}$ -48.1 (c, 0.33 in $CHCl_3$).
Marrero, J. *et al., J.O.C.*, 2003, **68**, 4977-4979 (*isol, pmr, cmr, cryst struct*)

Kapakahine A K-37

[181862-46-4]



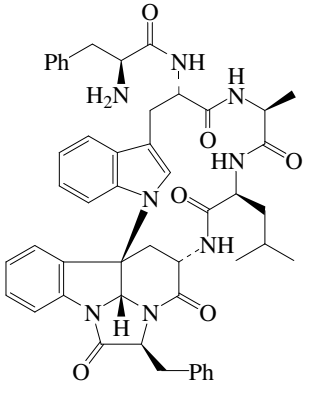
$C_{58}H_{72}N_{10}O_9$ 1053.268

Cyclic peptide. Isol. from the sponge *Cribrochalina olemda*. Protein phosphatase inhibitor. Amorph. solid. $[\alpha]_D^{20}$ -131 (c,1 in MeOH). λ_{max} 206 (ϵ 39000); 232 (ϵ 19000); 274 (ϵ 9500) (MeOH).

Yeung, B.K.S. *et al., J.O.C.*, 1996, **61**, 7168 (*isol, uv, pmr, cmr*)

Kapakahine B K-38

[165406-94-0]



Absolute Configuration

$C_{49}H_{52}N_8O_6$ 849

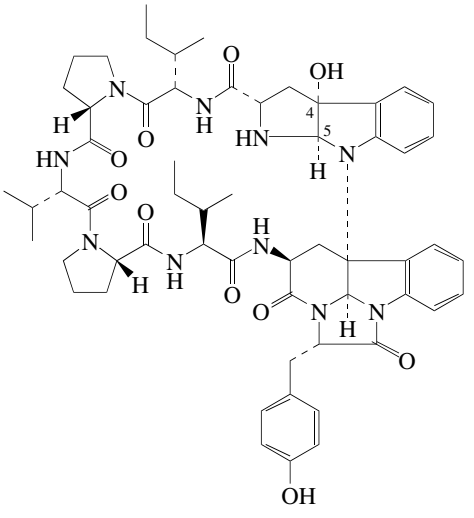
Cyclic hexapeptide antibiotic. Isol. from the sponge *Cribrochalina olemda*. Cytotoxic agent. Amorph. solid. Sol. MeOH, EtOAc; poorly sol. hexane. $[\alpha]_D^{20}$ -70 (c, 0.3 in MeOH). λ_{max} 214 (ϵ 21000); 250 (ϵ 8400); 280 (ϵ 5600); 294 (ϵ 4000) (MeOH).

N-*De(2-amino-3-phenylpropanoyl):* ***Kapakahine F***
$C_{40}H_{43}N_7O_5$ 701.824
Isol. from *Cribrochalina olemda*.

Nakao, Y. *et al., J.A.C.S.*, 1995, **117**, 8271-8272 (*isol, uv, ir, pmr, cmr*)
Yeung, B.K.S. *et al., J.O.C.*, 1996, **61**, 7168-7173 (*abs config*)
Nakao, Y. *et al., Org. Lett.*, 2003, **5**, 1387-1390 (*Kapakahine F*)

Kapakahine C K-39

[181862-47-5]



$C_{58}H_{72}N_{10}O_{10}$ 1069.268

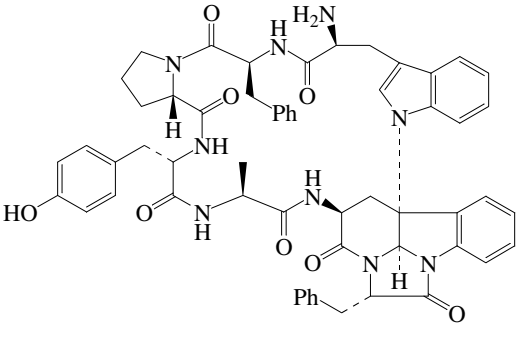
Cyclic peptide. Isol. from the sponge *Cribrochalina olemda*. Amorph. solid. $[\alpha]_D^{20}$ -120 (c, 0.5 in MeOH). λ_{max} 208 (ϵ 44000); 253 (ϵ 12000); 279 (ϵ 41000); 305 (ϵ 1200) (MeOH).

4,5-Diepimer: ***Kapakahine D***
[182074-03-9]
$C_{58}H_{72}N_{10}O_{10}$ 1069.268
Isol. from *Cribrochalina olemda*. Amorph. solid. $[\alpha]_D^{20}$ -30.7 (c, 0.9 in MeOH). λ_{max} 206 (ϵ 35000); 247 (ϵ 9000); 279 (ϵ 2800); 304 (ϵ 690) (MeOH).

Yeung, B.K.S. *et al., J.O.C.*, 1996, **61**, 7168 (*isol, uv, ir, pmr, cmr*)

Kapakahine E K-40

[530097-81-5]

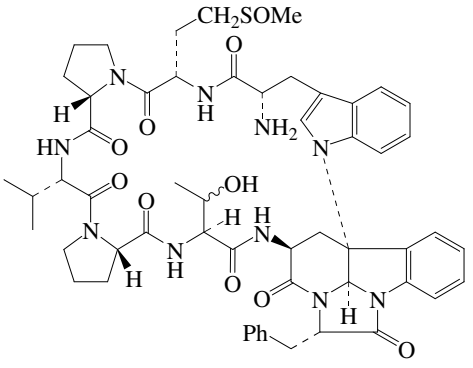


$C_{57}H_{57}N_9O_8$ 996.133
Isol. from the sponge *Cribrochalina olemda*. Cytotoxic.

Nakao, Y. *et al., Org. Lett.*, 2003, **5**, 1387-1390 (*isol, pmr, cmr, ms*)

Kapakahine G K-41

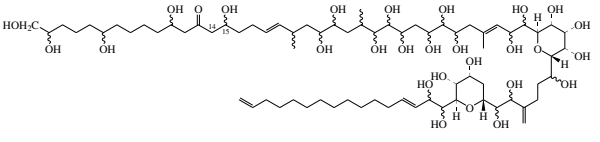
[530097-83-7]



$C_{55}H_{66}N_{10}O_{10}S$ 1059.253
Isol. from the sponge *Cribrochalina olemda*.

Nakao, Y. *et al., Org. Lett.*, 2003, **5**, 1387-1390 (*isol, pmr, cmr, ms*)

Karatungiol A K-42



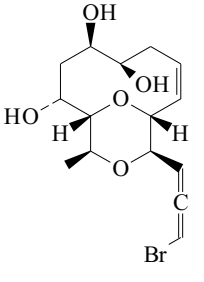
$C_{73}H_{132}O_{28}$ 1457.829
Isol. from *Amphidinium* sp. Antifungal agent. Pale yellow solid. $[\alpha]_D^{17}$ +13.6 (c, 0.1 in MeOH).

*15-Deoxy, 14,15-didehydro(*E-*):* ***Karatungiol B***
$C_{73}H_{130}O_{27}$ 1439.814
Isol. from *Amphidinium* sp. Pale yellow solid. $[\alpha]_D^{15}$ +24 (c, 0.1 in MeOH). λ_{max} 228 (ϵ 16300) (no solvent reported).

Washida, K. *et al., Tet. Lett.*, 2006, **47**, 2521-2525 (*isol, pmr, cmr*)

Kasallene K-43

[137609-72-4]

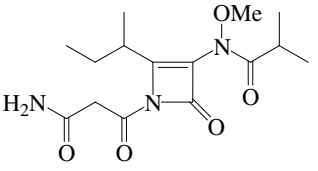


$C_{15}H_{21}BrO_5$ 361.232
Isol. from the red alga *Laurencia obtusa*. Cryst.
Mp 206-208° dec. $[\alpha]_D^{25}$ -200 (c, 0.1 in $CHCl_3$).

Oztunc, A. *et al., Tet. Lett.*, 1991, **32**, 4377 (*isol, pmr, cmr*)

Kasarin K-44

[272109-43-0]

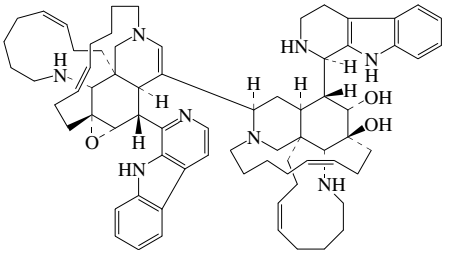


$C_{15}H_{23}N_3O_5$ 325.364
Monobactam antibiotic. Isol. from a marine *Hypomyces* sp. isol. from a *Zoanthus* sp. Antibacterial agent. Oil. $[\alpha]_D^{26}$ +22 (c, 0.3 in $CHCl_3$).

Suenaga, K. *et al., Heterocycles*, 2000, **52**, 1033-1036 (*isol, pmr, cmr*)

Kauluamine K-45

[170474-99-4]

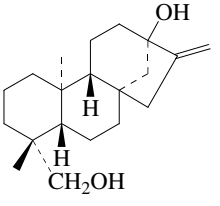


Absolute Configuration

$C_{72}H_{94}N_8O_3$ 1119.586
Alkaloid from an Indonesian marine sponge, *Prianos* sp. Shows mod. immunosuppressive activity. Unstable pale yellow solid. Sol. MeOH, $CHCl_3$, CH_2Cl_2. $[\alpha]_D$ +0.7 (c, 0.18 in $CHCl_3$).

Ohtani, I.I. *et al., J.A.C.S.*, 1995, **117**, 10743-10744 (*isol, ir, pmr, cmr, struct*)

16-Kaurene-13,19-diol K-46



$C_{20}H_{32}O_2$ 304.472

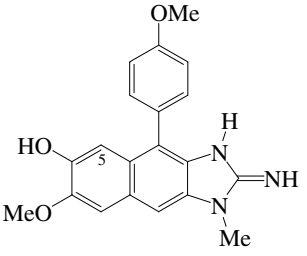
ent-form [38231-75-3]
Constit. of *Bruguiera gymnorrhiza*.
Cryst. ($C_6H_6/CHCl_3$).
Mp 255-257°. $[\alpha]_D^{30}$ -47 (c, 0.1 in MeOH).

19-Aldehyde: ***13-Hydroxy-16-kauren-19-al***
[238431-76-0]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Bruguiera gymnorrhiza*. Needles (hexane).
Mp 120°. $[\alpha]_D^{30}$ -59 (c, 0.1 in $CHCl_3$).

19-Carboxylic acid: See 13-Hydroxy-16-kauren-19-oic acid in *The Combined Chemical Dictionary.*

Subrahmanyam, C. *et al., Phytochemistry*, 1999, **51**, 83-90 (*isol, pmr, cmr*)

Kealiinine A K-47



$C_{20}H_{19}N_3O_3$ 349.388
Alkaloid from the sponge *Leucetta chagosensis*. Cytotoxic. Yellow-brown powder. λ_{max} 250; 314; 338 (MeOH).

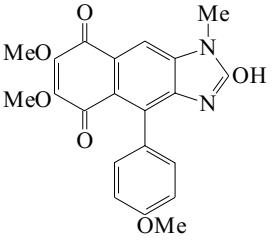
6-Me ether: ***Kealiinine B***
$C_{21}H_{21}N_3O_3$ 363.415
Alkaloid from *Leucetta chagosensis*. Dark brown solid. λ_{max} 250; 314; 338 (MeOH).

5-Methoxy, 6-Me ether: ***Kealiinine C***
$C_{22}H_{23}N_3O_4$ 393.441
Alkaloid from *Leucetta chagosensis*. Dark brown solid. λ_{max} 250; 314; 338 (MeOH).

Hassan, W. *et al., J. Nat. Prod.*, 2004, **67**, 817-822 (*isol, pmr, cmr, ms*)

Kealiiquinone K-48

*6,7-Dimethoxy-4-(4-methoxyphenyl)-1-methyl-1*H*-naphth[2,3-d]imidazole-2,5,8(3*H*)-trione, 9CI*
[124535-78-0]



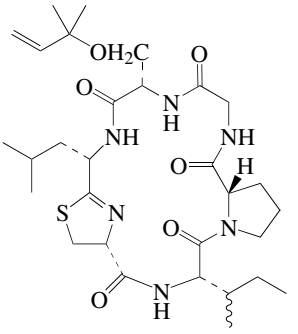
$C_{21}H_{18}N_2O_6$ 394.383
CAS registry no. refers to the trioxo tautomer. Alkaloid from the sponge *Leucetta* sp. Long red needles ($MeOH/CH_2Cl_2$/hexane). Mp 300° dec. λ_{max} 230 (ϵ 15100); 296 (ϵ 22400); 388 (ϵ 1380) (MeOH) (Derep).

2-Deoxy, 2-amino: ***2-Amino-2-deoxykealiiquinone****. 2-Deoxy-2-aminokealiiquinone*
[189748-83-2]
$C_{21}H_{19}N_3O_5$ 393.398
Alkaloid from the sponge *Leucetta chagosensis*. Red needles ($MeOH/CH_2Cl_2$).
Mp >250° dec. λ_{max} 220 (log ϵ 4.49); 294 (log ϵ 4.57); 382 (log ϵ 3.73) (MeOH).

Akee, R.K. *et al., J.O.C.*, 1990, **55**, 1944 (*isol, uv, ir, pmr, cmr, cryst struct*)
Kawasaki, I. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1393-1398 (*synth, uv, ir, pmr, cmr, cryst struct*)
Fu, X. *et al., J. Nat. Prod.*, 1997, **60**, 497 (*2-Deoxy-2-aminokealiiquinone*)

Keenamide A K-49

[177742-52-8]

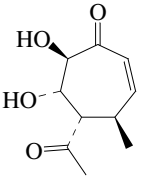


$C_{30}H_{48}N_6O_6S$ 620.812
Isol. from the marine mollusc *Pleurobranchus forskalii*. Cytotoxic agent. Off-white powder. $[\alpha]_D$ +24 (c, 0.3 in MeOH).

Wesson, K.J. *et al., J. Nat. Prod.*, 1996, **59**, 629-631 (*isol, ir, pmr, cmr, ms*)

Keisslone K-50

5-Acetyl-6,7-dihydroxy-4-methyl-2-cyclohepten-1-one



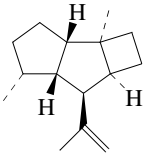
Absolute Configuration

$C_{10}H_{14}O_4$ 198.218
Prod. by the marine fungus *Keissleriella* sp. YS4108. Antifungal agent. Gum. $[\alpha]_D^{20}$ +181.8 (c, 0.1 in $CHCl_3$). λ_{max} 242 ($CHCl_3$).

Liu, C.H. *et al., Planta Med.*, 2003, **69**, 481-483 (*isol, pmr, cmr*)

Kelsoene K-51

[190663-65-1]

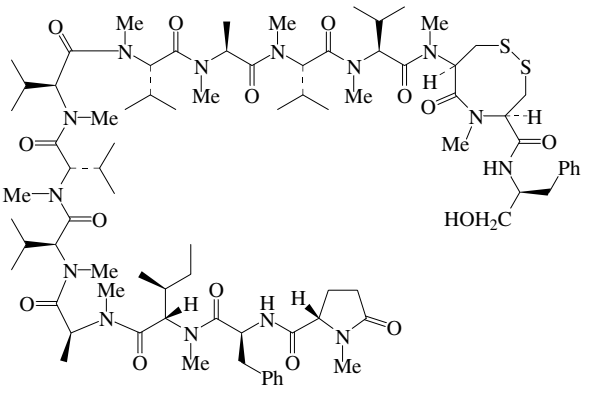


Absolute Configuration

$C_{15}H_{24}$ 204.355
Constit. of *Cymbastela hooperi*. Oil. $[\alpha]_D$ +78.1 (c, 1.98 in $CHCl_3$).

König, G.M. *et al., J.O.C.*, 1997, **62**, 3837-3840 (*isol, pmr, cmr*)
Nabeta, K. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 1772-1776 (*abs config*)
Mehta, G. *et al., Tet. Lett.*, 1999, **40**, 4877-4880 (*synth*)
Nabeta, K. *et al., J.C.S. Perkin 1*, 2000, 2703-2708 (*biosynth*)
Fietz-Razavian, S. *et al., Chem. Comm.*, 2001, 2154-2155 (*synth*)
Piers, E. *et al., Synthesis*, 2001, 2138-2142 (*synth, pmr, cmr*)
Mehta, G. *et al., Tet. Lett.*, 2001, **42**, 2855-2857 (*synth*)
Zhang, L. *et al., Org. Lett.*, 2002, **4**, 3755-3758 (*synth*)

Kendarimide A K-52



$C_{83}H_{134}N_{14}O_{15}S_2$ 1632.188

Isol. from the sponge *Haliclona* sp. Modulator of multidrug resistance in tumour cells. Powder. $[\alpha]_D^{25}$ -273 (c, 0.3 in MeOH).

Aoki, S. *et al., Tetrahedron*, 2004, **60**, 7053-7059 (*isol, pmr, cmr*)
Kotoku, N. *et al., Heterocycles*, 2005, **65**, 563-578 (*abs config*)

Kenojeinin I K-53

$C_{139}H_{233}N_{45}O_{32}$ 3046.652

Isol. from skin of fermented skate *Raja kenojei*. Shows antimicrobial activity.

Cho, S.H. *et al., Peptides (N.Y.)*, 2005, **26**, 581-587 (*isol*)

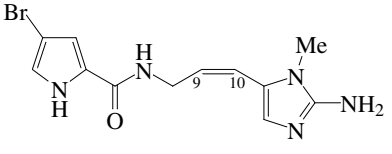
Kentin K-54

Basic polypeptide with MW *ca*. 18000 Da. Isol. from the sea anemone *Stoichactis kenti*. Cytolytic toxin.

Bernheimer, A.W. *et al., Toxicon*, 1985, **23**, 791-799 (*isol*)

Keramadine K-55

[88839-97-8]



$C_{12}H_{14}BrN_5O$ 324.18

Isol. from the Okinawan sea sponge *Agelas* sp. Antagonist of serotonergic receptors. Powder. Sol. MeOH, $CHCl_3$.
Mp 183-187°. λ_{max} 269 (ϵ 21400) (MeOH) (Derep).

9,10-Dihydro: ***9,10-Dihydrokeramadine***

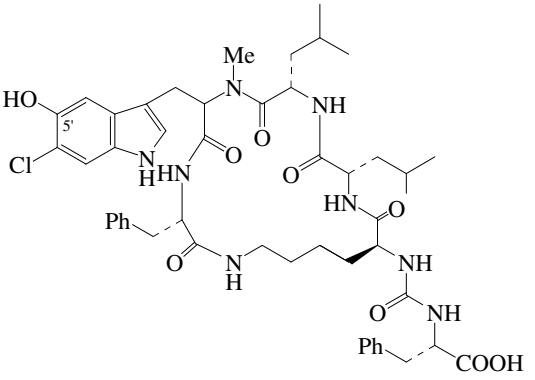
$C_{12}H_{16}BrN_5O$ 326.195

Isol. from an *Agelas* sp. Amorph. solid. λ_{max} 202 (ϵ 21200); 280 (ϵ 19700) (MeOH).

Nakamura, H. *et al., Tet. Lett.*, 1984, **25**, 2475-2478 (*isol, uv, ir, pmr, cmr, ms*)
Daninos-Zeghal, S. *et al., Tetrahedron*, 1997, **53**, 7605-7614 (*synth*)
Cafieri, F. *et al., J. Nat. Prod.*, 1998, **61**, 122-125 (*isol, pmr*)
Lindel, T. *et al., Tet. Lett.*, 1998, **39**, 2541-2544 (*synth, pmr*)
Endo, T. *et al., J. Nat. Prod.*, 2004, **67**, 1262-1267 (*9,10-Dihydrokeramadine*)

Keramamide A K-56

[137529-91-0]



$C_{49}H_{63}ClN_8O_9$ 943.538

Cyclic peptide. Isol. from the marine sponge *Theonella* sp. $[\alpha]_D^{20}$ -190 (c, 0.03 in MeOH). λ_{max} 213 (ϵ 26000); 287 (ϵ 5600); 303 (ϵ 5200); 315 (sh) (ϵ) (MeOH) (Derep). λ_{max} 213 (ϵ 26000); 287 (ϵ 5600); 303 (ϵ 5200) (MeOH) (Berdy).

5′-Deoxy: ***Keramamide L***

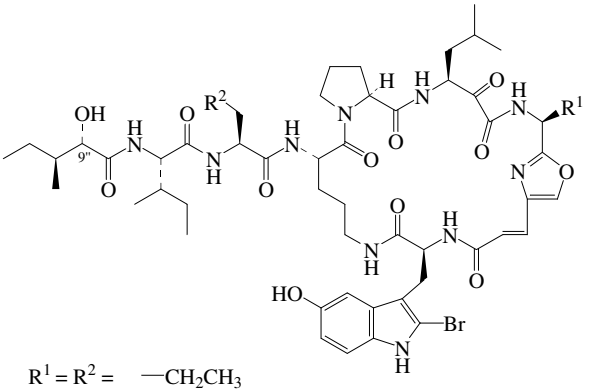
$C_{49}H_{63}ClN_8O_8$ 927.538

Isol. from *Theonella* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{22}$ -60 (c, 0.1 in MeOH). λ_{max} 213 (ϵ 18000) (MeOH). λ_{max} 213 (ϵ 18000); 285 (ϵ 2300); 297 (ϵ 1800) (MeOH) (Berdy).

Kobayashi, J. *et al., J.C.S. Perkin 1*, 1991, 2609 (*isol*)
Uemoto, H. *et al., Tetrahedron*, 1998, **54**, 6719-6724 (*Keramamide L*)

Keramamide B K-57

[137041-25-9]



$R^1 = R^2 =$ —CH_2CH_3

$C_{54}H_{77}BrN_{10}O_{12}$ 1138.166

Cyclic peptide. Isol. from the marine sponge *Theonella* sp. $[\alpha]_D^{23}$ -50 (c, 0.7 in MeOH). λ_{max} 267 (ϵ 23500); 312 (ϵ 4300) (MeOH) (Derep). λ_{max} 267 (ϵ 23500); 312 (ϵ 4300) (MeOH) (Berdy).

Kobayshi, J. *et al., J.A.C.S.*, 1991, **113**, 7812-7813 (*isol, pmr, cmr*)
Shioiri, T. *et al., Heterocycles*, 2003, **61**, 23-29 (*synth*)

Keramamide C K-58

[137041-26-0]

As Keramamide B, K-57 with

R^1 = –CH_2CH_3, R^2 = –CH_3

$C_{53}H_{75}BrN_{10}O_{12}$ 1124.139

Cyclic peptide. Isol. from the marine sponge *Theonella* sp. λ_{max} 267 (ϵ 23500); 312 (ϵ 4300) (MeOH) (Derep).

Kobayashi, J. *et al., J.A.C.S.*, 1991, **113**, 7812 (*isol*)

Keramamide D K-59

[137041-27-1]

As Keramamide B, K-57 with

$R^1 = R^2 = -CH_3$

$C_{52}H_{73}BrN_{10}O_{12}$ 1110.112

Cyclic peptide. Isol. from the marine sponge *Theonella* sp. λ_{max} 267 (ϵ 23500); 312 (ϵ 4300) (MeOH) (Derep).

9″-O-Sulfate: ***Keramamide M***

$C_{52}H_{73}BrN_{10}O_{15}S$ 1190.177

Isol. from a *Theonella* sp. Amorph. solid. λ_{max} 269 (ϵ 20000) (MeOH).

Kobayashi, J. *et al., J.A.C.S.*, 1991, **113**, 7812-7813 (*isol*)

Tsuda, M. *et al., Tetrahedron*, 1999, **55**, 12543-12548 (*Keramamide M*)

Keramamide E K-60

[161995-32-0]

As Keramamide B, K-57 with

R^1=CH_3, R^2=CH_2CH_3

$C_{53}H_{75}BrN_{10}O_{12}$ 1124.139

Cyclic peptide. Isol. from the sponge *Theonella* sp. Solid. $[\alpha]_D^{22}$ -39 (c, 0.1 in MeOH). λ_{max} 269 (ϵ 30900); 310 (sh) (MeOH). λ_{max} 269 (ϵ 30900); 310 (MeOH) (Berdy).

9″-O-Sulfate: ***Keramamide N***

$C_{53}H_{75}BrN_{10}O_{15}S$ 1204.204

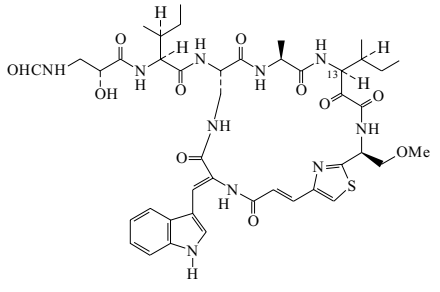
Isol. from a *Theonella* sp. Amorph. solid. λ_{max} 270 (ϵ 18000) (MeOH).

Kobayashi, J. *et al., Tetrahedron*, 1995, **51**, 2525-2532 (*isol, uv, ir, pmr, cmr, ms*)

Tsuda, M. *et al., Tetrahedron*, 1999, **55**, 12543-12548 (*Keramamide N*)

Keramamide F K-61

[143330-97-6]



$C_{43}H_{56}N_{10}O_{11}S$ 921.042

Cyclic thiopeptide antibiotic. Isol. from a *Theonella* sp. Amorph. Mp 187° dec. $[\alpha]_D^{21}$ -25 (c, 0.86 in MeOH). λ_{max} 209 (ϵ 30800); 220 (ϵ 30800); 275 (ϵ 23200); 339 (ϵ 9800) (MeOH) (Berdy).

13-Epimer: ***Keramamide G***

[162063-07-2]

$C_{43}H_{56}N_{10}O_{11}S$ 921.042

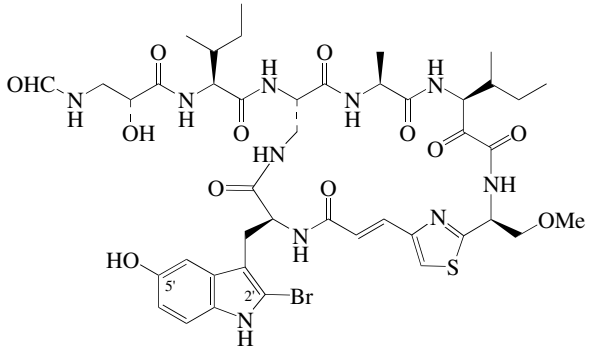
Isol. from a *Theonella* sp. Solid. $[\alpha]_D^{21}$ +10 (c, 0.1 in MeOH). λ_{max} 224 (ϵ 26500); 279 (ϵ 21200); 340 (ϵ 11700) (MeOH) (Berdy).

Itagaki, F. *et al., J.O.C.*, 1992, **57**, 5540 (*isol, pmr, cmr, struct*)

Kobayashi, J. *et al., Tetrahedron*, 1995, **51**, 2525 (*Keramamide G*)

Keramamide H K-62

[161995-33-1]



$C_{43}H_{57}BrN_{10}O_{12}S$ 1017.953

Cyclic peptide. Isol. from the sponge *Theonella* sp. Solid. $[\alpha]_D^{20}$ -42 (c, 0.05 in MeOH). λ_{max} 233; 277 (ϵ 23100) (MeOH). λ_{max} 277 (ϵ 23100) (MeOH) (Berdy).

2′-Debromo, 5′-deoxy: ***Keramamide J***

[161995-34-2]

$C_{43}H_{58}N_{10}O_{11}S$ 923.058

Isol. from *Theonella* sp. Solid. $[\alpha]_D^{18}$ +8.4 (c, 0.1 in MeOH). λ_{max} 222 (ϵ 45200); 278 (ϵ 27200) (MeOH). λ_{max} 228 (ϵ 45200); 278 (ϵ 27200) (MeOH) (Berdy).

2′-Debromo, 5′-deoxy, $N^{1'}$*-Me:* ***Keramamide K***

$C_{44}H_{60}N_{10}O_{11}S$ 937.084

Isol. from the sponge *Theonella* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{28}$ -25 (c, 0.1 in MeOH). λ_{max} 269 (ϵ 20000) (MeOH). λ_{max} 269 (ϵ 20000) (MeOH) (Berdy).

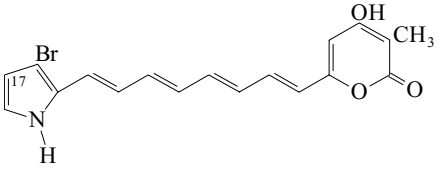
Kobayashi, J. *et al., Tetrahedron*, 1995, **51**, 2525-2532 (*isol, uv, ir, pmr, cmr, ms*)

Uemoto, H. *et al., Tetrahedron*, 1998, **54**, 6719-6724 (*Keramamide K*)

Sowinski, J.A. *et al., Chem. Comm.*, 1999, 981-982 (*synth, Keramamide J*)

Keronopsin B_1 K-63

[158182-29-7]



$C_{18}H_{16}BrNO_3$ 374.233

Alkaloid from the marine ciliate *Pseudokeronopsis rubra*. Chemical defence substance. Black cryst. (Me_2CO).

Mp 135-139°. λ_{max} 229 (ϵ 14454); 266 (ϵ 18620); 421 (ϵ 70794) (MeOH) (Berdy).

O-*Sulfate:* ***Keronopsin A_1***

[158182-31-1]

$C_{18}H_{16}BrNO_6S$ 454.297

Alkaloid from *Pseudokeronopsis rubra*. Brick-red amorph. powder (as Na salt). Unstable in the crude extract. Converted into Keronopsin B_1 with traces of acid. In dry state may polymerise spontaneously. CAS no. refers to Na salt. λ_{max} 221; 267; 325; 339; 439 (MeOH) (Berdy).

17-Bromo: ***Keronopsin B_2***

[158182-30-0]

$C_{18}H_{15}Br_2NO_3$ 453.129

Alkaloid from *Pseudokeronopsis rubra*. Brown-red amorph. powder. λ_{max} 229 (ϵ 15850); 439 (ϵ 61659) (MeOH) (Berdy).

17-Bromo, O-*sulfate:* ***Keronopsin A_2***

[158182-32-2]

$C_{18}H_{15}Br_2NO_6S$ 533.194

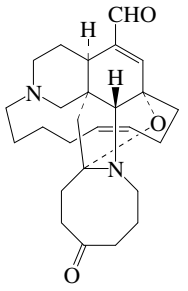
Alkaloid from *Pseudokeronopsis rubra*. Unstable in the crude

extract. Converted into Keronopsin B_2 with traces of acid. CAS no. refers to Na salt. λ_{max} 222; 269; 326; 434 (MeOH) (Berdy).

Höfle, G. *et al., Angew. Chem., Int. Ed.*, 1994, **33**, 1495-1497 (*isol, uv, ir, pmr, cmr, ms, struct*)

31-Keto-12,34-oxa-32,33-dihydroircinal A K-64

[721429-61-4]



Absolute Configuration

$C_{26}H_{36}N_2O_3$ 424.582

Related to Ircinol A, I-100. Isol. from an *Acanthostrongylophora* sp. Powder (MeOH).
Mp 164° dec. $[\alpha]_D^{25}$ +44 (c, 0.1 in $CHCl_3$). λ_{max} 235 (log ϵ 3.93) (MeOH).

Yousaf, M. *et al., J. Med. Chem.*, 2004, **47**, 3512-3517 (*isol, pmr, cmr*)

Keyhole limpet hemocyanin K-65

Immucothel. Vacmune^R*. KLH*

Cu-containing respiratory protein. Consists of 2 struct. and physiol. distinct isoforms KLH1 and KLH2. Isol. from the marine mollusc *Megathura crenulata*. Immunomodulator, antineoplastic agent. Hapten carrier and generalised vaccine component used in the diagnosis of schistosomiasis. Used in combination with the mucin antigen, sialyl-Tn (STn) as the therapeutic cancer vaccine, Theratope.

Harris, J.R. *et al., Micron*, 1997, **28**, 31-41; 43-56; 1999, **30**, 597-623 (*rev, struct, props, pharmacol*)
Kurokawa, T. *et al., Eur. J. Biochem.*, 2002, **269**, 5459-5473 (*bibl*)
Drugs RD, 2003, **4**, 236-240 (*theratope*)
Hartmann, H. *et al., J. Biol. Chem.*, 2004, **279**, 2841-2845 (*conformn*)
Geyer, H. *et al., J. Biol. Chem.*, 2005, **280**, 40731-40748 (*struct, use*)

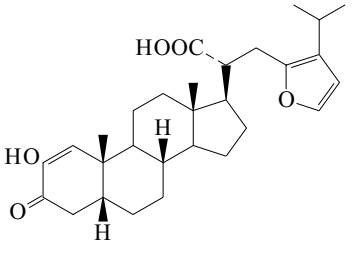
KHEYLRF amide K-66

Peptide AF2
[146269-94-5]
H-Lys-His-Glu-Tyr-Leu-Arg-Phe-NH_2
$C_{47}H_{70}N_{14}O_{10}$ 991.158
Isol. from *Achatina fulica*, *Ascaris suum*, *Caenorhabditis elegans*, *Haemonchus contortus* and *Panagrellus redivivus*. Neuromuscular transmitter.

Koch, G. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1993, **106**, 359 (*isol, struct*)
Cowden, C. *et al., Peptides (N.Y.)*, 1993, **14**, 423 (*isol, struct*)
Maule, A.G. *et al., Parasitology*, 1994, **109**, 351-356 (*isol*)
Marks, N.J. *et al., Biochem. Biophys. Res. Commun.*, 1995, **217**, 845 (*isol*)

Kiheisterone A K-67

[144436-06-6]



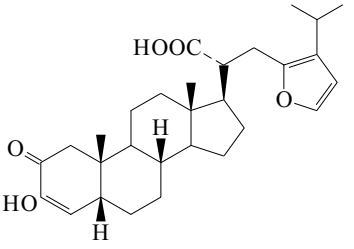
$C_{29}H_{40}O_5$ 468.632

Constit. of the sponge *Strongylacidon* sp. Glass. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D$ +144 (c, 1.72 in MeOH). λ_{max} 266 (ϵ 10300) (MeOH) (Derep). λ_{max} 266 (ϵ 10900) (MeOH) (Berdy).

Carney, J.R. *et al., J.O.C.*, 1992, **57**, 6637-6640 (*isol, pmr, cmr*)

Kiheisterone B K-68

[144436-07-7]

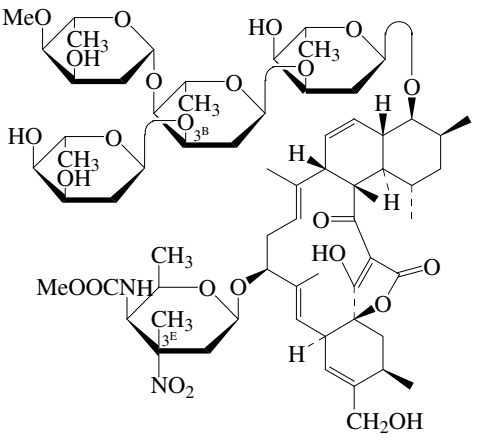


$C_{29}H_{40}O_5$ 468.632
Constit. of the sponge *Strongylacidon* sp. Needles. Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 223-225°. $[\alpha]_D$ +19 (c, 0.7 in $CHCl_3$). λ_{max} 266 (ϵ 10300) (MeOH) (Derep).

Carney, J.R. *et al., J.O.C.*, 1992, **57**, 6637-6640 (*isol, pmr, cmr*)

Kijanimicin K-69

Sch 25663. Antibiotic Sch 25663
[78798-08-0]



$C_{67}H_{100}N_2O_{24}$ 1317.526

Nitroaminoglycoside antibiotic. From *Actinomadura kijaniata*. Active against gram-positive bacteria and fungi. Amorph. solid. Sol. MeOH, Me_2CO; poorly sol. H_2O, hexane, Et_2O.
Mp 174.5°. $[\alpha]_D^{26}$ -124.2 (c, 0.2 in MeOH). pK_a 5. λ_{max} 215 (ϵ 13200); 239 (ϵ 12100); 267 (ϵ 9870); 274 (ϵ 8550) (MeOH) (Derep). λ_{max} 200 (ϵ 42832); 241 (ϵ 8946); 274 (ϵ 9446) (MeOH) (Berdy). λ_{max} 205 (ϵ 38313); 258 (ϵ 9881) (MeOH-HCl) (Berdy). λ_{max} 236 (ϵ 14677); 276 (ϵ 12002) (MeOH-NaOH) (Berdy). λ_{max} 199 (E1%/1cm 328); 242 (E1%/1cm 56.2); 264 (E1%/1cm 63.1); 274 (E1%/1cm 60.7) (EtOH) (Berdy).
▶ LD_{50} (mus, scu) 1000 mg/kg. OB8650500

3^B*-O-Deglycosyl:* ***Antibiotic U 64815***. *U 64185. 3*^{B}*-De-O-digitoxosylkijanimicin. Lobophorin B*
[78798-30-8]
[89492-38-6]
$C_{61}H_{90}N_2O_{21}$ 1187.383
Prod. by *Streptomyces microspinosus*. Also prod. by a marine actinomycete obt. from the alga *Lobophora variegata*. Powder. Sol. MeOH, DMSO, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D$ -129.5 (c, 0.3 in MeOH). λ_{max} 215; 240; 267 (EtOH). λ_{max} 204 (ϵ 40000);

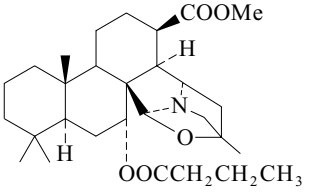
239 (ϵ 14000); 265 (ϵ 11000); 277 (ϵ 10000) (MeOH). λ_{max} 213; 261 (EtOH-HCl) (Berdy). λ_{max} 218; 239; 265; 280 (EtOH-NaOH) (Berdy).

3^B-O-Deglycosyl, 3^E-amino, 3^E-denitro: ***Lobophorin A***
[247171-46-6]
$C_{61}H_{92}N_2O_{19}$ 1157.4
Prod. by a marine actinomycete obt. from the alga *Lobophora variegata*.
$[\alpha]_D^{22}$ -175 (c, 0.28 in MeOH). λ_{max} 204 (ϵ 36000); 241 (ϵ 13000); 268 (ϵ 11000); 280 (ϵ 10000) (MeOH).

Waitz, J.A. *et al., J. Antibiot.*, 1981, **34**, 1101 (*isol*)
Mallams, A.K. *et al., J.A.C.S.*, 1981, **103**, 3938; 3940 (*struct*)
Mallams, A.K. *et al., J.C.S. Perkin 1*, 1983, 1497 (*isol, uv, ir, pmr, cmr, cryst struct*)
U.S. Pat., 1984, 4 427 776; *CA*, **100**, 155203a (*U 64815*)
Thiem, J. *et al., Tetrahedron*, 1990, **46**, 113 (*synth*)
Koepper, S. *et al., Annalen*, 1994, 581 (*pmr, conformn*)
Jiang, Z.-D. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 2003-2006 (*Lobophorins*)

Kimbasine A K-70

[135626-55-0]



$C_{29}H_{45}NO_5$ 487.678
Norsesterterpene alkaloid from the sponge *Igernella notabilis*. Cytotoxic. $[\alpha]_D$ -69.1 (c, 1.1 in $CHCl_3$).

O-*Debutanoyl,* O-*Ac:* ***Kimbasine B***
[135626-56-1]
$C_{27}H_{41}NO_5$ 459.625
Alkaloid from *Igernella notabilis*. Cytotoxic agent. $[\alpha]_D$ -64.1 (c, 0.1 in $CHCl_3$).

Cardellina, J.H. *et al., Tet. Lett.*, 1991, **32**, 2347 (*isol, pmr, cmr, struct*)

Penaeus vannamei Kinins K-71

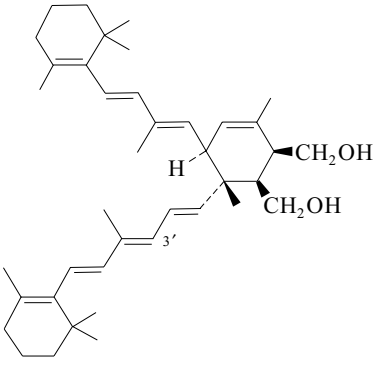
Asp-Ser-Phe-Ser-Pro-Trp-Gly-NH_2
Struct. of Pev-kinin 1 shown. Isol. from brain of the white shrimp *Penaeus vannamei*. Myotropic neuropeptides.

Pev-kinin 1 [212468-49-0]
$C_{36}H_{47}N_9O_9$ 749.822

Pev-kinin 2 [212468-51-4]
$C_{33}H_{42}N_8O_9$ 694.743

Nieto, J. *et al., Biochem. Biophys. Res. Commun.*, 1998, **248**, 406-411 (*isol*)

Kitol A K-72



$C_{40}H_{60}O_2$ 572.913

(All-*E*)-*form* [4626-00-0]
Constit. of whale liver and other liver oils.
Cryst. (Me or Et formate).
Mp 138-139°. $[\alpha]_D^{20}$ -2.6 (c, 1.1 in $CHCl_3$). λ_{max} 190 (ϵ 12000); 286 (ϵ 39000); 295 (ϵ 39000) (hexane).

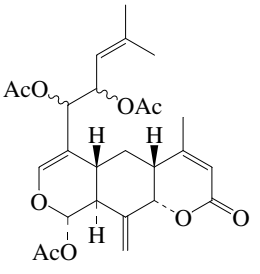
Di-Ac:
Cryst. (CH_2Cl_2/Et formate). Mp 150-151°. $[\alpha]_D^{20}$ -4 (c, 2.4 in $CHCl_3$).

(3′*Z*)-*form*
Kitol B
[75464-32-3]
Constit. of whale liver.

Burger, B.V. *et al., J.C.S. Perkin 1*, 1973, 590
Tsukida, K. *et al., J. Nutr. Sci. Vitaminol.*, 1980, **26**, 319 (*struct, Kitol B*)

Kitungolide A K-73

[676132-32-4]

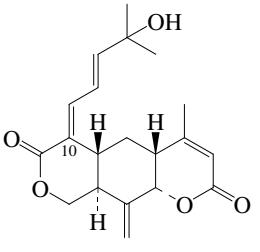


$C_{26}H_{32}O_9$ 488.533
Constit. of a soft coral. Oil. $[\alpha]_D^{21}$ +36.5 (c, 0.71 in $CHCl_3$).

Chill, L. *et al., Org. Lett.*, 2004, **6**, 755-758 (*isol, pmr, cmr*)

Kitungolide B K-74

[676132-33-5]



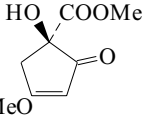
$C_{20}H_{24}O_5$ 344.407
Constit. of a soft coral. Oil. $[\alpha]_D^{21}$ +70.6 (c, 0.11 in $CHCl_3$).

10Z-Isomer: ***Kitungolide C***
[676132-34-6]
$C_{20}H_{24}O_5$ 344.407
Constit. of a soft coral. Oil. $[\alpha]_D^{21}$ +54.5 (c, 0.07 in $CHCl_3$).

Chill, L. *et al., Org. Lett.*, 2004, **6**, 755-758 (*isol, pmr, cmr*)

Kjellmanianone K-75

Methyl 1-hydroxy-4-methoxy-2-oxo-3-cyclopentene-1-carboxylate, 9CI



(*R*)–*form*

$C_8H_{10}O_5$ 186.164
Abs. config. revised in 1994. Natural Kjellmanianone is largely racemic. λ_{max} 242 (ϵ 14300) (MeOH) (Derep).

(*R*)-*form* [81369-90-6] Synthetic. Mp 157-158°. $[\alpha]_D$ -113 (c, 1.15 in $CHCl_3$).

(*S*)-*form* [76280-92-7]
Isol. from the marine alga *Sargassum kjellmanianum*. Shows mod. activity against gram-positive bacteria, *E. coli* and *Bacillus subtilis.*
Cryst.
Mp 139-139.5°. $[\alpha]_D$ +1.6 (c, 1.8 in $CHCl_3$). $[\alpha]_D$ +99.1 ($CHCl_3$) (calc.).

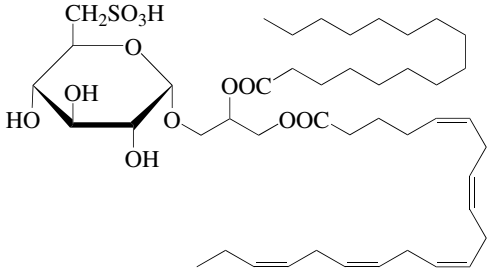
(±)-*form* [78738-68-8]
Mp 126-128°.

Ac:
Pale yellow solid. Mp 113-115°.

Nakayama, N. *et al., Chem. Lett.*, 1980, 1243 (*isol, struct*)
Boschelli, D. *et al., Tet. Lett.*, 1981, 4385 (*synth*)
Chen, B.-C. *et al., Tetrahedron*, 1991, **47**, 173 (*synth, cd*)
Zhu, J. *et al., Tetrahedron*, 1994, **50**, 10597 (*synth, abs config*)
Demir, A.S. *et al., Turk. J. Chem.*, 1996, **20**, 244-248 (*synth*)
Christoffers, J. *et al., Chem. Eur. J.*, 2004, **10**, 1042-1045 (*synth*)

KM043 K-76

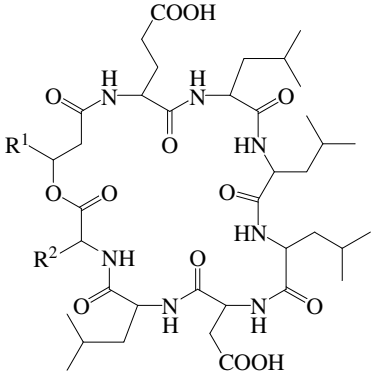
(6-Sulfoquinovopyranosyl)-(1→3′)-1′-(5,8,11,14,17-eicosapentaenoyl)-2′-hexadecanoylglycerol



$C_{45}H_{76}O_{12}S$ 841.154
Isol. from the red alga *Gigartina tenella*. Potent inhibitor of eukaryotic DNA polymerases and HIV-reverse transcriptase type 1. Cytotoxic agent. Amorph. solid. $[\alpha]_D$ +57 (c, 0.1 in MeOH).

Ohta, K. *et al., Chem. Pharm. Bull.*, 1998, **46**, 684-686 (*isol, pmr, cmr*)

Bacillus pumilus KMM 1364 Lipodepsipeptides K-77



A, R^1 = -$(CH_2)_8CH(CH_3)CH_2CH_3$, R^2 = -$CH(CH_3)_2$
B, R^1 = -$(CH_2)_9CH(CH_3)_2$, R^2 = -$CH(CH_3)_2$
C, R^1 = -$(CH_2)_8CH(CH_3)CH_2CH_3$, R^2 = -$CH(CH_3)CH_2CH_3$
D, R^1 = -$(CH_2)_9CH(CH_3)_2$, R^2 = -$CH(CH_3)CH_2CH_3$
E, R^1 = -$(CH_2)_{11}CH(CH_3)_2$, R^2 = -$CH(CH_3)_2$
F, R^1 = -$(CH_2)_{10}CH(CH_3)CH_2CH_3$, R^2 = -$CH(CH_3)CH_2CH_3$
G, R^1 = -$(CH_2)_{11}CH(CH_3)_2$, R^2 = -$CH(CH_3)CH_2CH_3$

Lipodepsipeptide antibiotic complex related to Surfactin and Bacircines, B-5. The individual components are not separately named in the ref. Named here as KMM 1364A-G. Prod. by *Bacillus pumilus* (KMM 1364) isol. from the ascidian *Halocynthia aurantium*.

KMM 1364A [464900-34-3]
$C_{53}H_{93}N_7O_{13}$ 1036.357

KMM 1364B [464900-27-4]
$C_{53}H_{93}N_7O_{13}$ 1036.357

KMM 1364C [464900-36-5]

KMM 1364D [464900-29-6]

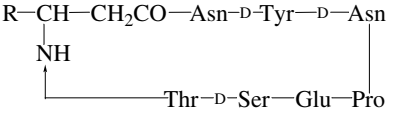
KMM 1364E [464900-31-0]

KMM 1364F [464900-38-7]
$C_{56}H_{99}N_7O_{13}$ 1078.437

KMM 1364G [464900-32-1]

Kalinovskaya, N.I. *et al., Mar. Biotechnol.*, 2002, **4**, 179-188 (*isol*)

Bacillus subtilis KMM 457 Peptide 1 K-78



R = -$(CH_2)_{10}CH_3$

$C_{47}H_{76}N_{10}O_{15}$ 1021.175
Isol. from a marine-derived *Bacillus subtilis* KMM 457. Antifungal agent.

Oleinikova, G.K. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2001, **50**, 2231-2235

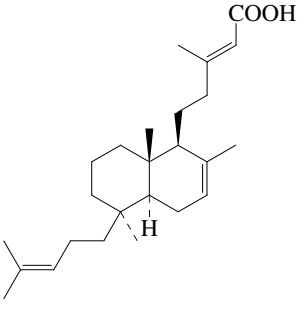
Bacillus subtilis KMM 457 Peptide 2 K-79

As *Bacillus subtilis* KMM 457 Peptide 1, K-78 with
R = -$(CH_2)_9CH(CH_3)_2$
$C_{48}H_{78}N_{10}O_{15}$ 1035.202
Isol. from a marine *Bacillus subtilis* strain KMM 457. Antifungal agent.

Oleinikova, G.K. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2001, **50**, 2231-2235

Kohamaic acid A K-80

[334829-38-8]

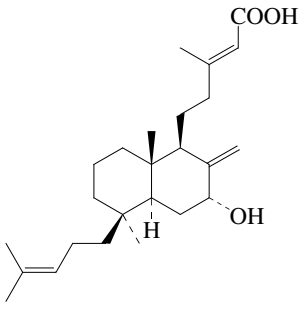


$C_{25}H_{40}O_2$ 372.59
Constit. of an *Ircinia* sponge.
$[\alpha]_D^{31}$ -3 (c, 0.42 in $CHCl_3$).

Kokubo, S. *et al., Chem. Lett.*, 2001, 176-177 (*isol, pmr, cmr*)

Kohamaic acid B K-81

[334829-39-9]

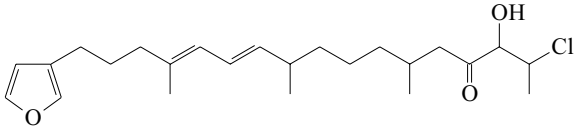


$C_{25}H_{40}O_3$ 388.589
Constit. of an *Ircinia* sponge.
$[\alpha]_D^{30}$ -4.7 (c, 0.082 in $CHCl_3$).

Kokubo, S. *et al., Chem. Lett.*, 2001, 176-177 (*isol, pmr, cmr*)

Konakhin K-82

[132970-80-0]

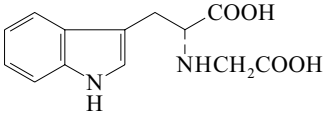


$C_{24}H_{37}ClO_3$ 409.007
Constit. of a marine Dictyoceratid sponge. Oil. $[\alpha]_D^{20}$ +6 (c, 0.1 in $CHCl_3$). λ_{max} 238 (ϵ 22000) (MeOH) (Derep).

N'diaye, I. *et al., Chem. Comm.*, 1991, 97-98 (*isol, pmr, cmr*)

Konbamidin K-83

N-*(Carboxymethyl)tryptophan, 9CI*



(*R*)–*form*

$C_{13}H_{14}N_2O_4$ 262.265

(*R*)-*form*

D-form
[160955-40-8]
Alkaloid from the Okinawan marine sponge *Ircinia* sp. Exhibits cytotoxicity against HeLa cells *in vitro*. Powder. $[\alpha]_D^{21}$ +15 (c, 0.27 in MeOH). λ_{max} 228 (ϵ 18200); 281 (ϵ 3310); 290 (ϵ 2690) (MeOH) (Berdy).

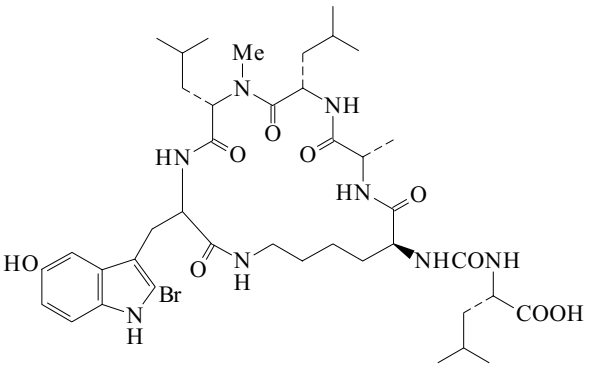
(*S*)-*form*

L-form
Synthetic. Not significantly cytotoxic. $[\alpha]_D^{21}$ -12.6 (c, 1.9 in MeOH).

Shinonaga, H. *et al., J. Nat. Prod.*, 1994, **57**, 1603 (*isol, uv, ir, pmr, cmr, synth, struct*)

Konbanamide K-84

Konbamide
[136466-02-9]

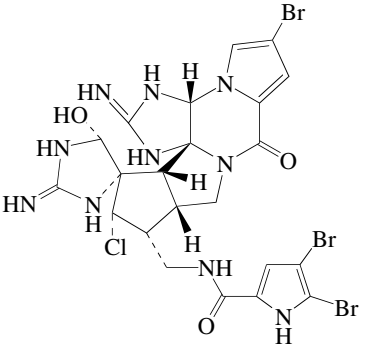


$C_{40}H_{61}BrN_8O_9$ 877.874
Cyclic hexapeptide. Proposed struct. shown is incorrect. Constit. of the sponge *Theonella* sp. Calmodulin antagonist. $[\alpha]_D^{21}$ -43 (c, 0.042 in MeOH). λ_{max} 222 (ϵ 18000); 278 (ϵ 5800); 298 (ϵ 4200); 310 (ϵ 2900) (MeOH) (Derep).

Kobayashi, J. *et al., Chem. Comm.*, 1991, 1050 (*isol, pmr, cmr*)
Schmidt, U. *et al., Angew. Chem., Int. Ed.*, 1996, **35**, 1336 (*synth, pmr, struct*)

Konbuacidin A K-85

[200207-22-3]

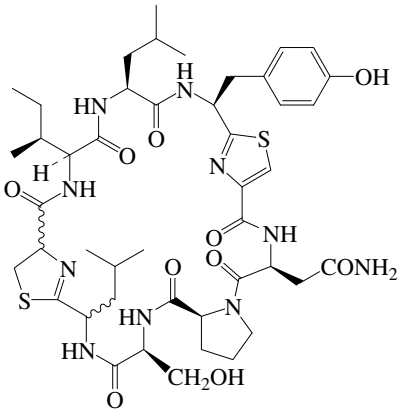


$C_{22}H_{22}Br_3ClN_{10}O_3$ 749.646
The imidazole ring systems are delocalised. Alkaloid from the sponge *Hymeniacidon* sp. Cyclin dependent kinase 4 inhibitor. Amorph. solid. $[\alpha]_D^{24}$ -45 (c, 0.5 in MeOH). λ_{max} 277 (ϵ 13000) (MeOH).

Kobayashi, J. *et al., Tetrahedron*, 1997, **53**, 15681-15684 (*isol, uv, ir, pmr, cmr, ms*)

Kororamide K-86

[261373-26-6]

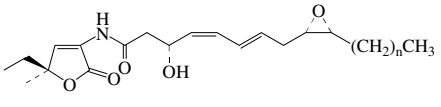


$C_{45}H_{64}N_{10}O_{10}S_2$ 969.194
Isol. from *Lyngbya majuscula*. Amorph. solid. λ_{max} 238 (ϵ 6400) (MeOH).

Mitchell, S.S. *et al., J. Nat. Prod.*, 2000, **63**, 279-282 (*isol, pmr, cmr, cd, uv*)

Korormicin A K-87

[200433-05-2]



Absolute Configuration

n = 7

$C_{25}H_{39}NO_5$ 433.587
Prod. by the marine bacterium *Pseudoalteromonas* sp. F-420 isol. from an alga. Active against marine gram-negative bacteria. Oil. $[\alpha]_D^{26}$ -24.4 (c, 0.3 in EtOH). λ_{max} 233 (log ϵ 4.8) (EtOH).

Yoshikawa, K. *et al., J. Antibiot.*, 1997, **50**, 949-953; 1999, **52**, 182-185 (*isol, uv, ir, pmr, cmr, activity*)
Uehara, H. *et al., Tet. Lett.*, 1999, **40**, 8641-8645 (*synth, abs config*)
Kobayashi, Y. *et al., Eur. J. Org. Chem.*, 2001, 1873-1881 (*synth, abs config*)

Korormicin B K-88

As Korormicin A, K-87 with
n = 5

$C_{23}H_{35}NO_5$ 405.533

Stereochem. not confirmed. Prod. by *Pseudoalteromonas* sp. F-420. Oil. λ_{max} 232 (log ϵ 4.55) (EtOH).

Yoshikawa, K. *et al., J. Antibiot.*, 2003, **56**, 866-870

Korormicin C K-89

As Korormicin A, K-87 with
n = 6

$C_{24}H_{37}NO_5$ 419.56
Prod. by *Pseudoalteromonas* sp. F-420. Oil. Stereochem. not confirmed. λ_{max} 232 (log ϵ 4.59) (EtOH).

Yoshikawa, K. *et al., J. Antibiot.*, 2003, **56**, 866-870

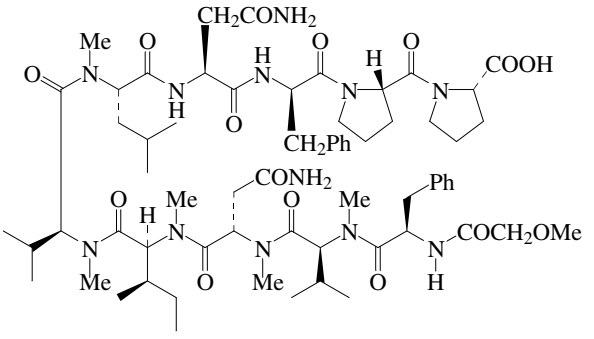
Korormicin D K-90

As Korormicin A, K-87 with
n = 8

$C_{26}H_{41}NO_5$ 447.614
Prod. by *Pseudoalteromonas* sp. F-420. Oil. Stereochem. not confirmed. λ_{max} 233 (log ϵ 4.43) (EtOH).

Yoshikawa, K. *et al., J. Antibiot.*, 2003, **56**, 866-870

Koshikamide A_1 K-91



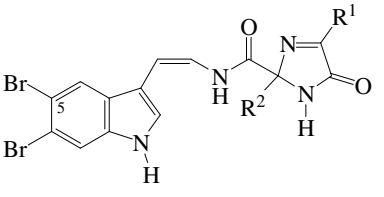
$C_{66}H_{100}N_{12}O_{15}$ 1301.587
Peptide antibiotic. Isol. from the sponge, *Theonella* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{25}$ -156 (c, 0.19 in MeOH). λ_{max} 212 (ϵ 29000) (MeOH).

L-Arginine amide: ***Koshikamide A_2***
$C_{72}H_{112}N_{16}O_{16}$ 1457.774
Isol. from a *Theonella* sp. Amorph. solid. $[\alpha]_D^{24}$ -130 (c, 0.1 in MeOH). λ_{max} 209 (ϵ 19000) (MeOH).

Fusetani, N. *et al., Tet. Lett.*, 1999, **40**, 4687-4690 (*Koshikamide A_1*)
Araki, T. *et al., Biosci., Biotechnol., Biochem.*, 2005, **69**, 1318-1322 (*Koshikamide A_2*)

Kottamide A K-92

[446862-69-7]



R^1 = -CH(CH$_3$)CH$_2$CH$_3$, R^2 = -CH(CH$_3$)$_2$

$C_{21}H_{24}Br_2N_4O_2$ 524.254
Isol. from the New Zealand ascidian *Pycnoclavella kottae*. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{20}$ +160 (c, 0.2 in MeOH). λ_{max} 236 (log ϵ 4.46); 284 (log ϵ 4.14) (MeOH).

5-Debromo: ***Kottamide B***
[446862-70-0]
$C_{21}H_{25}BrN_4O_2$ 445.358
Isol. from the New Zealand ascidian *Pycnoclavella kottae*. Amorph. solid. $[\alpha]_D^{20}$ +245 (c, 0.2 in MeOH). Obt. as a mixt. with Kottamide C to which data refers. λ_{max} 232 (log ϵ 4.44); 286 (log ϵ 4.13) (MeOH).

6-Debromo: ***Kottamide C***
[446862-71-1]
$C_{21}H_{25}BrN_4O_2$ 445.358
Isol. from *Pycnoclavella kottae*. Obt. as a mixt. with Kottamide B.

Appleton, D.R. *et al., J.O.C.*, 2002, **67**, 5402-5404 (*isol, pmr, cmr, N-15 nmr, ms*)

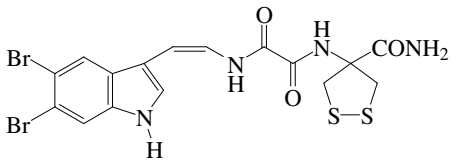
Kottamide D K-93

[446862-72-2]
As Kottamide A, K-92 with
R^1 = CH_3, R^2 = -CH(CH$_3$)CH$_2$CH$_3$

$C_{19}H_{20}Br_2N_4O_2$ 496.201
Isol. from the New Zealand ascidian *Pycnoclavella kottae*. Antiinflammatory and cytotoxic agent. Amorph. solid. $[\alpha]_D^{20}$ +150 (c, 0.2 in MeOH). λ_{max} 237 (log ϵ 4.39); 286 (log ϵ 4.11) (MeOH).

Appleton, D.R. *et al., J.O.C.*, 2002, **67**, 5402-5404 (*isol, pmr, cmr, N-15 nmr, ms*)

Kottamide E K-94



$C_{16}H_{14}Br_2N_4O_3S_2$ 534.252
Alkaloid from the ascidian *Pycnoclavella kottae*. Amorph. solid. λ_{max} 202 (log ϵ 4.36); 239 (log ϵ 4.41); 305 (log ϵ 3.92) (MeOH).

Appleton, D.R. *et al., Tet. Lett.*, 2003, **44**, 8963-8965 (*isol, pmr, cmr*)

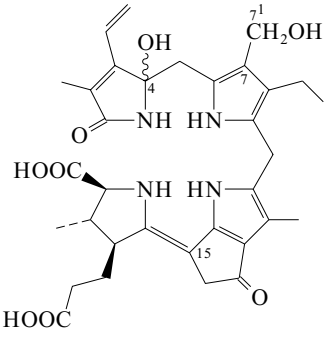
KPSFVRF amide K-95

H-Lys-Pro-Ser-Phe-Val-Arg-Phe-NH_2
$C_{43}H_{66}N_{12}O_8$ 879.07
Isol. from the nematode *Caenorhabditis elegans*. Neuropeptide.

Marks, N.J. *et al., Biochem. Biophys. Res. Commun.*, 1999, **254**, 222-230 (*isol*)

Krill fluorescent substance F K-96

Krill luciferin. Euphausia *Luciferin*
[121295-09-8]



$C_{33}H_{40}N_4O_8$ 620.701
Isol. from *Euphausia pacifica*. Unstable. Readily oxidises.

4,7[1]-Dideoxy: **Pyrocystis *Luciferin***
[121295-11-2]
$C_{33}H_{40}N_4O_6$ 588.702
Isol. from the dinoflagellate *Pyrocystis lunula*.

[122564-61-8]

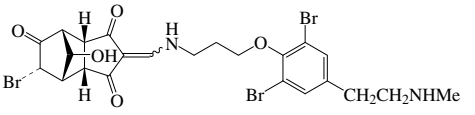
Nakamura, H. *et al., J.A.C.S.*, 1988, **110**, 2683; 1989, **111**, 7607 (*isol, struct, props*)
Stojanovic, M.N. *et al., Tet. Lett.*, 1994, **35**, 9343; 9347 (*Pyrocystis Luciferin*)
Wu, C. *et al., Tet. Lett.*, 2003, **44**, 1263-1266 (*biosynth*)

KSAYMRF amide K-97

Peptide AF8. *Peptide CF1*. *Peptide PF3*
[155455-76-8]
H-Lys-Ser-Ala-Tyr-Met-Arg-Phe-NH_2
$C_{41}H_{64}N_{12}O_9S$ 901.098
Isol. from the nematodes *Ascaris suum*, *Panagrellus redivivus*, *Haemonchus contortus* and *Caenorhabditis elegans*. Mycoactive peptide.

Maule, A.G. *et al., Biochem. Biophys. Res. Commun.*, 1994, **200**, 973-980 (*isol, struct*)
Marks, N.J. *et al., Biochem. Biophys. Res. Commun.*, 1998, **248**, 422-425 (*isol*)
Marks, N.J. *et al., Mol. Biochem. Parasitol.*, 1999, **100**, 185-194 (*isol*)

Kuchinoenamine K-98



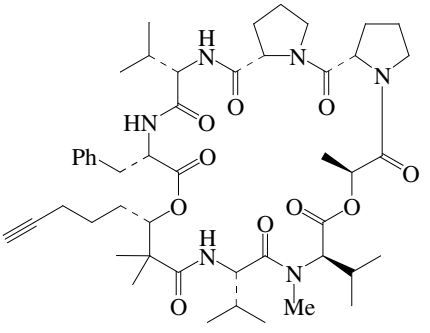
Relative Configuration

$C_{23}H_{25}Br_3N_2O_5$ 649.173
Alkaloid from the sponge *Hexadella* sp. Antibacterial agent. Amorph. solid. $[\alpha]_D^{21}$ +21 (c, 0.05 in MeOH). λ_{max} 244 (ϵ 8620); 310 (ϵ 12730) (MeOH).

Matsunaga, S. *et al., J.O.C.*, 2005, **70**, 1893-1896 (*isol, pmr, cmr*)

Kulokainalide 1 K-99

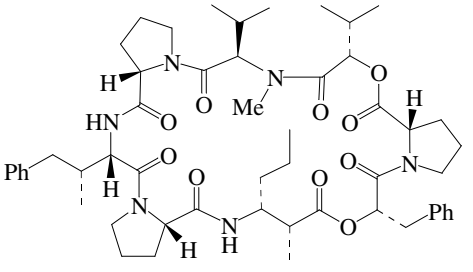
[206184-14-7]



$C_{48}H_{70}N_6O_{10}$ 891.115
Depsipeptide antibiotic. Related to Kulolide 1, K-102. Isol. from the mollusc *Philinopsis speciosa*. Amorph. solid. $[\alpha]_D^{20}$ -56 (c, 1 in MeOH). λ_{max} 260 (sh) (MeOH).

Nakao, Y. *et al., J.O.C.*, 1998, **63**, 3272-3280 (*isol, pmr, cmr*)

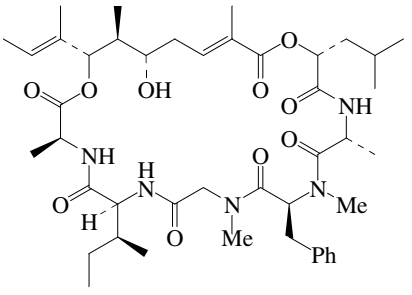
Kulokekahilide 1 K-100



$C_{53}H_{74}N_6O_{10}$ 955.202
Isol. from the mollusc *Philinopsis speciosa*. Cytotoxic. Amorph. solid. $[\alpha]_D$ +22 (c, 0.07 in MeOH). λ_{max} 205 (ϵ 14000); 235 (ϵ 3200) (MeOH).

Kimura, J. *et al., J.O.C.*, 2002, **67**, 1760-1767 (*isol, pmr, cmr*)

Kulokekahilide 2 K-101



Absolute Configuration

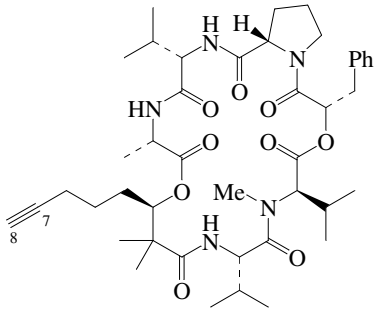
$C_{44}H_{67}N_5O_{10}$ 826.041

Isol. from the mollusc *Philinopsis speciosa*. Cytotoxic. Amorph. solid. $[\alpha]_D$ -15 (c, 0.04 in MeOH). λ_{max} 205 (ϵ 15000) (MeOH).

Nakao, Y. *et al., J. Nat. Prod.*, 2004, **67**, 1332-1340 (*isol, pmr, cmr*)

Kulolide 1 K-102

[183731-38-6]



$C_{43}H_{63}N_5O_9$ 793.999

Depsipeptide antibiotic. Isol. from the mollusc *Philinopsis speciosa*. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{20}$ -102 (c, 1 in MeOH). λ_{max} 215 (ϵ 16000); 254 (ϵ 460); 260 (ϵ 450); 266 (ϵ 350) (MeOH) (Berdy).

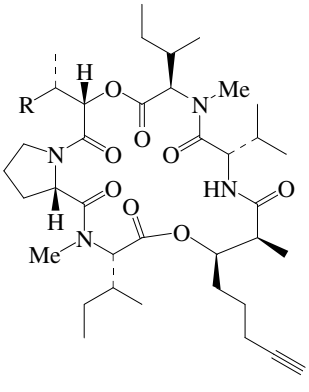
7,8-Dihydro: ***Kulolide 2***
$C_{43}H_{65}N_5O_9$ 796.015
Isol. from *Philinopsis speciosa*. Amorph. solid. $[\alpha]_D^{31}$ -59 (c, 1 in MeOH). λ_{max} 206 (ϵ 4300); 270 (ϵ 210) (MeOH).

7,7,8,8-Tetrahydro: ***Kulolide 3***
$C_{43}H_{67}N_5O_9$ 798.03
Isol. from *Philinopsis speciosa*. Amorph. solid. $[\alpha]_D^{31}$ -95.2 (c, 1.11 in MeOH). λ_{max} 208 (ϵ 20400); 213 (ϵ 17300); 287 (ϵ 700) (MeOH).

Reese, M.T. *et al., J.A.C.S.*, 1996, **118**, 11081-11084 (*isol, uv, ir, pmr, cmr*)
Nakao, Y. *et al., J.O.C.*, 1998, **63**, 3272-3280 (*Kulolide 2, Kukolide 3*)

Kulomoopunalide 1 K-103

[206184-15-8]



R = CH_2CH_3

$C_{39}H_{64}N_4O_8$ 716.957

Depsipeptide. Isol. from the mollusc *Philinopsis speciosa*. Amorph. solid. $[\alpha]_D^{31}$ -63 (c, 0.67 in MeOH). λ_{max} 206 (ϵ 14700); 276 (ϵ 300) (MeOH).

Nakao, Y. *et al., J.O.C.*, 1998, **63**, 3272-3280 (*isol, uv, ir, pmr, cmr*)

Kulomoopunalide 2 K-104

[206184-16-9]

As Kulomoopunalide 1, K-103 with

R = CH_3

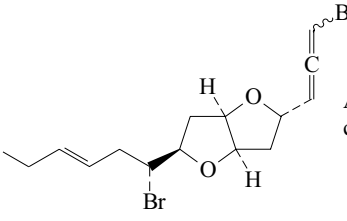
$C_{38}H_{62}N_4O_8$ 702.93

Depsipeptide. Isol. from the mollusc *Philinopsis speciosa*. Amorph. solid. $[\alpha]_D^{31}$ -45 (c, 1.36 in MeOH). λ_{max} 208 (ϵ 14100); 212 (ϵ 12900); 269 (ϵ 150); 284 (ϵ 130) (MeOH).

Nakao, Y. *et al., J.O.C.*, 1998, **63**, 3272-3280 (*isol, uv, ir, pmr, cmr*)

Kumausallene K-105

[87980-56-1]



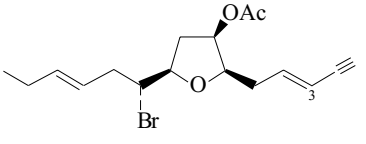
Absolute configuration

$C_{15}H_{20}Br_2O_2$ 392.13

Constit. of the red alga *Laurencia nipponica*. Cryst. (hexane). Mp 52-54°. $[\alpha]_D^{20}$ -150 (c, 1.00 in $CHCl_3$).

Suzuki, T. *et al., Chem. Lett.*, 1983, 1639
Grese, T.A. *et al., J.O.C.*, 1993, **58**, 2468-2477 (*synth*)
Lee, E. *et al., Tet. Lett.*, 1998, **39**, 317-318 (*synth*)
Evans, P.A. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 3175-3177 (*synth*)
Fernandez de la Pradilla, R. *et al., J.O.C.*, 2005, **70**, 10693-10700 (*synth*)

Kumausyne K-106



$C_{17}H_{23}BrO_3$ 355.271

(3*E*)-*form* [88034-94-0]
Constit. of the red alga *Laurencia nipponica*.
Oil. $[\alpha]_D^{26}$ -2.3 (c, 0.62 in $CHCl_3$).

O-*De-Ac:* ***Deacetylkumausyne***
[88034-95-1]
$C_{15}H_{21}BrO_2$ 313.234
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D^{20}$ +6.5 (c, 1.08 in $CHCl_3$).

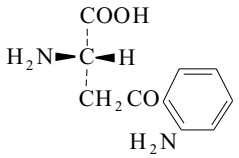
(3*Z*)-*form* [87980-57-2]
Constit. of *Laurencia nipponica*.
Oil. $[\alpha]_D^{25}$ -3.2 (c, 1.03 in $CHCl_3$).

O-*De-Ac:* [87980-61-8]
Constit. of *Laurencia nipponica*.
Oil. $[\alpha]_D^{20}$ +10.8 (c, 1.88 in $CHCl_3$).

Suzuki, T. *et al., Chem. Lett.*, 1983, 1643
Brown, M.J. *et al., J.A.C.S.*, 1991, **113**, 5378-5384 (*synth*)
Osumi, K. *et al., Tet. Lett.*, 1995, **36**, 5789-5792 (*synth*)
Martin, T. *et al., J.O.C.*, 1997, **62**, 1570-1571 (*synth*)
Boukouvalas, J. *et al., J.O.C.*, 1998, **63**, 916-917 (*synth*)
Gadikota, R.R. *et al., J.O.C.*, 2002, **66**, 9046-9051 (*synth*)
Fernandez de la Pradilla, R. *et al., J.O.C.*, 2005, **70**, 10693-10700 (*synth*)
Chandler, C.L. *et al., Org. Lett.*, 2005, **7**, 3493-3495 (*synth*)

Kumepaloxane K-107

[122666-10-8]



(S)–form

$C_{12}H_{20}BrClO$ 295.646

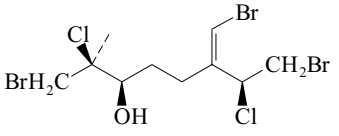
Constit. of bubble shell *Haminoea cymbalum*. Fish antifeedant. Ichthyotoxin. Oil. $[\alpha]_D$ +22.6 (c, 0.32 in $CHCl_3$).

Poiner, A. *et al., Tetrahedron*, 1989, **45**, 617-622 (*isol, pmr*)

Kurodainol K-108

1,8-Dibromo-6-(bromomethylene)-2,7-dichloro-2-methyl-3-octanol, 9CI

[81720-12-9]

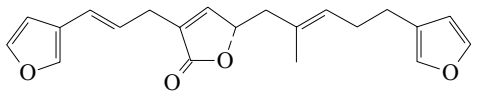


$C_{10}H_{15}Br_3Cl_2O$ 461.845

Constit. of *Aplysia kurodai*. Oil. $[\alpha]_D^{16}$ -1.7 (c, 7.6 in CCl_4).

Katayama, A. *et al., Agric. Biol. Chem.*, 1982, **46**, 859-860 (*Kurodainol*)

Kurospongin K-109



$C_{21}H_{22}O_4$ 338.402

(+)-*form*

ent-*Kurospongin*

[627893-98-5]

Constit. of a *Sarcotragus* sp.

Yellow oil. $[\alpha]_D^{21}$ +33.4 (c, 0.03 in $CHCl_3$).

(-)-*form* [115722-54-8]

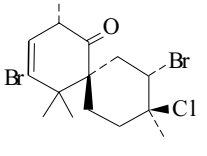
Constit. of *Spongia* sp. Ichthyotoxin, fish antifeedant. Unstable yellow oil. $[\alpha]_D$ -16.8 (c, 1.24 in $CHCl_3$). λ_{max} 213 (ε 19000) (MeOH).

Tanaka, J. *et al., Tetrahedron*, 1988, **44**, 2805 (*struct, abs config*)

Liu, Y. *et al., J. Nat. Prod.*, 2003, **66**, 1451-1456 (*ent-Kurospongin*)

Kylinone K-110

[72036-07-8]



$C_{15}H_{21}Br_2ClO$ 412.591

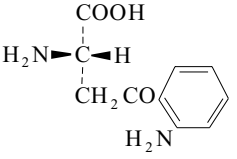
Constit. of *Laurencia pacifica*. Oil. $[\alpha]_D^{25}$ +31 (c, 1.9 in MeOH).

Selover, S.J. *et al., J.O.C.*, 1980, **45**, 69

Kynurenine K-111

α,2-Diamino-γ-oxobenzenebutanoic acid, 9CI. 3-(2-Aminobenzoyl)alanine. 2-Amino-3-(2-aminobenzoyl)propanoic acid. 3-Anthraniloylalanine

[343-65-7]



(S)–form

$C_{10}H_{12}N_2O_3$ 208.216

(*R*)-*form*

D-form

[13441-51-5]

Occurs free in *Viscum album*.

Mp 191°. $[\alpha]_D^{25}$ +30.

Sulfate:

Cryst. + $1H_2O$. Mp 178°. $[\alpha]_D^{25}$ -9.5.

(*S*)-*form*

L-form

[2922-83-0]

Occurs in the urine of various animals incl. as sex pheromone of *Oncorhynchus masou*. Intermed. in the metab. of tryptophan and in biosynth. of ommochromes, e.g. Xanthommatin, X-2 in crabs and insects.

Cryst. (EtOH).

Mp 194° (191°). $[\alpha]_D^{25}$ -30.5 (c, 1 in H_2O). Forms a hydrate with $^1/_3$ H_2O, Mp 180-90° dec.

Sulfate:

Needles + $1H_2O$ (EtOH aq.). Mp 179-180° dec. $[\alpha]_D^{25}$ +9.7 (c, 1 in H_2O).

$N^{2'}$-Formyl: α-Amino-2-(formylamino)-γ-oxobenzenebutanoic acid, 9CI. Formylkynurenine

[3978-11-8]

[1022-31-7]

$C_{11}H_{12}N_2O_4$ 236.227

Prod. of tryptophan metab.; intermed. in nicotinic acid biosynth.

Di-Ac:

Needles. Mp 198°.

(±)-*form* [3039-10-9]

Yellow cryst. Mp 219° dec.

Sulfate: [17268-44-9]

Cryst. + $1H_2O$ (EtOH aq.). Mp 194° dec. (173°), darkens at 166°.

[32999-58-9]

Biochem. Prep., 1953, **3**, 108 (*synth*)

Auerbach, V.H. *et al., Methods Enzymol.*, 1957, **3**, 620 (*synth*)

Vester, F. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1960, **322**, 273 (*isol*)

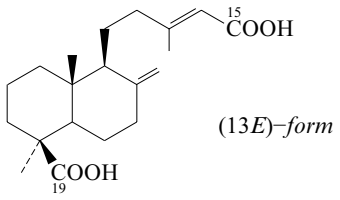
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 2723 (*isol, synth*)

Benassi, C.A. *et al., Gazz. Chim. Ital.*, 1967, **97**, 3 (*synth*)

Brown, K.S. *et al., Tet. Lett.*, 1967, 1721 (*ms*)

Yambe, H. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2006, **103**, 15370-15374 (*marine, isol*)

8(17),13-Labdadiene-15,19-dioic acid L-1



(13*E*)–*form*

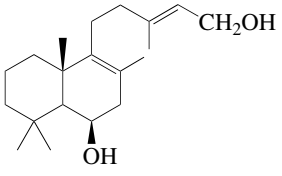
$C_{20}H_{30}O_4$ 334.455

13*E*-*form*

Agathic acid. *Agathenedicarboxylic acid. Kauric acid. Copaldicarboxylic acid. Agathenic acid*
[640-28-8]
Constit. of *Agathis australis* and *Agathis microstachya*. Prod. by the marine-derived *Chromocleista* sp. strain R721.
Cryst. (MeOH).
Mp 203-204°. $[\alpha]_D$ +56.1 (EtOH).

Bory, S. *et al., Bull. Soc. Chim. Fr.*, 1963, 2310 (*struct*)
Carman, R.M. *et al., Aust. J. Chem.*, 1966, **19**, 2403 (*isol*)
Bastard, J. *et al., J. Nat. Prod.*, 1984, **47**, 592 (*cmr*)
Park, Y.C. *et al., J. Nat. Prod.*, 2006, **69**, 580-584 (*Chromocleista, isol*)

8,13-Labdadiene-6,15-diol L-2



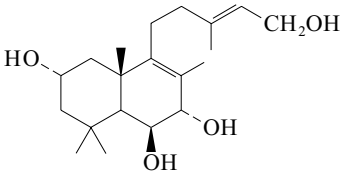
$C_{20}H_{34}O_2$ 306.487

(6β,13*E*)-*form*

6-Ac:
$C_{22}H_{36}O_3$ 348.525
Constit. of *Trimusculus peruvianus*. Oil. Error in diag. in ref.

San-Martín, A. *et al., Can. J. Chem.*, 1996, **74**, 2471-2475 (*isol, pmr, cmr*)

8,13-Labdadiene-2,6,7,15-tetrol L-3



$C_{20}H_{34}O_4$ 338.486

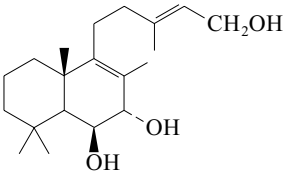
(2α,6β,7α,13*E*)-*form*

2,6,7-Tri-Ac: [273212-72-9]
$C_{26}H_{40}O_7$ 464.598
Constit. of *Trimusculus costatus*.

6-O-*(3-Methylbutanoyl), 2,7-di-Ac:* [111602-92-7]
$C_{29}H_{46}O_7$ 506.678
Constit. of marine pulmonate *Trimusculus reticulatus*. Oil. $[\alpha]_D$ +41.2 (c, 0.35 in $CHCl_3$).

Manker, D.C. *et al., Tetrahedron*, 1987, **43**, 3677
Gray, C.A. *et al., Nat. Prod. Lett.*, 1998, **12**, 47-53 (*2,6,7-tri-Ac*)

8,13-Labdadiene-6,7,15-triol L-4



$C_{20}H_{34}O_3$ 322.487

(6β,7α,13*E*)-*form*

6-Ac: [143913-61-5]
$C_{22}H_{36}O_4$ 364.524
Isol. from *Trimusculus peruvianus*.

6,7-Di-Ac: [273212-70-7]
$C_{24}H_{38}O_5$ 406.561
Constit. of tunicate *Trimusculus peruvianus* and *Trimusculus costatus*. Yellow oil. $[\alpha]_D^{27}$ +92.9 (c, 0.7 in $CHCl_3$).

7,15-Di-Ac:
$C_{24}H_{38}O_5$ 406.561
Constit. of *Trimusculus peruvianus*. Oil.

Tri-Ac:
$C_{26}H_{40}O_6$ 448.598
Constit. of *Trimusculus peruvianus*. Yellow oil.

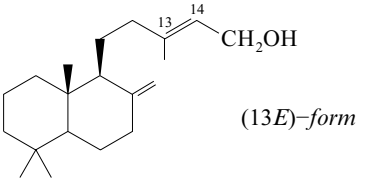
O^6-*(3-Methylbutanoyl):*
$C_{25}H_{42}O_4$ 406.604
Constit. of marine pulmonate *Trimusculus reticulatus* and its defensive mucus. Larvicide. Oil. $[\alpha]_D$ +38.7 (c, 0.83 in $CHCl_3$).

15-Carboxylic acid: 6,7-Dihydroxy-8,13-labdadien-15-carboxylic acid
$C_{20}H_{32}O_4$ 336.47

15-Carboxylic acid, 7-O-*(3-methylbutanoyl), 6-Ac:*
$C_{27}H_{42}O_6$ 462.625
Isol. from *Trimusculus conica* and *Trimusculus reticulatus*.

Manker, D.C. *et al., Tetrahedron*, 1987, **43**, 3677-3680 (*isol*)
Rovirosa, J. *et al., Bol. Soc. Chil. Quim.*, 1992, **37**, 143-145 (*6-Ac, isol*)
San-Martin, A. *et al., Can. J. Chem.*, 1996, **74**, 2471-2475 (*isol, pmr, cmr*)
Manker, D.C. *et al., J. Chem. Ecol.*, 1996, **22**, 23-35 (*carboxylic acid deriv*)
Gao, W.-G. *et al., Tet. Lett.*, 1996, **37**, 7071 (*synth*)
Gray, C.A. *et al., Nat. Prod. Lett.*, 1998, **12**, 47-53 (*Trimusculus costatus constit*)
Pathak, A. *et al., J.O.C.*, 2005, **70**, 4184-4187 (*synth*)

8(17),13-Labdadien-15-ol L-5



(13*E*)–*form*

$C_{20}H_{34}O$ 290.488

(13*E*)-*form*

Copalol
[10395-43-4]
Constit. of *Dacrydium kirkii*.
Oil. Bp_1 172-173°. $[\alpha]_D$ +33.2.

*15-Carboxylic acid: 8(17),13*E*-Labdadien-15-oic acid.* ***Anticopalic acid***. *Copaiferic acid B*
[24470-48-2]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Oxystigma oxyphyllum* and *Pinus monticola*. Oil. $Bp_{0.4}$ 171° (as Me ester). $[\alpha]_D^{22}$ +46 (c, 0.5 in MeOH) (Me ester).

13ξ,14ξ-Epoxide: ***13,14-Epoxy-8(17)-labden-15-ol***
[28762-95-0]
$C_{20}H_{34}O_2$ 306.487
Constit. of *Hemizonia lutescens*. Gum. $[\alpha]_D^{24}$ +7 (c, 0.4 in $CHCl_3$).

(13*Z*)-*form*

15-Carboxylic acid: ***Copaiferic acid A***
[10395-36-5]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Ceroplastes rubens*. Pale yellow oil. $[\alpha]_D$ -4.6 (c, 0.4 in $CHCl_3$). λ_{max} 222 (log ϵ 4.04) (no solvent reported).

(*ent*-13*E*)-*form* [21738-29-4]
Constit. of *Ruppia maritima*.
Oil. $[\alpha]_D$ -15.5 (c, 0.46 in $CHCl_3$).

15-Carboxylic acid: ent-*8(17),13*E-*Labdadien-15-oic acid.* ***Copalic acid***
[20257-75-4]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Trachylobium verrucosum* and *Hymenaea courbaril* (copinol). Oil. $Bp_{0.005}$ 160°. $[\alpha]_D$ -6.9 (c, 1.15 in $CHCl_3$).

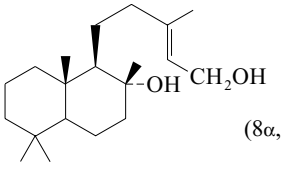
*15-Carboxylic acid, (3-acetoxy-2*S*-hydroxypropyl) ester:* ***Verrucosin 5***
[188405-18-7]
$C_{25}H_{40}O_5$ 420.588
Constit. of *Doris verrucosa*. Oil. $[\alpha]_D$ -15.9 (c, 0.27 in $CHCl_3$). λ_{max} 224 (ϵ 5320) (MeOH).

(±-13*E*)-*form* [80657-12-1]
Isol. from trunk resin of *Eperua purpurea*.
Needles (Me_2CO aq.).
Mp 105-107°.

[14022-42-5]

Nakano, T. *et al., J.O.C.*, 1961, **26**, 167 (*Copalic acid*)
Sandermann, W. *et al., Tet. Lett.*, 1967, 2685 (*isol*)
Bevan, C.W.L. *et al., J.C.S.(C)*, 1968, 1067 (*struct*)
Cambie, R.C. *et al., Aust. J. Chem.*, 1969, **22**, 1691 (*isol*)
Overton, K.H. *et al., J.C.S.(C)*, 1971, 312 (*synth*)
Zinkel, D.F. *et al., Phytochemistry*, 1971, **10**, 1161 (*isol*)
Manh, D.D.K. *et al., Tetrahedron*, 1975, **31**, 1903 (*synth*)
Imamura, P.M. *et al., Phytochemistry*, 1977, **16**, 1842 (*cmr*)
De Santis, V. *et al., J. Nat. Prod.*, 1981, **44**, 370 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 2383 (*epoxide*)
Yee, N.K.N. *et al., J.O.C.*, 1992, **57**, 4598 (*synth*)
San Feliciano, A. *et al., Fitoterapia*, 1993, **64**, 184 (*cmr*)
Carman, R.M. *et al., Aust. J. Chem.*, 1995, **48**, 1357-1366 (*Copaiferic acids, synth, pmr, cmr, ms*)
Atencio, R. *et al., Acta Cryst. C*, 1997, **53**, 1068-1070 (*cryst struct*)
Gavagnin, M. *et al., Tetrahedron*, 1997, **53**, 1491-1504 (*Verrucosin 5*)
DellaGreca, M. *et al., Phytochemistry*, 2000, **55**, 909-913 (*Ruppia maritima constit*)
Toshima, H. *et al., Tetrahedron*, 2000, **56**, 8443-8450 (*synth*)

13-Labdene-8,15-diol L-6



(8α,13*E*)–*form*

$C_{20}H_{36}O_2$ 308.503

(8β,13*E*)-*form*
Leoheteronin D
[25532-83-6]
Constit. of *Leonurus heterophyllus*.
Cryst.
Mp 134-135°. $[\alpha]_D^{25}$ 0 (c, 0.2 in $CHCl_3$).

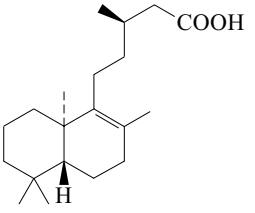
15-Aldehyde: Constit. of *Pleurobranchaea meckelii*.
Oil. $[\alpha]_D^{25}$ -28.2 (c, 0.27 in $CHCl_3$). λ_{max} 230 (ϵ 11186); 257 (ϵ 10120) (MeOH) (Berdy).

(8β,13*Z*)-*form*

15-Aldehyde: Constit. of *Pleurobranchaea meckelii*.
Oil. $[\alpha]_D^{25}$ -35.2 (c, 0.3 in $CHCl_3$). λ_{max} 230 (ϵ 11150); 259 (ϵ 10320) (MeOH) (Berdy).

Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 275 (*aldehyde*)
San Filiciano, A. *et al., Phytochemistry*, 1988, **27**, 2241 (*aldehyde*)
Ciavatta, M.L. *et al., Tet. Lett.*, 1995, **36**, 8673 (*15-aldehydes*)

8-Labden-15-oic acid L-7



$C_{20}H_{34}O_2$ 306.487

(*ent*-13*S*)-*form*

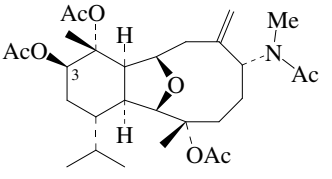
*(2-Acetoxy-3-hydroxypropyl) ester (*S-*):* [138909-51-0]
$C_{25}H_{42}O_5$ 422.604
Constit. of *Austrodoris kerguelensis*. Oil. $[\alpha]_D$ -48 (c, 0.66 in $CHCl_3$). Struct. revised in 2003.

*(3-Acetoxy-2-hydroxypropyl) ester (*S-*):* [138909-52-1]
$C_{25}H_{42}O_5$ 422.604
Constit. of *Austrodoris kerguelensis*. Oil. $[\alpha]_D$ -53 (c, 0.34 in $CHCl_3$).

Davies-Coleman, M.T. *et al., Tetrahedron*, 1991, **47**, 9743-9750 (*isol, pmr, cmr*)
Gavagnin, M. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 2647-2650 (*abs config*)
Gavagnin, M. *et al., Tetrahedron*, 2003, **59**, 5579-5583 (*isol, pmr, cmr, struct*)

Labiatamide A L-8

[174285-78-0]

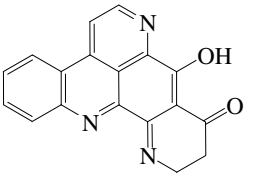


$C_{29}H_{45}NO_8$ 535.676
Constit. of *Eunicella labiata*. Oil. $[\alpha]_D$ +12.8 (c, 0.6 in $CHCl_3$).

3-Deacetoxy: ***Labiatamide B***
[174285-79-1]
$C_{27}H_{43}NO_6$ 477.64
Constit. of *Eunicella labiata*. Oil. $[\alpha]_D$ -6 (c, 0.2 in $CHCl_3$).
Roussis, V. *et al., Tetrahedron*, 1996, **52**, 2735 (*isol, pmr, cmr*)

Labuanine A L-9

*10,11-Dihydro-8-hydroxy-9*H-*benzo[*b*]pyrido[4,3,2-*de*][1,10]phenanthrolin-9-one*

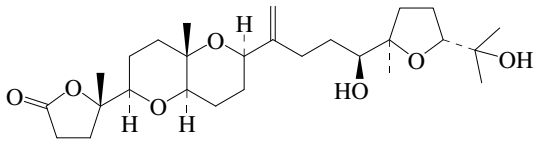


$C_{18}H_{11}N_3O_2$ 301.304
Isol. from the marine sponge *Biemna fortis*. Neuronal differentiation inducer. Amorph. yellow solid. λ_{max} 227 (ϵ 18000); 288 (ϵ 7720); 317 (ϵ 5190); 357 (ϵ 6070) (MeOH).

Aoki, S. *et al., Bioorg. Med. Chem.*, 2003, **11**, 1969-1973 (*isol, pmr, cmr*)

Lactodehydrothyrsiferol L-10

[477867-58-6]



$C_{27}H_{44}O_7$ 480.64
Constit. of *Laurencia viridis*. Amorph. solid. $[\alpha]_D^{25}$ +4.3 (c, 0.21 in $CHCl_3$).

Souto, M.L. *et al., Tetrahedron*, 2002, **58**, 8119-8125 (*isol, pmr, cmr*)

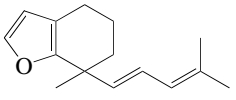
Lactyltrimethylarsonium betaine L-11

(2-Carboxy-2-hydroxyethyl)trimethylarsonium hydroxide inner salt, 9CI. β-Trimethylarsonium lactate
[68688-60-8]
$Me_3As^{\oplus}CH_2CH(OH)COO^{\ominus}$
$C_6H_{13}AsO_3$ 208.088
Component of phospholipids of marine algae e.g. *Dunaliella tertiolecta*. Also occurs as a phosphatidyl deriv. in the marine diatom *Chaetoceros concavicornis*. Occurs free in the lobster *Homarus americanus*. Plates (EtOH/Et_2O).
Mp 199-201°.

Cooney, R.V. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1978, **75**, 4262
Cooney, R.V. *et al., Chemosphere*, 1980, **9**, 335 (*biosynth*)
Summons, R.E. *et al., Phosphorus Sulfur Relat. Elem.*, 1982, **13**, 133 (*synth, ms, ir*)

Laevidiene L-12

[165337-78-0]

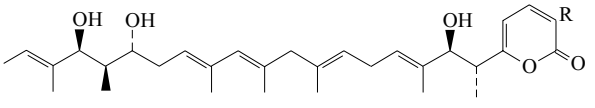


$C_{15}H_{20}O$ 216.322
Constit. of *Cadlina pellucida* and *Cadlina laevis*.
$[\alpha]_D$ -4.5 (c, 0.1 in $CHCl_3$). λ_{max} 216 (ϵ 8420); 240 (ϵ 11142) (EtOH).

Fontana, A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1995, **111**, 283-290 (*isol, pmr, cmr*)

Lagunapyrone A L-13

[175448-21-2]



R = CH_3

$C_{32}H_{48}O_5$ 512.728
Isol. from a marine sediment bacterium, *Actinomyces* sp.
Cytotoxic agent. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{20}$ +40.1 (c, 2 in MeOH). λ_{max} 225 (log ϵ 3.98); 298 (log ϵ 3.82) (CH_2Cl_2). λ_{max} 225 (ϵ 9506); 298 (ϵ 6546) (MeOH) (Berdy).

Lindel, T. *et al., Tet. Lett.*, 1996, **37**, 1327-1330 (*Lagunapyrone A*)

Lagunapyrone B L-14

[175448-22-3]
As Lagunapyrone A, L-13 with
R = $CH_2CH_2CH_3$
$C_{34}H_{52}O_5$ 540.782
Isol. from a marine sediment bacterium, *Actinomyces* sp.
Cytotoxic agent. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{20}$ +10.9 (c, 4 in CH_2Cl_2). λ_{max} 229 (log ϵ 3.95); 298 (log ϵ 3.72) (CH_2Cl_2). λ_{max} 229 (ϵ 8912); 298 (ϵ 5272) (MeOH) (Berdy).

Lindel, T. *et al., Tet. Lett.*, 1996, **37**, 1327-1330 (*Lagunapyrone B*)

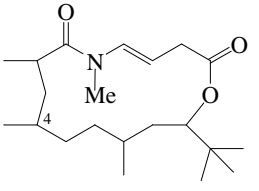
Lagunapyrone C L-15

[175448-23-4]
As Lagunapyrone A, L-13 with
R = $CH_2CH_2CH_2CH_3$
$C_{35}H_{54}O_5$ 554.809
Isol. from a marine sediment bacterium, *Actinomyces* sp.
Cytotoxic agent. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{20}$ +46 (c, 1.5 in MeOH). λ_{max} 227 (log ϵ 4.02); 298 (log ϵ 3.86) (CH_2Cl_2). λ_{max} 227 (ϵ 10495); 298 (ϵ 7278) (MeOH) (Berdy).

Lindel, T. *et al., Tet. Lett.*, 1996, **37**, 1327-1330 (*Lagunapyrone C*)

Laingolide L-16

[182801-62-3]

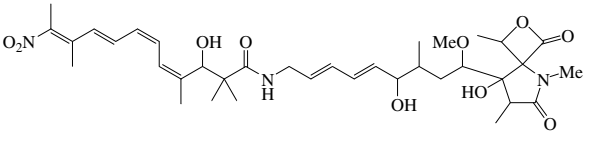


$C_{21}H_{37}NO_3$ 351.528
Macrolide. Isol. from *Lyngbya bouillonii*. Oil. λ_{max} 240 (ϵ 10650) (MeOH).

4-Demethyl: ***Laingolide A***
[230975-43-6]
$C_{20}H_{35}NO_3$ 337.501
Isol. from *Lyngbya bouillonii*. Amorph. solid.

Klein, D. *et al., Tet. Lett.*, 1996, **37**, 7519-7520 (*isol, uv, ir, pmr, cmr*)
Klein, D. *et al., J. Nat. Prod.*, 1999, **62**, 934-936 (*Laingolide A*)

Lajollamycin L-17

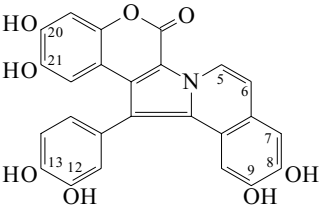


$C_{36}H_{53}N_3O_{10}$ 687.829
Closely related to Oxazolomycin. Prod. by the marine-derived *Streptomyces nodosus* (NPS007994). Antibacterial. Bright yellow solid.
Mp 92-95°. $[\alpha]_D^{25}$ +75 (c, 0.00002 in MeOH). λ_{max} 229 (ϵ 63000); 306 (ϵ 40000); 375 (ϵ 22000) (MeOH).

Manam, R.R. *et al., J. Nat. Prod.*, 2005, **68**, 240-243 (*isol, pmr, cmr*)

Lamellarin H L-18

[115982-22-4]



$C_{25}H_{15}NO_8$ 457.395
Authors' numbering scheme shown. Alkaloid from the marine

ascidian *Didemnum chartaceum*. Amorph. solid. λ_{max} 208 (ϵ 31000); 282 (ϵ 24000); 303 (sh); 324 (sh); 340 (ϵ 6000); 370 (ϵ 9000); 389 (ϵ 12000) (MeOH) (Derep). λ_{max} 218 (ϵ 30000); 244 (sh); 297 (ϵ 20000); 316; 402 (ϵ 13000) (MeOH/NaOH) (Derep). λ_{max} 205 (ϵ 44000); 298 (ϵ 20000); 405 (ϵ 13000) (MeOH/NaOH) (Berdy).

9,12,21-Tri-Me ether: ***Lamellarin D***
[97614-65-8]
$C_{28}H_{21}NO_8$ 499.476
Isol. from *Lamellaria* sp. Inhibitor of cell division in fertilised sea urchin eggs. Pale yellow powder. Sol. MeOH, EtOAc; poorly sol. H_2O. λ_{max} 218 (ϵ 30000); 244 (sh); 297 (ϵ 20000); 316; 402 (ϵ 13000) (MeOH/NaOH) (Derep). λ_{max} 208 (ϵ 31000); 282 (ϵ 24000); 303 (sh); 324 (sh); 340 (ϵ 6000); 370 (ϵ 9000); 389 (ϵ 12000) (MeOH) (Derep). λ_{max} 212; 280; 368; 387 (MeOH) (Berdy).

9,13,21-Tri-Me ether: ***Lamellarin N***
[149379-26-0]
$C_{28}H_{21}NO_8$ 499.476
Alkaloid from the unidentified *Didemnum* sp. and a *Lamellaria* sp. Needles (MeOH) (as tri-Ac).
Mp 283-285° (tri-Ac). λ_{max} 204 (ϵ 29500); 279 (ϵ 22500); 365 (ϵ 6000); 386 (ϵ 4000) (MeOH) (Berdy). λ_{max} 204 (ϵ 50000); 295 (ϵ 16800); 402 (ϵ 11300) (MeOH/NaOH) (Berdy).

*8,9,12,21-Tetra-Me ether, 20-*O*-sulfate:* ***Lamellarin α 20-sulfate***
[229956-47-2]
$C_{29}H_{23}NO_{11}S$ 593.567
Isol. from *Lamellaria* sp. HIV-1 integrase inhibitor. Solid (as Na salt).
Mp 145-148° (Na salt). λ_{max} 204 (ϵ 31500); 276 (ϵ 19500); 303 (ϵ 16000); 324 (sh); 338 (sh); 364 (ϵ 5500); 386 (ϵ 7000) (MeOH).

8,9,13,21-Tetra-Me ether: ***Lamellarin α***
[475232-29-2]
$C_{29}H_{23}NO_8$ 513.503
Alkaloid from *Didemnum obscurum*. Amorph. solid.
Mp 228-230°. λ_{max} 206 (log ϵ 1.99); 281 (log ϵ 1.91); 302 (log ϵ 1.79); 323 (log ϵ 1.54) (MeOH).

8,9,12,13,21-Penta-Me ether: ***Lamellarin η***
$C_{30}H_{25}NO_8$ 527.529
Alkaloid from *Didemnum obscurum*. Amorph. solid.
Mp 265-269°. λ_{max} 236 (log ϵ 0.76); 308 (log ϵ 0.55) (MeOH).

5,6-Dihydro, 9-Me ether: ***Lamellarin S***
[181423-71-2]
$C_{26}H_{19}NO_8$ 473.438
Metab. from an Australian tunicate, *Didemnum* sp. Oil. $[\alpha]_D$ +66.5 (c, 0.84 in MeOH). CAS name is defective. First example of this structural class to show atropisomerism. Abs config. not determined. Slowly racemises.

5,6-Dihydro, 13-Me ether: ***Lamellarin β***
[425381-27-7]
$C_{26}H_{19}NO_8$ 473.438
Isol. from a *Didemnum* sp. Cytotoxic. Amorph. solid. λ_{max} 205 (ϵ 43000); 268 (sh); 278 (ϵ 23000); 315 (ϵ 17000); 336 (ϵ 17000) (MeOH).

5,6-Dihydro, 9,20-di-Me ether: ***Lamellarin Z***
[221169-77-3]
$C_{27}H_{21}NO_8$ 487.465
Alkaloid from *Didemnum chartaceum*. Amorph. solid. λ_{max} 207 (ϵ 31000); 265 (sh) (ϵ 16000); 276 (ϵ 18000); 314 (ϵ 16000); 333 (ϵ 15000); 348 (sh) (ϵ 14000); 352 (sh) (ϵ 11000) (MeOH).

5,6-Dihydro, 9,12,21-tri-Me ether, 8,13,20-tri-Ac: ***Lamellarin χ***
$C_{34}H_{29}NO_{11}$ 627.603
Isol. from *Didemnum obscurum*. Amorph. solid.
Mp 164-166°. λ_{max} 208 (log ϵ 0.55); 274 (log ϵ 0.32) (MeOH).

5,6-Dihydro, 8,13,21-tri-Me ether, 20-sulfate: ***Lamellarin Y 20-sulfate***
[189084-06-8]
$C_{28}H_{23}NO_{11}S$ 581.556
Alkaloid from an unidentified ascidian. Powder (as Na salt). CAS no. refers to Na salt. λ_{max} 204 (ϵ 35000); 265 (sh); 273 (ϵ 23000); 309 (ϵ 21000); 328 (sh) (MeOH) (Na salt).

5,6-Dihydro, 9,13,20-tri-Me ether: ***Lamellarin G***
[115982-21-3]
$C_{28}H_{23}NO_8$ 501.492
Alkaloid from *Didemnum chartaceum*. Prisms (DMSO).
Mp 263-265°. λ_{max} 204 (ϵ 55000); 278 (ϵ 12000); 324 (ϵ 12000); 346 (ϵ 8000); 368 (sh) (MeOH/NaOH) (Derep). λ_{max} 206 (ϵ 46000); 267 (sh); 276 (ϵ 25000); 314 (ϵ 21000); 334 (ϵ 21000) (MeOH) (Derep).

5,6-Dihydro, 9,13,20-tri-Me ether, 8-sulfate: ***Lamellarin G 8-sulfate***
[221169-76-2]
$C_{28}H_{23}NO_{11}S$ 581.556
Alkaloid from *Didemnum chartaceum*. Amorph. solid. λ_{max} 205 (ϵ 46000); 225 (sh) (ϵ 35000); 266 (sh) (ϵ 24000); 275 (ϵ 28000); 301 (sh) (ϵ 20000); 314 (ϵ 27000); 336 (ϵ 22000) (MeOH).

5,6-Dihydro, 9,13,21-tri-Me ether: ***Lamellarin L***
[149378-57-4]
$C_{28}H_{23}NO_8$ 501.492
Alkaloid from an unidentified *Didemnum* sp. Immunomodulator. Amorph. powder.
Mp 285-287°.

5,6-Dihydro, 9,13,21-tri-Me ether, 20-sulfate: ***Lamellarin L 20-sulfate***
[221169-75-1]
$C_{28}H_{23}NO_{11}S$ 581.556
Alkaloid from *Didemnum chartaceum*. Amorph. solid. λ_{max} 203 (ϵ 32000); 221 (sh) (ϵ 21000); 267 (sh) (ϵ 16000); 276 (ϵ 19000); 314 (ϵ 16000); 338 (sh) (ϵ 14000) (MeOH).

5,6-Dihydro, 8,9,13,21-tetra-Me ether: ***Lamellarin U***
[189083-79-2]
$C_{29}H_{25}NO_8$ 515.518
Alkaloid from an unidentified ascidian.
Mp 200-204°.

5,6-Dihydro, 8,9,13,21-tetra-Me ether, 20-sulfate: Lamellarin U 20-sulfate
[189084-01-3]
$C_{29}H_{25}NO_{11}S$ 595.583
Alkaloid from an unidentified ascidian.
Mp 222-226°. λ_{max} 202 (ϵ 40000); 265 (sh); 273 (ϵ 23500); 309 (ϵ 20000); 327 (sh) (MeOH).

5,6-Dihydro, 9,12,13,21-tetra-Me ether: ***Lamellarin J***
[149355-76-0]
$C_{29}H_{25}NO_8$ 515.518
Alkaloid from the unidentified *Didemnum* sp. and a *Lamellaria* sp. Immunomodulator. Amorph. powder.
Mp 216-220°.

5,6-Dihydro, 8,9,12,13,21-penta-Me ether: ***Lamellarin F***
[115982-20-2]
$C_{30}H_{27}NO_8$ 529.545
Alkaloid from *Didemnum chartaceum*. Prisms (DMSO).
Mp 273-276° dec. λ_{max} 205 (ϵ 64000); 265 (sh); 288 (ϵ 28000); 323 (ϵ 23000) (MeOH/NaOH) (Derep). λ_{max} 208 (ϵ 48000); 268 (sh); 278 (ϵ 38000); 310 (ϵ 23000); 330 (sh) (MeOH) (Derep). λ_{max} 210 (ϵ 47000); 278 (ϵ 21000); 312 (ϵ 28000) (MeOH) (Berdy). λ_{max} 207 (ϵ 52000); 290 (ϵ 28000); 322 (ϵ 31000) (MeOH/NaOH) (Berdy).

5,6-Dihydro, 5ξ,7-dihydroxy, 7,8,9,12,20-penta-Me ether: ***Lamellarin A***
[97614-62-5]
$C_{30}H_{27}NO_{10}$ 561.544
Metab. of *Lamellaria* sp. MDR inhibitor, immunomodulator. Pale yellow prisms (MeOH).
Mp 168-172° dec. Consists of a 1:1 mixt. of geom. isomers generated by restricted rotn. around the pyrrole-aryl bond. Opt. inactive, prob. due to rapid interconversion at C-5 through an open-chain tautomer. λ_{max} 218 (ϵ 46000); 287 (ϵ 33000); 319 (ϵ 36000); 378 (ϵ 9000) (MeOH/NaOH) (Derep). λ_{max} 215 (ϵ 41000); 275 (ϵ 33000); 309 (ϵ 28000); 325 (sh); 326 (ϵ 25000) (MeOH) (Derep).

7-Hydroxy, 8,9,12,21-tetra-Me ether: ***Lamellarin M***
[149378-58-5]
$C_{29}H_{23}NO_9$ 529.502
Alkaloid from the unidentified *Didemnum* sp. and a *Lamellaria* sp. Immunomodulator. Amorph. powder.

7-Hydroxy, 8,9,13,21-tetra-Me ether: ***Lamellarin X***
[189083-94-1]
$C_{29}H_{23}NO_9$ 529.502
Alkaloid from an unidentified ascidian. Powder. λ_{max} 204 (ϵ 30000); 276 (ϵ 15000); 303 (ϵ 14000); 324 (sh); 338 (sh); 365 (sh) (MeOH).

7-Hydroxy, 7,8,9,12,21-penta-Me ether: ***Lamellarin B***
[97614-63-6]
$C_{30}H_{25}NO_9$ 543.529
Isol. from the marine prosobranch mollusc *Lamellaria* sp. Dehydration prod. of Lamellarin A. Immunomodulator. Pale yellow needles (MeOH).
Mp 258-259°. λ_{max} 218 (ϵ 30000); 244 (sh); 297 (ϵ 20000); 316; 402 (ϵ 13000) (MeOH/NaOH) (Derep). λ_{max} 208 (ϵ 31000); 282 (ϵ 24000); 303 (sh); 324 (sh); 340 (ϵ 6000); 370 (ϵ 9000); 389 (ϵ 12000) (MeOH) (Derep).

7-Hydroxy, 7,8,9,12,21-penta-Me ether, 20-sulfate: ***Lamellarin B 20-sulfate***
[221169-73-9]
$C_{30}H_{25}NO_{12}S$ 623.593
Alkaloid from *Didemnum chartaceum*. Amorph. solid. λ_{max} 202 (ϵ 31000); 224 (sh) (ϵ 18000); 283 (ϵ 27000); 301 (sh) (ϵ 21000); 321 (sh) (ϵ 11000); 365 (ϵ 8000); 386 (ϵ 10000) (MeOH).

7-Hydroxy, 8,9,12,13,21-penta-Me ether: ***Lamellarin ϵ***
$C_{30}H_{25}NO_9$ 543.529
Alkaloid from *Didemnum obscurum*. Amorph. solid.
Mp 271-275°. λ_{max} 209 (log ϵ 2.61); 277 (log ϵ 2.37); 304 (log ϵ 2.33); 325 (log ϵ 2.1); 367 (log ϵ 1.69) (MeOH).

7-Hydroxy, 5,6-dihydro, 8,9,12,21-tetra-Me ether: ***Lamellarin K***
[149378-56-3]
$C_{29}H_{25}NO_9$ 531.518
Alkaloid from an unidentified *Didemnum* sp. Immunomodulator. Amorph. powder.
Mp 196-198°. λ_{max} 203 (ϵ 40000); 278 (ϵ 23000); 312 (ϵ 20000); 337 (ϵ 17000) (MeOH) (Berdy).

7-Hydroxy, 5,6-dihydro, 8,9,13,21-tetra-Me ether: ***Lamellarin E***
[115982-19-9]
$C_{29}H_{25}NO_9$ 531.518
Alkaloid from *Didemnum chartaceum*. Prisms (MeOH).
Mp 228-232°. λ_{max} 205 (ϵ 64000); 265 (sh); 288 (ϵ 28000); 323 (ϵ 23000) (MeOH/NaOH) (Derep). λ_{max} 208 (ϵ 48000); 268 (sh); 278 (ϵ 38000); 310 (ϵ 23000); 330 (sh) (MeOH) (Derep).

7-Hydroxy, 5,6-dihydro, 7,8,9,12,21-penta-Me ether: ***Lamellarin C****. Dihydrolamellarin B*
[97614-64-7]
$C_{30}H_{27}NO_9$ 545.545
Metab. of a *Lamellaria* sp. Needles (MeOH). Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 225-230°. λ_{max} 218 (ϵ 46000); 287 (ϵ 33000); 319 (ϵ 36000); 378 (ϵ 9000) (MeOH/NaOH) (Derep). λ_{max} 215 (ϵ 41000); 275 (ϵ 33000); 309 (ϵ 28000); 325 (sh); 326 (ϵ 25000) (MeOH) (Derep).

7-Hydroxy, 5,6-dihydro, 7,8,9,12,21-penta-Me ether, 20-sulfate: ***Lamellarin C 20-sulfate***
[221169-74-0]
$C_{30}H_{27}NO_{12}S$ 625.609
Alkaloid from *Didemnum chartaceum*. Amorph. solid. λ_{max} 205 (ϵ 45000); 225 (sh) (ϵ 31000); 265 (sh) (ϵ 21000); 276 (ϵ 25000); 310 (ϵ 22000); 337 (sh) (17000) (MeOH).

7-Hydroxy, 5,6-dihydro, 7,8,9,12,13,21-hexa-Me ether: ***Lamellarin I***
[149355-75-9]
$C_{31}H_{29}NO_9$ 559.571
Alkaloid from an unidentified *Didemnum* sp. MDR inhibitor. Off-white irregular prisms (MeOH).
Mp 218-220°.

7-Methoxy, 8,12,21-tri-Me ether, 9,13,20-tri-Ac: ***Lamellarin ϕ***
$C_{35}H_{29}NO_{12}$ 655.614
Isol. from *Didemnum obscurum*. Amorph. solid.
Mp 276-279°. λ_{max} 224 (log ϵ 0.44); 298 (log ϵ 0.32) (MeOH).

7-Methoxy, 8,9,13,21-tetra-Me ether: ***Lamellarin W***
[189083-85-0]
$C_{30}H_{25}NO_9$ 543.529
Alkaloid from an unidentified ascidian. Pale yellow solid.
Mp 224-228°. λ_{max} 205 (ϵ 30000); 279 (ϵ 15000); 302 (ϵ 13000); 336 (sh); 364 (ϵ 5000); 385 (ϵ 6000) (MeOH).

7-Methoxy, 8,9,12,13,21-penta-Me ether: ***Lamellarin ζ***
$C_{31}H_{27}NO_9$ 557.556
Alkaloid from *Didemnum obscurum*. Amorph. solid.
Mp 268-272°. λ_{max} 230 (log ϵ 0.36); 404 (log ϵ 0.23) (MeOH).

7-Methoxy, 5,6-dihydro, 8,9,13,21-tetra-Me ether: ***Lamellarin T***
[189083-78-1]
$C_{30}H_{27}NO_9$ 545.545
Alkaloid from an unidentified ascidian. Powder.
Mp 214-218°.

7-Methoxy, 5,6-dihydro, 8,9,13,21-tetra-Me ether, 20-sulfate: Lamellarin T 20-sulfate
[189084-00-2]
$C_{30}H_{27}NO_{12}S$ 625.609
Alkaloid from an unidentified ascidian. Powder (as Na salt). CAS no. refers to Na salt. λ_{max} 204 (ϵ 47000); 265 (sh) (ϵ 19350); 274 (ϵ 24000); 309 (ϵ 21000); 330 (sh) (ϵ 16600) (MeOH) (Na salt).

7-Methoxy, 5,6-dihydro, 5ξ-hydroxy, 8,9,13,21-tetra-Me ether: ***Lamellarin V***
[189083-80-5]
$C_{30}H_{27}NO_{10}$ 561.544
Alkaloid from an unidentified ascidian. Powder.
Mp 162-166°.

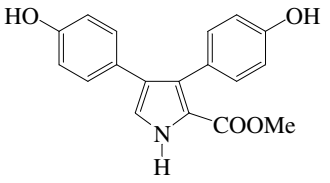
7-Methoxy, 5,6-dihydro, 5ξ-hydroxy, 8,9,13,21-tetra-Me ether, 20-sulfate: Lamellarin V 20-sulfate
[189084-02-4]
$C_{30}H_{27}NO_{13}S$ 641.608
Alkaloid from an unidentified ascidian.
Mp 174-178°. λ_{max} 202 (ϵ 29000); 264 (sh); 273 (ϵ 17000); 304 (ϵ 14000); 328 (sh) (MeOH).

14-Methoxy, 13-deoxy, 7-hydroxy, 5,6-dihydro, 8,9,12,21-tetra-Me ether: ***Lamellarin γ***
$C_{30}H_{27}NO_9$ 545.545
Alkaloid from *Didemnum obscurum*. Amorph. solid.
Mp 163-165°. λ_{max} 206 (log ϵ 1.88); 278 (log ϵ 1.65); 310 (log ϵ 1.63); 331 (log ϵ 1.55); 365 (log ϵ 0.87) (MeOH).

Andersen, R.J. *et al., J.A.C.S.*, 1985, **107**, 5492-5495 (*Lamellarins A-D*)
Lindquist, N. *et al., J.O.C.*, 1988, **53**, 4570-4574 (*Lamellarins E-H*)
Carroll, A.R. *et al., Aust. J. Chem.*, 1993, **46**, 489-501 (*Lamellarins I-N*)
Urban, S. *et al., Aust. J. Chem.*, 1996, **49**, 711-713 (*Lamellarin S*)
Heim, A. *et al., Angew. Chem., Int. Ed.*, 1997, **36**, 155-156 (*Lamellarin G, synth*)
Banwell, M. *et al., Chem. Comm.*, 1997, 2259-2260 (*Lamellarin K, synth*)
Pat. Coop. Treaty (WIPO), 1997, (*Pharma Mar*)97 01336; *CA*, **1327**, 166474 (*activity*)
Reddy, M.V.R. *et al., Tetrahedron*, 1997, **53**, 3457-3466 (*Lamellarins T-Y*)
Ishibashi, F. *et al., Tetrahedron*, 1997, **53**, 5951-5962 (*synth*)
Reddy, M.V.R. *et al., J. Med. Chem.*, 1999, **42**, 1901-1907 (*Lamellarin α 20-sulfate*)
Davis, R.A. *et al., J. Nat. Prod.*, 1999, 419-424 (*Didemnum chartaceum constits*)
Steglich, W. *et al., Chem. Eur. J.*, 2000, **6**, 1147-1152 (*Lamellarin L, synth*)
Ruchirawat, S. *et al., Tet. Lett.*, 2001, **42**, 1205-1208 (*Lamellarin G, synth*)
Ham, J. *et al., Bull. Korean Chem. Soc.*, 2002, **23**, 163-166 (*Lamellarin β*)
Iwao, M. *et al., Tet. Lett.*, 2003, **44**, 4443-4446 (*Lamellarin G, synth*)
Ploypradith, P. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 866-868 (*Lamellarins K,L, synth*)
Krishnaiah, P. *et al., J. Nat. Prod.*, 2004, **67**, 1168-1171 (*Lamellarins α,γ,ϵ*)
Handy, S.T. *et al., J.O.C.*, 2004, **69**, 2362-2366 (*Lamellarin G, synth*)
Reddy, S.M. *et al., Tetrahedron*, 2005, **61**, 9242-9247 (*Lamellarins ζ,η,ϕ,χ*)
Yamaguchi, T. *et al., Tet. Lett.*, 2006, **47**, 3755-3757 (*Lamellarin α 20-sulfate, synth*)
Fujikawa, N. *et al., Tetrahedron*, 2006, **62**, 594-604 (*Lamellarins D,L,N, synth*)

Lamellarin Q L-19

*Methyl 3,4-bis(4-hydroxyphenyl)-1*H*-pyrrole-2-carboxylate*
[168010-02-4]



$C_{18}H_{15}NO_4$ 309.321
Isol. from the sponge *Dendrilla cactos*. Pale yellow oil. λ_{max} 240 (ϵ 14000); 287 (ϵ 12000) (EtOH).

N-*(4-Hydroxyphenyl)*: ***Lamellarin R***
[168010-03-5]
$C_{24}H_{19}NO_5$ 401.418
Isol. from the sponge *Dendrilla cactos*. Green oil. λ_{max} 229 (ϵ 13500); 283 (ϵ 6000); 336 (ϵ 2200); 418 (ϵ 1200) (EtOH).

N-*[2-(4-Methoxyphenyl)-2-oxoethyl]*: ***Lamellarin O***
[158402-61-0]
$C_{27}H_{23}NO_6$ 457.482
Isol. from the Australian marine sponge *Dendrilla cactos*. Unstable pale yellow oil; pale yellow cryst. (as di-Me ether). Mp 55-58° (di-Me ether). λ_{max} 277 (ϵ 5200) (EtOH) (Berdy).

N-*[2-(2-Hydroxy-4-methoxyphenyl)-2-oxoethyl]*: ***Lamellarin P***
[158402-60-9]
$C_{27}H_{23}NO_7$ 473.481
From *Dendrilla cactos*. Moderately stable pale yellow oil. λ_{max} 231 (ϵ 5800); 276 (ϵ 6200); 305 (ϵ 3000) (EtOH) (Berdy).

Urban, S. *et al., Aust. J. Chem.*, 1994, **47**, 1919-1924; 1995, **48**, 1491-1494 (*isol, pmr, cmr, ms, struct, uv, ir*)
Fürstner, A. *et al., J.O.C.*, 1995, **60**, 6637 (*synth*)
Banwell, M.G. *et al., Chem. Comm.*, 1997, 207 (*synth*)
Boger, D.L. *et al., J.A.C.S.*, 1999, **121**, 54-62 (*synth*)
Marfil, M. *et al., Tetrahedron*, 2004, **60**, 8659-8668 (*Lamellarin O,Q, synth*)

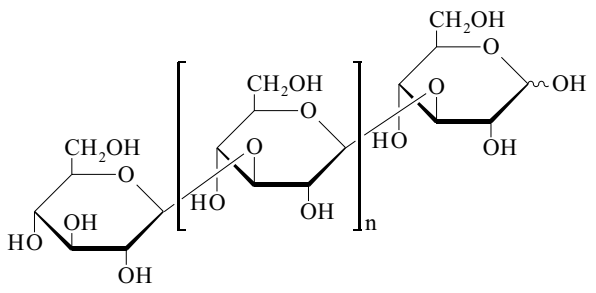
Laminaribiose phosphorylase L-20

E.C. 2.4.1.31. 3-β-D-Glucosyl-D-glucose:phosphate α-D-glucosyltransferase
[37257-29-7]
Hexosyltransferase enzyme. Isol. from *Euglena gracilis*. Catalyses the reversible reaction of 3-*O*-β-D-Glucopyranosyl-D-glucose, G-100 with orthophosphate to give D-glucose and α-D-glucose 1-phosphate.

Kitaoka, M. *et al., Arch. Biochem. Biophys.*, 1993, **304**, 508-514

Laminarin, 9CI L-21

Laminaran, 9CI, 8CI. Lamariose
[9008-22-4]



$C_6H_{10}O_5$ 162.142
General term for low M.W. water-soluble reserve glucans from phaephyte algae. Soluble and insoluble forms were earlier recognised, but laminarans differ considerably in struct. There are different degrees of chain branching caused by additional substitution at C-6, and the chain termini are mostly substituted with Mannitol, M-83. The proportion of mannitol is mostly responsible for the difference between soluble and insoluble forms. Anticoagulant. Antilipemic agent.

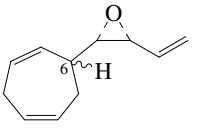
Soluble-*form*
Found in brown algae especially the Laminaria subgroup; isol. from *Laminaria digitata*. Sol. H_2O, pptd. by addn. of EtOH. $[\alpha]_D^{18}$ -11.9 (c, 2.1 in H_2O).
Per-Ac: $[\alpha]_D^{17}$ -64.6 (c, 0.9 in $CHCl_3$).
Per-carbanilate: Mp 175-185°. $[\alpha]_D^{20}$ -7 ($CHCl_3$). $[\alpha]_D^{20}$ -52 (Py).

Insoluble-*form*
Found in brown algae especially the Laminaria subgroup; isol. from *Laminaria cloustoni*. Insol. H_2O. $[\alpha]_D^{16}$ -13.4 (c, 0.9 in H_2O).
Per-Ac: $[\alpha]_D^{15}$ -65.6 (c, 0.45 in $CHCl_3$).

Peat, S. *et al., J.C.S.*, 1958, 724 (*struct*)
Annan, W.D. *et al., J.C.S.*, 1965, 885 (*constit*)
Black, W.A.P. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 159 (*synth*)
Black, W.A.P. *et al., Ind. Gums*, 2nd Ed., Academic Press, 1973, 137 (*rev*)
Colson, P. *et al., J.A.C.S.*, 1974, **96**, 8081 (*cmr*)
Zyvagintseva, T.N. *et al., Carbohydr. Res.*, 1999, **322**, 32-39 (***isol, bibl***)
Kim, Y.T. *et al., Carbohydr. Res.*, 2000, **328**, 331-341 (*nmr*)

Lamoxirene L-22

2-(2,5-Cycloheptadien-1-yl)-3-ethenyloxirane, 9CI. 1-(1,2-Epoxy-3-butenyl)-2,5-cycloheptadiene
[92675-19-9]
[183072-86-8, 183072-87-9]



$C_{11}H_{14}O$ 162.231
Pheromone from *Laminaria digitata*. Isol. as a mixt. of C-6 epimers.

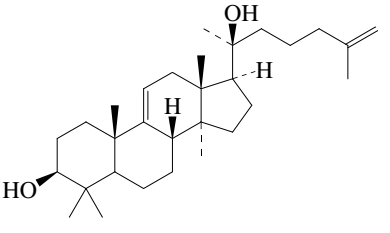
Marner, F.-J. *et al., Z. Naturforsch., C*, 1984, **39**, 689-691 (*isol, pmr, ms*)
Maier, I. *et al., Naturwissenschaften*, 1996, **83**, 378-379 (*abs config*)

Lamprey corticostatin-related peptide L-23

LCRP
[179667-65-3]
H-Cys-Pro-Cys-Gly-Arg-Arg-Arg-Cys-Cys-Val-Arg-Gly-Leu-Asn-Val-Tyr-Cys-Cys-Phe-OH
$C_{89}H_{140}N_{32}O_{22}S_6$ 2202.682
Primary struct. shown. All Cys residues are linked. Isol. from the skin of *Petromyzon marinus*.

Conlon, J.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1996, **114**, 133 (*isol, struct*)

Lanosta-9(11),25-diene-3,20-diol L-24

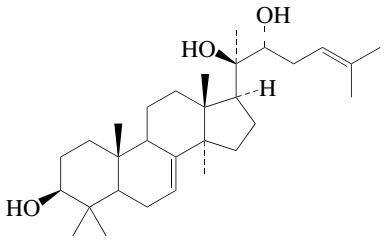


$C_{30}H_{50}O_2$ 442.724

(3β,20*S*)-*form*
3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]*: ***DS-Penaustroside B***
[143572-16-1]
$C_{59}H_{98}O_{24}$ 1191.409
Desulfated saponin from *Pentacta australis*. Powder.

Mp 220-225°. $[\alpha]_D^{23}$ -3 (c, 0.6 in Py).
Miyamoto, T. *et al., J. Nat. Prod.*, 1992, **55**, 940-946 (*isol, pmr, cmr*)

Lanosta-7,24-diene-3,20,22-triol L-25

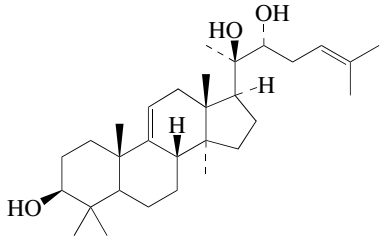


$C_{30}H_{50}O_3$ 458.723

(3β,20*R*,22*R*)-*form*

22-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Frondoside A_2-8***
[890152-38-2]
$C_{61}H_{100}O_{29}S$ 1329.51
Constit. of *Cucumaria frondosa*. Powder.
Mp 224-226°. $[\alpha]_D^{20}$ -33 (c, 0.1 in Py).
Silchenko, A.S. *et al., Can. J. Chem.*, 2005, **83**, 2120-2126 (*Frondoside A_2-8*)

Lanosta-9(11),24-diene-3,20,22-triol L-26



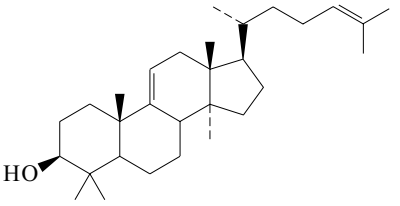
$C_{30}H_{50}O_3$ 458.723

(3β,20*R*,22*R*)-*form*

22-Ac, 3-O-*[3*-O-*methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Frondoside A_2-7***
[890152-28-0]
$C_{61}H_{100}O_{29}S$ 1329.51
Constit. of *Cucumaria frondosa*. Powder.
Mp 216-217°. $[\alpha]_D^{20}$ -10 (c, 0.1 in Py).

22-Ac, 3-O-*[3*-O-*methyl-6-sulfo-β-D-glucopyranosyl-(1→3)-6-sulfo-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4-sulfo-β-D-xylopyranoside]:* ***Frondoside C***
[208764-60-7]
$C_{61}H_{100}O_{35}S_3$ 1489.638
Constit. of *Cucumaria frondosa*. Shows strong cytotoxic activity.
Avilov, S.A. *et al., Can. J. Chem.*, 1998, **76**, 137-141 (*Frondoside C, activity*)
Silchenko, A.S. *et al., Can. J. Chem.*, 2005, **83**, 2120-2126 (*Frondoside A_2-7*)

Lanosta-9(11),24-dien-3-ol L-27

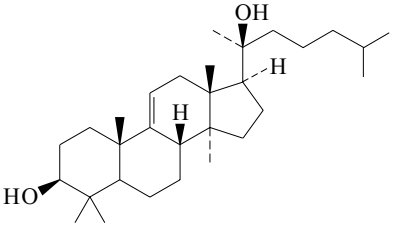


$C_{30}H_{50}O$ 426.724

3β-*form*

Parkeol
[514-45-4]
Constit. of *Butyrospermum parkii* (preferred genus name *Vitellaria*). Present in the sea cucumber *Holothuria arenicola* and in *Eupentacta fraudatrix*. Intermed. in the unusual non-Lanosterol steroid biosynthetic route shown by echinoderms. Cryst. (Et_2O/MeOH).
Mp 162-165°. $[\alpha]_D$ +76.8 (c, 1 in $CHCl_3$).
Schreiber, K. *et al., Tetrahedron*, 1964, **20**, 1803 (*struct*)
v. Tamelen, E.E. *et al., J.A.C.S.*, 1972, **94**, 8225 (*synth*)
Itoh, T. *et al., Steroids*, 1976, **27**, 275 (*pmr*)
Cordiero, M.L. *et al., Tet. Lett.*, 1988, **29**, 2159-2162 (*biosynth*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*biosynth*)

Lanost-9(11)-ene-3,20-diol L-28



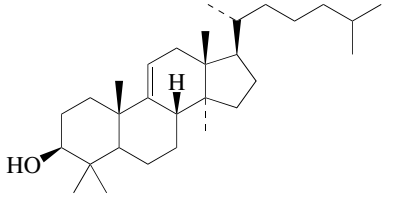
$C_{30}H_{52}O_2$ 444.74

(3β,20*S*)-*form*

Penaustrol
[143572-19-4]
Sapogenin from *Pentacta australis.*
Needles.
Mp 142-144°. $[\alpha]_D^{25}$ +18.7 (c, 0.075 in $CHCl_3$).

3-O-*[3*-O-*Methyl-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranoside]:* ***DS-Penaustroside A***
[143572-15-0]
$C_{59}H_{100}O_{24}$ 1193.425
Desulfated saponin from *Pentacta australis.* Powder.
Mp 292-296°. $[\alpha]_D^{24}$ -2.3 (c, 0.5 in Py).
Miyamoto, T. *et al., J. Nat. Prod.*, 1992, **55**, 940-946 (*isol, pmr, cmr*)

Lanost-9(11)-en-3-ol L-29

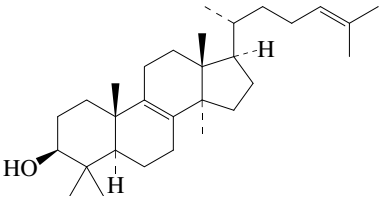


$C_{30}H_{52}O$ 428.74

(3β,5α)-*form*
Dihydroparkeol
[28032-52-2]
Constit. of *Holothuria scabra*.
Me ether: ***3-Methoxylanost-9(11)-ene***
[443965-53-5]
$C_{31}H_{54}O$ 442.767
Constit. of *Brachiaria decumbens*.
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*isol, pmr, ms*)
Pires, V.S. *et al., J. Braz. Chem. Soc.*, 2002, **13**, 135-139 (*Me ether*)

Lanosterol L-30

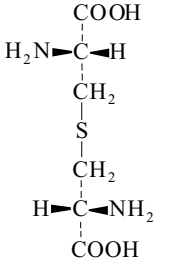
Lanosta-8,24-dien-3-ol. 4,4,14-Trimethylcholesta-8,24-dien-3-ol. Kryptosterol. Cryptosterol
[79-63-0]



$C_{30}H_{50}O$ 426.724
Major component of the "isocholesterol" sterol portion of wool fat. Also from yeast and some other fungi and *Euphorbia regis-jubae* and some other plants. Intermed. in the biosynth. of steroids in echinoderms, e.g. *Eupentacta fraudatrix*. Cryst. (MeOH/Me_2CO).
Mp 140-141°. $[\alpha]_D^{17}$ +58 ($CHCl_3$).
▶ OE3360000
3-O-*Sulfate:*
$C_{30}H_{50}O_4S$ 506.789
Mp 199-200° (as K salt).
Ac:
$C_{32}H_{52}O_2$ 468.762
Mp 131-133°. $[\alpha]_D^{20}$ +62.5 (c, 1.12 in $CHCl_3$).
Sobel, A.E. *et al., J.A.C.S.*, 1941, **63**, 1259 (*sulfate*)
Voser, W. *et al., Helv. Chim. Acta*, 1952, **35**, 66; 2414 (*struct*)
Hemmert, F. *et al., Bull. Soc. Chim. Fr.*, 1966, 976 (*pmr*)
Legrand, M. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1966, **262**, 1290 (*cd*)
Barton, D.H.R. *et al., J.C.S.(C)*, 1969, **332**, (*synth*)
Shishibori, T. *et al., Chem. Lett.*, 1973, 1289 (*biosynth*)
Boar, R.B. *et al., J.C.S. Perkin 1*, 1973, 1583-1588 (*synth, purifn*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*biosynth, echinoderms*)
Corey, E.J. *et al., J.A.C.S.*, 1995, **117**, 11819 (*biosynth*)
Joubert, B.M. *et al., Org. Lett.*, 2000, **2**, 339-341 (*biosynth*)
Hess, B.A. *et al., J.A.C.S.*, 2002, **124**, 10286-10287 (*biosynth*)
Hess, B.A. *et al., Org. Lett.*, 2003, **5**, 165-167 (*biosynth*)

Lanthionine L-31

S-*(2-Amino-2-carboxyethyl)cysteine, 9CI. β,β′-Diamino-β,β′-dicarboxydiethyl sulfide*
[496-98-0]
[3183-08-2]



(*R,R*)–*form*

$C_6H_{12}N_2O_4S$ 208.238
Present in normal and pathological brain tissue. Isol. from the red alga *Hypnea musciformis*.

(*R,R*)-*form*
L-*form*
[922-55-4]
Isol. from pupae of silkworm, *Bombyx mori*.
Hexagonal plates. $[\alpha]_D^{22}$ +8.6 (c, 5 in 2.4*M* NaOH). Dec. at 293-5° (darkening from 245°).

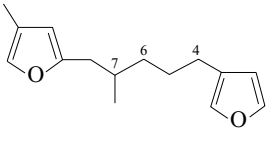
(*S,S*)-*form*
D-*form*
$[\alpha]_D^{21}$ -8 (c, 5 in 2.4*M* NaOH). Dec. at 293-5°.

(*RS,RS*)-*form*
(±)-*form*
Dec. at 286-92°.

(*RS,SR*)-*form*
meso-*form*
[922-56-5]
Isol. by alkaline hydrol. of wool. Also a residue in the antibiotics Nisin, Duramycin and Lanthiopeptin. Present in pollen of *Lilium candidum*.
Plates. Spar. sol. H_2O, insol. $CHCl_3$, Et_2O. Dec. at 304° (softening from 270°).
Dibenzoyl:
$C_{20}H_{20}N_2O_6S$ 416.454
Mp 205-206°.
Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 502C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 595D (*ir*)
Hom, M.J. *et al., J. Biol. Chem.*, 1941, **138**, 141 (*isol*)
du Vigneaud, V. *et al., J. Biol. Chem.*, 1941, **138**, 151
Brown, G.B. *et al., J. Biol. Chem.*, 1941, **140**, 767 (*abs config*)
Rossetti, V. *et al., Ann. Chim. (Rome)*, 1966, **56**, 935 (*isol*)
Rao, D.R. *et al., Biochemistry*, 1967, **6**, 1208 (*isol*)
Bartle, K.D. *et al., Biochim. Biophys. Acta*, 1968, **160**, 106 (*pmr*)
Ingram, L.C. *et al., Biochim. Biophys. Acta*, 1969, **184**, 216
Gross, E. *et al., J.A.C.S.*, 1971, **93**, 4634
Gross, E. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1973, **354**, 799; 810
Rosenfeld, R.E. *et al., J.A.C.S.*, 1974, **96**, 1925 (*cryst struct*)
Glówka, M.L. *et al., Acta Cryst. C*, 1986, **42**, 620 (*cryst struct*)
Desiraju, G.R. *et al., Acta Cryst. C*, 1990, **46**, 627 (*cryst struct*)
Friedman, M. *et al., J. Agric. Food Chem.*, 1999, **47**, 1295-1319 (*rev, food chem*)

Lasiosperman L-32

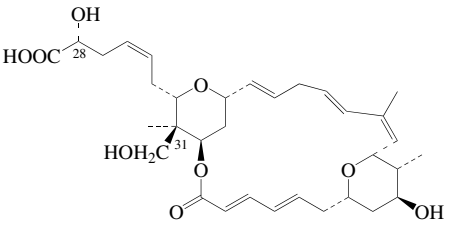
2-[5-(3-Furanyl)-2-methylpentyl]-4-methylfuran, 9CI
[33853-92-8]



$C_{15}H_{20}O_2$ 232.322
Constit. of *Lasiospermum radiatum*. Oil.
*6,7*E-*Didehydro:* ***Dehydrolasiosperman***
[33853-91-7]
$C_{15}H_{18}O_2$ 230.306
Constit. of *Lasiospermum radiatum* and mollusc *Ceratosoma brevicaudatum*. Oil. $Bp_{0.01}$ 90°.
4-Oxo: ***4-Oxolasiosperman***. *10-Oxolasiosperman*
[68776-21-6]
$C_{15}H_{18}O_3$ 246.305
Constit. of *Eumorphia* spp. Oil.
*6,7-Didehydro(*E-*), 5-(3-methylbutanoyloxy):* ***5-Isovaleryloxydehydrolasiosperman***
$C_{20}H_{26}O_4$ 330.423
Constit. of *Ursinia sericea*.
Bornowski, H. *et al., Tetrahedron*, 1971, **27**, 4101 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1155 (*4-Oxolasiosperman*)
Ksebati, M.B. *et al., J. Nat. Prod.*, 1988, **51**, 857
Jefford, C.W. *et al., Tet. Lett.*, 1990, **31**, 5741 (*synth*)

Jakupovic, J. *et al., Phytochemistry*, 1992, **31**, 863 (*Isovaleryloxydehydrolasiosperman*)

Lasonolide F L-33



Absolute Configuration

$C_{33}H_{46}O_9$ 586.721

Macrolide antibiotic. Stereochem. revised in 2003. Isol. from the marine sponge *Forcepia* sp. Cytotoxic agent. Oil. $[\alpha]_D^{20}$ -23.5 (c, 0.23 in MeOH). λ_{max} 248 (3.9); 268 (sh) (3.7) (MeOH).

Et ester: ***Lasonolide E***
$C_{35}H_{50}O_9$ 614.775
Isol. from a *Forcepia* sp. Oil. $[\alpha]_D^{20}$ -18 (c, 0.3 in MeOH/$CHCl_3$). λ_{max} 248 (log ϵ 4); 268 (sh) (log ϵ 3.9) (MeOH/$CHCl_3$).

(5-Methyl-2-methylenehexyl) ester: ***Lasonolide A***
[400710-54-5]
[157075-57-5]
$C_{41}H_{60}O_9$ 696.92
Isol. from the marine sponge *Forcepia*. Also in *Acarnus* sp., *Hemitedania* sp., *Tedania* sp. and *Lissodendoryx* sp. Cytotoxic agent. Signal transduction agent, cell adhesion inhibitor. Pale orange solid. $[\alpha]_D^{10}$ +24.2 (c, 0.20 in $CHCl_3$).

(3ξ-Hydroxy-5-methyl-2-methylenehexyl) ester: ***Lasonolide C***
$C_{41}H_{60}O_{10}$ 712.919
Isol. from a *Forcepia* sp. Powder. $[\alpha]_D^{20}$ -9.8 (c, 0.32 in $CHCl_3$). λ_{max} 248 (log ϵ 4.2); 268 (log ϵ 4.1) ($CHCl_3$).

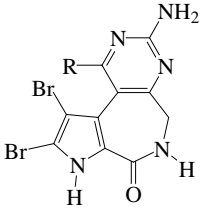
(4ξ-Hydroxy-3ξ-methyl-2-methylenehexyl) ester: ***Lasonolide B***
[186183-65-3]
$C_{41}H_{60}O_{10}$ 712.919
Isol. from a marine sponge, *Forcepia* sp. Cytotoxic agent.

31-O-Dodecanoyl, (3ξ-hydroxy-5-methyl-2-methylenehexyl) ester: ***Lasonolide G***
$C_{53}H_{82}O_{11}$ 895.224
Isol. from a *Forcepia* sp. Tan oil. $[\alpha]_D^{20}$ -18 (c, 0.5 in MeOH).

Decarboxy: ***Lasonolide D***
$C_{32}H_{46}O_7$ 542.711
Isol. from a *Forcepia* sp. Oil. $[\alpha]_D^{20}$ -5.3 (c, 0.34 in MeOH/$CHCl_3$). Has -CH_2OH terminal group. λ_{max} 248 (log ϵ 3.9); 268 (sh) (log ϵ 3.8) (MeOH/$CHCl_3$).

Horton, P.A. *et al., J.A.C.S.*, 1994, **116**, 6015-6016 (*Lasonolide A*)
U.S. Pat., 1997, 5 684 036; *CA*, **128**, 7300t (*Lasonolide B*)
Kang, S.H. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 4779-4782 (*Lasonolide A, synth*)
Song, H.Y. *et al., J.O.C.*, 2003, **68**, 8080-8087 (*synth, abs config*)
Wright, A.E. *et al., J. Nat. Prod.*, 2004, **67**, 1351-1355 (*Lasonolides A-F, isol, pmr, cmr*)
Kang, S.H. *et al., Synthesis*, 2004, 1102-1114 (*synth, pmr, cmr*)
Yoshimura, T. *et al., Org. Lett.*, 2006, **8**, 475-478 (*Lasonolide A, synth*)

Latonduine A L-34



R = H

$C_{10}H_7Br_2N_5O$ 373.006

Alkaloid from *Stylissa carteri*. Pale yellow solid. Dec. at 290°. λ_{max} 245 (ϵ 19830); 284 (ϵ 14220) (MeOH).

Linington, R.G. *et al., Org. Lett.*, 2003, **5**, 2735-2738 (*isol, synth, pmr, cmr*)

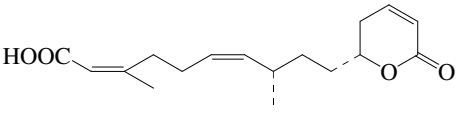
Latonduine B L-35

As Latonduine A, L-34 with
R = -COOH

$C_{11}H_7Br_2N_5O_3$ 417.016
Alkaloid from *Stylissa carteri*. Pale yellow cryst. (as Et ester). Mp 228-231° (Et ester). λ_{max} 203 (ϵ 24130); 252 (ϵ 25920); 284 (sh); 348 (ϵ 5890) (MeOH).

Linington, R.G. *et al., Org. Lett.*, 2003, **5**, 2735-2738 (*isol, pmr, cmr*)

Latrunculeic acid L-36

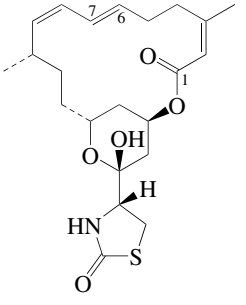


$C_{17}H_{24}O_4$ 292.374
Isol. from the sponge *Negombata magnifica*. Oil. $[\alpha]_D$ -50.9 (c, 0.05 in MeOH).

Vilozny, B. *et al., J. Nat. Prod.*, 2004, **67**, 1055-1057 (*isol, pmr, cmr, ms*)

Latrunculin A† L-37

[76343-93-6]



Absolute Configuration

$C_{22}H_{31}NO_5S$ 421.557
Toxin from the Red Sea sponge *Latrunculia magnifica* and *Latrunculia corticata*. Also found in three Pacific sponges, *Spongia mycofijiensis*, *Hyatella* sp., an unidentified specimen, and in *Chromodoris hamitoni*, *Chromodoris lochii* and *Chromodoris elisabethina*. Ichthyotoxin, inhibitor of protein kinase C, shows cytochalasin-like activity, potential antiglaucoma agent. Oil. Poorly sol. H_2O. $[\alpha]_D^{24}$ +152 (c, 1.2 in $CHCl_3$). λ_{max} 218 (ϵ 23500); 268 (sh) (MeOH) (Derep).

Me ether:
Cryst. (C_6H_6). Mp 164-165°. $[\alpha]_D^{24}$ +315 (c, 0.33 in $CHCl_3$).

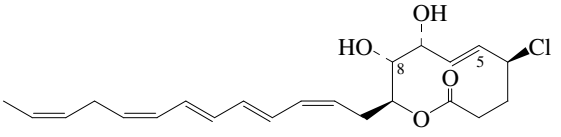
N-*(Hydroxymethyl):* ***Latrunculin G***
[122876-69-1]
$C_{23}H_{33}NO_6S$ 451.583
Isol. from *Latrunculia magnifica* plus formaldehyde. Cell division inhibitor. Oil. $[\alpha]_D^{25}$ +70 (c, 2.2 in $CHCl_3$).

6,7-Epoxide: ***6,7-Epoxylatrunculin A***
[122876-48-6]
$C_{22}H_{31}NO_6S$ 437.556
Constit. of *Latrunculia magnifica* and *Spongia* sp. Oil. Sol. MeOH. $[\alpha]_D^{25}$ +37 (c, 1.2 in $CHCl_3$). λ_{max} 218 (ϵ 23500); 268 (sh) (MeOH) (Derep).

Kashman, Y. *et al., Tet. Lett.*, 1980, **21**, 3629-3632 (*isol, uv, pmr, cmr, ms, cryst struct*)
Groweiss, A. *et al., J.O.C.*, 1983, **48**, 3512-3516 (*Latrunculin A, cryst struct*)
Spector, I. *et al., Science (Washington, D.C.)*, 1983, **219**, 493 (*rev*)
Okuda, R.K. *et al., Experientia*, 1985, **41**, 1355-1356
Kashman, Y. *et al., Tetrahedron*, 1985, **41**, 1905 (*abs config*)
Blasberger, D. *et al., Annalen*, 1989, 1171 (*epoxide*)

U.S. Pat., 1989, 4 857 538; *CA*, **112**, 30647q (*Latrunculin G*)
White, J.D. *et al., J.O.C.*, 1992, **57**, 5292 (*synth, bibl*)
Jefford, C.W. *et al., Tet. Lett.*, 1996, **37**, 159 (*abs config, cryst struct, bibl*)
Fürstner, A. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 3462-3466 (*synth*)

Latrunculin A† L-38



$C_{22}H_{29}ClO_4$ 392.921
Oil. $[\alpha]_D^{23}$ +36 (c, 0.09 in EtOH). λ_{max} 313 (log ϵ 4.94) (EtOH).

8-O-*[2,3,6-Trideoxy-α-L*-erythro-*hexopyranosyl-(1→4)-2,6-dideoxy-β-D*-arabino-*hexopyranosyl-(1→4)-2,6-dideoxy-β-L*-ribo-*hexopyranoside]:* ***Latrunculinoside A***
$C_{40}H_{59}ClO_{12}$ 767.352
Isol. from the Red Sea sponge *Latrunculia corticata*. Powder. $[\alpha]_D^{23}$ +72 (c, 0.13 in MeOH). λ_{max} 307 (log ϵ 4.82) (EtOH).

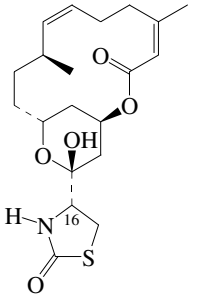
(5Z)-Isomer: ***Latrunculin B†***
$C_{22}H_{29}ClO_4$ 392.921
Oil. $[\alpha]_D^{23}$ -9 (c, 0.08 in MeOH). λ_{max} 312 (log ϵ 4.73) (EtOH).

(5Z)-Isomer, 8-O-*[2,6-dideoxy-β-D*-lyxo-*hexopyranosyl-(1→3)-2,6-dideoxy-β-D*-lyxo-*hexopyranoside]:* ***Latrunculinoside B***
$C_{34}H_{49}ClO_{10}$ 653.208
Isol. from the Red Sea sponge *Latrunculia corticata*. Powder. $[\alpha]_D^{22}$ -18.5 (c, 0.09 in MeOH).

Rezanka, T. *et al., Eur. J. Org. Chem.*, 2003, 2144-2152 (*isol, pmr, cmr, ms*)

Latrunculin B† L-39

[76343-94-7]



Absolute Configuration

$C_{20}H_{29}NO_5S$ 395.519
Isol. from the Red Sea sponge *Latrunculia magnifica*; also from *Latrunculia corticata*, *Spongia* sp., *Glossodoris quadricolor* and *Chromodoris hamiltonii*. Strongly ichthyotoxic; actin polym. inhibitor; shows insecticidal props. $[\alpha]_D^{24}$ +112 (c, 0.48 in $CHCl_3$). λ_{max} 212 (ϵ 17300); 269 (sh) (MeOH) (Derep).

Me ether: ***15-O-Methyllatrunculin B***
[105917-28-0]
$C_{21}H_{31}NO_5S$ 409.546
Isol. from *Negombata magnifica*.
$[\alpha]_D^{25}$ +108 (c, 1.5 in $CHCl_3$).

N-*Ac:* **N-*Acetyllatrunculin B***
$C_{22}H_{31}NO_6S$ 437.556
Isol. from *Negombata magnifica*. Oil. $[\alpha]_D^{25}$ +48 (c, 0.05 in EtOH).

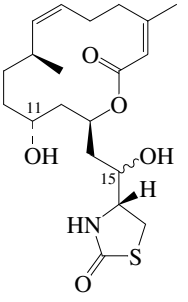
N-*(Hydroxymethyl):* ***Latrunculin H***
[122876-74-8]
$C_{21}H_{31}NO_6S$ 425.545
Isol. from *Latrunculia magnifica* plus formaldehyde. Cell division inhibitor. Oil.

16-Epimer: ***16-Epilatrunculin B***
$C_{20}H_{29}NO_5S$ 395.519
Isol. from the sponge *Negombata magnifica*.

Kashman, Y. *et al., Tet. Lett.*, 1980, **21**, 3629 (*isol, uv, ir, pmr, cmr, ms, struct*)
Groweiss, A. *et al., J.O.C.*, 1983, **48**, 3512 (*isol, uv, ir, pmr, cmr, ms, struct*)
Spector, I. *et al., Science (Washington, D.C.)*, 1983, **219**, 493 (*rev*)
Mebs, D. *et al., J. Chem. Ecol.*, 1985, **11**, 713 (*isol*)
Kashman, Y. *et al., Tetrahedron*, 1985, **41**, 1905 (*pmr, cmr*)
U.S. Pat., 1989, 4 857 538; *CA*, **112**, 30647q (*Latrunculin H*)
Hoye, T.R. *et al., J.A.C.S.*, 2002, **124**, 7405-7410 (*16-Epilatrunculin B*)
Vilozny, B. *et al., J. Nat. Prod.*, 2004, **67**, 1055-1057 (*15-O-Methyllatrunculin B*)
El Sayed, K.A. *et al., J. Nat. Prod.*, 2006, **69**, 219-223 (*N-Acetyllatrunculin B*)

Latrunculin C L-40

[76376-32-4]



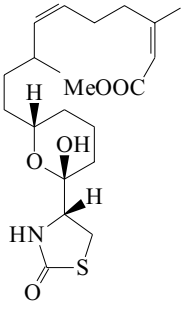
$C_{20}H_{31}NO_5S$ 397.535
Macrolide. Structs. originally reported for Latrunculins C and D were reversed. Isol. from the Red Sea Sponge *Latrunculia magnifica*. Ichthyotoxin. Oil. λ_{max} 212 (ϵ 17300); 269 (sh) (MeOH) (Derep).

15-Ketone, 11-Me ether: ***Latrunculin D***
[98155-17-0]
$C_{21}H_{31}NO_5S$ 409.546
From *Latrunculia magnifica*. Ichthyotoxin. Oil. Sol. MeOH, hexane; poorly sol. H_2O. λ_{max} 212 (ϵ 17300); 269 (sh) (MeOH) (Derep).

Kashman, Y. *et al., Tetrahedron*, 1985, **41**, 1905-1914 (*isol, uv, ir, pmr, cmr, ms, struct*)
Smith, A.B. *et al., J.A.C.S.*, 1992, **114**, 2995-3007 (*synth*)
Fürstner, A. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 5358-5360 (*synth*)

Latrunculin M L-41

[122876-49-7]

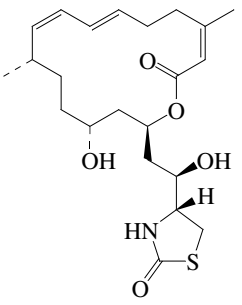


$C_{21}H_{33}NO_5S$ 411.561
Minor constit. of the Red Sea sponge *Latrunculia magnifica*. Oil. Sol. MeOH. $[\alpha]_D^{25}$ +11 (c, 0.2 in $CHCl_3$).

Blasberger, D. *et al., Annalen*, 1989, 1171 (*isol, ir, pmr, cmr, ms, struct*)

Latrunculin S L-42

[175992-99-1]

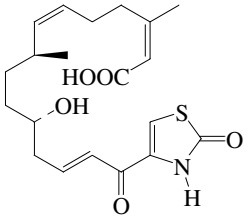


$C_{22}H_{33}NO_5S$ 423.572

Macrolide antibiotic. Isol. from the sponge *Fasciospongia rimosa*. Cytotoxic agent. $[\alpha]_D^{26}$ +110 (c, 0.2 in $CHCl_3$).

Tanaka, J. *et al., Chem. Lett.*, 1996, 255 (*isol, ir, pmr, cmr*)

Latrunculin T L-43



Absolute Configuration

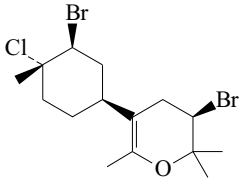
$C_{20}H_{27}NO_5S$ 393.503

Isol. from *Negombata magnifica*. Antimicrobial agent. Oil. $[\alpha]_D^{25}$ +109.5 (c, 0.11 in EtOH).

El Sayed, K.A. *et al., J. Nat. Prod.*, 2006, **69**, 219-223 (*isol, pmr, cmr*)

Laucapyranoid A L-44

[124193-05-1]



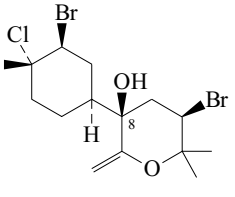
$C_{15}H_{23}Br_2ClO$ 414.607

Constit. of *Laurencia caespitosa* and *Aplysia dactylomela*. Cryst. Mp 118-120°. $[\alpha]_D$ +0.5 (c, 0.87 in $CHCl_3$). $[\alpha]_D$ +25.4 (c, 0.13 in $CHCl_3$).

Chang, M. *et al., Phytochemistry*, 1989, **28**, 1417-1424 (*isol, pmr, cmr*)
Wessels, M. *et al., J. Nat. Prod.*, 2000, **63**, 920-928 (*isol*)

Laucapyranoid B L-45

[124192-95-6]



$C_{15}H_{23}Br_2ClO_2$ 430.606

Constit. of *Laurencia caespitosa*. Cryst. Mp 97-98°. $[\alpha]_D$ +11 (c, 1.12 in $CHCl_3$).

8-Epimer: ***Laucapyranoid C***

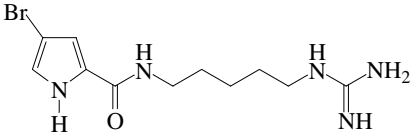
[124264-18-2]

$C_{15}H_{23}Br_2ClO_2$ 430.606

Constit. of *Laurencia caespitosa*. Unstable.

Chang, M. *et al., Phytochemistry*, 1989, **28**, 1417

Laughine L-46



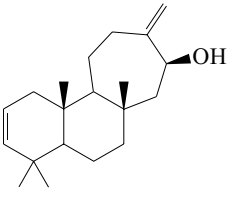
$C_{11}H_{18}BrN_5O$ 316.2

Isol. from the sponge *Eurypon laughlini*. Pale yellow oil. λ_{max} 206 (ϵ 3800); 265 (ϵ 4020) (MeOH).

Williams, D.E. *et al., J. Nat. Prod.*, 2005, **68**, 327-330 (*isol, pmr, cmr*)

Laukarlaol L-47

[168301-27-7]



$C_{20}H_{32}O$ 288.472

Constit. of *Laurencia karlae*. Needles.

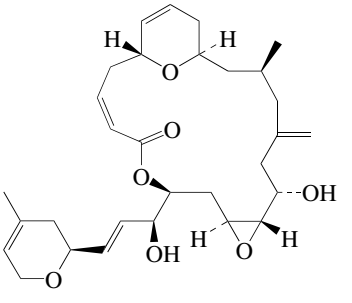
Mp 128-129°. $[\alpha]_D^{20}$ -52 (c, 0.025 in $CHCl_3$).

Su, J.-Y. *et al., Phytochemistry*, 1995, **40**, 195 (*isol, pmr, cmr*)
Justicia, J. *et al., J.A.C.S.*, 2005, **127**, 14911-14921 (*synth*)

Laulimalide L-48

Fijianolide B. Laulamide

[114995-73-2]



$C_{30}H_{42}O_7$ 514.658

Macrolide antibiotic. Isol. from sponges *Spongia mycofijiensis* and *Hyatella* sp. and from *Chromodoris lochi*. Potent cytotoxin. Oil. $[\alpha]_D^{20}$ -8 (c, 0.04 in $CHCl_3$). λ_{max} 208 (ϵ 10500) (MeOH) (Derep).

Di-Ac: $[\alpha]_D^{20}$ -8 (c, 0.04 in $CHCl_3$).

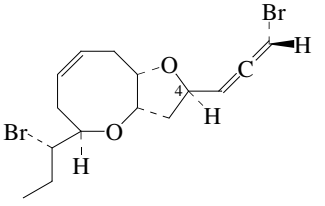
[115268-43-4]

Quiñoà, E. *et al., J.O.C.*, 1988, **53**, 3642 (*isol, pmr, cmr, struct*)
Corley, D.G. *et al., J.O.C.*, 1988, **53**, 3644-3646 (*isol, struct, pmr, cmr, ir, uv*)
Tanaka, J. *et al., Chem. Lett.*, 1996, 255 (*isol, struct*)
Jefford, C.W. *et al., Tet. Lett.*, 1996, **37**, 159 (*abs config*)
Mulzer, J. *et al., Angew. Chem., Int. Ed.*, 2001, **40**, 3842-3846 (*synth*)
Paterson, I. *et al., Org. Lett.*, 2001, **3**, 3149-3152 (*synth*)
Ghosh, A.K. *et al., Tet. Lett.*, 2001, **42**, 3399-3401 (*synth*)
Wender, P.A. *et al., J.A.C.S.*, 2002, **124**, 4956-4957 (*synth*)
Crimmins, M.T. *et al., J.A.C.S.*, 2002, **124**, 5958-5959 (*synth*)

Nelson, S.G. *et al., J.A.C.S.*, 2002, **124**, 13654-13655 (*synth*)
Ghosh, A.K. *et al., J.O.C.*, 2002, **66**, 8973-8982 (*synth*)
Mulzer, J. *et al., Tet. Lett.*, 2002, **43**, 3381-3383 (*synth*)
Williams, D.R. *et al., Tet. Lett.*, 2002, **43**, 4841-4844 (*synth*)
Ahmed, A. *et al., J.O.C.*, 2003, **68**, 3026-3042 (*synth, bibl*)
Uenishi, J. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 2756-2760 (*synth*)
Thepchatri, P. *et al., J.A.C.S.*, 2005, **127**, 12838-12846 (*conformn*)
Paterson, I. *et al., Tet. Lett.*, 2005, **46**, 3677-3682 (*pmr, struct*)

Laurallene L-49

*2-(3-Bromo-1,2-propanediyl)-5-(1-bromopropyl)-3,3*a*,5,6,9,9*a*-hexahydro-2*H*-furo[3,2-*b*]oxocin, 9CI. 1,13-Dibromo-4,7:6,12-diepoxy-1,2,9-pentadecatriene*
[72719-97-2]



$C_{15}H_{20}Br_2O_2$ 392.13

Structs. not yet clear, and assignment of CAS nos. is confused.
Constit. of *Laurencia nipponica*. Cryst. (hexane).
Mp 58.9-59.4° (53-54°). $[\alpha]_D$ +173.6 (c, 1.13 in $CHCl_3$).

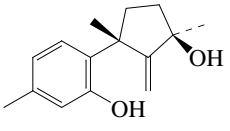
4-Epimer(?): ***Panosallene***
$C_{15}H_{20}Br_2O_2$ 392.13
Isol. from the red alga *Laurencia pannosa*. Needles. $[\alpha]_D^{26}$ +64.3 (c, 0.07 in $CHCl_3$). Struct. shown was originally assigned to Epilaurallene. The CAS no. [85761-64-4] has been applied to both.

Stereoisomer(?): ***Epilaurallene***
[85761-64-4]
$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of *Laurencia nipponica*. Cryst.
Mp 51-52°. $[\alpha]_D^{25}$ +175 (c, 1 in $CHCl_3$). Assigned struct. (1983) is incorrect. May be a stereoisomer or polymorph of Laurallene.

Fukuzawa, A. *et al., Tet. Lett.*, 1979, 2797-2800 (*Laurallene*)
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 715-718 (*Epilaurallene*)
Suzuki, M. *et al., Phytochemistry*, 1996, **41**, 1101-1103 (*Panosallene*)
Ishihara, J. *et al., Tetrahedron*, 1997, **53**, 8371-8382 (*biosynth*)
Crimmins, M.T. *et al., J.A.C.S.*, 2000, **122**, 5473-5476 (*synth*)
Saitoh, T. *et al., Tet. Lett.*, 2003, **44**, 3175-3178 (*synth*)

5(13),6,8,10-Lauratetraene-4,7-diol L-50

11-Laurene-1,10-diol



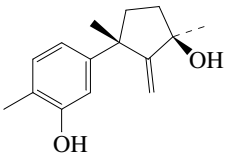
$C_{15}H_{20}O_2$ 232.322

(1R,4R)-form [861251-20-9]
Constit. of *Laurencia tristicha*.
Cryst. (MeOH).
Mp 95-97°. $[\alpha]_D^{20}$ -93.8 (c, 0.08 in MeOH).

Sun, J. *et al., J. Nat. Prod.*, 2005, **68**, 915-919 (*Laurencia tristicha constit*)

5(13),6,8,10-Lauratetraene-4,8-diol L-51

11-Laurene-2,10-diol



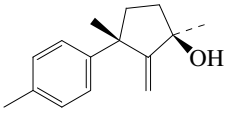
$C_{15}H_{20}O_2$ 232.322

(1R,4R)-form [861251-18-5]
Constit. of *Laurencia tristicha*.
Cryst. (MeOH).
Mp 99-100°. $[\alpha]_D^{20}$ -70.5 (c, 0.19 in MeOH).

Sun, J. *et al., J. Nat. Prod.*, 2005, **68**, 915-919 (*Laurencia tristicha constit*)

5(13),6,8,10-Lauratetraen-4-ol L-52

11-Lauren-10-ol



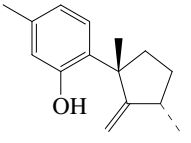
$C_{15}H_{20}O$ 216.322

(1R,4R)-form [861251-19-6]
Constit. of *Laurencia tristicha*.
Cryst. (MeOH).
Mp 62-63°. $[\alpha]_D^{20}$ -32.7 (c, 0.56 in MeOH).

Sun, J. *et al., J. Nat. Prod.*, 2005, **68**, 915-919 (*Laurencia tristicha constit*)

5(13),6,8,10-Lauratetraen-7-ol L-53

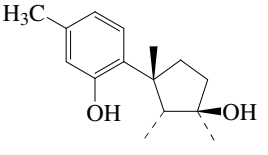
[62003-49-0]



$C_{15}H_{20}O$ 216.322
Constit. of *Laurencia majuscula*.

Masuda, M. *et al., Phycol. Res.*, 1997, **45**, 59-64; *CA*, **127**, 133150

6,8,10-Lauratriene-4,7-diol L-54



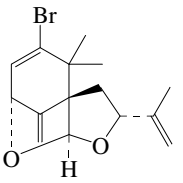
$C_{15}H_{22}O_2$ 234.338

(1R,4R,5R)-form
3,7-Dihydroxydihydrolaurene
[874193-55-2]
Constit. of *Laurencia obtusa*.
Oil. $[\alpha]_D^{20}$ -12 (c, 0.15 in CH_2Cl_2). λ_{max} 204 (log ϵ 4.4); 231 (log ϵ 3.6); 287 (log ϵ 3.3) (hexane).

Kladi, M. *et al., Tetrahedron*, 2006, **62**, 182-189

Laureacetal A L-55

[66347-80-6]

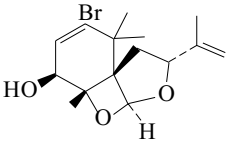


$C_{15}H_{19}BrO_2$ 311.218
Constit. of *Laurencia nipponica*. Cryst. (diisopropyl ether).
Mp 82-83°. $[\alpha]_D$ +98 (c, 1 in $CHCl_3$).

Suzuki, T. *et al., Tet. Lett.*, 1977, **18**, 3731-3734 (*isol, pmr, cmr, cryst struct*)

Laureacetal B L-56

[69369-25-1]

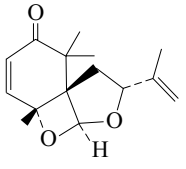


$C_{15}H_{21}BrO_3$ 329.233
Constit. of *Laurencia nipponica*. Cryst. (isopropyl ether/hexane).
Mp 105-106°. $[\alpha]_D$ +8.4 (c, 1 in $CHCl_3$).

Suzuki, T. *et al., Chem. Lett.*, 1979, 301

Laureacetal C L-57

[84744-66-1]



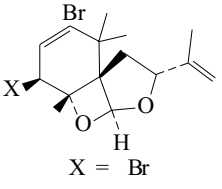
Absolute configuration

$C_{15}H_{20}O_3$ 248.321
Constit. of red alga *Laurencia nipponica*. Cryst. (diisopropyl ether).
Mp 118-119°. $[\alpha]_D$ +9.8 (c, 1.53 in $CHCl_3$).

Kurata, K. *et al., Chem. Lett.*, 1983, 29

Laureacetal D L-58

[85933-22-8]



Absolute configuration

X = Br

$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of red alga *Laurencia nipponica*. Cryst. (hexane/diisopropyl ether).
Mp 126-127°. $[\alpha]_D$ +166 (c, 0.25 in $CHCl_3$).

Kurata, K. *et al., Chem. Lett.*, 1983, 557 (*cryst struct*)

Laureacetal E L-59

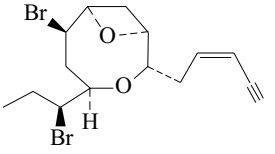
[85933-21-7]
As Laureacetal D, L-58 with
X = Cl

$C_{15}H_{20}BrClO_2$ 347.678
Constit. of red alga *Laurencia nipponica*. Cryst. (hexane/diisopropyl ether). Mp 119-120°. $[\alpha]_D$ +99.5 (c, 0.42 in $CHCl_3$).

Kurata, K. *et al., Chem. Lett.*, 1983, 557 (*cryst struct*)

Laureatin L-60

6-Bromo-4-(1-bromopropyl)-2-(2-penten-4-ynyl)-3,8-dioxabicyclo[5.1.1]nonane, 9CI. 10,13-Dibromo-6,12:7,9-diepoxypentadec-3-en-1-yne
[18762-30-6]



Absolute configuration

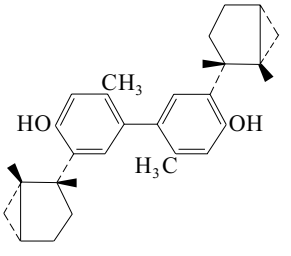
$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of *Laurencia nipponica*. Sol. MeOH, CCl_4, C_6H_6, $CHCl_3$; poorly sol. H_2O.
Mp 82-83°. $[\alpha]_D$ +96 (CCl_4). λ_{max} 223 (ϵ 12800) (EtOH) (Berdy).

(E)-Isomer: ***(3E)-Laureatin***
$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of *Laurencia nipponica*. Cryst. (MeOH).
Mp 77-78°. $[\alpha]_D^{18}$ +36.6 (c, 0.95 in $CHCl_3$).

Irie, T. *et al., Tetrahedron*, 1970, **26**, 851-870 (*isol, ir, uv, pmr, ms, struct*)
Kurosawa, E. *et al., Tet. Lett.*, 1973, 3875 (*cryst struct*)
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 3791 (*isol*)
Fukuzawa, A. *et al., Tet. Lett.*, 1992, **33**, 2017 (*synth*)

Laurebiphenyl L-61

[97649-04-2]

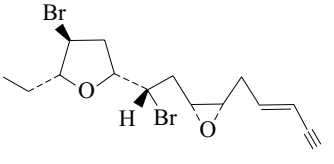


$C_{30}H_{38}O_2$ 430.629
Constit. of *Laurencia nidifica*. Cryst. (C_6H_6/hexane).
Mp 232-232.5°. $[\alpha]_D^{25}$ +15.2 (c, 0.092 in $CHCl_3$).

Shizuri, Y. *et al., Phytochemistry*, 1985, **24**, 1385

Laureepoxide L-62

Laurepoxide
[73328-63-9]

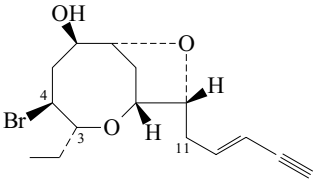


$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D$ +25 (c, 1.0 in $CHCl_3$).

Fukuzawa, A. *et al., Tet. Lett.*, 1980, 1471

Laurefucin L-63

4-Bromo-3,9:7,10-diepoxy-12-pentadecen-14-yn-6-ol
[36431-73-9]



$C_{15}H_{21}BrO_3$ 329.233

Revised struct. Constit. of *Laurencia nipponica*.
Mp 107-108°. $[\alpha]_D$ -80. λ_{max} 225 (ϵ 17900); 232 (sh) (ϵ 14100) (MeOH) (Derep).

Ac: ***Acetyllaurefucin***
$C_{17}H_{23}BrO_4$ 371.27
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D$ -126.5. λ_{max} 225 (ϵ 17900); 232 (sh) (ϵ 14100) (MeOH) (Derep).

Debromo, 3,4-didehydro: 3,9:7,10-Diepoxy-3,12-pentadecadien-14-yn-6-ol. ***Dehydrobromolaurefucin***
[157659-24-0]
$C_{15}H_{20}O_3$ 248.321
Constit. of *Laurencia* sp. cf. *Laurencia gracilis*. Oil. $[\alpha]_D^{25}$ -26.3 (c, 0.7 in $CHCl_3$).

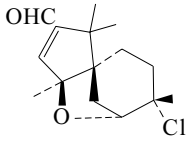
Debromo, 3,4-didehydro, 11-hydroxy: 6,9:7,13-Diepoxy-3,11-pentadecadien 1-yne-5,10-diol. ***5-Hydroxydehydrobromolaurefucin***
[157580-67-1]
$C_{15}H_{20}O_4$ 264.321
Constit. of *Laurencia* sp. cf. *Laurencia gracilis*. Oil. $[\alpha]_D^{25}$ -22 (c, 0.5 in $CHCl_3$).

6,7,9,10-Tetraepimer, 10-Me ether: ***Isolaurefucin methyl ether***
[150415-51-3]
$C_{16}H_{23}BrO_3$ 343.26
Isol. from the red alga *Dasyphila plumariodes*. Mobile yellow oil. $[\alpha]_D$ +8 (c, 0.3 in $CHCl_3$).

Furusaki, A. *et al., Tet. Lett.*, 1973, 4579 (*struct*)
de Nys, R. *et al., Aust. J. Chem.*, 1993, **46**, 1073 (*Isolaurefucin*)
Koenig, G.M. *et al., J. Nat. Prod.*, 1994, **57**, 477 (*derivs*)

Laurencial L-64

[86330-91-8]

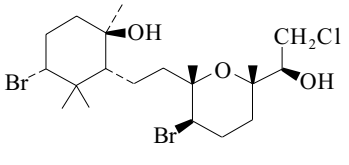


$C_{15}H_{21}ClO_2$ 268.782
Constit. of red alga *Laurencia nipponica*. Cryst. (hexane/diisopropyl ether).
Mp 124-126°. $[\alpha]_D$ +11.2 (c, 0.25 in $CHCl_3$).

Kurata, K. *et al., Chem. Lett.*, 1983, 299 (*isol, cryst struct*)
Miyasita, K. *et al., Tetrahedron*, 1998, **54**, 1395-1406 (*synth*)

Laurencianol L-65

[84323-26-2]



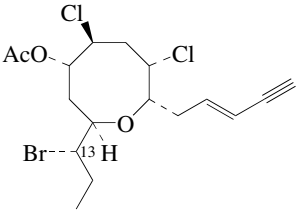
Absolute configuration

$C_{20}H_{35}Br_2ClO_3$ 518.755
Constit. of marine alga *Laurencia obtusa*. Antibacterial agent.
Cryst. (C_6H_6/hexane). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O, hexane.
Mp 114-116°.

Caccamese, S. *et al., Tet. Lett.*, 1982, **23**, 3415 (*isol, cryst struct*)

Laurencienyne L-66

2-(1-Bromopropyl)-5,7-dichloro-8-(2-penten-4-ynyl)-4-oxocanol acetate, 9CI. 10-Acetoxy-13-bromo-7,9-dichloro-6,12-epoxy-3-pentadecen-1-yne
[75179-72-5]



$C_{17}H_{23}BrCl_2O_3$ 426.176
Constit. of *Laurencia obtusa*. Cytotoxic agent. Toxic to brine shrimp larvae. Cryst. (C_6H_6/hexane).
Mp 119-120°. $[\alpha]_D^{24}$ +50.3 (c, 1.1 in $CHCl_3$). λ_{max} 225 (ϵ 15000) (MeOH) (Berdy).

Z-Isomer: ***Laurencienyne B***
[229623-92-1]
$C_{17}H_{23}BrCl_2O_3$ 426.176
Isol. from *Laurencia obtusa*. Oil. $[\alpha]_D^{20}$ +16.2 (CH_2Cl_2). λ_{max} 224 (ϵ 11302) (hexane).

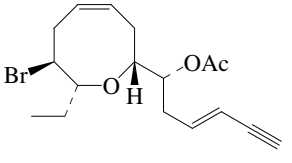
13-Epimer: ***13-Epilaurencienyne***
$C_{17}H_{23}BrCl_2O_3$ 426.176
Isol. from *Laurencia obtusa*. Toxic on brine shrimp larvae. Cytotoxic.

13-Epimer, 3Z-isomer: ***13-Epilaurencienyne B***
$C_{17}H_{23}BrCl_2O_3$ 426.176
Isol. from *Laurencia obtusa*. Oil. $[\alpha]_D^{20}$ +37.5 (c, 0.11 in $CHCl_3$). λ_{max} 225 (log ϵ 4.01) (hexane).

Caccamese, S. *et al., Tet. Lett.*, 1980, 2299 (*cryst struct, abs config*)
Imre, S. *et al., Pharmazie*, 1997, **52**, 883-885 (*13-Epilaurencienyne, activity*)
Mihopoulos, N. *et al., Nat. Prod. Lett.*, 1999, **13**, 151-156 (*Laurencienyne B*)
Iliopoulou, D. *et al., Phytochemistry*, 2002, **59**, 111-116 (*3Z-13-Epilaurencienyne*)

Laurencin L-67

7-Bromo-8-ethyl-3,6,7,8-tetrahydro-α-(2-penten-4-ynyl)-2H-oxocin-2-methanol acetate, 8CI. 6-Acetoxy-12-bromo-7,13-epoxy-3,9-pentadecadien-1-yne
[3442-58-8]



(+)-*form*

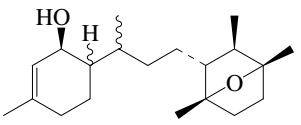
$C_{17}H_{23}BrO_3$ 355.271
Constit. of *Laurencia glandulifera*. Sol. MeOH, CCl_4, C_6H_6, $CHCl_3$; poorly sol. H_2O.
Mp 73-74°. $[\alpha]_D^{23}$ +70.2 (c, 1.0 in $CHCl_3$). λ_{max} 224 (ϵ 16400); 232 (sh) (ϵ 11000) (MeOH) (Derep).

O-*De-Ac:* ***Deacetyllaurencin***
[3352-02-1]
$C_{15}H_{21}BrO_2$ 313.234
Constit. of *Laurencia* sp. Oil. $[\alpha]_D^{17}$ +46.1 (c, 1.1 in $CHCl_3$).

Irie, T. *et al., Tetrahedron*, 1968, **24**, 4193 (*isol, pmr, ms*)
Cameron, A.F. *et al., J.C.S.(B)*, 1969, 559 (*cryst struct*)
Murai, A. *et al., Tet. Lett.*, 1977, 2507 (*synth*)
Tsushima, K. *et al., Tet. Lett.*, 1992, **33**, 4345 (*synth*)

Robinson, R.A. *et al., J.A.C.S.*, 1993, **115**, 10400; 1996, **118**, 6806 (*synth*)
Koenig, G.M. *et al., J. Nat. Prod.*, 1994, **57**, 477 (*de-Ac*)
Bratz, M. *et al., J.A.C.S.*, 1995, **117**, 5958 (*synth*)
Burton, J.W. *et al., J.A.C.S.*, 1997, **119**, 7483-7498 (*synth*)
Krueger, J. *et al., J.A.C.S.*, 1997, **119**, 7499-7504 (*synth*)
Crimmins, M.T. *et al., Org. Lett.*, 1999, **1**, 2029-2032 (*synth*)
Baek, S. *et al., Org. Lett.*, 2005, **7**, 75-77 (*synth*)
Fujiwara, K. *et al., Tet. Lett.*, 2005, **46**, 6819-6822 (*synth*)

Laurenditerpenol L-68

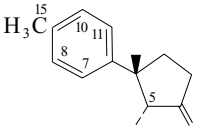


$C_{20}H_{34}O_2$ 306.487
Constit. of *Laurencia intricata*. Oil. $[\alpha]_D^{26}$ -158.8 (c, 0.34 in $CHCl_3$). λ_{max} 206 (log ϵ 3.39); 230 (log ϵ 2.37) (MeOH).

Mohammed, K.A. *et al., J. Nat. Prod.*, 2004, **67**, 2002-2007 (*isol, pmr, cmr*)

Laurene L-69

1,2-Dimethyl-3-methylene-1-(4-methylphenyl)cyclopentane
[18452-41-0]



$C_{15}H_{20}$ 200.323
Constit. of *Laurencia glandulifera*. Oil. Bp_{21} 131-133°. $[\alpha]_D^{23}$ +48.7 (EtOH).

7,8-Dihydro: ***Dihydrolaurene***
[62311-77-7]
$C_{15}H_{22}$ 202.339
Constit. of *Laurencia filiformis*. Pale yellow oil.

8,11-Dihydro: ***Isodihydrolaurene***
[82486-70-2]
$C_{15}H_{22}$ 202.339
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D$ +33.5 (c, 1.24 in $CHCl_3$).

7-Hydroxy: ***7-Hydroxylaurene***
[63181-28-2]
$C_{15}H_{20}O$ 216.322
Isol. from *Laurencia subopposita*. Shows antibiotic props. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{20}$ +45 (c, 2.5 in $CHCl_3$).

7-Hydroxy, 10-bromo: ***Allolaurinterol***
[62311-74-4]
$C_{15}H_{19}BrO$ 295.218
Constit. of *Laurencia filiformis* and *Laurencia subopposita*. Shows antimycobacterial activity. Pale yellow viscous oil. $[\alpha]_D$ +22 (c, 1.7 in $CHCl_3$). λ_{max} 240 (ϵ 30000) (EtOH) (Derep).

7-Acetoxy, 10-bromo: ***Allolaurinterol acetate***
[62573-44-8]
$C_{17}H_{21}BrO_2$ 337.256
Isol. from *Aplysia dactylomela*. Cytotoxic against P388 cells. Glass. $[\alpha]_D^{20}$ +47 (c, 0.07 in MeOH).

7-Hydroxy, 10-bromo, 11-iodo: ***10-Bromo-7-hydroxy-11-iodolaurene***
[72008-57-2]
$C_{15}H_{18}BrIO$ 421.115
Constit. of *Laurencia nana*. Cryst.
Mp 147-153° dec. $[\alpha]_D$ +225 (c, 0.24 in $CHCl_3$).

15-Hydroxy: ***Laurenol***
[82486-71-3]
$C_{15}H_{20}O$ 216.322
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D$ +34.7 (c, 0.20 in $CHCl_3$).

15-Acetoxy: ***Laurenol acetate***
[82486-74-6]
$C_{17}H_{22}O_2$ 258.36
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D$ +23.6 (c, 0.42 in $CHCl_3$).

15-Hydroxy, 8,11-dihydro: ***Isodihydrolaurenol***
[82486-69-9]
$C_{15}H_{22}O$ 218.338
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D$ +40 (c, 1.52 in $CHCl_3$).

15-Acetoxy, 8,11-dihydro: O-*Acetylisodihydrolaurenol*
[82486-73-5]
$C_{17}H_{24}O_2$ 260.375
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D$ +40 (c, 0.21 in $CHCl_3$).

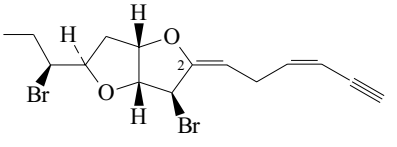
15-Oxo: ***Laurenal***
[82486-72-4]
$C_{15}H_{18}O$ 214.307
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D$ +33.2 (c, 0.23 in $CHCl_3$).

5-Epimer: ***Epilaurene***
[18452-45-4]
$C_{15}H_{20}$ 200.323
From *Laurencia glandulifera* and *Laurencia nipponica*. Oil. $[\alpha]_D$ -31 (c, 2.1 in $CHCl_3$).

Irie, T. *et al., Tetrahedron*, 1969, **25**, 459-468 (*struct*)
McMurry, J.E. *et al., Tetrahedron*, 1974, **30**, 2027-2032 (*synth*)
Kazlauskas, R. *et al., Aust. J. Chem.*, 1976, **29**, 2533-2539 (*Allolaurinterol, Dihydrolaurene*)
Wratten, S.J. *et al., J.O.C.*, 1977, **42**, 3343-3349 (*7-Hydroxylaurene, Allolaurinterol*)
Posner, G.H. *et al., Tet. Lett.*, 1977, 3215-3218 (*synth*)
Izae, R.R. *et al., J.A.C.S.*, 1979, **101**, 6136-6137 (*10-Bromo-7-hydroxy-11-iodolaurene*)
Taber, D.F. *et al., Tet. Lett.*, 1980, 2779-2782 (*synth*)
Suzuki, T. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 1561-1563 (*Laurenol, Laurenol acetate, Laurenal, Isodihydrolaurene, O-Acetylisodihydrolaurenol*)
Schmitz, F.J. *et al., J.A.C.S.*, 1982, **104**, 6415 (*Allolaurinterol acetate*)
Gewali, M.B. *et al., J.O.C.*, 1982, **47**, 2792-2795 (*synth, Allolaurinterol*)
Kametani, T. *et al., J.C.S. Perkin 1*, 1988, 193-199 (*synth*)
Nemoto, H. *et al., J.C.S. Perkin 1*, 1993, 2329-2332 (*synth*)
Schwarz, J.B. *et al., J.O.C.*, 1995, **60**, 6511-6514 (*synth*)
Bailey, W.F. *et al., J.O.C.*, 1995, **60**, 7791-7795 (*synth*)
Kulkarni, M.G. *et al., J.C.S. Perkin 1*, 1997, 3127-3128 (*synth*)
Konig, G.M. *et al., Planta Med.*, 1997, **63**, 186-187 (*Allolaurinterol, cmr*)
Avila-Zárraga, J.G. *et al., Chem. Lett.*, 2000, 512-513 (*synth*)
Koenig, G.M. *et al., Planta Med.*, 2000, 337-342 (*activity*)
Kojima, S. *et al., Tet. Lett.*, 2000, **41**, 4409-4413 (*synth*)
Oh, C.H. *et al., Tet. Lett.*, 2000, **41**, 8365-8370 (*synth*)
Appleton, D.R. *et al., Tetrahedron*, 2001, **57**, 10181-10189 (*Allolaurinterol, acetate, isol, pmr, cmr*)

Laurenenyne A L-70

3-Bromo-5-(1-bromopropyl)-2-(3-hexen-5-ynylidene)hexahydrofuro[3,2-b]furan, 9CI. 8,13-Dibromo-7,10:9,12-diepoxy-3,6-pentadecadien-1-yne
[149998-02-7]



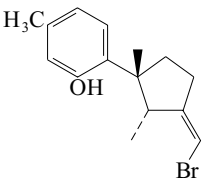
$C_{15}H_{18}Br_2O_2$ 390.114
Acetogenin. Constit. of the red alga *Laurencia* sp. Oil. $[\alpha]_D^{20}$ -151 (estimated). Obt. as an inseparable mixt. with Laurenenyne B.

2Z-Isomer: ***Laurenenyne B***
[150133-26-9]
$C_{15}H_{18}Br_2O_2$ 390.114
Constit. of *Laurencia* sp. Oil. $[\alpha]_D^{20}$ -168 (estimated).

Suzuki, M. *et al., Tetrahedron*, 1993, **49**, 2033 (*isol, pmr, cmr*)

Laurenisol L-71

[23526-39-8]



$C_{15}H_{19}BrO$ 295.218
Constit. of *Laurencia nipponica*. Unstable oil. $[\alpha]_D$ +85.9 ($CHCl_3$). λ_{max} 278 (ϵ 2605); 285 (ϵ 2600) (EtOH) (Derep).

Ac: Laurenisol acetate
[93236-40-9]
$C_{17}H_{21}BrO_2$ 337.256
Constit. of *Aplysia dactyomela*. Cryst.
Mp 102.5-103°. $[\alpha]_D$ +85.1 ($CHCl_3$).

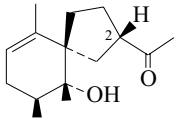
10-Bromo: ***10-Bromolaurenisol***
[72782-83-3]
$C_{15}H_{18}Br_2O$ 374.115
Constit. of *Laurencia glandulifera*. Oil. $[\alpha]_D^{22}$ +74 (c, 0.6 in $CHCl_3$).

E-*Isomer:* ***Isolaurenisol***†
[157659-25-1]
$C_{15}H_{19}BrO$ 295.218
Constit. of a *Laurencia* sp. Oil. $[\alpha]_D^{23}$ +48.1 (c, 0.42 in $CHCl_3$). See also Isolaurenisol, I-191. λ_{max} 275 (ϵ 2560); 281 (ϵ 2420) (EtOH) (Derep).

Irie, T. *et al., Tet. Lett.*, 1969, 1343-1346 (*isol, pmr, uv*)
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 3349-3351 (*10-Bromolaurenisol*)
Capon, R.J. *et al., J. Nat. Prod.*, 1988, **51**, 1302-1304 (*10-Bromolaurenisol*)
Rovirosa, J. *et al., Bol. Soc. Chil. Quim.*, 1991, **36**, 152 (*Ac*)
König, G. *et al., J. Nat. Prod.*, 1994, **57**, 477-485 (*Isolaurenisol*)

Laurenone A L-72

[93552-60-4]

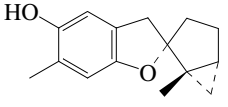


$C_{15}H_{24}O_2$ 236.353
Constit. of red alga *Laurencia nipponica*. Oil. $[\alpha]_D$ +152 ($CHCl_3$).

2-Epimer: ***Laurenone B***
[93603-63-5]
$C_{15}H_{24}O_2$ 236.353
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D$ +58.2 ($CHCl_3$).
Fukuzawa, A. *et al., Chem. Lett.*, 1986, 1349 (*cryst struct*)

Laurentristich-4-ol L-73

[861394-32-3]

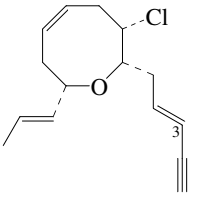


$C_{15}H_{18}O_2$ 230.306
Constit. of *Laurencia tristicha*. Gum. $[\alpha]_D^{20}$ -13.7 (c, 0.005 in MeOH).

Sun, J. *et al., J. Nat. Prod.*, 2005, **68**, 915-919 (*Laurencia tristicha constit*)

Laurenyne L-74

3-Chloro-3,4,7,8-tetrahydro-2-(2-penten-4-ynyl)-8-(1-propenyl)-2H-oxocin, 9CI. 7-Chloro-6,12-epoxy-3,9,13-pentadecatrien-1-yne
[77182-65-1]



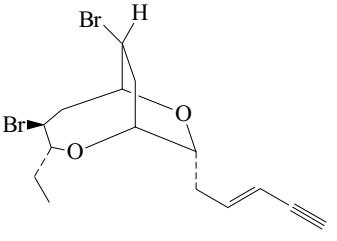
$C_{15}H_{19}ClO$ 250.767
Constit. of *Laurencia obtusa*. Cryst. (petrol).
Mp 78-80°. $[\alpha]_D^{17}$ +22.64 (c, 2.35 in $CHCl_3$).

3Z-Isomer:
$C_{15}H_{19}ClO$ 250.767
Constit. of *Laurencia yonaguniensis*. Needles.
Mp 46-48°. $[\alpha]_D^{28}$ +30.4 (c, 0.63 in $CHCl_3$).

Falshaw, C.P. *et al., Tet. Lett.*, 1980, 4951-4954 (*cryst struct, abs config*)
Takahashi, Y. *et al., J. Nat. Prod.*, 2002, **65**, 395-398 (*Z-isomer*)
Boeckman, R.K. *et al., Org. Lett.*, 2002, **4**, 3891-3894 (*synth*)

Laureoxanyne L-75

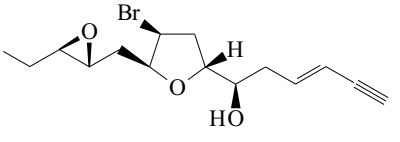
[125428-09-3]



$C_{15}H_{20}Br_2O_2$ 392.13
Metab. of *Laurencia nipponica*. Oil. $[\alpha]_D^{24}$ +20.9 (c, 0.31 in $CHCl_3$).

Fukuzawa, A. *et al., Tet. Lett.*, 1990, **31**, 4895 (*isol, struct*)

Laureoxolane L-76

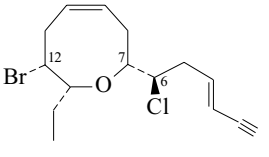


$C_{15}H_{21}BrO_3$ 329.233
Metab. of *Laurencia nipponica*. Unstable oil. $[\alpha]_D^{24}$ +21.9 (c, 0.32 in $CHCl_3$). λ_{max} 224 (ϵ 8600); 230 (sh) (ϵ 7700) (EtOH) (Derep).

Fukuzawa, A. *et al., Tet. Lett.*, 1989, **30**, 3665

Laurepinnacin L-77

[81176-29-6]



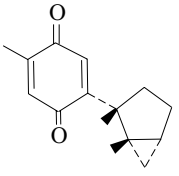
$C_{15}H_{20}BrClO$ 331.679
Constit. of *Laurencia pinnata*. Has insecticidal activity. Oil. Sol. MeOH, Et_2O. $[\alpha]_D$ -35.3 ($CHCl_3$).

12-Epimer, 3Z-isomer: ***Intricenyne***
[68252-61-9]
Isol. from *Laurencia intricata*.
Oil. $[\alpha]_D^{25}$ +60 (c, 0.5 in $CHCl_3$).

White, R.H. *et al., Phytochemistry*, 1978, **17**, 939 (*Intricenyne*)
Fukuzawa, A. *et al., Tet. Lett.*, 1981, **22**, 4081
Blunt, J.W. *et al., Aust. J. Chem.*, 1984, **37**, 1545 (*Intricenyne*)
Kotsuki, H. *et al., J.O.C.*, 1989, **54**, 5153 (*abs config*)

Laurequinone L-78

[94418-42-5]

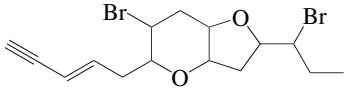


$C_{15}H_{18}O_2$ 230.306
Constit. of *Laurencia nidifica*. Pale-yellow oil. $[\alpha]_D^{23}$ -53.5 (c, 0.91 in $CHCl_3$).

Shizuri, Y. *et al., Phytochemistry*, 1984, **23**, 2672
Takahashi, H. *et al., Chem. Lett.*, 1998, 485-486 (*synth*)

Laurobtusin L-79

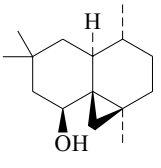
6-Bromo-2-(1-bromopropyl)hexahydro-5-(2-penten-4-ynyl)-2H-furo[3,2-b]pyran, 9CI. 7,13-Dibromo-6,10;9,12-diepoxy-3-pentadecen-1-yne
[114746-98-4]



$C_{15}H_{20}Br_2O_2$ 392.13
Constit. of *Laurencia obtusa*.

Imre, S. *et al., CA*, 1988, **109**, 146573e (*isol, struct*)

Laurobtusol L-80

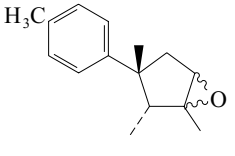


$C_{15}H_{26}O$ 222.37
Constit. of *Laurencia obtusa*. Amorph. powder.
Mp 121-122°. $[\alpha]_D^{25}$ +28.7 (c, 0.9 in EtOH). The proposed struct. and several stereoisomers have been synthesised. None of the synthetic isomers is identical to the natural product.

Caccamese, S. *et al., Tetrahedron*, 1991, **47**, 10101 (*isol, pmr, cmr*)
Blanchfield, J.T. *et al., Aust. J. Chem.*, 2004, **57**, 673-676 (*synth*)

Laurol L-81

[131815-25-3]



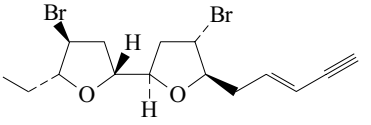
$C_{15}H_{20}O$ 216.322

Constit. of *Laurencia pinnatifida*. Amorph. powder.

Ahmad, V.U. *et al., Sci. Pharm.*, 1990, **58**, 299 (*isol, pmr*)

Lauroxane L-82

4,4′-Dibromo-5-ethyloctahydro-5′-(2-penten-4-ynyl)-2,2′-bifuran
[122261-54-5]



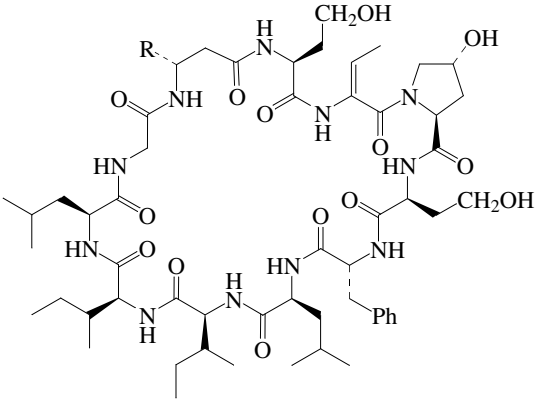
Relative configuration

$C_{15}H_{20}Br_2O_2$ 392.13
Metab. of alga *Laurencia majuscula*.

Kim, I.K. *et al., Tet. Lett.*, 1989, **30**, 1757 (*isol, pmr, cmr*)

Laxaphycin A L-83

[145680-51-9]



R = -$(CH_2)_4CH_3$

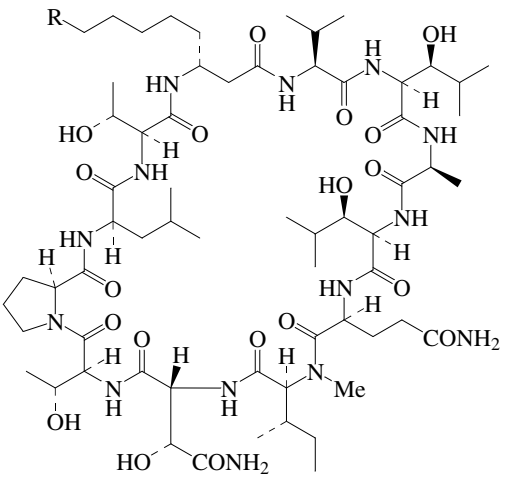
$C_{60}H_{97}N_{11}O_{14}$ 1196.492
Struct. and relationship with Hormothamnin A confirmed in 1997. Prod. by the blue-green alga *Anabaena laxa* and the marine cyanobacterium *Lyngbya majuscula*. Cytotoxic agent. Powder.

(Z)-Isomer: ***Hormothamnin A***
[120500-21-2]
Prod. by the marine cyanobacterium *Hormothamnion enteromorphoides*. Cytotoxic. Powder. λ_{max} 240 (ϵ 9500); 270 (ϵ 400) (no solvent reported).

Frankmoelle, W.P. *et al., J. Antibiot.*, 1992, **45**, 1451-1457; 1458-1466 (*isol, pmr, cmr, activity*)
Gerwick, W.H. *et al., Tetrahedron*, 1992, **48**, 2313-2324; 5755 (*Hormothamnin A*)
Bonnard, I. *et al., Lett. Pept. Sci.*, 1997, **4**, 289-292 (*struct*)

Laxaphycin B **L-84**

[144941-08-2]



R = CH_2CH_3

$C_{65}H_{114}N_{14}O_{19}$ 1395.698

Cyclic peptide antibiotic. Isol. from the blue-green alga *Anabaena laxa* and the marine cyanobacterium *Lyngbya majuscula*. Antifungal agent. Cytotoxic. Powder.

Frankmoelle, W.P. *et al., J. Antibiot.*, 1992, **45**, 1451-1457; 1458-1466 (*isol, pmr, cmr, activity*)
Bonnard, I. *et al., Lett. Pept. Sci.*, 1997, **4**, 289-292 (*stereochem*)

Laxaphycin C **L-85**

[144941-09-3]

$C_{65}H_{114}N_{14}O_{18}$ 1379.699

Cyclic peptide antibiotic. Struct. not determined. Prod. by the blue-green alga *Anabaena laxa*. Antifungal and cytotoxic agent. Powder.

Frankmolle, W.P. *et al., J. Antibiot.*, 1992, **45**, 1451-1457; 1458-1466

Leconotide, INN **L-86**

Omega-conopeptide MVIIA. *ω-Conopeptide MVIIA*. *ω-Conotoxin C VID*

[247207-64-3]

Cys-Lys-Ser-Lys-Gly-Ala-Lys-Cys-Ser-Lys-Leu-Met-Tyr-Asp-Cys-Cys-Ser-Gly-Ser-Cys-Ser-Gly-Thr-Val-Gly-Arg-Cys-NH_2

$C_{107}H_{179}N_{35}O_{36}S_7$ 2756.266

Reduced form shown. Isol. from venom of *Conus catus*. Analgesic.

[247208-09-9]

Pat. Coop. Treaty (WIPO), 1999, (*Univ. Queensland, Australia*)99 54 350; *CA*, **131**, 332121k (*synth, use*)
Lewis, R.J. *et al., J. Biol. Chem.*, 2000, **275**, 35335-35344 (*isol*)

***Aphrocallistes vastus* Lectin** **L-87**

Glycoprotein. Isol. from the hexactinellid sponge *Aphrocallistes vastus*. C-type lectin.

Gundacker, D. *et al., Glycobiology*, 2001, **11**, 21-29 (*isol*)

***Bryothamnion triquetrum* Lectin** **L-88**

Peptide containing 91 amino acid residues and 2 disulfide bonds. Isol. from the marine red alga *Bryothamnion triquetrum*. Lectin.

Calvete, J.J. *et al., Cell Mol. Life Sci.*, 2000, **57**, 343-350 (*isol*)

***Cancer antennarius* Lectin** **L-89**

Protein, MW *ca*. 36 kDa. Isol. from the haemolymph of the Californian coastal crab *Cancer antennarius*. *O*-Acetylsialic acid-specific lectin.

Ravindranath, M.H. *et al., J. Biol. Chem.*, 1985, **260**, 8850-8856 (*isol*)

***Cerianthus membranaceus* Lectin** **L-90**

Cerianthin lectin

Non-glycosylated protein, consisting of a single protein chain with no disulfide bonds. Isol. from the marine metazoan *Cerianthus membranaceus*. Lectin.

Koch, O.M. *et al., Immunobiology (Stuttgart)*, 1982, **163**, 53-62 (*isol*)

***Cucumaria japonica* Lectin** **L-91**

Protein consisting of 2 identical subunits. Isol. from the coelomic fluid of the holothurian *Cucumaria japonica*. Mannan-binding lectin.

Bulgakov, A.A. *et al., Biochemistry (Engl. Transl.)*, 2000, **65**, 933-939 (*isol*)

***Desmapsamma anchorata* Lectin** **L-92**

Glycoprotein with 2 subunits with MW *ca*. 18 and 36 kDa. Isol. from the marine sponge *Desmapsamma anchorata*. Mitogenic lectin for human lymphocytes.

Atta, A.M. *et al., Braz. J. Med. Biol. Res.*, 1990, **23**, 191-194 (*isol*)

***Geodia cydonium* Lectin I** **L-93**

Glycoprotein consisting of 3 subunits, two of which are linked by one disulfide bond. Isol. from the sponge *Geodia cydonium*. D-Galactose-specific lectin.

Muller, W.E. *et al., Eur. J. Biochem.*, 1983, **133**, 263-267 (*isol*)

***Gerardia savaglia* Lectin** **L-94**

Protein composed of 2 polypeptide chains which are not linked by disulfide bonds. Isol. from the coral *Gerardia savaglia*.

Kljajic, Z. *et al., Eur. J. Biochem.*, 1987, **169**, 97-104 (*isol*)

***Haliclona cratera* Lectin** **L-95**

Protein. Isol. from the Adriatic sponge *Haliclona cratera*. Lectin.

Pajic, I. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 2002, **132**, 213-221 (*isol*)

***Megabalanus rosa* Lectin** **L-96**

Multimeric glycoprotein with a subunit consisting of 173 amino acid residues and one carbohydrate chain; each subunit has 2 intrachain disulfide bonds and 1 interchain disulfide bond. Isol. from the acorn barnacle *Megabalanus rosa*. Lectin.

Muramoto, K. *et al., Biochim. Biophys. Acta*, 1990, **1039**, 42-51; 52-60 (*isol, struct*)

***Pellina semitubulosa* Lectin** **L-97**

Protein, prob. a hexamer of polypeptide chains covalently linked through disulfide bridges. Isol. from the sponge *Pellina semitubulosa*. Galactose- and arabinose-specific lectin.

Engel, M. *et al., Biochimie*, 1992, **74**, 527-537 (*isol*)

***Pinctada fucata* Lectin** **L-98**

Multimeric protein composed of identical subunits. Isol. from haemolymph of the pearl oyster *Pinctada fucata martensii*. Lectin.

Suzuki, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **92**, 455-462 (*isol*)

***Polyandrocarpa misakiensis* Lectin** **L-99**

Polypeptide containing 125 amino acid residues with 2 intrachain disulfide bonds. Isol. from the tunicate *Polyandrocarpa misakiensis*. Lectin with strong antibacterial activity.

Suzuki, T. *et al., J. Biol. Chem.*, 1990, **265**, 1274-1281 (*isol, struct*)

***Ptilota filicina* Lectin** **L-100**

Trimeric protein with apparently identical subunits. Isol. from the red marine alga *Ptilota filicina*. Galactose-specific lectin.

Sampaio, A.H. *et al., Phytochemistry*, 1998, **45**, 765-769 (*isol*)

Ruditapes philippinarum Lectin L-101

Protein consisting of 74-, 34- and 30-kDa subunits. Isol. from the Manila clam *Ruditapes philippinarum*. $Ca^{2\oplus}$-dependent lectin.

Bulgakov, A.A. *et al., Fish Shellfish Immunol.*, 2004, **16**, 487-499 (*isol*)

Scylla serrata Lectin L-102

Protein containing 2 subunits (30 kDa and 25 kDa). Isol. from haemolymph of the marine crab *Scylla serrata*. *N*- Glycolylneuraminic acid-specific lectin.

Mercy, P.D. *et al., Eur. J. Biochem.*, 1993, **215**, 697-704 (*isol*)

Sinularia lochmodes Lectin L-103

Glycoprotein consisting of 8 identical 15-kDa subunits. Isol. from the octocoral *Sinularia lochmodes*. D-Galactose-binding lectin.

Jimbo, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2000, **125**, 227-236 (*isol*)
Jimbo, M. *et al., Biochem. Biophys. Res. Commun.*, 2005, **330**, 157-162 (*struct*)

Tachypleus gigas Lectin L-104

Protein consisting of 13 identical 31-kDa subunits. Isol. from haemolymph of the horseshoe crab *Tachypleus gigas*. Sialic acid-specific lectin.

Tsuboi, I. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1237-1242 (*isol*)

Toxopneustes pileolus Lectin L-105

Sea urchin lectin I

Monomeric protein containing 294 amino acid residues. Isol. from the large globiferous pedicellariae of the sea urchin *Toxopneustes pileolus*. D-Galactose-binding lectin.

Nakagawa, H. *et al., Adv. Exp. Med. Biol.*, 1996, **391**, 213-223 (*isol, struct*)
Nakagawa, H. *et al., J. Nat. Toxins*, 1999, **8**, 297-308 (*isol*)

Tridacna derasa Lectin L-106

Protein consisting of 2 subunits (23 and 46 kDa) linked by disulfide bridges; the larger subunit may be a homodimer of the smaller one. Isol. from the haemolymph of the photosymbiotic marine bivalve *Tridacna derasa*. $Ca^{2\oplus}$-dependent lectin.

Odo, S. *et al., J. Biochem. (Tokyo)*, 1995, **117**, 965-973 (*isol*)

Lectin L6 L-107

Protein with 221 residues including 15 cysteines (7 disulfide bonds). Prod. by *Limulus* sp. Shows antimicrobial activity; lipopolysaccharide-binding.

Saito, T. *et al., J. Biol. Chem.*, 1995, **270**, 14493-14499 (*isol, struct*)

Aaptos Lectins L-108

Three polypeptides of MW 18-21000 containing no significant carbohydrate component. *Aaptos* Lectin I differs from II and III in amino acid composition; II and III are very similar. Isol. from sponge *Aaptos papillata*.

Bretting, H. *et al., Biochemistry*, 1976, **15**, 5029-5038 (*isol*)

Anadara granosa Lectins L-109

Anadarin P

Protein consisting of 2 subunits (MW 17000 and 16000) which are non-covalently bound. Isol. from the plasma of the marine blood clam *Anadara granosa*. Galactosyl-binding lectin.

***Anadara* Foot lectin**

Tetrameric protein. Isol. from the foot muscles of *Anadara granosa*. *N*-Glycolylneuraminic acid-specific lectin.

Dam, T.K. *et al., Mol. Cell. Biochem.*, 1992, **117**, 1-9 (*Anadarin P*)
Dam, T.K. *et al., Biochem. Biophys. Res. Commun.*, 1993, **196**, 422-429 (*Foot lectin*)

Axinella polypoides Lectins L-110

Four lectins: the structs. of Lectins I and II have been detd. Lectin I is a homodimer with each subunit comprising 144 amino acids and one intrachain disulfide bridge. Lectin II has 65% homology with Lectin I. Isol. from the sponge *Axinella polypoides*. D-Galactose-binding lectins.

Phillips, S.G. *et al., J. Immunol.*, 1976, **117**, 1226-1232 (*isol*)
Buck, F. *et al., Biochim. Biophys. Acta*, 1992, **1159**, 1-8 (*Lectin I, struct*)
Buck, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **121**, 153-160 (*Lectin II, struct*)

Bugula neritina Lectins L-111

Two proteins, BnA-I and BnA-II. Isol. from the marine bryozoan *Bugula neritina*. Lectins.

BnA-I

Hexameric homopolymer. Appears in animal extracts prepd. in the spring.

BnA-II

Monomer, MW 65-70 kDa. Expressed only during the summer and winter.

Colon-Urban, R. *et al., J. Exp. Zool.*, 1990, **254**, 138-143 (*isol*)

Cucumaria echinata Lectins L-112

Four proteins. Isol. from the marine invertebrate *Cucumaria echinata*. $Ca^{2\oplus}$-dependent lectins specific for *N*-acetylgalactosamine/galactose.

CEL-I

Protein consisting of 2 identical subunits with 140 amino acid residues. There are 2 intrachain and one interchain disulfide bonds.

CEL-II

Protein with estimated MW 35 kDa.

CEL-III

Protein containing 432 amino acid residues.

CEL-IV

Protein containing 157 amino acid residues with one interchain and 2 intrachain disulfide bonds.

Hatakeyama, T. *et al., J. Biochem. (Tokyo)*, 1994, **116**, 209-214 (*isol*)
Hatakeyama, T. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1314-1317 (*CEL-IV, struct*)
Nakano, M. *et al., Biochim. Biophys. Acta*, 1999, **1435**, 167-176 (*CEL-III, struct*)
Hatakeyama, T. *et al., Acta Cryst. D*, 2002, **58**, 143-144 (*CEL-I, cryst struct*)
Hatakeyama, T. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 157-163 (*CEL-I, struct*)
Uchida, T. *et al., J. Biol. Chem.*, 2004, **279**, 37133-37141 (*CEL-III, cryst struct*)

Didemnum candidum Lectins L-113

Two proteins (DCL-I and DCL-II) consisting of 4 equal-sized subunits. Isol. from plasma of the ascidian *Didemnum candidum*. Galactosyl-specific lectins.

Vasta, G.R. *et al., J. Biol. Chem.*, 1986, **261**, 9174-9181; 9182-9186 (*isol*)

Gracilaria Lectins L-114

***Gracilaria cornea* Lectin**

Monomeric glycoprotein. Isol. from the marine red alga *Gracilaria cornea*. Lectin.

***Gracilaria ornata* Lectin**

Monomeric glycoprotein. Isol. from the marine red alga *Gracilaria ornata*. Lectin.

Leite, Y.F. *et al., Biochim. Biophys. Acta*, 2005, **1724**, 137-145 (*Gracilaria ornata lectin*)
Lima, M.E. *et al., J. Agric. Food Chem.*, 2005, **53**, 6414-6419 (*Gracilaria cornea lectin*)

Halichondria okadai Lectins L-115

Two proteins, HOL-I and HOL-II. Isol. from the marine sponge *Halichondria okadai*.

HOL-I

Protein, possibly consisting of 4 identical subunits. *N*-Acetylsugar-specific lectin.

HOL-II

Monomeric protein. *N*-Acetyllactosamine-specific lectin.

Kawagishi, H. *et al., J. Biol. Chem.*, 1994, **269**, 1375-1379 (*isol*)

Hypnea Lectins L-116

Two lectins (HML and HCA) consisting of a mixt. of a 90-residue polypeptide containing 7 intrachain disulfide bonds and 2 disulfide-bonded subunits generated by cleavage between residues 50 and 51. Lectins. HML and HCA show 55% sequence identity (80% similarity).

***Hypnea musciformis* Lectin**

HML

Isol. from the red marine alga *Hypnea musciformis*.

***Hypnea cervicornis* Agglutinin**

HCA

Isol. from the red marine alga *Hypnea cervicornis*.

Nagano, C.S. *et al., Protein Pept. Lett.*, 2002, **9**, 159-166 (*HML, isol*)
Nagano, C.S. *et al., Acta Cryst. F*, 2005, **61**, 997-999 (*HML, cryst struct*)
Nagano, C.S. *et al., Protein Sci.*, 2005, **14**, 2167-2176 (*struct*)
Nascimento, K.S. *et al., Biochem. Cell Biol.*, 2006, **84**, 49-54 (*HCA, isol*)

Stichopus japonicus Lectins L-117

Two proteins SJL-I and SJL-II. Isol. from the sea cucumber *Stichopus japonicus*. $Ca^{2\oplus}$-dependent lectins. Two other lectins, SPL-I and SPL-II, have been isol. from the coelomic fluid of *S. japonicus*.

SJL-I

Protein consisting of 143 amino acid residues. Agglutinates rabbit and human erythrocytes.

SJL-II

Protein. Agglutinates rabbit but not human erythrocytes.

Hatakeyama, T. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1736-1739 (*isol*)
Himeshima, T. *et al., J. Biochem. (Tokyo)*, 1994, **115**, 689-692 (*SJL-I, struct*)
Matsui, T. *et al., J. Biochem. (Tokyo)*, 1994, **116**, 1127-1133 (*isol*)

Leech excitatory peptide L-118

LEP

[193148-49-1]

Ala-Lys-Cys-Glu-Gly-Glu-Trp-Ala-Ile-His-Ser-Cys-Leu-Gly-Gly-Asn-NH_2

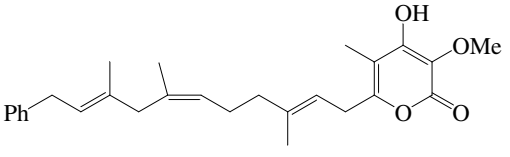
$C_{70}H_{106}N_{22}O_{22}S_2$ 1671.874

A member of the GGNG peptide family; struct. of reduced form shown. Isol. from the leech *Hirudo nipponia*. Myoactive.

Minakata, H. *et al., FEBS Lett.*, 1997, **410**, 437-442 (*isol*)

Lehualide A L-119

*4-Hydroxy-3-methoxy-5-methyl-6-(3,7,9-trimethyl-11-phenyl-2,6,9-undecatrienyl)-2*H*-pyran-2-one*



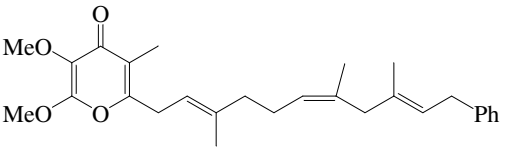
$C_{27}H_{34}O_4$ 422.563

Isol. from a *Plakortis* sp. Oil. λ_{max} 242 (log ϵ 3.77); 292 (log ϵ 3.63) (MeOH).

Sata, N. *et al., J. Nat. Prod.*, 2005, **68**, 1400-1403 (*isol, pmr, cmr*)

Lehualide B L-120

*2,3-Dimethoxy-5-methyl-6-(3,7,9-trimethyl-11-phenyl-2,6,9-undecatrienyl)-4*H*-pyran-4-one*



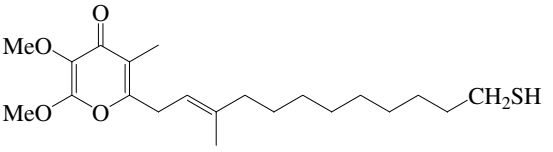
$C_{28}H_{36}O_4$ 436.59

Isol. from a *Plakortis* sp. Cytotoxic. Oil. λ_{max} 292 (log ϵ 3.92) (MeOH).

Sata, N. *et al., J. Nat. Prod.*, 2005, **68**, 1400-1403 (*isol, pmr, cmr*)

Lehualide D L-121

*2-(12-Mercapto-3-methyl-2-dodecenyl)-5,6-dimethoxy-3-methyl-4*H*-pyran-4-one*



$C_{21}H_{34}O_4S$ 382.563

Isol. from a *Plakortis* sp. Cytotoxic. Oil. λ_{max} 252 (log ϵ 3.92) (MeOH).

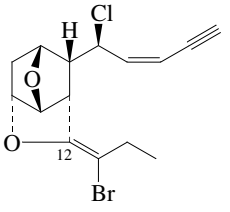
S-*Ac:* ***Lehualide C***

$C_{23}H_{36}O_5S$ 424.6

Isol. from a *Plakortis* sp. Oil. λ_{max} 240 (log ϵ 3.92) (MeOH).

Sata, N. *et al., J. Nat. Prod.*, 2005, **68**, 1400-1403 (*isol, pmr, cmr*)

Lembyne A L-122



Relative Configuration

$C_{15}H_{16}BrClO_2$ 343.647

Isol. from a *Laurencia* sp.

Mp 95-96°. $[\alpha]_D^{24}$ +197.6 (c, 0.7 in $CHCl_3$).

*12*E-*Isomer:* ***12E-Lembyne A***

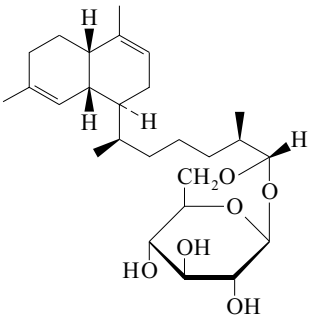
$C_{15}H_{16}BrClO_2$ 343.647

Isol. from *Laurencia mariannensis*. Oil. $[\alpha]_D^{24}$ +42 (c, 0.02 in $CHCl_3$).

Vairappan, C.S. *et al., Phytochemistry*, 2001, **58**, 291-297; 517-523

Lemnabourside L-123

[136825-98-4]



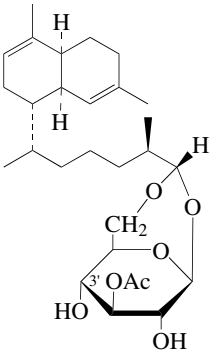
$C_{26}H_{42}O_6$ 450.614

Struct. revised in 1994. Constit. of *Lemnalia bournei*. Needles. Mp 90-90.5°. $[\alpha]_D^{22.5}$ +33.3 (c, 0.03 in EtOH).

Zhang, M. *et al., J. Nat. Prod.*, 1994, **57**, 155 (*isol, pmr, cmr*)

Lemnabourside B L-124

[214059-20-8]



$C_{28}H_{44}O_7$ 492.651

Constit. of *Lemnalia bournei*. Amorph. solid.

Mp 66.5-67.5°. $[\alpha]_D^{22.5}$ +10.3 (c, 0.029 in EtOH).

2′-De-Ac, 3′-Ac: ***Lemnabourside C***

[214059-21-9]

$C_{28}H_{44}O_7$ 492.651

Constit. of *Lemnalia bournei*. Amorph. solid.

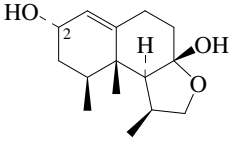
Mp 69-70.2°. $[\alpha]_D^{22.5}$ +25 (c, 0.02 in EtOH).

Zhang, M. *et al., J. Nat. Prod.*, 1998, **61**, 1300-1301 (*isol, pmr, cmr*)

Lemnacarnol L-125

1,4,5,7,8,9,9a,9b-Octahydro-1,9,9a-trimethylnaphtho[2,1-b]furan-3a,7(2H)-diol, 9CI. 7,12-Epoxy-1(10)-nardosinene-2,7-diol

[55890-26-1]



Absolute Configuration

$C_{15}H_{24}O_3$ 252.353

Constit. of *Lemnalia carnosa*. Cryst. (Et_2O).

Mp 160-163°.

2-Ac: ***Lemnacarnol acetate***

[143705-29-7]

$C_{17}H_{26}O_4$ 294.39

Constit. of *Parerythropodium fulvum*. Oil. $[\alpha]_D$ -20 (c, 0.05 in CH_2Cl_2).

2-Ketone: 7,12-Epoxy-7-hydroxy-1(10)-nardosinen-2-one. 2-Oxolemnacarnol (incorr.)

[63043-71-0]

$C_{15}H_{22}O_3$ 250.337

Constit. of soft coral *Parerythropodium fulvum*. Oil. $[\alpha]_D$ +9 (c, 0.26 in MeOH).

2-Deoxy: 7,12-Epoxy-1(10)-nardosinen-7-ol. ***2-Deoxylemnacarnol***

[63043-65-2]

$C_{15}H_{24}O_2$ 236.353

Constit. of *Lemnalia africana*, *Lemnalia laevis* and *Paralemnalia thyrsoides*. Cryst.

Mp 101-103°. $[\alpha]_D$ -165 (c, 0.1 in $CHCl_3$).

2-Deoxy, 12-oxo: 7-Hydroxy-1(10)-nardosinen-12,7-olide. ***2-Deoxy-12-oxolemnacarnol***

[63043-66-3]

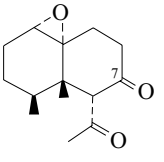
$C_{15}H_{22}O_3$ 250.337

Constit. of *Paralemnalia thyrsoides*. Cryst. $[\alpha]_D$ -20 ($CHCl_3$).

Tursch, B. *et al., Bull. Soc. Chim. Belg.*, 1975, **84**, 81-82 (*isol*)
Karlsson, R. *et al., Acta Cryst. B*, 1976, **32**, 1614-1616 (*abs config*)
Losman, D. *et al., Acta Cryst. B*, 1977, **33**, 1959-1962 (*cryst struct, 2-deoxy-12-oxo*)
Daloze, D. *et al., Bull. Soc. Chim. Belg.*, 1977, **86**, 47-54 (*2-Deoxylemnacarnol, 2-Deoxy-12-oxolemnacarnol*)
Bowden, B.F. *et al., Tet. Lett.*, 1980, **21**, 3105-3108 (*2-Ac, 2-ketone*)
Green, D. *et al., J. Nat. Prod.*, 1992, **55**, 1186-1196 (*Lemnacarnol acetate*)

Lemnaliadione L-126

1,10-Epoxy-13-nor-7,11-nardosinanedione



$C_{14}H_{20}O_3$ 236.31

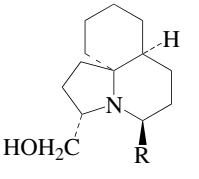
Constit. of *Paralemnalia thyrsoides* and *Lemnalia africana*. Cryst.

Mp 87-89°. $[\alpha]_D$ -298 (c, 1.0 in $CHCl_3$).

Izac, R.R. *et al., Tet. Lett.*, 1982, **23**, 817-820 (*isol, pmr, cmr*)

Lepadiformine A L-127

[155944-27-7]



Absolute Configuration

R = $-(CH_2)_5CH_3$

$C_{19}H_{35}NO$ 293.492

Struct. revised in 2002. Alkaloid from the ascidians *Clavelina lepadiformis* and *Clavelina moluccensis*. Exhibits moderate cytotoxicity. Oil. λ_{max} 206 (log ϵ 2.74); 310 (log ϵ 1.56) (EtOH).

Biard, J.F. *et al., Tet. Lett.*, 1994, **35**, 2691-2694 (*isol, pmr, cmr*)
Werner, K.M. *et al., J.O.C.*, 1999, **64**, 686-687 (*synth*)
Greshock, T.J. *et al., Org. Lett.*, 2001, **3**, 3511-3514 (*synth*)
Sun, P. *et al., J.O.C.*, 2002, **67**, 4337-4345 (*synth, abs config*)
Kibayashi, C. *et al., Bull. Chem. Soc. Jpn.*, 2003, **76**, 2059-2074 (*synth*)
Liu, J.L. *et al., Org. Lett.*, 2004, **6**, 3989-3992 (*synth*)
Abe, H. *et al., J.A.C.S.*, 2005, **127**, 1473-1480 (*synth*)
Sauviat, M.-P. *et al., J. Nat. Prod.*, 2006, **69**, 558-562 (*isol, pmr, cmr, activity*)
Lee, M. *et al., Org. Lett.*, 2006, **8**, 745-748 (*synth*)
Šchär, P. *et al., Org. Lett.*, 2006, **8**, 1569-1571 (*synth*)

Lepadiformine B L-128

As Lepadiformine A, L-127 with
R = -$(CH_2)_3CH_3$

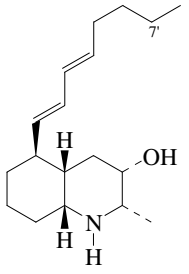
$C_{17}H_{31}NO$ 265.438
Alkaloid from *Clavelina moluccensis*. Pale yellow oil. $[\alpha]_D$ +3 (c, 1 in $CHCl_3$). λ_{max} 215 (log ϵ 2.98); 296 (log ϵ 2.55) (EtOH).

Deoxy: ***Lepadiformine C***
$C_{17}H_{31}N$ 249.439
Alkaloid from *Clavelina moluccensis*. Pale yellow oil. $[\alpha]_D$ +11 (c, 1 in $CHCl_3$). λ_{max} 205 (log ϵ 2.57); 275 (log ϵ 1.63) (EtOH).

Sauviat, M.-P. *et al., J. Nat. Prod.*, 2006, **69**, 558-562 (*isol, pmr, cmr, activity*)

Lepadin B L-129

[168434-12-6]



Absolute Configuration

$C_{18}H_{31}NO$ 277.449
Alkaloid from the flatworm *Prostheceraeus villatus* and its tunicate prey *Clavelina lepadiformis*. Exhibits significant *in vitro* cytotoxicity against human cancer cell lines. Oil. $[\alpha]_D$ -96 (MeOH). *Prostheceraeus villatus* appers to be an authors' misspelling of *P. vittatus*.

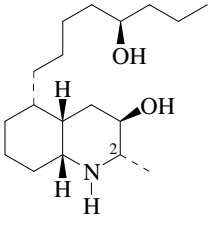
O-*(Hydroxyacetyl):* ***Lepadin A***
[141544-70-9]
$C_{20}H_{33}NO_3$ 335.486
Alkaloid from *Prostheceraeus villatus* and *Clavelina lepadiformis*. Exhibits significant *in vitro* cytotoxicity against human cancer cell lines. Oil. $[\alpha]_D$ -8.5 (c, 0.002 in $CHCl_3$).

7'-Oxo, O-*(hydroxyacetyl):* ***Lepadin C***
[168434-13-7]
$C_{20}H_{31}NO_4$ 349.469
Alkaloid from *Prostheceraeus villatus* and *Clavelina lepadiformis*. Oil. $[\alpha]_D$ -25 (MeOH).

Steffan, B. *et al., Tetrahedron*, 1991, **47**, 8729-8732 (*Lepadin A, isol, pmr, cmr, struct*)
Kubanek, J. *et al., Tet. Lett.*, 1995, **36**, 6189-6192 (*Lepadin B, Lepadin C*)
Toyooka, N. *et al., Tetrahedron*, 1999, **55**, 10673-10684 (*synth*)
Ozawa, T. *et al., J.O.C.*, 2001, **66**, 3338-3347 (*synth*)
Pu, X.-T. *et al., J.O.C.*, 2006, **71**, 6562-6572 (*synth, abs config*)

Lepadin D L-130

Decahydro-3-hydroxy-5-(5-hydroxyoctyl)-2-methylquinoline
[444914-17-4]
[444914-18-5 (quaternary salt)]



Absolute Configuration

$C_{18}H_{35}NO_2$ 297.48
Alkaloid from a *Didemnum* sp. Oil. $[\alpha]_D^{22}$ +3 (c, 0.2 in MeOH). $[\alpha]_D^{22}$ -14.4 (c, 0.27 in MeOH) (quaternary salt). Isol. also in oily cationic form (counterion not specified).

*3-*O*-(2*E*-Octenoyl):* ***Lepadin E***
[444914-21-0]
$C_{26}H_{47}NO_3$ 421.662
Alkaloid from a *Didemnum* sp. Oil. $[\alpha]_D^{22}$ -2 (c, 0.1 in MeOH). λ_{max} 263 (ϵ 2110) (MeOH).

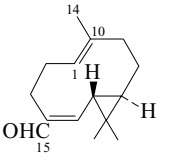
*3-*O*-(2*E*,4*E*-Octadienoyl):* ***Lepadin H***
[412328-25-7]
$C_{26}H_{45}NO_3$ 419.646
Alkaloid from *Aplidium tabascum*. Red gum. $[\alpha]_D$ +8.2 (c, 0.75 in CH_2Cl_2). Unstable. λ_{max} 261 (ϵ 16000) (MeOH).

*2-Epimer, 3-*O*-(2*E*-octenoyl):* ***Lepadin F***
[412328-23-5]
[444914-19-6]
$C_{26}H_{47}NO_3$ 421.662
Alkaloid from *Aplidium tabascum* and *Didemnum* sp. Antiplasmodial and antitrypanosomal agent. Red gum or clear oil. $[\alpha]_D$ +5.5 (c, 0.12 in CH_2Cl_2). $[\alpha]_D$ -1.5 (c, 0.1 in $CHCl_3$). Unstable. λ_{max} 262 (ϵ 3000) (MeOH). λ_{max} 261 (ϵ 16000) (MeOH).

*2-Epimer, 3-*O*-(2*E*,4*E*-octadienoyl):* ***Lepadin G***
[412328-24-6]
$C_{26}H_{45}NO_3$ 419.646
Alkaloid from the ascidian *Aplidium tabascum*. Red gum. $[\alpha]_D$ +12.5 (c, 0.31 in CH_2Cl_2). Unstable. λ_{max} 263 (ϵ 24000) (MeOH).

Wright, A.D. *et al., J. Med. Chem.*, 2002, **45**, 3067-3072 (*isol, pmr, cmr*)
Davis, R.A. *et al., J. Nat. Prod.*, 2002, **65**, 454-457 (*isol, pmr, cmr*)
Pu, X.-T. *et al., J.O.C.*, 2006, **71**, 6562-6572 (*synth, abs config*)

1(10),4-Lepidozadien-15-al L-131



Absolute configuration

$C_{15}H_{22}O$ 218.338

(1(10)E,4E,6S,7R)-form
Lepidozenal*. Lepidozienal*
[74033-93-5]
Constit. of *Lepidozia vitrea* and *Anthopleura pacifica*. Phytotoxic. Oil. $[\alpha]_D$ -169 (c, 1.11 in $CHCl_3$). λ_{max} 265 (ϵ 14000) (MeOH) (Berdy).

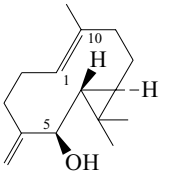
15-Alcohol: 1(10),4-Lepidozadien-15-ol. ***Lepidozenol****. Lepidozienol*
[74033-95-7]
$C_{15}H_{24}O$ 220.354
Constit. of *Anthopleura pacifica*. Oil. $[\alpha]_D$ -104 (c, 1.75 in $CHCl_3$). λ_{max} 211 (ϵ 6700) (MeOH) (Berdy).

Deoxo: 3,7,11,11-Tetramethylbicyclo[8.1.0]undeca-2,6-diene, 9CI. 1(10),4-Lepidozadiene. ***Lepidozene***
[133005-43-3]
$C_{15}H_{24}$ 204.355
Constit. of *Lepidozia vitrea* and the gorgonian *Lophogorgia ruberrima*. Oil. $[\alpha]_D^{25}$ +223 (c, 0.9 in $CHCl_3$).

Matsuo, A. *et al., J.C.S. Perkin 1*, 1984, 203-214 (*isol, pmr*)
Zheng, G.C. *et al., J.O.C.*, 1990, **55**, 3677-3679 (*Lepidozenal, isol, pmr, cmr, activity*)
Norte, M. *et al., Tetrahedron*, 1990, **46**, 8237-8242 (*Lepidozene*)

1(10),4(15)-Lepidozadien-5-ol L-132

[127062-42-4]



$C_{15}H_{24}O$ 220.354

(5β,1(10)E)-form

Constit. of *Anthopleura pacifica*. Ichthyotoxic agent. Oil. $[\alpha]_D$ -35 (c, 0.24 in EtOH).

1α,10α-Epoxide: ***1,10-Epoxy-4(15)-lepidozen-5-ol***
[126979-97-3]
$C_{15}H_{24}O_2$ 236.353
Constit. of *Anthopleura pacifica*. Oil. $[\alpha]_D$ -76 (c, 0.09 in $CHCl_3$).

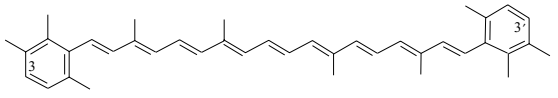
5-Hydroperoxide: ***5-Hydroperoxy-1(10),4(15)-lepidozadiene***
[126979-98-4]
$C_{15}H_{24}O_2$ 236.353
Constit. of *Anthopleura pacifica*. Oil. $[\alpha]_D$ -20.4 (c, 0.23 in EtOH).

5-Hydroperoxide, 1α,10α-epoxide: ***1,10-Epoxy-5-hydroperoxy-4(15)-lepidozene***
[126979-96-2]
$C_{15}H_{24}O_3$ 252.353
Constit. of *Anthopleura pacifica*. Oil. $[\alpha]_D$ -68.1 (c, 0.07 in EtOH).

Zheng, G.-C. *et al., J.O.C.*, 1990, **55**, 3677 (*isol, pmr, cmr*)

Leprotene L-133

Isorenieratene. ϕ,ϕ-Carotene. Streptoxanthin. Leprotin. Isorenieratin
[524-01-6]



$C_{40}H_{48}$ 528.819
Constit. of various mycobacteria, from the sponge *Reniera japonica*, the nudibranches *Anisodoris nobilis*, *Dendrodoris fulva*, *Doriopsilla albopunctata* and from *Phaeobium* spp. Purple needles (C_6H_6/petrol).
Mp 200-201°. λ_{max} 428; 452; 479 (petrol).

3-Hydroxy: ***3-Hydroxyleprotene****. 3-Hydroxyisorenieratene. ϕ,ϕ-Caroten-3-ol*
[23394-40-3]
$C_{40}H_{48}O$ 544.819
Isol. from *Streptomyces mediolani* and *Brevibacterium linens*.
Amorph. powder.
Mp 180-185° (178°).

3,3′-Dihydroxy: ***3,3′-Dihydroxyleprotene****. 3,3′-Dihydroxyisorenieratene. ϕ,ϕ-Carotene-3,3′-diol*
[23394-41-4]
$C_{40}H_{48}O_2$ 560.818
From *Streptomyces mediolani* and *Brevibacterium linens*. Amorph. red solid.
Mp 200° dec. (229°).

7Z-Isomer: ***Isorenieracistene***
[84773-18-2]
$C_{40}H_{48}$ 528.819
Constit. of *Tethya amamensis*.

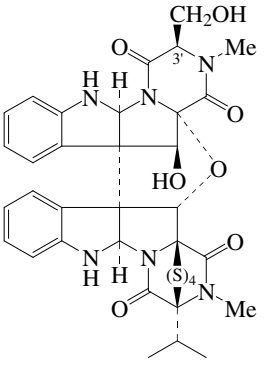
7Z,7′Z-Isomer: ***Isorenieradicistene***
[92934-56-0]
$C_{40}H_{48}$ 528.819
Constit. of *Suberites sericeus*.

7Z,9′Z-Isomer: [105118-23-8]
$C_{40}H_{48}$ 528.819
Constit. of *Polymastia granulosa*. Possibly artifact.

Goodwin, T.W. *et al., Biochem. J.*, 1956, **62**, 269-275 (*uv*)
Yamaguchi, M. *et al., Bull. Chem. Soc. Jpn.*, 1958, **31**, 51-55 (*struct*)
Cooper, R.D.G. *et al., J.C.S.*, 1963, 5637-5641 (*synth*)
Jensen, S.L. *et al., Acta Chem. Scand.*, 1964, **18**, 1562-1564; 1965, **19**, 1025-1030 (*isol*)
Arcamone, F. *et al., Experientia*, 1969, **25**, 241-242 (*3-hydroxy, 3,3′-dihydroxy, isol*)
Arcamone, F. *et al., Gazz. Chim. Ital.*, 1970, **100**, 581-590 (*3-Hydroxyleprotene, 3,3′-Dihydroxyleprotene*)
McBeth, J.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1972, **41**, 55-67 (*isol*)
Schaeflé, J. *et al., Tet. Lett.*, 1977, 3673-3676 (*isol, pmr, ms*)
Akiyama, S. *et al., Tet. Lett.*, 1979, 2813-2816 (*synth*)
Tanaka, Y. *et al., Nippon Suisan Gakkaishi*, 1982, **48**, 1651; *CA*, **98**, 86548t (*Isorenieracistene*)
Kohl, W. *et al., Phytochemistry*, 1983, **22**, 207-210 (*3,3′-dihydroxy, isol*)
Matsuno, T. *et al., Nippon Suisan Gakkaishi*, 1984, **50**, 1071; *CA*, **101**, 207839e (*Isorenieradicistene*)
Hertzberg, S. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 801-814 (*Polymastia granulosa constit*)
Valla, A.R. *et al., Helv. Chim. Acta*, 2003, **86**, 3314-3319 (*synth*)

Leptosin I L-134

[160472-96-8]



Relative Configuration

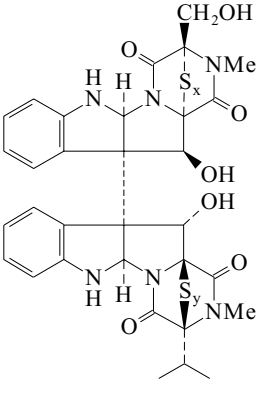
$C_{32}H_{32}N_6O_7S_4$ 740.905
Metab. from a strain of *Leptosphaeria* sp. originally isol. from the marine alga *Sargassum tortile*. Cytotoxic agent. Pale yellow powder. Sol. DMSO, $CHCl_3$, MeOH; poorly sol. H_2O, hexane. Mp 218-220°. $[\alpha]_D^{24}$ +212 (c, 0.13 in $CHCl_3$). λ_{max} 209 (log ϵ 4.45); 240 (log ϵ 3.91); 305 (log ϵ 3.45) (EtOH).

3′-Epimer: ***Leptosin J***
[160550-15-2]
$C_{32}H_{32}N_6O_7S_4$ 740.905
From *Leptosphaeria* sp. Cytotoxic agent. Pale yellow powder. Sol. DMSO, MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 215-216°. $[\alpha]_D^{24}$ +188 (c, 0.21 in $CHCl_3$). λ_{max} 209 (log ϵ 4.45); 240 (log ϵ 3.94); 298 (log ϵ 3.44) (EtOH).

Takahashi, C. *et al., J. Antibiot.*, 1994, **47**, 1242 (*isol, uv, ir, pmr, cmr, cd, struct*)

Leptosin A L-135

[159518-74-8]



Absolute configuration

x = 4, *y* = 2

$C_{32}H_{32}N_6O_7S_6$ 805.037
Metab. from a strain of *Leptosphaeria* sp. originally isol. from the marine alga *Sargassum tortile*. Exhibits potent cytotoxicity against P388 lymphocytic leukaemia cells and significant antitumour activity against Sarcoma 180 ascites. Pale yellow powder. Sol. MeOH, $CHCl_3$; poorly sol. hexane.

Mp 216-218°. $[\alpha]_D$ +237 (c, 0.49 in $CHCl_3$). λ_{max} 209 (ϵ 40700); 242 (ϵ 15500); 298 (ϵ 6750) (EtOH) (Berdy).

Takahashi, C. *et al., J.C.S. Perkin 1*, 1994, 1859 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)

Leptosin B L-136

[159518-75-9]
As Leptosin A, L-135 with
x = 3, *y* = 2
$C_{32}H_{32}N_6O_7S_5$ 772.971
Metab. from a strain of *Leptosphaeria* sp. Exhibits potent cytotoxicity against P388 lymphocytic leukaemia cells. Pale yellow powder. Sol. MeOH, $CHCl_3$; poorly sol. hexane.
Mp 210-213°. $[\alpha]_D$ +392 (c, 0.50 in $CHCl_3$). λ_{max} 208 (ϵ 28200); 244 (ϵ 10000); 299 (ϵ 4800) (EtOH) (Berdy).

Takahashi, C. *et al., J.C.S. Perkin 1*, 1994, 1859 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)

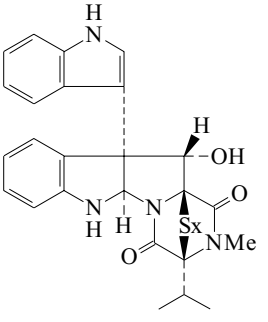
Leptosin C L-137

[159518-76-0]
As Leptosin A, L-135 with
x = 2, y = 2
$C_{32}H_{32}N_6O_7S_4$ 740.905
Metab. from a strain of *Leptosphaeria* sp. and a *Sesquicillium* sp. Exhibits potent cytotoxicity against P388 lymphocytic leukaemia cells and significant antitumour activity against Sarcoma 180 ascites. Pale yellow powder. Sol. MeOH, $CHCl_3$; poorly sol. hexane.
Mp 208-210°. $[\alpha]_D$ +237 (c, 0.36 in $CHCl_3$). λ_{max} 206 (ϵ 60400); 283 (ϵ 17000); 301 (ϵ 5150) (EtOH) (Berdy).

Takahashi, C. *et al., J.C.S. Perkin 1*, 1994, 1859 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)

Leptosin D L-138

[159518-77-1]



Absolute configuration

x = 2

$C_{25}H_{24}N_4O_3S_2$ 492.622
Metab. from the mycelium of a strain of *Leptosphaeria* sp. attached to the marine alga *Sargassum tortile*. Also from *Sesquicillium* sp. Shows potent cytotoxicity against P388 lymphocytic leukaemia cells. Pale yellow powder. Sol. MeOH, $CHCl_3$; poorly sol. hexane.
Mp 190-192°. $[\alpha]_D$ +436 (c, 0.51 in $CHCl_3$). λ_{max} 206 (ϵ 39800); 219 (ϵ 41600); 240 (ϵ 11450); 272 (ϵ 5900); 282 (ϵ 6750); 290 (ϵ 6750) (EtOH) (Berdy).

Takahashi, C. *et al., J.C.S. Perkin 1*, 1994, 1859 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)

Leptosin E L-139

[159518-78-2]
As Leptosin D, L-138 with
x = 3
$C_{25}H_{24}N_4O_3S_3$ 524.688
Metab. from a strain of *Leptosphaeria* sp. and by *Sesquicillium* sp. Exhibits potent cytotoxicity against P388 lymphocytic leukaemia cells. Pale yellow powder. Sol. MeOH, $CHCl_3$; poorly sol. hexane.
Mp 229-231°. $[\alpha]_D$ +563 (c, 0.32 in $CHCl_3$). λ_{max} 206 (ϵ 42600); 218 (ϵ 44700); 240 (ϵ 13150); 273 (ϵ 6700); 282 (ϵ 6920); 291 (ϵ 6490) (EtOH) (Berdy).

Takahashi, C. *et al., J.C.S. Perkin 1*, 1994, 1859 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)

Leptosin F L-140

[159518-79-3]
As Leptosin D, L-138 with
x = 4
$C_{25}H_{24}N_4O_3S_4$ 556.754
Metab. from a strain of *Leptosphaeria* sp. and *Sesquicillium* sp. Exhibits potent cytotoxicity against P388 lymphocytic leukaemia cells. Pale yellow powder. Sol. MeOH, $CHCl_3$; poorly sol. hexane.
Mp 219-221°. $[\alpha]_D$ +452 (c, 0.39 in $CHCl_3$). λ_{max} 206 (ϵ 45700); 216 (ϵ 49000); 240 (ϵ 15500); 272 (ϵ 7550); 281 (ϵ 7950); 290 (ϵ 7950) (EtOH) (Berdy).

Takahashi, C. *et al., J.C.S. Perkin 1*, 1994, 1859 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)

Leptosin G_1 L-141

[162232-33-9]
As Leptosin A, L-135 with
x = 3, y = 3
$C_{32}H_{32}N_6O_7S_6$ 805.037
Metab. from a strain of *Leptosphaeria* sp. and *Sargassum tortile*. Exhibits cytotoxicity against P388 lymphocytic leukaemia cells. Powder.
Mp 210-212°. $[\alpha]_D^{24}$ +558 (c, 0.45 in $CHCl_3$). λ_{max} 210 (ϵ 52480); 240 (ϵ 13800); 296 (ϵ 6166) (EtOH) (Berdy).

Takahashi, C. *et al., Phytochemistry*, 1995, **38**, 155 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)

Leptosin G_2 L-142

[159334-39-1]
As Leptosin A, L-135 with
x = 2, y = 3
$C_{32}H_{32}N_6O_7S_5$ 772.971
Metab. from a strain of *Leptosphaeria* sp.and *Sargassum tortile*. Exhibits cytotoxicity against P388 lymphocytic leukaemia cells. Pale yellow powder.
Mp 210-215°. $[\alpha]_D^{24}$ +303 (c, 0.58 in $CHCl_3$). λ_{max} 206 (ϵ 58000); 240 (ϵ 20417); 296 (ϵ 6310) (EtOH) (Berdy).

Takahashi, C. *et al., Phytochemistry*, 1995, **38**, 155 (*isol, uv, ir, pmr, ms, cd, struct*)

Leptosin G L-143

[159334-43-7]
As Leptosin A, L-135 with
x = 4, y = 3
$C_{32}H_{32}N_6O_7S_7$ 837.103
Metab. of a strain of *Leptosphaeria* sp. and *Sargassum tortile*. Exhibits cytotoxicity against P388 lymphocytic leukaemia cells. Pale yellow powder.
Mp 205-210°. $[\alpha]_D^{24}$ +481 (c, 0.40 in $CHCl_3$). λ_{max} 206 (ϵ 81283); 240 (ϵ 26300); 296 (ϵ 8130) (EtOH) (Berdy).

Takahashi, C. *et al., Phytochemistry*, 1995, **38**, 155 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)

Leptosin H L-144

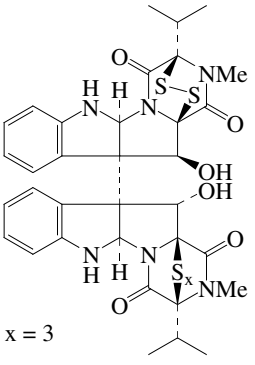
[159334-40-4]
As Leptosin A, L-135 with
x = 2, y = 4
$C_{32}H_{32}N_6O_7S_6$ 805.037
Metab. from a strain of *Leptosphaeria* sp. and *Sargassum tortile*. Exhibits cytotoxicity against P388 lymphocytic leukaemia cells.

Pale yellow powder.
Mp 214-215°. $[\alpha]_D^{24}$ +298 (c, 0.47 in $CHCl_3$). λ_{max} 207 (ϵ 64565); 240 (ϵ 23442); 302 (ϵ 7080) (EtOH) (Berdy).

Takahashi, C. *et al., Phytochemistry*, 1995, **38**, 155 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)

Leptosin K_1 L-145

[159334-36-8]



Absolute Configuration

$C_{34}H_{36}N_6O_6S_5$ 785.025
Metab. from a strain of *Leptosphaeria* sp. Exhibits potent cytotoxicity against P388 lymphocytic leukaemia cells. Pale yellow powder.
Mp 209-212°. $[\alpha]_D$ +88.9 (c, 0.32 in $CHCl_3$). λ_{max} 207 (ϵ 51286); 237 (ϵ 19500); 300 (ϵ 5495) (EtOH) (Berdy).

Takahashi, C. *et al., Tetrahedron*, 1995, **51**, 3483 (*isol, uv, ir, pmr, ms, cd, cryst struct*)

Leptosin K_2 L-146

[159334-37-9]
As Leptosin K_1, L-145 with
x = 4
$C_{34}H_{36}N_6O_6S_6$ 817.091
Metab. from a strain of *Leptosphaeria* sp. Exhibits potent cytotoxicity against P388 lymphocytic leukaemia cells. Pale yellow powder.
Mp 214-216°. $[\alpha]_D$ +482.8 (c, 0.44 in $CHCl_3$). λ_{max} 205 (ϵ 34950); 242 (ϵ 14125); 296 (ϵ 4365) (EtOH) (Berdy).

Takahashi, C. *et al., Tetrahedron*, 1995, **51**, 3483 (*isol, uv, ir, pmr, cmr, ms, cd, cryst struct*)

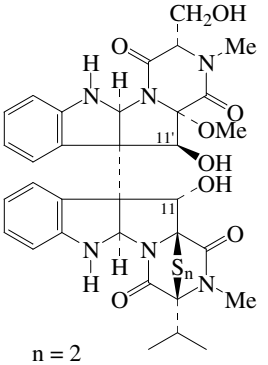
Leptosin K L-147

[159334-35-7]
As Leptosin K_1, L-145 with
x = 2
$C_{34}H_{36}N_6O_6S_4$ 752.959
Metab. from a strain of *Leptosphaeria* sp. OUPS-4 originally isolated from the marine alga *Sargassum tortile*. Exhibits potent cytotoxicity against P388 lymphocytic leukaemia cells. Prisms (EtOAc).
Mp 222-224°. $[\alpha]_D$ +76.7 (c, 0.37 in $CHCl_3$). λ_{max} 206 (ϵ 60256); 240 (ϵ 19050); 302 (ϵ 6025) (EtOH).

Takahashi, C. *et al., Tetrahedron*, 1995, **51**, 3483-3498 (*isol, uv, ir, pmr, cmr, ms, cd, cryst struct*)

Leptosin M_1 L-148

[406213-88-5]



Absolute Configuration

$C_{33}H_{36}N_6O_8S_2$ 708.815
Metab. of *Leptosphaeria* sp. OUPS-4. Pale yellow powder.
Mp 219-222°. $[\alpha]_D$ +140 (c, 0.18 in $CHCl_3$). λ_{max} 212 (log ϵ 4.73); 238 (log ϵ 4.3); 300 (log ϵ 3.83) (EtOH).

Yamada, T. *et al., Tetrahedron*, 2002, **58**, 479-487

Leptosin M L-149

[406213-87-4]
As Leptosin M_1, L-148 with
n = 4
$C_{33}H_{36}N_6O_8S_4$ 772.947
Metab. of *Leptosphaeria* sp. OUPS-4 isol. from the marine alga *Sargassum tortile*. Pale yellow powder.
Mp 223-226°. $[\alpha]_D$ +478 (c, 0.1 in $CHCl_3$). λ_{max} 206 (log ϵ 4.64); 243 (log ϵ 4.08); 304 (log ϵ 3.62) (EtOH).

11,11′-Diepimer: ***Leptosin N***
[406213-89-6]
$C_{33}H_{36}N_6O_8S_4$ 772.947
Metab. of *Leptosphaeria* sp. OUPS-4. Pale yellow powder.
Mp 226-228°. $[\alpha]_D$ +276 (c, 0.16 in $CHCl_3$). λ_{max} 212 (log ϵ 4.75); 240 (log ϵ 4.36); 302 (log ϵ 3.86) (EtOH).

Yamada, T. *et al., Tetrahedron*, 2002, **58**, 479-487 (*isol, uv, pmr, cmr, cd, struct*)

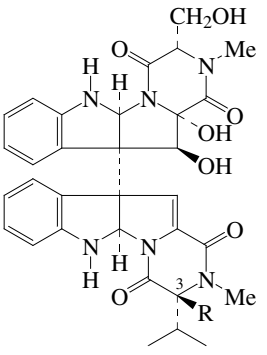
Leptosin N_1 L-150

[406213-90-9]
As Leptosin M, L-149 with
n = 3
$C_{33}H_{36}N_6O_8S_3$ 740.881
Metab. of *Leptosphaeria* sp. OUPS-4. Pale yellow powder.
Mp 227-229°. $[\alpha]_D$ +347 (c, 0.14 in $CHCl_3$). λ_{max} 212 (log ϵ 4.74); 240 (log ϵ 4.34); 302 (log ϵ 3.82) (EtOH).

Yamada, T. *et al., Tetrahedron*, 2002, **58**, 479-487

Leptosin O L-151

[721960-15-2]



R = -S-S-Me

$C_{33}H_{36}N_6O_7S_2$ 692.815
Metab. of *Leptosphaeria* sp. OUPS-N80 isol. from *Sargassum tortile*. Cytotoxic. Pale yellow powder.
Mp 220-222°. $[\alpha]_D$ -99 (c, 0.08 in $CHCl_3$). λ_{max} 211 (log ϵ 4.76); 238 (log ϵ 4.58); 265 (log ϵ 4.3); 298 (log ϵ 4.08) (EtOH).

3-Epimer: ***Leptosin P***
[721960-16-3]
$C_{33}H_{36}N_6O_7S_2$ 692.815
Metab. of *Leptosphaeria* sp. OUPS-N80 from *Sargassum tortile*. Cytotoxic. Pale yellow powder.
Mp 233-235°. $[\alpha]_D$ +35 (c, 0.17 in $CHCl_3$). λ_{max} 209 (log ϵ 4.49); 238 (log ϵ 4.3); 270 (log ϵ 3.99); 300 (log ϵ 3.78) (EtOH).

Yamada, T. *et al., Heterocycles*, 2004, **63**, 641-652 (*isol, cd, pmr, cmr, ms*)

Leptosin Q L-152

[721960-17-4]
As Leptosin O, L-151 with
R = -SMe
$C_{33}H_{36}N_6O_7S$ 660.749
Metab. of *Leptosphaeria* sp. OUPS-N80 isol. from *Sargassum tortile*. Pale yellow powder.
Mp 231-233°. $[\alpha]_D$ -92 (c, 0.07 in $CHCl_3$). λ_{max} 212 (log ϵ 4.76); 238 (log ϵ 4.32); 268 (log ϵ 4.02); 299 (log ϵ 3.75) (EtOH).

3-Epimer: ***Leptosin R***
[721960-18-5]
$C_{33}H_{36}N_6O_7S$ 660.749
Metab. of *Leptosphaeria* sp. OUPS-N80 isol. from *Sargassum tortile*. Pale yellow powder.
Mp 221-223°. $[\alpha]_D$ -24 (c, 0.1 in $CHCl_3$). λ_{max} 212 (log ϵ 4.95); 238 (log ϵ 4.72); 267 (log ϵ 4.35); 298 (log ϵ 4.14) (EtOH).

Yamada, T. *et al., Heterocycles*, 2004, **63**, 641-652 (*isol, pmr, cmr, ms*)

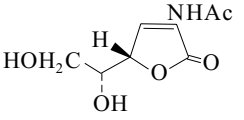
Leptosin S L-153

[721960-19-6]
As Leptosin O, L-151 with
R = NH_2
$C_{32}H_{35}N_7O_7$ 629.671
Metab. of *Leptosphaeria* sp. OUPS-N80 isol. from *Sargassum tortile*. Pale yellow powder.
Mp 231-233°. $[\alpha]_D$ -56 (c, 0.07 in $CHCl_3$). λ_{max} 212 (log ϵ 4.77); 238 (log ϵ 4.61); 270 (log ϵ 4.1); 300 (log ϵ 4.04) (EtOH).

Yamada, T. *et al., Heterocycles*, 2004, **63**, 641-652 (*isol, pmr, cmr, ms*)

Leptosphaerin L-154

2-(Acetylamino)-2,3-dideoxy-erythro-*hex-2-enonic acid γ-lactone, 9CI. 3-Acetamido-5-(1,2-dihydroxyethyl)-2(5*H*)-furanone*
[76022-72-5]

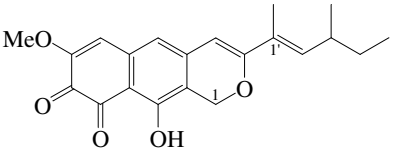


$C_8H_{11}NO_5$ 201.179
Isol. from *Leptosphaeria oraemaris*. Cryst.
Mp 189.5-190.5°. $[\alpha]_D$ +40 (c, 0.2 in H_2O). λ_{max} 246 (solvent not reported) (Derep). λ_{max} 246 (MeOH) (Berdy).

Ruzic-Toros, Z. *et al., Acta Cryst. B*, 1978, **34**, 854
Schiehser, G.A. *et al., Tet. Lett.*, 1986, **27**, 5587 (*isol, cryst struct*)
Pallenberg, A.J. *et al., Tet. Lett.*, 1986, **27**, 5591 (*synth*)
Rollin, P. *et al., Tet. Lett.*, 1987, **28**, 3813 (*synth*)
White, J.D. *et al., Tetrahedron*, 1989, **45**, 6631 (*synth, abs config*)
Pedersen, C. *et al., Carbohydr. Res.*, 1999, **315**, 192-197 (*synth*)

Leptosphaerodione L-155

*3-(1,3-Dimethyl-1-pentenyl)-10-hydroxy-7-methoxy-1*H*-naphtho[2,3-*c*]pyran-8,9-dione, 9CI. Obioninene*
[138039-33-5]



$C_{21}H_{22}O_5$ 354.402
Azaphilone antibiotic. Isol. from the marine-derived *Leptosphaeria oraemaris* and from *Stagonospora* spp. Phytotoxin.
Deep red solid. $[\alpha]_D^{20}$ -53.3 (c, 0.02 in MeOH).

1′ξ,2-Dihydro: ***Obionin A***
[125287-04-9]
$C_{21}H_{24}O_5$ 356.418
Metab. of the marine fungus *Leptosphaeria obiones*. Brown-red solid.
Mp 168-169°. $[\alpha]_D$ +28.5 (c, 0.01 in $CHCl_3$). λ_{max} 264 (ϵ 5400); 350 (ϵ 2090); 530 (ϵ 1600) (MeOH/NaOH) (Derep). λ_{max} 280 (ϵ 4640); 464 (ϵ 2090) (MeOH) (Derep).

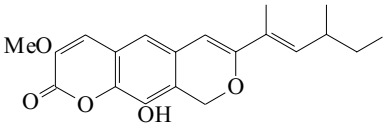
1-Methoxy: ***Laccaridione A***
$C_{22}H_{24}O_6$ 384.428
Prod. by *Laccaria amethystea*. Protease inhibitor. Deep red solid.
Mp 164-165°. λ_{max} 239 (ϵ 19300); 298 (ϵ 17000); 481 (ϵ 12800) (MeOH).

1-Ethoxy: ***Laccaridione B***
$C_{23}H_{26}O_6$ 398.455
Prod. by *Laccaria amethystea*. Protease inhibitor. Deep red solid.
Mp 178-179°. λ_{max} 239 (ϵ 19000); 299 (ϵ 16500); 480 (ϵ 12100) (MeOH).

Poch, G.K. *et al., Tet. Lett.*, 1989, **30**, 3483 (*Obionin A*)
Guerriero, A. *et al., Helv. Chim. Acta*, 1991, **74**, 1445-1450 (*Leptosphaerodione*)
Nicolet, B. *et al., CA*, 2000, **132**, 134414 (*isol, activity*)
Berg, A. *et al., J. Antibiot.*, 2000, **53**, 1313-1316 (*Laccaridiones*)

Leptosphaerolide L-156

[138039-35-7]



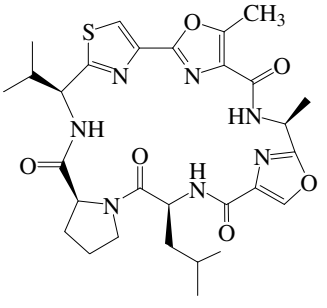
$C_{20}H_{22}O_5$ 342.391

Polyketide lactone antibiotic. Metab. of the marine ascomycete *Leptosphaeria oraemaris*. Yellow semi-solid. $[\alpha]_D^{20}$ +39 (c, 0.13 in MeOH). λ_{max} 228 (ϵ 9800); 244 (ϵ 9500); 301 (ϵ 22750) (MeOH) (Berdy). λ_{max} 238 (ϵ 12500); 314 (ϵ 4600) (MeOH/NaOH) (Berdy).

Guerriero, A. *et al., Helv. Chim. Acta*, 1991, **74**, 1445 (*isol, pmr, cmr*)

Leucamide A L-157

[447461-16-7]



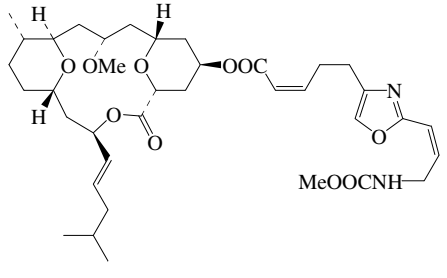
$C_{29}H_{37}N_7O_6S$ 611.721

Isol. from the Australian sponge *Leucetta microraphis*. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{23}$ -69.3 (c, 0.6 in $CHCl_3$). λ_{max} 246 (ϵ 9270) ($CHCl_3$).

Kehraus, S. *et al., J.O.C.*, 2002, **67**, 4989-4992 (*isol, pmr, cmr*)
Wang, W. *et al., J.O.C.*, 2003, **68**, 1636-1639 (*synth*)

Leucascandrolide A L-158

[175448-18-7]



Absolute Configuration

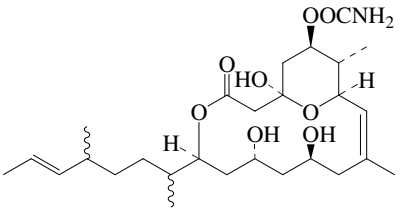
$C_{38}H_{56}N_2O_{10}$ 700.868

Isol. from the marine sponge *Leucascandra caveolata*. Shows potent antifungal activity against *Candida albicans*; shows strong cytotoxicity. Amorph. solid. Sol. MeOH, $CHCl_3$, CH_2Cl_2, EtOH; poorly sol. H_2O. $[\alpha]_D^{20}$ +41 (EtOH). λ_{max} 205 (ϵ 15000); 262 (ϵ 11000) (EtOH).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1996, **79**, 51-60 (*isol, uv, ir, pmr, cmr, ms, cryst struct, activity*)
Hornberger, K.R. *et al., J.A.C.S.*, 2000, **122**, 12894-12895 (*synth, activity*)
Wang, Y. *et al., J.A.C.S.*, 2002, **124**, 13670-13671 (*synth*)
Williams, D.R. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 3934-3938 (*synth*)
Fettes, A. *et al., J.O.C.*, 2003, **68**, 9274-9283 (*synth*)
Crimmins, M.T. *et al., Org. Lett.*, 2003, **5**, 4641-4644 (*synth*)
Williams, D.R. *et al., Org. Lett.*, 2003, **5**, 5035-5038 (*synth*)
Paterson, I. *et al., Tetrahedron*, 2003, **59**, 6833-6849 (*synth*)
Su, Q. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 1223-1225 (*synth*)

Leucascandrolide B L-159

[228092-28-2]



Relative Configuration

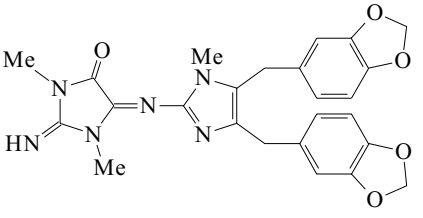
$C_{27}H_{45}NO_8$ 511.654

Isol. from the sponge *Leucascandra caveolata*.
$[\alpha]_D^{20}$ -2 (c, 0.19 in $CHCl_3$).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1999, **82**, 347-353

Leucettamidine L-160

[147395-97-9]



$C_{25}H_{24}N_6O_5$ 488.502

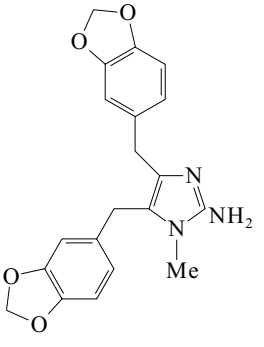
Alkaloid from the marine sponge *Leucetta microraphis*. Exhibits significant leukotriene B4 receptor binding activity. Antiinflammatory agent. λ_{max} 205 (ϵ 4200); 285 (ϵ 800); 386 (ϵ 6000) ($CHCl_3$/MeOH) (Derep). λ_{max} 205; 237; 363 (MeOH) (Berdy).

Chan, G.W. *et al., J. Nat. Prod.*, 1993, **56**, 116 (*isol, pmr, struct*)

Leucettamine A L-161

*4,5-Bis(1,3-benzodioxol-5-ylmethyl)-1-methyl-1*H*-imidazol-2-amine, 9CI*

[147395-95-7]



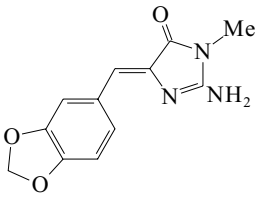
$C_{20}H_{19}N_3O_4$ 365.388

Alkaloid from the marine sponge *Leucetta microraphis*. Exhibits potent leukotriene B4 receptor binding activity. Antiinflammatory agent. Yellowish amorph. solid. λ_{max} 205 (ϵ 4280); 285 (ϵ 796) (MeOH) (Derep).

Boehm, J.C. *et al., J. Med. Chem.*, 1993, **36**, 3333 (*synth*)
Chan, G.W. *et al., J. Nat. Prod.*, 1993, **56**, 116 (*isol, uv, ir, pmr, cmr, ms, struct, activity*)

Leucettamine B L-162

[147395-96-8]



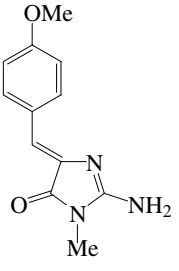
$C_{12}H_{11}N_3O_3$ 245.237

Alkaloid from the marine sponge *Leucetta microraphis*. Cream solid. λ_{max} 205 (ϵ 2320); 237 (ϵ 1830); 363 (ϵ 3710) (MeOH) (Derep).

Chan, G.W. *et al., J. Nat. Prod.*, 1993, **56**, 116 (*isol, uv, ir, pmr, cmr, ms, struct*)
Molina, P. *et al., Tet. Lett.*, 1994, **35**, 2235 (*synth*)
Roue, N. *et al., Tetrahedron*, 1999, **55**, 14729-14738 (*synth*)

Leucettamine C L-163

*2-Amino-3,5-dihydro-5-[(4-methoxyphenyl)methylidene]-3-methyl-4*H*-imidazol-4-one, 9CI*
[497085-85-5]



$C_{12}H_{13}N_3O_2$ 231.254

Alkaloid from the sponge *Leucetta* sp. Amorph. yellow powder. λ_{max} 207 (log ϵ 4.26); 230 (log ϵ 4.1); 368 (log ϵ 4.4) (MeOH).

Crews, P. *et al., J. Nat. Prod.*, 2003, **66**, 177-182 (*isol, pmr, cmr*)

Leu-contryphan P L-164

[245113-78-4]

H-Gly-Cys-Val-D-Leu-Leu-Pro-Trp-Cys-OH

$C_{41}H_{61}N_9O_9S_2$ 888.12

Peptide containing a D-leucine residue; struct. of reduced form shown. Isol. from the venom of *Conus purpurascens*.

Jacobsen, R.B. *et al., J. Pept. Res.*, 1999, **54**, 93-99 (*isol*)

Leu-contryphan Tx L-165

[354530-27-1]

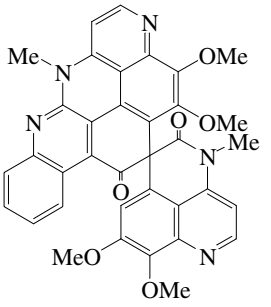
Cys-Val-D-Leu-Tyr-Pro-Trp-Cys-NH_2

$C_{42}H_{57}N_9O_8S_2$ 880.1

Isol. from venom ducts of *Conus textile*.

Jimenez, E.C. *et al., Toxicon*, 2001, **39**, 803-808 (*isol*)

Lihouidine L-166



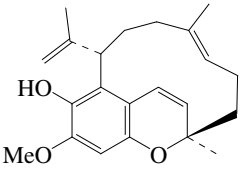
$C_{36}H_{27}N_5O_6$ 625.639

Alkaloid from the marine sponge *Suberea* sp. nov. Purple-red prisms (MeCN).

Mp >330°. Racemic. λ_{max} 210 (ϵ 54400); 246 (ϵ 74200); 287 (sh) (ϵ 24000); 314 (ϵ 19000); 340 (ϵ 14700); 406 (ϵ 5100); 430 (ϵ 5600); 444 (ϵ 5600); 514 (ϵ 10500); 543 (sh) (ϵ 10200) (EtOH).

Bowden, B.F. *et al., J.O.C.*, 2004, **69**, 7791-7793 (*isol, uv, pmr, cmr, cryst struct*)

Likonide A L-167



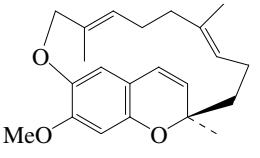
Absolute Configuration

$C_{22}H_{28}O_3$ 340.461

Isol. from the Kenyan sponge *Hyatella* sp. Oil. $[\alpha]_D$ +85 (c, 0.56 in MeOH).

Rudi, A. *et al., Org. Lett.*, 2004, **6**, 4013-4016 (*isol, cd, pmr, cmr*)

Likonide B L-168



Absolute Configuration

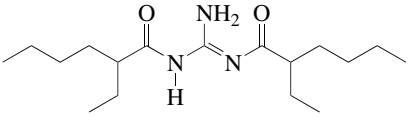
$C_{22}H_{28}O_3$ 340.461

Isol. from the Kenyan sponge *Hyatella* sp. Oil. $[\alpha]_D$ +27 (c, 0.08 in MeOH).

Rudi, A. *et al., Org. Lett.*, 2004, **6**, 4013-4016 (*isol, cd, pmr, cmr*)

Limaciamine L-169

N,N′-Carbonimidoylbis[2-ethylhexanamide], 9CI. N,N′-Bis(2-ethylhexanoyl)guanidine
[202747-40-8]



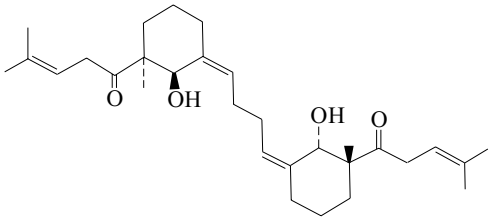
$C_{17}H_{33}N_3O_2$ 311.467

Isol. from the skin extracts of nudibranch *Limacia clavigera*. Glass. Related to Triophamine, T-750.

Graziani, E.I. *et al., J. Nat. Prod.*, 1998, **61**, 285-286 (*isol, pmr, cmr, ms*)

Limatulone L-170

[97764-35-7]



$C_{30}H_{46}O_4$ 470.691

The nat. material is an opt. inactive mixture of *meso*- (illus.) and (±)-stereoisomers. Defensive substance from *Collisella limatula*. Ichtyotoxic, feeding inhibitor. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. λ_{max} 222 (ϵ 14000) (MeOH) (Berdy).

meso-form

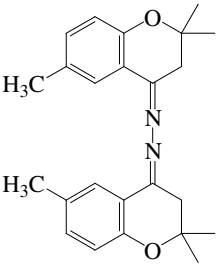
Rods. Mp 95-97°.

Albizati, K.F. *et al., J.O.C.*, 1985, **50**, 3428-3430 (*Collisella limulata constit*)
Mori, K. *et al., J.C.S. Perkin 1*, 1993, 169-179 (*synth*)
Mori, K. *et al., J. Synth. Org. Chem., Jpn.*, 1995, **53**, 952 (*config, bibl*)

Limnazine L-171

*4,4′-Azinobis[3,4-dihydro-2,2,6-trimethyl-2*H*-1-benzopyran]. 2,2,6-Trimethyl-4-chromanone azine*

[474955-54-9]



$C_{24}H_{28}N_2O_2$ 376.497

Prod. by the marine *Bacillus* sp. GW90a. Light yellow cryst. Mp 204°. λ_{max} 271 (log ϵ 3.96); 280 (log ϵ 3.97); 307 (log ϵ 3.93); 350 (log ϵ 4.08) ($CHCl_3$).

Asolkar, R.N. *et al., J. Nat. Prod.*, 2002, **65**, 1664-1666 (*isol, synth, pmr, cmr, ms*)

Limulin L-172

Limulus polyphemus *Lectin*

Glycoprotein with MW *ca*. 500,000 and consisting of 2 non-identical subunits with MW 18,000 and 24,000. Isol. from haemolymph of the horseshoe crab *Limulus polyphemus*. Sialic acid-binding lectin.

Roche, A.C. *et al., Biochim. Biophys. Acta*, 1974, **371**, 242-254 (*isol*)
Kaplan, R. *et al., Biochemistry*, 1977, **16**, 4297-4303 (*struct*)
Barondes, S.H. *et al., Methods Enzymol.*, 1978, **50**, 302-305 (*isol*)
Robey, F.A. *et al., J. Biol. Chem.*, 1981, **256**, 969-975 (*isol*)
Muresan, V. *et al., J. Histochem. Cytochem.*, 1982, **30**, 938-946 (*isol*)

Limulus factor D L-173

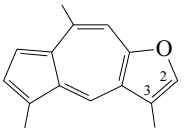
Glycoprotein, MW 43 kDa; a serine protease homologue. Isol. from haemocytes of the horseshoe crab *Tachypleus tridentatus*. Shows antimicrobial activity.

Kawabata, S. *et al., FEBS Lett.*, 1996, **398**, 146-150 (*isol*)

Linderazulene L-174

*3,5,8-Trimethylazuleno[6,5-*b*]furan, 9CI. 8,12-Epoxy-1,3,5,7,9,11-guaiahexaene*

[489-79-2]



$C_{15}H_{14}O$ 210.275

Pigment of the sea gorgonian *Paramuricea chamaeleon* and a *Acalycigorgia* Sp. Dehydrogenation prod. of sesquiterpenoids. Immunodepressant. Lustrous violet-black plates (2-propanol). Mp 106-107°. λ_{max} 280; 287; 292; 300; 315; 321; 361; 372; 380; 391; 563; 601; 612; 644 (sh); 673 (hexane) (Derep).

2,3-Dihydro: 2,3-Dihydrolinderazulene. ***11,12-Dihydrolinderazulene****. 8,12-Epoxy-1,3,5,7,9-guaiapentaene*

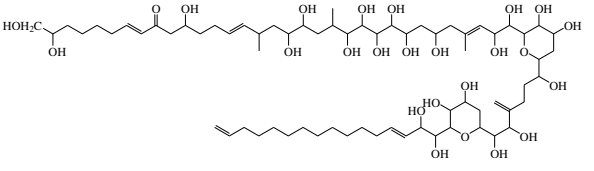
[110207-64-2]

$C_{15}H_{16}O$ 212.291

Constit. of an *Acalycigorgia* sp. Immunostimulant. Purple oil. $[\alpha]_D$ +800 (c, 0.05 in $CHCl_3$).

Takeda, K. *et al., J.C.S.*, 1964, 2591-2597 (*synth, bibl*)
Imre, S. *et al., Experientia*, 1981, **37**, 442-443 (*isol*)
Sakemi, S. *et al., Experientia*, 1987, **43**, 624-625 (*2,3-dihydro*)

Lingshuiol L-175

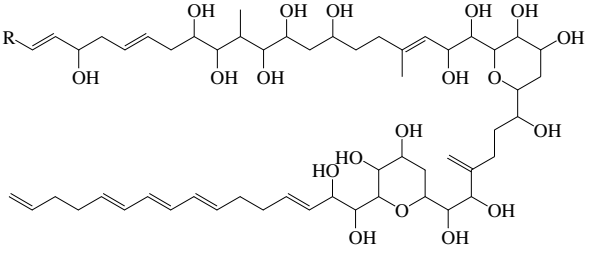


$C_{69}H_{122}O_{25}$ 1351.708

Related to Amphidinol, A-436. Isol. from an *Amphidinium* sp. Cytotoxic. Pale yellow solid. $[\alpha]_D^{25}$ -8 (c, 0.28 in MeOH). λ_{max} 226 (ϵ 13800) (MeOH).

Huang, X.-C. *et al., Bioorg. Med. Chem. Lett.*, 2004, **14**, 3117-3120 (*isol, pmr, cmr*)

Lingshuiol A L-176



R = -$CH_2CH(OH)(CH_2)_3CH(OH)(CH_2)_3CH(OH)CH_2OH$

$C_{66}H_{112}O_{23}$ 1273.597

Related to Amphidinol, A-436. Isol. from *Amphidinium* sp. Pale yellow amorph. solid. $[\alpha]_D^{25}$ -2.8 (c, 0.4 in MeOH). λ_{max} 259 (ϵ 11200); 269 (ϵ 18400) (MeOH).

Huang, X.-C. *et al., Tet. Lett.*, 2004, **45**, 5501-5504 (*isol*)

Lingshuiol B L-177

As Lingshuiol A, L-176 with

R = -$(CH_2)_4CH_2OSO_3H$

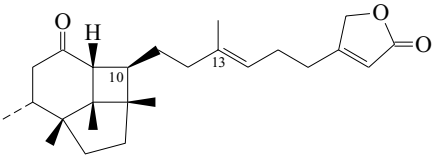
$C_{60}H_{100}O_{23}S$ 1221.502

Isol. from *Amphidinium* sp. Pale yellow amorph. solid. $[\alpha]_D^{25}$ +2.5 (c, 0.5 in MeOH). λ_{max} 259 (ϵ 14600); 269 (ϵ 22600); 280 (ϵ 14900) (MeOH).

Huang, X.-C. *et al., Tet. Lett.*, 2004, **45**, 5501-5504

Lintenone L-178

[145176-85-8]



$C_{25}H_{36}O_3$ 384.558
Constit. of *Cacospongia* cf. *linteiformis*. Antifeedant. Ichthyotoxic agent. Macrophage activation modulator. Toxic to brine shrimp. Oil. $[\alpha]_D^{25}$ -75.5 (c, 0.004 in $CHCl_3$). λ_{max} 215 (ϵ 10000) (MeOH) (Derep).

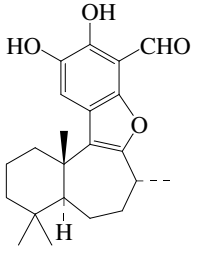
13Z-Isomer:
$C_{25}H_{36}O_3$ 384.558
Constit. of *Cacospongia* cf. *linteiformis*. Antifeedant. Ichthyotoxic agent. $[\alpha]_D^{25}$ -75 (c, 0.03 in $CHCl_3$).

10-Epimer:
$C_{25}H_{36}O_3$ 384.558
Constit. of *Cacospongia* cf. *linteiformis*. Antifeedant. Ichthyotoxic agent. Macrophage activation modulator. $[\alpha]_D^{25}$ -70 (c, 0.04 in $CHCl_3$).

Fattorusso, E. *et al., J.O.C.*, 1992, **57**, 6921 (*isol, pmr, cmr*)
Carotenuto, A. *et al., Tetrahedron*, 1995, **51**, 10751 (*deriv*)

Liphagal L-179

[874292-32-7]

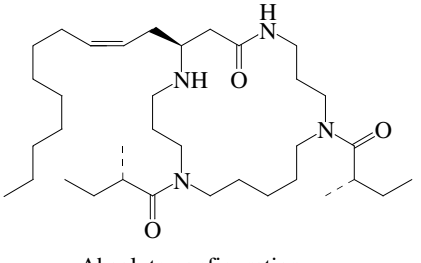


$C_{22}H_{28}O_4$ 356.461
Constit. of *Aka coralliphaga*. Amorph. yellow solid. $[\alpha]_D^{25}$ +12 (c, 3.7 in MeOH).

Marion, F. *et al., Org. Lett.*, 2006, **8**, 321-324 (*Liphagal, isol, synth*)

Lipogrammistin A L-180

[151756-67-1]



Absolute configuration

$C_{35}H_{66}N_4O_3$ 590.931

Isol. from the mucus secreted by the soapfish *Diploprion bifasciatum*. Shows haemolytic activity and exhibits erythrocyte transformation. Ichthyotoxic. $[\alpha]_D$ +18.5 (c, 0.86 in MeOH). Exists in soln. as a mixt. of 4 conformers.

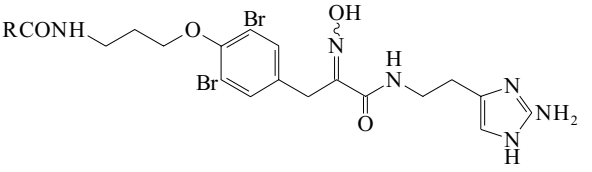
Onuki, H. *et al., J.O.C.*, 1998, **63**, 3925-3932 (*synth, abs config*)
Kobayashi, Y. *et al., Bioorg. Med. Chem.*, 1999, **7**, 2073-2081 (*activity*)
Kan, T. *et al., Tetrahedron*, 2002, **58**, 6267-6276 (*synth*)

Shewanella pacifica Lipooligosaccharide L-181

Non-stoichiometric glycosphingolipid complex with 7 sugar residues substituted by phosphate groups. Generic struct. determined. Isol. from the marine bacterium *Shewanella pacifica*.

Silipo, A. *et al., Eur. J. Org. Chem.*, 2005, 2281-2291 (*isol, pmr, cmr, P-31 nmr, ms*)

Lipopurealins L-182



Lipopurealin A; R = $(CH_2)_{12}CH_3$
B; R = $(CH_2)_{11}CH(CH_3)_2$
C; R = $(CH_2)_{14}CH_3$
D; R = $(CH_2)_7CH{=}CH(CH_2)_4CH(CH_3)_2$ (*Z*–)
E; R = $(CH_2)_{17}CH_3$

Metabs. of the Okinawan marine sponge *Psammaplysilla purea*.

Lipopurealin A [101541-48-4]
$C_{31}H_{48}Br_2N_6O_4$ 728.566
$Na^{\oplus}$ and $K^{\oplus}$-ATPase inhibitor. Amorph. solid (as hydrochloride). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 94-95° (hydrochloride). CAS no. refers to hydrochloride. λ_{max} 284 (ϵ 970) (MeOH) (Berdy).

Lipopurealin B [101541-49-5]
$C_{32}H_{50}Br_2N_6O_4$ 742.593
$Na^{\oplus}$ and $K^{\oplus}$-ATPase inhibitor. Amorph. solid (as hydrochloride). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 93-95° (hydrochloride). CAS no. refers to hydrochloride. λ_{max} 284 (ϵ 930) (MeOH) (Berdy).

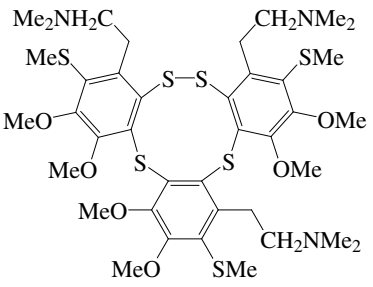
Lipopurealin C [101541-50-8]
$C_{33}H_{52}Br_2N_6O_4$ 756.62
$Na^{\oplus}$ and $K^{\oplus}$-ATPase inhibitor. Amorph. solid (as hydrochloride). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 108-110° (hydrochloride). CAS no. refers to hydrochloride. λ_{max} 284 (ϵ 910) (MeOH) (Berdy).

Lipopurealin D [164301-28-4]
$C_{34}H_{52}Br_2N_6O_4$ 768.631
Amorph. solid. Oxime has *E*-config.

Lipopurealin E [164301-29-5]
$C_{36}H_{58}Br_2N_6O_4$ 798.7
Amorph. solid. Oxime has *E*-config.

Wu, H. *et al., Experientia*, 1986, **42**, 855 (*Lipopurealins A-C*)
Kobayashi, J. *et al., J. Nat. Prod.*, 1995, **58**, 467 (*Lipopurealins D-E*)

Lissoclibadin 1 L-183

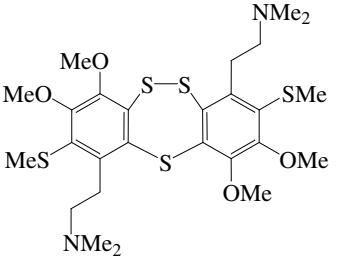


$C_{39}H_{57}N_3O_6S_7$ 888.358

Isol. from *Lissoclinum* cf. *badium*. Active against *Ruegeria atlantica*. $[\alpha]_D$ -3.6 (c, 0.1 in $CHCl_3$) (as tris(TFA) salt). λ_{max} 279 (ϵ 134300); 318 (sh) (ϵ 26500) (tris(TFA) salt).

Liu, H. *et al., Tetrahedron*, 2005, **61**, 8611-8615 (*isol, pmr, cmr*)

Lissoclibadin 2 L-184

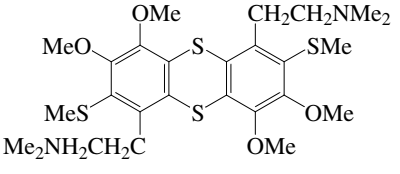


$C_{26}H_{38}N_2O_4S_5$ 602.927

Disulfide analogue of Lissoclibadin 3, L-185. Isol. from *Lissoclinum* cf *badium*. λ_{max} 270 (ϵ 14300); 316 (ϵ 6500) (as bis(trifluoroacetate)).

Liu, H. *et al., Tetrahedron*, 2005, **61**, 8611-8615 (*isol, pmr, cmr*)

Lissoclibadin 3 L-185



$C_{26}H_{38}N_2O_4S_4$ 570.861

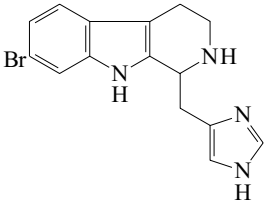
Isomeric with Lissoclinotoxin E, L-196. Isol. from *Lissoclinum* cf. *badium*. Cytotoxic. Amorph. (as bis-TFA salt). λ_{max} 274 (ϵ 13300); 318 (ϵ 4500) (MeOH) (bis-TFA salt).

Liu, H. *et al., Tetrahedron*, 2005, **61**, 8611-8615 (*isol, pmr, cmr*)

Lissoclin C L-186

*7-Bromo-2,3,4,9-tetrahydro-1-(1*H*-imidazol-4-ylmethyl)-1*H*-pyrido[3,4-*b*]indole, 9CI*

[158761-14-9]



$C_{15}H_{15}BrN_4$ 331.214

Alkaloid from the tropical ascidian *Lissoclinum* sp. Isol. as a virtual racemate, prob. by racemisation during isol. λ_{max} 231 (ϵ 21900); 285 (ϵ 4170) (MeOH) (TFA salt).

*Debromo: 2,3,4,9-Tetrahydro-1-(1*H*-imidazol-4-ylmethyl)-1*H*-pyrido[3,4-*b*]indole.* ***Haploscleridamine***

[426258-83-5]

$C_{15}H_{16}N_4$ 252.318

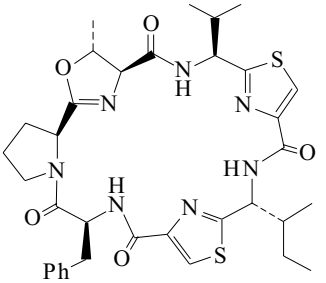
Alkaloid from a sponge of the order Haploscleridae. Cathepsin K inhibitor. Gum. $[\alpha]_D$ -3.4 (c, 0.78 in MeOH). Racemate or virtual racemate. λ_{max} 235 (log ϵ 3.72); 270 (log ϵ 3.41); 278 (log ϵ 3.55); 288 (log ϵ 3.06) (MeOH).

Searle, P.A. *et al., J.O.C.*, 1994, **59**, 6600-6605 (*isol, uv, ir, pmr, cmr, struct*)
Patil, A.D. *et al., J. Nat. Prod.*, 2002, **65**, 628-629 (*Haploscleridamine*)

Lissoclinamide 1 L-187

14-Demethyl-7-de(1-methylpropyl)-7-(1-methylethyl)-14-(1-methylpropyl)ulicyclamide, 9CI

[87411-84-5]



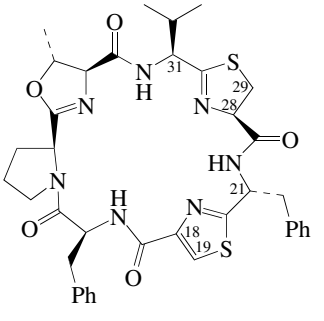
$C_{35}H_{43}N_7O_5S_2$ 705.901

Cyclic peptide alkaloid. Isol. from the marine tunicate *Lissoclinum patella*. Related to Ulicyclamide, U-6.

Wasylyk, J.M. *et al., J.O.C.*, 1983, **48**, 4445-4449 (*isol, ir, pmr, ms, struct*)

Lissoclinamide 4 L-188

[120853-16-9]



$C_{38}H_{43}N_7O_5S_2$ 741.934

Cyclopeptide from the ascidian *Lissoclinum patella*. Exhibits marked cytotoxicity. Powder (Et_2O).

Mp 152-154°. $[\alpha]_D$ +45 (c, 0.7 in $CHCl_3$).

18α,19-Dihydro: ***Lissoclinamide 7***

[126297-39-0]

$C_{38}H_{45}N_7O_5S_2$ 743.949

Isol. from *Lissoclinum patella*. Shows selective metal binding props. Cytotoxic.

28,29-Didehydro: ***Lissoclinamide 5***

[120853-17-0]

$C_{38}H_{41}N_7O_5S_2$ 739.918

From *Lissoclinum patella*. Cytotoxic (less than Lissoclinamide 4 by two orders of magnitude).

21-Epimer: ***Lissoclinamide 6***

[121209-53-8]

$C_{38}H_{43}N_7O_5S_2$ 741.934

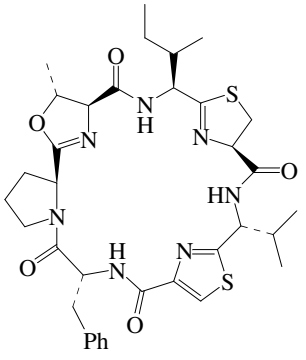
Trace constit. of *Lissoclinum patella*. Cytotoxic. Possibly an artifact.

Stereoisomer: ***Lissoclinamide 8***
[126452-98-0]
$C_{38}H_{43}N_7O_5S_2$ 741.934
Isol. from *Lissoclinum patella*. Cytotoxic. Full config. not detd.

Degnan, B.M. *et al., J. Med. Chem.*, 1989, **32**, 1349-1354 (*isol, pmr, cmr, struct*)
Schmitz, F.J. *et al., J.O.C.*, 1989, **54**, 3463-3472 (*isol, ir, pmr, cmr, struct*)
Hawkins, C.J. *et al., J. Med. Chem.*, 1990, **33**, 1634-1638 (*Lissoclinamides 7 and 8*)
Wipf, P. *et al., J.A.C.S.*, 1996, **118**, 12358-12367; 1998, **120**, 4105-4112 (*Lissoclinamide 7, synth, abs config, conformn*)
Boden, C.D.J. *et al., J.C.S. Perkin 1*, 2000, 875-882 (*synth, abs config*)
Morris, L.A. *et al., Tetrahedron*, 2001, **57**, 3199-3207 (*activity*)

Lissoclinamide 9 L-189

[309963-07-3]



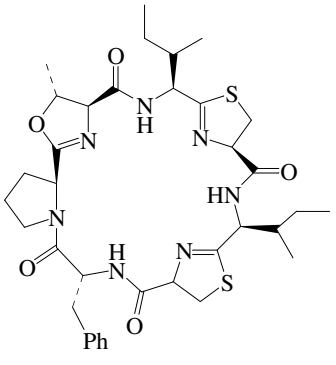
Absolute Configuration

$C_{35}H_{45}N_7O_5S_2$ 707.916
Isol. from *Lissoclinum patella*. Pale yellow oil. λ_{max} 308 (ϵ 3370) ($CHCl_3$).

Morris, L.A. *et al., Tetrahedron*, 2000, **56**, 8345-8353 (*isol, pmr, cmr, cd*)

Lissoclinamide 10 L-190

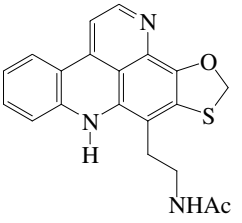
[309963-08-4]



$C_{36}H_{49}N_7O_5S_2$ 723.959
Isol. from *Lissoclinum patella*. Pale yellow oil. λ_{max} 308 (ϵ 2900) ($CHCl_3$).

Morris, L.A. *et al., Tetrahedron*, 2000, **56**, 8345-8353 (*isol, pmr, cmr, cd*)

Lissoclinidine L-191

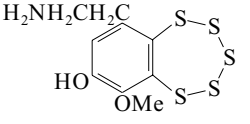


$C_{20}H_{17}N_3O_2S$ 363.439
Alkaloid from the ascidian *Lissoclinum notti*. Hygroscopic purple solid (as TFA salt). λ_{max} 218 (log ϵ 4.41); 281 (log ϵ 4.26); 295 (log ϵ 4.21); 310 (log ϵ 4.1); 384 (log ϵ 3.61); 548 (log ϵ 3.4) (MeOH/TFA).

Appleton, D.R. *et al., Tetrahedron*, 2002, **58**, 9779-9783 (*isol*)

Lissoclinotoxin A L-192

9-(2-Aminoethyl)-6-methoxy-7-benzopentathiepinol
[133883-05-3]



$C_9H_{11}NO_2S_5$ 325.521
Originally reported with an incorrect trithiane struct. Chiral molecule exhibiting unusual stereoisomerism due to restricted inversion, although isol. samples are racemic. Isol. from the tunicate *Lissoclinum perforatum*. Exhibits potent antimicrobial and antifungal activity. Amorph. yellow solid. Fairly sol. MeOH, DMSO; poorly sol. butanol, hexane.
Mp 245-250°. λ_{max} 215 (ϵ 10400); 246 (ϵ 8870) (EtOH) (Derep). λ_{max} 213 (ϵ 14100) (MeOH) (Berdy).

Me ether: 8,9-Dimethoxy-6-benzopentathiepinethanamine, 9CI. ***Varacin***
[134029-48-4]
$C_{10}H_{13}NO_2S_5$ 339.548
Isol. from the ascidians *Lissoclinum vareau* and *Polycitor* sp. Exhibits potent antifungal and antimicrobial activity. Cytotoxic towards the human colon cancer HCT 116. Light yellow powder (also descr. as a glass).
Mp 258-260° dec. λ_{max} 214; 244 (MeOH) (Derep). λ_{max} 212; 244 (EtOH) (Berdy).

Me ether, N-*Ac:*
Light yellow cryst. (MeOH). Mp 136-137°.

O-*De-Me: 9-(2-Aminoethyl)-6,7-benzopentathiepindiol, 9CI.* ***Dide-O-methylvaracin***. *De*-O-*methyllissoclinotoxin A*
[159645-89-3]
$C_8H_9NO_2S_5$ 311.495
Isol. from a *Eudistoma* sp. Yellow powder.

8-(Methylthio), Me ether: 9-(2-Aminoethyl)-6,7-dimethoxy-8-(methylthio)benzopentathiepin. ***5-(Methylthio)varacin***
[159645-87-1]
$C_{11}H_{15}NO_2S_6$ 385.641
Isol. from a *Lissoclinum* sp. CAS no. refers to trifluoroacetate.

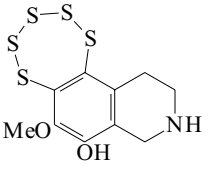
8-(Methylthio), N,N,O-*tri-Me: 6-Amino-8,9-dimethoxy*-N,N-*dimethyl-7-(methylthio)benzopentathiepin.* **N,N-*Dimethyl-5-(methylthio)varacin***
[159645-83-7]
$C_{13}H_{19}NO_2S_6$ 413.695
Isol. from *Lissoclinum japonicum*. Pale yellow oil (as trifluoroacetate). CAS no. refers to trifluoroacetate. λ_{max} 211 (ϵ 16500) (MeOH).

Davidson, B.S. *et al., J.A.C.S.*, 1991, **113**, 4709-4710 (*Varacin*)
Litaudon, M. *et al., Tet. Lett.*, 1991, **32**, 911-914 (*isol, pmr, cmr*)
Ford, P.W. *et al., J.O.C.*, 1994, **59**, 5955-5960 (*synth, struct*)
Searle, P.A. *et al., J.O.C.*, 1994, **59**, 6600-6605 (*isol, uv, ir, pmr, cmr*)

Litaudon, M. *et al., Tetrahedron*, 1994, **50**, 5323-5334 (*uv, pmr, ms, struct*)
Compagnone, R.S. *et al., Tetrahedron*, 1994, **50**, 12785-12792 (*isol, uv, pmr, cmr*)
Makarieva, T.N. *et al., J. Nat. Prod.*, 1995, **58**, 254 (*Varacin*)
Greer, A. *et al., J.A.C.S.*, 2001, **123**, 10379-10386 (*Varacin, struct*)

Lissoclinotoxin B L-193

8,9,10,11-Tetrahydro-6-methoxy-1,2,3,4,5-pentathiepino[6,7-f]isoquinolin-7-ol, 9CI
[157536-34-0]

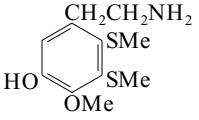


$C_{10}H_{11}NO_2S_5$ 337.532
Minor constit. of the tunicate *Lissoclinum perforatum*. Exhibits antimicrobial activity. Antiplasmodial agent. Pale yellow powder. Fairly sol. MeOH; poorly sol. $CHCl_3$, CH_2Cl_2.
Mp 310-313°. λ_{max} 215 (ϵ 20000); 246 (ϵ 6500) (MeOH) (Berdy).

Litaudon, M. *et al., Tetrahedron*, 1994, **50**, 5323 (*isol, uv, ir, pmr, cmr, struct*)

Lissoclinotoxin C L-194

5-(2-Aminoethyl)-2-methoxy-3,4-bis(methylthio)phenol, 9CI. 5-Hydroxy-4-methoxy-2,3-bis(methylthio)phenethylamine
[158761-15-0]

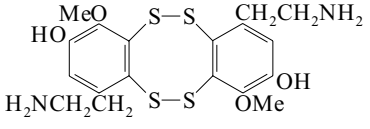


$C_{11}H_{17}NO_2S_2$ 259.393
Alkaloid from the tropical ascidian *Lissoclinum* sp.

Searle, P.A. *et al., J.O.C.*, 1994, **59**, 6600-6605 (*isol, pmr, struct*)

Lissoclinotoxin D L-195

4,10-Bis(2-aminoethyl)-1,7-dimethoxydibenzo[c,g][1,2,5,6]-tetrathiocin-2,8-diol, 9CI
[158761-16-1]

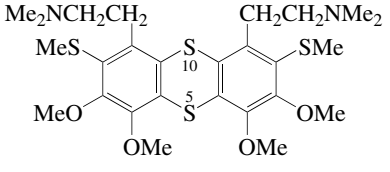


$C_{18}H_{22}N_2O_4S_4$ 458.647
Alkaloid from the tropical ascidian *Lissoclinum* sp. Exhibits antifungal activity.

Searle, P.A. *et al., J.O.C.*, 1994, **59**, 6600-6605 (*isol, pmr, struct*)

Lissoclinotoxin E L-196

Lissoclin

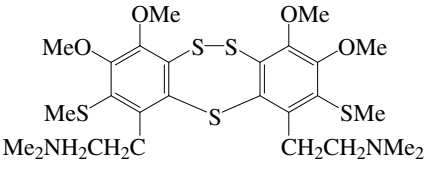


$C_{26}H_{38}N_2O_4S_4$ 570.861
Struct. revised from, and isomeric with Lissoclibadin 3, L-185 in 2005. Isol. from *Lissoclinum* cf. *badium* and an unidentified Philippine ascidian. Cytotoxic. λ_{max} 210 (ϵ 15000); 232 (sh) (ϵ 9000); 254 (ϵ 7000); 272 (ϵ 12000) (MeOH).

5,10-Dioxide: ***Lissoclin disulfoxide***
[195303-92-5]
$C_{26}H_{38}N_2O_6S_4$ 602.86
Isol. from a *Lissoclinum* sp. Inhibitor of interleukin-8 receptors. Yellow solid. λ_{max} 243; 266; 318 (MeOH).

Patil, A.D. *et al., Nat. Prod. Lett.*, 1997, **10**, 225-229 (*Lissoclin disulfoxide*)
Davies, R.A. *et al., Tetrahedron*, 2003, **59**, 2855-2859 (*isol, pmr, cmr*)
Liu, H. *et al., Tetrahedron*, 2005, **61**, 8611-8615 (*isol, struct*)

Lissoclinotoxin F L-197

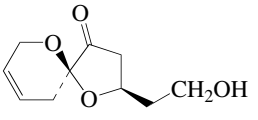


$C_{26}H_{38}N_2O_4S_5$ 602.927
Isol. from a Philippine didemnid ascidian. Cytotoxic. Light brown film (as bis-TFA salt). λ_{max} 210 (ϵ 13000); 238 (sh) (ϵ 11000); 268 (ϵ 11000); 320 (ϵ 3000) (MeOH).

Davis, R.A. *et al., Tetrahedron*, 2003, **59**, 2855-2859 (*isol, pmr, cmr*)

Lissoketal L-198

2-(2-Hydroxyethyl)-1,6-dioxaspiro[4.5]dec-8-en-4-one
[186416-50-2]



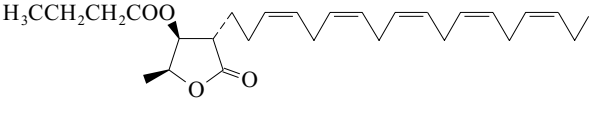
Relative Configuration

$C_{10}H_{14}O_4$ 198.218
Isol. from the ascidian *Lissoclinum voeltzkowi*. Oil. $[\alpha]_D$ +2 (c, 0.1 in MeOH).

Hopmann, C. *et al., Tet. Lett.*, 1997, **38**, 169-170 (*isol, ir, pmr, cmr*)

Litophytolide A L-199

[119979-77-0]



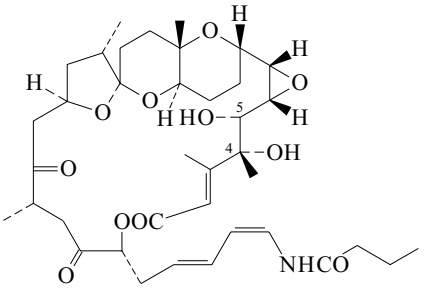
$C_{27}H_{40}O_4$ 428.611
Constit. of a *Litophyton* sp. Oil. $[\alpha]_D^{18}$ -17.2 (c, 0.1 in EtOH).

Deacyl, Ac: ***Litophytolide B***
[119979-78-1]
$C_{25}H_{36}O_4$ 400.557
Constit. of a *Litophyton* sp. Oil. $[\alpha]_D^{22}$ -25.4 (c, 0.24 in $CHCl_3$).

Ochi, M. *et al., Heterocycles*, 1989, **29**, 39 (*isol, pmr, cmr*)

Lituarine C L-200

[143621-77-6]



$C_{38}H_{55}NO_{11}$ 701.853
Isol. from the sea pen *Lituaria australasiae*. Shows antifungal, cytotoxic and antineoplastic activities. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 153-157°. λ_{max} 269 (ϵ 22419) (MeOH) (Berdy).

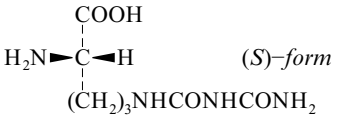
5-Ac: ***Lituarine B***
[143621-76-5]
$C_{40}H_{57}NO_{12}$ 743.89
From *Lituaria australasiae*. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 126-129°. λ_{max} 269 (ϵ 26604) (MeOH) (Berdy).

4,5-Dideoxy: ***Lituarine A***
[143621-75-4]
$C_{38}H_{55}NO_9$ 669.854
From *Lituaria australasiae*. Cryst.
Mp 83-85°. λ_{max} 270 (ϵ 15857) (MeOH) (Berdy).

Vidal, J.-P. *et al., J.O.C.*, 1992, **57**, 5857 (*isol, pmr, cmr, struct*)

Lividine L-201

N^5-*[[(Aminocarbonyl)amino]carbonyl]ornithine, 9CI*. N^{ω}-*Carbamoylcitrulline*



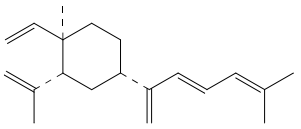
$C_7H_{14}N_4O_4$ 218.212

(S)-form
L-form
[89499-15-0]
Isol. from the red alga *Grateloupia livida*.
Mp 225-228° dec. $[\alpha]_D^{14}$ +20 (c, 0.66 in 2*M* HCl).

Wakamiya, T. *et al., Tetrahedron*, 1984, **40**, 235 (*isol, pmr, cmr, struct, synth*)

8,10,13,15,17-Lobapentaene L-202

[213907-89-2]

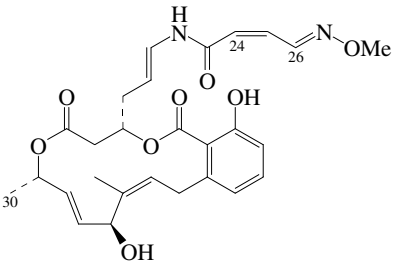


$C_{20}H_{30}$ 270.457
Constit. of *Lobophytum pauciflorum*. Oil. $[\alpha]_D$ +17.8 (c, 0.1 in $CHCl_3$).

Babu, U.V. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 576-578

Lobatamide A L-203

[200563-47-9]



Absolute Configuration

$C_{27}H_{32}N_2O_8$ 512.558
Isol. from the tunicate *Aplidium lobatum*. Cytotoxic agent. $[\alpha]_D$ -7.9 (c, 0.2 in MeOH). λ_{max} 273 (log ϵ 4.22) (MeOH).

30-Hydroxy: ***Lobatamide D***
[215722-31-9]
$C_{27}H_{32}N_2O_9$ 528.558
Isol. from *Aplidium lobatum*.
$[\alpha]_D$ -35 (c, 0.08 in MeOH). λ_{max} 281 (log ϵ 4.23) (MeOH).

*24*E-*Isomer:* ***Lobatamide C***
[215722-30-8]
$C_{27}H_{32}N_2O_8$ 512.558
Isol. from *Aplidium lobatum*.
$[\alpha]_D$ -15.5 (c, 0.11 in MeOH). λ_{max} 280 (log ϵ 4.04) (MeOH).

*24*E-*Isomer, 30-hydroxy:* ***Lobatamide F***
[215722-35-3]
$C_{27}H_{32}N_2O_9$ 528.558
Isol. from *Aplidium lobatum*.
$[\alpha]_D$ -19.2 (c, 0.07 in MeOH). λ_{max} 280 (log ϵ 4.17) (MeOH).

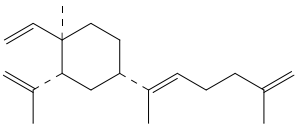
26Z-Isomer: ***Lobatamide B***
[200563-48-0]
$C_{27}H_{32}N_2O_8$ 512.558
Isol. from *Aplidium lobatum*. Cytotoxic agent. $[\alpha]_D$ -15 (c, 0.03 in MeOH). λ_{max} 281 (log ϵ 4.55) (MeOH).

26Z-Isomer, 30-hydroxy: ***Lobatamide E***
[215722-32-0]
$C_{27}H_{32}N_2O_9$ 528.558
Isol. from *Aplidium lobatum*.
$[\alpha]_D$ -26.7 (c, 0.06 in MeOH). λ_{max} 282 (log ϵ 4.25) (MeOH).

Stereoisomer (?): ***Antibiotic YM 75518***. *YM 75518*
[199165-90-7]
$C_{27}H_{32}N_2O_8$ 512.558
Prod. by *Pseudomonas* sp. Q38009. Antifungal agent. Amorph. powder.
Mp 126-128°. $[\alpha]_D^{25}$ -13.9 (c, 3.7 in MeOH). λ_{max} 211 (log ϵ 4.04); 282 (log ϵ 3.95) (EtOH).

Suzumura, K. *et al., Tet. Lett.*, 1997, **38**, 7573-7576 (*YM 75518*)
McKee, T.C. *et al., J.O.C.*, 1998, **63**, 7805-7810 (*isol, uv, ir, pmr, cmr, ms*)
Shen, R. *et al., J.A.C.S.*, 2002, **124**, 5650-5651; 2003, **125**, 7889-7901 (*synth, abs config*)

8,10,13(15),18-Lobatetraene L-204

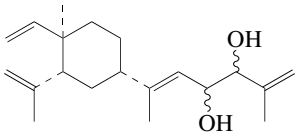


$C_{20}H_{32}$ 272.473

13(15)*E-form*
Ineleganene
[274683-41-9]
Constit. of *Sinularia inelegans*.
Oil. $[\alpha]_D^{25}$ +9.6 (c, 0.1 in $CHCl_3$).

Chai, M.-C. *et al., J. Nat. Prod.*, 2000, **63**, 843-844 (*isol, pmr, cmr*)

8,10,13(15),18-Lobatetraene-16,17-diol L-205

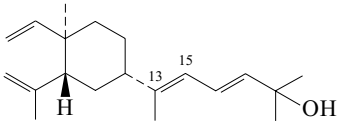


$C_{20}H_{32}O_2$ 304.472
Isol. from *Lobophytum microlobulatum*. Oil. $[\alpha]_D^{25}$ +20.6 (c, 1 in $CHCl_3$).

Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 1294-1303 (*isol, ir, pmr, cmr*)

8,10,13(15),16-Lobatetraen-18-ol L-206

Fuscol
[70206-91-6]



$C_{20}H_{32}O$ 288.472
Constit. of *Eunicea fusca*. Oil. $[\alpha]_D$ +17.6 (c, 0.9 in $CHCl_3$). λ_{max} 240 (ϵ 40000) (MeOH) (Derep).

O-*β*-D-*Arabinopyranosyl:* ***Fuscoside B***
[133470-56-1]
$C_{25}H_{40}O_5$ 420.588
Constit. of *Eunicea fusca*. Antiinflammatory agent. Oil. $[\alpha]_D$ -90 (c, 1 in $CHCl_3$). λ_{max} 241 (ϵ 44000) (MeOH) (Derep).

13ξ,15ξ-Epoxide (isomer 1), O-*β*-D-*arabinopyranosyl:* ***Fuscoside C***
[133470-58-3]
$C_{25}H_{40}O_6$ 436.587
Constit. of *Eunicea fusca*. Antiinflammatory agent.

13ξ,15ξ-Epoxide (isomer 2), O-*β*-D-*arabinopyranosyl:* ***Fuscoside D***
$C_{25}H_{40}O_6$ 436.587
Constit. of *Eunicea fusca*. Antiinflammatory agent.

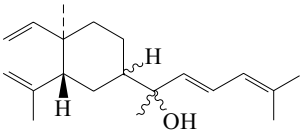
Me ether: ***Fuscol methyl ether***
[171297-73-7]
$C_{21}H_{34}O$ 302.499
Constit. of *Lobophytum pauciflorum*. Toxic to brine shrimp. Oil. $[\alpha]_D^{25}$ +14.9 (c, 0.9 in $CHCl_3$). $[\alpha]_D$ -2.6 (c, 0.33 in $CHCl_3$). λ_{max} 199 (ϵ 8690) (hexane). λ_{max} 199 (ϵ 8690); 240 (ϵ 1710) (MeOH) (Berdy).

13ξ,15ξ-Epoxide: 13,15-Epoxy-8,10,16-lobatrien-18-ol
$C_{20}H_{32}O_2$ 304.472
Constit. of *Lobophytum hirsutum*. Oil. Mixt. of C-13, C-15-diastereoisomers.

Gopichand, Y. *et al., Tet. Lett.*, 1978, 3641
Shin, J. *et al., J.O.C.*, 1991, **56**, 3153 (*isol, pmr, cmr*)
Iwashima, M. *et al., Tet. Lett.*, 1992, **33**, 81 (*synth*)
Raju, B.L. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 221 (*epoxide*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 1074 (*Me ether*)
Edrada, R.A. *et al., J. Nat. Prod.*, 1998, **61**, 358-361 (*Me ether*)
Kosugi, H. *et al., J.C.S. Perkin 1*, 1998, 217-222 (*synth*)

8,10,15,17-Lobatetraen-13-ol L-207

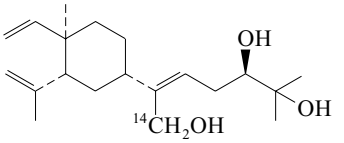
Isofuscol
[105377-88-6]



$C_{20}H_{32}O$ 288.472
Isol. from *Eunicea fusca*. Oil. $[\alpha]_D$ +8.3 (c, 0.5 in $CHCl_3$). Possibly an artifact derived from 8,10,13(15),16-Lobatetraen-18-ol, L-206.

Coll, J.C. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 815 (*isol, pmr*)

8,10,13(15)-Lobatriene-14,17,18-triol L-208



$C_{20}H_{34}O_3$ 322.487

(17*R*)-*form*
Lobatrientriol
[139579-30-9]
Constit. of *Sinularia flexibilis.*
Oil. $[\alpha]_D^{25}$ +15 (c, 0.2 in $CHCl_3$).

14-Ac: [71593-04-9]
$C_{22}H_{36}O_4$ 364.524
Constit. of *Lobophytum* sp. Yellow oil.

14,17-Di-Ac: [71593-08-3]
$C_{24}H_{38}O_5$ 406.561
Constit. of *Lobophytum* sp. Yellow oil. $[\alpha]_D^{25}$ +60 (c, 0.13 in $CHCl_3$).

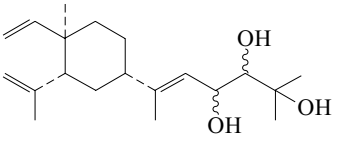
14-Deoxy: ***8,10,13(15)-Lobatriene-17,18-diol***
[71593-07-2]
$C_{20}H_{34}O_2$ 306.487
Constit. of *Lobophytum* sp. Cryst. (EtOAc). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 195.3-197.1°. $[\alpha]_D^{25}$ +25.9 (c, 0.34 in $CHCl_3$).

14-Deoxy, 17-Ac: [203798-91-8]
$C_{22}H_{36}O_3$ 348.525
Constit. of *Lobophytum pauciflorum*. Yellow viscous oil. $[\alpha]_D$ +52.7 (c, 1.56 in $CHCl_3$). λ_{max} 199 (ϵ 4350) (hexane).

Dunlop, R.W. *et al., Aust. J. Chem.*, 1979, **32**, 1345
Hamada, T. *et al., Chem. Lett.*, 1992, 33 (*isol, pmr, cmr*)
Nagaoka, H. *et al., Chem. Pharm. Bull.*, 1992, **40**, 556 (*synth*)
Edrada, R.A. *et al., J. Nat. Prod.*, 1998, **61**, 358-361 (*14-deoxy-17-Ac*)
Kato, M. *et al., J.C.S. Perkin 1*, 1999, 783-788 (*synth*)

8,10,13(15)-Lobatriene-16,17,18-triol L-209

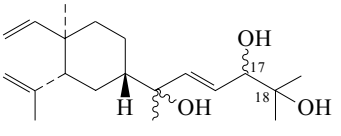
[150312-95-1]



$C_{20}H_{34}O_3$ 322.487
Constit. of a *Lobophytum* sp. Cryst.
Mp 73-75°. $[\alpha]_D$ -14.1 (c, 1 in $CHCl_3$).

Raju, B.L. *et al., J. Nat. Prod.*, 1993, **56**, 961 (*isol, pmr, cmr*)

8,10,15-Lobatriene-13,17,18-triol L-210

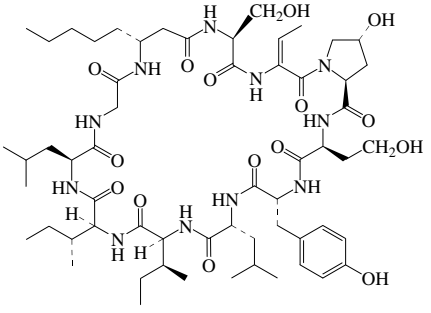


$C_{20}H_{34}O_3$ 322.487

(13ξ,15*E*,17ξ)-*form* [185223-58-9]
Constit. of a *Lobophytum* sp.

17,18-Di-Ac: [171297-72-6]
$C_{24}H_{38}O_5$ 406.561
Constit. of a *Lobophytum* sp. Oil.
Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 1071-1073; 1996, **35**, 1294 (*isol, pmr, cmr*)

Lobocyclamide A L-211

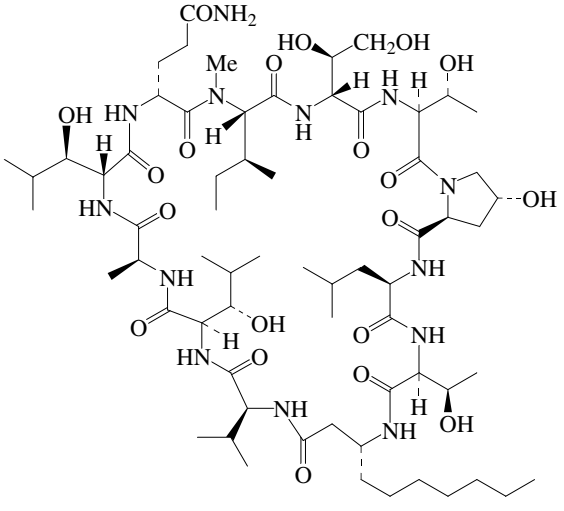


Absolute Configuration

$C_{59}H_{95}N_{11}O_{15}$ 1198.464
Closely related to Laxaphycin A, L-83. Isol. from *Lyngbya confervoides*. Shows moderate antifungal activity. Amorph. powder. $[\alpha]_D$ +33 (c, 0.17 in MeOH).
MacMillan, J.B. *et al., J.O.C.*, 2002, **67**, 8210-8215 (*isol, pmr, cmr*)

Lobocyclamide B L-212

[440103-61-7]

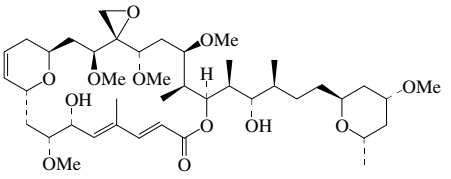


$C_{65}H_{115}N_{13}O_{20}$ 1398.699
Isol. from *Lyngbya confervoides*. Shows moderate antifungal activity. Amorph. powder. $[\alpha]_D$ -13 (c, 0.22 in MeOH).
MacMillan, J.B. *et al., J.O.C.*, 2002, **67**, 8210-8215 (*isol, pmr, cmr*)

Lobocyclamide C L-213

As Lobocyclamide B, L-212 with
R = $-(CH_2)_4CH_3$
$C_{63}H_{111}N_{13}O_{20}$ 1370.645
Isol. from *Lyngbya confervoides*. Amorph. powder. $[\alpha]_D$ -16 (c, 0.2 in MeOH).
MacMillan, J.B. *et al., J.O.C.*, 2002, **67**, 8210-8215 (*isol, pmr, cmr*)

Lobophorolide L-214

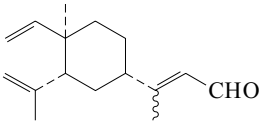


Absolute Configuration

$C_{42}H_{70}O_{12}$ 767.008
Macrolide antibiotic. Similar to Tolytoxin, T-356. Isol. from the brown alga *Lobophora variegata*. Antifungal agent. Amorph. solid. $[\alpha]_D^{25}$ -33 (c, 0.07 in MeOH). λ_{max} 262 (log ϵ 4) (MeOH).
Kubanek, J. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2003, **100**, 6916-6921 (*isol, cd, pmr, cmr, ms*)

Lobophytal L-215

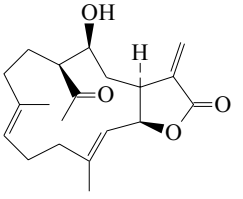
[139694-47-6]



$C_{16}H_{24}O$ 232.365
Constit. of *Lobophytum pauciflorum*. Pale yellow oil. $[\alpha]_D^{25}$ +33 (c, 1 in $CHCl_3$). Not related to Lobophytol, L-216. λ_{max} 240 ($CHCl_3$).
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 1074-1079 (*isol, pmr, cmr*)

Lobophytol L-216

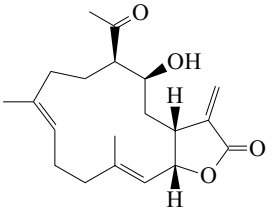
[134175-15-8]



$C_{20}H_{28}O_4$ 332.439
Struct. revised in 1991. Constit. of *Lobophytum pauciflorum*. Cryst.
Mp 147-149°. $[\alpha]_D$ -12.5 (c, 0.8 in $CHCl_3$).
Ac: Lobophytol acetate
$C_{22}H_{30}O_5$ 374.476
Constit. of *Lobophytum pauciflorum*. Cryst.
Mp 119°. $[\alpha]_D$ -82 (c, 1.7 in $CHCl_3$).
Yamada, Y. *et al., Chem. Pharm. Bull.*, 1979, **27**, 2394 (*isol*)
Iguchi, K. *et al., Chem. Lett.*, 1991, 319 (*isol, pmr, cmr, struct*)

Lobophytum lactone L-217

[77449-20-8]



$C_{20}H_{28}O_4$ 332.439

Constit. of *Lobophytum pauciflorum*. Cryst. (MeOH).
Mp 147-149°. $[\alpha]_D$ -12.5 (c, 0.8 in $CHCl_3$).

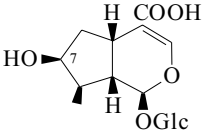
Ac: [77449-19-5]
$C_{22}H_{30}O_5$ 374.476
Constit. of *Lobophytum pauciflorum*. Cryst. (MeOH).
Mp 119°. $[\alpha]_D$ -82 (c, 1.7 in $CHCl_3$).

[67240-44-2, 72629-70-0]

Yamada, Y. *et al., Chem. Pharm. Bull.*, 1979, **27**, 2394 (*isol*)
Yamada, Y. *et al., Tet. Lett.*, 1980, 3911 (*struct*)

Loganic acid L-218

[22255-40-9]

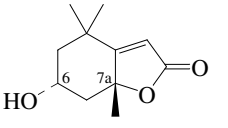


$C_{16}H_{24}O_{10}$ 376.36
Constit. of *Swertia caroliniensis* and *Dipsacus asperoides*. Powder.
Mp 168° dec. $[\alpha]_D^{26}$ -86.2 (c, 0.5 in H_2O).

*8-Epimer, 7-*O*-(5-phenyl-2,4-pentadienoyl)(*E,E*-), Me ester:* ***7-O-(5-Phenyl-2,4-pentadienoyl)-8-epiloganin***
[97857-27-7]
$C_{28}H_{34}O_{11}$ 546.57
Constit. of *Avicennia marina*. λ_{max} 308 (log ε 4.3) (MeOH).
Koenig, G. *et al., Phytochemistry*, 1985, **24**, 1245-1248 (*Phenylpentadienoylepiloganin*)

Loliolide L-219

*5,6,7,7*a*-Tetrahydro-6-hydroxy-4,4,7*a*-trimethyl-2(4*H*)-benzofuranone, 9CI. Digiprolactone. Calendin*
[10481-90-0, 33824-59-8]



(6*R*,7a*R*)-*form*

$C_{11}H_{16}O_3$ 196.246
λ_{max} 214 (ε 14800) (MeOH) (Derep).

(6R,7aR)-form [147730-52-7]
Isol. from *Viburnum dilatum*.
Needles (Et_2O/hexane).
Mp 121.5-122.5°. $[\alpha]_D^{21}$ -89.6 ($CHCl_3$).

(6R,7aS)-form [81444-64-6]
Isol. from *Cystophora moniliformis*.
Needles (EtOAc/hexane).
Mp 153.5-154°. $[\alpha]_D^{20}$ +105.5 ($CHCl_3$).

(6S,7aR)-form [5989-02-6]
Constit. of *Lolium perenne* and many other plants incl. *Eucommia ulmoides*, *Digitalis lanata*, *Fumaria officinalis*, *Nicandra physaloides*, *Digitalis purpurea*, *Xanthoxylum setulosum*, *Undaria pinnatifida*, *Cystophora moniliformis*, *Calendula officinalis*, *Euphorbia supina*, *Acanthospermum hispidum*, *Acanthosyris paulo-alvini*, *Malachra fasciata*, also from the mollusc *Dolabella ecaudata* and the brown alga *Sargassum crassifolium*,. Germination inhibitor, cytostatic against carcnoma and leukaemia cells, and a repellent for ants (*Atta cephalotes*). Needles (EtOAc/hexane).
Mp 152.5-153°. $[\alpha]_D^{20}$ -107.2 (c, 1 in $CHCl_3$). λ_{max} 214 (ε 10830); 217 (ε 11000) (EtOH) (Berdy).

O-*β*-*D*-*Glucopyranoside:* [82395-89-9]
$C_{17}H_{26}O_8$ 358.388
Constit. of flue-dried tobacco *Nicotiana tabacum*.
$[\alpha]_D$ -21.25 (c, 0.08 in EtOH).

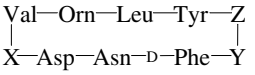
Ac: $[\alpha]_D^{15}$ -65.2 ($CHCl_3$).

6-Ketone: ***Dehydrololiolide***
[1133-04-6]
$C_{11}H_{14}O_3$ 194.23
Constit. of *Nicotiana tabacum*.

(6S,7aS)-form
Isololiolide. Epiloliolide
[38274-00-9]
Constit. of *Eirmocephala megaphylla* (preferred genus name *Vernonia*), the brown alga *Sargassum crassifolium*, the marine sponge *Tedania ignis*, and Greek tobacco. Phytotoxin. Needles (Et_2O/hexane). Sol. $CHCl_3$.
Mp 122-122.5°. $[\alpha]_D^{22}$ +91.4 ($CHCl_3$). λ_{max} 214 (ε 7409) (MeOH) (Berdy).

Hodges, R. *et al., Tetrahedron*, 1964, **20**, 1463-1467 (*6S,7aR-form, isol, uv, ir, pmr, ms*)
Marx, J.N. *et al., Tetrahedron, Suppl.*, No. 8, 1966, 1-7 (*synth*)
Isoe, S. *et al., Tet. Lett.*, 1972, 2517-2520 (*abs config*)
Cadosch, H. *et al., Helv. Chim. Acta*, 1974, **57**, 1466-1472 (*cd*)
Kienzle, F. *et al., Helv. Chim. Acta*, 1978, **61**, 2616-2627 (*6S,7aR-form, synth*)
Uegaki, R. *et al., Agric. Biol. Chem.*, 1979, **43**, 1149-1150 (*Dehydrololiolide*)
Petit, G.R. *et al., J. Nat. Prod.*, 1980, **43**, 752-755 (*isol, activity*)
Kodama, H. *et al., Agric. Biol. Chem.*, 1982, **46**, 1409-1411 (*glucoside*)
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 171-182 (*6R,7aS-form, isol*)
Takazawa, O. *et al., Chem. Lett.*, 1983, 63-64 (*synth*)
Rouessac, F. *et al., Tet. Lett.*, 1983, **24**, 2247-2250 (*synth*)
Zamarlik, H. *et al., Can. J. Chem.*, 1984, **62**, 2326-2329 (*synth*)
Mori, K. *et al., Annalen*, 1993, 77-82 (*isomers, synth*)
Tamura, H. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1902-1903 (*Dehydrololiolide, synth*)
Okada, N. *et al., Phytochemistry*, 1994, 37; 281-282 (*6S,7aR-form, isol, pmr*)
Borkosky, S. *et al., Phytochemistry*, 1996, **42**, 1637-1639 (*Epiloliolide*)
Hiraga, Y. *et al., Nat. Prod. Lett.*, 1997, **10**, 181-186 (*pmr, cmr*)
Jones, L. *et al., Fitoterapia*, 2000, **71**, 580-583 (*Calendin, pmr, cmr*)
Kuba, M. *et al., Chem. Lett.*, 2002, 1248-1249 (*6S,7aR-form, synth*)

Loloatins L-220



Loloatin A	X = Tyr, Y = Phe, Z = Pro
Loloatin B	X = Trp, Y = Phe, Z = Pro
Loloatin C	X = Y = Trp, Z = Pro
Loloatin D	X = Trp, Y = Phe, Z = 4*R*-Hydroxy-Pro

Cyclic decapeptide antibiotic complex. Prod. by a marine bacterium; possibly a *Bacillus* sp. Antibacterial agents. λ_{max} 220 (ε 43000); 280 (ε 5900) (MeOH) (Berdy).

Loloatin A
$C_{65}H_{84}N_{12}O_{15}$ 1273.45
Powder. $[\alpha]_D$ -88 (EtOH). λ_{max} 224 (ε 21000); 278 (ε 3400) (MeOH) (Berdy).

Loloatin B [182422-45-3]
$C_{67}H_{85}N_{13}O_{14}$ 1296.487
Mp 229-233°. $[\alpha]_D$ -80 (EtOH). λ_{max} 220 (ε 43000); 280 (ε 5900) (EtOH).

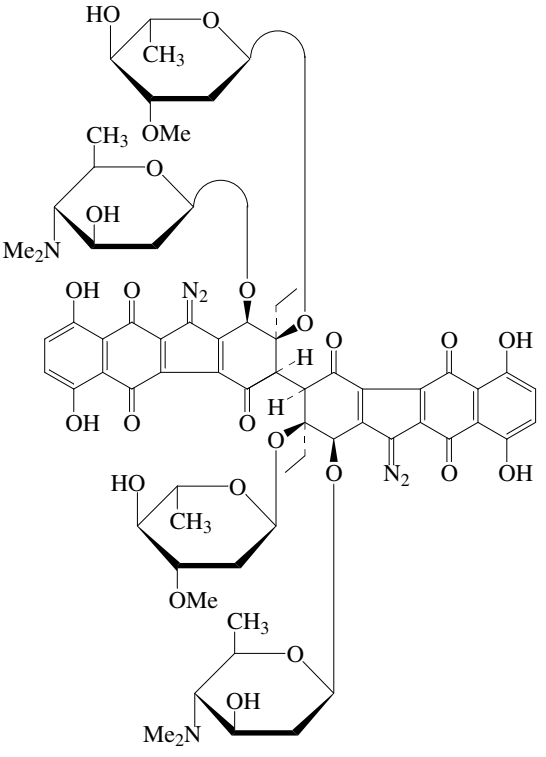
Loloatin C
$C_{69}H_{86}N_{14}O_{14}$ 1335.524
Mp 239-243°. $[\alpha]_D$ -76 (EtOH). λ_{max} 223 (ε 66000); 280 (ε 10000) (EtOH). λ_{max} 223 (ε 66000); 280 (ε 10000) (MeOH) (Berdy).

Loloatin D
$C_{67}H_{85}N_{13}O_{15}$ 1312.487
Powder.

Gerard, J.M. *et al., J. Nat. Prod.*, 1999, **62**, 80-85 (*isol, uv, ir, pmr, cmr, ms*)

Scherkenbeck, J. *et al., Eur. J. Org. Chem.*, 2002, 2350-2355 (*synth*)
Chen, H. *et al., Eur. J. Org. Chem.*, 2004, 31-37 (*Loloatin C, pmr, conformn*)

Lomaiviticin A L-221

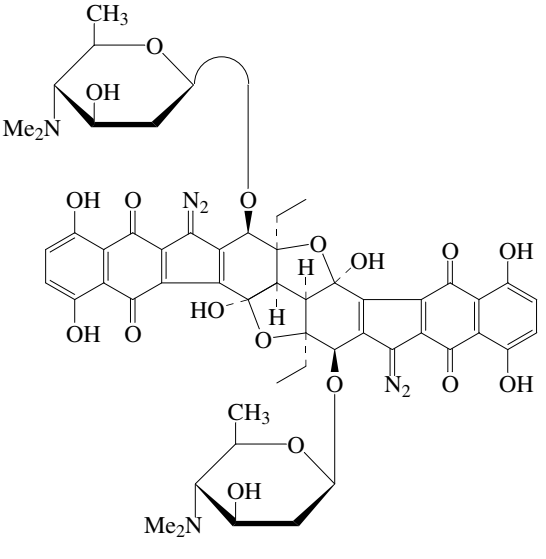


$C_{68}H_{80}N_6O_{24}$ 1365.406

Related to Kinamycin F. Prod. by the marine-derived *Micromonospora lomaivitiensis* (strain LL-37I366). Potent antitumour agent and active against gram-positive bacteria. Amorph. red powder. $[\alpha]_D$ -101.4 (c, 0.07 in MeOH).

He, H. *et al., J.A.C.S.*, 2001, **123**, 5362-5363

Lomaiviticin B L-222



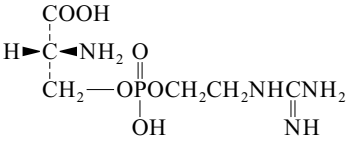
$C_{54}H_{56}N_6O_{18}$ 1077.066

Prod. by the marine-derived *Micromonospora lomaivitiensis* (strain LL-37I366). Potent antitumour agent and active against gram-positive bacteria. Amorph. red powder. $[\alpha]_D$ -71.4 (c, 0.07 in MeOH).

He, H. *et al., J.A.C.S.*, 2001, **123**, 5362-5363

Lombricine L-223

Serine 2-[(aminoiminomethyl)amino]ethyl hydrogen phosphate (ester), 9CI. O^3*-(2-Guanidinoethoxyphosphinicoserine). Lumbricine*



(*R*)–*form*

$C_6H_{15}N_4O_6P$ 270.181

(*R*)-*form*

D-form

Constit. of *Ophelia bicornis* muscle.

Mp 229-230°. $[\alpha]_D^{25.4}$ +14.4 (c, 0.917 in H_2O).

$N^{(\omega)}$*-Phosphonyl:* ***Phospholombricine***. N-*Phosphoryllombricine. Lombricine phosphate*

[25540-15-2]

$C_6H_{16}N_4O_9P_2$ 350.161

Isol. from *Lumbricus terrestris* and other earthworms. High-energy phosphate regulator.

Characterised as a cryst. $NH_4^{\oplus}$ salt and as other salts.

(*S*)-*form*

L-form

[18416-85-8]

Constit. of the body wall muscle of the echiuroid worm *Thalassema neptuni.*

Cryst. (EtOH aq.).

Mp 233°. $[\alpha]_D^{25}$ -11.3 (c, 0.380 in H_2O). pK_{a1} 2; pK_{a2} 8.9 (20°).

α-N,N-*Di-Me:* ***Thalassemine***

[40524-74-1]

$C_8H_{19}N_4O_6P$ 298.235

Constit. of viscera of *Thalassema neptuni*. Cryst. + $1H_2O$ (H_2O).

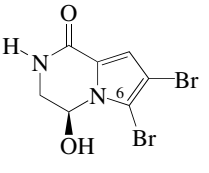
Mp 184°. $[\alpha]_D^{26}$ -11.3 (c, 0.919 in H_2O).

[18555-02-7]

Thoai, N.-V. *et al., Biochim. Biophys. Acta*, 1954, **14**, 76 (*isol*)
Pant, R. *et al., Biochem. J.*, 1959, **73**, 30 (*isol*)
Ennor, A.H. *et al., Biochem. J.*, 1962, **83**, 14 (*Phospholombricine*)
Dubey, S.S. *et al., Indian J. Chem.*, 1963, **1**, 453 (*isol*)
Beatty, I.M. *et al., J.C.S.*, 1965, 12 (*synth, Phospholombricine*)
Thoai, N.-V. *et al., Biochemistry*, 1972, **11**, 3890 (*isol*)
Everby, M.R. *et al., J. Chromatogr.*, 1988, **445**, 433

Longamide† L-224

*6,7-Dibromo-3,4-dihydro-4-hydroxypyrrolo[1,2-*a*]pyrazin-1(2*H*)-one, 9CI*



$C_7H_6Br_2N_2O_2$ 309.945

(*S*)-*form* [170891-48-2]

Isol. from the Caribbean sponge *Agelas longissima* and by *Homaxinella* sp. Shows moderate antibacterial activity. Sol. MeOH, butanol. $[\alpha]_D$ +86 (c, 0.001 in MeOH). λ_{max} 209 (ε 16200); 230 (ε 8100); 276 (ε 7700) (MeOH) (Berdy).

(±)-*form* [219783-00-3]

Alkaloid from the sponge *Homaxinella* sp.

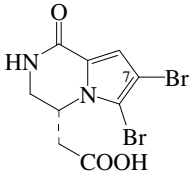
(ξ)-*form*

6-Debromo: 6-Debromolongamide. ***Mukanadine C***
[203579-34-4]
$C_7H_7BrN_2O_2$ 231.049
Isol. from the sponge *Axinella carteri* and *Agelas nakamurai*. Yellow powder. $[\alpha]_D$ -6 (c, 0.08 in MeOH). Stereochem. not determined for either isolate.

Cafieri, F. *et al., Tet. Lett.*, 1995, **36**, 7893-7896 (*isol, uv, ir, pmr, cmr, cd, struct*)
Li, C.-J. *et al., J. Nat. Prod.*, 1998, **61**, 387-389 (*deriv, isol, pmr, cmr*)
Umeyama, A. *et al., J. Nat. Prod.*, 1998, **61**, 1433-1434 (*isol*)
Uemoto, H. *et al., J. Nat. Prod.*, 1999, **62**, 1581-1583 (*Mukanadine C*)
Marchais, S. *et al., Tet. Lett.*, 1999, **40**, 5519-5522 (*synth*)

Longamide B L-225

*6,7-Dibromo-1,2,3,4-tetrahydro-1-oxopyrrolo[1,2-*a*]pyrazine-4-acetic acid, 9CI*



(*R*)-*form*

$C_9H_8Br_2N_2O_3$ 351.982

(*R*)-*form*

Me ester: [219782-99-7]
$C_{10}H_{10}Br_2N_2O_3$ 366.009
Alkaloid from the sponge *Agelas ceylonica*.
$[\alpha]_D$ +7 (c, 1 in MeOH).

7-Debromo, Me ester: [335022-79-2]
$C_{10}H_{11}BrN_2O_3$ 287.113
Alkaloid from the sponge *Axinella tenuidigitata*. Solid. $[\alpha]_D^{25}$ +8.2 (c, 0.5 in MeOH). λ_{max} 220 (ϵ 29600); 244 (ϵ 12100); 303 (ϵ 8130) (MeOH).

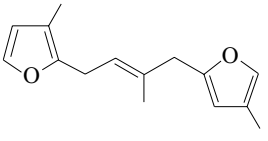
(±)-*form* [200264-70-6]
Isol. from the sponge *Agelas dispar*.
Amorph. solid. λ_{max} 210 (ϵ 12100); 230 (ϵ 8500); 280 (ϵ 7700) (MeCN). λ_{max} 210 (ϵ 12100); 230 (ϵ 7700); 280 (ϵ 8500) (MeOH) (Berdy).

Et ester: ***Hanishin***
[196303-62-5]
$C_{11}H_{12}Br_2N_2O_3$ 380.035
Alkaloid from the sponges *Acanthella carteri* and *Homaxinella* sp. Semisolid. λ_{max} 203 (ϵ 17800); 230 (ϵ 10000); 280 (ϵ 6500) (MeOH).

Mancini, I. *et al., Tet. Lett.*, 1997, **38**, 6271-6274 (*Hanishin*)
Cafieri, F. *et al., J. Nat. Prod.*, 1998, **61**, 122-125 (*Hanishin*)
Umeyama, A. *et al., J. Nat. Prod.*, 1998, **61**, 1433-1434 (*Hanishin*)
Reddy, N.S. *et al., Biochem. Syst. Ecol.*, 2000, **28**, 1035-1037 (*Me ester, isol*)
Reddy, N.S. *et al., Indian J. Chem., Sect. B*, 2000, **39**, 971-972 (*7-debromo Me ester*)
Patel, J. *et al., J.O.C.*, 2005, **70**, 9081-9084 (*synth, abs config*)

Longifolin L-226

3-Methyl-2-[3-methyl-4-(4-methyl-2-furanyl)-2-butenyl]furan, 9CI
[39007-94-8]

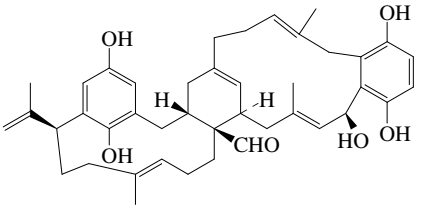


$C_{15}H_{18}O_2$ 230.306
Constit. of *Actinodaphne longifolia*, also from sponge *Pleraplysilla spinifera* and its predator *Glossodoris gracilis.* Oil.

Hayashi, N. *et al., Chem. Ind. (London)*, 1972, 572
Cimino, G. *et al., Bull. Soc. Chim. Belg.*, 1980, **89**, 1069-1073 (*isol*)

Longithorol B L-227

[245738-15-2]



Relative Configuration

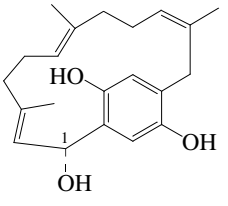
$C_{42}H_{52}O_6$ 652.869
Constit. of *Aplidium longithorax*. Amorph. powder (as penta-Ac). $[\alpha]_D$ +20.3 (c, 1.8 in MeOH) (penta-Ac).

Stereoisomer: ***Longithorol A***
[245738-14-1]
$C_{42}H_{52}O_6$ 652.869
Constit. of *Aplidium longithorax*. Amorph. solid (as penta-Ac). $[\alpha]_D$ +114.3 (c, 2 in MeOH) (penta-Ac). Stereochem. not fully resolved.

Fu, X. *et al., J. Nat. Prod.*, 1999, **62**, 1306-1310 (*isol, pmr, cmr*)

Longithorol C L-228

[247921-70-6]



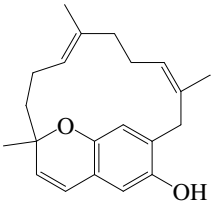
$C_{21}H_{28}O_3$ 328.45
Constit. of *Aplidium longithorax*. Yellow gum. $[\alpha]_D$ -136 (c, 0.613 in MeOH). λ_{max} 207 (ϵ 11000); 234 (sh) (ϵ 5000); 301 (ϵ 2000) (MeOH).

1-Me ether: ***Longithorol D***
[247921-71-7]
$C_{22}H_{30}O_3$ 342.477
Constit. of *Aplidium longithorax*. Yellow gum. $[\alpha]_D$ -125 (c, 0.013 in MeOH). λ_{max} 203 (ϵ 7000); 229 (sh) (ϵ 4000); 304 (ϵ 1000) (MeOH).

Davis, R.A. *et al., J. Nat. Prod.*, 1999, **62**, 1405-1409 (*isol, pmr, cmr, abs config*)

Longithorol E L-229

[247921-72-8]

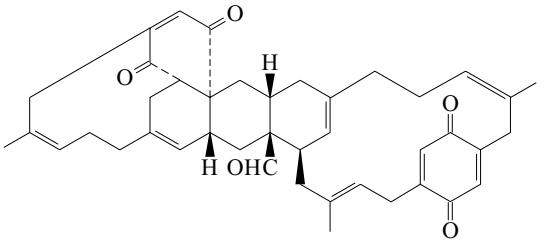


$C_{21}H_{26}O_2$ 310.435
Constit. of *Aplidium longithorax*. Yellow gum. $[\alpha]_D$ +135 (c, 0.127 in MeOH). λ_{max} 203 (ϵ 7000); 228 (ϵ 6000); 271 (sh) (ϵ 2000); 327 (ϵ 1000) (MeOH).

Davis, R.A. *et al., J. Nat. Prod.*, 1999, **62**, 1405-1409 (*isol, pmr, cmr*)

Longithorone A L-230

[159736-39-7]



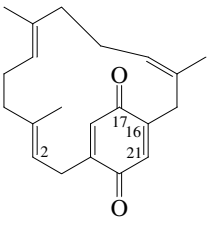
$C_{42}H_{46}O_5$ 630.822

Dimeric prenylated quinone. Isol. from the tunicate *Aplydium longithorax*. Weak cytotoxic agent. Cryst. ($MeOH/CH_2Cl_2$). Mp 195-196°. $[\alpha]_D$ -87.5 (c, 2.7 in $CHCl_3$). λ_{max} 250 (ϵ 14700); 300 (ϵ 3500) (EtOH) (Derep).

Fu, X. *et al., J.A.C.S.*, 1994, **116**, 12125-12126 (*isol, uv, ir, pmr, cmr, cryst struct*)
Fu, X. *et al., J.O.C.*, 1997, **62**, 3810-3819 (*cmr*)
Layton, M.E. *et al., J.A.C.S.*, 2002, **124**, 773-775 (*synth*)
Nicolaou, K.C. *et al., Classics in Total Synthesis II: More Targets, Strategies, Methods*, Wiley-VCH, 2003, 465 (*rev, synth*)
Morales, C.A. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2004, **101**, 12036-12041 (*synth*)

Longithorone B L-231

[190837-20-8]



$C_{21}H_{26}O_2$ 310.435

Isol. from the tunicate *Aplidium longithorax*. Cryst. ($MeOH/CH_2Cl_2$).
Mp 80-82°. $[\alpha]_D$ -92.4 (c, 0.57 in CH_2Cl_2). λ_{max} 258 (ϵ 14228) (EtOH).

(2Z)-Isomer: ***Longithorone C***
[190913-23-6]
$C_{21}H_{26}O_2$ 310.435
Isol. from *Aplidium longithorax*.
$[\alpha]_D$ -15 (c, 0.07 in CH_2Cl_2). λ_{max} 260 (ϵ 15125) (EtOH).

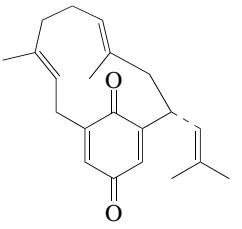
16α,21-Dihydro: ***Longithorone K***
$C_{21}H_{28}O_2$ 312.451
Isol. from *Aplidium longithorax*. Unstable pale yellow gum. $[\alpha]_D$ +61 (c, 0.05 in CH_2Cl_2). λ_{max} 237 (ϵ 6600) (MeOH).

16α,21-Dihydro, 17β-alcohol: ***Longithorone J***
$C_{21}H_{30}O_2$ 314.467
Isol. from *Aplidium longithorax*. Unstable solid. $[\alpha]_D$ +170 (c, 0.08 in CH_2Cl_2). λ_{max} 233 (ϵ 6800) (MeOH).

Fu, X. *et al., J.O.C.*, 1997, **62**, 3810-3819 (*isol, uv, ir, pmr, cmr, cryst struct*)
Davis, R.A. *et al., J. Nat. Prod.*, 1999, **62**, 158-160 (*Longithorones J-K*)
Kato, T. *et al., Tet. Lett.*, 1999, **40**, 1941-1944 (*synth*)

Longithorone D L-232

[190313-24-7]



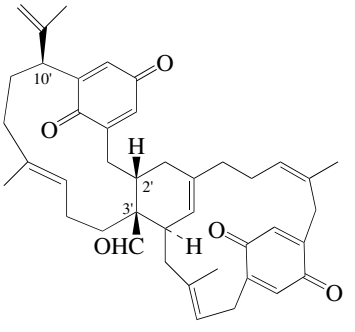
$C_{21}H_{26}O_2$ 310.435

Apparently incorrectly indexed in CA. Isol. from the tunicate *Aplidium longithorax*. Cryst. ($MeOH/CH_2Cl_2$).
Mp 127-129°. $[\alpha]_D$ -305.3 (c, 0.23 in CH_2Cl_2). λ_{max} 256 (ϵ 10370) (EtOH).

Fu, X. *et al., J.O.C.*, 1997, **62**, 3810-3819 (*isol, uv, ir, pmr, cmr, cryst struct*)

Longithorone E L-233

[190837-55-9]



$C_{42}H_{48}O_5$ 632.838

Constit. of *Aplydium longithorax*. Yellow needles.
Mp >230° dec. $[\alpha]_D$ -35.4 (c, 0.48 in $CHCl_3$). λ_{max} 258 (ϵ 23920) (EtOH).

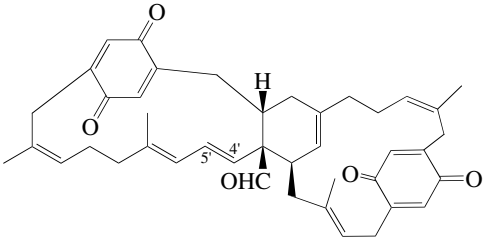
Atropisomer: ***Longithorone F***
[190913-25-8]
$C_{42}H_{48}O_5$ 632.838
Constit. of *Aplydium longithorax*. Amorph. powder. $[\alpha]_D$ -65.2 (c, 0.89 in $CHCl_3$). λ_{max} 258 (ϵ 24940) (EtOH).

2′,3′,10′-Triepimer: ***Longithorone G***
[190913-26-9]
$C_{42}H_{48}O_5$ 632.838
Constit. of *Aplydium longithorax*. Amorph. powder. $[\alpha]_D$ +73.5 (c, 0.34 in $CHCl_3$). λ_{max} 258 (ϵ 25698) (EtOH).

Fu, X. *et al., J.O.C.*, 1997, **62**, 3810-3819 (*isol, pmr, cmr, cryst struct, uv, ir*)

Longithorone H L-234

[190838-19-8]



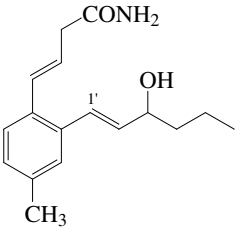
$C_{42}H_{46}O_5$ 630.822

Isol. from the tunicate *Aplidium longithorax*. Amorph. powder. $[\alpha]_D$ -51 (c, 0.2 in $CHCl_3$). λ_{max} 240 (ϵ 11340); 260 (ϵ 15360) ($CHCl_3$).

4′,5′-Dihydro: ***Longithorone I***
[190838-01-8]
$C_{42}H_{48}O_5$ 632.838
Isol. from *Aplidium longithorax*.
$[\alpha]_D$ -49.5 (c, 0.07 in CH_2Cl_2). λ_{max} 256 (ϵ 10930) (EtOH).
Fu, X. *et al., J.O.C.*, 1997, **62**, 3810-3819 (*isol, uv, ir, pmr, cmr*)

Lorneamide A L-235

4-[2-(3-Hydroxy-1-hexenyl)-4-methylphenyl]-3-butenamide
[313951-44-9]

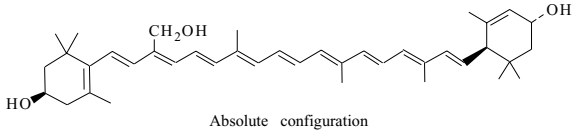


$C_{17}H_{23}NO_2$ 273.374
Alkaloid from a marine actinomycete (MST-MA190). Glass. $[\alpha]_D^{19}$ -7.2 (c, 0.2 in MeOH). λ_{max} 239 (log ϵ 4.09); 263 (log ϵ 3.96) (MeOH).

1′,2′-Dihydro, 3′-ketone: 4-[4-Methyl-2-(3-oxohexyl)phenyl]-3-butenamide. ***Lorneamide B***
[313951-45-0]
$C_{17}H_{23}NO_2$ 273.374
Alkaloid from a marine actinomycete (MST-MA190). Glass. λ_{max} 209 (log ϵ 4); 253 (log ϵ 3.8) (MeOH).
Capon, R.J. *et al., J. Nat. Prod.*, 2000, **63**, 1682-1683 (*Lorneamides A,B*)

Loroxanthin L-236

β,ϵ-Carotene-3,3′,19-triol. 19-Hydroxylutein. Trollein
[27637-71-4]

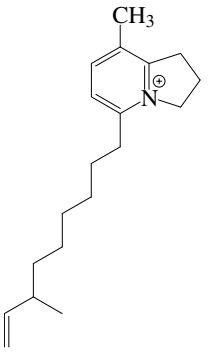


Absolute configuration

$C_{40}H_{56}O_3$ 584.881
Constit. of *Scenedesmus obliquus* and *Chlorella vulgaris*. May be identical with Pyrenoxanthin, P-740.

19-(2-Dodecenoyl):
$C_{52}H_{76}O_4$ 765.17
Constit. of *Pyramimonas parkeae*. λ_{max} 445; 471 (MeOH).
Aitzetmüller, K. *et al., Phytochemistry*, 1969, **8**, 1761 (*isol, struct, ir, pmr, ms, uv*)
Walton, T.J. *et al., Phytochemistry*, 1970, **9**, 2545 (*synth*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1983, **66**, 1175 (*abs config*)
Fiksdahl, A. *et al., Phytochemistry*, 1984, **23**, 649 (*synth*)
Sasa, T. *et al., Plant Cell Physiol.*, 1992, **33**, 921 (*dodecenoyl*)

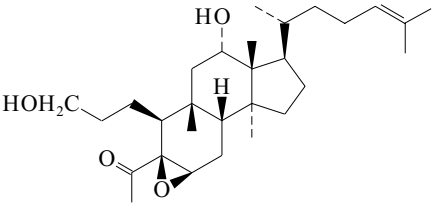
Louludinium(1+) L-237



$C_{19}H_{30}N^{\oplus}$ 272.453
Isol. from the blue-green alga *Lyngbya gracilis*. Cryst. (as chloride). $[\alpha]_D^{23}$ +97 (c, 0.6 in MeOH). Mp. >300° dec. (chloride). λ_{max} 204 (ϵ 1700); 218 (ϵ 1200); 278 (ϵ 800) (MeOH).
Yoshida, W.Y. *et al., Heterocycles*, 1998, **47**, 1023-1027 (*isol, uv, ir, pmr, cmr*)

Lovenone L-238

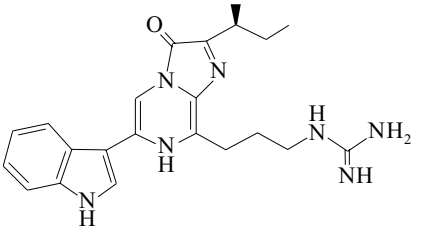
[162232-41-9]



$C_{29}H_{48}O_4$ 460.696
A secocucurbitane. Constit. of *Adalaria loveni*. Glass. $[\alpha]_D$ -38 ($CHCl_3$).
Graziani, E.I. *et al., Tet. Lett.*, 1995, **36**, 1763-1766 (*isol, pmr, cmr*)

Cypridina Luciferin L-239

Cypridina luciferin
[7273-34-9]



$C_{22}H_{27}N_7O$ 405.502
Isol. from *Cypridina (Vargula) hilgendorfii*. Cryst. (MeOH) (as dihydrobromide).
Mp 252-254° (dec.) (dihydrobromide). λ_{max} 218 (ϵ 27500); 270 (ϵ 17000); 310 (sh) (ϵ 11500); 435 (ϵ 9000) (MeOH aq.) (dihydrobromide). λ_{max} 221 (ϵ 29000); 243 (sh) (ϵ 12000); 275 (ϵ 14500); 307 (ϵ 20000); 320 (sh) (ϵ 6000) (MeOH/HBr aq.) (dihydrobromide).
Shimomura, O. *et al., Bull. Chem. Soc. Jpn.*, 1957, **30**, 929-933 (*isol, uv*)
Kishi, Y. *et al., Tet. Lett.*, 1966, 3427-3436; 3437-3444; 3445-3450 (*struct, synth*)
Nakamura, H. *et al., Tet. Lett.*, 2000, **41**, 2185-2188 (*synth*)
Kato, S.-I. *et al., Tetrahedron*, 2004, **60**, 11427-11434 (*biosynth, ms*)
Wu, C. *et al., Tet. Lett.*, 2006, **47**, 753-756 (*synth*)

Luciferin monooxygenases L-240

Luciferases
Oxidoreductase enzymes.

***Cypridina* Luciferin 2-monooxygenase**
E.C. 1.13.12.6. Cypridina-*Luciferin:oxygen 2-oxidoreductase (decarboxylating)*. Cypridina *Luciferase*
[61969-99-1]
Isol. from the marine ostracod crustacean *Cypridina hilgendorfii*. Catalyses the reaction of *Cypridina* Luciferin, L-239 with O_2 to give oxidised *Cypridina luciferin*, CO_2 and light.

***Photinus* Luciferin 4-monooxygenase (ATP-hydrolysing)**
E.C. 1.13.12.7. Photinus-*Luciferin:oxygen 4-oxidoreductase (decarboxylating, ATP-hydrolysing)*. *Firefly luciferase*. Photinus *Luciferase*
[61970-00-1]
Isol. from the firefly *Photinus pyralis*. Catalyses the reaction of with O_2 and ATP to give oxidised *Photinus* luciferase, CO_2, H_2O, AMP, pyrophosphate and light.

***Renilla* Luciferin 2-monooxygenase**
E.C. 1.13.12.5. Renilla-*Luciferin:oxygen 2-oxidoreductase (decarboxylating)*. Renilla *Luciferase*
[61869-41-8]
Isol. from the soft coral *Renilla reniformis*. Catalyses the reaction of, 4′-Deoxy with O_2 to give Coelenteramide, C-718, CO_2 and light (480 nm).

***Watasenia* Luciferin 2-monooxygenase**
E.C. 1.13.12.8. Watasenia-*Luciferin:oxygen 2-oxidoreductase (decarboxylating)*. Watasenia *Luciferase*
Isol. from the luminous squid *Watasenia scintillans*. Catalyses the reaction of *Watasenia* luciferin with O_2 to give *Watasenia* Oxyluciferin, O-185 , CO_2 and light.

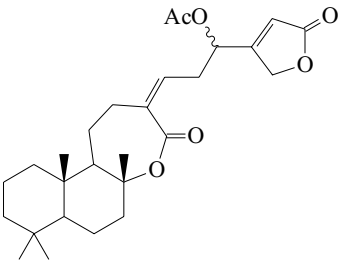
***Oplophorus* Luciferin 2-monooxygenase**
E.C. 1.13.12.13. Oplophorus-*Luciferin:oxygen 2-oxidoreductase (decarboxylating)*. Oplophorus *Luciferase*
Isol. from the deep sea shrimp *Oplophorus gracilorostris*. Catalyses the reaction of Coelenterazine, C-720 with O_2 to give oxidised *Oplophorus* luciferin, CO_2 and light.

***Latia* Luciferin monooxygenase (demethylating)**
E.C. 1.14.99.21. Latia-*Luciferin, hydrogen-donor:oxygen oxidoreductase (demethylating)*. Latia *Luciferase*
[62213-54-1]
Isol. from the bioluminescent mollusc *Latia neritoides*. Catalyses the reaction of *Latia* Luciferin with an electron donor substrate and O_2 to give oxidised *Latia* luciferin, CO_2, formate, the oxidised donor, H_2O and light. Flavin-dependent.

McElroy, W.D. *et al., Methods Enzymol.*, 1955, **2**, 851-856; 1963, **6**, 445-448 (*Cypridina, Photinus*)
Tsugi, F.I. *et al., J. Cell. Comp. Physiol.*, 1961, **58**, 113-123 (*Cyrpidina*)
Shimomura, O. *et al., Biochemistry*, 1968, **7**, 1734-1738 (*Latia*)
Karkhanis, Y.D. *et al., Biochemistry*, 1971, **10**, 317-326 (*Renilla*)
Shimomura, O. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1972, **69**, 2086-2089 (*Latia*)
Tsugi, F.I. *et al., Biochemistry*, 1974, **13**, 5204-5209 (*Cypridina*)
Cormier, M.J. *et al., Biochim. Biophys. Acta*, 1974, **346**, 137-164 (*Renilla, rev*)
De Luca, M. *et al., Adv. Enzymol. Relat. Areas Mol. Biol.*, 1976, **44**, 37-68 (*Photinus, rev*)
Inoue, S. *et al., Tet. Lett.*, 1976, **34**, 2971-2974 (*Watasenia*)
Matthews, J.C. *et al., Biochemistry*, 1977, **16**, 85-91 (*Renilla*)
Shimomura, O. *et al., Biochemistry*, 1978, **17**, 994-998 (*Oplophorus*)
De Luca, M. *et al., Methods Enzymol.*, 1978, **57**, 3-15 (*Photinus*)
Anderson, J.M. *et al., Methods Enzymol.*, 1978, **57**, 244-257 (*Renilla*)
Tsuji, F.I. *et al., Methods Enzymol.*, 1978, **57**, 364-372 (*Cypridina*)
Charbonneau, H. *et al., J. Biol. Chem.*, 1979, **254**, 769-780 (*Renilla*)
Kricka, L.J. *et al., Anal. Biochem.*, 1988, **175**, 14-21 (*Photinus, rev*)
Wood, K.V. *et al., J. Biolumin. Chemilumin.*, 1989, **4**, 298-301 (*Photinus, rev*)
Tsuji, F.I. *et al., Biochim. Biophys. Acta*, 2002, **1564**, 189-197 (*Watasenia*)
Greer, R.F. *et al., Luminescence*, 2002, **17**, 43-74 (*rev*)

Luffalactone L-241

[140389-49-7]

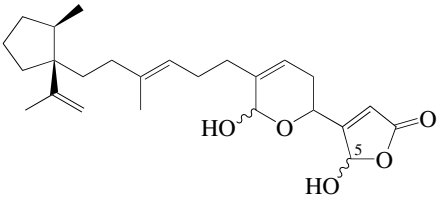


$C_{27}H_{38}O_6$ 458.594
Constit. of *Luffariella variabilis*. Oil. $[\alpha]_D$ +18.8 (c, 0.48 in C_6H_6).

Potts, B.C.M. *et al., J.O.C.*, 1992, **57**, 2965 (*isol, pmr, cmr*)

Luffariellin A L-242

[108663-77-0]



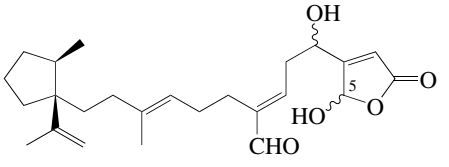
$C_{25}H_{36}O_5$ 416.556
Isol. from the marine sponge *Luffariella variabilis*. Phospholipase A_2 inhibitor. Calcium homeostasis modifier. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ +40.1 (c, 0.01 in $CHCl_3$). λ_{max} 230 (ϵ 4800) (MeOH).

5-Deoxy: ***Luffariellin C***
[114076-51-6]
$C_{25}H_{36}O_4$ 400.557
Metab. of *Chromodoris funerea*.

Kernan, M.R. *et al., J.O.C.*, 1987, **52**, 3081 (*isol, uv, ir, pmr, cmr*)
Kernan, M.R. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1988, **89**, 275 (*isol*)

Luffariellin B L-243

[108663-78-1]



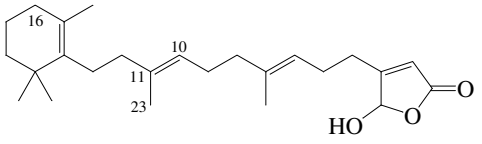
$C_{25}H_{36}O_5$ 416.556
Isol. from the marine sponge *Luffariella variabilis*. Phospholipase A_2 inhibitor. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ -5.5 (c, 0.03 in $CHCl_3$). λ_{max} 226 (ϵ 10000) (MeOH).

5-Deoxy: ***Luffariellin D***
[114076-52-7]
$C_{25}H_{36}O_4$ 400.557
Metab. of *Chromodoris funerea*.

Kernan, M.R. *et al., J.O.C.*, 1987, **52**, 3081 (*isol, uv, ir, pmr, cmr*)
Kernan, M.R. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1988, **89**, 275 (*isol*)

Luffariellolide L-244

[111149-87-2]



$C_{25}H_{38}O_3$ 386.573
Constit. of sponges *Luffariella* sp., *Cacospongia* sp. and *Fascaplysinopsis reticulata*. Phospholipase A_2 inhibitor. Antiinflammatory agent. Oil. Sol. MeOH, hexane; poorly sol. H_2O. λ_{max} 253 (ϵ 4400) (MeOH/NaOH) (Derep). λ_{max} 214 (ϵ 10000) (MeOH) (Derep).

Me ether: ***25-O-Methylluffariellolide***
[799808-36-9]
$C_{26}H_{40}O_3$ 400.6
Constit. of *Acanthodendrilla* sp. Oil. $[\alpha]_D$ -55 (c, 1 in $CHCl_3$). λ_{max} 214 (MeOH).

Et ether: ***25-O-Ethylluffariellolide***
[799808-38-1]
$C_{27}H_{42}O_3$ 414.627
Constit. of an *Acanthodendrilla* sp. Oil. $[\alpha]_D$ -61 (c, 1 in $CHCl_3$). λ_{max} 218 (MeOH).

16ξ-Hydroxy: ***16-Hydroxyluffariellolide***
[863493-03-2]
$C_{25}H_{38}O_4$ 402.573
Constit. of a *Thorectandra* sp. Oil. $[\alpha]_D^{24}$ +17 (c, 0.16 in MeOH). λ_{max} 210; 260 (sh) (MeOH).

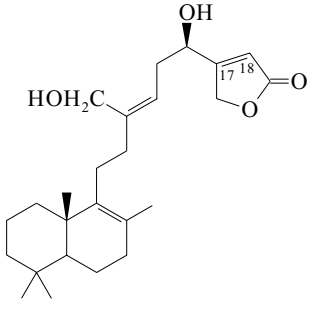
16-Oxo: ***Acantholide B****. 16-Oxoluffariellolide*
[799808-28-9]
$C_{25}H_{36}O_4$ 400.557
Constit. of an *Acanthodendrilla* sp. and a *Thorectandra* sp. Oil. $[\alpha]_D$ -44.5 (c, 1 in $CHCl_3$). λ_{max} 203; 252 (MeOH).

$\Delta^{11(23)}$-Isomer, 10ξ-hydroxy: ***Acantholide A***
$C_{25}H_{38}O_4$ 402.573
Constit. of an *Acanthodendrilla* sp. Oil. $[\alpha]_D$ -20.8 (c, 1 in $CHCl_3$). λ_{max} 222 (MeOH).

Albizati, K.F. *et al., Experientia*, 1987, **43**, 949 (*Luffariellolide*)
Potts, B.C.M. *et al., J.A.C.S.*, 1992, **114**, 5093-5100 (*Luffariellolide, activity*)
Elkhayat, E. *et al., J. Nat. Prod.*, 2004, **67**, 1809-1817 (*Acantholides A,B, Me ether, Et ether*)
Cao, S. *et al., Bioorg. Med. Chem.*, 2005, **13**, 5094-5098 (*Thorectandra constits*)

Luffarin I L-245

[145398-63-6]



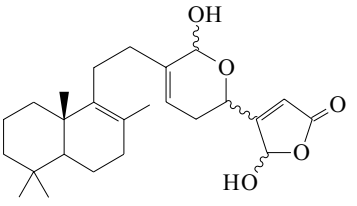
$C_{25}H_{38}O_4$ 402.573
Constit. of *Luffariella geometrica*. Oil. $[\alpha]_D^{20}$ +64.3 (c, 1.4 in $CHCl_3$).

17,18-Dihydro: ***Luffarin J***
[145398-64-7]
$C_{25}H_{40}O_4$ 404.589
Constit. of *Luffariella geometrica*. Oil. $[\alpha]_D^{20}$ +33.1 (c, 0.29 in $CHCl_3$).

Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705 (*isol, pmr, cmr*)

Luffarin A L-246

[145398-59-0]

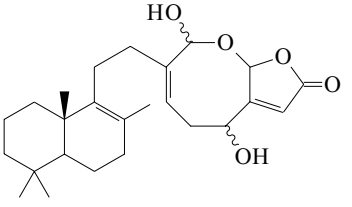


$C_{25}H_{36}O_5$ 416.556
Constit. of *Luffariella geometrica*. Solid. $[\alpha]_D^{20}$ +101 (c, 1.7 in $CHCl_3$). λ_{max} 208 (ϵ 6509) (EtOH) (Berdy).

Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705 (*isol, pmr, cmr*)

Luffarin B L-247

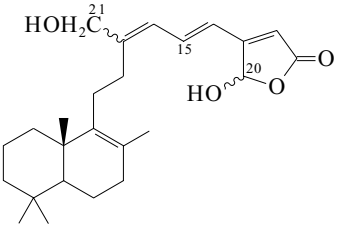
[145427-70-9]



$C_{25}H_{36}O_5$ 416.556
Constit. of *Luffariella geometrica*. Oil. $[\alpha]_D^{20}$ +85.7 (c, 0.16 in $CHCl_3$).

Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705 (*isol, pmr, cmr*)

Luffarin E L-248



$C_{25}H_{36}O_4$ 400.557
Constit. of *Luffariella geometrica*. Pale yellow oil. $[\alpha]_D^{20}$ +49.9 (c, 1.1 in $CHCl_3$). λ_{max} 324 (ϵ 23000) (EtOH) (Berdy).

21-Aldehyde: ***Luffarin C***
$C_{25}H_{34}O_4$ 398.541
Constit. of *Luffariella geometrica*. Yellow oil. $[\alpha]_D^{20}$ +47.1 (c, 1.3 in $CHCl_3$). λ_{max} 204 (ϵ 10500); 318 (ϵ 24000) (EtOH) (Berdy).

21-Aldehyde, di-Me acetal: ***Luffarin D***
[145398-60-3]
$C_{27}H_{40}O_5$ 444.61
Constit. of *Luffariella geometrica*. Yellow oil. $[\alpha]_D^{20}$ +26.4 (c, 0.3 in $CHCl_3$). λ_{max} 205 (ϵ 10100); 315 (ϵ 15500) (EtOH) (Berdy).

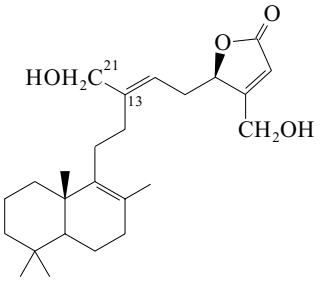
20-Deoxy: ***Luffarin G***
[145398-62-5]
$C_{25}H_{36}O_3$ 384.558
Constit. of *Luffariella geometrica*. Pale yellow oil. $[\alpha]_D^{20}$ +41.1 (c, 0.8 in $CHCl_3$).

15Z-Isomer: ***Luffarin F***
$C_{25}H_{36}O_4$ 400.557
Constit. of *Luffariella geometrica*. Pale yellow oil. $[\alpha]_D^{20}$ +43.4 (c, 0.7 in $CHCl_3$). λ_{max} 327 (ϵ 15000) (EtOH) (Berdy).

15Z-Isomer, 20-deoxy: ***Luffarin H***
[145512-19-2]
$C_{25}H_{36}O_3$ 384.558
Constit. of *Luffariella geometrica*. Pale yellow oil. $[\alpha]_D^{20}$ +48.2 (c, 0.4 in $CHCl_3$).
[145514-35-8]
Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705 (*isol, pmr, cmr*)

Luffarin K L-249

[145427-72-1]



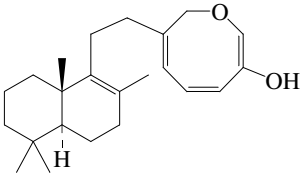
$C_{25}H_{38}O_4$ 402.573
Constit. of *Luffariella geometrica*. Oil. $[\alpha]_D$ +25.2 (c, 2.8 in $CHCl_3$). λ_{max} 216 (ϵ 7350) (EtOH) (Berdy).

21-Aldehyde: ***Luffarin M***
[145398-61-4]
$C_{25}H_{36}O_4$ 400.557
Constit. of *Luffariella geometrica*. Oil. $[\alpha]_D$ +23 (c, 1 in $CHCl_3$). λ_{max} 222 (ϵ 10300) (EtOH) (Berdy).

13Z-Isomer: ***Luffarin L***
[145514-36-9]
$C_{25}H_{38}O_4$ 402.573
Constit. of *Luffariella geometrica*. Oil. $[\alpha]_D$ +25.1 (c, 2.1 in $CHCl_3$). λ_{max} 216 (ϵ 1000) (EtOH) (Berdy).
[145514-35-8]
Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705 (*isol, pmr, cmr*)

Luffarin O L-250

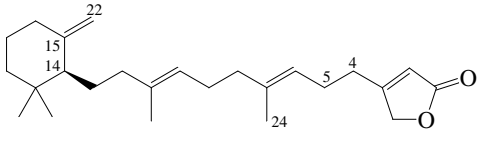
[145398-67-0]



$C_{23}H_{34}O_2$ 342.52
Tautomeric. Enol-form predominant. Constit. of *Luffariella geometrica*. Pale yellow oil. $[\alpha]_D^{20}$ +40.5 (c, 0.83 in $CHCl_3$). λ_{max} 208 (ϵ 7200) (EtOH).
Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705-1743 (*isol, pmr, cmr, ms*)

Luffarin P L-251

[145398-68-1]

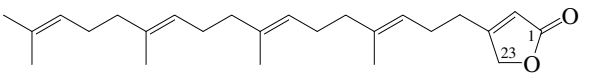


$C_{25}H_{38}O_2$ 370.574
Constit. of *Luffariella geometrica*. Oil. $[\alpha]_D^{20}$ +5 (c, 0.1 in $CHCl_3$).

*24-Acetoxy, 14-hydroxy, 4,5*E*-didehydro, 15,22-dihydro:* [882693-47-2]
$C_{27}H_{40}O_5$ 444.61
Constit. of *Fasciospongia cavernosa*. Amorph. solid. $[\alpha]_D$ -5.1 (c, 0.01 in $CHCl_3$). λ_{max} 257 (log ϵ 3.76) (MeOH).
Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705-1743 (*Luffarin P*)
De Rosa, S. *et al., Tetrahedron*, 2006, **62**, 2845-2849 (*Fasciospongia cavernosa constit*)

Luffarin Q L-252

[145398-69-2]

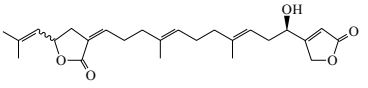


$C_{25}H_{38}O_2$ 370.574
Constit. of *Luffariella geometrica* and *Thorecta horridus*. Shows antiinflammatory props. Oil.

1-Deoxo, 21-oxo:
$C_{25}H_{38}O_2$ 370.574
Constit. of *Thorecta horridus*.
Fattorusso, E. *et al., Bioorg. Med. Chem. Lett.*, 1991, **1**, 639-644 (*isol, cmr*)
Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705 (*isol, pmr, cmr*)

Luffarin R L-253

[145427-73-2]

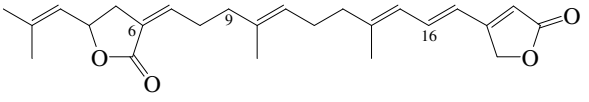


$C_{25}H_{34}O_5$ 414.541
Constit. of *Luffariella geometrica*. Pale yellow oil. $[\alpha]_D^{20}$ -13.7 (c, 4.41 in $CHCl_3$).

Ac: ***Luffarin S***
[145398-70-5]
$C_{27}H_{36}O_6$ 456.578
Constit. of *Luffariella geometrica*. Oil. $[\alpha]_D^{20}$ -12.5 (c, 0.9 in $CHCl_3$).
Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705 (*isol, pmr, cmr*)

Luffarin T L-254

[145398-71-6]



$C_{25}H_{32}O_4$ 396.525
Constit. of *Luffariella geometrica*. Yellow oil. $[\alpha]_D^{20}$ -30.3 (c, 1.7 in $CHCl_3$).

16,17-Dihydro: ***6Z-Luffarin V***
[198208-71-8]
$C_{25}H_{34}O_4$ 398.541
Constit. of *Fasciospongia cavernosa*.
$[\alpha]_D$ -18 (c, 0.1 in $CHCl_3$). λ_{max} 220 (ϵ 10500) (MeOH).

*6*E*-Isomer, 16,17-dihydro:* ***Luffarin V***
[145398-72-7]
$C_{25}H_{34}O_4$ 398.541
Constit. of *Luffariella geometrica*. Oil. $[\alpha]_D^{20}$ -30 (c, 0.1 in $CHCl_3$).

16Z-Isomer: ***Luffarin U***
[145512-20-5]
$C_{25}H_{32}O_4$ 396.525
Constit. of *Luffariella geometrica*. Yellow oil. $[\alpha]_D^{20}$ -28 (c, 0.3 in $CHCl_3$).

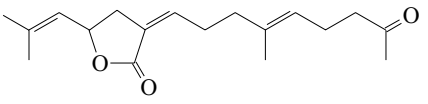
9β-Acetoxy, 16,17-dihydro: [882693-46-1]
$C_{27}H_{36}O_6$ 456.578

Constit. of *Fasciospongia cavernosa*. Amorph. solid. $[\alpha]_D$ -34.6 (c, 0.2 in $CHCl_3$). λ_{max} 220 (log ϵ 3.64) (MeOH).

Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705-1743 (*Luffariella geometrica constits*)
De Rosa, S. *et al., Nat. Prod. Lett.*, 1997, **10**, 267-274 (*6Z-Luffarin V*)
De Rosa, S. *et al., Tetrahedron*, 2006, 2845-2849 (*Fasciospongia cavernosa constit*)

Luffarin Z L-255

[145398-76-1]

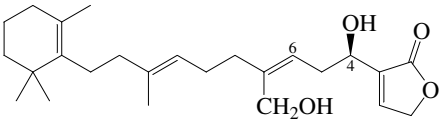


$C_{18}H_{26}O_3$ 290.402
Constit. of *Luffariella geometrica*. Oil. $[\alpha]_D^{20}$ -30 (c, 0.05 in $CHCl_3$).

Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705 (*isol, pmr, cmr*)

Luffariolide B L-256

[141394-71-0]

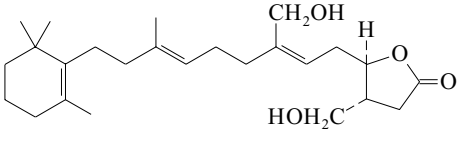


$C_{25}H_{38}O_4$ 402.573
Constit. of a *Luffariella* sp. Oil. $[\alpha]_D^{25}$ +20 (c, 1.0 in $CHCl_3$). λ_{max} 218 (ϵ 7400) (EtOH) (Derep).

*6*E-*Isomer, 4-deoxy, 4,5-didehydro:* ***Luffariolide A***
[141321-12-2]
$C_{25}H_{36}O_3$ 384.558
Constit. of *Luffariella* sp. Oil. λ_{max} 325 (ϵ 25000) (EtOH) (Derep).
Tsuda, M. *et al., J.O.C.*, 1992, **57**, 3503 (*isol, pmr, cmr*)

Luffariolide C L-257

[141394-72-1]

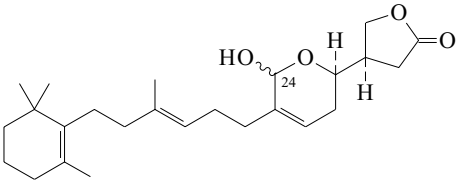


$C_{25}H_{40}O_4$ 404.589
Constit. of *Luffariella* sp. Oil. $[\alpha]_D^{25}$ +4.4 (c, 1.6 in $CHCl_3$).

Tsuda, M. *et al., J.O.C.*, 1992, **57**, 3503 (*isol, pmr, cmr*)

Luffariolide D L-258

[141321-13-3]

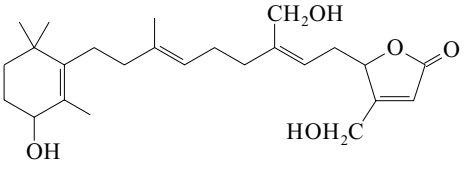


$C_{25}H_{38}O_4$ 402.573
Constit. of a *Luffariella* sp. Oil. $[\alpha]_D^{20}$ +9 (c, 0.15 in $CHCl_3$).

24-Ketone: ***Luffariolide E***
[141344-10-7]
$C_{25}H_{36}O_4$ 400.557
Constit. of a *Luffariella* sp. Oil. $[\alpha]_D^{17}$ +7.1 (c, 0.42 in $CHCl_3$). λ_{max} 230 (ϵ 7500) (MeOH) (Derep). λ_{max} 230 (ϵ 7500) (EtOH) (Berdy).
Tsuda, M. *et al., J.O.C.*, 1992, **57**, 3503 (*isol, pmr, cmr*)

Luffariolide F L-259

[147663-78-3]

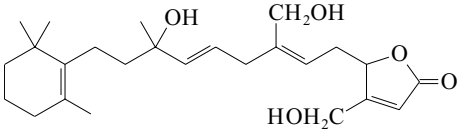


$C_{25}H_{38}O_5$ 418.572
Constit. of a *Luffariella* sp. Oil. $[\alpha]_D^{19}$ -5.9 (c, 0.67 in MeOH). λ_{max} 210 (ϵ 15000) (MeOH) (Berdy).

Kobayashi, J. *et al., J. Nat. Prod.*, 1993, **56**, 436 (*isol, pmr, cmr*)

Luffariolide G L-260

[147663-79-4]

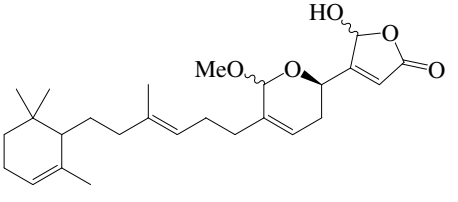


$C_{25}H_{38}O_5$ 418.572
Constit. of a *Luffariella* sp. Oil. $[\alpha]_D^{24}$ -9.5 (c, 0.2 in MeOH). λ_{max} 210 (ϵ 8300) (MeOH) (Berdy).

Kobayashi, J. *et al., J. Nat. Prod.*, 1993, **56**, 436 (*isol, pmr, cmr*)

Luffariolide H L-261

[472958-09-1]

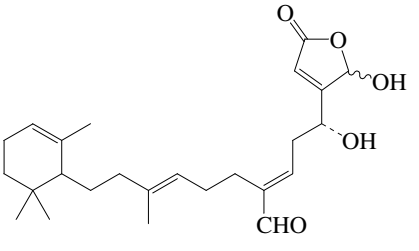


$C_{26}H_{38}O_5$ 430.583
Constit. of a *Luffariella* sponge. Oil. λ_{max} 230 (sh) (MeOH).

Tsuda, M. *et al., J. Nat. Prod.*, 2002, **65**, 1507-1508 (*isol, pmr, cmr*)

Luffariolide J L-262

[472958-10-4]

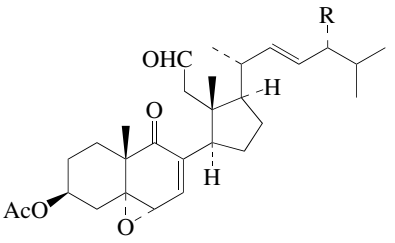


$C_{25}H_{36}O_5$ 416.556
Constit. of a *Luffariella* sponge. Oil. λ_{max} 230 (sh) (MeOH).

Tsuda, M. *et al., J. Nat. Prod.*, 2002, **65**, 1507-1508 (*isol, pmr, cmr*)

Luffasterol B L-263

[185520-90-5]



R = CH_3

$C_{30}H_{44}O_5$ 484.675
Constit. of a *Luffariella* sp. Solid. $[\alpha]_D$ -27.8 (c, 0.047 in $CHCl_3$). λ_{max} 256 (ϵ 4400) (CH_2Cl_2).

O-*De-Ac:* ***3-Deacetylluffasterol B***
[201213-02-7]
$C_{28}H_{42}O_4$ 442.637
Constit. of *Spongia agaricina*. Amorph. solid. $[\alpha]_D^{25}$ -21.4 (c, 0.1 in $CHCl_3$). λ_{max} 258 (ϵ 4920) (MeOH).

22,23-Dihydro, 24,28-didehydro, O-*de-Ac:* [201213-03-8]
$C_{28}H_{42}O_4$ 442.637
Constit. of *Spongia agaricina*. Amorph. solid. $[\alpha]_D^{25}$ -29 (c, 0.1 in $CHCl_3$). λ_{max} 259 (ϵ 4756) (MeOH).

Reddy, M.V.R. *et al., J. Nat. Prod.*, 1997, **60**, 41 (*isol, pmr, cmr*)
Rueda, A. *et al., J. Nat. Prod.*, 1998, **61**, 258-261 (*Spongia agaricina constits*)

Luffasterol C L-264

[185520-91-6]
As Luffasterol B, L-263 with
R = H

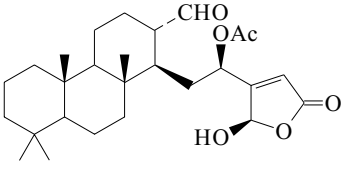
$C_{29}H_{42}O_5$ 470.648
Constit. of *Luffariella* sp. Amorph. solid. $[\alpha]_D$ -22 (c, 0.16 in $CHCl_3$). λ_{max} 255 (ϵ 4200) (CH_2Cl_2).

22,23-Dihydro: ***Luffasterol A***
[185520-89-2]
$C_{29}H_{44}O_5$ 472.664
Constit. of *Luffariella* sp. Needles (EtOAc/hexane).
Mp 139-141°. $[\alpha]_D$ -33.5 (c, 0.35 in $CHCl_3$). λ_{max} 255 (ϵ 4100) (CH_2Cl_2).

Reddy, M.V.R. *et al., J. Nat. Prod.*, 1997, **60**, 41-43 (*isol, pmr, cmr*)

Luffolide L-265

[121449-94-3]

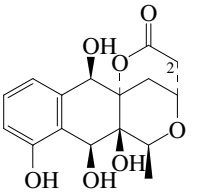


$C_{27}H_{40}O_6$ 460.609
Constit. of *Luffariella* sp. Cryst. ($CDCl_3$).
Mp 123°.

Kernan, M.R. *et al., Experientia*, 1989, **45**, 388 (*isol, pmr, cryst struct*)
Basabe, P. *et al., J.O.C.*, 2005, **70**, 9480-9485 (*synth*)

Luisol A L-266

[225110-59-8]



Relative Configuration

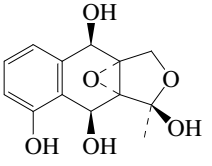
$C_{16}H_{18}O_7$ 322.314
Prod. by a marine *Streptomyces* sp. (isolate CNH-370). Gum. $[\alpha]_D^{25}$ -29.2 (c, 0.5 in MeOH). λ_{max} 275 (ϵ 1960) (MeOH).

2ξ-Hydroxy: ***2-Hydroxyluisol A***
$C_{16}H_{18}O_8$ 338.313
Prod. by the marine actinomycete ACT 7617.

Cheng, X.C. *et al., J. Nat. Prod.*, 1999, **62**, 608-610 (*isol, uv, ir, pmr, cmr*)
Laatsch, H. *et al., Dissertation*, Univ. of Göttingen, 2005, (*2-Hydroxyluisol A*)

Luisol B L-267

[225110-61-2]



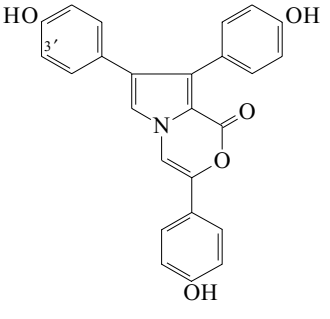
Relative Configuration

$C_{13}H_{14}O_6$ 266.25
Prod. by a marine *Streptomyces* sp. (isolate CNH-370). Cryst. Mp 125-127°. $[\alpha]_D^{25}$ -2.4 (c, 2 in MeOH). λ_{max} 275 (ϵ 1500) (MeOH).

Cheng, X.C. *et al., J. Nat. Prod.*, 1999, **62**, 608-610 (*isol, uv, ir, pmr, cmr*)

Lukianol A L-268

*3,7,8-Tris(4-hydroxyphenyl)-1*H*-pyrrolo[2,1-*c*][1,4]oxazin-1-one, 9CI*
[144398-24-3]



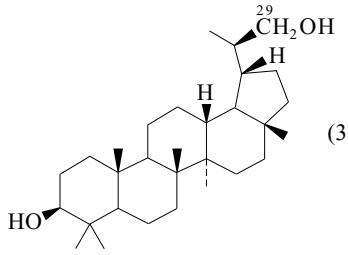
$C_{25}H_{17}NO_5$ 411.413
Isol. from an unidentified tunicate. Cytotoxic; MDR reversing agent. Amorph. powder (MeOH).
Mp 264-266°. Mp refers to crystalline synthetic material. λ_{max} 206 (ϵ 33113); 282 (ϵ 35481); 344 (ϵ 14125) (MeOH) (Berdy).

3′-Iodo: ***Lukianol B***
[144398-25-4]
$C_{25}H_{16}INO_5$ 537.31
Minor constit. from the unidentified tunicate. Cytotoxic. Off-white powder (MeOH).

Yoshida, W.Y. *et al., Helv. Chim. Acta*, 1992, **75**, 1721 (*isol, uv, pmr, cmr, struct*)
Fürstner, A. *et al., J.O.C.*, 1995, **60**, 6637 (*synth*)
Banwell, M.G. *et al., Chem. Comm.*, 1997, 207 (*synth*)

Boger, D.L. *et al., J.A.C.S.*, 1999, **121**, 54-62 (*synth*)
Gupton, J.T. *et al., Tetrahedron*, 1999, **55**, 14515-14522 (*synth*)
Liu, J.-H. *et al., J.O.C.*, 2000, **65**, 3587-3595 (*synth, pmr, cmr*)

3,29-Lupanediol L-269



(3β,20*R*)–*form*

$C_{30}H_{52}O_2$ 444.74

(3β,20*R*)-*form*
Cryst. Mp 235°. $[\alpha]_D^{20}$ -14.09 (c, 1.22 in $CHCl_3$).

29-Carboxylic acid: 3β-Hydroxy-29-lupanoic acid. ***Gymnosporic acid***
[65527-04-0]
$C_{30}H_{50}O_3$ 458.723
Isol. from *Gymnosporia wallichiana* and *Ceriops decandra*. Cryst.
Mp 290°. $[\alpha]_D$ -44 (c, 1 in $CHCl_3$/EtOH).

(3β,20*S*)-*form*
Wallichianol
[65556-58-3]
Constit. of *Gymnosporia wallichiana* and *Lawsonia inermis*.
Cryst. (EtOH).
Mp 266°. $[\alpha]_D^{20}$ -5.79 (c, 0.95 in $CHCl_3$).

Di-Ac:
Cryst. Mp 218-220°.

29-Carboxylic acid: ***Wallichianic acid***
[65527-05-1]
$C_{30}H_{50}O_3$ 458.723
Isol. from *Gymnosporia wallichiana*. Cryst.
Mp 280°. $[\alpha]_D$ +28 (c, 1 in $CHCl_3$/EtOH).

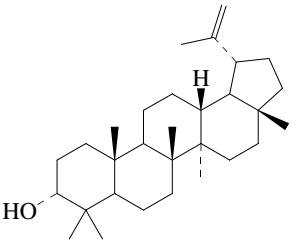
29-Carboxylic acid, 3-Ac: ***Wallichianic acid acetate***
[105645-77-0]
$C_{32}H_{52}O_4$ 500.76
Constit. of aerial roots of *Ficus microcarpa*. Cryst.
Mp 287-290°. $[\alpha]_D^{29}$ +18.9 (c, 0.7 in $CHCl_3$).

(3β,20ξ)-*form* [30854-30-9]
Isol. from *Lithocarpus polystachya, Mallotus apelta* and *Pseudocyphellaria rubella*.
Mp 238-240°.

29-Aldehyde, 3-Ac: ***3β-Acetoxy-29-lupanal***
$C_{32}H_{52}O_3$ 484.761
Metab. of *Pseudocyphellaria rubella*. Cryst.
Mp 175-180°.

Kulshreshtha, D.K. *et al., Phytochemistry*, 1977, **16**, 1783-1785 (*isol, pmr*)
Corbett, R.E. *et al., J.C.S. Perkin 1*, 1985, 2051 (*synth, abs config, bibl*)
Corbett, R.E. *et al., Aust. J. Chem.*, 1987, **40**, 461 (*isol, bibl*)
Chiang, Y.-M. *et al., J. Nat. Prod.*, 2001, **64**, 436-439 (*Wallichianic acid acetate*)
Thongdeeying, P. *et al., Acta Cryst. E*, 2005, **61**, 01861-o1863 (*cryst struct*)

20(29)-Lupen-3-ol L-270



3α-*form*

$C_{30}H_{50}O$ 426.724

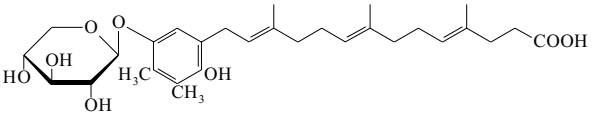
3β-*form*
Lupeol. *Monogynol B. Fagarasterol. β-Viscol. Cautchicol. Xanthosterin. Clerodol*
[545-47-1]
Occurs in many plants, e.g. *Ficus*, *Manilkara* spp. First isol. in 1889 from *Lupinus luteus*. One of the most widespread of the pentacyclic triterpenes. Antineoplastic agent. Trypsin and chymotrypsin inhibitor. Cryst. (Me_2CO/MeOH aq.).
Mp 215-216°. $[\alpha]_D$ +26.4 ($CHCl_3$). Log P 10.51 (uncertain value) (calc).

3-O-[α-L-Arabinofuranosyl-(1→4)-β-D-glucuronopyranoside]:
[78657-53-1]
$C_{41}H_{66}O_{11}$ 734.966
Constit. of *Acanthus illicifolius*. Cryst. (MeOH).
Mp 262-264° dec.

Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 2023 (*occur*)
Minocha, P.K. *et al., Phytochemistry*, 1981, **20**, 135-137 (*arabinosylglucuronide*)

Lurlenic acid L-271

Lurlene L
[160925-88-2]



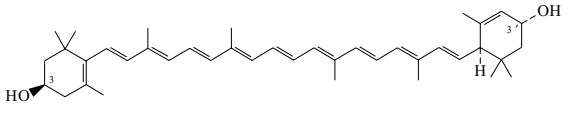
$C_{30}H_{44}O_8$ 532.673
Lurlene was the former name. Sexual pheromone of *Chlamydomonas allensworthii*. Glassy solid. λ_{max} 282 (ε 2700) (H_2O). λ_{max} 282 (ε 3642) (MeOH) (Berdy).

1-Alcohol: ***Lurlenol***. *Lurlene C*
[184091-97-2]
$C_{30}H_{46}O_7$ 518.689
Mating pheromone of a *Chlamydomonas allensworthii*. Fine needles ($CHCl_3$).
Mp 68-69° (65°). $[\alpha]_D^{25}$ -17 (c, 0.4 in MeOH). λ_{max} 283 (ε 4500) (H_2O).

Jaenicke, L. *et al., Annalen*, 1995, 1343 (*isol, pmr, cmr*)
Starr, R.C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1995, **92**, 41 (*isol, pmr, cmr, ms, props*)
Jaenicke, L. *et al., Eur. J. Biochem.*, 1996, **241**, 581-585 (*Lurlenol, isol, pmr, ms*)
Mori, K. *et al., Tet. Lett.*, 1996, **37**, 1821 (*synth*)
Takanashi, S. *et al., Liebigs Ann./Recl.*, 1997, 825 (*synth, ir, pmr, cmr*)

Lutein† L-272

Xanthophyll. β,ε-Carotene-3,3′-diol. Lutein A
[127-40-2]



$C_{40}H_{56}O_2$ 568.881

Pigment from egg yolk and leaves. Found in all higher plants, e.g. *Mimosa invasiva*, *Cosmos caudatus*, and also in microorganisms e.g. *Staphylococcus aureus*, green algae, *Porphyra* spp and in animals, e.g river crab *Potamon dehaani* and marine invertebrates. Antioxidant. Shows antitumour, antimutagenic and a wide range of antimicrobial activity. Potentially useful for treating macular degeneration. Coppery cryst. (MeOH).
Mp 196°. $[\alpha]_{643.9}^{18}$ +160 ($CHCl_3$). λ_{max} 420; 444; 472 (MeOH) (Berdy).

Dihexadecanoyl: ***Xantofyl palmitate, INN****. Helenien, JAN. Adaptinol. Aptinol. Heligal. Xantophyll dipalmitate. E161b*
[547-17-1]
$C_{72}H_{116}O_4$ 1045.706
Constit. of *Helenium autumnale* and other flowers, esp. in the Compositae. Retinal oxygenising agent. Red cryst. (EtOH).
Mp 92°.

Di-Me ether: 3,3′-Dimethoxy-β,ϵ-carotene. Lutein dimethyl ether. Xanthophyll dimethyl ether
[53779-13-8]
$C_{42}H_{60}O_2$ 596.935
Nat. occurring, isol. descr. in a thesis. Cryst. (MeOH/Et_2O).
Mp 162-163° (155°). λ_{max} 267; 428; 433; 480 (dioxan).

3′-Ketone: 3-Hydroxy-β,ϵ-caroten-3′-one. ***Philosamixanthin****. 3′-O-Didehydrolutein*
[97134-08-2]
$C_{40}H_{54}O_2$ 566.865
Isol. from marine fish eggs, silkworm haemolymph and other sources. Red needles (petrol).
Mp 168-170°. λ_{max} 449; 477 (Me_2CO).

5,6-Epoxide: See Lutein epoxide in *The Combined Chemical Dictionary.*

7′,8′-Dihydro: ***7′,8′-Dihydrolutein***
[169275-78-9]
$C_{40}H_{58}O_2$ 570.897
Constit. of *Bathycoccus prasinos*, *Mantoniella squamata* and the catfish *Parasilurus asotus.*

3′-Epimer: ***3′-Epilutein****. Calthaxanthin*
[52842-48-5]
$C_{40}H_{56}O_2$ 568.881
Isol. from plants, e.g. *Rosa* spp., *Caltha palustris*, and animals, e.g. river crab *Potamon dehaani*, yellowtail fish *Seriola quinquerodiata*.
Mp 162-163°. $[\alpha]_D^{20}$ +88 (EtOH). λ_{max} 420; 444; 472 (no solvent reported).

6′-Epimer: [97169-07-8]
$C_{40}H_{56}O_2$ 568.881
Isol. from eggs of dolphin and flying fish. λ_{max} 420; 444; 472 (petrol).

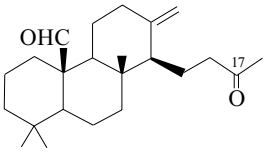
3′,6′-Diepimer: 3′,6′-Diepilutein. ***Lutein D***
[89673-72-3]
$C_{40}H_{56}O_2$ 568.881
Isol. from eggs of dolphin and flying fish. λ_{max} 420; 444; 472 (petrol).

[15904-92-4, 105452-20-8]

Kuhn, R. *et al., Naturwissenschaften*, 1930, **18**, 754 (*isol*)
Ohta, T. *et al., Chem. Pharm. Bull.*, 1959, **7**, 254-255 (*isol*)
Jensen, S.L. *et al., Acta Chem. Scand.*, 1966, **20**, 1703-1709 (*di-Me ether*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, nos. 1844; 1845 (*occur*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1974, **57**, 631-656; 1979, **62**, 2817-2824 (*abs config, synth, di-Me ether, synth*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97-102 (*cmr*)
Weedon, B.C.L. *et al., Pure Appl. Chem.*, 1976, **47**, 161-171 (*synth*)
Davies, B.H. *et al., Int. Rev. Biochem.*, 1977, **14**, 51 (*rev*)
Mayer, H. *et al., Helv. Chim. Acta*, 1980, **63**, 1451-1455 (*synth*)
Baranyai, M. *et al., Tetrahedron*, 1981, **37**, 203-207 (*cmr*)
Vecchi, M. *et al., Helv. Chim. Acta*, 1982, **65**, 1050-1058 (*Calthaxanthin, hplc, pmr*)
Milborrow, B.V. *et al., Phytochemistry*, 1982, **21**, 2853-2857 (*synth, Philosamixanthin*)
Miki, W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 195-201 (*Calthaxanthin, occur, biosynth*)
Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 779-789 (*stereoisomers, Philosamixanthin*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 133; 136; 232; 302 (*bibl*)
Chopra, M. *et al., Ann. N.Y. Acad. Sci.*, 1993, **691**, 246-249 (*pharmacol*)
Bui, M.H. *et al., J. Chromatogr., B: Biomed. Appl.*, 1994, **654**, 129 (*hplc*)
Egeland, E.S. *et al., Phytochemistry*, 1995, **40**, 515 (*7′,8′-Dihydrolutein*)
Sliwka, H.-R. *et al., Acta Chem. Scand.*, 1996, **50**, 637-639 (*synth*)
Okai, Y. *et al., Cancer Lett. (Shannon, Irel.)*, 1996, **100**, 235-240; *CA*, **128**, 223350u (*activity*)
Largo, G. *et al., Philipp. J. Sci.*, 1997, **126**, 107-115; *CA*, **128**, 306237w (*activity*)
Ragasa, C.Y. *et al., Philipp. J. Sci.*, 1997, **126**, 199-206; *CA*, **129**, 313379 (*activity*)
Deli, J. *et al., Helv. Chim. Acta*, 1998, **81**, 1815-1819 (*Lutein, pmr, cmr*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 999
Tsushima, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2002, **133**, 331-336; 2003, **136**, 147-148 (*7′,8′-Dihydrolutein*)
Linden, A. *et al., Helv. Chim. Acta*, 2004, **87**, 1254-1269 (*cryst struct, abs config*)

Luteone† L-273

[80902-35-8]



Relative configuration

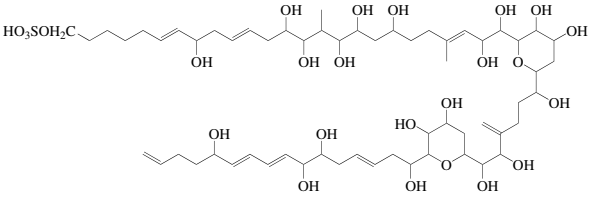
$C_{23}H_{36}O_2$ 344.536
Constit. of the nudibranch *Cadlina luteomarginata*. Cryst. $[\alpha]_D^{25}$ +12 ($CHCl_3$). λ_{max} 244 (log ϵ 2.42) ($CHCl_3$).

17-(2,4-Dinitrophenylhydrazone):
Cryst. (MeOH). Mp 84-86°.

Hellou, J. *et al., Tetrahedron*, 1982, **38**, 1875 (*cryst struct*)
Dumdei, E.J. *et al., Can. J. Chem.*, 1997, **75**, 773-789 (*isol, pmr, cmr*)
Kubanek, J. *et al., J.O.C.*, 1997, **62**, 7239-7246 (*biosynth*)

Luteophanol A L-274

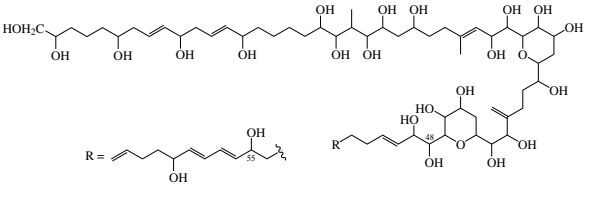
[184024-71-3]



$C_{60}H_{102}O_{25}S$ 1255.517
Isol. from the marine dinoflagellate *Amphidinium* sp. Y-52 symbiotic with *Pseudaphanostoma luteocoloris*. Phycotoxin. Amorph. solid. $[\alpha]_D^{29}$ -7.6 (c, 1 in MeOH). Genus name given in the lit., apparently incorrectly, as Pseudoaphanostoma. λ_{max} 232 (ϵ 2700) (MeOH).

Doi, Y. *et al., J.O.C.*, 1997, **62**, 3820-3823 (*isol, uv, ir, pmr, cmr, ms*)

Luteophanol B L-275



$C_{67}H_{116}O_{25}$ 1321.638

Isol. from the marine dinoflagellate *Amphidinium* sp. symbiotic with *Pseudaphanostoma luteocoloris*. Amorph. solid. $[\alpha]_D^{20}$ +3.4 (c, 0.21 in MeOH). Genus name given in the lit. as Pseudoaphanostoma, apparently incorrectly. λ_{max} 232 (ϵ 21300) (MeOH).

Kubota, T. *et al., Tetrahedron*, 1998, **54**, 14455-14464 (*isol*)

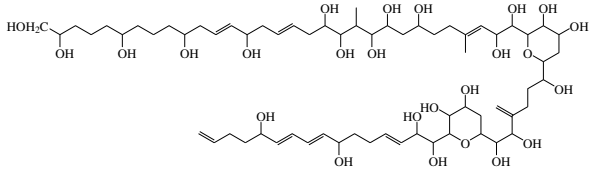
Luteophanol C **L-276**

As Luteophanol B, L-275 with
R = $H_2C{=}CHCH_2CH_2CH_2CH(OH)CH{=}CHCH{=}CHCH(OH)$-

$C_{67}H_{116}O_{25}$ 1321.638
Isol. from *Amphidinium* sp. Amorph. solid. $[\alpha]_D^{20}$ +12 (c, 0.19 in MeOH). λ_{max} 233 (ϵ 23500) (MeOH).

Kubota, T. *et al., Tetrahedron*, 1998, **54**, 14455-14464

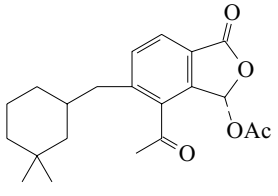
Luteophanol D **L-277**



$C_{66}H_{114}O_{25}$ 1307.612
Isol. from an *Amphidinium* sp. Amorph. solid. $[\alpha]_D^{23}$ +4.7 (c, 0.25 in MeOH). λ_{max} 232 (ϵ 22800) (MeOH).

Kubota, T. *et al., Mar. Drugs*, 2005, **3**, 113-118 (*isol, pmr, cmr*)

Luteorosin **L-278**

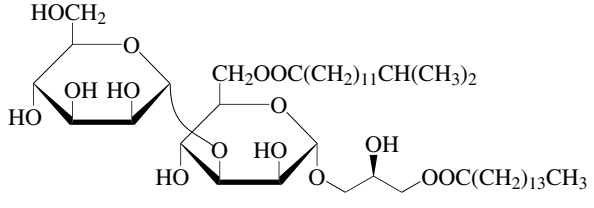


$C_{21}H_{26}O_5$ 358.433
Constit. of *Chromodoris luteorosea*. Ichthyotoxic. λ_{max} 215 (ϵ 19000); 243 (ϵ 11200) (MeOH) (Berdy).

Cimino, G. *et al., J. Nat. Prod.*, 1990, **53**, 102-106 (*isol, pmr, cmr*)
Gavagnin, M. *et al., J. Nat. Prod.*, 1992, **55**, 368-371 (*isol*)

Lutoside **L-279**

[195702-39-7]

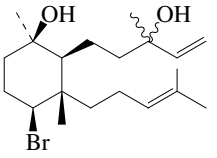


$C_{45}H_{84}O_{15}$ 865.15
Isol from *Micrococcus luteus* found on the sponge *Xestospongia* sp. Amorph. solid.
Mp 88°. $[\alpha]_D$ +8.6 (c, 0.5 in MeOH).

Bultel-Ponce, V. *et al., Tet. Lett.*, 1997, **38**, 5805-5808 (*isol, pmr, cmr*)

Luzodiol **L-280**

[866453-24-9]

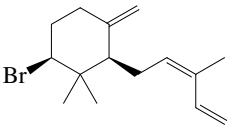


$C_{20}H_{35}BrO_2$ 387.399
Constit. of *Laurencia luzonensis*. Amorph. solid. $[\alpha]_D$ +13.7 (c, 0.12 in $CHCl_3$).

Kuniyoshi, M. *et al., J. Nat. Prod.*, 2005, **68**, 1314-1317 (*Luzodiol*)

Luzonensin **L-281**

[350483-19-1]

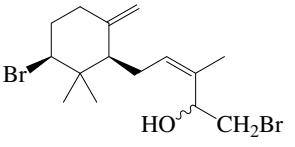


$C_{15}H_{23}Br$ 283.251
Constit. of *Laurencia luzonensis*. Oil. $[\alpha]_D^{25}$ +3 (c, 0.16 in $CHCl_3$).

Kuniyoshi, M. *et al., J. Nat. Prod.*, 2001, **64**, 696-700 (*isol, pmr, cmr*)

Luzonensol **L-282**

[350483-17-9]

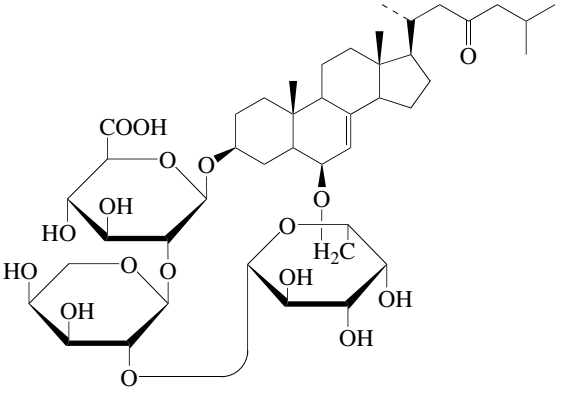


$C_{15}H_{24}Br_2O$ 380.162
Constit. of *Laurencia luzonensis*. Oil. $[\alpha]_D^{27}$ -39.6 (c, 2.26 in $CHCl_3$).

Ac: ***Luzonensol acetate***
[350483-18-0]
$C_{17}H_{26}Br_2O_2$ 422.199
Constit. of *Laurencia luzonensis*. Oil. $[\alpha]_D^{25}$ -13 (c, 0.23 in $CHCl_3$).
Kuniyoshi, M. *et al., J. Nat. Prod.*, 2001, **64**, 696-700 (*isol, pmr, cmr*)

Luzonicoside A **L-283**

[81001-97-0]



$C_{44}H_{68}O_{17}$ 869.011
Constit. of *Echinaster luzonicus*.
$[\alpha]_D$ -66 (H_2O).

Riccio, R. *et al., Experientia*, 1982, **38**, 68-70 (*isol, pmr, cmr*)

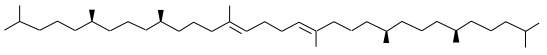
LVL 1 L-284

Glycoprotein composed of covalently bonded subunits of 53 kDa. Isol. from the soft coral *Lobophytum variatum*. Lectin.

Goto-Nance, R. *et al., Fish. Sci.*, 1996, **62**, 297-301 (*isol*)

Lycopadiene L-285

1,1′,2,2′,5,5′,6,6′,7,7′,8,8′,9,9′,10,10′,11,11′,12,12′,15,15′-Docosahydrolycopene
[111051-86-6]

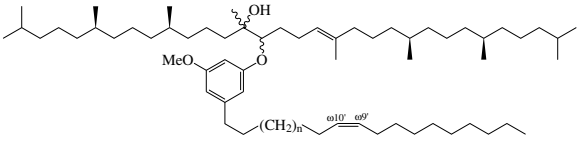


$C_{40}H_{78}$ 559.056
Constit. of green alga *Botryococcus braunii*.

*13*R,*14*R:*13′*S,*14′*S-*Diepoxide:* ***Diepoxylycopane***
[220676-63-1]
$C_{40}H_{78}O_2$ 591.055
Constit. of *Botryococcus braunii*. Oil. $[\alpha]_D$ -2.8 (c, 3.9 in heptane). Nonstandard numbering used in the lit.

Metzger, P. *et al., Tet. Lett.*, 1987, **28**, 3931
Metzger, P. *et al., Tetrahedron*, 1999, **55**, 167-176 (*diepoxide*)

Lycopanerol I L-286



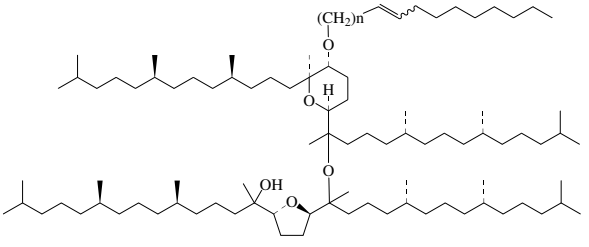
n = 6,8,10,12,14,16

A series of homologues, some with ω9′, ω10′-dihydro. Constit. of *Botryococcus braunii*.

[565430-00-4, 565430-01-5, 565430-02-6, 565430-03-7, 565430-04-8, 565430-05-9, 565430-06-0, 565430-07-1, 565430-08-2, 565430-09-3]

Metzger, P. *et al., J. Nat. Prod.*, 2003, **66**, 772-778 (*isol, pmr, cmr*)

Lycopanerol A L-287



Series of polyether homologues isol. from *Botryococcus braunii*. $[\alpha]_D^{20}$ -6.9 (c, 4.58 in heptane). Both *E*- and *Z*- double bonds present.

n = 18 [190778-22-4]
[190778-45-1]
$C_{108}H_{212}O_5$ 1590.86

n = 20 [190778-76-8]
[190778-93-9]
$C_{110}H_{216}O_5$ 1618.913

Epoxide: ***Lycopanerol B***
[295342-58-4]
$C_{110}H_{216}O_6$ 1634.913
Constit. of *Botryococcus braunii*. Mixt. of homologues with n = 20, 22.

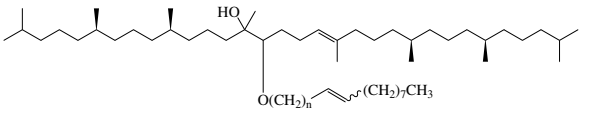
n = 22 [190778-97-3]
[190779-02-3]
$C_{112}H_{220}O_5$ 1646.967

Epoxide: [295342-71-1]
$C_{112}H_{220}O_6$ 1662.966
Constit. of *Botryococcus braunii*.

Metzger, P. *et al., Tet. Lett.*, 1997, **38**, 2977-2980 (*Lycopanerols A*)
Rager, M.-N. *et al., Phytochemistry*, 2000, **54**, 427-437 (*Lycopanerols B*)

Lycopanerol C L-288

[295342-73-3]
[295342-74-4]

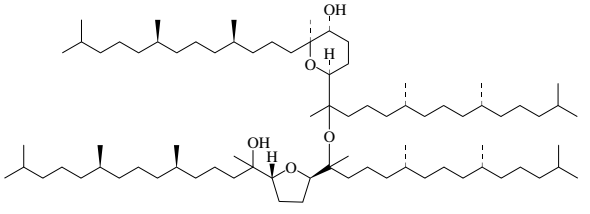


$C_{70}H_{138}O_2$ 1011.859
Isol. as mixt. of homologues, n = 18, 20, 22. MF and CAS refer to homologue with n = 20. Isol. from *Botryococcus braunii*. Both *E*- and *Z*- double bonds present.

Rager, M.-N. *et al., Phytochemistry*, 2000, **54**, 427-437 (*isol, pmr, cmr*)

Lycopanerol D L-289

[295342-60-8]

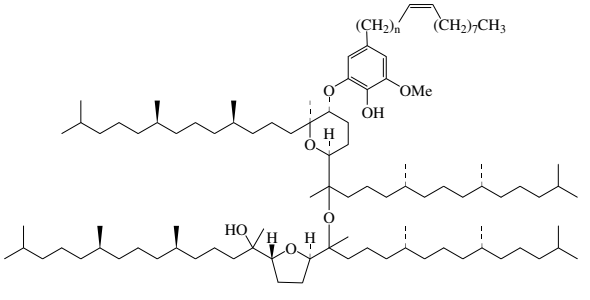


$C_{80}H_{158}O_5$ 1200.125
Isol. from *Botryococcus braunii*. Oil. $[\alpha]_D^{20}$ -1.7 (c, 7.5 in $CHCl_3$).

Rager, M.-N. *et al., Phytochemistry*, 2000, **54**, 427-437 (*isol, pmr, cmr*)

Lycopanerol E L-290

[295342-61-9]
[295342-70-0, 295342-72-2]

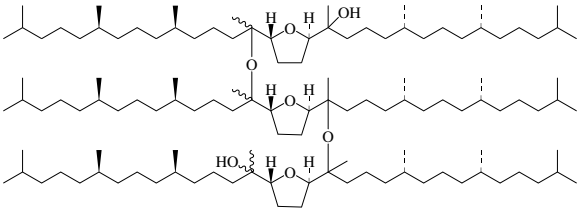


$C_{114}H_{216}O_7$ 1698.956
Isol. as series of homologues, n = 17, 21, 25. MF and CAS no. refer to lowest homologue with n = 17. Isol. from *Botryococcus braunii*.

Rager, M.-N. *et al., Phytochemistry*, 2000, **54**, 427-437 (*isol, pmr, cmr*)

Lycopanerol F L-291

[295342-62-0]

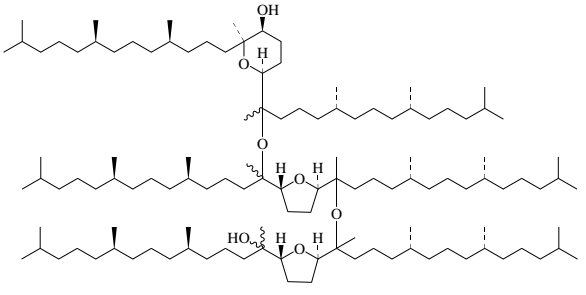


$C_{120}H_{236}O_7$ 1791.18
Constit. of *Botryococcus braunii*. Oil. $[\alpha]_D^{20}$ -2.4 (c, 5 in $CHCl_3$).

Rager, M.-N. *et al., Phytochemistry*, 2000, **54**, 427-437 (*isol, pmr, cmr*)

Lycopanerol G L-292

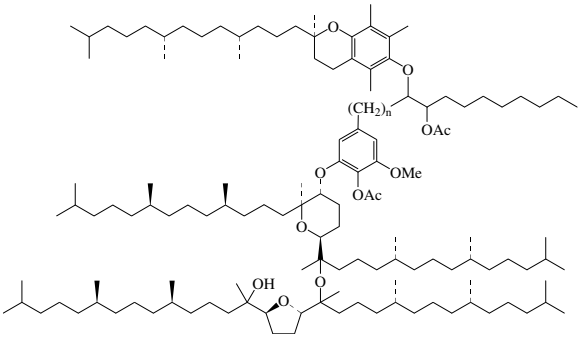
[295342-63-1]



$C_{120}H_{236}O_7$ 1791.18
Constit. of *Botryococcus braunii*. Oil. $[\alpha]_D^{20}$ -7.4 (c, 6.3 in $CHCl_3$).

Rager, M.-N. *et al., Phytochemistry*, 2000, **54**, 427-437 (*isol, pmr, cmr*)

Lycopanerol H L-293



A mixt. of homologues with n = 21, 23. Isol. from *Botryococcus braunii*.

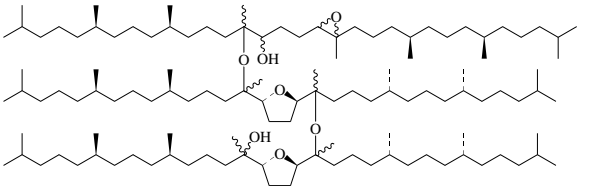
n = 21 [436805-17-3]
$C_{151}H_{278}O_{12}$ 2285.85

n = 23 [436805-18-4]
$C_{153}H_{282}O_{12}$ 2313.904

Metzger, P. *et al., Tet. Lett.*, 2002, **43**, 2377-2380

Lycopanerol J L-294

[565430-10-6]

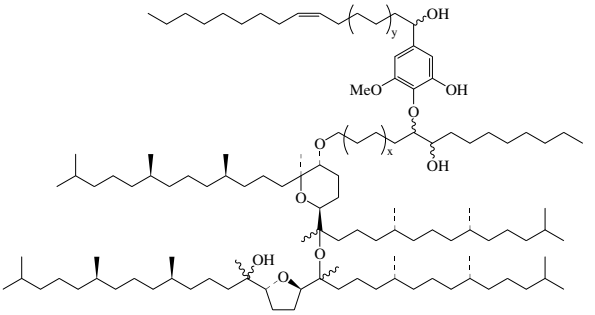


$C_{120}H_{236}O_7$ 1791.18
Constit. of *Botryococcus braunii*.

Metzger, P. *et al., J. Nat. Prod.*, 2003, **66**, 772-778 (*isol, pmr, cmr*)

Lycopanerol K L-295

[565430-11-7]
[565430-12-8]



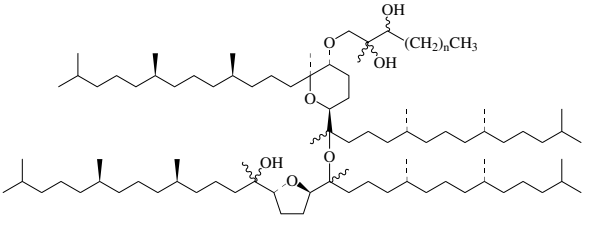
x = 8-11, y = 6-8

Series of homologues. Constit. of *Botryococcus braunii*.

Metzger, P. *et al., J. Nat. Prod.*, 2003, **66**, 772-778 (*isol, pmr, cmr*)

Lycopanerol L L-296

[565430-13-9, 565430-14-0]



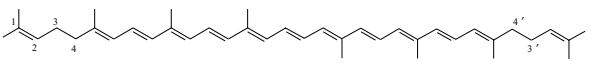
n = 24,28

Mixt. of homologues. Prod. by *Botryococcus braunii*.

Metzger, P. *et al., J. Nat. Prod.*, 2003, **66**, 772-778 (*isol, pmr, cmr*)

Lycopene L-297

2,6,10,14,19,23,27,31-Octamethyl-2,6,8,10,12,14,16,18,20,22,24,26,30-dotriacontatridecaene. ψ,ψ-Carotene, 9CI. Solanorubin. Dicarotene. Lycopine. E160



$C_{40}H_{56}$ 536.882
Used as food colouring.

(all-E)-form [502-65-8]
Constit. of tomatoes and many other fruits. Also occurs in bacteria and fungi. Widely distributed in marine algae (red, green and brown).

Long red needles or prisms (petrol).
Mp 175°.

*1,2*S-*Epoxide:* ***1,2-Epoxy-1,2-dihydrolycopene****. 1,2-Epoxy-1,2-dihydro-ψ,ψ-carotene*
[51599-09-8]
$C_{40}H_{56}O$ 552.882
Isol. from tomatoes.

5,6-Epoxide: ***5,6-Epoxy-5,6-dihydrolycopene****. 5,6-Epoxy-5,6-dihydro-ψ,ψ-carotene*
[51599-10-1]
$C_{40}H_{56}O$ 552.882
Constit. of tomatoes.

3,4-Didehydro: Monodehydrolycopene. 3,4-Dehydrolycopene. 3,4-Didehydro-ψ,ψ-carotene
$C_{40}H_{54}$ 534.867
Isol. from *Neurospora* spp., *Lycogala epidendron* and other microorganisms. Fine violet needles (C_6H_6/petrol).
Mp 196°.

(7*Z*,7′*Z*,9*Z*,9′*Z*)-*form*
Prolycopene
[2361-24-2]
Constit. of tomatoes (*Lycopersicon esculentum*). Also in other fruits.
Red prisms (C_6H_6/MeOH); red-orange flaky cryst. (hexane/EtOH).
Mp 111°. λ_{max} 232; 255; 295; 437 (hexane).

(5*Z*)-*form*
Synthetic.
Red cryst. (CH_2Cl_2/MeOH). Mp 143°. λ_{max} 362; 443; 470; 502 (hexane/CH_2Cl_2).

(7*Z*)-*form*
Synthetic.
Red cryst. (hexane). Mp 126°. λ_{max} 362; 443; 469; 499 (hexane/CH_2Cl_2).

(15*Z*)-*form*
Synthetic. Mp 100° approx. λ_{max} 360; 441; 499 (hexane/CH_2Cl_2).

(5*Z*,5′*Z*)-*form*
Synthetic.
Deep red cryst. (CH_2Cl_2/MeOH). Mp 152-153°. λ_{max} 362; 443; 470; 502 (hexane/CH_2Cl_2).

(7*Z*,7′*Z*)-*form*
Synthetic.
Red-orange cryst. Mp 133°. λ_{max} 466; 493 (hexane/CH_2Cl_2).

(7*Z*,9*Z*)-*form*
Synthetic.
Sensitive, red-orange cryst. (CH_2Cl_2/MeOH). Mp 78-79°. λ_{max} 444; 470 (hexane/CH_2Cl_2).

(9*Z*,9′*Z*)-*form*
Synthetic.
Red cryst. (hexane). Mp 135°. λ_{max} 360; 433; 459; 490 (hexane/CH_2Cl_2).

(9*Z*)-*form* [64727-64-6]
Synthetic. Identified by pmr.

(13*Z*)-*form*
Synthetic. Identified by pmr.

(5*Z*,9′*Z*)-*form*
Synthetic. Identified by pmr.

(9*Z*,13′*Z*)-*form*
Synthetic. Identified by pmr.

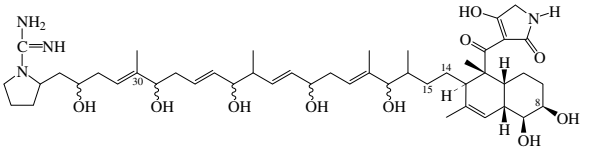
(5*Z*,9*Z*,5′*Z*)-*form*
Synthetic. Identified by pmr.

(5*Z*,13*Z*,5′*Z*)-*form*
Synthetic. Identified by pmr.

Karrer, P. *et al., Helv. Chim. Acta*, 1950, **33**, 1349 (*synth*)
Isler, O. *et al., Helv. Chim. Acta*, 1956, **39**, 463 (*synth*)
Winterstein, A. *et al., Chem. Ber.*, 1960, **93**, 2951 (*derivs*)
Surmatis, J.D. *et al., J.O.C.*, 1963, **28**, 2735 (*synth, Dehydrolycopene*)
Jensen, S.L. *et al., Phytochemistry*, 1965, **4**, 925 (*Monodehydrolycopene*)
Enzell, C.R. *et al., Acta Chem. Scand.*, 1969, **23**, 727 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, nos. 1818; 1820 (*occur*)
Ben-Aziz, A. *et al., Phytochemistry*, 1973, **12**, 2759 (*isol*)
Clough, J.M. *et al., J.C.S. Perkin 1*, 1983, 3011 (*Prolycopene*)
Pfander, H. *et al., Helv. Chim. Acta*, 1984, **67**, 964; 968 (*epoxide, isol, synth*)
Ritacco, R.P. *et al., J. Agric. Food Chem.*, 1984, **32**, 296
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 31 (*bibl*)
Pattenden, G. *et al., Tet. Lett.*, 1987, **28**, 5751 (*synth*)
Hengartner, U. *et al., Helv. Chim. Acta*, 1992, **75**, 1848 (*synth*)
Stahl, W. *et al., Arch. Biochem. Biophys.*, 1996, **336**, 1-9 (*rev*)
Bramley, P. M. *et al., Phytochemistry*, 2000, **54**, 233-236 (*rev*)
Bruno, R.S. *et al., Handbook of Nutraceuticals and Functional Foods*, (ed. Wildman, R.E.C.) CRC Press, 2001, 157-168
Eguchi, T. *et al., Tetrahedron*, 2005, **61**, 2027-2035 (*synth*)

Lydicamycin L-298

[133352-27-9]



$C_{47}H_{74}N_4O_{10}$ 855.122
Prod. by *Streptomyces lydicus* SANK 60390. Active against gram-positive bacteria. Powder. Sol. MeOH, butanol; poorly sol. H_2O. Mp 161-166°. $[\alpha]_D^{18}$ +75.1 (c, 1 in MeOH). λ_{max} 207 (ϵ 18900); 250 (sh) (ϵ 6600); 282 (ϵ 9900) (MeOH/HCl) (Derep). λ_{max} 208 (ϵ 19900); 245 (ϵ 9700); 281 (ϵ 9600) (MeOH/NaOH) (Derep). λ_{max} 207 (ϵ 19600); 245 (ϵ 9900); 282 (ϵ 10000) (MeOH) (Derep).

8-Deoxy: ***8-Deoxylydicamycin****. Antibiotic TPU 0037D. TPU 0037D*
$C_{47}H_{74}N_4O_9$ 839.123
Prod. by the marine-derived *Streptomyces platensis* TP-A0598. Active against gram-positive bacteria incl. MRSA. Powder. Mp 161-163°. $[\alpha]_D^{28}$ +50.3 (c, 1 in MeOH). λ_{max} 203 (log ϵ 4.31); 244 (log ϵ 3.95); 282 (log ϵ 3.96) (MeOH).

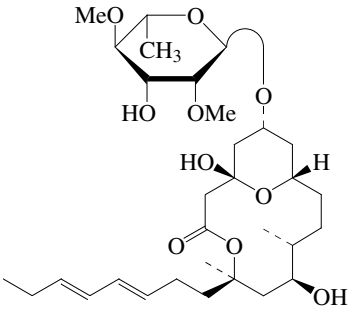
8-Deoxy, 14,15-didehydro: ***14,15-Didehydro-8-deoxylydicamycin****. Antibiotic TPU 0037B. TPU 0037B*
$C_{47}H_{72}N_4O_9$ 837.107
Prod. by the marine-derived *Streptomyces platensis* TP-A0598. Active against gram-positive bacteria incl. MRSA. Powder. Mp 162-164°. $[\alpha]_D^{28}$ +105.5 (c, 1 in MeOH). λ_{max} 207 (log ϵ 4.31); 244 (log ϵ 3.95); 283 (log ϵ 3.97) (MeOH).

30-Demethyl: ***30-Demethyllydicamycin****. Antibiotic TPU 0037A. TPU 0037A*
$C_{46}H_{72}N_4O_{10}$ 841.096
Prod. by the marine-derived *Streptomyces platensis* TP-A0598. Active against gram-positive bacteria incl. MRSA. Powder. Mp 151-153°. $[\alpha]_D^{28}$ +57.5 (c, 1 in MeOH). λ_{max} 204 (log ϵ 4.31); 247 (log ϵ 3.95); 282 (log ϵ 3.95) (MeOH).

30-Demethyl, 8-deoxy: ***30-Demethyl-8-deoxylydicamycin****. Antibiotic TPU 0037C. TPU 0037C*
$C_{46}H_{72}N_4O_9$ 825.096
Prod. by the marine-derived *Streptomyces platensis* TP-A0598. Active against gram-positive bacteria incl. MRSA. Powder. Mp 161-163°. $[\alpha]_D^{28}$ +52 (c, 0.76 in MeOH). λ_{max} 207 (log ϵ 4.31); 244 (log ϵ 3.96); 281 (log ϵ 3.97) (MeOH).

Hayakawa, Y. *et al., J. Antibiot.*, 1991, **44**, 282-287; 288-292 (*isol, props*)
Hayakawa, Y. *et al., Tet. Lett.*, 1991, **32**, 213-216 (*pmr, cmr, ms*)
Furuma, T. *et al., J. Antibiot.*, 2002, **55**, 873-880 (*TPU 0037 antibiotics*)

Lyngbouilloside L-299



Relative Configuration

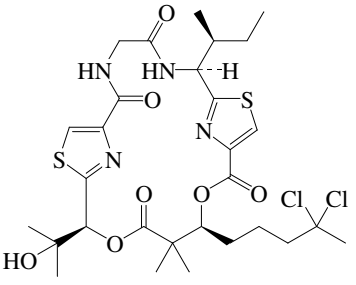
$C_{31}H_{52}O_{10}$ 584.746

Similar to Dolastatin 19, D-1213. Relative stereochem. of aglycone and sugar portions were not correlated. Isol. from *Lyngbya bouillonii*. Moderate cytotoxic agent. Amorph. solid. $[\alpha]_D^{25}$ -38 (c, 0.46 in $CHCl_3$). λ_{max} 235 (ϵ 26200) (EtOH).

Tan, L.T. *et al., J. Nat. Prod.*, 2002, **65**, 925-928 (*isol, pmr, cmr*)

Lyngbyabellin A L-300

[273202-85-0]



$C_{29}H_{40}Cl_2N_4O_7S_2$ 691.695

Depsipeptide antibiotic. Related to Dolabellin, D-1180. Isol. from *Lyngbya majuscula*. Potent disruptor of the cellular microfilament network. Cytotoxic agent. Cryst. (CH_2Cl_2/6-methylheptane).

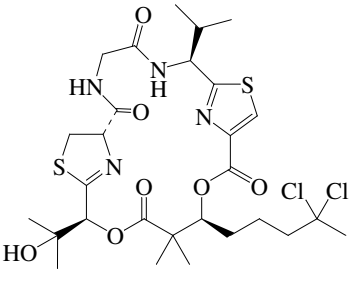
Mp 150-152°. $[\alpha]_D^{27}$ -74 (c, 0.5 in $CHCl_3$). λ_{max} 202 (log ϵ 4.48); 236 (log ϵ 4.08) (MeOH).

Luesch, H. *et al., J. Nat. Prod.*, 2000, **63**, 611-615 (*isol*)
Yokokawa, F. *et al., Tetrahedron*, 2002, **58**, 9445-9458 (*synth*)

Lyngbyabellin B L-301

Tortugamide

[300830-53-9]



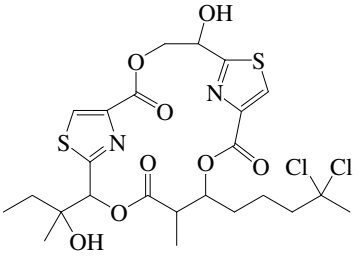
$C_{28}H_{40}Cl_2N_4O_7S_2$ 679.684

Isol. from *Lyngbya majuscula*. Cytotoxic and antifungal agent. Amorph. solid. $[\alpha]_D^{25}$ -152 (c, 0.06 in $CHCl_3$). $[\alpha]_D$ +33 (c, 0.2 in CH_2Cl_2). Isol. simultaneously by 2 groups. λ_{max} 200 (log ϵ 4.49); 224 (log ϵ 4.06); 236 (sh) (log ϵ 3.93) (MeOH).

Luesch, H. *et al., J. Nat. Prod.*, 2000, **63**, 1437-1439
Milligan, K.E. *et al., J. Nat. Prod.*, 2000, **63**, 1440-1443
Yokokawa, F. *et al., Tetrahedron*, 2002, **58**, 9445-9458 (*synth*)

Lyngbyabellin C L-302

[479482-34-3]



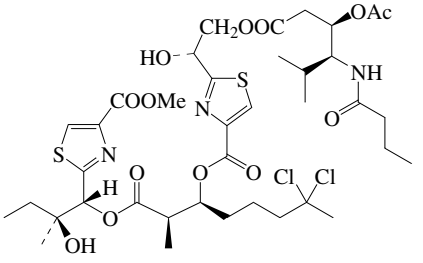
$C_{24}H_{30}Cl_2N_2O_8S_2$ 609.547

Isol. from a *Lyngbya* sp. Cytotoxic. Amorph. solid. $[\alpha]_D^{25}$ -10 (c, 0.1 in $CHCl_3$). λ_{max} 202 (log ϵ 4.47); 235 (log ϵ 4.04) (MeOH).

Luesch, H. *et al., Tetrahedron*, 2002, **58**, 7959-7966 (*isol, pmr, cmr*)

Lyngbyabellin D L-303

[532427-69-3]



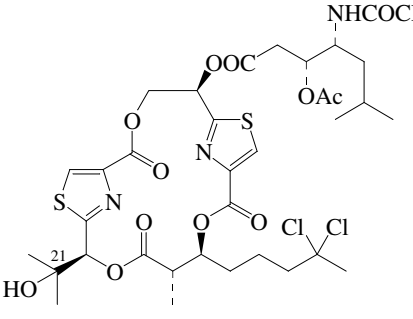
Absolute Configuration

$C_{38}H_{55}Cl_2N_3O_{13}S_2$ 896.902

Isol. from a *Lyngbya* sp. Cytotoxic. Powder. $[\alpha]_D^{25}$ +20 (c, 0.4 in MeOH). λ_{max} 202 (log ϵ 7.31); 223 (log ϵ 6.81) (MeOH).

Williams, P.G. *et al., J. Nat. Prod.*, 2003, **66**, 595-598 (*isol, pmr, cmr*)

Lyngbyabellin E L-304



Absolute Configuration

$C_{37}H_{51}Cl_2N_3O_{12}S_2$ 864.86

Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{26}$ -31 (c, 0.7 in MeOH). λ_{max} 240 (log ϵ 4.18) (MeOH).

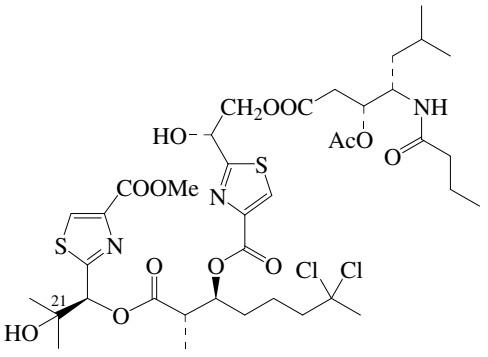
21-Deoxy: ***Lyngbyabellin H***

$C_{37}H_{51}Cl_2N_3O_{11}S_2$ 848.861

Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{26}$ -53 (c, 0.08 in MeOH). λ_{max} 242 (log ϵ 4.15) (MeOH).

Han, B. *et al., Tetrahedron*, 2005, **61**, 11723-11729 (*isol, pmr, cmr*)

Lyngbyabellin F L-305

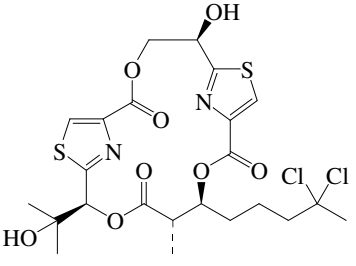


$C_{38}H_{55}Cl_2N_3O_{13}S_2$ 896.902
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{26}$ -6.5 (c, 0.2 in MeOH). λ_{max} 238 (log ϵ 4) (MeOH).

21-Deoxy: ***Lyngbyabellin I***
$C_{38}H_{55}Cl_2N_3O_{12}S_2$ 880.903
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{26}$ -25 (c, 0.04 in MeOH). λ_{max} 238 (log ϵ 4.28) (MeOH).

Han, B. *et al., Tetrahedron*, 2005, **61**, 11723-11729 (*isol, pmr, cmr*)

Lyngbyabellin G L-306



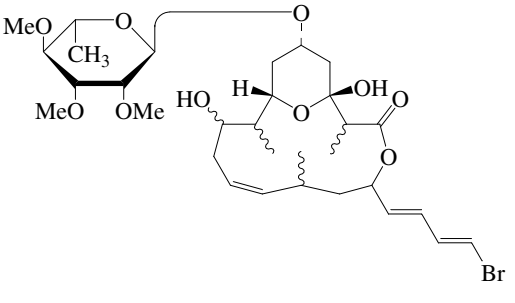
Absolute Configuration

$C_{23}H_{28}Cl_2N_2O_8S_2$ 595.52
Isol. from *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{26}$ -26 (c, 0.2 in MeOH). λ_{max} 238 (log ϵ 3.75) (MeOH).

Han, B. *et al., Tetrahedron*, 2005, **61**, 11723-11729 (*isol, pmr, cmr*)

Lyngbyaloside L-307

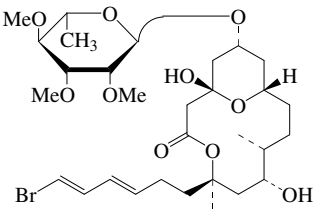
[196874-10-9]



$C_{31}H_{49}BrO_{10}$ 661.626
Isol. from *Lyngbya bouillonii*. Amorph. solid. λ_{max} 199 (ϵ 10700); 240 (ϵ 25700) (hexane).

Klein, D. *et al., J. Nat. Prod.*, 1997, **60**, 1057-1059 (*isol, uv, pmr, cmr, ms*)

Lyngbyaloside B L-308



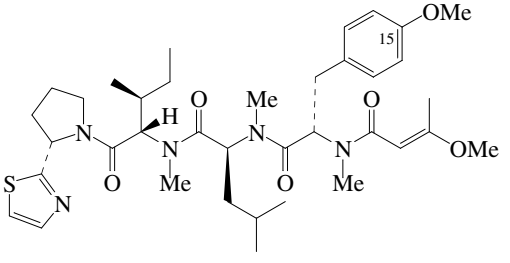
Probable Absolute Configuration

$C_{30}H_{49}BrO_{10}$ 649.615
Isol. from a Palauan marine cyanobacterium, *Lyngbya* sp. Weakly cytotoxic. Amorph. solid. $[\alpha]_D^{25}$ -20 (c, 0.1 in $CHCl_3$). λ_{max} 233 (log ϵ 3.66); 240 (log ϵ 3.66); 246 (sh) (log ϵ 3.55) (MeOH).

Luesch, H. *et al., J. Nat. Prod.*, 2002, **65**, 1945-1948 (*isol, pmr, cmr, ms*)

Lyngbyapeptin A L-309

[221531-83-5]



Absolute Configuration

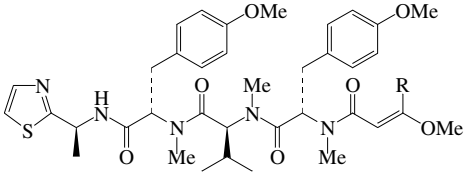
$C_{37}H_{55}N_5O_6S$ 697.937
Isol. from *Lyngbya bouillonii* and *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{25}$ -235 (c, 0.58 in MeOH). λ_{max} 201 (log ϵ 4.55); 225 (log ϵ 4.3); 240 (sh) (log ϵ 4.09) (MeOH).

15-O-*De-Me:* ***15-Norlyngbyapeptin A***
[532427-68-2]
$C_{36}H_{53}N_5O_6S$ 683.911
Isol. from a *Lyngbya* sp. Powder. $[\alpha]_D^{22}$ -31 (c, 0.4 in MeOH). λ_{max} 201 (log ϵ 4.2); 226 (log ϵ 4.02) (MeOH).

Klein, D. *et al., Tet. Lett.*, 1999, **40**, 695-696 (*isol, pmr, cmr*)
Luesch, H. *et al., J.O.C.*, 2000, **63**, 1437-1439 (*abs config*)
Williams, P.G. *et al., J. Nat. Prod.*, 2003, **66**, 595-598 (*15-Norlyngbyapeptin A*)

Lyngbyapeptin B L-310

[479482-35-4]



R = CH_3

Absolute Configuration

$C_{38}H_{51}N_5O_7S$ 721.916
Isol. from a *Lyngbya* sp. Amorph. solid. $[\alpha]_D^{25}$ -50 (c, 0.23 in MeOH). λ_{max} 200 (log ϵ 4.53); 227 (log ϵ 4.24); 245 (sh) (log ϵ 4) (MeOH).

Luesch, H. *et al., Tetrahedron*, 2002, **58**, 7959-7966 (*isol, pmr, cmr*)

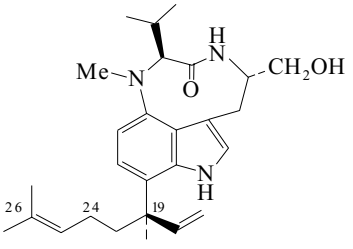
Lyngbyapeptin C L-311

[479482-36-5]
As Lyngbyapeptin B, L-310 with
R = CH_2CH_3
$C_{39}H_{53}N_5O_7S$ 735.943
Isol. from a *Lyngbya* sp. Amorph. solid. $[\alpha]_D^{25}$ -52 (c, 0.09 in MeOH). λ_{max} 200 (log ϵ 4.53); 227 (log ϵ 4.26); 245 (sh) (log ϵ 4) (MeOH).

Luesch, H. *et al., Tetrahedron*, 2002, **58**, 7959-7966 (*isol, pmr, cmr*)

Lyngbyatoxin A L-312

Teleocidin A_1
[70497-14-2]



$C_{27}H_{39}N_3O_2$ 437.624
Numbering as given by Aimi *et al*. Isol. from lipid extracts of a Hawaiian shallow-water variety of the marine blue-green alga *Lyngbya majuscula*. Also prod. by *Streptomyces mediocidicus*. Nematocide and acaricide. Potent tumour promoter.
Mp 61°. $[\alpha]_D$ -110 (MeOH). $[\alpha]_D$ -171 (c, 1.8 in $CHCl_3$). Closely related to Teleocidin B_1. λ_{max} 233 (ϵ 34700); 287 (ϵ 9770); 298 (sh) (ϵ 8130) (MeOH) (Derep).

▶ Highly inflammatory and vesicatory. Tumour promoter. Causes dermatitis. Very toxic. LD_{50} (mus, orl) 2mg/kg. WY1981000

14-Ac: **O-*Acetyllyngbyatoxin A***
[70497-15-3]
$C_{29}H_{41}N_3O_3$ 479.661
Isol. from the sea hare *Stylocheilus longicauda*. Oil. $[\alpha]_D$ -4 (c, 0.4 in MeOH). λ_{max} 229 (ϵ 4260); 297 (ϵ 1270) (MeOH).

N-*De-Me:* **N^{13}-*Demethylteleocidin A_1***
$C_{26}H_{37}N_3O_2$ 423.597
From *Streptoverticillium blastmyceticum*. No phys. props. reported. Sol. MeOH, EtOAc; poorly sol. H_2O. λ_{max} 228 (ϵ 25900); 285 (ϵ 7600); 295 (ϵ 6800) (MeOH) (Derep).

▶ Tumour promoter.

Me ether: **5-O-*Methylteleocidin A_1***
[114774-86-6]
$C_{28}H_{41}N_3O_2$ 451.651
From *Streptoverticillium blastmyceticum*. Gummy solid. Sol. MeOH, Me_2CO, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{18}$ -198 (c, 0.21 in $CHCl_3$). λ_{max} 230 (ϵ 27000); 286 (ϵ 8400); 301 (ϵ 9200) (MeOH) (Berdy).

▶ Tumour promoter.

24ξ-Hydroxy, Δ^{26}-isomer: ***Lyngbyatoxin B***
[133084-52-3]
$C_{27}H_{39}N_3O_3$ 453.623
Isol. from *Lyngbya majuscula*. TPA binding inhibitor. Amorph.

▶ Skin irritant.

26-Hydroxy, Δ^{24}-isomer: ***Lyngbyatoxin C***
[133084-53-4]
$C_{27}H_{39}N_3O_3$ 453.623
Isol. from *Lyngbya majuscula*. TPA binding inhibitor. Amorph.

▶ Skin irritant.

19-Epimer: ***Teleocidin A_2***
[102209-77-8]
$C_{27}H_{39}N_3O_2$ 437.624
From *Streptoverticillium mediocidicus*.
$[\alpha]_D^{18}$ -185.1 (c, 0.18 in MeOH). λ_{max} 233 (ϵ 34700); 287 (ϵ 9770); 298 (sh) (ϵ 8130) (MeOH) (Derep).

▶ Potent tumour promoter.

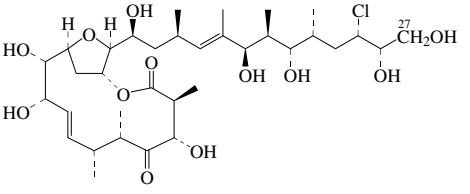
Takashima, M. *et al., Agric. Biol. Chem.*, 1962, **26**, 660 (*isol, props*)
Cardellina, J.H. *et al., Science (Washington, D.C.)*, 1979, **204**, 193 (*isol, pmr, cmr, cd, struct*)
Moore, R.E. *et al., Pure Appl. Chem.*, 1982, **54**, 1919 (*rev*)
Sakai, S.-I. *et al., Tet. Lett.*, 1986, **27**, 5219
Muratake, H. *et al., Tet. Lett.*, 1987, **28**, 2265 (*synth*)
Hagiwara, N. *et al., Agric. Biol. Chem.*, 1988, **52**, 641 (*isol, deiv*)
Irie, K. *et al., Agric. Biol. Chem.*, 1988, **52**, 3193 (*deriv*)
Aimi, N. *et al., J. Nat. Prod.*, 1990, **53**, 1593 (*Lyngbyatoxin B, Lyngbyatoxin C*)
Irie, K. *et al., Tetrahedron*, 1990, **46**, 2773 (*biosynth*)
Muratake, H. *et al., Tetrahedron*, 1991, **47**, 8535; 8545; 8559 (*synth*)
Gallimore, W.A. *et al., J. Nat. Prod.*, 2000, **63**, 1022-1026 (*O-Acetyllyngbyatoxin A*)

Lytechinastatin L-313

[80893-08-9]
Glycoprotein. Isol. from the sea urchin *Lytechinus variegatus*. Shows antitumour activity. Fairly sol. H_2O; poorly sol. hexane.

Pettit, G.R. *et al., J. Nat. Prod.*, 1981, **44**, 713-716 (*isol*)

Lytophilippine A L-314



Absolute Configuration

$C_{34}H_{57}ClO_{12}$ 693.27
Isol. from the Red Sea hydroid *Lytocarpus philippinus*. Powder. $[\alpha]_D^{23}$ -45.8 (c, 0.04 in MeOH). λ_{max} 282 (log ϵ 2.07) (MeOH).

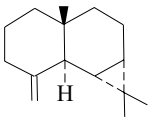
27-O-*Hexadecanoyl:* ***Lytophilippine B***
$C_{50}H_{87}ClO_{13}$ 931.682
Isol. from *Lytocarpus philippinus*. Powder. $[\alpha]_D^{23}$ -37.4 (c, 0.009 in MeOH). λ_{max} 282 (log ϵ 1.98) (MeOH).

27-O-*(9Z-Octadecenoyl):* ***Lytophilippine C***
$C_{52}H_{89}ClO_{13}$ 957.72
Isol. from *Lytocarpus philippinus*. Powder. $[\alpha]_D^{23}$ -44.2 (c, 0.008 in MeOH). λ_{max} 282 (log ϵ 2.07) (MeOH).

Rezanka, T. *et al., Tetrahedron*, 2004, **60**, 12191-12199 (*isol, pmr, cmr*)

γ-Maaliene M-1

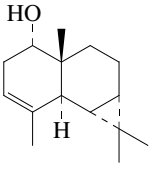
[20071-49-2]



$C_{15}H_{24}$ 204.355
Constit. of *Pseudopterogorgia americana*. Oil. $[\alpha]_D^{25}$ +10.9 (c, 1.2 in hexane).

Weinheimer, A.J. *et al., Chem. Comm.*, 1968, 1070

3-Maalien-1-ol M-2



$C_{15}H_{24}O$ 220.354

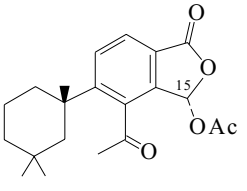
1α-*form* [680210-16-6]
Constit. of *Clavularia koellikeri*.
Oil. $[\alpha]_D^{25}$ -3.8 (c, 0.15 in $CHCl_3$).

Ac: [680210-15-5]
$C_{17}H_{26}O_2$ 262.391
Constit. of *Clavularia koellikeri*. Oil. $[\alpha]_D^{25}$ +21.9 (c, 0.08 in $CHCl_3$).

Iguchi, K. *et al., J. Nat. Prod.*, 2004, **67**, 577-583 (*isol, pmr, cmr*)

Macfarlandin A M-3

[102396-21-4]



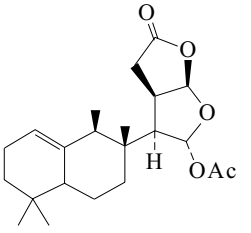
$C_{21}H_{26}O_5$ 358.433
Constit. of *Chromodoris macfarlandi* and *Chromodoris luteorosea*. Ichthyotoxic, antimicrobial. Cryst. (Et_2O/hexane). Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. H_2O.
Mp 183-184°. $[\alpha]_D$ +189 (c, 0.65 in $CHCl_3$). λ_{max} 216 (ϵ 17200); 246 (ϵ 15800) (MeOH) (Derep). λ_{max} 216 (ϵ 17200); 246 (ϵ 15800) (MeOH) (Berdy).

15-Epimer: ***Macfarlandin B***
[102396-22-5]
$C_{21}H_{26}O_5$ 358.433
From *Chromodoris macfarlandi*. Antimicrobial. Glass. Sol. MeOH, $CHCl_3$, Me_2CO; poorly sol. H_2O. $[\alpha]_D$ -128 (c, 0.99 in $CHCl_3$). λ_{max} 216 (ϵ 17200); 246 (ϵ 15800) (MeOH) (Derep). λ_{max} 209
(ϵ 18400); 245 (ϵ 12000) (MeOH) (Berdy).

Molinski, T.F. *et al., J.O.C.*, 1986, **51**, 2601
Cimino, G. *et al., J. Nat. Prod.*, 1990, **53**, 102

Macfarlandin C M-4

[105064-35-5]

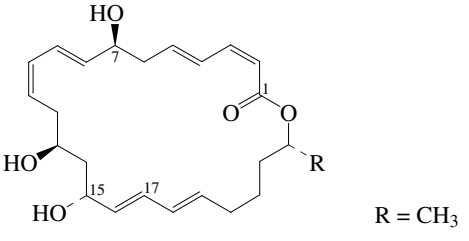


$C_{22}H_{32}O_5$ 376.492
Constit. of *Chromodoris macfarlandi*. Cryst. (Et_2O/hexane). Mp 195-196°. $[\alpha]_D$ -29.1 (c, 0.75 in $CHCl_3$).

Molinski, T.F. *et al., J.O.C.*, 1986, **51**, 4564-4567 (*isol*)

Macrolactin A M-5

[122540-27-6]



$C_{24}H_{34}O_5$ 402.53
Macrolide antibiotic. Isol. from an unclassifiable marine bacterium. Also prod. by a *Actinomadura* sp. and *Bacillus* sp. PP19-H3. Antiviral and cytotoxic agent. Plates (EtOAc/2,3,3-trimethylpentane). Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 75-78°. $[\alpha]_D$ -9.6 (c, 1.86 in MeOH). λ_{max} 227 (ϵ 49200); 261 (ϵ 18700) (MeOH) (Derep).

7-O-*β*-D-*Glucopyranoside:* ***Macrolactin B***
[122540-28-7]
$C_{30}H_{44}O_{10}$ 564.672
From a marine bacterium. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D$ -42 (c, 3.8 in MeOH). λ_{max} 229 (ϵ 55900); 261 (ϵ 20800) (MeOH) (Derep).

7-O-*(6*-O-*Succinoyl-β*-D-*glucopyranoside):* ***Macrolactin D***
[122540-30-1]
$C_{34}H_{48}O_{13}$ 664.745
From a marine bacterium. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D$ -29.2 (c, 0.96 in MeOH). λ_{max} 228 (ϵ 43500); 261 (ϵ 19200) (MeOH) (Derep).

15-O-*β*-D-*Glucopyranoside:* ***Macrolactin C***
[122540-29-8]
$C_{30}H_{44}O_{10}$ 564.672
From a marine bacterium. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D$ -21 (c, 0.87 in MeOH). λ_{max} 229 (ϵ 55900); 261 (ϵ 20800) (MeOH) (Derep). λ_{max} 228 (ϵ 60800); 261 (ϵ 23100) (MeOH) (Berdy).

7-O-*(3-Carboxypropanoyl):* ***7-O-Succinoylmacrolactin A***
$C_{28}H_{38}O_8$ 502.603
Prod. by the marine *Bacillus* sp. Sc026. Amorph. solid. $[\alpha]_D^{25}$ -9.6 (c, 0.18 in MeOH). λ_{max} 229 (log ϵ 4.57); 261 (log ϵ 4.18) (MeOH).

15-Ketone: ***Macrolactin E***
[122540-31-2]
$C_{24}H_{32}O_5$ 400.514
From a marine bacterium. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D$ +21.8 (c, 0.44 in MeOH). λ_{max} 234 (ϵ 19000); 261 (ϵ 23700) (MeOH) (Derep).

16,17-Dihydro, 15-ketone: ***Macrolactin F***
[122540-32-3]
$C_{24}H_{34}O_5$ 402.53
From a marine bacterium. Shows antibacterial activity. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D$ -30.1 (c, 1.31 in MeOH). λ_{max} 234 (ϵ 19000); 261 (ϵ 23700) (MeOH) (Derep). λ_{max} 234 (ϵ 16600); 261 (ϵ 15400) (MeOH) (Berdy).

*16,17-Dihydro, 15-ketone, 7-*O*-(3-carboxypropanoyl):* ***7-O-Succinoylmacrolactin F***
$C_{28}H_{38}O_8$ 502.603
Prod. by the marine *Bacillus* sp. Sc026. Amorph. solid. $[\alpha]_D^{25}$ -24.4 (c, 0.5 in MeOH). λ_{max} 235 (log ϵ 4.17); 261 (log ϵ 4.23) (MeOH).

*7-Deoxy, 9-hydroxy, 7,8-didehydro(*E*-), 8,9-dihydro:* ***Macrolactin G***
$C_{24}H_{34}O_5$ 402.53
Prod. by *Bacillus* sp. PP19-H3.
$[\alpha]_D^{25}$ -109.1 (c, 0.03 in MeOH). λ_{max} 231 (ϵ 36500); 262 (ϵ 19000) (MeOH).

*10*E*-Isomer:* ***Macrolactin I***
$C_{24}H_{34}O_5$ 402.53
Prod. by *Bacillus* sp. PP19-H3.
$[\alpha]_D^{25}$ -137.7 (c, 0.17 in MeOH). λ_{max} 226 (ϵ 26000); 262 (ϵ 9500) (MeOH).

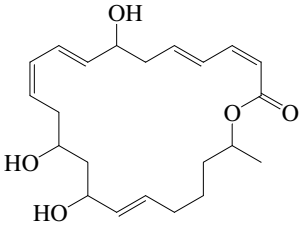
*10*E*-Isomer, 16,17-dihydro, 15-ketone:* ***Macrolactin K***
$C_{24}H_{34}O_5$ 402.53
Prod. by *Bacillus* sp. PP19-H3.
$[\alpha]_D^{25}$ -169.8 (c, 0.11 in MeOH). λ_{max} 234 (ϵ 17800); 263 (ϵ 11500) (MeOH).

18Z-Isomer: ***Macrolactin J***
$C_{24}H_{34}O_5$ 402.53
Prod. by *Bacillus* sp. PP19-H3.
$[\alpha]_D^{25}$ -85.5 (c, 0.08 in MeOH). λ_{max} 231 (ϵ 20100); 263 (ϵ 8300) (MeOH).

Gustafson, K. *et al., J.A.C.S.*, 1989, **111**, 7519 (*isol, pmr, cmr, struct*)
Rychnovsky, S.D. *et al., J.A.C.S.*, 1992, **114**, 671 (*struct*)
Norcross, R.D. *et al., Chem. Rev.*, 1995, **95**, 2041 (*rev, synth*)
Smith, A.B. *et al., J.A.C.S.*, 1996, **118**, 13095 (*synth*)
Boyce, R.J. *et al., Tet. Lett.*, 1996, **37**, 3501 (*synth*)
Smith, A.B. *et al., J.A.C.S.*, 1998, **120**, 3935-3948 (*synth*)
Jaruchoktaweechai, C. *et al., J. Nat. Prod.*, 2000, **63**, 984-986 (*Macrolactin F, 7-Succinoylmacrolactins, activity*)
Nagao, T. *et al., J. Antibiot.*, 2001, **54**, 333-339 (*Macrolactins G,I,J,K*)
Marino, J.P. *et al., J.A.C.S.*, 2002, **124**, 1664-1668 (*Macrolactin A, synth*)

Macrolactin H M-6

[196403-93-7]

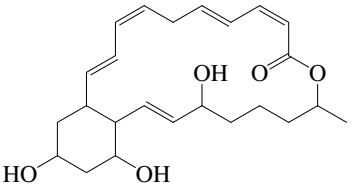


$C_{22}H_{32}O_5$ 376.492
Macrolide antibiotic. Prod. by a marine *Bacillus* sp. PP19-H3.
$[\alpha]_D^{25}$ -92.2 (c, 0.06 in MeOH). λ_{max} 235 (ϵ 18700); 262 (ϵ 13100) (MeOH).

Nagao, T. *et al., J. Antibiot.*, 2001, **54**, 333-339

Macrolactin L M-7

[196403-92-6]



$C_{24}H_{34}O_5$ 402.53
Macrolide antibiotic. Prod. by a marine *Bacillus* sp. PP19-H3.
$[\alpha]_D^{25}$ -139.5 (c, 0.04 in MeOH). λ_{max} 230 (ϵ 26800); 262 (ϵ 13000) (MeOH).

Nagao, T. *et al., J. Antibiot.*, 2001, **54**, 333-339

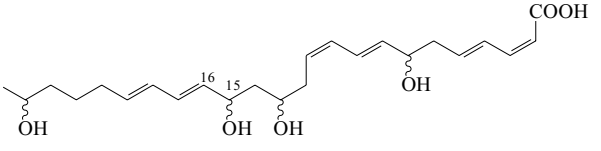
Macrolactin M M-8

24-Ethyl-8,14,16-trihydroxyoxacyclotetracosa-3,5,9,11,17,19-hexaen-2-one, 9CI
[200625-26-9]
As Macrolactin A, M-5 with
R = CH_2CH_3
$C_{25}H_{36}O_5$ 416.556
Prod. by a marine *Bacillus* sp. PP19-H3. Antibacterial agent.
$[\alpha]_D^{25}$ -43.2 (c, 0.04 in MeOH). λ_{max} 228 (ϵ 33700); 263 (ϵ 13400) (MeOH).

Japan. Pat., 1997, 97 301 970; *CA*, **128**, 74381h (*isol*)
Nagao, T. *et al., J. Antibiot.*, 2001, **54**, 333-339

Macrolactinic acid M-9

7,13,15,23-Tetrahydroxy-2,4,8,10,16,18-tetracosahexaenoic acid
[122540-33-4]



$C_{24}H_{36}O_6$ 420.545
Isol. from an unclassifiable marine bacterium.
$[\alpha]_D$ -13.9 (c, 0.58 in MeOH). Also see Macrolactin A, M-5.
λ_{max} 230 (ϵ 53400); 261 (ϵ 28400) (MeOH) (Berdy).

16,17-Dihydro, 15-ketone: ***Isomacrolactinic acid***
[122540-34-5]
$C_{24}H_{36}O_6$ 420.545
From a marine bacterium.
$[\alpha]_D$ -9.3 (c, 0.22 in MeOH). λ_{max} 234 (E1%/1cm 25300); 261 (E1%/1cm 18300) (MeOH) (Berdy).

Gustafson, K. *et al., J.A.C.S.*, 1989, **111**, 7519 (*isol, pmr, cmr, struct*)
Smith, A.B, *et al., J.A.C.S.*, 1999, **120**, 3935-3948 (*synth*)

Hypoxylon oceanicum Macrolide antibiotic M-10

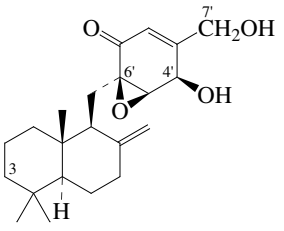
$C_{31}H_{36}O_{15}$ 648.616
Macrolide antibiotic. Struct. unknown. Prod. by the marine fungus *Hypoxylon oceanicum*. Antifungal agent.

Deoxy:
$C_{31}H_{36}O_{14}$ 632.617
Prod. by the marine fungus *Hypoxylon oceanicum*. Antifungal agent.

Int. Mycol. Congr. Vancouver, 6th, 1994, 76
Eur. Pat., 1996, 745 680; *CA*, **126**, 73849p

Macrophorin A M-11

[85754-70-7]



$C_{22}H_{32}O_4$ 360.492

Prod. by *Macrophoma* fruit rot of apple. Active against *Staphylococcus aureus, Trichophyton* sp. and LS 178y mouse tumours. Cryst. (Me_2CO/C_6H_6).

Mp 127-128°. $[\alpha]_D^{20}$ +29 (MeOH). λ_{max} 237 (MeOH).

4′-O-*Malonyl:* ***Macrophorin G***

[220229-94-7]

$C_{25}H_{34}O_7$ 446.539

Prod. by *Botryosphaeria berengeriana*. Amorph. solid.

7′-O-*Malonyl:* ***Macrophorin E***

[220229-90-3]

$C_{25}H_{34}O_7$ 446.539

Prod. by *Botryosphaeria berengeriana*. Antifungal agent. Amorph. solid. $[\alpha]_D$ +24 (c, 0.5 in MeOH).

7′-O-*(3-Hydroxy-3-methylglutaroyl)(*S-*):* ***Macrophorin D***

[92279-92-0]

$C_{28}H_{40}O_8$ 504.619

From *Macrophoma* fruit rot. Shows self-growth inhibiting activity. Gum. Sol. MeOH, EtOAc, bases; poorly sol. H_2O, hexane. $[\alpha]_D^{21}$ +31 (c, 1.7 in MeOH). λ_{max} 231 (MeOH) (Berdy). λ_{max} 235 (MeOH/NaOH) (Berdy).

1′-Alcohol, 7′-O-*(3-hydroxy-3-methylglutaroyl):* ***Antibiotic F 12436B****. F 12436 B*

[191599-25-4]

$C_{28}H_{42}O_8$ 506.635

Prod. by *Dasyscyphella nivea* SANK 26995. Antibacterial agent. Stereochem. not defined.

4′-Ketone: ***4′-Oxomacrophorin A****. EC-B*

[349147-29-1]

$C_{22}H_{30}O_4$ 358.477

Metab. of *Eupenicillium crustaceum*. Yellow oil. $[\alpha]_D$ +10.2 (c, 0.3 in MeOH). λ_{max} 219 (log ϵ 3.87); 268 (sh) (log ϵ 3.33) (MeOH).

4′-Ketone, 7′-O-*(3-hydroxy-3-methylglutaroyl)(*S-*):* ***4′-Oxomacrophorin D****. EC-A*

[349147-28-0]

$C_{28}H_{38}O_8$ 502.603

Metab. of *Eupenicillium crustaceum*. Yellow oil. $[\alpha]_D^{25}$ +35.5 (c, 0.3 in MeOH). λ_{max} 221 (log ϵ 3.97); 260 (sh) (log ϵ 3.47) (MeOH).

3-Oxo: ***Macrophorin B***

[85764-12-1]

$C_{22}H_{30}O_5$ 374.476

From *Macrophoma* fruit rot. Shows self-growth inhibiting activity. Cryst.

Mp 107-110°. $[\alpha]_D$ +11.5 (MeOH).

3β-Hydroxy: ***Macrophorin C***

[85764-11-0]

$C_{22}H_{32}O_5$ 376.492

From *Macrophoma* fruit rot. Cryst.

Mp 113-116°. $[\alpha]_D$ +23 (MeOH).

Sassa, T. *et al., Agric. Biol. Chem.*, 1983, **47**, 187-189; 1984, **48**, 1923-1925 (*isol, struct*)

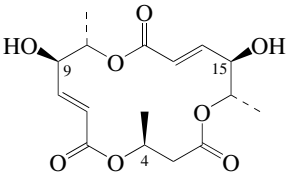
Japan. Pat., 1997, 9 176 091; *CA*, **127**, 80239p (*F 12436B*)

Sassa, T. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 2260-2262 (*Macrophorins E,G*)

Fujimoto, H. *et al., J. Nat. Prod.*, 2001, **64**, 1234-1237 (*4′-Oxomacrophorin A, 4′-Oxomacrophorin D, abs config*)

Macrosphelide A M-12

[172923-77-2]



Absolute configuration

$C_{16}H_{22}O_8$ 342.345

Macrolide antibiotic. Prod. by *Microsphaeropsis* sp. FO-5050. Inhibitor of cell-cell adhesion. Antimetastatic agent. Needles. Sol. MeOH, $CHCl_3$, Me_2CO, EtOAc; poorly sol. H_2O. Mp 141-142°. $[\alpha]_D^{23}$ +84.1 (c, 0.6 in MeOH). λ_{max} 207 (ϵ 13200) (MeOH).

15-Ketone: ***Macrosphelide B***

[172923-78-3]

$C_{16}H_{20}O_8$ 340.329

From *Microsphaeropsis* sp. FO-5050. Inhibitor of cell-cell adhesion. Plates. Sol. MeOH, Me_2CO, $CHCl_3$, EtOAc; poorly sol. H_2O.

Mp 148-150°. $[\alpha]_D^{23}$ +4.1 (c, 1 in MeOH). λ_{max} 210 (ϵ 14120) (MeOH).

9-Deoxy: ***Macrosphelide C***

[199731-56-1]

$C_{16}H_{22}O_7$ 326.346

Prod. by *Microsphaeropsis* sp. FO-5050. Inhibitor of cell-cell adhesion. Needles.

Mp 80-84°. $[\alpha]_D^{20}$ +29.5 (c, 0.1 in MeOH). λ_{max} 207 (log ϵ 4.22) (MeOH).

13-Methoxy, 13,14-dihydro, 15-ketone: ***Macrosphelide J***

$C_{17}H_{24}O_9$ 372.371

Prod. by *Microsphaeropsis* sp. FO-5050IV. Oil. $[\alpha]_D$ -41 (c, 0.2 in MeOH). λ_{max} 211 (log ϵ 4.02) (MeOH).

13-Ethoxy, 13,14-dihydro, 15-ketone: ***Macrosphelide K***

$C_{18}H_{26}O_9$ 386.398

Prod. by *Microsphaeropsis* sp. FO-5050IV. Oil. $[\alpha]_D^{20}$ -59 (c, 0.2 in MeOH). λ_{max} 210 (log ϵ 3.98) (MeOH).

4-Epimer: ***Macrosphelide E***

[200335-76-8]

$C_{16}H_{22}O_8$ 342.345

Prod. by a strain of *Periconia byssoides* isol. from *Aplysia kurodai*. Oil. $[\alpha]_D$ +56.8 (c, 0.5 in EtOH). λ_{max} 213 (log ϵ 4.18) (EtOH).

4-Epimer, 15-ketone: ***Macrosphelide L***

$C_{16}H_{20}O_8$ 340.329

Prod. by *Periconia byssoides* isol. from *Aplysia kurodai*. Inhibitor of cell adhesion. Oil. $[\alpha]_D^{21}$ -24.2 (c, 0.33 in EtOH). λ_{max} 218 (log ϵ 3.75) (EtOH).

4-Epimer, 13,14-dihydro: ***Macrosphelide I***

$C_{16}H_{24}O_8$ 344.361

Prod. by a strain of *Periconia byssoides* isol. from *Aplysia kurodai*. Oil. $[\alpha]_D$ +10.3 (c, 0.31 in EtOH). λ_{max} 215 (log ϵ 3.76) (EtOH).

4-Epimer, 9-deoxy: ***Macrosphelide F***

[200335-77-9]

$C_{16}H_{22}O_7$ 326.346

Prod. by a strain of *Periconia byssoides* isol. from *Aplysia kurodai*. Oil. $[\alpha]_D$ +23.3 (c, 0.09 in MeOH). λ_{max} 216 (log ϵ 4.15) (EtOH).

4-Epimer, 15-deoxy: ***Macrosphelide G***

[200335-78-0]

$C_{16}H_{22}O_7$ 326.346

Prod. by a strain of *Periconia byssoides* isol. from *Aplysia kurodai*. Oil. $[\alpha]_D$ +66.7 (c, 0.5 in EtOH). λ_{max} 217 (4.17) (EtOH).

Stereoisomer: ***Macrosphelide D***

[199731-57-2]

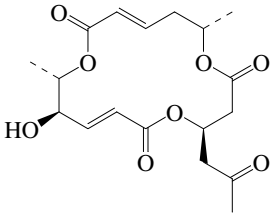
$C_{16}H_{22}O_8$ 342.345

Prod. by *Microsphaeropsis* sp. FO-5050. Inhibitor of cell-cell adhesion. Oil. $[\alpha]_D$ +65.3 (c, 0.3 in MeOH). λ_{max} 207 (log ϵ 4.21) (MeOH).

Hayashi, M. *et al., J. Antibiot.*, 1995, **48**, 1435-1439 (*isol, props*)
Takamatsu, S. *et al., J. Antibiot.*, 1996, **49**, 95-98; 1997, **50**, 878-880 (*isol, uv, ir, pmr, cmr*)
Sunazuka, T. *et al., J.A.C.S.*, 1997, **119**, 10247-10248 (*synth, abs config*)
Fukami, A. *et al., J. Antibiot.*, 1999, **52**, 501-504 (*Macrosphelides J,K*)
Yamada, T. *et al., J.C.S. Perkin 1*, 2001, 3046-3053 (*isol, uv, pmr, cmr, abs config*)
Kobayashi, Y. *et al., J.O.C.*, 2001, **66**, 2011-2018 (*synth*)
Ono, M. *et al., Chem. Pharm. Bull.*, 2002, **50**, 692-696 (*synth*)
Nakamura, H. *et al., Heterocycles*, 2002, **57**, 327-336 (*synth*)
Yamada, T. *et al., J. Antibiot.*, 2002, **55**, 147-154 (*Macrosphelide L*)
Sharma, G.V.M. *et al., Tet. Lett.*, 2002, **43**, 9159-9161 (*synth*)
Kawaguchi, T. *et al., J.O.C.*, 2004, **69**, 505-509 (*synth*)
Matsuya, Y. *et al., Heterocycles*, 2005, **65**, 1741-1749 (*rev, synth*)
Kobayashi, Y. *et al., Lett. Org. Chem.*, 2005, **1**, 297-307 (*Macrosphelides C,F,G, synth*)
Paek, S.-M. *et al., Org. Lett.*, 2005, **7**, 3159-3162 (*synth*)
Sunazuka, T. *et al., Tetrahedron*, 2005, **61**, 3789-3803 (*synth, abs config*)

Macrosphelide H M-13

[200335-79-1]



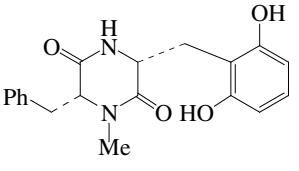
Absolute Configuration

$C_{18}H_{24}O_8$ 368.383
Prod. by a strain of *Periconia byssoides* isol. from *Aplysia kurodai.* Oil. $[\alpha]_D$ +41.7 (c, 0.2 in EtOH). λ_{max} 214 (log ϵ 4.19) (EtOH).

Numata, A. *et al., Tet. Lett.*, 1997, **38**, 8215-8218 (*isol, uv, pmr, cmr*)
Yamada, T. *et al., J.C.S. Perkin 1*, 2001, 3046-3053 (*synth*)
Yamada, T. *et al., J. Antibiot.*, 2002, **55**, 147-154 (*abs config*)
Kobayashi, Y. *et al., Lett. Org. Chem.*, 2005, **1**, 297-307 (*synth*)

Mactanamide M-14

[278171-44-1]



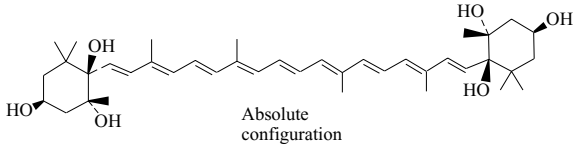
Absolute Configuration

$C_{19}H_{20}N_2O_4$ 340.378
Absolute stereochem. incorrectly shown in paper. Prod. by a marine *Aspergillus* sp. isol. from a *Sargassum* sp. Cryst. (MeOH).
Mp 241-243°. $[\alpha]_D$ -42.8 (c, 0.93 in MeOH). λ_{max} 205 (ϵ 28400); 272 (ϵ 1400); 276 (ϵ 1300) (MeOH).

Lorenz, P. *et al., Nat. Prod. Lett.*, 1998, **12**, 55-60 (*isol*)

Mactraxanthin M-15

5,5′,6,6′-Tetrahydro-β,β-carotene-3,3′,5,5′,6,6′-hexol
[86105-69-3]



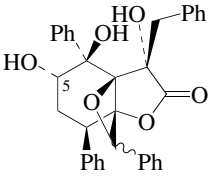
Absolute configuration

$C_{40}H_{60}O_6$ 636.91
Constit. of Japanese edible surf clam (*Mactra chinensis*). Deep orange needles.
Mp 232-233°.

Matsuno, T. *et al., Tet. Lett.*, 1983, **24**, 911
Buchecker, R. *et al., Helv. Chim. Acta*, 1984, **67**, 2043 (*synth, struct*)

Maculalactone I M-16

[199600-41-4]



Relative Configuration

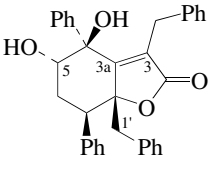
$C_{34}H_{30}O_6$ 534.607
Isol. from the cyanobacterium *Kyrtuthrix maculans.* Oil. $[\alpha]_D$ +52 (c, 0.1 in $CHCl_3$).

5-Ketone: ***Maculalactone K***
[199600-43-6]
$C_{34}H_{28}O_6$ 532.592
Isol. from *Kyrtuthrix maculans.* Oil. $[\alpha]_D$ +40.2 (c, 0.04 in $CHCl_3$).

Lee, S.-C. *et al., J. Nat. Prod.*, 1998, **61**, 29-33 (*isol, ir, pmr, cmr*)

Maculalactone E M-17

[199600-37-8]



Relative Configuration

$C_{34}H_{30}O_4$ 502.609
Isol. from the cyanobacterium *Kyrtuthrix maculans.* Oil. $[\alpha]_D$ +84.7 (c, 0.2 in $CHCl_3$).

4-Deoxy: ***Maculalactone D***
[199600-36-7]
$C_{34}H_{30}O_3$ 486.609
Isol. from *Kyrtuthrix maculans.* Oil. $[\alpha]_D$ -47.1 (c, 0.07 in $CHCl_3$).

4-Epimer, 5-ketone: ***Maculalactone F***
[199600-38-9]
$C_{34}H_{28}O_4$ 500.593
Isol. from *Kyrtuthrix maculans.* Oil.

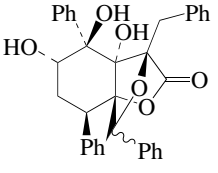
3α,3aα-Epoxide: ***Maculalactone G***
[199600-39-0]
$C_{34}H_{30}O_5$ 518.608
Isol. from *Kyrtuthrix maculans.* Oil. $[\alpha]_D$ +19.2 (c, 0.4 in $CHCl_3$).

3α,3aα-Epoxide, 1′ξ-hydroxy: ***Maculalactone H***
[199600-40-3]
$C_{34}H_{30}O_6$ 534.607
Isol. from *Kyrtuthrix maculans.* Solid. $[\alpha]_D$ +43.8 (c, 0.3 in $CHCl_3$). Dec. at 230°.

Lee, S.-C. *et al., J. Nat. Prod.*, 1998, **61**, 29-33 (*isol, ir, pmr, cmr*)

Maculalactone J M-18

[199600-42-5]



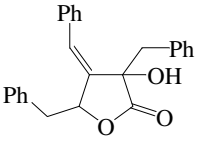
Relative Configuration

$C_{34}H_{30}O_6$ 534.607
Isol. from the cyanobacterium *Kyrtuthrix maculans.*

Lee, S.-C. *et al., J. Nat. Prod.*, 1998, **61**, 29-33 (*isol, pmr, cmr*)

Maculalactone L M-19

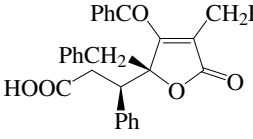
3,5-Dibenzyl-4-benzylidenedihydro-3-hydroxy-2(3H)-furanone



$C_{25}H_{22}O_3$ 370.447
Isol. from the cyanobacterium *Kyrtuthrix maculans.*
$[\alpha]_D$ +12.5 (c, 0.04 in $CHCl_3$).

Lee, S.-C. *et al., Phytochemistry*, 1999, **52**, 537-540 (*isol, ir, pmr, cmr, ms*)

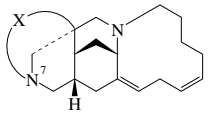
Maculalactone M M-20



$C_{34}H_{28}O_5$ 516.592
Isol. from the marine cyanobacterium *Kyrtuthrix maculans.* Pale green gum. $[\alpha]_D$ +26.8 (c, 0.2 in $CHCl_3$). λ_{max} 204; 252; 280 (sh) (MeOH).

Wong, H.-F. *et al., Phytochemistry*, 2002, **60**, 425-429 (*isol, pmr, cmr*)

Madangamines M-21



Madangamine A X = N^7-$CH_2CH_2CH{=}^{Z}CHCH_2CH{=}^{Z}CHCH_2CH{=}^{Z}CHCH_2CH_2$-
B X = N^7-$CH_2CH_2CH{=}^{Z}CHCH_2CH{=}^{Z}CHCH_2CH_2CH{=}^{E}CHCH_2$-
C X = N^7-$(CH_2)_6CH{=}^{Z}CHCH_2CH_2$-
D X = -$(CH_2)_{11}$-
E X = -$(CH_2)_{10}$-

Madangamine A [155944-26-6]
$C_{30}H_{44}N_2$ 432.691
Alkaloid from the marine sponge *Xestospongia ingens.* Cytotoxic agent. Glass. $[\alpha]_D$ +319 (c, 1 in EtOAc).

Madangamine B [203060-01-9]
$C_{30}H_{44}N_2$ 432.691
Alkaloid from the marine sponge *Xestospongia ingens.* Cytotoxic agent. Glass. $[\alpha]_D$ +150.7 (c, 0.07 in EtOAc).

Madangamine C [203060-06-4]
$C_{28}H_{44}N_2$ 408.669
Alkaloid from the marine sponge *Xestospongia ingens.* Cytotoxic agent. Glass. $[\alpha]_D$ +140.8 (c, 0.09 in EtOAc).

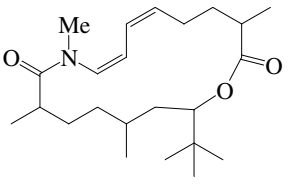
Madangamine D [203060-15-5]
$C_{29}H_{48}N_2$ 424.712
Alkaloid from the marine sponge *Xestospongia ingens.* Cytotoxic agent. Isol. as an inseparable mixt. with Madangamine E.

Madangamine E [203060-37-1]
$C_{28}H_{46}N_2$ 410.685
Alkaloid from the marine sponge *Xestospongia ingens.* Cytotoxic agent. Isol. as an inseparable mixt. with Madangamine D.

Kong, F. *et al., J.A.C.S.*, 1994, **116**, 6007-6008 (*isol, pmr, cmr, struct*)
Kong, F. *et al., J. Nat. Prod.*, 1998, **61**, 267-271 (*isol, pmr, cmr, ms*)
Matzanke, N. *et al., Org. Prep. Proced. Int.*, 1998, **30**, 3-51 (*rev*)

Madangolide M-22

[230975-42-5]

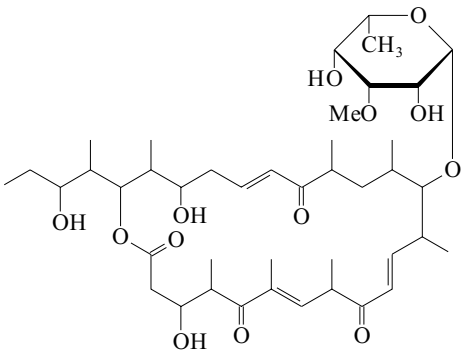


$C_{23}H_{39}NO_3$ 377.566
Isol. from *Lyngbya bouillonii.* Amorph. solid. λ_{max} 200 (ϵ 16600); 244 (ϵ 24400) (MeOH).

Klein, D. *et al., J. Nat. Prod.*, 1999, **62**, 934-936 (*isol, uv, pmr, cmr, ms*)

Maduralide M-23

[135288-70-9]

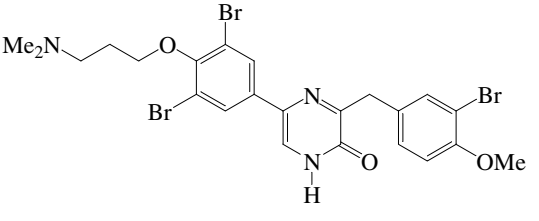


$C_{42}H_{68}O_{13}$ 780.991
Macrolide antibiotic. Prod. by a marine bacterium (Actinomycetales). Exhibits weak antibacterial activity. Oil. $[\alpha]_D$ -46.3 (c, 0.32 in $CHCl_3$). λ_{max} 229 (MeOH) (Derep).

Pathirana, C. *et al., Tet. Lett.*, 1991, **32**, 2323 (*isol, pmr, cmr, struct*)

Maedamine A M-24

[310396-69-1]



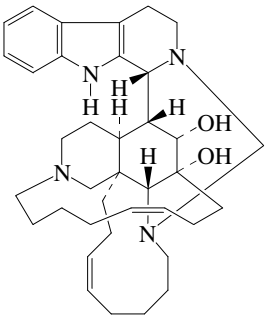
$C_{23}H_{24}Br_3N_3O_3$ 630.173
Alkaloid from the sponge *Suberea* sp. Cytotoxic agent. Amorph. yellow solid. λ_{max} 285 (ϵ 4000); 350 (ϵ 1000) (MeOH).

N-*De-Me:* ***Maedamine B***
[310396-70-4]
$C_{22}H_{22}Br_3N_3O_3$ 616.146
Alkaloid from *Suberea* sp. Cytotoxic agent. Amorph. yellow solid. λ_{max} 285 (ϵ 5000); 350 (ϵ 1200) (MeOH).

Hirano, K. *et al., Tetrahedron*, 2000, **56**, 8107-8110 (*Maedamines A,B*)

Maeganedin A M-25

[205247-54-7]



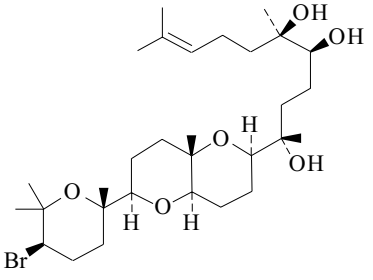
$C_{37}H_{52}N_4O_2$ 584.843

Related to Manzamine A, M-95. Alkaloid from the sponge *Amphimedon* sp. Amorph. solid. $[\alpha]_D^{25}$ +47 (c, 0.4 in MeOH). λ_{max} 205 (ϵ 13000); 223 (ϵ 2500); 274 (ϵ 2500); 322 (ϵ 4000) (MeOH).

Tsuda, M. *et al., Tet. Lett.*, 1998, **39**, 1207-1210 (*isol, uv, ir, pmr, cmr*)

Magireol A M-26

[109063-83-4]



$C_{30}H_{53}BrO_6$ 589.649

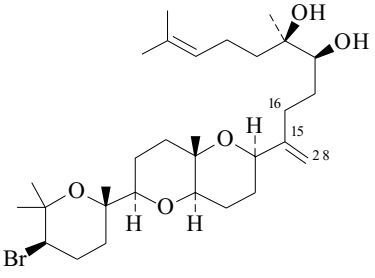
Constit. of red alga *Laurencia obtusa*. Cytotoxic. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 98.5-100°. $[\alpha]_D$ 0.

Suzuki, T. *et al., Chem. Lett.*, 1987, 361

Magireol B M-27

[109063-84-5]



$C_{30}H_{51}BrO_5$ 571.634

Constit. of red alga *Laurencia obtusa*. Cytotoxic. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 64.5-66°. $[\alpha]_D$ +7.8 (c, 1.00 in $CHCl_3$).

Δ^{15}-Isomer: ***Magireol C***

[109028-21-9]

$C_{30}H_{51}BrO_5$ 571.634

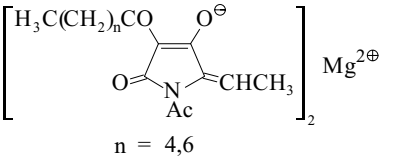
Constit. of *Laurencia obtusa*. Cytotoxic. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 67-69°. $[\alpha]_D$ +6.4 (c, 1.00 in $CHCl_3$).

Suzuki, T. *et al., Chem. Lett.*, 1987, 361

Magnesidin M-28

[52081-52-4]



n = 4,6

A mixt. of Mg salts of 2 tetramic acids. Obt. from *Pseudomonas magnesiorubra* ATCC 21856 and a marine *Vibrio gazogenes*. Active against gram-positive bacteria, particularly the spore bearers. Sol. MeOH, Et_2O; poorly sol. H_2O. Mol. formula $C_{28}H_{36}MgN_2O_8/C_{32}H_{44}MgN_2O_8$. λ_{max} 257 (ϵ 19800) (MeOH) (Derep). λ_{max} 261 (E1%/1cm 928) (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 50 mg/kg. OM2457600

Gandhi, N.M. *et al., J. Antibiot.*, 1973, **26**, 797 (*isol*)
U.K. Pat., 1977, 1 478 643; *CA*, **88**, 168480 (*synth, props*)
Imamura, N. *et al., J. Antibiot.*, 1994, **47**, 257-261 (*isol, pmr, cmr, ms*)

Magnificalysins M-29

Two proteins, Magnificalysin I and Magnificalysin II, MW approx. 19000. Isol. from the tropical sea anemone *Heteractis magnifica*. Cytolysins.

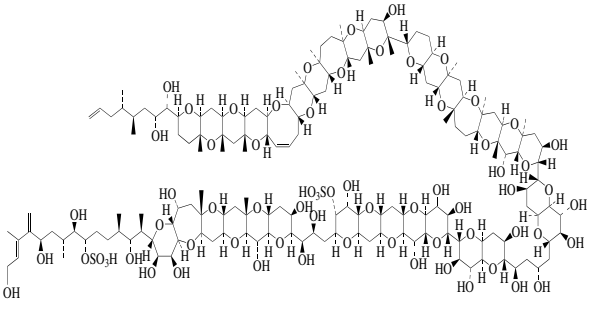
[155123-75-4, 155123-76-5]

Khoo, K.S. *et al., Toxicon*, 1993, **31**, 1567-1569 (*isol*)
Anderluh, G. *et al., Toxicon*, 2002, **40**, 111-124 (*rev*)

Maitotoxin M-30

MTX

[59392-53-9]



$C_{164}H_{258}O_{68}S_2$ 3381.933

Polyether antibiotic. Possesses highest molecular weight of any known nat. products, except biopolymers. Constit. of the dinoflagellate *Gambierdiscus toxicus*. One of the most potent non-proteinaceous toxins. Phycotoxin. Neurotoxic agent. Calcium channel and protein kinase activator. Amorph. solid (as di-Na salt). Sol. H_2O.

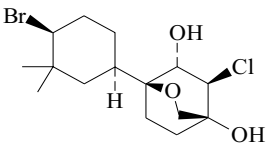
▶ LD_{50} (mus, ipr) .17 mg/kg. OM5470000

[131594-69-9]

Yokoyama, A. *et al., J. Biochem. (Tokyo)*, 1988, **104**, 184 (*isol, props*)
Yasumoto, T. *et al., Chem. Rev.*, 1993, **93**, 1978 (*rev*)
Yasumoto, T. *et al., Gazz. Chim. Ital.*, 1993, **123**, 367 (*rev*)
Murata, M. *et al., J.A.C.S.*, 1993, **115**, 2060; 1994, **116**, 7098 (*struct, pmr, stereochem*)
Sasaki, M. *et al., Angew. Chem., Int. Ed.*, 1996, **35**, 1672; 1675 (*abs config*)
Zheng, W. *et al., J.A.C.S.*, 1996, **118**, 7946 (*stereochem*)
Kishi, Y. *et al., Pure Appl. Chem.*, 1998, **70**, 339-344 (*rev, struct*)
Food Sci. Technol., Seafood and Freshwater Toxins, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*revs*)

Majapol A **M-31**

[174158-70-4]

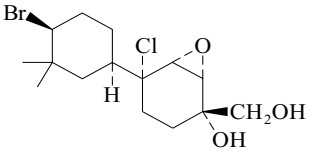


$C_{15}H_{24}BrClO_3$ 367.709
Constit. of *Laurencia majuscula*. Oil.

Erickson, K.L. *et al., J. Nat. Prod.*, 1996, **58**, 1848 (*isol, pmr, cmr*)

Majapol B **M-32**

[174158-71-5]

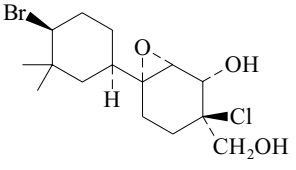


$C_{15}H_{24}BrClO_3$ 367.709
Constit. of *Laurencia majuscula*. Oil.

Erickson, K.L. *et al., J. Nat. Prod.*, 1996, **58**, 1848 (*isol, pmr, cmr*)

Majapol C **M-33**

[174158-72-6]

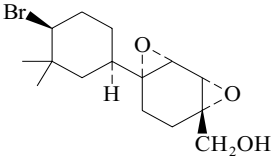


$C_{15}H_{24}BrClO_3$ 367.709
Constit. of *Laurencia majuscula*. Oil.

Erickson, K.L. *et al., J. Nat. Prod.*, 1996, **58**, 1848 (*isol, pmr, cmr*)

Majapol D **M-34**

[174158-73-7]

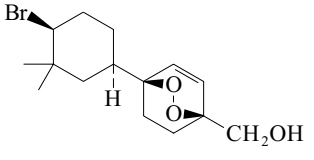


$C_{15}H_{23}BrO_3$ 331.249
Constit. of *Laurencia majuscula*. Oil.

Erickson, K.L. *et al., J. Nat. Prod.*, 1996, **58**, 1848 (*isol, pmr, cmr*)

Majapolene A **M-35**

[174158-67-9]

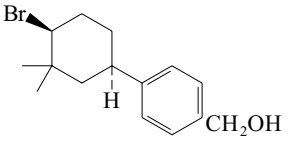


$C_{15}H_{23}BrO_3$ 331.249
Constit. of *Laurencia majuscula*. Cryst. $[\alpha]_D$ -20 (c, 0.2 in $CHCl_3$).

Erickson, K.L. *et al., J. Nat. Prod.*, 1996, **55**, 1848 (*isol, pmr, cmr*)

Majapolene B **M-36**

[174158-68-0]

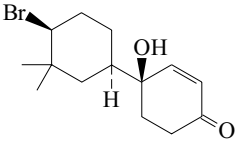


$C_{15}H_{21}BrO$ 297.234
Constit. of *Laurencia majuscula*. Cryst. $[\alpha]_D$ -14.6 (c, 3.8 in $CHCl_3$).

Erickson, K.L. *et al., J. Nat. Prod.*, 1996, **58**, 1848 (*isol, pmr, cmr*)

Majapolone **M-37**

[174158-69-1]

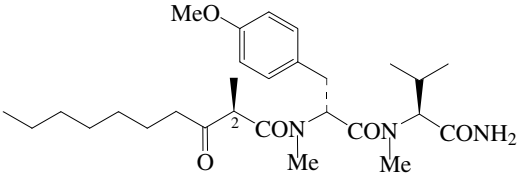


$C_{14}H_{21}BrO_2$ 301.223
Constit. of *Laurencia majuscula*. Oil.

Erickson, K.L. *et al., J. Nat. Prod.*, 1996, **58**, 1848 (*isol, pmr, cmr*)

Majusculamide A **M-38**

N,O-*Dimethyl*-N-*(2-methyl-1,3-dioxodecyl)*-D-tyrosyl-N^2-*methyl*-L-*valinamide*
[62758-06-9]



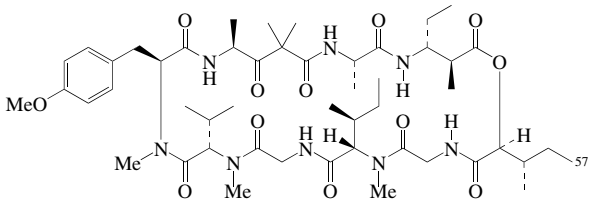
$C_{28}H_{45}N_3O_5$ 503.681
Lipodipeptide from a shallow-water variety of the marine blue-green alga *Lyngbya majuscula*. Needles + $1H_2O$ (MeOH aq.). Sol. MeOH.
Mp 96-97°. $[\alpha]_D^{26}$ +19.3 (c, 1.14 in EtOH). λ_{max} 224 (ϵ 7400); 277 (ϵ 900); 283 (ϵ 720) (EtOH) (Derep).

2-Epimer: ***Majusculamide B***
[62840-08-8]
$C_{28}H_{45}N_3O_5$ 503.681
Isol. from a shallow-water variety of *Lyngbya majuscula*. Needles + $1H_2O$ (MeOH aq.). Sol. MeOH.
Mp 102-103°. $[\alpha]_D^{26}$ +14.6 (c, 0.82 in EtOH). λ_{max} 224 (ϵ 7400); 277 (ϵ 900); 283 (ϵ 720) (EtOH) (Derep).

Marner, F.-J. *et al., J.O.C.*, 1977, **42**, 2815-2819 (*isol, uv, ir, pmr, ms, cryst struct, abs config*)

Majusculamide C M-39

[83712-17-8]



$C_{50}H_{80}N_8O_{12}$ 985.228

Depsipeptide antibiotic. Similar to Dolastatin 11, D-1205. Isol. from *Lyngbya majuscula* (deep water variety) and *Ptilocaulis trachys*. Cytotoxic. Active against plant pathogenic fungi. Solid. $[\alpha]_D$ -96 (c, 2.5 in CH_2Cl_2). Isolate from *L. majuscula* shown to be a mixt. of C-15 epimers in 2003. λ_{max} 225 (ϵ 6610); 277 (ϵ 2190); 283 (ϵ 1900) (MeOH) (Derep). λ_{max} 230 (ϵ 5900); 278 (ϵ 1420) (MeOH) (Berdy).

57-Nor: ***57-Normajusculamide C***

[119264-85-6]

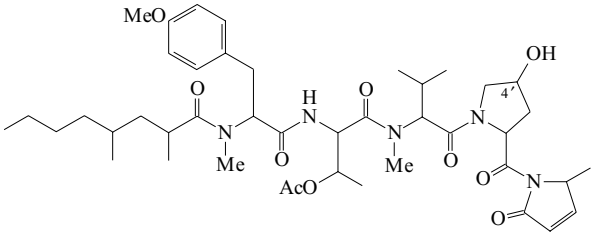
$C_{49}H_{78}N_8O_{12}$ 971.202

Minor cyclic depsipeptide from a deep-water variety of *Lyngbya majuscula*. Exhibits antimycotic activity.

U.S. Pat., 1982, 4 342 751; *CA*, **97**, 214251 (*isol*)
Carter, D.C. *et al., J.O.C.*, 1984, **49**, 236 (*struct, spectra*)
Mynderse, J.S. *et al., J. Nat. Prod.*, 1988, **51**, 1299 (*57-Normajusculamide C*)
Williams, D.E. *et al., J. Nat. Prod.*, 1993, **56**, 545 (*isol, struct*)
Bates, R.B. *et al., J.A.C.S.*, 1997, **119**, 2111 (*abs config*)
Williams, P.G. *et al., J. Nat. Prod.*, 2003, **66**, 1356-1363 (*isol, config*)
Ali, M.A. *et al., Bioorg. Med. Chem.*, 2005, **13**, 4138-4152 (*synth*)

Majusculamide D M-40

[119603-16-6]



$C_{43}H_{65}N_5O_{10}$ 812.014

Lipopeptide antibiotic. Isol. from *Lyngbya majuscula*. Cytotoxic.

4′-Deoxy: ***Deoxymajusculamide D***

[118063-78-8]

$C_{43}H_{65}N_5O_9$ 796.015

From *Lyngbya majuscula*. Cytotoxic.

Moore, R.E. *et al., Phytochemistry*, 1988, **27**, 3101 (*isol, struct*)

Majusculoic acid M-41

2-(6-Bromo-3,5-nonadienyl)cyclopropanepropanoic acid. 11-Bromo-4,5-methylene-8,10-tetradecadienoic acid

Relative Configuration

$C_{15}H_{23}BrO_2$ 315.25

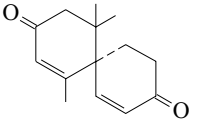
Isol. from a marine cyanobacterial mat assemblage. Antifungal agent. Amorph. solid. $[\alpha]_D$ -15.8 (c, 0.1 in MeOH).

MacMillan, J.B. *et al., J. Nat. Prod.*, 2005, **68**, 604-606 (*isol, pmr, cmr*)

Majusculone M-42

1,5,5-Trimethylspiro[5.5]undeca-1,7-diene-3,9-dione, 9CI. 15-Nor-1,7-chamigradiene-3,9-dione

[112642-49-6]



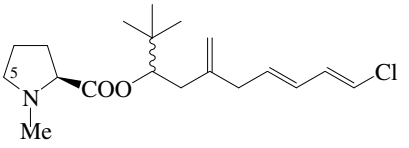
$C_{14}H_{18}O_2$ 218.295

Constit. of the red alga *Laurencia majuscula*. Cryst. (diisopropyl ether).

Mp 91.1-92°. $[\alpha]_D^{19}$ +145 (c, 0.965 in $CHCl_3$).

Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 3795

Makalika ester M-43



$C_{19}H_{30}ClNO_2$ 339.904

Isol. from the sea hare *Stylocheilus longicauda*. Oil. $[\alpha]_D$ -39 (c, 0.1 in MeOH). λ_{max} 214 (ϵ 45000); 220 (ϵ 45000); 223 (ϵ 11995); 229 (ϵ 45000); 245 (ϵ 12810) (MeOH).

5-Oxo: ***Makalikone ester***

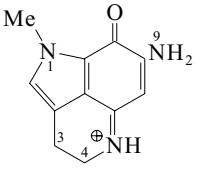
$C_{19}H_{28}ClNO_3$ 353.888

Isol. from *Stylocheilus longicauda*. Oil. $[\alpha]_D$ -23 (c, 0.14 in MeOH). λ_{max} 203 (ϵ 15910); 207 (ϵ 13130); 234 (ϵ 7575); 357 (ϵ 4645) (MeOH).

Gallimore, W.A. *et al., J. Nat. Prod.*, 2000, **63**, 1022-1026

Makaluvamine A M-44

[146555-78-4]



$C_{11}H_{12}N_3O^{\oplus}$ 202.235

Isol. from the sponges *Zyzzya fuliginosa* and *Histodermella* sp. Also isol. from the myxomycete *Didymium bahiense*. Cytotoxic. Inhibitor of topoisomerase II. Green solid (as trifluoroacetate). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 220 (ϵ 17400); 330 (ϵ 16100) (MeOH/NaOH) (Derep). λ_{max} 242 (ϵ 24000); 348 (ϵ 15500) (MeOH) (Derep).

N^5*-Me:* ***Makaluvamine H***. *NSC 700647*

[174232-34-9]

$C_{12}H_{14}N_3O^{\oplus}$ 216.262

Metab. from the sponge *Zyzzya fuliginosa*. Red-brown solid (as trifluoroacetate). Sol. MeOH. λ_{max} 240 (ϵ 19400); 345 (ϵ 13500); 522 (ϵ 1100) (MeOH) (Berdy).

N^9*-(4-Hydroxyphenethyl):* ***Makaluvamine K***

[174232-36-1]

$C_{19}H_{20}N_3O_2^{\oplus}$ 322.386

From *Zyzzya fuliginosa*. Shows cytotoxic activity. Red-brown solid (as trifluoroacetate). Sol. MeOH. λ_{max} 222 (ϵ 18000); 246 (ϵ 29800); 347 (ϵ 19200); 536 (ϵ 2600) (MeOH) (Berdy).

N^9*-(4-Hydroxyphenethyl),* N^5*-Me:* ***Makaluvamine P***

$C_{20}H_{22}N_3O_2^{\oplus}$ 336.413

Isol. from *Zyzzya fuliginosa*. Cytotoxic. Violet solid. Counterion not specified. λ_{max} 222 (ϵ 7470); 248 (ϵ 7750); 361 (ϵ 5075) (MeOH).

N^9-*(4-Hydroxyphenylethenyl)(*E-*):* ***Makaluvamine E***
[146555-82-0]
$C_{19}H_{18}N_3O_2^{\oplus}$ 320.37
Isol. from *Zyzzya fuliginosa*. Cytotoxic. Inhibitor of topoisomerase II. Green solid (as trifluoroacetate). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 314 (ϵ 8600); 607 (ϵ 5000) (MeOH/NaOH) (Derep). λ_{max} 226 (ϵ 6200); 278 (ϵ 8700); 333 (ϵ 6800); 448 (ϵ 4900); 626 (ϵ 5700) (MeOH) (Derep).

N^9-*(4-Hydroxyphenylethenyl)(*E-*),* N^5-*Me:* ***Makaluvamine G***
[152273-69-3]
$C_{20}H_{20}N_3O_2^{\oplus}$ 334.397
Metab. from the Indonesian sponge *Histodermella* sp. and the micronesian sponge *Zyzzya fuliginosa*. Cytotoxic. Moderate inhibitor of topoisomerase I. Immunomodulator. Protein, DNA and RNA synthesis inhibitor. Green-black powder.
Mp 250°. λ_{max} 250 (ϵ 13850); 346 (ϵ 12590); 450 (ϵ 7940); 624 (ϵ 10000) (MeOH) (Berdy). λ_{max} 286 (ϵ 12590); 612 (ϵ 12590) (MeOH/NaOH) (Berdy).

N^1-*De-Me:* ***Makaluvamine I***
[138087-43-1]
$C_{10}H_{10}N_3O^{\oplus}$ 188.208
Isol. from *Zyzzya fuliginosa*. Green solid (as trifluoroacetate). Sol. MeOH. λ_{max} 240 (ϵ 23900); 340 (ϵ 13500); 534 (ϵ 1000) (MeOH) (Berdy).

N^1-*De-Me,* N^1-*β-D-ribofuranosyl:* ***N^1-β-D-Ribofuranosylmakaluvamine I***
$C_{15}H_{18}N_3O_5^{\oplus}$ 320.324
Isol. from the sponge *Strongylodesma aliwaliensis*. Orange-brown solid. $[\alpha]_D^{14}$ +5.3 (c, 0.19 in MeOH). λ_{max} 242 (ϵ 7815); 342 (ϵ 4110); 532 (ϵ 190) (MeOH).

N^1-*De-Me,* N^5-*Me:* ***Makaluvamine C***
[146555-80-8]
$C_{11}H_{12}N_3O^{\oplus}$ 202.235
Isol. from *Zyzzya fuliginosa*. Cytotoxic. Inhibitor of topoisomerase II. Green solid (as trifluoroacetate). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 246 (ϵ 20400); 355 (ϵ 16900) (MeOH/NaOH) (Derep). λ_{max} 241 (ϵ 25300); 358 (ϵ 19100) (MeOH) (Derep).

N^1-*De-Me,* N^9-*(4-hydroxyphenethyl):* ***Makaluvamine D***
[146555-81-9]
$C_{18}H_{18}N_3O_2^{\oplus}$ 308.359
Isol. from *Zyzzya fuliginosa*. Cytotoxic. Inhibitor of topoisomerase II. Brown solid (as trifluoroacetate). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 243 (ϵ 16800); 339 (ϵ 12100) (MeOH/NaOH) (Derep). λ_{max} 245 (ϵ 22000); 348 (ϵ 10600) (MeOH) (Derep).

N^1-*De-Me,* N^9-*(4-hydroxyphenethyl),* N^5-*Me:* ***Makaluvamine J***
[174232-35-0]
$C_{19}H_{20}N_3O_2^{\oplus}$ 322.386
Isol. from *Zyzzya fuliginosa*. Red-brown solid (as trifluoroacetate). Sol. MeOH. λ_{max} 220 (ϵ 11600); 241 (ϵ 18600); 354 (ϵ 13900); 534 (ϵ 1400) (MeOH) (Berdy).

N^1-*De-Me,* N^9-*(4-hydroxystyryl)(*E-*):* ***Makaluvamine M***
[174232-41-8]
$C_{18}H_{16}N_3O_2^{\oplus}$ 306.343
Trace metab. from *Zyzzya fuliginosa*. Green solid (as trifluoroacetate). Sol. MeOH. λ_{max} 274 (ϵ 14900); 330 (ϵ 11000); 445 (ϵ 8400); 623 (ϵ 9200) (MeOH) (Berdy).

N^1-*De-Me,* N^9-*(4-hydroxystyryl)(*E-*),* N^5-*Me:* ***Makaluvamine L***
[174232-37-2]
$C_{19}H_{18}N_3O_2^{\oplus}$ 320.37
From *Zyzzya fuliginosa*. Green solid (as trifluoroacetate). Sol. MeOH. λ_{max} 276 (ϵ 10500); 344 (ϵ 11700); 451 (ϵ 9200); 638 (ϵ 10400) (MeOH) (Berdy).

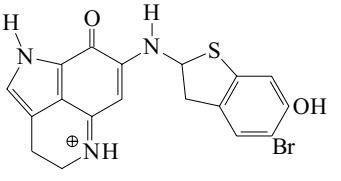
3,4-Didehydro: ***Makaluvamine B***
[146555-79-5]
$C_{11}H_{10}N_3O^{\oplus}$ 200.219
Isol. from *Zyzzya fuliginosa*. Cytotoxic. Inhibitor of topoisomerase II. Red solid (as trifluoroacetate). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 204 (ϵ 17200); 419 (ϵ 4800) (MeOH/NaOH) (Derep). λ_{max} 228 (ϵ 9600); 442 (ϵ 4800) (MeOH) (Derep).

6-Bromo, N^1-*de-Me:* ***Makaluvamine N***
[187964-02-9]
$C_{10}H_9BrN_3O^{\oplus}$ 267.105
Isol. from *Zyzzya fuliginosa*. Cytotoxic against human colon tumour cells. Inhibitor of topoisomerase II. Reddish-brown solid. Counterion not specified. λ_{max} 242 (ϵ 52966); 344 (ϵ 35116); 390 (ϵ 18806); 544 (ϵ 2274) (MeOH).

Radisky, D.C. *et al., J.A.C.S.*, 1993, **115**, 1632 (*isol, uv, ir, pmr, cmr, struct*)
Carney, J.R. *et al., Tetrahedron*, 1993, **49**, 8483 (*Makaluvamine G*)
White, J.D. *et al., J.A.C.S.*, 1994, **116**, 1831 (*synth, Makaluvamine D*)
Izawa, T. *et al., Tetrahedron*, 1994, **50**, 13593 (*synth, Makaluvamines A-E*)
Yamada, F. *et al., Heterocycles*, 1995, **41**, 1905 (*synth, Makaluvamine A*)
Schmidt, E.W. *et al., J. Nat. Prod.*, 1995, **58**, 1861 (*Makaluvamines H-M*)
Sadanandan, E.V. *et al., J.O.C.*, 1995, **60**, 1800 (*synth, Makaluvamine D*)
Fu, X. *et al., J. Nat. Prod.*, 1996, **59**, 1104-1106 (*activity*)
Peat, A.J. *et al., J.A.C.S.*, 1996, **118**, 1028 (*synth, Makaluvamine C*)
Venables, D.A. *et al., J. Nat. Prod.*, 1997, **60**, 408 (*Makaluvamine N*)
Roberts, D. *et al., J.O.C.*, 1997, **62**, 568 (*synth, Makaluvamines A-D*)
Kraus, G.A. *et al., J.O.C.*, 1998, **63**, 9846-9849 (*synth, Makaluvanine C*)
Iwao, M. *et al., Tetrahedron*, 1998, **54**, 8999-9010 (*synth*)
Ishibashi, M. *et al., J. Nat. Prod.*, 2001, **64**, 108-110 (*isol, pmr, cmr*)
Casapullo, A. *et al., J. Nat. Prod.*, 2001, **64**, 1354-1356 (*Makaluvamine P*)
Keyzers, R.A. *et al., Tet. Lett.*, 2004, **45**, 9415-9418 (N^1-*Ribofuranosylmakaluvamine I*)
Dijoux, M.-G. *et al., Bioorg. Med. Chem.*, 2005, **13**, 6035-6044 (*isol, activity*)
Harayama, Y. *et al., Curr. Org. Chem.*, 2005, **9**, 1567-1588 (*rev, synth*)

Makaluvamine F M-45

[146555-83-1]

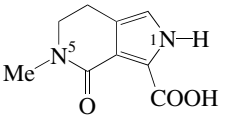


$C_{18}H_{15}BrN_3O_2S^{\oplus}$ 417.305
Metab. of the Fijian sponge *Zyzzya* cf. *marsailis*. Cytotoxic. Inhibitor of topoisomerase II. Orange solid (as trifluoroacetate). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -475.8 (c, 0.0248 in MeOH). λ_{max} 324 (ϵ 17700) (MeOH/NaOH) (Derep). λ_{max} 246 (ϵ 30200); 311 (ϵ 10800); 344 (ϵ 14100) (MeOH) (Derep).

Radisky, D.C. *et al., J.A.C.S.*, 1993, **115**, 1632 (*isol, uv, ir, pmr, cmr, struct*)
Kita, Y. *et al., Chem. Comm.*, 1999, 143-144 (*synth*)
Kita, Y. *et al., Synthesis*, 1999, 885-897 (*synth, ir, uv, pmr, cmr*)

Makaluvic acid A M-46

[184023-18-5]



$C_9H_{10}N_2O_3$ 194.19
Alkaloid from the marine sponge *Zyzzya fuliginosis*. Cryst. (MeOH). Mp not reported. λ_{max} 268 (ϵ 12684); 285 (ϵ 11086) (MeOH).

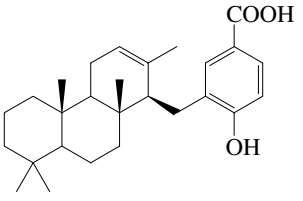
N^5-*De-Me:* ***Makaluvic acid C***
$C_8H_8N_2O_3$ 180.163
Alkaloid from the sponge *Strongylodesma aliwaliensis*. Brown solid. λ_{max} 200 (log ϵ 4.3); 260 (log ϵ 4.02); 289 (log ϵ 3.94) (MeOH).

N^5-*De-Me,* N^1-*β-D-ribofuranosyl:* N′-*β-D-Ribofuranosylmakaluvic acid C*
$C_{13}H_{16}N_2O_7$ 312.279
Alkaloid from *Strongylodesma aliwaliensis*. Brown solid. $[\alpha]_D^{26}$ +41.2 (c, 0.0003 in MeOH). λ_{max} 210 (log ϵ 3.93); 260 (log ϵ 3.7); 286 (log ϵ 3.61) (MeOH).

N^1-*Me,* N^5-*de-Me:* ***Makaluvic acid B***
[184023-37-8]
$C_9H_{10}N_2O_3$ 194.19
From *Zyzzya fuliginosis.* λ_{max} 268 (ϵ 12497); 288 (ϵ 11386) (MeOH).
Fu, X. *et al., J. Nat. Prod.*, 1996, **59**, 1104 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Keyzers, R.A. *et al., J. Nat. Prod.*, 2005, **68**, 506-510 (*Makaluvic acid C*)

Makassaric acid M-47

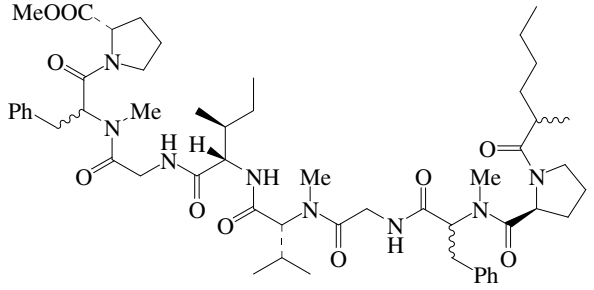
[827348-07-2]



$C_{27}H_{38}O_3$ 410.595
Constit. of an *Acanthodendrilla* sp. Oil. $[\alpha]_D^{25}$ +7.3 (c, 5.4 in MeOH). λ_{max} 217 (ϵ 9711); 254 (ϵ 8715) (MeOH).
Williams, D.E. *et al., J. Nat. Prod.*, 2004, **67**, 2127-2129 (*isol, pmr, cmr*)

Malevamide A M-48

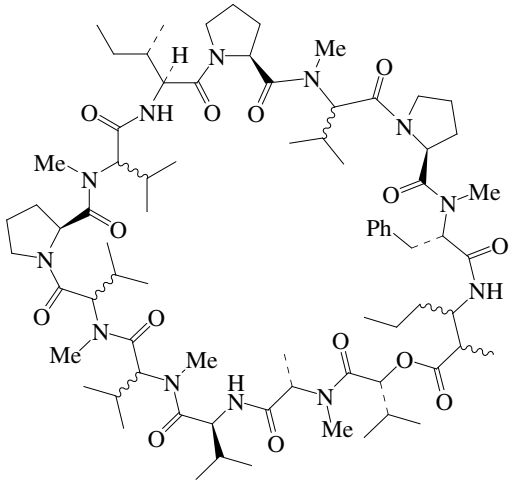
[268544-67-8]



$C_{54}H_{80}N_8O_{10}$ 1001.274
Isol. from the cyanobacterium *Symploca laete-viridis.* Amorph. solid. $[\alpha]_D$ +25 (c, 0.13 in MeOH). $[\alpha]_D$ +26 (c, 0.13 in $CHCl_3$). λ_{max} 209 (log ϵ 4.48); 259 (log ϵ 2.55) (no solvent reported).
Horgen, F.D. *et al., J. Nat. Prod.*, 2000, **63**, 461-467,

Malevamide B M-49

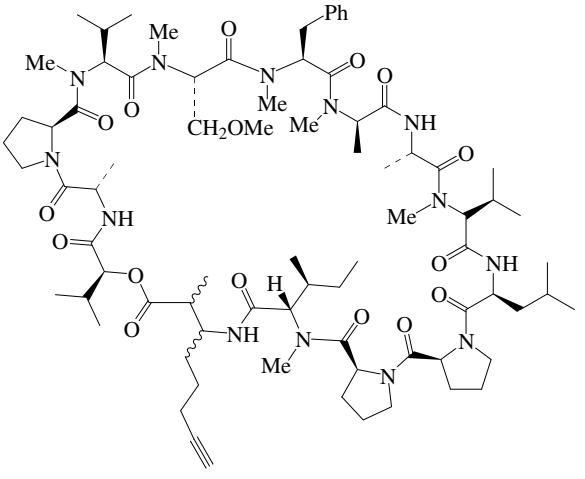
[268544-68-9]



$C_{76}H_{124}N_{12}O_{14}$ 1429.888
Isol. from the cyanobacterium *Symploca laete-viridis.* Amorph. solid. $[\alpha]_D$ -193 (c, 0.19 in MeOH). $[\alpha]_D$ -178 (c, 0.19 in $CHCl_3$). λ_{max} 208 (log ϵ 4.72); 236 (sh) (log ϵ 3.98) (no solvent reported).
Horgen, F.D. *et al., J. Nat. Prod.*, 2000, **63**, 461-467,

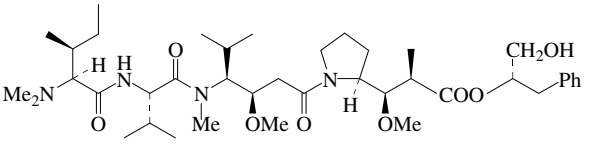
Malevamide C M-50

[268544-69-0]



$C_{79}H_{125}N_{13}O_{16}$ 1512.934
Isol. from the cyanobacterium *Symploca laete-viridis.* Amorph. solid. $[\alpha]_D$ -199 (c, 0.15 in MeOH). $[\alpha]_D$ -198 (c, 0.15 in $CHCl_3$). λ_{max} 207 (log ϵ 4.72); 236 (sh) (log ϵ 3.97) (no solvent reported).
Horgen, F.D. *et al., J. Nat. Prod.*, 2000, **63**, 461-467,

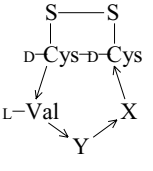
Malevamide D M-51



$C_{40}H_{68}N_4O_8$ 732.999
Peptide antibiotic. Closely related to Isodolastatin H, I-170. Isol. from the cyanobacterium *Symploca hydnoides.* Cytotoxic. Oil. $[\alpha]_D^{26}$ -55 (c, 0.1 in MeOH). λ_{max} 206 (ϵ 21800) (no solvent reported).
Horgen, F.D. *et al., J. Nat. Prod.*, 2002, **65**, 487-491 (*isol, pmr, cmr, ms*)

Malformin M-52

[53571-13-4]



malformin	A_1	X =	L–Ile,	Y =	D–Leu
	A_2	X =	L–Val,	Y =	D–Leu
	A_4	X =	L–Val,	Y =	D–Ile
	B_{1a}	X =	L-*allo*–Ile,	Y =	D–Leu
	B_{1b}	X =	L–Leu,	Y =	D–Leu
	B_2	X =	L–Leu,	Y =	D–Val
	B_3	X =	L–Leu,	Y =	D–Ile
	B_4	X =	L–Ile ,	Y =	D–Ile
	B_5	X =	L–Ile ,	Y =	D–Val
	C	X =	L–Leu,	Y =	D–Leu

Cyclic peptide antibiotic complex. Prod. by *Aspergillus niger*. Isol. from mould damaged rice. Causes deformities in bean seedlings. Antibacterial agent and toxin.

Malformin A, 9CI

Malformin A_1. Cyclic (D-cysteinyl-D-cysteinyl-L-valyl-D-leucyl-L-isoleucyl)cyclic(1→2)-disulfide, 9CI

[3022-92-2]

$C_{23}H_{39}N_5O_5S_2$ 529.724

Sol. MeOH, butanol; fairly sol. Me_2CO, EtOAc; poorly sol. $CHCl_3$, H_2O, hexane. Mp 300° dec. $[\alpha]_D^{24}$ +58.6 (c, 0.5 in DMF). $[\alpha]_D^{25}$ -39 (2-methoxyethanol). Major component of Malformin complex. Contains 12% Malformin A_2 which is biol. inactive. λ_{max} 252 (ϵ 475) (EtOH) (Derep). λ_{max} 220 (ϵ 4100) (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 3.1 mg/kg. ON7050000

Malformin A_2 [83680-20-0]

$C_{22}H_{37}N_5O_5S_2$ 515.697

$[\alpha]_D$ -49.5 (c, 0.73 in 2-methoxyethanol).

Malformin A_4

$C_{22}H_{37}N_5O_5S_2$ 515.697

Malformin B_1 [138875-32-8]

$C_{23}H_{39}N_5O_5S_2$ 529.724

$[\alpha]_D^{25}$ -40.3 (c, 0.72 in 2-methoxyethanol). Minor component. Has been separated into 2 components B_{1a} and B_{1b}.

Malformin B_2 [138797-31-6]

$C_{22}H_{37}N_5O_5S_2$ 515.697

Amorph. Sol. EtOH, MeOH, EtOAc; poorly sol. H_2O, hexane. λ_{max} 220 (MeOH) (Berdy).

Malformin B_3 [149596-54-3]

$C_{23}H_{39}N_5O_5S_2$ 529.724

Malformin B_4 [149596-55-4]

$C_{23}H_{39}N_5O_5S_2$ 529.724

Malformin B_5 [149596-56-5]

$C_{22}H_{37}N_5O_5S_2$ 515.697

Malformin C

Malformin A_3

[59926-78-2]

$C_{23}H_{39}N_5O_5S_2$ 529.724

Prod. by a marine-derived *Aspergillus niger*. Shows antitumour activity. Amorph.

Mp 300° dec. $[\alpha]_D^{25}$ -37.4 (c, 1.01 in DMSO). Poss. identical with B_{1b}.

▶ LD_{50} (mus, ipr) 0.9 mg/kg. ON7060000

[11004-48-1, 130392-01-7, 130392-02-8]

Curtis, R.W. *et al., Science (Washington, D.C.)*, 1958, **128**, 661-662 (*activity*)

Tekeuchi, S. *et al., Phytochemistry*, 1967, **6**, 287-292 (*Malformins B, isol*)

Bodanszky, M. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1974, **71**, 2791-2794 (*Malformin A, struct, synth*)

Bodanszky, M. *et al., Bioorg. Chem.*, 1975, **4**, 93-105 (*Malformin A, synth, cd, activity*)

Bodanszky, M. *et al., J. Antibiot.*, 1976, **29**, 549-553 (*ms*)

Anderegg, R.J. *et al., J.A.C.S.*, 1976, **98**, 3365-3370 (*Malformin C, isol, ir, pmr, ms, struct*)

Bodanszky, M. *et al., Int. J. Pept. Protein Res.*, 1982, **20**, 16-25 (*struct, bibl, conformn*)

Hall, D. *et al., J. Comput. Chem.*, 1982, **3**, 89 (*conformn*)

Chandrasekaran, R. *et al., Conform. Biol.*, (Srinivasan, R., Ed.,), Adenine Press, New York, 1983, (*conformn, rev*)

Sugawara, F. *et al., Tet. Lett.*, 1990, **31**, 4337-4340 (*pmr, struct*)

Kim, K.W. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 240-243; 787-791 (*Malformins A,B, isol, pmr, struct*)

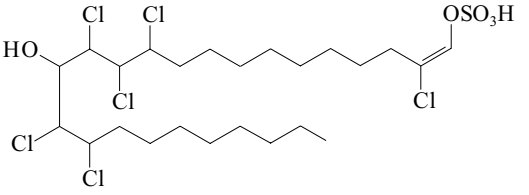
Varoglu, M. *et al., J. Nat. Prod.*, 2000, **63**, 41-43 (*Malformin C, isol, pmr, cmr, activity*)

Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 671; 673; 675; 678

Malhamensilipin A **M-53**

2,11,12,13,15,16-Hexachloro-1-sulfooxy-1-tetracosen-14-ol

[156281-16-2]



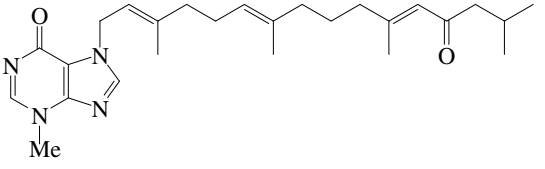
$C_{24}H_{42}Cl_6O_5S$ 655.375

Proposed regiochemistry. Constit. of the cultured chrysophyte of *Poterioochromonas malhamensis*. Inhibitor of protein tyrosine kinase. Oil. $[\alpha]_D$ +28 (c, 0.5 in MeOH). λ_{max} 206 (ϵ 13200) (MeOH).

Chen, J.L. *et al., J. Nat. Prod.*, 1994, **57**, 524 (*isol, uv, ir, pmr, cmr, ms*)

Malonganenone A **M-54**

[882403-69-2]



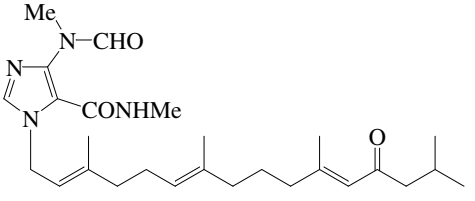
$C_{26}H_{38}N_4O_2$ 438.612

Isol. from *Leptogorgia gilchristi*. Cytotoxic. Glass. λ_{max} 221 (ϵ 30900); 252 (ϵ 28800) (no solvent reported).

Keyzers, R.A. *et al., Tetrahedron*, 2006, **62**, 2200-2206 (*Malonganenone A*)

Malonganenone B **M-55**

[882403-70-5]



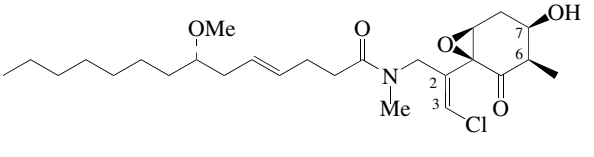
$C_{27}H_{42}N_4O_3$ 470.654

Isol. from *Leptogorgia gilchristi*. Cytotoxic. Glass. λ_{max} 238 (ϵ 14400) (MeOH).

Keyzers, R.A. *et al., Tetrahedron*, 2006, **62**, 2200-2206 (*isol, pmr, cmr*)

Malyngamide I **M-56**

[170894-27-6]



$C_{26}H_{42}ClNO_5$ 484.074

Alkaloid from a marine cyanobacterium *Lyngbya majuscula*. Ichthyotoxin. $[\alpha]_D^{30}$ +20.5 (c, 1.53 in EtOH).

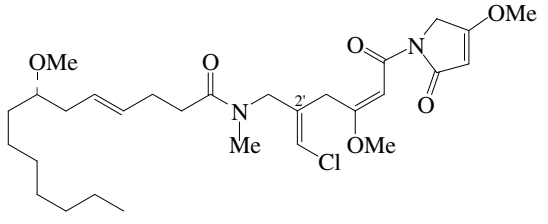
Ac: ***Stylocheilamide***
[69121-74-0]
$C_{28}H_{44}ClNO_6$ 526.111
Constit. of the sea hare *Stylocheilus longicauda* and alga *Gracilaria coronopifolia*. Noncryst. $[\alpha]_D^{28}$ +10.6 (c, 28.2 in MeOH). Struct. revised in 1995.

7-Deoxy, 6,7-didehydro: ***Malyngamide N****. Deacetoxystylocheilamide*
[69121-75-1]
$C_{26}H_{40}ClNO_4$ 466.059
From *Stylocheilus longicauda* and *Gracilaria coronopifolia*. $[\alpha]_D^{25}$ -11.3 (c, 15.7 in MeOH). Struct. of Deacetoxysylocheilamide revised here following struct. revision of Stylocheilamide. The trivial name Deacetoxystylochielamide is now misleading. λ_{max} 241 (ϵ 6800) (MeOH) (Derep). λ_{max} 237 (MeOH) (Berdy).

Rose, A.F. *et al., J.A.C.S.*, 1978, **100**, 7665-7670 (*isol, uv, ir, pmr, cmr, ms*)
Todd, J.S. *et al., Tet. Lett.*, 1995, **36**, 7837-7840 (*Malyngamide I, struct*)
Kan, Y. *et al., J. Nat. Prod.*, 1998, **61**, 152-155 (*isol, abs config*)

Malyngamide A M-57

N-*[2-(Chloromethylene)-6-(2,5-dihydro-4-methoxy-2-oxo-1*H*-pyrrol-1-yl)-4-methoxy-6-oxo-4-hexenyl]-7-methoxy*-N*-methyl-4-tetradecenamide, 9CI*
[69778-82-1]

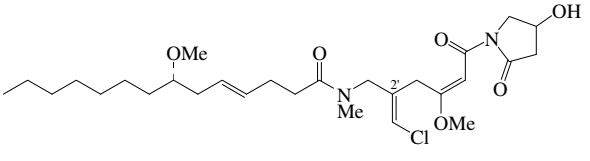


$C_{29}H_{45}ClN_2O_6$ 553.137
Constit. of shallow-water varieties of the marine blue-green alga *Lyngbya majuscula*. Shows antifeedant activity. Oil. $[\alpha]_D^{25}$ -6.5 (c, 0.77 in CH_2Cl_2). λ_{max} 213 (ϵ 15700); 265 (ϵ 17600) (EtOH) (Derep).

*2′*Z*-Isomer:* ***Isomalyngamide A***
$C_{29}H_{45}ClN_2O_6$ 553.137
Isol. from *Lyngbya majuscula*.
$[\alpha]_D^{29}$ -4.8 (c, 2.9 in CH_2Cl_2).

Cardellina, J.H. *et al., Phytochemistry*, 1978, **17**, 2091 (*isol, uv, pmr, ms, struct*)
Cardellina, J.H. *et al., J.A.C.S.*, 1979, **101**, 240 (*isol, uv, pmr, ms, struct*)
Kan, Y. *et al., J. Nat. Prod.*, 2000, **63**, 1599-1602 (*Isomalyngamide A*)

Malyngamide B M-58



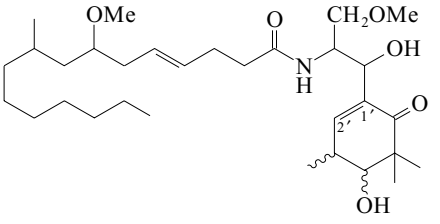
$C_{28}H_{45}ClN_2O_6$ 541.126
Metab. from a shallow-water variety of the marine blue-green alga *Lyngbya majuscula*.

*2′*Z*-Isomer:* ***Isomalyngamide B***
$C_{28}H_{45}ClN_2O_6$ 541.126
Isol. from *Lyngbya majuscula*.
$[\alpha]_D^{27}$ +46 (c, 0.4 in $CHCl_3$).

Cardellina, J.H. *et al., Phytochemistry*, 1978, **17**, 2091 (*isol, pmr, ms*)
Christophersen, C. *et al., Alkaloids (N.Y.)*, 1985, **24**, 57 (*struct*)
Kan, Y. *et al., J. Nat. Prod.*, 2000, **63**, 1599-1602 (*Isomalyngamide B*)

Malyngamide E M-59

N-*[2-Hydroxy-2-(4-hydroxy-3,5,5-trimethyl-6-oxo-1-cyclohexen-1-yl)-1-(methoxymethyl)ethyl]-7-methoxy-9-methyl-4-hexadecenamide, 9CI*
[67488-05-5]



$C_{31}H_{55}NO_6$ 537.779
Constit. of *Lyngbya majuscula*. Shows mild antibiotic activity against *Mycobacterium smegmatis* and *Bacillus subtilis*. $[\alpha]_D^{24}$ +24.2 (c, 0.6 in $CHCl_3$). λ_{max} 235 (ϵ 6500) (MeOH) (Derep).

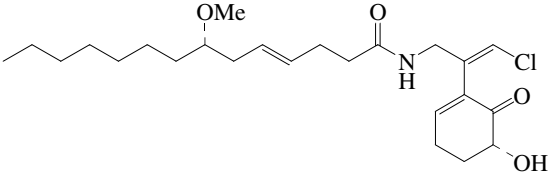
Di-Ac: $[\alpha]_D^{25}$ +37.5 (c, 0.12 in $CHCl_3$).

1′,2′-Dihydro, 2′-hydroxy: ***Malyngamide D***†
[67488-04-4]
$C_{31}H_{57}NO_7$ 555.794
Metab. from *Lyngbya majuscula*. Shows similar prop. as parent. $[\alpha]_D^{25}$ -33 (c, 0.53 in $CHCl_3$). Appears to be different from Malyngamide D descr. under Malyngamide F, M-60. λ_{max} 235 (ϵ 6500) (MeOH) (Derep).

Mynderse, J.S. *et al., J.O.C.*, 1978, **43**, 4359 (*pmr, ms, cmr, ir, uv, struct*)

Malyngamide F M-60

Malyngamide D†
[109897-54-3]



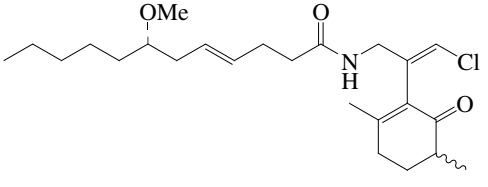
$C_{24}H_{38}ClNO_4$ 440.021
Erroneously described as Malyngamide D but subsequently renamed. See under Malyngamide E, M-59. Isol. from the marine cyanobacterium *Lyngbya majuscula*. Shows mild cytotoxic activity. $[\alpha]_D^{25}$ +17 (c, 0.9 in $CHCl_3$).

O-*Ac:* ***Malyngamide F acetate****. Malyngamide D acetate*
[109897-55-4]
$C_{26}H_{40}ClNO_5$ 482.058
From *Lyngbya majuscula*. Oil. $[\alpha]_D^{25}$ -15.1 (c, 3.6 in $CHCl_3$). λ_{max} 252 (ϵ 1760) (MeOH) (Berdy).

Gerwick, W.H. *et al., Phytochemistry*, 1987, **26**, 1701-1704; 3381 (*isol, uv, ir, pmr, cmr, ms, struct, deriv*)

Malyngamide G M-61

[153146-47-5]

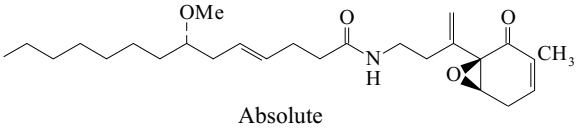


$C_{24}H_{38}ClNO_3$ 424.022
Isol. from *Lyngbya majuscula*. Yellow oil. $[\alpha]_D$ +16.2 (c, 1.1 in $CHCl_3$). λ_{max} 230 (ϵ 7300) (MeOH).

Praud, A. *et al., Tet. Lett.*, 1993, **34**, 5437-5440 (*isol, uv, ir, pmr, cmr, ms*)

Malyngamide H M-62

7-Methoxy-N-*[3-(3-methyl-2-oxo-7-oxabicyclo[4.1.0]hept-3-en-1-yl)-3-butenyl]-4-tetradecenamide, 9CI*
[165337-92-8]



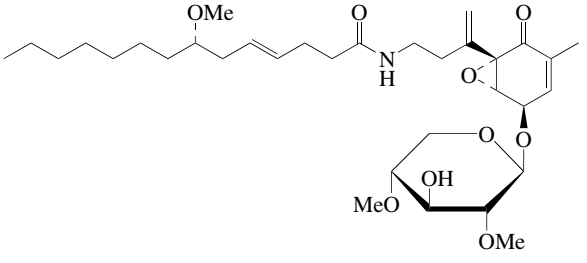
Absolute configuration

$C_{26}H_{41}NO_4$ 431.614
Isol. from the Caribbean cyanobacterium *Lyngbya majuscula*. Ichthyotoxic. Yellowish oil. $[\alpha]_D^{26}$ +26.1 (c, 0.5 in $CHCl_3$). λ_{max} 243 (ϵ 6460) (MeOH) (Berdy).

Orjala, J. *et al., J. Nat. Prod.*, 1995, **58**, 764 (*isol, uv, ir, pmr, cmr, ms, struct*)

Malyngamide J M-63

[200409-60-5]

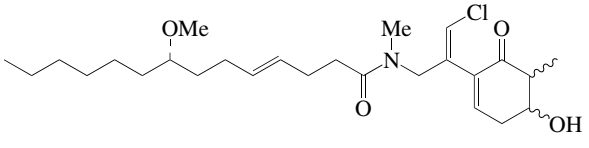


$C_{33}H_{53}NO_9$ 607.783
Isol. from the cyanobacterium *Lyngbya majuscula*. Ichthyotoxic. $[\alpha]_D$ +64 (c, 0.1 in $CHCl_3$). λ_{max} 240 (ϵ 5600) (MeOH).

Wu, M. *et al., Tetrahedron*, 1997, **53**, 15986-15990 (*isol, uv, ir, cd, pmr, cmr, ms*)

Malyngamide L M-64

[200409-81-0]

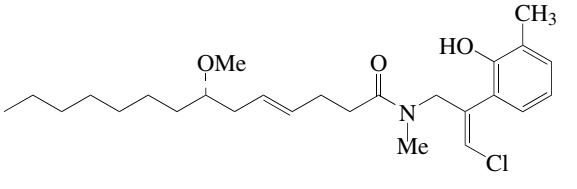


$C_{26}H_{42}ClNO_4$ 468.075
Isol. from the cyanobacterium *Lyngbya majuscula*. Oil. $[\alpha]_D$ +17.3 (c, 0.1 in EtOH). λ_{max} 206 (ϵ 31000) (MeOH).

Wu, M. *et al., Tetrahedron*, 1997, **53**, 15983-15990 (*isol, uv, ir, pmr, cmr, ms*)

Malyngamide M M-65

[200716-67-2]

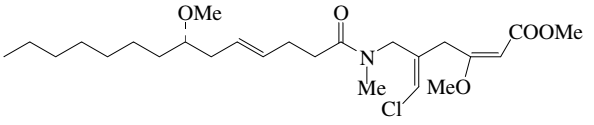


$C_{26}H_{40}ClNO_3$ 450.06
Isol. from the red alga *Gracilaria coronopifolia*.
$[\alpha]_D$ -35 (c, 0.06 in MeOH). λ_{max} 279 (ϵ 3940); 302 (ϵ 3410); 317 (ϵ 3050) (MeOH).

Kan, Y. *et al., J. Nat. Prod.*, 1998, **61**, 152-155 (*isol, uv, ir, pmr, cmr*)

Malyngamide O M-66

[298184-52-8]

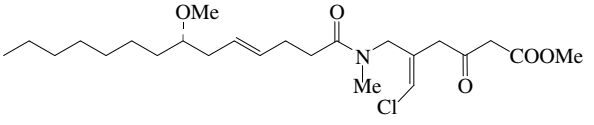


$C_{25}H_{42}ClNO_5$ 472.063
Isol. from the sea hare *Stylocheilus longicauda*. Pale yellow oil. $[\alpha]_D$ -55.6 (c, 0.02 in MeOH). λ_{max} 212 (ϵ 13080); 240 (ϵ 9680) (MeOH).

Gallimore, W.A. *et al., J. Nat. Prod.*, 2000, **63**, 1422-1424

Malyngamide P M-67

[298184-53-9]

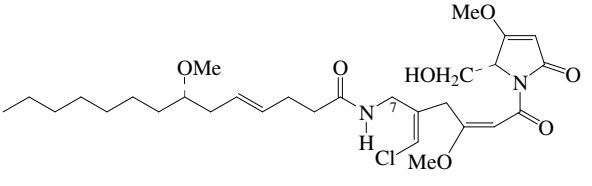


$C_{24}H_{40}ClNO_5$ 458.036
Isol. from the sea hare *Stylocheilus longicauda*. Oil. $[\alpha]_D$ -75 (c, 0.02 in MeOH). λ_{max} 208 (ϵ 9030); 275 (ϵ 3090) (MeOH).

Gallimore, W.A. *et al., J. Nat. Prod.*, 2000, **63**, 1422-1424

Malyngamide Q M-68

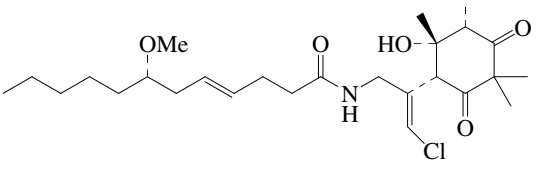
[280114-13-8]



$C_{29}H_{45}ClN_2O_7$ 569.136
Isol. from *Lyngbya majuscula*. Pale yellow oil. $[\alpha]_D^{25}$ +2.1 (c, 0.8 in MeOH). λ_{max} 264 (log ϵ 4.18) (MeOH).

7-N-*Me:* ***Malyngamide R***
[280114-14-9]
$C_{30}H_{47}ClN_2O_7$ 583.163
Isol. from *Lyngbya majuscula*. Pale yellow oil. $[\alpha]_D^{25}$ +2 (c, 0.9 in MeOH). λ_{max} 258 (log ϵ 4.18) (MeOH).
Milligan, K.E. *et al., J. Nat. Prod.*, 2000, **63**, 965-968

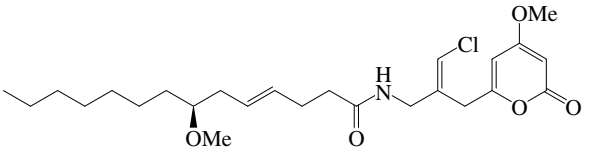
Malyngamide S M-69



$C_{26}H_{42}ClNO_5$ 484.074
Isol. from the sea hare *Bursatella leachii*. Exhibits cytotoxic and antiinflammatory activities. Oil. $[\alpha]_D^{20}$ -8 (c, 1.5 in MeOH). λ_{max} 204 (log ϵ 4.25); 275 (log ϵ 2.3) (MeOH).

Appleton, D.R. *et al., J. Nat. Prod.*, 2002, **65**, 630-631 (*isol, pmr, cmr*)

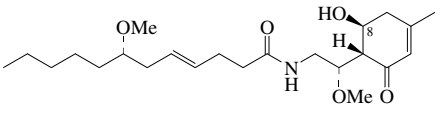
Malyngamide T M-70



$C_{25}H_{38}ClNO_5$ 468.032
Isol. from *Lyngbya majuscula*. Pale yellow oil. $[\alpha]_D^{22}$ -13.5 (c, 0.2 in $CHCl_3$). λ_{max} 218 (log ϵ 4.45); 284 (log ϵ 4.14) (MeOH).

Nogle, L.M. *et al., J. Nat. Prod.*, 2003, **66**, 217-220 (*isol, pmr, cmr, ms*)

Malyngamide U M-71



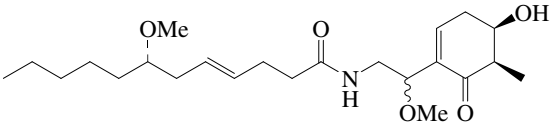
Relative Configuration

$C_{23}H_{39}NO_5$ 409.565
Isol. from *Lyngbya majuscula*. Oil. $[\alpha]_D^{18}$ -15.8 (c, 0.12 in $CHCl_3$). λ_{max} 203 (log ϵ 3.48); 233 (log ϵ 3.54) (MeOH).

8-Epimer: ***Malyngamide V***
$C_{23}H_{39}NO_5$ 409.565
Isol. from *Lyngbya majuscula*. Oil. $[\alpha]_D^{18}$ +4.3 (c, 0.12 in $CHCl_3$). λ_{max} 203 (log ϵ 3.48); 231 (log ϵ 3.48) (MeOH).

McPhail, K.L. *et al., J. Nat. Prod.*, 2003, **66**, 132-135 (*isol*)

Malyngamide W M-72

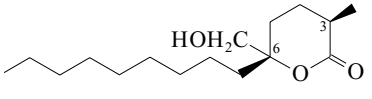


$C_{23}H_{39}NO_5$ 409.565
Isol. from *Lyngbya majuscula*. Pale yellow oil. $[\alpha]_D^{18}$ -15 (c, 0.06 in $CHCl_3$). λ_{max} 203 (log ϵ 4.08); 227 (log ϵ 3.88) (MeOH).

McPhail, K.L. *et al., J. Nat. Prod.*, 2003, **66**, 132-135 (*isol, pmr, cmr*)

Malyngolide M-73

*Tetrahydro-6-(hydroxymethyl)-3-methyl-6-nonyl-2*H*-pyran-2-one, 9CI*



(3*R*,6*S*)*-form*

$C_{16}H_{30}O_3$ 270.411

(3*R*,6*S*)*-form* [71582-80-4]
Isol. from *Lyngbya majuscula*. Active against *Mycobacterium smegmatis* and *Streptococcus pyogenes*. Cryst.
Mp 36-37°. $[\alpha]_D$ -13 (c, 2 in $CHCl_3$).

Ac:
Oil. $[\alpha]_D^{29}$ -17 (c, 1 in $CHCl_3$).

(3*S*,6*S*)*-form*
Epimalyngolide
[76023-93-3]
Cryst. Mp 29-30°. $[\alpha]_D^{25}$ +19.1 (c, 1.13 in $CHCl_3$).

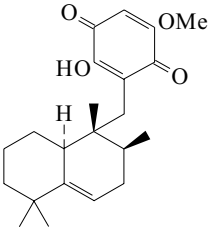
(3*RS*,6*RS*)*-form* [76984-84-4] $Bp_{0.01}$ 144-146°.

(3*RS*,6*SR*)*-form* [74742-19-1] $Bp_{0.01}$ 144-146°.

Cardellina, J.H. *et al., J.O.C.*, 1979, **44**, 4039 (*isol*)
Matsuo, Y. *et al., Chem. Pharm. Bull.*, 1981, **29**, 3047; 3070 (*synth*)
Pougny, J.-R. *et al., Tet. Lett.*, 1982, 4929 (*synth, bibl*)
Cardellina, J.H. *et al., J. Nat. Prod.*, 1983, **46**, 196 (*purifn*)
Sato, T. *et al., Chem. Lett.*, 1988, 1739 (*synth*)
Ichimoto, I. *et al., Agric. Biol. Chem.*, 1990, **54**, 657 (*synth*)
Honda, T. *et al., J.C.S. Perkin 1*, 1990, 2677 (*synth, bibl*)
Floerke, H. *et al., Annalen*, 1996, 147 (*synth, bibl*)
Enders, D. *et al., Tetrahedron*, 1996, **52**, 5805 (*synth, bibl*)
Konno, H. *et al., Tet. Lett.*, 1997, **38**, 6023 (*synth*)
Matsuo, K. *et al., Heterocycles*, 1998, **48**, 1213-1220 (*synth, bibl*)
Ohira, S. *et al., J.C.S. Perkin 1*, 1998, 293-297 (*synth*)
Winter, E. *et al., Tetrahedron*, 1998, **54**, 10329-10338 (*synth, bibl*)
Maezaki, N. *et al., Tetrahedron*, 1998, **54**, 13087-13104 (*synth*)
Wan, Z. *et al., J.A.C.S.*, 2000, **122**, 10470-10471 (*synth*)
Trost, B.M. *et al., Org. Lett.*, 2000, **2**, 4013-4015 (*synth*)
Mizutani, H. *et al., Tetrahedron*, 2002, **58**, 8926-8936 (*synth*)
Carda, M. *et al., Tetrahedron*, 2003, **59**, 858-864 (*synth*)
Miyamoto, H. *et al., Heterocycles*, 2005, **66**, 61-68 (*synth*)

Mamanuthaquinone M-74

[138843-20-6]

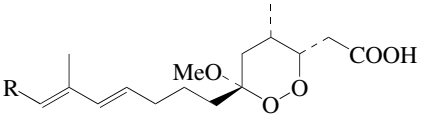


$C_{22}H_{30}O_4$ 358.477
Metab. of a *Fasciospongia* sp. Reverse transcriptase inhibitor. Orange oil. $[\alpha]_D$ -31 (c, 0.058 in $CHCl_3$). λ_{max} 298 (ϵ 1440); 430 (ϵ 620) (prob. $CHCl_3$) (Derep). λ_{max} 298 (ϵ 1435); 430 (ϵ 620) (MeOH) (Berdy).

Swersey, J.C. *et al., Tet. Lett.*, 1991, **32**, 6687 (*isol, pmr, cmr*)

Manadic acid A M-75

6-Methoxy-4-methyl-6-(6-methyl-4,6-octadienyl)-1,2-dioxane-3-acetic acid, 9CI
[170894-34-5]



R = CH_3

$C_{17}H_{28}O_5$ 312.405
Isol. from the sponge *Plakortis* sp. Cytotoxic agent. Oil. $[\alpha]_D^{18}$ +83.9 (MeOH). λ_{max} 232 (ϵ 30500) (MeOH).

Ichiba, T. *et al., Tetrahedron*, 1995, **51**, 12195; 1996, **52**, 14079 (*isol, uv, ir, pmr, cmr, ms*)

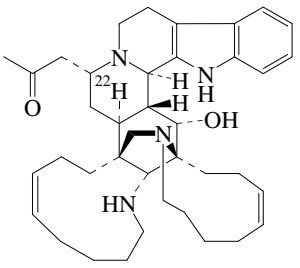
Manadic acid B M-76

6-Methoxy-4-methyl-6-(6-methyl-4,6-nonadienyl)-1,2-dioxane-3-acetic acid, 9CI
[170894-35-6]
As Manadic acid A, M-75 with
R = CH_2CH_3

$C_{18}H_{30}O_5$ 326.432
Isol. from the sponge *Plakortis* sp. Cytotoxic agent. Oil. $[\alpha]_D^{18}$ +130.3 (c, 4 in MeOH).

Ichiba, T. *et al., Tetrahedron*, 1995, **51**, 12195; 1996, **52**, 14079 (*isol, uv, ir, pmr, cmr, ms*)

Manadomanzamine A M-77



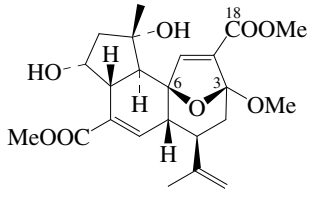
$C_{39}H_{54}N_4O_2$ 610.881
Isol. from the Indonesian sponge *Acanthostrongylophora* sp. Active against HIV-1 and mycobacteria. Powder. $[\alpha]_D$ -19 (c, 0.11 in MeOH). λ_{max} 282 (ϵ 7700) (no solvent reported).

22-Epimer: ***Manadomanzamine B***
$C_{39}H_{54}N_4O_2$ 610.881
Isol. from *Acanthostrongylophora* sp. Powder. $[\alpha]_D$ -18 (c, 0.11 in MeOH). λ_{max} 282 (ϵ 7200) (no solvent reported).

Peng, J. *et al., J.A.C.S.*, 2003, **125**, 13382-13386 (*isol, cd, pmr, cmr*)

Mandapamate M-78

[157143-53-8]



$C_{23}H_{30}O_8$ 434.485
Constit. of *Sinularia dissecta*. Oil. $[\alpha]_D$ +147 (c, 0.25 in $CHCl_3$). λ_{max} 217 (ϵ 10000) (MeOH) (Derep).

3,6-Diepimer: ***Isomandapamate***
[169738-53-8]
$C_{23}H_{30}O_8$ 434.485
Constit. of *Sinularia maxima*. Oil. $[\alpha]_D^{27}$ +84.7.

3,6-Diepimer, 3-O-de-Me, O^3*-Et, 18-Et ester analogue:* ***Bishomoisomandapamate***
[250261-01-9]
$C_{25}H_{34}O_8$ 462.539
Constit. of a *Sinularia* sp.

3,6-Diepimer, 3-O-de-Me, O^3*-Et, 20-Et ester analogue:* ***Confertdiate***
[851706-23-5]
$C_{25}H_{34}O_8$ 462.539
Constit. of *Sinularia conferta*. Oil. $[\alpha]_D^{20}$ +124 (c, 0.4 in MeOH).

Venkateswarlu, Y. *et al., Tet. Lett.*, 1994, **35**, 2249 (*isol, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., Tetrahedron*, 1995, **51**, 10997-11010 (*Isomandapamate*)
Ammanamanchi, *et al., J. Chem. Res., Synop.*, 1999, 600-601 (*Bishomoisomandapamate*)
Su, J.-Y. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 107-113 (*Confertdiate*)

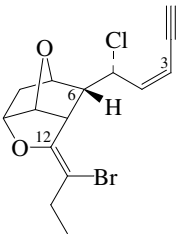
Mandibular organ-inhibiting hormone M-79

MOIH
Two peptides (MOIH-1 and -2) containing 78 amino acid residues and 3 intrachain disulfide bridges; members of the crustacean hyperglycaemic hormone family. Isol. from the eyestalk of the crab *Cancer pagarus*. Regulates synth. of Me farnesoate in the mandibular organs of crustaceans.

[219481-34-2, 252028-11-8, 252207-18-4]

Wainwright, G. *et al., J. Biol. Chem.*, 1996, **271**, 12749-12754 (*isol, struct*)

Maneonenes M-80



(3*Z*,5*R*,6*R*,12*E*)-*form*

$C_{15}H_{16}BrClO_2$ 343.647

(3*Z*,5*R*,6*R*,12*E*)-*form*
Maneonene C
[62624-86-6]
Constit. of *Laurencia nidifica*.
Oil. $[\alpha]_D^{21}$ +336 (c, 1.46 in $CHCl_3$).

(3*Z*,5*R*,6*S*,12*E*)-*form*
Maneonene A
[61661-24-3]
From *Laurencia nidifica*.
Oil. $[\alpha]_D^{21}$ +39 (c, 1 in $CHCl_3$).

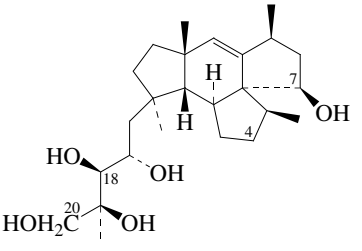
(3*E*,5*R*,6*S*,12*Z*)-*form*
(E)-Maneonene B
[61688-65-1]
From *Laurencia nidifica*.
Oil. $[\alpha]_D^{21}$ -25 (c, 0.4 in $CHCl_3$).

(3*Z*,5*R*,6*S*,12*Z*)-*form*
(Z)-Maneonene B
[61661-25-4]
From *Laurencia nidifica*.
Oil. $[\alpha]_D^{21}$ -49 (c, 3.6 in $CHCl_3$).

Waraskiewicz, S.M. *et al., J.O.C.*, 1978, **43**, 3194 (*isol, struct*)
Holmes, A.B. *et al., Chem. Comm.*, 1983, 415; 1984, 1594 (*synth*)
Sakai, R. *et al., Helv. Chim. Acta*, 1986, **69**, 91 (*Maneonene C*)

Mangicol A M-81

[293735-53-2]



$C_{25}H_{42}O_5$ 422.604
Metab. of marine-derived *Fusarium heterosporum*. Cryst. Mp 86-88°. $[\alpha]_D$ +80 (c, 0.2 in MeOH). λ_{max} 203 (ϵ 3000) (MeOH).

18-Ketone: ***Mangicol C***
[293735-55-4]
$C_{25}H_{40}O_5$ 420.588
Metab. of marine-derived *Fusarium heterosporum*. Amorph. solid. $[\alpha]_D$ -11 (c, 0.4 in MeOH). Error in struct. diag. in ref. λ_{max} 202 (ϵ 5900) (MeOH).

7-Deoxy: ***Mangicol D***
[293735-56-5]
$C_{25}H_{42}O_4$ 406.604
Metab. of marine-derived *Fusarium heterosporum*. Amorph. solid. $[\alpha]_D$ +76 (c, 1 in MeOH). λ_{max} 203 (ϵ 3000) (MeOH).

7-Deoxy, 18-ketone: ***Mangicol E***
[293735-57-6]
$C_{25}H_{40}O_4$ 404.589

Constit. of marine-derived *Fusarium heterosporum*. Amorph. solid. $[\alpha]_D$ -16 (c, 0.42 in MeOH). λ_{max} 202 (ϵ 5900) (MeOH).

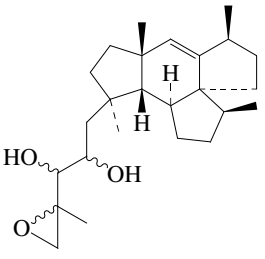
7-Deoxy, 4α-hydroxy: ***Mangicol B***
[293735-54-3]
$C_{25}H_{42}O_5$ 422.604
Metab. of marine-derived *Fusarium heterosporum*. Amorph. solid. $[\alpha]_D$ +61 (c, 0.33 in MeOH). λ_{max} 203 (ϵ 2800) (MeOH).

7,20-Dideoxy, 18-ketone: ***Mangicol F***
[293735-58-7]
$C_{25}H_{40}O_3$ 388.589
Constit. of marine-derived *Fusarium heterosporum*. Amorph. solid. $[\alpha]_D$ +14 (c, 0.75 in MeOH). λ_{max} 202 (ϵ 6000) (MeOH).

Renner, M.K. *et al., J.O.C.*, 2000, **65**, 4843-4852 (*isol, pmr, cmr*)

Mangicol G M-82

[293735-59-8]

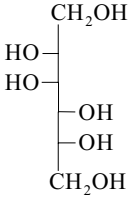


$C_{25}H_{40}O_3$ 388.589
Constit. of marine-serived *Fusarium heterosporum*. Amorph. solid. $[\alpha]_D$ +48 (c, 0.68 in MeOH). λ_{max} 204 (ϵ 3200) (MeOH).

Renner, M.K. *et al., J.O.C.*, 2000, **65**, 4843-4852 (*isol, pmr, cmr*)

Mannitol M-83

Mannite. manno-*Hexitol. Kurrine (obsol.)*
[87-78-5]



D–*form*

$C_6H_{14}O_6$ 182.173
▶ OP2050000

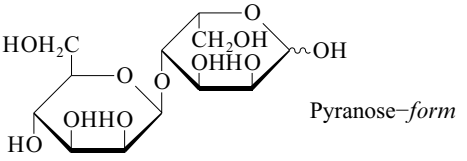
D-*form*
Cordycepic acid. Manita. Osmitrol. Resectisol. E421
[69-65-8]
Cordycepic acid was originally given the struct. of a stereoisomer of quinic acid. Widespread in plants and their exudates particularly olive and plane trees. Obt. from manna and seaweeds. Obt. industrially from Fructose. Used as solid in alkalimetric titration of boric acid and Ge(*IV*); masking agent for metals. Reference material used in elemental microanalysis. Inexpensive starting material for synthesis. Sweetening agent. Food additive, used as anticaking agent, lubricant, for stabiliser and thickener, and for other uses in food processing. Energy reserve in brown algae. Diagnostic aid (renal function determination); diuretic. Tablet and capsule diluent. Needles. Sol. H_2O, Py; sl. sol. EtOH; insol. Et_2O.
Mp 166°. $Bp_{3.5}$ 295°. $[\alpha]_D^{25}$ -0.21 (c, 17.6 in H_2O). $[\alpha]_D^{25}$ +28.61 (c, 10 in 12.8% borax aq.). pK_{a1} 13.29 (25°). Log P -4.67 (calc). Often occurs as boric ester conjugates in brown algae.
▶ Human systemic effects when used therapeutically, LD_{50} (rat, orl) 13500 mg/kg. OP2060000

[45007-61-2, 61453-77-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 186C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 289C; 401A; 401B; 404A (*nmr*)
Lohmar, R. *et al., Carbohydr. Res.*, 1949, **4**, 211 (*rev*)
Wright, L. *et al., J.O.C.*, 1961, **26**, 1588 (*synth*)
Brimacombe, J.S. *et al., The Carbohydrates*, Academic Press, 1972, **1A**, 479
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **1**, 754 (*rev*)
Matsuhiro, B. *et al., Carbohydr. Res.*, 1981, **89**, 326 (*cmr*)
Chuda, Y. *et al., Phytochemistry*, 1997, **46**, 209-213 (*occur, borates*)
Fronezck, F.R. *et al., Acta Cryst. C*, 2003, **59**, o567-o570 (*D-form, cryst struct*)

4-*O*-β-D-Mannopyranosyl-L-gulose, 8CI M-84

[20237-61-0]



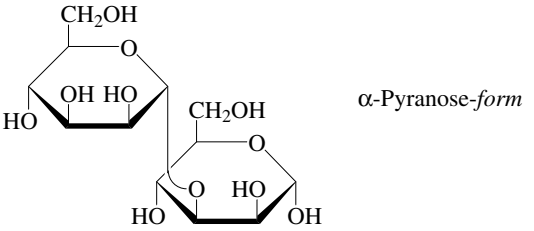
Pyranose–*form*

$C_{12}H_{22}O_{11}$ 342.299
Formed by the partial acid hydrolysis of a chemically reacted alginic acid, extracted from *Laminaria digitata*. Cryst. (EtOH/EtOAc).
Mp 201-203°. $[\alpha]_D$ -23.2 (c, 0.83 in H_2O).

Hirst, E.L. *et al., J.C.S.*, 1964, 1493 (*synth*)
Percival, E. *et al., Carbohydr. Res.*, 1967, **4**, 441 (*glc*)

3-*O*-α-D-Mannopyranosyl-D-mannose, 9CI, 8CI M-85

[34141-02-1]



α-Pyranose-*form*

$C_{12}H_{22}O_{11}$ 342.299
Constit. of the unsulfated α-D-mannan isol. from an aqueous extract of *Urospora penicilliformis*.
$[\alpha]_D^{27}$ +40 (c, 1.55 in MeOH). $[\alpha]_D$ +50 (c, 2.86 in MeOH).

α-Pyranose-*form* [50499-35-9]

*Octa-Ac: 1,2,4,6-Tetra-*O*-acetyl-3-*O*-(2,3,4,6-tetra-*O*-acetyl-α-D-mannopyranosyl)-α-D-mannopyranose*
[65877-61-4]
$C_{28}H_{38}O_{19}$ 678.597
Mp 170-172°. $[\alpha]_D^{22}$ +37.6 (c, 0.51 in $CHCl_3$).

*Me glycoside: Methyl 3-*O*-α-D-mannopyranosyl-α-D-mannopyranoside*
[72028-62-7]
$C_{13}H_{24}O_{11}$ 356.326
Amorph. powder + $5H_2O$. $[\alpha]_D^{25}$ +94.8 (c, 0.31 in H_2O).

*Me glycoside, tetra-Ac: Methyl 3-*O*-(2,3,4,6-tetra-*O*-acetyl-α-D-mannopyranosyl)-α-D-mannopyranoside*
[71978-78-4]
$C_{21}H_{32}O_{15}$ 524.475
Foam. $[\alpha]_D$ +70 (c, 0.43 in EtOH).

*Me glycoside, hepta-Ac: Methyl 2,4,6-tri-*O*-acetyl-3-*O*-(2,3,4,6-tetra-*O*-acetyl-α-D-mannopyranosyl)-α-D-mannopyranoside*
[71978-79-5]
$C_{27}H_{38}O_{18}$ 650.586
Syrup. $[\alpha]_D$ +39 (c, 0.9 in $CHCl_3$).

*Me glycoside, tetrabenzyl: Methyl 2,4-di-*O*-benzyl-3-*O*-(2,4-di-*O*-benzyl-α-D-mannopyranosyl)-α-D-mannopyranoside*
[79218-61-4]

$C_{41}H_{48}O_{11}$ 716.824
$[\alpha]_D^{25}$ +30.8 (c, 0.35 in $CHCl_3$).

*Benzyl glycoside, hexabenzyl: Benzyl 2,4,6-tri-*O*-benzyl-3-*O*-(2,4,6-tri-*O*-benzyl-α-D-mannopyranosyl)-α-D-mannopyranoside*
$C_{61}H_{64}O_{11}$ 973.17
$[\alpha]_D$ +16 (c, 0.60 in $CHCl_3$).

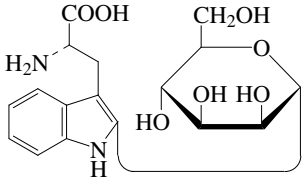
β-Pyranose-*form* [50499-34-8]

Hexa-Ac, 1,2-methylorthoacetate: [81555-83-1]
$C_{27}H_{38}O_{18}$ 650.586
Mp 96-97°. $[\alpha]_D^{26}$ -45 (c, 0.22 in $CHCl_3$).

Jones, J.K.N. *et al., J.C.S.*, 1958, 27 (*isol*)
Jeanes, A. *et al., Can. J. Chem.*, 1962, **40**, 2256 (*isol*)
Gorin, P.A.J. *et al., Can. J. Chem.*, 1973, **51**, 2375 (*cmr*)
Bourne, E.J. *et al., J. Carbohydr., Nucleosides, Nucleotides*, 1974, 235 (*isol*)
Ponpipom, M.M. *et al., Carbohydr. Res.*, 1977, **59**, 311 (*synth*)
Lee, E.E. *et al., Carbohydr. Res.*, 1979, **75**, 322 (*Me gly*)
Ogawa, T. *et al., Carbohydr. Res.*, 1981, **97**, 205; **93**, 53 (*Me gly, cmr, deriv, synth*)
Winnick, F.M. *et al., Carbohydr. Res.*, 1982, **103**, 15-28 (*α-Me-pyr*)
Winnick, F.M. *et al., J.O.C.*, 1982, **47**, 2701-2707 (*hexa-Ac, octa-Ac*)
Brisson, J.R. *et al., J. Carbohydr. Chem.*, 1983, **2**, 41-55 (*Me gly, pmr*)
Ogawa, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 475 (*synth, α-benzyl-pyr hexabenzyl*)
Garegg, P.J. *et al., Carbohydr. Res.*, 1990, **200**, 475 (*α-Me pyr derivs*)
Ajisaka, K. *et al., Carbohydr. Res.*, 1995, **270**, 123-130 (*enzymic synth*)

2-α-D-Mannopyranosyltryptophan M-86

[180509-18-6]



$C_{17}H_{22}N_2O_7$ 366.37
Isol. from human urine. Found in human RNase and several glycoproteins of the complement system. Also isol. from the marine ascidians *Leptoclinides dubius* and *Pharyngodictyon cauliflos.* Amorph. solid. $[\alpha]_D$ +50 (c, 0.0004 in MeOH).

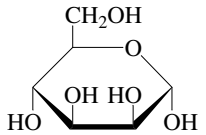
N$^{\alpha}$-Me: 2-α-D-Mannopyranosyl-N$^{\alpha}$-methyltryptophan
[296762-84-0]
$C_{18}H_{24}N_2O_7$ 380.397
Isol. from the marine ascidian *Ritterella rete.* Amorph. solid. $[\alpha]_D$ +95 (c, 0.007 in MeOH).

[252187-40-9, 358718-00-0]

Gutsche, B. *et al., Biochem. J.*, 1999, **343**, 11-19 (*isol, pmr, cmr*)
Manabe, S. *et al., J.A.C.S.*, 1999, **121**, 9754-9755 (*synth, pmr, cmr*)
Garcia, A. *et al., Org. Lett.*, 2000, **2**, 2765-2767 (*isol, pmr, cmr*)
Nishikawa, T. *et al., Synlett*, spec. issue, 2001, 945-947 (*synth, pmr, cmr*)

Mannuronic acid, 9CI, 8CI M-87

[6814-36-4]



α-D-Pyranose-*form*

$C_6H_{10}O_7$ 194.141

D-*form* [1986-14-7]
A hydrol. prod. of alginic acids from algae, e.g. *Macrocystis pyrifera*.
V. hygroscopic cryst.
Mp 165-167°. $[\alpha]_D$ -50 → -20 (H_2O, equilib.). Crystallises spontaneously as the 6,3-lactone. The variable opt. rotn. values of the acid and its readily-formed lactone are difficult to interpret.

6,3-Lactone: D-Mannuronolactone. Mannurone
[7424-09-1]
$C_6H_8O_6$ 176.126
Cryst. (dimorph.). Mp 143-144° Mp 191-192°. $[\alpha]_D^{21}$ +57.7 → +92.2 (30 min) (H_2O).

α-D-Pyranose-*form*

Me glycoside: Methyl α-D-mannopyranosiduronic acid
$C_7H_{12}O_7$ 208.168
Monohydrate. Mp 108°. $[\alpha]_D^{19}$ +65.6 (c, 1.2 in H_2O).

Me glycoside, Me ester: Methyl (methyl α-D-mannopyranosid)uronate
$C_8H_{14}O_7$ 222.194
Syrup. $[\alpha]_D^{25}$ +78.8 (c, 1.04 in H_2O).

Me glycoside, amide: Methyl α-D-mannopyranosiduronamide
$C_7H_{13}NO_6$ 207.183
Prisms (Me_2CO aq.). Mp 182-183°. $[\alpha]_D^{18}$ +66 (c, 1.1 in H_2O).

*Me glycoside, 2,3,4-tri-Ac: Methyl 2,3,4-tri-*O*-acetyl-α-D-mannopyranosiduronic acid*
$C_{13}H_{18}O_{10}$ 334.279
Syrup. $[\alpha]_D^{20}$ +41 (c, 1.1 in $CHCl_3$).

*Me glycoside, 2,3,4-tri-Me, Me ester: Methyl (methyl 2,3,4-tri-*O*-methyl-α-D-mannopyranosid)uronate*
$C_{11}H_{20}O_7$ 264.275
$Bp_{0.02}$ 118°. $[\alpha]_D^{20}$ +74 (c, 1 in MeOH). $[\alpha]_D$ +64.1 (c, 1 in $CHCl_3$).

Me glycoside, 6,3-lactone: Methyl α-D-mannopyranosidurono-6,3-lactone
$C_7H_{10}O_6$ 190.152
Cryst. (MeOH). Mp 186°. $[\alpha]_D^{20}$ +80 (c, 1.1 in H_2O).

β-D-Pyranose-*form*

*6→1Lactone, tri-Ac: 2,3,4-Tri-*O*-acetyl-β-D-mannopyranurono-6,1-lactone*
[141989-99-3]
$C_{12}H_{14}O_9$ 302.237
Syrup. $[\alpha]_D^{20}$ +7.9 (c, 0.8 in $CHCl_3$).

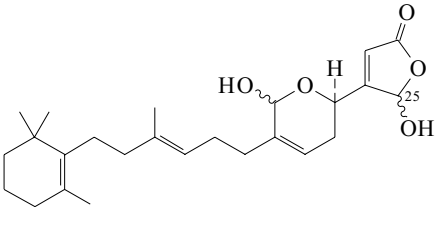
L-*form*
Mp 143-144°. $[\alpha]_D^{27}$ -92 (H_2O).
Semicarbazone: Mp 189°.

[35898-49-8]

Nelson, W.L. *et al., J.A.C.S.*, 1932, **54**, 3409 (*D-lactone, isol*)
Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate, 4th edn., J.A. Barth*, 1935, 322; 325 (*rev*)
Stacey, M. *et al., J.C.S.*, 1944, 587 (*D-lactone, α-D-Me pyr tri-Ac, α-D-Me pyr lactone*)
Isbell, H.S. *et al., J. Res. Natl. Bur. Stand. (U.S.)*, 1946, **37**, 43; 321 (*D-lactone, isol, struct*)
Edington, R.A. *et al., J.C.S.*, 1955, 2281 (*α-D-Me pyr amide*)
Whistler, R.L. *et al., Methods Carbohydr. Chem.*, 1963, **2**, 35 (*D-lactone, isol*)
Schmidt, H.W.H. *et al., Tet. Lett.*, 1967, 235 (*α-D-Me pyr Me ester*)
Morris, E.R. *et al., J.C.S. Perkin 2*, 1975, 1418 (*cd*)
Vogel, C. *et al., J. Carbohydr. Chem.*, 1992, **11**, 287-303 (*6,1-lactone tri-Ac*)
Shalaby, M.A. *et al., Carbohydr. Res.*, 1994, **265**, 197 (*cryst struct, lactone*)

Manoalide M-88

[75088-80-1]



$C_{25}H_{36}O_5$ 416.556
Constit. of *Luffariella variabilis*, *Smenospongia* sp. and *Hyrtios erecta*. Shows some antibacterial activity. Cytotoxic agent. Antiinflammatory and antipsoriatic agent. Potent analgesic.

Imhibitor of ornithine decarboxylase and phospholipase A2. Amorph. Sol. MeOH, Me_2CO, EtOAc. λ_{max} 227 (ϵ 5000) (MeOH) (Derep). λ_{max} 246 (ϵ 7700) (MeOH/NaOH) (Berdy).

25-Ac: ***Manoalide 25-acetate***
[75088-81-2]
$C_{27}H_{38}O_6$ 458.594
Constit. of *Thorectandra excavatus*. Flakes (CH_2Cl_2/hexane). Mp 117-119°. $[\alpha]_D^{17}$ +34 (c, 1 in $CHCl_3$). λ_{max} 239 (ϵ 1600) (MeOH).

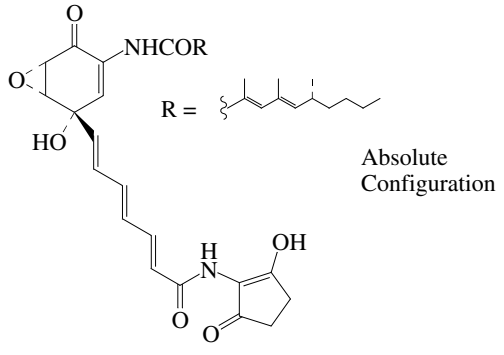
*24-Me ether (24*R*-): 24-*O*-Methylmanoalide*
[690267-88-0]
$C_{26}H_{38}O_5$ 430.583
Constit. of a *Luffariella* sp.

*24-Me ether (24*S*-):* [690267-89-1]
$C_{26}H_{38}O_5$ 430.583
Constit. of a *Luffariella* sp.
$[\alpha]_D^{23}$ +20.4 (c, 0.3 in CH_2Cl_2).

De Silva, E.D. *et al., Tet. Lett.*, 1980, 1611-1614; 1981, **22**, 3147-3150 (*isol, struct*)
Katsumura, S. *et al., Tet. Lett.*, 1985, **26**, 5827-5830 (*synth*)
Jacobs, R.S. *et al., Tetrahedron*, 1985, **41**, 981-984 (*rev*)
Cambie, R.C. *et al., J. Nat. Prod.*, 1988, **51**, 331-334 (*25-Ac, isol, pmr, cmr, uv*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 265-270 (*abs config, pmr, cmr*)
Bury, P. *et al., Tetrahedron*, 1994, **50**, 8793-8808 (*synth*)
Pommier, A. *et al., Chem. Comm.*, 1997, 1139-1140 (*synth*)
Gauvin, A. *et al., Riv. Ital. EPPOS*, (spec. no.), 1998, 622-626 (*activity*)
Soriente, A. *et al., Eur. J. Org. Chem.*, 2000, 947-953 (*abs config*)
Pommier, A. *et al., J.O.C.*, 2003, **68**, 4008-4013 (*synth*)
Namikoshi, M. *et al., Fish. Sci.*, 2004, **70**, 152-158; *CA*, **140**, 420871w (*24-Me ether*)

Manumycin A M-89

Antibiotic TMC 1F. TMC 1F. UCF1C. Antibiotic UCF1C
[52665-74-4]



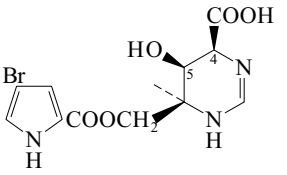
$C_{31}H_{38}N_2O_7$ 550.65

Abs. config. revised in 1999. Isol. from *Streptomyces parvulus* Tü 64 and a marine *Streptomyces* sp. Active against gram-positive bacteria. Inhibits protein-farnesyl transferase. Shows antiprotozoal activity. Cryst. (MeOH aq.). Sol. MeOH, MeCN, C_6H_6, bases; poorly sol. H_2O, hexane.
Mp 139-141° dec. $[\alpha]_D^{20}$ -185 (c, 0.4 in $CHCl_3$). Similar to Asukamycin. λ_{max} 270 (ϵ 31700); 328 (ϵ 32300) (MeOH/HCl) (Derep). λ_{max} 261 (ϵ 40200) (MeOH/NaOH) (Derep). λ_{max} 278 (ϵ 36400); 314 (ϵ 34600) (MeOH) (Derep).

Zeeck, A. *et al., J. Antibiot.*, 1987, **40**, 1530; 1541; 1549 (*isol, abs config, props, bibl*)
Thiericke, R. *et al., J.A.C.S.*, 1990, **112**, 3979 (*biosynth*)
Hara, M. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1993, **90**, 2281-2285 (*UCF1C*)
Kohno, J. *et al., J. Antibiot.*, 1996, **49**, 1212 (*TMC 1F*)
Alcaraz, L. *et al., J.O.C.*, 1998, **63**, 3526-3527 (*synth, config*)
Sattler, I. *et al., Nat. Prod. Rep.*, 1998, **15**, 221-240 (*rev*)
Alcaraz, L. *et al., Tetrahedron*, 1999, **55**, 3707-3716 (*synth, abs config*)
Pat. Coop. Treaty (WIPO), 2001, 01 05 384; *CA*, **134**, 110443q (*activity*)
Li, F. *et al., J. Nat. Prod.*, 2005, **68**, 349-353 (*isol, cmr*)

Manzacidin B M-90

[134029-42-8]



$C_{12}H_{14}BrN_3O_5$ 360.164
Alkaloid from the marine sponge *Hymeniacidon* sp. Oil. $[\alpha]_D^{22}$ -71 (c, 0.43 in MeOH). λ_{max} 209 (ϵ 5100); 272 (ϵ 5800) (MeOH) (Derep).

5-Deoxy: ***Manzacidin A***
[134029-41-7]
$C_{12}H_{14}BrN_3O_4$ 344.164
From the sponge *Hymeniacidon* sp. Oil. $[\alpha]_D^{27}$ -28 (c, 0.67 in MeOH). λ_{max} 209 (ϵ 5100); 272 (ϵ 5800) (MeOH) (Derep).

Debromo, 5-deoxy, N^1*-Me:* ***Manzacidin D***
[192197-62-9]
$C_{13}H_{17}N_3O_4$ 279.295
Alkaloid from the sponge *Astrosclera willeyana*. Viscous oil. $[\alpha]_D^{25}$ +14.5 (c, 0.3 in $CHCl_3$). λ_{max} 225 (ϵ 5980); 270 (ϵ 7980) (no solvent reported).

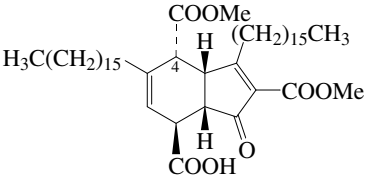
4-Epimer, 5-deoxy: ***Manzacidin C***
[134107-38-3]
$C_{12}H_{14}BrN_3O_4$ 344.164
From the sponge *Hymeniacidon* sp. Oil. $[\alpha]_D^{22}$ +37 (c, 0.23 in MeOH). λ_{max} 209 (ϵ 5100); 272 (ϵ 5800) (MeOH) (Derep).

4-Epimer, 5-deoxy, N^1*-Me:* ***N^1-Methylmanzacidin C***
$C_{13}H_{16}BrN_3O_4$ 358.191
Isol. from the sponge *Axinella brevistyla*. Antifungal and cytotoxic agent. $[\alpha]_D^{23}$ +36.4 (c, 0.17 in MeOH). λ_{max} 202 (log ϵ 3.7); 220 (log ϵ 3.7); 273 (log ϵ 3.7) (MeOH).

Kobayashi, J. *et al., J.O.C.*, 1991, **56**, 4574 (*isol, uv, ir, pmr, cmr, ms*)
Jahn, T. *et al., Tet. Lett.*, 1997, **38**, 3883 (*Manzacidin D*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 2001, **64**, 1576-1578 (*N^1-Methylmanzacidin C*)
Wehn, P.M. *et al., J.A.C.S.*, 2002, **124**, 12950-12951 (*Manzacidin A, C, synth*)
Drouin, C. *et al., Tet. Lett.*, 2004, **45**, 7197-7199 (*Manzacidin D, synth*)
Lanter, J.C. *et al., Org. Lett.*, 2005, **7**, 5905-5907 (*Mancacidin C, synth*)
Kano, T. *et al., J.A.C.S.*, 2006, **128**, 2174-2175 (*Manzacidin A, synth*)

Manzamenone A M-91

[143430-08-4]



$C_{46}H_{78}O_7$ 743.118
Stereochem. revised in 2000. Isol. from the sponge *Plakortis* sp. Protein kinase C inhibitor. Oil. $[\alpha]_D^{17}$ -3 (c, 1.3 in $CHCl_3$). λ_{max} 229 (ϵ 10000) (EtOH) (Derep).

Me ester: [143430-13-1]
Solid. Mp 63-64°.

Et ester: ***Manzamenone C***
[143430-09-5]
$C_{48}H_{82}O_7$ 771.172
Isol. from *Plakortis* sp. Oil. $[\alpha]_D^{17}$ -1 (c, 0.54 in $CHCl_3$). λ_{max} 224 (ϵ 10400) (EtOH) (Derep).

Butyl ester: ***Manzamenone F***
[143430-12-0]
$C_{50}H_{86}O_7$ 799.225
Isol. from *Plakortis* sp. Oil. $[\alpha]_D^{19}$ -3.3 (c, 1.0 in MeOH). λ_{max} 224 (ϵ 10400) (EtOH) (Derep).

Amide: ***Manzamenone D***
[143430-10-8]
$C_{46}H_{79}NO_6$ 742.133
Isol. from *Plakortis* sp. Oil. $[\alpha]_D^{17}$ -9.5 (c, 1.4 in $CHCl_3$). λ_{max} 229 (ϵ 10000) (EtOH) (Derep).

Valine amide(S-): ***Manzamenone E***
[143430-11-9]
$C_{51}H_{87}NO_8$ 842.25
Isol. from *Plakortis* sp. Oil. $[\alpha]_D^{19}$ +75 (c, 0.31 in $CHCl_3$). λ_{max} 227 (ϵ 9500) (EtOH) (Derep).

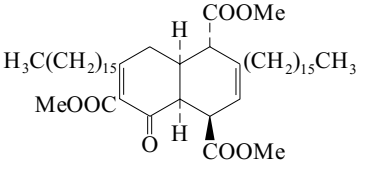
[2-(4-Hydroxyphenyl)ethyl]amide: ***Manzamenone H***
[151459-99-3]
$C_{54}H_{87}NO_7$ 862.284
Isol. from *Plakortis* sp. Oil. $[\alpha]_D^{27}$ -5.7 (c, 0.3 in MeOH). λ_{max} 226 (ϵ 9700) (EtOH) (Derep).

4-Epimer: ***Manzamenone B***
[143490-86-2]
$C_{46}H_{78}O_7$ 743.118
Isol. from *Plakortis* sp. Oil. $[\alpha]_D^{17}$ +7.7 (c, 0.26 in $CHCl_3$). λ_{max} 229 (ϵ 10000) (EtOH) (Derep).

Sachiko, T. *et al., J.O.C.*, 1992, **57**, 5255-5260 (*isol, ir, uv, pmr, cmr, ms, struct*)
Kobayashi, J. *et al., Tetrahedron*, 1993, **49**, 5955-5960 (*Manzamenone H*)
Takeuchi, S. *et al., Tetrahedron*, 1995, **51**, 5979-5986 (*abs config*)
Al-Busafi, S. *et al., Tet. Lett.*, 2000, **41**, 3467-3470 (*synth, abs config*)

Manzamenone G M-92

[151459-98-2]

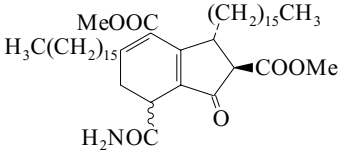


$C_{48}H_{82}O_7$ 771.172
Isol. from the sponge *Plakortis* sp. Oil. $[\alpha]_D^{19}$ -12 (c, 1.1 in $CHCl_3$). λ_{max} 225 (ϵ 10700) (EtOH) (Derep). λ_{max} 225 (ϵ 10700) (EtOH) (Berdy).

Kobayashi, J. *et al., Tetrahedron*, 1993, **49**, 5955 (*isol, uv, ir, pmr, cmr, ms*)

Manzamenone J M-93

[164473-24-9]



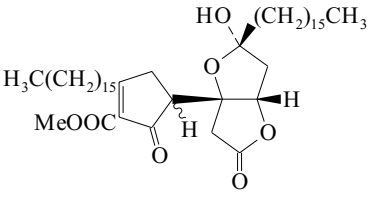
Relative configuration

$C_{46}H_{79}NO_6$ 742.133
Isol. from the sponge *Plakortis* sp. Oil. $[\alpha]_D^{17}$ -6.1 (c, 0.2 in MeOH). λ_{max} 220 (ϵ 39000); 317 (ϵ 23300) (MeOH).

Takeuchi, S. *et al., Tetrahedron*, 1995, **51**, 5979 (*isol, uv, ir, pmr, cmr, ms*)

Manzamenone K M-94

[164415-60-5]

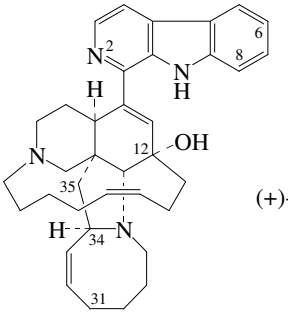


$C_{45}H_{78}O_7$ 731.107
Isol. from the sponge *Plakortis* spp. Oil. $[\alpha]_D^{17}$ -5.2 (c, 0.3 in MeOH). λ_{max} 225 (ϵ 1200) (MeOH).

Takeuchi, S. *et al., Tetrahedron*, 1995, **51**, 5979 (*isol, uv, ir, pmr, cmr, ms*)

Manzamine A M-95

Keramamine A



(+)-*form*

$C_{36}H_{44}N_4O$ 548.77

(+)-form [104196-68-1]
Alkaloid from the Okinawan marine sponges *Haliclona* sp., *Xestospongia* sp. and *Pellina* sp. Shows antitumour props. Exhibits weak cytotoxicity against KB cells, also insecticidal activity and activity against gram-positive and gram-negative bacteria. Exhibits strong antimalarial props. and activity against *Leishmania donovani*; also strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Cryst. (MeOH) (as hydrochloride).
Mp 240° dec. (hydrochloride). $[\alpha]_D^{20}$ +50 (c, 0.28 in $CHCl_3$) (hydrochloride). λ_{max} 238 (ϵ 15300); 278 (ϵ 9680); 290 (ϵ 8350); 346 (ϵ 4420); 358 (ϵ 4770) (hydrochloride). λ_{max} 219 (ϵ 22900); 236 (ϵ 18600); 280 (ϵ 10800); 290 (ϵ 11000); 346 (ϵ 5300); 357 (ϵ 5600) (MeOH).

*2-*N*-Oxide:* ***Manzamine A* N-*oxide***
[184361-76-0]
$C_{36}H_{44}N_4O_2$ 564.769
Alkaloid from the Phillipine marine sponge *Xestospongia ashmorica*. Cytotoxic agent. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Yellow cryst. powder.
$[\alpha]_D$ +18.6 (c, 0.35 in $CHCl_3$). λ_{max} 201 (ϵ 26000); 241 (ϵ 23000); 261 (ϵ 23000); 310 (ϵ 21000) (MeOH).

3,4-Dihydro: ***3,4-Dihydromanzamine A***
[162465-80-7]
$C_{36}H_{46}N_4O$ 550.786
Alkaloid from the Okinawan marine sponge *Amphimedon* sp. Cytotoxic against L-1210 and KB cells. Exhibits antibacterial activity. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Amorph. solid.
Mp 237-241°. $[\alpha]_D^{20}$ +86 (c, 0.25 in $CHCl_3$). λ_{max} 244 (ϵ 21000); 323 (ϵ 10000) (MeOH) (Berdy).

*3,4-Dihydro, 2-*N*-oxide:* ***3,4-Dihydromanzamine A* N-*oxide***
[184361-75-9]
$C_{36}H_{46}N_4O_2$ 566.785
Alkaloid from *Xestospongia ashmorica*. Cytotoxic agent. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$).

Yellow cryst. powder. $[\alpha]_D$ +34.1 (c, 0.59 in $CHCl_3$). λ_{max} 201 (ϵ 25000); 355 (ϵ 11000) (MeOH).

*1*R*,2,3,4-Tetrahydro:* ***Manzamine D***
[116477-23-7]
$C_{36}H_{48}N_4O$ 552.801
Alkaloid from the sponges *Haliclona, Ircinia* and *Amphimedon* spp. Cytotoxic agent. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{24}$ +44. λ_{max} 223 (ϵ 28800); 281 (ϵ 6700); 288 (ϵ 5400) (MeOH) (Berdy).

*1*S*,2,3,4-Tetrahydro:* ***1-Epimanzamine D***
[302327-68-0]
$C_{36}H_{48}N_4O$ 552.801
Alkaloid from a Palaun sponge. Cytotoxic agent. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Amorph. powder. $[\alpha]_D^{23}$ +77.3 (c, 0.16 in $CHCl_3$). λ_{max} 225 (log ϵ 4.23); 281 (log ϵ 3.79) (MeOH).

*1*S*,2,3,4-Tetrahydro,* N^2*-Me:* ***1-Epi-2-N-methylmanzamine D***
[302327-67-9]
$C_{37}H_{50}N_4O$ 566.828
Alkaloid from a Palaun sponge. Cytotoxic agent. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Cryst. (MeOH).
Mp 185-188°. $[\alpha]_D^{23}$ +91.4 (c, 0.27 in $CHCl_3$). λ_{max} 223 (log ϵ 4.24); 281 (log ϵ 3.74) (MeOH).

31,34-Epoxide, 32,33-dihydro: ***6-Deoxymanzamine X***
[184361-73-7]
$C_{36}H_{44}N_4O_2$ 564.769
Alkaloid from *Xestospongia ashmorica*. Cytotoxic agent. Active against *Leishmania donovani*. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Pale yellow amorph. powder. $[\alpha]_D$ +30.1 (c, 0.35 in $CHCl_3$). λ_{max} 210 (ϵ 26000); 260 (ϵ 11800); 312 (sh) (ϵ 10000); 378 (ϵ 3000) (MeOH).

6-Hydroxy: ***6-Hydroxymanzamine A***. *Manzamine Y*
[162465-79-4]
$C_{36}H_{44}N_4O_2$ 564.769
Alkaloid from the Okinawan marine sponge *Amphimedon* sp. and *Haliclona* sp. Cytotoxic against L-1210 and KB cells. Exhibits antibacterial activity. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Yellowish amorph. solid.
Mp 253°. $[\alpha]_D^{20}$ +139 (c, 1.1 in MeOH). $[\alpha]_D^{19}$ +33.2 (c, 2.50 in $CHCl_3$).

6-Hydroxy, 3,4-dihydro: ***3,4-Dihydro-6-hydroxymanzamine A***
[208392-25-0]
$C_{36}H_{46}N_4O_2$ 566.785
Alkaloid from *Amphimedon* sp. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Amorph. solid. $[\alpha]_D^{25}$ +28 (c, 1.2 in MeOH). λ_{max} 207 (ϵ 9000); 225 (ϵ 6500); 250 (ϵ 3500); 337 (ϵ 2500) (MeOH).

12-Deoxy, 12,28α-epoxy: ***12,28-Oxamanzamine A***
[721429-59-0]
$C_{36}H_{42}N_4O$ 546.754
Isol. from an *Acanthostrongylophora* sp. Amorph. solid.
Mp 148° dec. $[\alpha]_D^{25}$ +38 (c, 0.1 in $CHCl_3$). λ_{max} 253 (log ϵ 3.81); 274 (log ϵ 3.66); 352 (log ϵ 3.41) (MeOH).

12-Deoxy, 12,34-epoxy: ***12,34-Oxamanzamine A***
$C_{36}H_{42}N_4O$ 546.754
Alkaloid from an Indo-Pacific sponge. Shows activity against *Leishmania donovani*. Powder (MeOH).
Mp 164° dec. $[\alpha]_D^{25}$ +40 (c, 0.6 in $CHCl_3$). Not indexed in CA **138**. λ_{max} 252 (log ϵ 3.82); 271 (log ϵ 3.71); 358 (log ϵ 3.41) (MeOH).

31-Oxo, 32,33-dihydro: ***Manzamine E***
[117631-50-2]
$C_{36}H_{44}N_4O_2$ 564.769
Alkaloid from a *Xestospongia* sponge. Shows activity against *Mycobacterium tuberculosis* and *Leishmania donovani*. Cryst. (MeCN). Sol. MeOH, $CHCl_3$, EtOAc; poorly sol. H_2O, hexane.
Mp 174-176°. $[\alpha]_D$ +63.7 (c, 2.51 in $CHCl_3$). λ_{max} 238 (ϵ 15300); 278 (ϵ 9680); 290 (ϵ 8350); 346 (ϵ 4420); 358 (ϵ 4770) (as hydrochloride) (Derep). λ_{max} 219 (ϵ 22900); 236 (ϵ 18600); 280 (ϵ 10800); 290 (ϵ 11000); 346 (ϵ 5300); 357 (ϵ 5600) (MeOH) (Derep). λ_{max} 220 (ϵ 35800); 237 (ϵ 28100); 279 (ϵ 18000); 346 (ϵ 7700); 359 (ϵ 9300) (MeOH) (Berdy).

12-Deoxy, 31-oxo, 12,34-epoxy, 32,33-dihydro: ***12,34-Oxamanzamine E***
$C_{36}H_{42}N_4O_2$ 562.753
Alkaloid from the Indonesian sponge *Acanthostrongylophora* sp. Pale yellow powder (MeOH).
Mp 152° dec. $[\alpha]_D^{25}$ +44.3 (c, 0.6 in $CHCl_3$). λ_{max} 239 (log ϵ 3.38); 252 (log ϵ 3.82); 275 (log ϵ 3.65); 354 (log ϵ 3.41) (MeOH).

6-Hydroxy, 31β,34β-epoxide, 32,33-dihydro: ***Manzamine X***
[164301-23-9]
$C_{36}H_{44}N_4O_3$ 580.769
Alkaloid from sponge *Xestospongia* sp. Cytotoxic against L-1210 and KB cells. Exhibits antibacterial activity. Yellow prisms (hexane/Me_2CO).
Mp 250°. $[\alpha]_D^{19}$ +66.1 (c, 1.93 in $CHCl_3$). λ_{max} 215 (ϵ 29500); 300 (ϵ 17000); 378 (ϵ 4800) (MeOH) (Berdy).

6-Hydroxy, 31-oxo, 32,33-dihydro: ***6-Hydroxymanzamine E***
$C_{36}H_{44}N_4O_3$ 580.769
Alkaloid from the Indonesian sponge *Acanthostrongylophora* sp. Yellow powder ($CHCl_3$).
Fp *ca.* 198. $[\alpha]_D^{25}$ +34.4 (c, 0.2 in $CHCl_3$). λ_{max} 218 (log ϵ 3.64); 239 (log ϵ 3.63); 280 (log ϵ 3.25); 288 (log ϵ 3.09); 346 (log ϵ 3.42) (MeOH).

6-Hydroxy, 35-oxo, 32,33-dihydro: ***32,33-Dihydro-6-hydroxy-35-oxomanzamine A***
[581782-67-4]
$C_{36}H_{44}N_4O_3$ 580.769
Alkaloid from an Indonesian sponge. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Pale yellow powder.
Mp >200° dec. $[\alpha]_D^{25}$ +10 (c, 1 in MeOH). λ_{max} 219; 248; 268; 356; 395 (MeOH).

8-Hydroxy: ***Manzamine G***. *8-Hydroxymanzamine A*
[154466-37-2]
$C_{36}H_{44}N_4O_2$ 564.769
Alkaloid from an undescribed sponge *Pachypellina* sp. and by an *Amphimedon* sp. Exhibits antitumour, antimalarial and anti-HSV-II activities. Active against *Leishmania donovani*. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Pale yellow cryst.
Mp 230° dec. $[\alpha]_D$ +118.5 (c, 1.94 in $CHCl_3$). Obt. as a salt. Anion not specified. λ_{max} 222 (ϵ 32300); 245 (ϵ 30600); 268 (ϵ 14000); 360 (ϵ 8200) (EtOH) (Berdy).

*8-Hydroxy, 1*R*,2,3,4-tetrahydro:* ***1,2,3,4-Tetrahydro-8-hydroxymanzamine A***. *8-Hydroxymanzamine D*
[160070-84-8]
$C_{36}H_{48}N_4O_2$ 568.801
Alkaloid from the Papua New Guinea sponge *Petrosia contignata*. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$).

*8-Hydroxy, 1*R*,2,3,4-tetrahydro,* N^2*-Me:* ***1,2,3,4-Tetrahydro-2-N-methyl-8-hydroxymanzamine A***. *8-Hydroxy-2-*N*-methylmanzamine D*
[160070-83-7]
$C_{37}H_{50}N_4O_2$ 582.828
Alkaloid from the Papua New Guinea sponges *Petrosia contignata* and *Cribrochalina* sp. Cytotoxic to P388 leukemia cells. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Powder. $[\alpha]_D$ +46 (c, 0.006 in CH_2Cl_2). Props. refer to a salt (acid component not specified).

8-Hydroxy, 31-oxo, 32,33-dihydro: ***Manzamine F***. *Keramamine B*
[107900-75-4]
$C_{36}H_{44}N_4O_3$ 580.769
Isol. from a *Xestospongia* sponge and from a *Petrosia* sponge. Cytotoxic. Shows antimicrobial activity and strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Cryst. (MeCN).
Mp 200° dec. $[\alpha]_D$ +59.9 (c, 1.67 in $CHCl_3$). λ_{max} 245 (ϵ 25600); 268 (ϵ 12100); 353 (ϵ 6800); 360 (ϵ 6820) (as AcOH salt) (Derep). λ_{max} 220 (ϵ 36000); 244 (ϵ 31000); 265 (ϵ 13900); 355 (ϵ 8100) (MeOH) (Derep).

8-Hydroxy, 12-deoxy, 12,28α-epoxy: ***8-Hydroxy-12,28-oxamanzamine A***
[721429-60-3]
$C_{36}H_{42}N_4O_2$ 562.753
Isol. from an *Acanthostrongylophora* sp. Amorph. powder (EtOH).
Mp 160° dec. $[\alpha]_D^{25}$ +8 (c, 0.1 in $CHCl_3$). λ_{max} 251 (log ϵ 3.85); 273 (log ϵ 3.78); 356 (log ϵ 3.38) (MeOH).

31β-Hydroxy, 32,33-dihydro: ***32,33-Dihydro-31-hydroxymanzamine A***
[581782-65-2]
$C_{36}H_{46}N_4O_2$ 566.785
Alkaloid from an Indonesian sponge. Cryst. (MeOH). $[\alpha]_D^{25}$ +34.4 (c, 0.9 in $CHCl_3$). λ_{max} 215; 248; 281; 291; 352; 359 (MeOH).

6,31β-Dihydroxy, 32,33-dihydro: ***32,33-Dihydro-6,31-dihydroxymanzamine A***
[581782-71-0]
$C_{36}H_{46}N_4O_3$ 582.784
Alkaloid from an Indonesian sponge. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Pale yellow powder. $[\alpha]_D^{25}$ +25.9 (c, 0.5 in MeOH). λ_{max} 218; 240; 280; 291; 356; 359 (MeOH).

(-)-*form*

8-Hydroxy: **ent-*Manzamine G***
[403619-70-5]
$C_{36}H_{44}N_4O_2$ 564.769
Alkaloid from an undescribed sponge of the Petrosiidae. Exhibits activity against *Toxoplasma gondii* and strong antimalarial activity. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Yellowish powder (EtOH).
Mp 196-198° dec. $[\alpha]_D^{25}$ -112 (c, 0.12 in $CHCl_3$). λ_{max} 266 (log ϵ 2.95); 282 (log ϵ 2.94); 390 (log ϵ 2.85) (MeOH).

8-Hydroxy, 31-oxo, 32,33-dihydro: **ent-*Manzamine F***
[403619-71-6]
$C_{36}H_{44}N_4O_3$ 580.769
Alkaloid from an undescribed sponge of the Petrosiidae. Exhibits activity against *Toxoplasma gondii* and strong antimalarial activity. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Yellowish powder (EtOH).
Mp 194° dec. $[\alpha]_D$ -44.6 (c, 0.11 in $CHCl_3$). λ_{max} 266 (log ϵ 3.04); 300 (log ϵ 3.02); 380 (log ϵ 2.92) (MeOH).

12-Deoxy, 31-oxo, 12,34-epoxy, 32,33-dihydro: **ent-*12,34-Oxamanzamine E***
[479411-38-6]
$C_{36}H_{42}N_4O_2$ 562.753
Alkaloid from an Indo-Pacific sponge. Amorph. brown powder ($CHCl_3$).
Mp 152° dec. $[\alpha]_D^{25}$ -54.6 (c, 0.3 in $CHCl_3$). λ_{max} 252 (log ϵ 3.82); 275 (log ϵ 3.65); 354 (log ϵ 3.41) (MeOH).

8-Hydroxy, 12-deoxy, 31-oxo, 12,34-epoxy, 32,33-dihydro: **ent-*12,34-Oxamanzamine F***
[402935-15-3]
$C_{36}H_{42}N_4O_3$ 578.753
Alkaloid from an Indo-Pacific sponge. Shows strong activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Powder (MeOH).
Mp 164° dec. $[\alpha]_D^{25}$ +40 (c, 0.6 in $CHCl_3$). λ_{max} 252 (log ϵ 3.82); 271 (log ϵ 3.71); 358 (log ϵ 3.41) (MeOH).

Sakai, R. *et al., J.A.C.S.*, 1986, **108**, 6404-6405 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Nakamura, H. *et al., Tet. Lett.*, 1987, **28**, 621-624 (*isol, uv, pmr, cmr, cryst struct*)
Eur. Pat., 1988, 272 056; *CA*, **109**, 129416p (*Manzamine D*)
Ichiba, T. *et al., Tet. Lett.*, 1988, **29**, 3083-3086 (*Manzamines E, F*)
Baldwin, J.E. *et al., Tet. Lett.*, 1992, **33**, 2059-2062 (*biosynth*)
Ichiba, T. *et al., J. Nat. Prod.*, 1994, **57**, 168-170 (*8-Hydroxymanzamine A*)
Kobayashi, J. *et al., J. Nat. Prod.*, 1994, **57**, 1737-1740 (*3,4-Dihydromanzamine A, 6-Hydroxymanzamine A*)
Crews, P. *et al., Tetrahedron*, 1994, **50**, 13567-13574 (*1,2,3,4-Tetrahydro-8-hydroxymanzamine A, 1,2,3,4-Tetrahydro-2-N-methyl-8-hydroxymanzamine A*)
Kobayashi, M. *et al., Tetrahedron*, 1995, **51**, 3727-3736 (*Manzamine X, Manzamine Y, isol, uv, ir, pmr, cmr, cryst struct*)
Edrada, R.A. *et al., J. Nat. Prod.*, 1996, **59**, 1056-1060 (*Manzamine A N-oxide, 3,4-Dihydromanzamine A N-oxide, 6-Deoxymanzamine X*)
Tsuda, M. *et al., Tetrahedron*, 1996, **52**, 2319-2324 (*Manzamine D*)
Tsuda, M. *et al., Heterocycles*, 1997, **46**, 765-794 (*rev*)
Watanabe, D. *et al., J. Nat. Prod.*, 1998, **61**, 689-692 (*Dihydrohydroxymanzamine A*)
Winkler, J.D. *et al., J.A.C.S.*, 1998, **120**, 6425-6426 (*synth, Manzamine D*)
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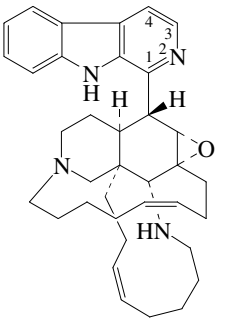
Magnier, E. *et al., Tetrahedron*, 1998, **54**, 6201-6258 (*rev, synth*)
Ang, K.K.H. *et al., Antimicrob. Agents Chemother.*, 2000, **44**, 1645-1649 (*activity*)
Zhou, B.-N. *et al., Tetrahedron*, 2000, **56**, 5781-5784 (*1-Epimanzamine D, N-Me-1-Epimanzamine D*)
El Sayed, K.A. *et al., J.A.C.S.*, 2001, **123**, 1804-1808 (*ent-Manzamine F, ent-Manzamine G, isol, activity*)
Humphrey, J.M. *et al., J.A.C.S.*, 2002, **124**, 8584-8592 (*synth*)
Yousaf, M. *et al., Tetrahedron*, 2002, **58**, 7397-7402 (*12,34-Oxamanzamines*)
Rao, K.V. Y*J. Nat. Prod.*, 2003, **66**, 823-828; 2004, **67**, 1314-1318 (*32,33-Dihydrohydroxymanzamines, 6-Hydroxymanzamine E, 12,34-Oxamanzamine E*)
Yousaf, M. *et al., J. Med. Chem.*, 2004, **47**, 3512-3517 (*12,28-Oxamanzamines*)

Manzamine B M-96

[112663-92-0]



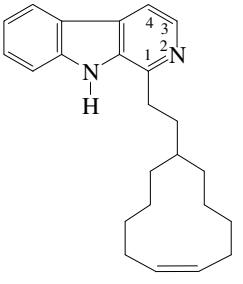
$C_{36}H_{46}N_4O$ 550.786
Alkaloid from the marine sponges *Haliclona*, *Amphimedon* and *Ircinia* spp. Shows activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Cryst. (EtOAc). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 198-203°. $[\alpha]_D^{20}$ +89 (c, 1.8 in $CHCl_3$). λ_{max} 212 (ϵ 18000); 235 (ϵ 22000); 240 (sh) (ϵ 20000); 250 (sh) (ϵ 15000); 282 (sh) (ϵ 6900); 288 (ϵ 11000); 338 (ϵ 3500); 351 (ϵ 3500) (MeOH) (Derep).

1β,2,3,4-Tetrahydro: ***1,2,3,4-Tetrahydromanzamine B***
$C_{36}H_{50}N_4O$ 554.817
Alkaloid from the sponge *Amphimedon* sp. Shows activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Amorph. solid. $[\alpha]_D^{25}$ -16 (c, 0.14 in MeOH). λ_{max} 225 (ϵ 9700); 273 (ϵ 2500); 280 (ϵ 2600); 289 (ϵ 2100) (MeOH).

Sakai, R. *et al., Tet. Lett.*, 1987, **28**, 5493-5496 (*isol, uv, ir, pmr, cmr, cryst struct*)
Baldwin, J.E. *et al., Tet. Lett.*, 1992, **33**, 2059-2062 (*biosynth*)
Tsuda, M. *et al., Heterocycles*, 1997, **46**, 765-794 (*rev*)
Tsuda, M. *et al., Heterocycles*, 1999, **50**, 485-488 (*Tetrahydromanzamine B*)
El Sayed, K.A. *et al., J.A.C.S.*, 2001, **123**, 1804-1808 (*activity*)

Manzamine C M-97

[112693-24-0]



$C_{23}H_{29}N_3$ 347.502

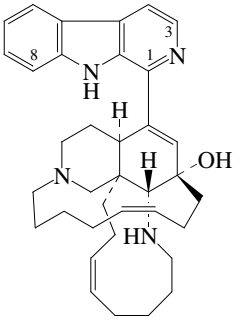
Alkaloid from the marine sponge *Haliclona* sp. and from *Amphimedon* sp. Shows activity against *Mycobacterium tuberculosis* ($H_{37}Rv$). Plates ($CHCl_3$/MeCN). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 77-82°. λ_{max} 212 (ϵ 13500); 234 (ϵ 22000); 239 (sh) (ϵ 21000); 248 (sh) (ϵ 14000); 282 (sh) (ϵ 6100); 287 (ϵ 9500); 335 (ϵ 3000); 350 (ϵ 3000) (MeOH) (Derep).

1ξ,2,3,4-Tetrahydro: ***Keramamine C***
[157207-88-0]
$C_{23}H_{33}N_3$ 351.534
Alkaloid from the Okinawan marine sponge *Amphimedon* sp. Plausible biogenetic precursor of Manzamine C, M-97. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ +20 (c, 0.92 in MeOH). λ_{max} 225 (sh) (ϵ); 271 (ϵ 5600); 285 (sh) (ϵ); 290 (sh) (ϵ) (MeOH) (Derep).

Sakai, R. *et al., Tet. Lett.*, 1987, **28**, 5493-5496 (*isol, uv, ir, pmr, cmr, cryst struct*)
Torisawa, Y. *et al., Tetrahedron*, 1991, **47**, 8067-8078 (*synth*)
Baldwin, J.E. *et al., Tet. Lett.*, 1992, **33**, 2059-2062 (*biosynth*)
Nowak, W. *et al., Annalen*, 1993, 153-159 (*synth*)
Seki, H. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1173-1176 (*pmr, cmr*)
Tsuda, M. *et al., Tet. Lett.*, 1994, **35**, 4387-4388 (*Keramamine C*)
Tsuda, M. *et al., Heterocycles*, 1997, **46**, 765-794 (*rev*)
Matzanke, N. *et al., Org. Prep. Proced. Int.*, 1998, **30**, 3-51 (*rev, synth*)
Magnier, E. *et al., Tetrahedron*, 1998, **54**, 6201-6258 (*rev, synth*)
MaGee, D.I. *et al., Can. J. Chem.*, 2000, **78**, 1060-1066 (*synth*)
El Sayed, K.A. *et al., J.A.C.S.*, 2001, **123**, 1804-1808 (*activity*)

Manzamine J M-98

[139975-58-9]



$C_{36}H_{46}N_4O$ 550.786
Alkaloid from the Okinawan marine sponge *Ircinia* sp. and the Philippine sponge *Xestospongia ashmorica*. Exhibits cytotoxicity against L1210 murine leukaemia cells and KB human epidermoid carcinoma cells. Shows antimycobacterial activity.
Mp 140°. $[\alpha]_D^{25}$ +47 (c, 2.0 in $CHCl_3$). λ_{max} 238 (ϵ 15300); 278 (ϵ 9680); 290 (ϵ 8350); 346 (ϵ 4420); 358 (ϵ 4770) (as HCl salt) (Derep). λ_{max} 219 (ϵ 22900); 236 (ϵ 18600); 280 (ϵ 10800); 290 (ϵ 11000); 346 (ϵ 5300); 357 (ϵ 5600) (MeOH) (Derep).

N^2*-Oxide:* ***Manzamine J* N*-oxide***
$C_{36}H_{46}N_4O_2$ 566.785
Alkaloid from *Xestospongia ashmorica*. Cytotoxic agent. Shows antimycobacterial activity. Insecticide. Yellow cryst. powder. $[\alpha]_D$ +15 (c, 0.40 in $CHCl_3$). λ_{max} 261 (ϵ 25000); 325 (ϵ 19000) (MeOH).

3,4-Dihydro: ***3,4-Dihydromanzamine J***
[208392-24-9]
$C_{36}H_{48}N_4O$ 552.801
Alkaloid from *Amphimedon* sp. Shows antimycobacterial activity. Amorph. solid. $[\alpha]_D^{30}$ +50 (c, 0.1 in MeOH). λ_{max} 209 (ϵ 13000); 242 (ϵ 9000); 322 (ϵ 4500) (MeOH).

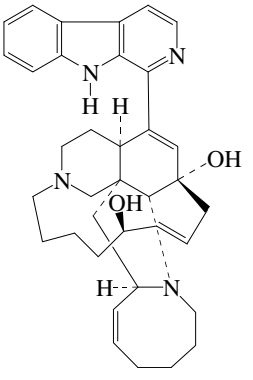
*1*R*,2,3,4-Tetrahydro:* ***Manzamine H***
[139975-57-8]
$C_{36}H_{50}N_4O$ 554.817
From *Ircinia* spp. and *Amphimedon* sp. Exhibits cytotoxicity against L1210 murine leukaemia cells and KB human epidermoid carcinoma cells. Shows antimycobacterial activity.
Mp 145°. $[\alpha]_D^{27}$ +17 (c, 1.1 in $CHCl_3$). λ_{max} 224 (ϵ 20000); 283 (ϵ 4600) (MeOH) (Derep). λ_{max} 225 (ϵ 29000); 277 (ϵ 6600); 282 (ϵ 6800); 290 (ϵ 5500) (MeOH) (Derep).

1S,2,3,4-Tetrahydro: ***Manzamine L***
[175274-50-7]
$C_{36}H_{50}N_4O$ 554.817
Alkaloid from the Okinawan marine sponge *Amphimedon* sp. Shows antimycobacterial activity. Amorph. solid.
Mp 143°. $[\alpha]_D^{24}$ -15 (c, 0.42 in $CHCl_3$). λ_{max} 223 (ϵ 34000); 283 (ϵ 6400) (MeOH) (Berdy).

8-Hydroxy: ***8-Hydroxymanzamine J***
$C_{36}H_{46}N_4O_2$ 566.785
Alkaloid from the Indonesian sponge *Acanthostrongylophora* sp. Pale yellow powder ($CHCl_3$). $[\alpha]_D^{25}$ +23.4 (c, 0.2 in $CHCl_3$). λ_{max} 251 (log ϵ 3.62); 274 (log ϵ 3.68); 358 (log ϵ 3.39) (MeOH).

Kondo, K. *et al., J.O.C.*, 1992, **57**, 2480 (*isol, uv, ir, pmr, cmr, ms, struct*)
Edrada, R.A. *et al., J. Nat. Prod.*, 1996, **59**, 1056 (*N-oxide*)
Tsuda, M. *et al., Tetrahedron*, 1996, **52**, 2319 (*Manzamine L*)
Watanabe, D. *et al., J. Nat. Prod.*, 1998, **61**, 689-692 (*3,4-Dihydromanzamine J*)
El Sayed, K.A. *et al., J.A.C.S.*, 2001, **123**, 1804-1808 (*activity*)
Rao, K.V. *et al., J. Nat. Prod.*, 2004, **67**, 1314-1318 (*8-Hydroxymanzamine J*)

Manzamine M M-99

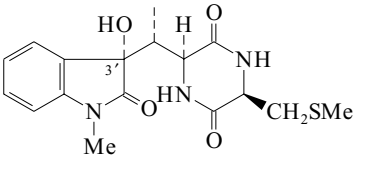


$C_{36}H_{44}N_4O_2$ 564.769
Alkaloid from the sponge *Amphimedon* sp. Amorph. solid.
$[\alpha]_D^{25}$ +16 (c, 0.48 in MeOH). λ_{max} 205 (ϵ 14000); 233 (ϵ 3000); 276 (ϵ 1500); 359 (ϵ 1000) (MeOH).

Watanabe, D. *et al., J. Nat. Prod.*, 1998, **61**, 689-692 (*isol, uv, ir, pmr, cmr*)

Maremycin A M-100

[165467-67-4]



$C_{17}H_{21}N_3O_4S$ 363.437
Probable abs. config. depicted. Isol. from the marine *Streptomyces* sp. B9173. Sol. MeOH, DMSO; fairly sol. $CHCl_3$, EtOAc, Me_2CO, CH_2Cl_2; poorly sol. H_2O.
Mp 229°. $[\alpha]_D^{20}$ -120.95 (c, 0.21 in MeOH). λ_{max} 209 (ϵ 33890); 257 (ϵ 3715) (MeOH) (Berdy). λ_{max} 208 (ϵ 35450); 257 (ϵ 3715) (MeOH/HCl) (Berdy). λ_{max} 212 (ϵ 27540); 248 (ϵ 3236) (MeOH/NaOH) (Berdy).

3′-Epimer: ***Maremycin B***
[165877-95-2]
$C_{17}H_{21}N_3O_4S$ 363.437
From *Streptomyces* sp. B9173. Shows sl. cytotoxicity. Sol. MeOH, DMSO; fairly sol. $CHCl_3$, CH_2Cl_2, EtOAc, Me_2CO; poorly sol. H_2O.
Mp 216°. $[\alpha]_D^{20}$ +2.94 (c, 0.21 in MeOH). λ_{max} 209 (ϵ 29510); 258 (ϵ 4265) (MeOH) (Berdy). λ_{max} 208 (ϵ 31620); 258 (ϵ 4265) (MeOH-HCl) (Berdy). λ_{max} 212 (ϵ 25700); 252 (ϵ 7943) (MeOH-NaOH) (Berdy).

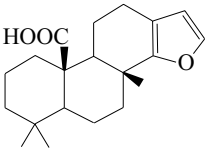
3′-Epimer, S-*oxide(*R-*):* ***Maremycin C_2***
[333997-43-6]
$C_{17}H_{21}N_3O_5S$ 379.436
Prod. by *Streptomyces* sp. strain GT 051237. Powder. $[\alpha]_D^{20}$ +20 (c, 0.58 in DMSO). Data given is for mixt. with Maremycin C_1. λ_{max} 215 (log ϵ 4.03); 258 (log ϵ 3.59); 293 (sh) (log ϵ 2.97) (EtOH).

3′-Epimer, S-*oxide(*S-*):* ***Maremycin C_1***
[333997-39-0]
$C_{17}H_{21}N_3O_5S$ 379.436
Prod. by *Streptomyces* sp. strain GT 051237. Obt. as a mixt. with Maremycin C_2.

Balk-Bindseil, W. *et al., Annalen*, 1995, 1291-1294 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)
Takayama, H. *et al., Tetrahedron*, 1999, **55**, 6841-6846 (*config*)
Tang, Y.-Q. *et al., Eur. J. Org. Chem.*, 2001, 261-267 (*Maremycin B, Maremycin C, activity*)

Marginatafuran M-101

[97640-44-3]

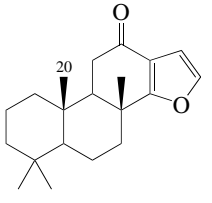


$C_{20}H_{28}O_3$ 316.439
Constit. of the dorid nudibranch *Cadlina luteomarginata*. Needles (hexane).
Mp 208°. $[\alpha]_D$ -102 (c, 0.22 in $CHCl_3$).

Gustafson, K. *et al., Tet. Lett.*, 1985, **26**, 2521 (*cryst struct*)
Dumdei, E.J. *et al., Can. J. Chem.*, 1997, **75**, 773-789 (*pmr, cmr*)

Marginatone M-102

[130221-24-8]



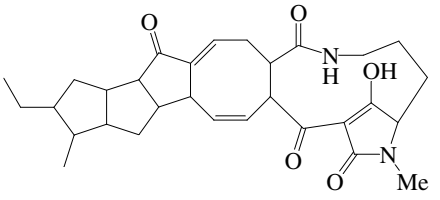
$C_{20}H_{28}O_2$ 300.44
Constit. of *Aplysilla glacialis*. Solid. $[\alpha]_D$ -16 (c, 0.4 in $CHCl_3$). CAS spelling is Marginotone.

20-Acetoxy: ***20-Acetoxymarginatone***
[194020-41-2]
$C_{22}H_{30}O_4$ 358.477
Constit. of *Cadlina luteomarginata*. Oil.

Tischler, M. *et al., J.O.C.*, 1991, **56**, 42-47 (*Marginatone, isol, pmr, cmr*)
Dumdei, E.J. *et al., Can. J. Chem.*, 1997, **75**, 773-789 (*20-Acetoxymarginatone*)
Kolympadi, M. *et al., Tetrahedron*, 2005, **61**, 2003-2010 (*synth*)

Marine *Streptomyces* $C_{30}H_{38}N_2O_5$ lactam M-103

[184348-39-8]



$C_{30}H_{38}N_2O_5$ 506.641
Related to Aburatubolactam A, A-30. Prod. by *Streptomyces* sp. SCRC A20. Cytotoxic agent.

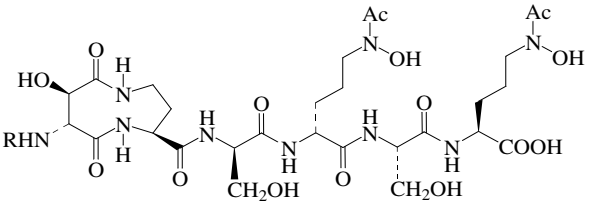
Japan. Pat., 1996, 96 245 625; *CA*, **126**, 17872d

Marine cell aggregation factor M-104

MAF
Large proteoglycan. Isol. from sponges, e.g. *Microciona prolifera*. Adhesion factor responsible for reaggregation of dissociated sponge cells.

Jumblatt, J.E. *et al., J. Biol. Chem.*, 1980, **19**, 1038
Deng, S. *et al., J. Carbohydr. Chem.*, 1998, **17**, 439-452 (*bibl*)

Marinobactins M-105



Marinobactin A R = $-CO(CH_2)_{10}CH_3$
" B R = $-CO(CH_2)_5CH\overset{z}{=}CH(CH_2)_5CH_3$
" C R = $-CO(CH_2)_{12}CH_3$
" D_1 R = $-CO(CH_2)_7CH\overset{z}{=}CH(CH_2)_5CH_3$
" D_2 R = $-CO(CH_2)_5CH\overset{z}{=}CH(CH_2)_7CH_3$
" E R = $-CO(CH_2)_{14}CH_3$

Isol. from *Marinobacter* sp. strains DS40M6 and DS40M8. Siderophores.

Marinobactin A [265319-69-5]
$C_{40}H_{69}N_9O_{16}$ 932.036

Marinobactin B [265319-73-1]
$C_{42}H_{71}N_9O_{16}$ 958.074

Marinobactin C [265319-74-2]
$C_{42}H_{73}N_9O_{16}$ 960.089

Marinobactin D_1 [265319-75-3]
$C_{44}H_{75}N_9O_{16}$ 986.127

Marinobactin D_2 [265319-76-4]
$C_{44}H_{75}N_9O_{16}$ 986.127

Marinobactin E [265319-77-5]
$C_{44}H_{77}N_9O_{16}$ 988.143

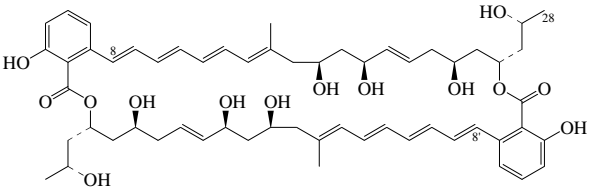
Martinez, J.S. *et al., Science (Washington, D.C.)*, 2000, **287**, 1245-1247 (*isol, struct*)

Marinocine M-106

Protein. Prod. by the bacterium *Marinomonas mediterranea*. Broad-spectrum antibacterial agent.

Lucas-Elio, P. *et al., Biochim. Biophys. Acta*, 2005, **1721**, 193-203 (*isol*)
Lucas-Elio, P. *et al., J. Bacteriol.*, 2006, **188**, 2493-2501 (*activity*)

Marinomycin A M-107



Absolute Configuration

$C_{58}H_{76}O_{14}$ 997.23

Macrodiolide antibiotic. Prod. by *Marinispora* sp. strain CNQ-140. Antibacterial agent. Cytotoxic. Yellow powder. $[\alpha]_D$ +180 (c, 0.11 in EtOH). λ_{max} 325 (sh) (ϵ 29000); 345 (sh) (ϵ 41600); 359 (ϵ 52300); 378 (ϵ 44000) (EtOH).

8Z-Isomer: ***Marinomycin C***
Prod. by *Marinispora* sp. strain CNQ-140.
Yellow powder. $[\alpha]_D$ -161 (c, 0.13 in EtOH). λ_{max} 319 (sh) (ϵ 40800); 345 (sh) (ϵ 48300); 358 (ϵ 53800); 375 (ϵ 41400) (EtOH).

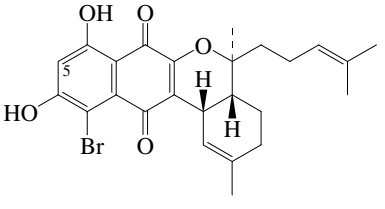
(8Z,8′Z)-Isomer: ***Marinomycin B***
$C_{58}H_{76}O_{14}$ 997.23
Prod. by *Marinispora* sp. strain CNQ-140. Yellow powder. $[\alpha]_D$ -245 (c, 0.15 in EtOH). λ_{max} 315 (ϵ 55300); 340 (ϵ 50300) (EtOH).

28-Methyl, (8Z,8′Z)-isomer: ***Marinomycin D***
$C_{59}H_{78}O_{14}$ 1011.257
Prod. by *Marinispora* sp. strain CNQ-140. Yellow powder. $[\alpha]_D$ -233 (c, 0.03 in EtOH). λ_{max} 315 (ϵ 58200); 340 (ϵ 50600) (EtOH).

Kwon, H.C. *et al., J.A.C.S.*, 2006, **128**, 1622-1632 (*isol, cd, uv, pmr, cmr, ms*)

Marinone M-108

[146488-63-3]



$C_{25}H_{27}BrO_5$ 487.389
Constit. of marine actinomycetes CNB-632 and CNH-099. Moderate cytotoxic agent. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{25}$ -170 (c, 0.15 in MeOH). λ_{max} 235 (ϵ 17400); 300 (ϵ 10500); 406 (ϵ 2290); 508 (ϵ 4100) (MeOH) (Derep). λ_{max} 202 (ϵ 18100); 268 (ϵ 6900); 307 (ϵ 5200); 395 (ϵ 1500); 435 (ϵ 1400) (MeOH + HCl). λ_{max} 298 (ϵ 9900); 335 (ϵ 5400); 385 (ϵ 2300); 510 (ϵ 3700) (MeOH + KOH).

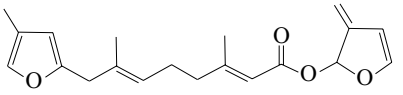
Debromo: ***Debromomarinone***
[146488-64-4]
$C_{25}H_{28}O_5$ 408.493
Constit. of a marine actinomycete (CNB-632). Sol. MeOH, EtOAc; poorly sol. H_2O. λ_{max} 226 (ϵ 16600); 269 (ϵ 10400); 299 (ϵ 9200); 388 (ϵ 2600); 488 (ϵ 2280) (MeOH) (Derep).

Debromo, 5-bromo: ***Isomarinone***
[272458-32-9]
$C_{25}H_{27}BrO_5$ 487.389
Constit. of a marine actinomycete (CNH-099). Moderate cytotoxic agent. $[\alpha]_D^{25}$ -120 (c, 0.2 in MeOH). λ_{max} 206 (ϵ 2600); 265 (ϵ 8000); 270 (ϵ 8100); 312 (ϵ 4700); 390 (ϵ 1500) (MeOH + HCl). λ_{max} 230 (ϵ 12200); 295 (ϵ 9500); 327 (ϵ 4100); 385 (ϵ 2000); 513 (ϵ 2000) (MeOH + KOH).

Pathirana, C. *et al., Tet. Lett.*, 1992, **33**, 7663 (*isol, pmr, cmr*)
Hardt, I.H. *et al., Tet. Lett.*, 2000, **41**, 2073-2076 (*isol, pmr, cmr*)

Marislin M-109

[78284-85-2]

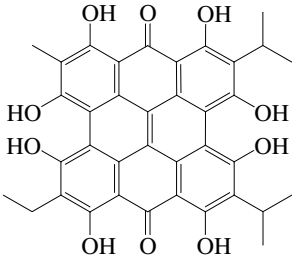


$C_{20}H_{24}O_4$ 328.407
Metab. of the shell-less mollusc *Chromodoris marislae*. Oil.

Hochlowski, J.E. *et al., Tet. Lett.*, 1981, **22**, 271-274 (*isol, ir, nmr*)

Maristentorin M-110

2-Ethyl-1,3,4,6,8,10,11,13-octahydroxy-5-methyl-9,12-bis(1-methylethyl)phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 9CI
[885123-41-1]

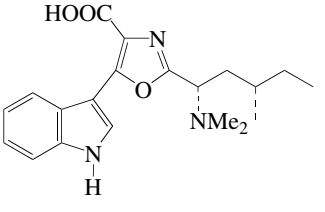


$C_{37}H_{30}O_{10}$ 634.638
Similar to Hypericin and Stentorin, S-373. Isol. from the marine ciliate *Maristentor dinoferus*.

Mukherjee, P. *et al., J. Phys. Chem. B*, 2006, **110**, 6359-6364 (*isol, uv, pmr, cmr, ms*)

Martefragine A M-111

[200809-93-4]
[188546-50-1]



Absolute configuration

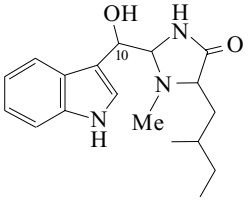
$C_{20}H_{25}N_3O_3$ 355.436
Alkaloid from the marine alga *Martensia fragilis*. Inhibitor of lipid peroxidation in rat microsome. Powder.
Mp 147-148°. $[\alpha]_D^{26}$ -20.3 (c, 0.76 in MeOH). λ_{max} 224 (ϵ 20200); 248 (sh) (ϵ 8600); 295 (sh) (ϵ 8800); 323 (ϵ 14200) (MeOH).

Takahashi, S. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1527-1529 (*isol, uv, ir, pmr, cmr, cryst struct*)
Nishida, A. *et al., Tet. Lett.*, 1998, **39**, 5983-5986 (*synth, cd, pmr, cmr, abs config*)

Martensine A M-112

*2-(Hydroxy-1*H*-indol-3-ylmethyl)-1-methyl-5-(2-methylbutyl)-4-imidazolidinone, 9CI*

[87168-35-2]



$C_{18}H_{25}N_3O_2$ 315.414

Alkaloid from the marine red alga *Martensia fragilis*. Shows antibiotic activity. $[\alpha]_D$ +42 (c, 0.34 in MeOH). λ_{max} 223 (ϵ 20900); 257 (sh) (ϵ 5200); 268 (sh) (ϵ 5500); 280 (ϵ 5800); 288 (ϵ 5200) (EtOH) (Derep). λ_{max} 260; 280; 288 (MeOH) (Berdy).

10-Epimer: ***10-Epimartensine A***

[87246-79-5]

$C_{18}H_{25}N_3O_2$ 315.414

Minor alkaloid from *Martensia fragilis*. λ_{max} 223 (ϵ 20900); 257 (sh) (ϵ 5200); 268 (sh) (ϵ 5500); 280 (ϵ 5800); 288 (ϵ 5200) (EtOH) (Derep).

10-Ketone: ***Martensine B***

[87168-37-4]

$C_{18}H_{23}N_3O_2$ 313.399

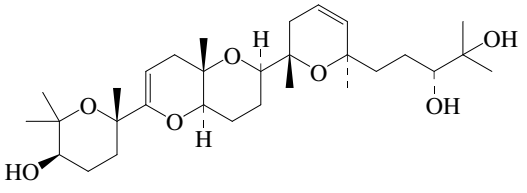
Alkaloid from *Martensia fragilis*.

Mp 184-186°. $[\alpha]_D$ -18 (c, 1.1 in Me_2CO). λ_{max} 267 (ϵ 10000); 335 (ϵ 10000) (EtOH/NaOH) (Derep). λ_{max} 215 (ϵ 10000); 244 (ϵ 11000); 261 (ϵ 8400); 303 (ϵ 10000) (EtOH) (Derep).

Kirkup, M.P. *et al., Tet. Lett.*, 1983, **24**, 2087 (*isol, uv, ir, pmr, cmr, ms, struct*)

Martiriol M-113

[346583-57-1]

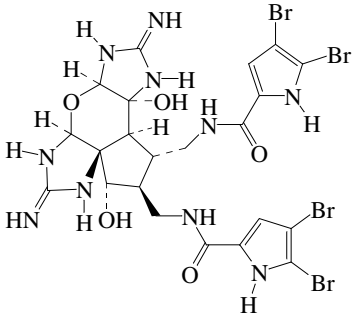


$C_{30}H_{50}O_7$ 522.721

Constit. of *Laurencia viridis*. Amorph. solid. $[\alpha]_D^{25}$ +4 (c, 0.03 in $CHCl_3$).

Manríquez, C.P. *et al., Tetrahedron*, 2001, **57**, 3117-3123 (*isol, pmr, cmr*)

Massadine M-114



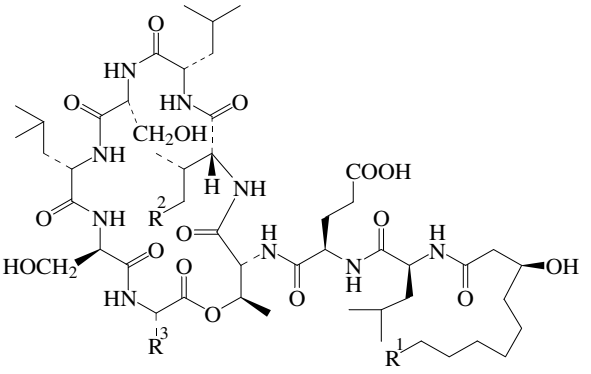
$C_{22}H_{24}Br_4N_{10}O_5$ 828.112

Alkaloid from the sponge *Stylissa* aff. *massa*. Yellow powder.

$[\alpha]_D^{17}$ -12 (c, 0.1 in MeOH). λ_{max} 278 (ϵ 20000) (MeOH).

Nishimura, S. *et al., Org. Lett.*, 2003, **5**, 2255-2257 (*isol, cd, pmr, cmr, ms*)

Massetolides M-115



Lipodepsipeptide antibiotics. Closely related to Viscosin. Prod. by *Pseudomonas* spp. from marine pseudomonads. Active against *Mycobacterium tuberculosis*.

Massetolide A [186409-57-4]

$C_{55}H_{97}N_9O_{16}$ 1140.422

Solid. Mp 237-238° dec. $[\alpha]_D$ +45.9 (EtOH). Has $R^1 = R^2 = CH_3$, $R^3 = CH(CH_3)CH_2CH_3$.

Diastereoisomer: ***Pseudophomin A***

$C_{55}H_{97}N_9O_{16}$ 1140.422

Prod. by *Pseudomonas fluorescens* strain BRG100. Cryst. + $1H_2O$ (CH_2Cl_2/MeOH). $[\alpha]_D^{26}$ -23 (c, 0.25 in EtOH).

Massetolide B [186409-58-5]

$C_{56}H_{99}N_9O_{16}$ 1154.449

Solid. Has $R^1 = CH_2CH_3$, $R^2 = CH_3$, $R^3 = CH(CH_3)CH_2CH_3$.

Massetolide C [186409-60-9]

$C_{57}H_{101}N_9O_{16}$ 1168.476

Solid. Has $R^1 = CH_2CH_2CH_3$, $R^2 = CH_3$, $R^3 = CH(CH_3)CH_2CH_3$.

Diastereoisomer: ***Pseudophomin B***

$C_{57}H_{101}N_9O_{16}$ 1168.476

Prod. by *Pseudomonas fluorescens* strain BRG100. Antifungal agent. Cryst. + $1H_2O$ (MeCN aq.). $[\alpha]_D^{16}$ -15 (c, 0.4 in EtOH).

Massetolide D [186409-62-1]

$C_{55}H_{97}N_9O_{16}$ 1140.422

Solid. Has $R^1 = R^2 = CH_3$, $R^3 = CH_2CH(CH_3)_2$.

Massetolide E [186409-63-2]

$C_{53}H_{93}N_9O_{16}$ 1112.368

Solid. Has $R^1 = CH_3$, $R^2 = H$, $R^3 = CH(CH_3)_2$.

Massetolide F [186409-64-3]

$C_{54}H_{95}N_9O_{16}$ 1126.395

Solid. Has $R^1 = CH_3$, $R^2 = H$, $R^3 = CH_2CH(CH_3)_2$.

Massetolide G [186409-65-4]

$C_{55}H_{97}N_9O_{16}$ 1140.422

Solid. Has $R^1 = CH_2CH_3$, $R^2 = H$, $R^3 = CH(CH_3)CH_2CH_3$.

Massetolide H [186409-66-5]

$C_{56}H_{99}N_9O_{16}$ 1154.449

Solid. Has $R^1 = CH_2CH_2CH_3$, $R^2 = H$, $R^3 = CH(CH_3)CH_2CH_3$.

Massetolide I [186409-67-6]

$C_{53}H_{93}N_9O_6$ 952.374

Unnatural analogue prod. by directed biosynth.

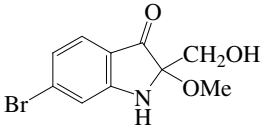
Massetolide J [186409-68-7]

$C_{53}H_{93}N_9O_{16}$ 1112.368

Unnatural analogue prod. by directed biosynth.

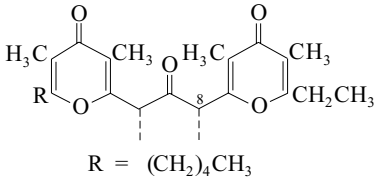
Massetolide K [186409-69-8]
$C_{54}H_{93}N_9O_{16}$ 1124.379
Unnatural analogue prod. by directed biosynth.
Gerard, J. *et al., J. Nat. Prod.*, 1997, **60**, 223-229 (*isol, pmr, cmr, ms*)
El Sayed, K.A. *et al., Tetrahedron*, 2000, **56**, 949 (*activity*)
Quail, J.W. *et al., Acta Cryst. C*, 2002, **58**, o268-o271 (*Pseudophomins*)
Pedras, M.S.C. *et al., Phytochemistry*, 2003, **62**, 1105-1114 (*Pseudophomins*)

Matemone **M-116**
*6-Bromo-1,2-dihydro-2-hydroxymethyl-2-methoxy-3*H*-indol-3-one*
[288849-91-2]



$C_{10}H_{10}BrNO_3$ 272.098
Isol. from the sponge *Iotrochota purpurea*. Mild cytotoxic agent. Yellow-green film. $[\alpha]_D^{25}$ +8.9 (c, 0.45 in MeOH). λ_{max} 228 (log ϵ 4.34); 245 (log ϵ 4.33); 273 (log ϵ 4.01); 399 (log ϵ 3.5) (MeOH).
Carletti, I. *et al., J. Nat. Prod.*, 2000, **63**, 981-983 (*isol, pmr, cmr, uv*)

Maurapyrone A **M-117**
[100082-10-8]



R = $(CH_2)_4CH_3$

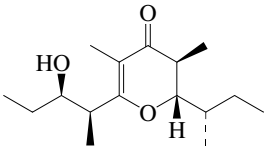
$C_{26}H_{36}O_5$ 428.567
Isol. from *Siphonaria maura*. Shows activity against *Vibrio anguillarum*. Cryst. Sol. MeOH, Me_2CO, EtOAc; poorly sol. H_2O. Mp 110-112°. λ_{max} 258 (ϵ 17000) (MeOH) (Derep).

8-Epimer: ***Maurapyrone B***
[100046-03-5]
From *Siphonaria maura*.
Wax. Sol. MeOH, Me_2CO, EtOAc; poorly sol. H_2O. λ_{max} 258 (ϵ 17000) (MeOH) (Derep). λ_{max} 257 (ϵ 19700) (MeOH) (Berdy).
Manker, D.C. *et al., J.O.C.*, 1986, **51**, 814 (*isol, cryst struct*)

Maurapyrone C **M-118**
[100046-04-6]
As Maurapyrone A, M-117 with
R = $-CH_2CH(CH_3)_2$
$C_{25}H_{34}O_5$ 414.541
Isol. from *Siphonaria maura*. Shows activity against *Vibrio anguillarum*. Wax. Sol. MeOH, Me_2CO, EtOAc; poorly sol. H_2O. λ_{max} 253 (ϵ 21600) (MeOH) (Derep).

8-Epimer: ***Maurapyrone D***
From *Siphonaria maura*. Active against *Vibrio anguillarum*. Oil. Sol. MeOH, EtOAc, Me_2CO; poorly sol. H_2O. λ_{max} 253 (ϵ 21600) (MeOH) (Derep). λ_{max} 253 (ϵ 17900) (MeOH) (Berdy).
Manker, D.C. *et al., J.O.C.*, 1986, **51**, 814-816 (*isol, cryst struct*)

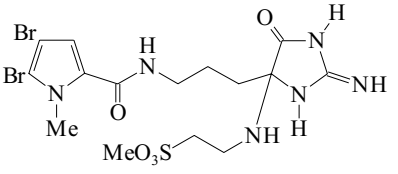
Maurenone **M-119**
*2,3-Dihydro-6-(2-hydroxy-1-methylbutyl)-3,5-dimethyl-2-(1-methylpropyl)-4*H*-pyran-4-one, 9CI*
[100046-02-4]



Absolute Configuration

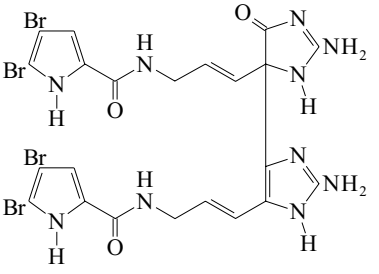
$C_{16}H_{28}O_3$ 268.395
Metab. of the mollusc *Siphonaria maura*. Oil. Related to Stegobiol. λ_{max} 276 (ϵ 13400) (MeOH) (Derep).
Manker, D.C. *et al., J.O.C.*, 1986, **51**, 814-816 (*isol, pmr*)
Crossman, J.S. *et al., J.O.C.*, 2006, **71**, 117-124 (*synth, pmr, cmr, abs config*)

Mauritamide A **M-120**
[155210-56-3]



$C_{15}H_{22}Br_2N_6O_5S$ 558.25
Alkaloid from the Fijian sponge *Agelas mauritiana*. Protein-tyrosine kinase inhibitor. Amorph. solid. $[\alpha]_D^{20}$ +1.3 (c, 0.003 in MeOH). λ_{max} 254 (ϵ 6200); 258 (ϵ 6110); 278 (ϵ 3910) (MeOH) (Derep).
Jiménez, C. *et al., Tet. Lett.*, 1994, **35**, 1375 (*isol, uv, ir, pmr, cmr, ms, struct*)

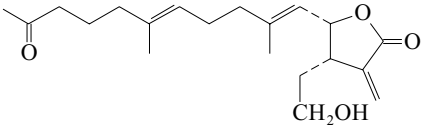
Mauritiamine **M-121**



$C_{22}H_{20}Br_4N_{10}O_3$ 792.081

(±)-*form* [175669-27-9]
Alkaloid from the marine sponge *Agelas mauritiana*. Antifouling substance. Exhibits moderate antibacterial activity. Solid. λ_{max} 272; 278 (ϵ 18400) (MeOH) (Berdy).
Tsukamoto, S. *et al., J. Nat. Prod.*, 1996, **59**, 501 (*isol, uv, ir, pmr, cmr, struct*)
Olofson, A. *et al., J.O.C.*, 1997, **62**, 7918-7919 (*synth*)

Mayolide A **M-122**
[114728-06-2]



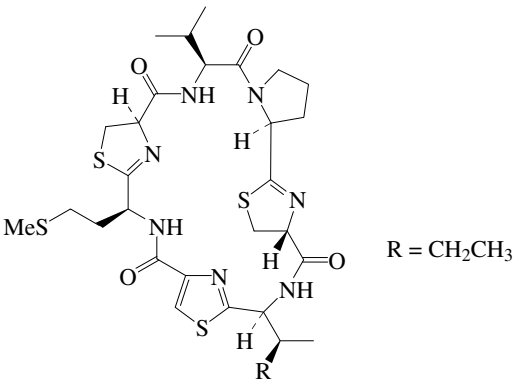
$C_{20}H_{30}O_4$ 334.455

Constit. of *Sinularia mayi*. Oil. $[\alpha]_D$ -56.4 ($CHCl_3$).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 488 (*isol, pmr, cmr*)
Nagaoka, H. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1742 (*synth, abs config*)

Mayotamide A M-123

[217449-23-5]

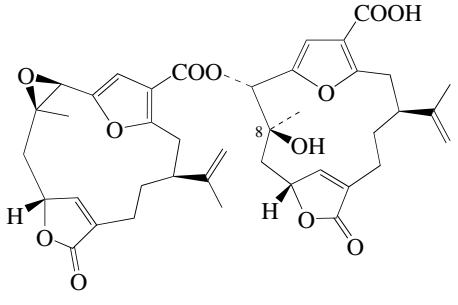


$C_{30}H_{43}N_7O_4S_4$ 693.978
Isol. from *Didemnum molle*. Cytotoxic agent. Amorph. powder. $[\alpha]_D$ +77 (c, 0.3 in MeOH).

Lower homologue: ***Mayotamide B***
[217449-24-6]
$C_{29}H_{41}N_7O_4S_4$ 679.951
Isol. from *Didemnum molle*. Cytotoxic agent. Amorph. powder. $[\alpha]_D$ +130 (c, 0.1 in MeOH). Has R = CH_3.
Rudi, A. *et al., Tetrahedron*, 1998, **54**, 13203-13210 (*isol, pmr, cmr, ms*)

Mayotolide A M-124

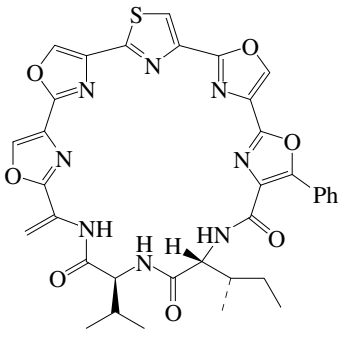
[208391-98-4]



$C_{40}H_{44}O_{12}$ 716.78
Constit. of *Sinularia erecta*. Oil. $[\alpha]_D$ +43 (c, 0.33 in MeOH).

8-Epimer: ***Mayotolide B***
[208391-99-5]
Constit. of *Sinularia erecta*.
Oil. $[\alpha]_D$ +48.5 (c, 0.23 in MeOH).
Rudi, A. *et al., J. Nat. Prod.*, 1998, **61**, 872-875 (*isol, pmr, cmr*)

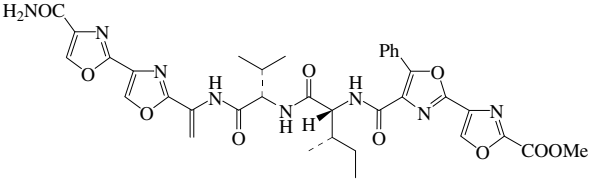
Mechercharmycin A M-125



$C_{35}H_{32}N_8O_7S$ 708.753
Prod. by the marine-derived *Thermoactinomyces* sp. YM3-251. Cytotoxic. Powder. $[\alpha]_D^{25}$ +110 (c, 0.04 in DMSO). λ_{max} 223 (log ϵ 4.71); 260 (log ϵ 4.73); 300 (sh) (MeOH).

Kanoh, K. *et al., J. Antibiot.*, 2005, **58**, 289-292 (*isol, pmr, cmr, cryst struct*)

Mechercharmycin B M-126

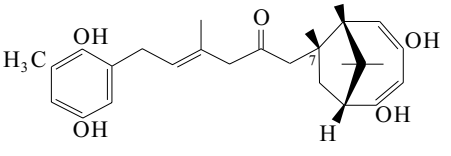


$C_{35}H_{36}N_8O_{10}$ 728.717
Prod. by the marine-derived *Thermoactinomyces* sp. YM3-251. Cytotoxic. Powder. $[\alpha]_D^{25}$ +56 (c, 0.06 in DMSO). λ_{max} 220 (log ϵ 4.65); 261 (log ϵ 4.62); 310 (sh) (MeOH).

Kanoh, K. *et al., J. Antibiot.*, 2005, **58**, 289-292 (*isol, pmr, cmr*)

Mediterraneol A M-127

[97730-98-8]



$C_{27}H_{36}O_5$ 440.578
Synthetic studies indicate that the structure requires revision (1995). Constit. of the alga *Cystoseira mediterranea*. Inhibitor of mitotic cell division of fertilized sea urchin eggs. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Exists as tautomeric mixt. λ_{max} 215 (ϵ 19000); 237 (sh) (ϵ); 289 (ϵ 2800) (MeOH) (Derep).

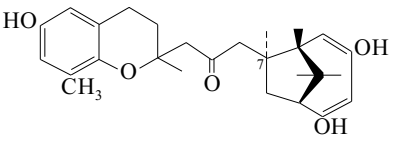
Tetra-Me ether:
Foam. $[\alpha]_D$ 0 (c, 2.5 in $CHCl_3$).

7-Epimer: ***Mediterraneol B***
[101141-34-8]
$C_{27}H_{36}O_5$ 440.578
From *Cystoseira mediterranea*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 215 (ϵ 19000); 237 (sh) (ϵ); 289 (ϵ 2800) (MeOH) (Derep).

Francisco, C. *et al., Tet. Lett.*, 1985, **26**, 2629 (*isol*)
Francisco, C. *et al., J.O.C.*, 1986, **51**, 1115 (*isol*)
Kakiuchi, K. *et al., J.O.C.*, 1995, **60**, 3318 (*synth*)

Mediterraneol C M-128

[100994-55-6]



$C_{27}H_{36}O_5$ 440.578

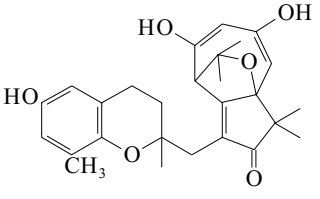
Constit. of *Cystoseira mediterranea*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 215 (ϵ 19000); 237 (sh) (ϵ); 289 (ϵ 2800) (MeOH) (Derep).

7-Epimer: ***Mediterraneol D***
[101053-52-5]
$C_{27}H_{36}O_5$ 440.578
From *Cystoseira mediterranea*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 215 (ϵ 19000); 237 (sh) (ϵ); 289 (ϵ 2800) (MeOH) (Derep).

Francisco, C. *et al., J.O.C.*, 1986, **51**, 1115

Mediterraneol E M-129

[135077-17-7]



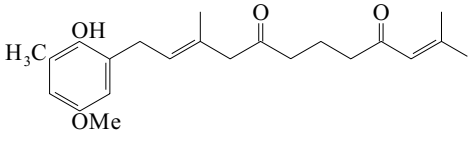
$C_{27}H_{32}O_6$ 452.546

Mixt. of diastereoisomers. Constit. of *Cystoseira mediterranea*. Foam. λ_{max} 215 (ϵ 13600); 248 (ϵ 8700); 289 (ϵ 2940) (MeOH) (Berdy).

Fadli, M. *et al., Tet. Lett.*, 1991, **32**, 2477 (*isol, pmr, cmr*)

Mediterraneone M-130

[133301-13-0]



$C_{22}H_{30}O_4$ 358.477

Metab. of *Cystoseira mediterranea*. Oil. λ_{max} 211 (ϵ 11020); 248 (ϵ 12700); 289 (ϵ 2390) (MeOH) (Berdy).

Fadli, M. *et al., J. Nat. Prod.*, 1991, **54**, 261 (*isol, pmr, cmr*)

Megabalanein A M-131

CdIP1
[207385-09-9]
H-Glu-Ile-Glu-Lys-Arg-Ala-Glu-Glu-Leu-Ser-Gly-Gln-Ile-Asp-Ser-OH

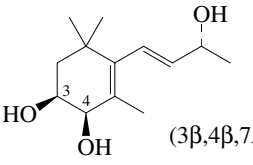
$C_{70}H_{118}N_{20}O_{29}$ 1703.819

Isol. from the barnacle *Megabalanus volcano*. Cadmium-inducible peptide.

1-(Serylglycylvalylglycyl): ***Megabalanein B****. CdIP2*
[220074-79-3]
$C_{82}H_{138}N_{24}O_{34}$ 2004.133
Isol. from *Megabalanus volcano*. Cadmium-inducible peptide.

Togi, A. *et al., Tet. Lett.*, 1998, **39**, 2775-2778 (*isol, cd, pmr, cmr*)
Togi, A. *et al., Tetrahedron*, 1998, **54**, 15581-15588

5,7-Megastigmadiene-3,4,9-triol M-132



(3β,4β,7*E*,9*R*)-*form*

$C_{13}H_{22}O_3$ 226.315

(3β,4β,7*E*,9*R*)-*form*

9-O-[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]: ***Ebracteatoside A***
[394692-97-8]
$C_{24}H_{40}O_{12}$ 520.573
Constit. of *Acanthus ebracteatus*. Amorph. powder. $[\alpha]_D^{22}$ -65.4 (c, 0.52 in MeOH).

Kanchanapoom, T. *et al., Phytochemistry*, 2001, **58**, 811-817 (*Ebracteatoside A*)

Melanin-concentrating hormone M-133

MCH
[67382-96-1]
H-Asp-Thr-Met-Arg-Cys-Met-Val-Gly-Arg-Val-Tyr-Arg-Pro-Cys-Trp-Glu-Val-OH

$C_{89}H_{139}N_{27}O_{24}S_4$ 2099.508

Peptide. Struct. of reduced form of salmon MCH shown; rat MCH has an *N*-terminal extension of 2 amino acids and 4 additional substitutions. Originally isol. from chub salmon pituitaries (*Oncorhynchus keta*); found in the hypothalamus of many vertebrates including mammals. Nonselective natural ligand for the human MCH receptor.

[85940-93-8, 87218-84-6, 123466-63-7, 128315-56-0]

Kiwauchis, H. *et al., Nature (London)*, 1983, **305**, 321-323 (*isol, salmon*)
Vaughan, J.M. *et al., Endocrinology (Baltimore)*, 1989, **125**, 1660-1665 (*rat, struct*)
Baker, B.I. *et al., Int. Rev. Cytol.*, 1991, **126**, 1-47 (*rev*)
Kiwauchi, H. *et al., Ann. N.Y. Acad. Sci.*, 1993, **680**, 64-77 (*rev*)
Kuigge, K.M. *et al., Peptides (N.Y.)*, 1996, **17**, 1063-1073 (*rev*)
Balm, P.H.M. *et al., Ann. N.Y. Acad. Sci.*, 1998, **839**, 205-209 (*rev, fish MCH*)
Bednarek, M.A. *et al., J. Biol. Chem.*, 2002, **277**, 13821-13826 (*activity*)
Marsh, D.J. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2002, **99**, 3240-3245 (*bibl*)

Melanodocin M-134

[81774-59-6]

$C_{44}H_{68}O_{13}S$ 837.079

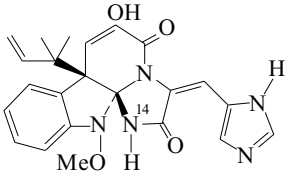
Stereo- or positional isomer of Acanthifolicin. Isol. from *Halichondria melanodocia*. Cytotoxic and antitumour agent. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Me ester: [81774-60-9]
$C_{45}H_{70}O_{13}S$ 851.106
From *Halichondria melanodocia*. Cytotoxic agent.

U.S. Pat., 1982, 4 314 057; *CA*, **96**, 205394 (*isol, struct, spectra*)

Meleagrin M-135

[71751-77-4]



Absolute configuration

$C_{23}H_{23}N_5O_4$ 433.466

Related to Cytochalasins. Isol. from *Penicillium meleagrinum* and a marine- derived *Penicillium chrysogenum*. Shows structural

similarity to tremorgenic mycotoxins. Pale yellow leaves ($CHCl_3$ or CH_2Cl_2).
Mp 250° dec. $[\alpha]_D$ -116 (c, 0.088 in $CHCl_3$). λ_{max} 232 (ϵ 27500); 285 (sh) (ϵ 8320); 349 (ϵ 27500) (EtOH) (Derep). λ_{max} 230 (ϵ 24500); 345 (ϵ 26200) (MeOH) (Berdy).

O-*Ac:*
Pale yellow cryst. powder (C_6H_6/petrol).

N^{14}-*Me:*
Pale yellow needles (MeOH). Mp 212° dec.

Me ether: ***Oxaline***
[55623-37-5]
$C_{24}H_{25}N_5O_4$ 447.493
Isol. from cultures of the toxicogenic fungus *Penicillium oxalicum*, and from *Penicillium* sp. Fg-234. Also prod. by a marine-derived fungus isol. from *Gracilaria verrucosa*. Cryst. (Me_2CO or $MeNO_2$). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 220-221° Mp 230-232° dec. λ_{max} 228 (ϵ 21300); 345 (ϵ 25200) (MeOH) (Derep). λ_{max} 228 (ϵ 20890); 347 (ϵ 24550) (MeOH) (Berdy).

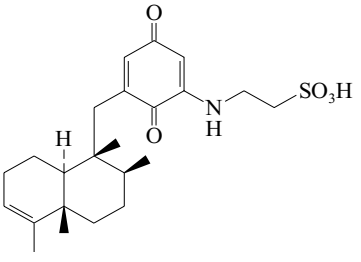
O,N^{14}-*Di-Me:*
Needles (hexane). Mp 217-218° (214-216°).

22,23-Dihydro, Me ether: Mp 254-255°.

Nagel, D.W. *et al., Tetrahedron*, 1976, **32**, 2625 (*Oxaline, cryst struct*)
Nozawa, K. *et al., J. Nat. Prod.*, 1979, **42**, 374 (*isol*)
Vleggaar, R. *et al., Chem. Comm.*, 1980, 160; 1983, 560 (*cmr, biosynth*)
Konda, Y. *et al., Chem. Pharm. Bull.*, 1980, **28**, 2987 (*Oxaline*)
Kawai, K. *et al., Chem. Pharm. Bull.*, 1984, **32**, 94 (*cryst struct, abs config*)
Reshetilova, T.A. *et al., Food Addit. Contam.*, 1995, **12**, 461-466 (*occur*)
Li, Y. *et al., Arch. Pharmacal Res.*, 2003, **26**, 21-23 (*Oxaline, marine isol*)
Bringmann, G. *et al., Tetrahedron*, 2005, **61**, 7252-7265 (*marine isol*)

Melemeleone A M-136

[144587-55-3]

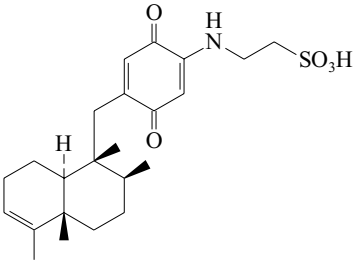


$C_{23}H_{33}NO_5S$ 435.583
Constit. of *Dysidea avara*. Red amorph. solid.
Mp 110-115°. $[\alpha]_D^{20}$ -20.1 (c, 0.006 in CH_2Cl_2). λ_{max} 214 (ϵ); 290 (ϵ); 483 (ϵ) (MeOH) (Derep).

Alvi, K.A. *et al., J.O.C.*, 1992, **57**, 6604 (*isol, pmr, cmr*)

Melemeleone B M-137

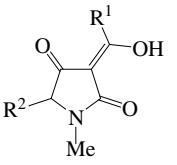
[144587-56-4]



$C_{23}H_{33}NO_5S$ 435.583
Constit. of *Dysidea avara*. Tyrosine kinase inhibitor. Red amorph. solid. Sol. MeOH.
Mp 190-200°. $[\alpha]_D^{20}$ -22 (c, 0.01 in CH_2Cl_2). λ_{max} 214 (ϵ); 290 (ϵ); 483 (ϵ) (MeOH) (Derep).

Abvi, K.A. *et al., J.O.C.*, 1992, **57**, 6604 (*isol, pmr, cmr*)

Melophlins M-138



Melophlin A $R^1 = -(CH_2)_{14}CH_3$, $R^2 = H$
B $R^1 = -CH_2CH_2CH(CH_3)(CH_2)_7CH_3$, $R^2 = CH_3$
C $R^1 = -(CH_2)_3CH(CH_3)(CH_2)_6CH_3$, $R^2 = CH_3$
D $R^1 = -(CH_2)_{13}CH_3$, $R^2 = H$
E $R^1 = -(CH_2)_{12}CH(CH_3)_2$, $R^2 = H$
F $R^1 = -(CH_2)_{11}CH(CH_3)CH_2CH_3$, $R^2 = H$
G $R^1 = -(CH_2)_{12}CH_3$, $R^2 = H$
H $R^1 = -(CH_2)_{11}CH(CH_3)_2$, $R^2 = H$
I $R^1 = -(CH_2)_{10}CH(CH_3)CH_2CH_3$, $R^2 = H$
J $R^1 = -(CH_2)_{12}CH_3$, $R^2 = CH_3$
K $R^1 = -(CH_2)_{10}CH(CH_3)_2$, $R^2 = H$
L $R^1 = -(CH_2)_{11}CH_3$, $R^2 = CH_3$
M $R^1 = -(CH_2)_{10}CH_3$, $R^2 = CH_3$
N $R^1 = -(CH_2)_9CH(CH_3)_2$, $R^2 = CH_3$
O $R^1 = -(CH_2)_8CH(CH_3)CH_2CH_3$, $R^2 = CH_3$
P $R^1 = -(CH_2)_{14}CH_3$, $R^2 = CH_3$
Q $R^1 = -(CH_2)_{11}CH(CH_3)_2$, $R^2 = CH_3$
R $R^1 = -(CH_2)_{10}CH(CH_3)CH_2CH_3$, $R^2 = CH_3$
S $R^1 = -(CH_2)_3CH(CH_3)(CH_2)_8CH_3$, $R^2 = CH_3$

Tetramic acid derivs. Enolised β-triketones. Isol. from the marine sponge *Melophlus sarassinorum*.

Melophlin A
3-(1-Hydroxyhexadecylidene)-1-methyl-2,4-pyrrolidinedione, 9CI
[268745-62-6]
$C_{21}H_{37}NO_3$ 351.528
Cytotoxic agent. Oil. λ_{max} 244 (ϵ 9000); 284 (ϵ 15000) (MeOH).

Melophlin B
3-(1-Hydroxy-4-methyldodecylidene)-1,5-dimethyl-2,4-pyrrolidinedione
[268745-63-7]
$C_{19}H_{33}NO_3$ 323.475
Cytotoxic. $[\alpha]_D$ -12.4 (c, 1.2 in MeOH). Has *S*-config. at C-5. λ_{max} 245 (ϵ 13800); 285 (ϵ 17000) (MeOH).

Melophlin C
3-(1-Hydroxy-5-methyldodecylidene)-1,5-dimethyl-2,4-pyrrolidinedione
[499136-46-8]
$C_{19}H_{33}NO_3$ 323.475
Antibacterial agent. Yellow oil. $[\alpha]_D$ -5.8 (c, 0.35 in MeOH). Isol. as a 1:2 mixt. of 5*R*- and 5*S*-enantiomers. λ_{max} 248 (log ϵ 3.9); 286 (log ϵ 4.12) (MeOH).

Melophlin D
3-(1-Hydroxypentadecylidene)-1-methyl-2,4-pyrrolidinedione
[499136-47-9]
$C_{20}H_{35}NO_3$ 337.501
Yellow oil. λ_{max} 247 (log ϵ 3.74); 286 (log ϵ 3.93) (MeOH).

Melophlin E
3-(1-Hydroxy-14-methylpentadecylidene)-1-methyl-2,4-pyrrolidinedione
[499136-48-0]
$C_{21}H_{37}NO_3$ 351.528
Yellow oil. λ_{max} 246 (log ϵ 4.08); 286 (log ϵ 4.2) (MeOH).

Melophlin F
3-(1-Hydroxy-13-methylpentadecylidene)-1-methyl-2,4-pyrrolidinedione
[499136-49-1]
$C_{21}H_{37}NO_3$ 351.528
Yellow oil. λ_{max} 245 (log ϵ 3.06); 285 (log ϵ 3.15) (MeOH).

Melophlin G
3-(1-Hydroxytetradecylidene)-1-methyl-2,4-pyrrolidinedione
[499136-50-4]
$C_{19}H_{33}NO_3$ 323.475
Yellow oil. λ_{max} 247 (log ϵ 4); 285 (log ϵ 4.19) (MeOH).

Melophlin H
3-(1-Hydroxy-13-methyltetradecylidene)-1-methyl-2,4-pyrrolidinedione
[499136-52-6]
$C_{20}H_{35}NO_3$ 337.501
Yellow oil. λ_{max} 247 (log ϵ 4.01); 285 (log ϵ 4.25) (MeOH).

Melophlin I
3-(1-Hydroxy-12-methyltetradecylidene)-1-methyl-2,4-pyrrolidinedione
[499136-55-9]
$C_{20}H_{35}NO_3$ 337.501
Yellow oil. $[\alpha]_D^{20}$ -2.6 (c, 0.34 in MeOH). λ_{max} 245 (log ϵ 3.27); 286 (log ϵ 3.47) (MeOH).

Melophlin J
3-(1-Hydroxytetradecylidene)-1,5-dimethyl-2,4-pyrrolidinedione
[499136-60-6]
$C_{20}H_{35}NO_3$ 337.501
Yellow oil. $[\alpha]_D^{20}$ -2.6 (c, 0.31 in MeOH). Isol. as a partial racemate, approx. 3:2 5*R*/5*S*-. λ_{max} 246 (log ϵ 3.11); 285 (log ϵ 3.25) (MeOH).

Melophlin K
3-(1-Hydroxy-12-methyltridecylidene)-1-methyl-2,4-pyrrolidinedione
[499136-61-7]
$C_{19}H_{33}NO_3$ 323.475
Yellow oil. λ_{max} 243 (log ϵ 3.04); 286 (log ϵ 3.09) (MeOH).

Melophlin L
3-(1-Hydroxytridecylidene)-1,5-dimethyl-2,4-pyrrolidinedione
[499136-75-3]
$C_{19}H_{33}NO_3$ 323.475
Yellow oil. $[\alpha]_D^{20}$ -3.8 (c, 0.16 in MeOH). Isol. as a partial racemate, approx. 1:2 5*R*/5*S*-. λ_{max} 245 (log ϵ 3); 286 (log ϵ 3.03) (MeOH).

Melophlin M
3-(1-Hydroxydodecylidene)-1,5-dimethyl-2,4-pyrrolidinedione
[499136-76-4]
$C_{18}H_{31}NO_3$ 309.448
Yellow oil. $[\alpha]_D^{20}$ -5 (c, 0.4 in MeOH). Isol. as a partial racemate, approx. 1:2 5*R*/5*S*-. λ_{max} 248 (log ϵ 3.53); 286 (log ϵ 3.69) (MeOH).

Melophlin N
3-(1-Hydroxy-11-methyldodecylidene)-1,5-dimethyl-2,4-pyrrolidinedione
[499136-77-5]
$C_{19}H_{33}NO_3$ 323.475
Yellow oil. Isol. as a partial racemate, approx. 1:2 5*R*/5*S*-. λ_{max} 248 (log ϵ 3.79); 286 (log ϵ 3.99) (MeOH).

Melophlin O
3-(1-Hydroxy-10-methyldodecylidene)-1,5-dimethyl-2,4-pyrrolidinedione
[499136-81-1]
$C_{19}H_{33}NO_3$ 323.475
Yellow oil. Isol. a partial racemate, approx. 1:2 5*R*/5*S*-. λ_{max} 248 (log ϵ 3.79); 286 (log ϵ 3.99) (MeOH).

Melophlin P
3-(1-Hydroxyhexadecylidene)-1,5-dimethyl-2,4-pyrrolidinedione
$C_{22}H_{39}NO_3$ 365.555
Yellowish oil. Racemate. λ_{max} 245 (log ϵ 3.8); 282 (log ϵ 4.1) (MeOH).

Melophlin Q
3-(1-Hydroxy-13-methyltetradecylidene)-1,5-dimethyl-2,4-pyrrolidinedione
$C_{21}H_{37}NO_3$ 351.528
Yellowish oil. Racemate. λ_{max} 246 (log ϵ 4.1); 283 (log ϵ 4.2) (MeOH).

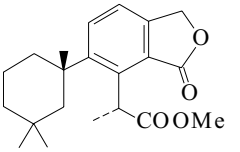
Melophlin R
3-(1-Hydroxy-12-methyltetradecylidene)-1,5-dimethyl-2,4-pyrrolidinedione
$C_{21}H_{37}NO_3$ 351.528
Yellowish oil. Racemate. λ_{max} 248 (log ϵ 4.2); 280 (log ϵ 4.2) (MeOH).

Melophlin S
3-(1-Hydroxy-5-methyltetradecylidene)-1,5-dimethyl-2,4-pyrrolidinedione
$C_{21}H_{37}NO_3$ 351.528
Yellowish oil. Racemate. λ_{max} 248 (log ϵ 3.8); 283 (log ϵ 4.5) (MeOH).

Aoki, S. *et al., Tetrahedron*, 2000, **56**, 1833-1836 (*Melophlins A,B*)
Wang, C.-Y. *et al., J. Nat. Prod.*, 2003, **66**, 51-56 (*Melophlins C-O*)
Xu, J. *et al., Chem. Pharm. Bull.*, 2006, **54**, 852-854 (*Melophlins P-S*)

Membranolide M-139

[106231-26-9]

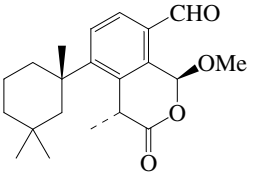


$C_{21}H_{28}O_4$ 344.45
Constit. of *Dendrilla membranosa*. Oil. Sol. CH_2Cl_2, 1-propanol. $[\alpha]_D$ -28.8 (c, 2.25 in $CHCl_3$). λ_{max} 211 (ϵ 20300); 231 (ϵ 5800); 285 (ϵ 1600); 293 (ϵ 1600) (MeOH) (Derep).

Molinski, T.F. *et al., J.O.C.*, 1987, **52**, 296 (*isol*)
Manriquez, V. *et al., Acta Cryst. C*, 1990, **46**, 2486 (*cryst struct*)

Membranolide B M-140

[732296-53-6]

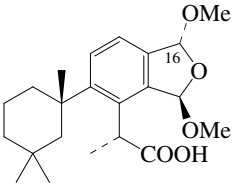


$C_{21}H_{28}O_4$ 344.45
Constit. of *Dendrilla membranosa*. Oil. $[\alpha]_D^{25}$ -121 (c, 0.6 in $CHCl_3$). λ_{max} 228 (log ϵ 3.9); 263 (log ϵ 3.95) (MeOH).

Ankisetty, S. *et al., J. Nat. Prod.*, 2004, **67**, 1172-1174 (*isol, pmr, cmr*)

Membranolide C M-141

[732296-54-7]



$C_{22}H_{32}O_5$ 376.492

Constit. of *Dendrilla membranosa*. Oil. $[\alpha]_D^{25}$ -100.8 (c, 0.6 in $CHCl_3$). λ_{max} 215 (log ϵ 3.93); 258 (log ϵ 3.38) (MeOH).

16-Epimer: ***Membranolide D***

[732296-55-8]

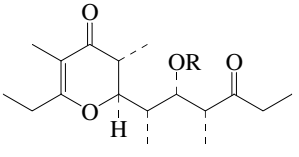
$C_{22}H_{32}O_5$ 376.492

Constit. of *Dendrilla membranosa*. Oil. $[\alpha]_D^{25}$ +6.5 (c, 0.6 in $CHCl_3$). λ_{max} 215 (log ϵ 3.91); 258 (log ϵ 3.36) (MeOH).

Ankisetty, S. *et al., J. Nat. Prod.*, 2004, **67**, 1172-1174 (*isol, pmr, cmr*)

Membrenone A M-142

[152273-81-9]



Absolute Configuration

R = -COCH(CH$_3$)CH$_2$CH$_3$ (*R*-)

$C_{22}H_{36}O_5$ 380.523

Abs. config. assigned in 2002 is based on that of Membrenone C, M-144. Constit. of the skin of the mollusc *Pleurobranchus membranaceus*. Feeding deterrent. Sol. MeOH, EtOH, EtOAc, butanol; poorly sol. H_2O. $[\alpha]_D^{20}$ +24.7 (c, 0.05 in $CHCl_3$). λ_{max} 272 (ϵ 4450) (MeOH) (Derep).

Ciavatta, M.L. *et al., Tet. Lett.*, 1993, **34**, 6791-6794 (*isol, struct*)
Sampson, R.A. *et al., Org. Lett.*, 2002, **4**, 1655-1658 (*synth, abs config*)

Membrenone B M-143

[152273-82-0]

As Membrenone A, M-142 with

R = –COCH$_2$CH$_3$

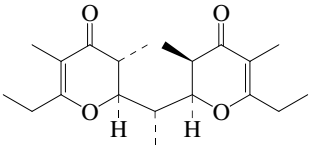
$C_{20}H_{32}O_5$ 352.47

Constit. of the skin of the mollusc *Pleurobranchus membranaceus*. Feeding deterrent. Sol. MeOH, EtOAc, EtOH, butanol; poorly sol. H_2O. $[\alpha]_D^{20}$ -24.8 (c, 0.2 in $CHCl_3$). λ_{max} 273 (ϵ 8120) (MeOH) (Derep). λ_{max} 216 (ϵ 25800); 258 (ϵ 12600); 272 (ϵ 4440); 301 (ϵ 4000) (MeOH) (Berdy).

Ciavatta, M.L. *et al., Tet. Lett.*, 1993, **34**, 6791-6794 (*isol, struct*)
Sampson, R.A. *et al., Org. Lett.*, 2002, **4**, 1655-1658 (*synth, abs config*)

Membrenone C M-144

[152273-83-1]



Absolute Configuration

$C_{20}H_{30}O_4$ 334.455

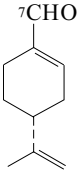
Abs. config. revised in 2002. An earlier opposite assignment made in 2001 was based on an incorrect report of a negative opt. rotn for natural Mesembrenone A. Constit. of the skin of the mollusc *Pleurobranchus membranaceus*. Feeding deterrent. Sol. MeOH, butanol, EtOAc, EtOH; poorly sol. H_2O. $[\alpha]_D^{20}$ +58.1 (c, 0.1 in $CHCl_3$). λ_{max} 273 (ϵ 8120) (MeOH) (Derep). λ_{max} 206 (ϵ 16700); 273 (ϵ 8216); 295 (ϵ 5800) (MeOH) (Berdy).

Ciavatta, M.L. *et al., Tet. Lett.*, 1993, **34**, 6791-6794 (*isol, struct*)
Perkins, M.V. *et al., Org. Lett.*, 2002, **4**, 1655-1658 (*synth, abs config*)
Marshall, J.A. *et al., Org. Lett.*, 2003, **5**, 1729-1732 (*synth*)
Yadav, J.S. *et al., Tet. Lett.*, 2006, **47**, 1603-1606 (*synth*)

p-Mentha-1,8-dien-7-al M-145

4-(1-Methylethenyl)-1-cyclohexene-1-carboxaldehyde, 9CI
. 4-Isopropenyl-1-cyclohexene-1-carboxaldehyde. ***Perillaldehyde****. Perillaaldehyde*

[2111-75-3]



(*R*)–*form*

$C_{10}H_{14}O$ 150.22

▶ Skin irritant. LD_{50} (mus, orl) 1720 mg/kg. GW2967000

(R)-form [5503-12-8]

Isol. from *Siler trilobum* (preferred genus name *Laserpitium*), *Sium latifolium*, *Citrus reticulata* and other plants.

Oil. Bp_9 99-104°. $[\alpha]_D$ +137.

Oxime:

Cryst. Mp 102°.

7-Carboxylic acid: p-*Mentha-1,8-dien-7-oic acid.* ***Perillic acid***

[7694-45-3]

$C_{10}H_{14}O_2$ 166.219

Isol. from *Salvia dorisiana*. Cryst. (EtOH).

Mp 132-133°. Bp_{10} 164-165°. $[\alpha]_D^{20}$ -146.

7-Carboxylic acid, Me ester: [54298-90-7] $Bp_{0.5}$ 81-83°.

7-Carboxylic acid, β-D-glucopyranosyl ester: ***Perilloside B***

$C_{16}H_{24}O_7$ 328.361

Constit. of perilla (*Perilla frutescens*). Aldose reductase inhibitor, antidiabetic agent. Needles ($CHCl_3$/Et_2O).

Mp 154-155°. $[\alpha]_D^{22}$ -57.1 (c, 0.645 in MeOH). λ_{max} 220 (ϵ 10500) (MeOH) (Berdy).

(S)-form [18031-40-8]

Constit. of *Perilla nankinensis* and gingergrass oils (*Cymbopogon* sp.).

Oil. Bp_{10} 104-105°. $[\alpha]_D^{20}$ -145.8.

▶ GW2967200

(E)-Oxime: Perilla sugar. Perillartine

[30950-27-7]

$C_{10}H_{15}NO$ 165.235

Sweetening agent. V. sweet cryst. Mp 102°. Bp_{12} 147-148°.

▶ LD_{50} (rat, orl) 2500 mg/kg. GW2975000

(Z)-Oxime:

Cryst. Mp 129°.

(ξ)-form

Occurs in Black Sea bryozoan *Conopeum seuratum*.

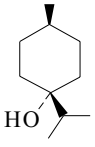
[6611-91-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 477A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 745C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 568A (*ir*)
Ritter, J.J. *et al., J.A.C.S.*, 1950, **72**, 2381 (*synth, Perillic acid*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1968, **45**, 615 (*synth*)
Acton, E.M. *et al., Experientia*, 1970, **26**, 473 (*struct*)
Suga, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 545 (*stereochem*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Tori, K. *et al., Tet. Lett.*, 1975, 2199 (*pmr*)
Regan, J.W. *et al., J. Agric. Food Chem.*, 1976, **24**, 377 (*Perillic acid*)
Hadjieva, P. *et al., Z. Naturforsch., C*, 1987, **42**, 1019-1022 (*occur, Conopeum*)

Tius, M.A. *et al., Synth. Commun.*, 1988, **18**, 1905 (*synth*)
Fujita, T. *et al., Phytochemistry*, 1993, **34**, 1545 (*Perilloside B*)
McGeady, P. *et al., J. Nat. Prod.*, 2002, **65**, 953-955 (*activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DKX100; PCJ000

p-Menthan-4-ol M-146

4-Methyl-1-(1-methylethyl)cyclohexanol. 1-Isopropyl-4-methylcyclohexanol
[470-65-5]



(1*RS*,4*RS*)–*form*

$C_{10}H_{20}O$ 156.267
Present in turpentine from *Pinus sylvestris* (Scotch pine) and isol. from *Mentha* spp. Present in the bryozoan *Conopeum seuratum*.

(1*RS*,4*RS*)-*form*
cis-*form*
[3239-02-9]
Cryst. Mp 52-53°.

Phenylurethane:
Cryst. Mp 131-141°.

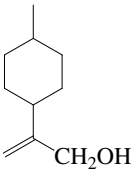
(1*RS*,4*SR*)-*form*
trans-*form*
[3239-03-0]
Oil.

Phenylurethane:
Cryst. Mp 99-100°.

Bowman, R.M. *et al., J.C.S.(C)*, 1966, 612 (*synth*)
Murphy, R. *et al., Aust. J. Chem.*, 1976, **29**, 617 (*synth*)
Hadjieva, P. *et al., Z. Naturforsch., B*, 1987, **42**, 1019-1022 (*occur, bryozoan*)

p-Menth-8-en-10-ol M-147

4-Methyl-β-methylenecyclohexaneethanol, 9CI
[5502-99-8]
[15714-12-2 *trans*-form]

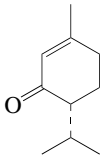


$C_{10}H_{18}O$ 154.252
Occurs in bryozoan *Conopeum seuratum*. Bp_5 130°. n_D^{30} 1.4760.

Camps, F. *et al., J.O.C.*, 1966, **31**, 3510-3513 (*synth*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1968, **45**, 615-627 (*synth*)
Khadzhieva, P. *et al., Z. Naturforsch., C*, 1987, **42**, 1019-1022 (*occur*)

p-Menth-1-en-3-one M-148

3-Methyl-6-(1-methylethyl)-2-cyclohexen-1-one. 6-Isopropyl-3-methyl-2-cyclohexen-1-one. ***Piperitone****. 3-Carvomenthenone*
[89-81-6]



(*R*)-*form*

$C_{10}H_{16}O$ 152.236
Flavouring ingredient. Antiasthmatic agent. Log P 2.5 (calc).
▶ Skin irritant. LD_{50} (rat, orl) 2450 mg/kg. OT0257000

(*R*)-*form* [4573-50-6]
Constit. of *Eucalyptus dives* oil and other *Eucalyptus* spp., *Mentha* spp. and *Zanthoxylum piperitum* (Japanese pepper tree) oil.
Mp -29°. Bp_{15} 110.5°. $[\alpha]_D^{20}$ -51.53.

(*S*)-*form*
D-Piperitone. FEMA 2910
[6091-50-5]
Constit. of oils from *Andropogon jwarancusa* and *Cymbopogon senarensis*. A common constit. of *Mentha* spp. oils. Alarm pheromone from *Tyrophagus similis* (acarid mite).
Oil with camphoraceous odour. Bp_{20} 116-118.5°. $[\alpha]_D^{20}$ +49.13.

Semicarbazone:
Cryst. Mp 193-194°. $[\alpha]_D^{20}$ -216.8.

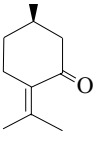
(ξ)-*form*
Present in Black Sea bryozoan *Conopeum seuratum*.

[6091-52-7]

Thomas, A.F. *et al., J.C.S.(B)*, 1967, 392 (*ms*)
Nagasawa, T. *et al., Agric. Biol. Chem.*, 1975, **39**, 2083 (*abs config*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 863 (*rev, tox*)
Burbott, A.J. *et al., Phytochemistry*, 1983, **22**, 2227-2230 (*isol, uv, cd, abs config*)
Kuwahara, Y. *et al., Agric. Biol. Chem.*, 1987, **51**, 3441 (*isol*)
Hadjieva, P. *et al., Z. Naturforsch., C*, 1987, **42**, 1019-1022 (*occur, Conopeum*)
Garcez, F.R. *et al., Phytochemistry*, 1988, **27**, 1079 (*isol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 679
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2230-2231
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MCF250

p-Menth-4(8)-en-3-one M-149

5-Methyl-2-(1-methylethylidene)cyclohexanone. 2-Isopropylidene-5-methylcyclohexanone. ***Pulegone****. β-Pulegone*
[15932-80-6]



(*R*)–*form*

$C_{10}H_{16}O$ 152.236
▶ LD_{50} (rat, orl) 470 mg/kg. Skin irritant. OT0260000

(*R*)-*form*
FEMA 2963
[89-82-7]
Occurs in oils of *Mentha* spp., *Hedeoma pulegioides* and many other essential oils. Fragrance and flavour ingredient.
Oil with pleasant peppermint odour. d_4^{20} 0.94. Bp 224°. $[\alpha]_D^{20}$ +23 (c, 5 in EtOH).
▶ OT0261000

Semicarbazone:
Cryst. (EtOH). Mp 174°.

(*S*)-*form* [3391-90-0]
Occurs in *Agastache formosanum* and *Glechoma hederacea*.
Oil. Bp_{22} 104-108°. $[\alpha]_D^{23}$ -22.5 (neat).

(ξ)-*form*
Identified by gc-ms in the Black Sea bryozoan *Conopeum seuratum*.

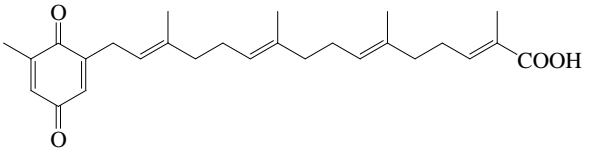
[3285-04-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 449A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 693B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 538D (*ir*)
Black, C. *et al., J.C.S.*, 1956, 2971 (*synth*)
Banthorpe, D.V. *et al., J.C.S. Perkin 1*, 1972, 1532 (*isol, biosynth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 549 (*occur*)

Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Corey, E.J. *et al., J.O.C.*, 1976, **41**, 380 (*synth*)
Allen, K.G. *et al., Phytochemistry*, 1976, **15**, 101 (*biosynth*)
Hadjieva, P. *et al., Z. Naturforsch., C*, 1987, **42**, 1019-1022 (*occur, Conopeum*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1407
Eisenreich, W. *et al., Tet. Lett.*, 1997, **38**, 3889-3892 (*biosynth*)
Bartoli, G. *et al., J.O.C.*, 2002, **67**, 9111-9114 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MCF500

Menzoquinone M-150

[755016-04-7]



$C_{27}H_{36}O_4$ 424.579
Constit. of *Desmarestia menziesii*. Oil. λ_{max} 253 (log ϵ 4.69) (MeOH).

Ankisetty, S. *et al., J. Nat. Prod.*, 2004, **67**, 1295-1302 (*isol, pmr, cmr*)

4-Mercapto-2-butanone, 8CI M-151

2-Thiahexan-5-one. 2-Keto-4-butanethiol. FEMA 3357
[34619-12-0]
$HSCH_2CH_2COCH_3$
C_4H_8OS 104.173
Flavouring ingredient. Oil. Bp_{15} 63-65°.

S-*Me: 4-(Methylthio)-2-butanone, 8CI. FEMA 3375*
[34047-39-7]
$C_5H_{10}OS$ 118.199
Isol. from an arctic marine bacterium. Flavouring ingredient. Bp_{55} 106° Bp_{16} 72-73°. n_D^{25} 1.4772.

S-*Me, 2,4-dinitrophenylhydrazone:*
Orange prisms (EtOH). Mp 100.5° (98.5-100°).

S-*Me, semicarbazone:*
Prisms ($CHCl_3$/petrol). Mp 127-128°.

S-*Me,* S-*oxide: 4-Methylsulfinyl-2-butanone*
$C_5H_{10}O_2S$ 134.199
Cryst. (petrol). Mp 28-29°.

S-*Me,* S,S-*dioxide: 4-Methylsulfonyl-2-butanone*
[68152-37-4]
$C_5H_{10}O_3S$ 150.198
Cryst. (2-propanol). Mp 88-89°.

S-*Me,* S,S-*dioxide, oxime:*
$C_5H_{11}NO_3S$ 165.213
Needles (2-propanol). Mp 107-108°.

S-*Et: 4-(Ethylthio)-2-butanone*
[61224-82-6]
$C_6H_{12}OS$ 132.226
Oil. Bp_{17} 118-120°.

S-*Ph:* See 4-(Phenylthio)-2-butanone in *The Combined Chemical Dictionary.*

S-*Ph,* S-*oxide: 4-(Phenylsulfinyl)-2-butanone*
[77657-95-5]
$C_{10}H_{12}O_2S$ 196.27
Oil.

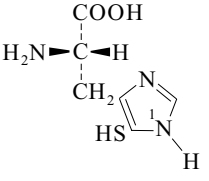
S-*Ph,* S,S-*dioxide: 4-(Phenylsulfonyl)-2-butanone*
[83802-87-3]
[24731-39-3]
$C_{10}H_{12}O_3S$ 212.269
Needles (petrol). Mp 88-89°.

S-*Ph, di-Me acetal,* S,S-*dioxide:* [85785-78-0]
$C_{12}H_{18}O_4S$ 258.338
Cryst. (Et_2O). Mp 65-66° (62-63°).

Cardwell, H.M.E. *et al., J.C.S.*, 1949, 715 (*S-Me, synth*)
Gill, N.S. *et al., J.A.C.S.*, 1952, **74**, 4923 (*synth, derivs*)
Böhme, H. *et al., Chem. Ber.*, 1953, **86**, 443 (*S,S-dioxide, synth*)
Pfister, K. *et al., J.A.C.S.*, 1955, **77**, 697 (*S-Me, synth*)
Murata, N. *et al., Kogyo Kagaku Zasshi*, 1956, **59**, 129 (*synth*)
Cain, M.E. *et al., J.C.S.*, 1962, 2959 (*derivs*)
McIntosh, J.M. *et al., Can. J. Chem.*, 1976, **54**, 1923 (*synth*)
Kuwajima, I. *et al., Synthesis*, 1976, 602-604 (*S-Ph, synth*)
Otera, J. *et al., Organometallics*, 1983, **2**, 332 (*S-Ph S,S-dioxide, pmr*)
Yusufoğlu, A. *et al., J.O.C.*, 1986, **51**, 3485-3487 (*S-Ph di-Me acetal S,S-dioxide*)
Clennan, E.L. *et al., J.O.C.*, 1992, **57**, 4477-4487 (*S-Ph, synth, pmr*)
Greenhalgh, R. *et al., Synlett*, 1992, 235-236 (*S-Ph S-oxide, synth*)
Ozaki, Y. *et al., Chem. Pharm. Bull.*, 1995, **43**, 734 (*S-Et*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 425; 570
Gibson, S.E. *et al., J.C.S. Perkin 1*, 1995, 2427 (*S-Ph S,S-dioxide, synth, ir, pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1522; 1868
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*marine isol*)

5-Mercaptohistidine, 9CI M-152

5-Thiolhistidine



$C_6H_9N_3O_2S$ 187.222

(S)-form
L-form
1-Me: ***5-Mercapto-1-methylhistidine***
[62982-24-5]
$C_7H_{11}N_3O_2S$ 201.249
Constit. of the unfertilised eggs of the sea urchin *Paracentrotus lividus*. Also a component of the struct. of adrenochrome, an Fe(III) contg. peptide from *Octopus vulgaris.*

1-Me, disulfide: ***5,5′-Dithiobis[1-methylhistidine], 9CI***
[83471-81-2]
$C_{14}H_{20}N_6O_4S_2$ 400.482
Isol. from the unfertilised eggs of *Paracentrotus lividus* and other echinoderms. Prisms (EtOH aq.).
Mp 202-205° (darkens). $[\alpha]_D^{20}$ +76 (c, 1.2 in 0.1*M* HCl).

3-Me: See 1-Methyl-4-mercaptohistidine, M-384

1,N^{α},N^{α}*-Tri-Me, disulfide:* ***5,5′-Dithiobis[N,N,1-trimethylhistidine], 9CI***
[91283-93-1]
$C_{18}H_{28}N_6O_4S_2$ 456.589
Isol. from the unfertilized eggs of *Sphaerechinus granularis.*
λ_{max} 257 (ϵ 6760) (H_2O).

Palumbo, A. *et al., Tet. Lett.*, 1982, **23**, 3207-3208 (*isol, uv, pmr, cmr*)
Palumbo, A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1984, **78**, 81-83 (*isol*)
Rossi, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 843-845 (*isol*)

1-Mercapto-3-undecanone M-153

$H_3C(CH_2)_7COCH_2CH_2SH$
$C_{11}H_{22}OS$ 202.36

S-*Ac:* S-*(3-Oxoundecyl) thioacetate*
[33796-36-0]
$C_{13}H_{24}O_2S$ 244.397
Constit. of *Dictyopteris plagiogramma*. Oil. $Bp_{0.0005}$ 80-85°.

Roller, P. *et al., Chem. Comm.*, 1971, 503 (*isol*)

1-Mercapto-5-undecen-3-ol M-154

$H_3C(CH_2)_4CH{=}CHCH_2CH(OH)CH_2CH_2SH$

$C_{11}H_{22}OS$ 202.36

O,S-*Di-Ac: Ethanethioic acid* S-*[3-(acetyloxy)-5-undecenyl] ester, 9CI. 3-Acetoxy-5-undecenyl thioacetate*
[36948-67-1]
$C_{15}H_{26}O_3S$ 286.435
Constit. of *Dictyopteris* spp. Liq. $[\alpha]_D$ -25 (CCl_4).

Disulfide, di-O-*Ac: Bis(3-acetoxy-5-undecenyl)disulfide*
[36948-66-0]
$C_{26}H_{46}O_4S_2$ 486.779
Constit. of *Dictyopteris* spp. Low-melting solid.

Moore, R.E. *et al., Chem. Comm.*, 1972, 326 (*isol, pmr, ms*)

1-Mercapto-4-undecen-3-one, 8CI M-155

$H_3C(CH_2)_5CH{=}CHCOCH_2CH_2SH$
$C_{11}H_{20}OS$ 200.344

(E)-form
S-*Ac:* S-*(3-Oxo-4-undecenyl) thioacetate*
[33783-84-5]
$C_{13}H_{22}O_2S$ 242.382
Constit. of *Dictyopteris plagiogramma*. Oil.

Roller, P. *et al., Chem. Comm.*, 1971, 503 (*isol*)

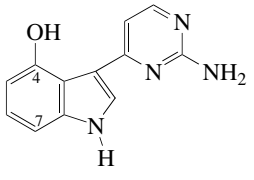
Mercenene M-156

[8057-77-0]
Struct. unknown; the active principle is a low-MW species loosely bound to a protein or glycoprotein. Isol. from the common clam *Mercenaria mercenaria* and from *Mercenaria campechiensis*. Shows antitumour activity. Sol. H_2O; poorly sol. MeOH, hexane. λ_{max} 214; 234; 250; 274 (H_2O) (Berdy).

Schmeer, M.R. *et al., Ann. N.Y. Acad. Sci.*, 1966, **136**, 211-218 (*isol*)
Schmeer, M.R. *et al., Life Sci.*, 1966, **5**, 1169-1178 (*isol*)
Schmer, A.C. *et al., Natl. Cancer Inst. Monogr.*, 1969, **31**, 581-591 (*antitumour activity*)

Meridianin A M-157

[213472-98-1]



$C_{12}H_{10}N_4O$ 226.237
Alkaloid from the tunicate *Aplidium meridianum*. Protein kinase inhibitor. Yellow needles (MeOH aq.).
Mp 164-168°. λ_{max} 248 (log ϵ 3.68); 356 (log ϵ 3.58) ($CHCl_3$).
λ_{max} 248 (ϵ 4786); 356 (ϵ 3800) (MeOH) (Berdy).

6-Bromo: ***Meridianin B***
[213472-99-2]
$C_{12}H_9BrN_4O$ 305.133
Alkaloid from *Aplidium meridianum*. Cytotoxic agent. Yellow powder (EtOAc).
Mp 190° dec. λ_{max} 246 (log ϵ 3.87); 354 (log ϵ 3.71) ($CHCl_3$).
λ_{max} 246 (ϵ 7413); 354 (ϵ 5128) (MeOH) (Berdy).

7-Bromo: ***Meridianin E***
[213473-03-1]
$C_{12}H_9BrN_4O$ 305.133
Alkaloid from *Aplidium meridianum*. Cytotoxic agent. Yellow cryst. (MeOH aq.).
Mp 172-175°. λ_{max} 224 (log ϵ 4.2); 358 (log ϵ 3.85) (MeOH).

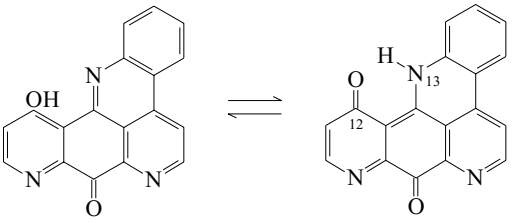
Deoxy, 5-bromo: ***Meridianin C***
[213473-00-8]
$C_{12}H_9BrN_4$ 289.134
Alkaloid from *Aplidium meridianum*. Cytotoxic agent. Yellow powder (MeOH aq.).
Mp 103-106°. λ_{max} 244 (log ϵ 4.06); 324 (log ϵ 4.1) ($CHCl_3$).
λ_{max} 246 (ϵ 11480); 324 (ϵ 12590) (MeOH) (Berdy).

Deoxy, 6-bromo: ***Meridianin D***
[213473-01-9]
$C_{12}H_9BrN_4$ 289.134
Alkaloid from *Aplidium meridianum*. Cytotoxic agent. Yellow powder (EtOAc/MeOH).
Mp 218-221°. λ_{max} 240 (log ϵ 4.17); 324 (log ϵ 4.14) ($CHCl_3$).
λ_{max} 240 (ϵ 14790); 324 (ϵ 13800) (MeOH) (Berdy).

Franco, L.H. *et al., J. Nat. Prod.*, 1998, **61**, 1130-1132 (*isol, uv, ir, pmr, cmr*)
Jiang, B. *et al., Heterocycles*, 2000, **53**, 1489-1498 (*Meridianin D, synth*)
Fresneda, P.M. *et al., Tetrahedron*, 2001, **57**, 2355-2363 (*synth*)
Gompel, M. *et al., Bioorg. Med. Chem. Lett.*, 2004, **14**, 1703-1707 (*activity*)
Karpov, A.S. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 6951-6956 (*synth*)

Meridine M-158

*12(13*H*)-Meridinone*
[129722-90-3]



$C_{18}H_9N_3O_2$ 299.288
Tautomeric system, both tautomers isolable. Alkaloid from the ascidian *Amphicarpa meridiana* and the marine sponge *Corticium* sp. Cytotoxic. Exhibits antifungal activity. Yellow amorph. solid.
Mp 250°.

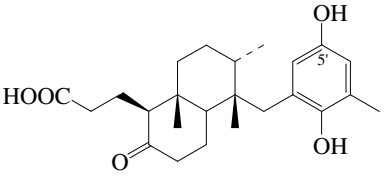
Oxo-*form*
Isomeridine
Separately isolable, tautom. to Meridine after 1-2 d. in $CDCl_3$ soln.

[129722-91-4]

Schmitz, F.J. *et al., Pure Appl. Chem.*, 1990, **62**, 1393-1396 (*Isomeridine*)
Schmitz, F.J. *et al., J.O.C.*, 1991, **56**, 804-808 (*isol, pmr, cmr, cryst struct*)
McCarthy, P.J. *et al., J. Nat. Prod.*, 1992, **55**, 1664-1668 (*isol, props*)
Kitahara, Y. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1363-1364 (*synth*)
Bontemps, N. *et al., Tetrahedron*, 1997, **53**, 1743-1750 (*synth*)
Kitahara, Y. *et al., Tetrahedron*, 1998, **54**, 8421-8432 (*synth, pmr, cmr*)

Stypopodium Meroterpenoid A M-159

[476478-79-2]



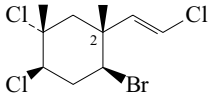
$C_{24}H_{34}O_5$ 402.53
Constit. of *Stypopodium zonale*. Yellow oil (as Me ester).
$[\alpha]_D^{25}$ +22.1 (c, 0.07 in $CHCl_3$) (Me ester). Not named in ref.

5′-Me ether: **Stypopodium *Meroterpenoid B***
[476478-78-1]
$C_{25}H_{36}O_5$ 416.556
Constit. of *Stypopodium zonale*. Yellow oil (as Me ester). $[\alpha]_D^{25}$ +7.5 (c, 0.13 in $CHCl_3$) (Me ester). Not named in ref.

Dorta, E. *et al., J. Nat. Prod.*, 2002, **65**, 1727-1730 (*isol, pmr, cmr*)

Mertensene M-160

2-Bromo-4,5-dichloro-1-(2-chloroethenyl)-1,5-dimethylcyclohexane. Mertensene 1
[66389-40-0]



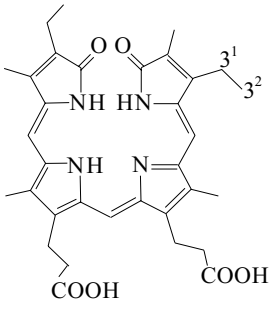
$C_{10}H_{14}BrCl_3$ 320.483
Constit. of *Plocamium mertensii*, *Plocamium hamatum* and *Aplysia punctata*. Shows antibacterial and antialgal props. Insecticide. Sedative, smooth muscle relaxant, anticonvulsant. Needles (hexane). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 105.5-106°. $[\alpha]_D$ +20 (c, 0.3 in $CHCl_3$).

2-Epimer: ***Coccinene***†
[95044-70-5]
$C_{10}H_{14}BrCl_3$ 320.483
Constit. of *Plocamium coccineum*. Cryst. (hexane).
Mp 65°. $[\alpha]_D^{25}$ -24 (c, 0.82 in $CHCl_3$).

Norton, R.S. *et al., Tet. Lett.*, 1977, 3905-3908 (*isol*)
Capon, R.J. *et al., Aust. J. Chem.*, 1984, **37**, 537-544 (*isol*)
Castedo, L. *et al., J. Nat. Prod.*, 1984, **47**, 724-726 (*Coccinene, isol*)
Crews, P. *et al., J.O.C.*, 1984, **49**, 1371-1377 (*cmr, struct*)
Sardina, F.J. *et al., Chem. Lett.*, 1985, 697-700 (*Coccinene, struct*)
Coll, J.C. *et al., Aust. J. Chem.*, 1988, **41**, 1743-1753 (*struct, cmr*)
Konig, G.M. *et al., Phytochemistry*, 1991, **52**, 1047-1053 (*isol, activity*)

Mesobiliverdin IXα M-161

*3,18-Diethyl-1,19,22,24-tetrahydro-2,7,13,17-tetramethyl-1,19-dioxo-21*H*-biline-8,12-dipropanoic acid, 9CI. Glaucobilin IXα. Glaucobilin. Mesobiliverdin*
[493-88-9]



$C_{33}H_{38}N_4O_6$ 586.686
Oxidn. prod. from Mesobilirubin. Bile pigment. Greenish-blue cryst. (MeOH).
Mp 304° (205-220°, 316° dec.).

Di-Me ester: [21059-15-4]
$C_{35}H_{42}N_4O_6$ 614.74
Bile pigment. Deep-blue-violet cryst. ($CHCl_3$).
Mp 216° (232°).

3^1-Hydroxy: 3^1-Hydroxymesobiliverdin IXα
$C_{33}H_{38}N_4O_7$ 602.686
Isol. from the red alga *Cyanidium caldarium*.

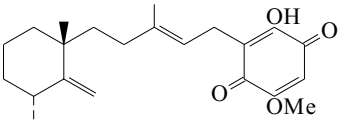
3^2-Hydroxy: 3^2-Hydroxymesobiliverdin IXα. ***Turboverdin***
[72436-15-8]
$C_{33}H_{38}N_4O_7$ 602.686
Isol. from the ovary of *Turbo cornutus*. Dark blue plates (as di-Me ester).
Mp 214-215° (di-Me ester).

[72436-16-9, 100776-56-5]

Fischer, H. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1932, **206**, 201
Siedel, W. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1935, **237**, 8 (*synth*)
Stoll, M.S. *et al., Biochem. J.*, 1977, **163**, 59 (*pmr, ms*)
Ogata, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1979, **63**, 239 (*Turboverdin*)
Benedikt, E. *et al., Z. Naturforsch., C*, 1985, **40**, 755 (*3′-Hydroxymesobiliverdin*)
Awruch, J. *et al., Tetrahedron*, 1986, **42**, 4137 (*synth*)
Saito, S. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 3539 (*synth*)
Benedikt, E. *et al., Eur. J. Biochem.*, 1988, **175**, 643 (*Turboverdin*)
Arciero, D.M. *et al., J. Biol. Chem.*, 1988, **263**, 18350 (*synth, pmr*)

Metachromin A M-162

[114466-74-9]

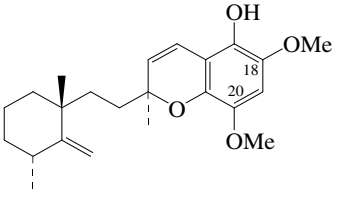


$C_{22}H_{30}O_4$ 358.477
Isol. from the sponge *Hippospongia* cf. *metachromia*. Orange cryst. (hexane).
Mp 80-82°. $[\alpha]_D^{27}$ -11 (c, 1 in $CHCl_3$). λ_{max} 220 (ϵ 36000); 289 (ϵ 12000); 520 (ϵ 1200) (MeOH/pH 10) (Derep). λ_{max} 206 (ϵ 15000); 286 (ϵ 14000); 435 (ϵ 500) (MeOH/pH 7) (Derep).

Ishibashi, M. *et al., J.O.C.*, 1988, **53**, 2855
Kobayashi, J. *et al., J.O.C.*, 1992, **57**, 5773 (*cmr*)
Almeida, W.P. *et al., Tet. Lett.*, 1994, **35**, 1367 (*synth*)
Almeida, W.P. *et al., J. Braz. Chem. Soc.*, 1999, **10**, 401-414 (*synth*)
Brüggeman, M. *et al., Eur. J. Org. Chem.*, 2001, 647-654 (*synth*)

Metachromin B M-163

[114466-75-0]



$C_{23}H_{32}O_4$ 372.503
Isol. from the sponge *Hippospongia* cf. *metachromia*. Oil. $[\alpha]_D^{24}$ +8 (c, 1 in $CHCl_3$). λ_{max} 221 (ϵ 31000); 289 (ϵ 5800); 354 (ϵ 2700) (MeOH/pH 11) (Derep). λ_{max} 207 (ϵ 15000); 223 (ϵ 15000); 278 (ϵ 7000); 334 (ϵ 1800) (MeOH/pH 7) (Derep).

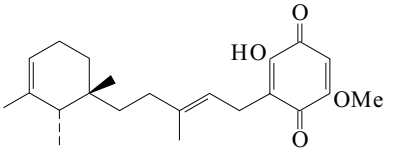
O^{19}-De-Me: ***Hippochromin A***
[348083-28-3]
$C_{22}H_{30}O_4$ 358.477
Constit. of *Hippospongia metachromia*.

O^{20}-De-Me: ***Hippochromin B***
[348083-29-4]
$C_{22}H_{30}O_4$ 358.477
Constit. of *Hippospongia metachromia*. λ_{max} 276 (log ϵ 3.67); 290 (log ϵ 3.7) (MeOH).

Ishibashi, M. *et al., J.O.C.*, 1988, **53**, 2855-2858 (*Metachromin B*)
Kobayashi, J. *et al., J.O.C.*, 1992, **57**, 5773-5776 (*cmr*)
Shen, Y.-C. *et al., J. Nat. Prod.*, 2001, **64**, 801-803 (*Hippochromins*)

Metachromin C M-164

[124596-50-5]



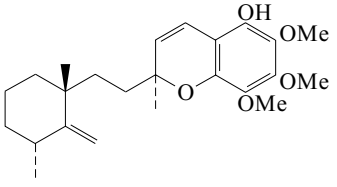
$C_{22}H_{30}O_4$ 358.477
Constit. of *Hippospongia metachromia*. Shoes coronary vasodilatory props. Yellow solid (hexane). Sol. MeOH, EtOAc; poorly sol. H_2O.

Mp 90-91°. $[\alpha]_D^{26}$ -29.7 (c, 0.2 in $CHCl_3$). λ_{max} 208 (ϵ 49500); 285 (ϵ 17200); 425 (ϵ 400) (MeOH) (Berdy). λ_{max} 206 (ϵ 49500); 290 (ϵ 11800); 515 (ϵ 900) (MeOH-NaOH) (Berdy).

Kobayashi, J. *et al., J. Nat. Prod.*, 1989, **52**, 1173 (*isol, pmr, cmr*)
Kobayashi, J. *et al., J.O.C.*, 1992, **57**, 5773 (*cmr*)

Metachromin D M-165

[143592-21-6]

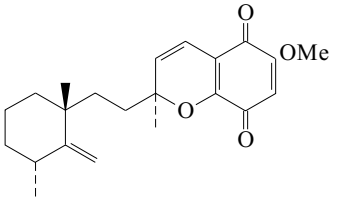


$C_{24}H_{34}O_5$ 402.53
Constit. of *Hippospongia metachroma*. Oil. $[\alpha]_D^{22}$ +15 (c, 0.7 in $CHCl_3$). λ_{max} 226 (ϵ 25000); 280 (ϵ 10000); 320 (ϵ 3000) (MeOH) (Berdy).

Kobayashi, J. *et al., J.O.C.*, 1992, **57**, 5773 (*isol, pmr, cmr*)

Metachromin E M-166

[143592-22-7]

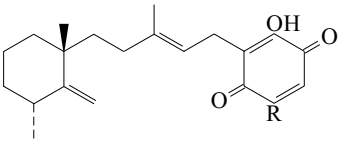


$C_{22}H_{28}O_4$ 356.461
Constit. of *Hippospongia metachroma*. Orange oil. $[\alpha]_D^{22}$ -54 (c, 0.3 in $CHCl_3$). λ_{max} 260 (ϵ 6000); 290 (ϵ 8700); 360 (ϵ 500); 483 (ϵ 300) (MeOH) (Berdy).

Kobayashi, J. *et al., J.O.C.*, 1992, **57**, 5773 (*isol, pmr, cmr*)

Metachromin F M-167

[143592-23-8]



R = $OCH_2CH_2CH_2CH_3$

$C_{25}H_{36}O_4$ 400.557
Consit. of *Hippospongia metachroma*. Yellow oil. $[\alpha]_D^{22}$ -4 (c, 0.2 in $CHCl_3$). λ_{max} 290 (ϵ 16400); 455 (ϵ 250) (MeOH) (Berdy).

Kobayashi, J. *et al., J.O.C.*, 1992, **57**, 5773 (*isol, pmr, cmr*)

Metachromin G M-168

[143592-24-9]
As Metachromin F, M-167 with
R = $NHCH_2CH_2Ph$
$C_{29}H_{37}NO_3$ 447.616
Constit. of *Hippospongia metachroma*. Purple oil. $[\alpha]_D^{20}$ -18 (c, 0.2 in C_6H_6). λ_{max} 211 (ϵ 29700); 324 (ϵ 14700); 508 (ϵ 800) (MeOH) (Berdy).

Kobayashi, J. *et al., J.O.C.*, 1992, **57**, 5773 (*isol, pmr, cmr*)

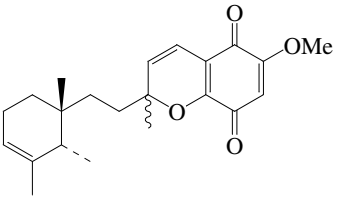
Metachromin H M-169

[143592-25-0]
As Metachromin F, M-167 with
R = $NHCH_2CH_2CH(CH_3)_2$
$C_{26}H_{39}NO_3$ 413.599
Constit. of *Hippospongia metachroma*. Purple oil. $[\alpha]_D^{19}$ -9 (c, 0.2 in C_6H_6). λ_{max} 324 (ϵ 12800); 512 (ϵ 700) (MeOH) (Berdy).

Kobayashi, J. *et al., J.O.C.*, 1992, **57**, 5773 (*isol, pmr, cmr*)

Metachromin J M-170

[882524-91-6]

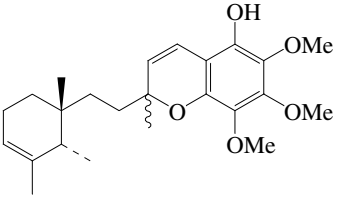


$C_{22}H_{28}O_4$ 356.461
Constit. of a *Spongia* sp. Red oil. $[\alpha]_D^{24}$ -38 (c, 0.2 in $CHCl_3$). λ_{max} 203 (ϵ 18000); 258 (ϵ 7000); 303 (ϵ 8300) (MeOH).

Takahashi, Y. *et al., Heterocycles*, 2006, **67**, 791-795

Metachromin K M-171

[882524-92-7]



$C_{24}H_{34}O_5$ 402.53
Constit. of a *Spongia* sp. Oil. $[\alpha]_D^{24}$ +13 (c, 0.3 in $CHCl_3$). λ_{max} 204 (ϵ 30000); 224 (ϵ 26000); 282 (ϵ 11000) (MeOH).

Takahashi, Y. *et al., Heterocycles*, 2006, **67**, 791-795

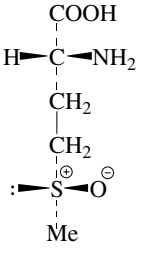
Metamorphosin A M-172

Pyroglutamylglutaminylprolylglycylleucyltryptophanamide
[157622-03-2]
H-5-OxoPro-Gln-Pro-Gly-Leu-Trp-NH_2
$C_{34}H_{47}N_9O_8$ 709.801
Isol. from the marine hydroid *Hydractinia echinata*. Induces morphogenesis in host.

Leitz, T. *et al., Dev. Biol.*, 1994, **163**, 440 (*isol, struct*)

Methionine sulfoxide M-173

2-Amino-4-(methylsulfinyl)butanoic acid, 9CI. Methionine S-*oxide*
[62697-73-8]



$(R)_c,(R)_s$-*form*

$C_5H_{11}NO_3S$ 165.213

(*R*)$_C$(*R*)$_S$-*form* [50896-97-4]
Mp 250-255° dec. $[\alpha]_D$ -100.2 (c, 0.6 in H_2O).

(*R*)$_C$(*S*)$_S$-*form* [50896-98-5]
Mp 235-240°. $[\alpha]_D$ +78 (c, 0.5 in H_2O) (>95% de).

N-*Phthaloyl:* [210167-64-9]
Mp 181-183°. $[\alpha]_D$ +63 (c, 0.8 in EtOH) (>95% de).

(*S*)$_C$(*R*)$_S$-*form* [3226-66-2]
[3226-65-1]
Isol. from various red algae incl. *Amphiroa beauvoisii* and *Grateloupia proteus.*
Cryst. (EtOH aq.).
Mp 239° dec. $[\alpha]_D^{25}$ -77 (c, 1 in H_2O). $[\alpha]_D^{25}$ -57.6 (1*M* HCl).

N-*Me:* **N-*Methylmethionine sulfoxide***
[53179-67-2]
$C_6H_{13}NO_3S$ 179.24
Isol. from various red algae incl. *Centroceras clavulatum*, *Grateloupia doryphora* and *Gelidium latifolium*. Cryst. (EtOH aq.).
Mp 224-227°. $[\alpha]_D^{20}$ -33.6 (c, 1 in H_2O).

(*S*)$_C$(*S*)$_S$-*form* [23631-84-7]
[3226-65-1]
Constit. of the blowfly *Phormia regina* and *Bombyx mori*.
Cryst. (MeOH aq.).
Mp 250-255° sinters. $[\alpha]_D^{20}$ +99.7 (c, 1 in H_2O). $[\alpha]_D^{20}$ +127 (1*M* HCl).

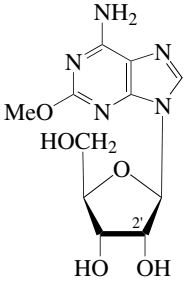
N-*Phthaloyl:* [23631-85-8]
Cryst. (MeOH). Mp 217-218°. $[\alpha]_D$ +12.5 (c, 1.2 in EtOH) (>98% de).

[454-41-1, 1118-85-0, 7530-67-8, 173239-84-4, 210167-66-1]

Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 2145 (*synth*)
Lucas, F. *et al., Biochem. J.*, 1966, **100**, 473-478 (*ir, ord, isol*)
Impellizzeri, G. *et al., Phytochemistry*, 1975, **14**, 1549-1557 (*algae, isol*)
Cancetti, A. *et al., Biol. Met.*, 1990, **3**, 125
Brot, N. *et al., BioFactors*, 1991, **3**, 91-96 (*biochem*)
Yang, J. *et al., Insect Biochem.*, 1995, **25**, 975-980 (*isol*)
Holland, H.L. *et al., Tetrahedron: Asymmetry*, 1998, **9**, 535-538 (*synth, N-phthaloyl*)
Simon-Colin, C. *et al., Phycol. Res.*, 2002, **50**, 125-128 (*Grateloupia doryphora constit, isol*)
Simon-Colin, C. *et al., Phytochem. Rev.*, 2005, **3**, 367-370 (*Grateloupia doryphora constit, isol, purif*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, ALF600

2-Methoxyadenosine M-174

Spongosine
[24723-77-1]



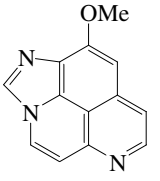
$C_{11}H_{15}N_5O_5$ 297.27
Isol. from the Caribbean sponge *Cryptotethia crypta* and from an unidentified Australian sponge (Tethyidae). Muscle relaxant; CNS depressant; cardioactive, antiinflammatory and hypothermic agent. Sol. H_2O, MeOH.
Mp 191-192°. $[\alpha]_D$ -43.5 (NaOH aq.). λ_{max} 248 (ϵ 7500); 275 (ϵ 11000) (pH 2) (Derep). λ_{max} 255 (sh) (ϵ); 268 (ϵ 12000) (pH 7) (Derep). λ_{max} 235; 267 (ϵ 14200) (MeOH) (Berdy). λ_{max} 269 (H_2O) (Berdy).

2′-Deoxy: ***2′-Deoxyspongosine****. 2′-Deoxy-2-methoxyadenosine*
[24757-70-8]
$C_{11}H_{15}N_5O_4$ 281.271
Isol. from an unidentified Australian sponge. Amorph. solid (H_2O).
Mp 174-175°. $[\alpha]_D$ -22.5 (c, 1 in DMSO). λ_{max} 267 (ϵ 13700) (MeOH) (Berdy).

Bergmann, W. *et al., J.O.C.*, 1951, **16**, 981-987; 1956, **21**, 226-228; 1957, **22**, 1575-1577 (*isol, struct, synth*)
Cook, A.F. *et al., J.O.C.*, 1980, **45**, 4020-4025 (*synth*)
Searle, P.A. *et al., J. Nat. Prod.*, 1994, **57**, 1452-1454 (*isol, uv, ir, pmr, cmr, ms*)

10-Methoxybenzimidazo[6,7,1-*def*][1,6]naphthyridine, 9CI M-175

[597553-94-1]

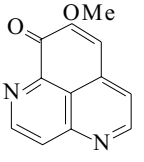


$C_{13}H_9N_3O$ 223.234
Alkaloid from a *Xestospongia* sp. Brown gum. λ_{max} 209 (ϵ 5845); 237 (ϵ 5250); 258 (ϵ 2980); 269 (ϵ 2770); 355 (ϵ 2015) (EtOH).

Calcul, L. *et al., Tetrahedron*, 2003, **59**, 6539-6544 (*isol, pmr, cmr*)

8-Methoxy-9*H*-benzo[*de*][1,6]naphthyridin-9-one, 9CI M-176

Demethyloxyaaptamine
[88839-99-0]



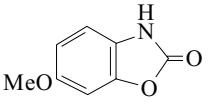
$C_{12}H_8N_2O_2$ 212.207
Alkaloid from the Okinawan marine sponge *Aaptos aaptos* and a *Xestospongia* sp. Cytotoxic. Exhibits potent antimicrobial activity against gram-positive and -negative bacteria. Fine bright yellow rods (EtOAc).
Mp 210-212° (198-200° dec.). λ_{max} 235 (ϵ 10600); 308 (ϵ 1740); 360 (sh) (ϵ 5540); 373 (ϵ 5040); 415 (sh) (ϵ 2310) (H_2O) (Derep).

Di-Me acetal: ***8,9,9-Trimethoxy-9H-benzo[de][1,6]naphthyridine***
$C_{14}H_{14}N_2O_3$ 258.276
Alkaloid from a *Xestospongia* sp. Brown gum. λ_{max} 205 (ϵ 7045); 229 (ϵ 11330); 350 (ϵ 4560) (EtOH).

Nakamura, H. *et al., J.C.S. Perkin 1*, 1987, 173 (*isol, uv, ir, pmr, cmr, struct*)
Pelletier, J.C. *et al., J.O.C.*, 1987, **52**, 616 (*synth, ir, pmr*)
Coutinho, A.F. *et al., Heterocycles*, 2002, **57**, 1265-1272 (*isol, pmr, cmr*)
Calcul, L. *et al., Tetrahedron*, 2003, **59**, 6539-6544 (*isol, pmr, cmr*)

6-Methoxy-2(3*H*)-benzoxazolone, 9CI M-177

6-Methoxy-2-benzoxazolinone, 8CI. Coixol. MBOA
[532-91-2]



$C_8H_7NO_3$ 165.148
Isol. from roots of *Coix lacryma jobi* (Job's tears) (Gramineae) and from seedlings of several cereal plants, e.g. wheat (*Triticum aestivum*), corn (*Zea mays*) and rye (*Secale cereale*). Also present in all plant parts of *Scoparia dulcis* (Scrophulariaceae)and isol

from a marine sponge *Oceanapia* sp. Disease and insect attack inhibitor in plants. Toxic to brine shrimp. Pink cryst. (MeOH aq.). Sol. bases, EtOH, Et_2O, C_6H_6; fairly sol. H_2O; poorly sol. hexane. Mp 160-161° (154-155°). λ_{max} 229; 286 (H_2O) (Berdy).

▶ DM5275200

N-*Ac:* [62655-08-7]
$C_{10}H_9NO_4$ 207.185
Needles. Mp 147.5°.

N-*Benzoyl:*
$C_{15}H_{11}NO_4$ 269.256
Needles. Mp 162-162.5°.

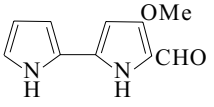
O-*De-Me:* ***6-Hydroxy-2(3H)-benzoxazolone, 9CI***. *6-Hydroxy-2-benzoxazolinone*
$C_7H_5NO_3$ 151.121
Alkaloid from *Acanthus arboreus*. Pale yellow cryst.
Mp 260°. λ_{max} 268; 302; 305; 340 (MeOH).

5-Chloro: 5-Chloro-6-methoxy-2(3H)-benzoxazolone. 5-Chloro-6-methoxy-2-benzoxazolinone
$C_8H_6ClNO_3$ 199.593
Isol. from *Zea mays*.

Koyama, T. *et al., Yakugaku Zasshi*, 1955, **75**, 699
Virtanen, A.I. *et al., Suom. Kemistil. B*, 1956, **29**, 143; 171
List, P.H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1959, **292**, 452
Allen, E.H. *et al., J.O.C.*, 1971, **36**, 2004 (*synth*)
Richey, J.D. *et al., Agric. Biol. Chem.*, 1976, **40**, 2413 (*synth*)
Kubo, I. *et al., Experientia*, 1983, **39**, 355 (*isol, synth*)
Sicher, D. *et al., Synthesis*, 1989, 875 (*synth*)
Maleski, R.J. *et al., J. Het. Chem.*, 1991, **28**, 1937 (***synth***)
Bjostad, L.B. *et al., J. Chem. Ecol.*, 1992, **18**, 931
Hayashi, T. *et al., Phytochemistry*, 1994, **37**, 1611 (*isol, occur*)
Kato-Noguchi, H. *et al., Phytochemistry*, 1998, **49**, 433-435 (*5-chloro*)
Venkateswarlu, Y. *et al., Biochem. Syst. Ecol.*, 1999, **27**, 519-520 (*isol, activity*)
Amer, M.E. *et al., J. Braz. Chem. Soc.*, 2004, **15**, 262-266 (*6-Hydroxybenzoxazolinone*)

4-Methoxy-2,2′-bipyrrole-5-carboxaldehyde M-178

5-Formyl-4-methoxy-2,2′-bipyrrole. Tambjamine aldehyde
[10476-41-2]

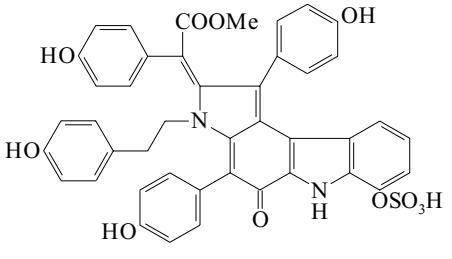


$C_{10}H_{10}N_2O_2$ 190.201
Isol. from the nembrothid nudibranchs *Roboastra tigris*, *Tambja eliora*, *Tambja abdere* and the bryozoan *Sessibugula translucens*. Cryst. (EtOH aq.).
Mp 263-265° dec. Artifact. λ_{max} 251 (ϵ 14700); 361 (ϵ 40300) (MeOH).

Rapoport, H. *et al., J.A.C.S.*, 1962, **84**, 635-642 (*synth, uv*)
Carté, B. *et al., J.O.C.*, 1983, **48**, 2314-2318 (*isol, uv, ir, pmr*)

37-(Methoxycarbonyl)dictyodendrin E M-179

[149444-92-8]



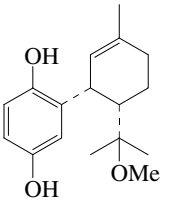
$C_{43}H_{32}N_2O_{11}S$ 784.799
Alkaloid from the marine sponge *Dictyodendrilla* sp. Potent aldose reductase inhibitor. Antidiabetic agent. Purple solid. Sol. MeOH, EtOAc.
Mp 300°. λ_{max} 231 (ϵ 41000); 281 (ϵ 21000); 482 (ϵ 23200) (EtOH) (Derep).

De(methoxycarbonyl): ***Dictyodendrin E***
$C_{41}H_{30}N_2O_9S$ 726.762
Alkaloid from *Dictyodendrilla verongiformis*. Amorph. red solid (as Na salt). λ_{max} 230 (ϵ 33900); 280 (ϵ 17700); 464 (ϵ 20600) (MeOH) (Na salt).

Sato, A. *et al., J.O.C.*, 1993, **58**, 7632 (*isol, uv, ir, pmr, cmr, struct*)
Warabi, K. *et al., J.O.C.*, 2003, **68**, 2765-2770 (*Dictyodendrin E*)
Fürstner, A. *et al., J.A.C.S.*, 2006, **128**, 8087-8094 (*synth*)

Methoxyconidiol M-180

[868391-32-6]

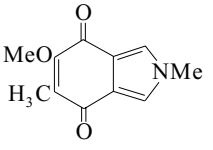


$C_{17}H_{24}O_3$ 276.375
Constit. of *Aplidium* aff. *densum*. Yellow oil. $[\alpha]_D^{23}$ +6.4 (c, 0.2 in $CHCl_3$).

Simon-Levert, A. *et al., J. Nat. Prod.*, 2005, **68**, 1412-1415 (*Methoxyconidiol*)

5-Methoxy-2,6-dimethyl-2*H*-isoindole-4,7-dione, 9CI M-181

2,5-Dimethyl-6-methoxy-4,7-isoindolequinone
[79664-59-8]

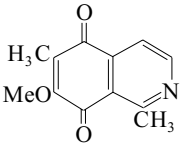


$C_{11}H_{11}NO_3$ 205.213
Found in *Reniera* sp. Active against gram-positive bacteria and marine pseudomonads.
Mp 153-154° Mp 167-168° (synthetic). First naturally-occurring isoindole. λ_{max} 224 (ϵ 13600); 233 (ϵ 12000); 275 (ϵ 11000); 362 (ϵ 3030) (MeOH) (Derep).

Frincke, J.M. *et al., J.A.C.S.*, 1982, **104**, 265 (*isol, struct*)
Parker, K.A. *et al., Tet. Lett.*, 1984, **25**, 4917 (*synth*)
Padwa, A. *et al., J.O.C.*, 1985, **50**, 4006 (*synth*)
Schubert-Zsilavecz, M. *et al., Annalen*, 1991, 973 (*synth*)

7-Methoxy-1,6-dimethyl-5,8-isoquinolinedione, 9CI M-182

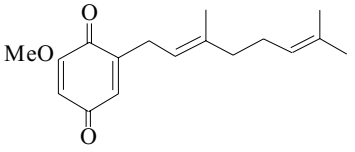
[79664-58-7]



$C_{12}H_{11}NO_3$ 217.224
Isol. from an unidentified *Reniera* sponge and an undescribed *Xestospongia* sp. Shows insecticidal activity and weak activity against gram-positive bacteria. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 188-190° dec. λ_{max} 223 (ϵ); 276 (ϵ); 283 (ϵ); 292 (ϵ) (MeOH) (Derep).

Frincke, J.M. *et al., J.A.C.S.*, 1982, **104**, 265 (*isol, uv, ir, pmr, cmr, ms, struct*)
Edrada, R.A. *et al., J. Nat. Prod.*, 1996, **59**, 973 (*isol, props*)
Molina, P. *et al., Synthesis*, 1997, 963-966 (*synth*)
Kuwabara, N. *et al., Tetrahedron*, 2004, **60**, 2943-2952 (*synth*)

6-Methoxy-2-(3,7-dimethyl-2,6-octadienyl)-1,4-benzoquinone M-183



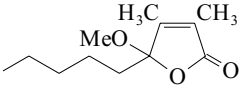
(*E*)–*form*

$C_{17}H_{22}O_3$ 274.359

(*E*)-*form*
Verapliquinone A
[31415-00-6]
Constit. of an *Aplidium* sp. λ_{max} 264 (ϵ 13500); 342 (ϵ 1370) ($CHCl_3$).

(*Z*)-*form*
Verapliquinone B
[109954-48-5]
Constit. of an *Aplidium* sp. λ_{max} 264 (ϵ 13500); 342 (ϵ 1370) ($CHCl_3$).
Guella, G. *et al., Helv. Chim. Acta*, 1987, **26**, 621-626 (*isol, pmr, cmr, uv*)

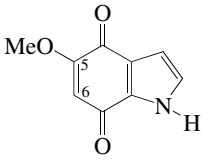
5-Methoxy-3,4-dimethyl-5-pentyl-2(5*H*)-furanone M-184
4-Methoxy-2,3-dimethyl-4-pentyl-2-butenolide
[75239-72-4]



$C_{12}H_{20}O_3$ 212.288

(±)-*form*
Constit. of the red alga *Ahnfeltia paradoxa*.
Oil.
Nomura, Y. *et al., Chem. Lett.*, 1980, 955 (*isol, ms*)

5-Methoxy-1*H*-indole-4,7-dione, 9CI M-185
[17606-06-3]

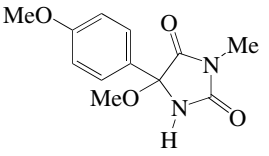


$C_9H_7NO_3$ 177.159
Alkaloid from the muricid gastropod *Drupella fragum*. Antimicrobial agent. Orange needles.
Mp 198-200° (natural) Mp 205-208° (synthetic). λ_{max} 222 (ϵ 18200); 281 (ϵ 19400); 324 (ϵ 2540); 432 (ϵ 1120) (EtOH).
Fukuyama, Y. *et al., Tetrahedron*, 1998, **54**, 10007-10016 (*isol, synth, ir, uv, pmr, cmr*)

6-Methoxy-1*H*-indole-4,7-dione, 9CI M-186
[137542-70-2]

$C_9H_7NO_3$ 177.159
Alkaloid from the muricid gastropod *Drupella fragum*. Antimicrobial agent. Orange prisms.
Mp 188-190° (natural) Mp 210-212° (synthetic). λ_{max} 222 (ϵ 17300); 282 (ϵ 16000); 326 (ϵ 3800); 424 (ϵ 880) (EtOH).
Fukuyama, Y. *et al., Tetrahedron*, 1998, **54**, 10007-10016 (*isol, synth, ir, uv, pmr, cmr*)

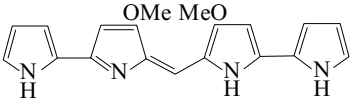
5-Methoxy-5-(4-methoxyphenyl)-3-methyl-2,4-imidazolidinedione M-187



$C_{12}H_{14}N_2O_4$ 250.254

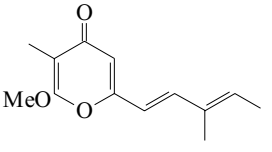
(±)-*form*
Metab. of Indian ocean ascidian *Polycarpa clavata*.
Amorph. solid. Prob. artifact. CAS no. not found 13-14CI. λ_{max} 203 (log ϵ 4.01); 225 (log ϵ 3.79); 277 (log ϵ 3.28); 292 (log ϵ 3.19) (MeOH).
Kang, H. *et al., Tet. Lett.*, 1996, **37**, 2369-2372 (*isol, ir, uv, pmr, cmr, struct*)

4-Methoxy-5-[(3-methoxy-5-pyrrol-2-yl-2*H*-pyrrol-2-ylidene)methyl]-2,2′-bipyrrole, 8CI M-188
[19369-65-4]
[19369-64-3]



$C_{19}H_{18}N_4O_2$ 334.377
Pyrrole antibiotic. Pigment from an Australian ascidian and from the bryozoan *Bugula dentata*, also prod. by a mutant strain of the bacterium *Serratia marcescens*, from *Streptomyces coelicolor* and from *Nembrotha kubaryana*. Shows mild activity against gram-positive bacteria. Blue cryst. (CH_2Cl_2/petrol)(as hydrochloride).
Mp 300° dec. (hydrochloride). Red colour in basic soln λ_{max} 555 (sh); 588 (HCl salt) (Derep). λ_{max} 326 (ϵ 26300); 556 (ϵ 2840); 599
(ϵ 103000) ($CHCl_3$) (Berdy).
Wasserman, H.H. *et al., Tet. Lett.*, 1968, 641 (*isol, pmr, struct, synth*)
Kazlauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 215 (*isol, uv, ir, pmr, cmr, ms*)
Matsunaga, S. *et al., Experientia*, 1986, **42**, 84 (*isol, uv, pmr, cmr*)
Karuso, P. *et al., Molecules*, 2002, **7**, 1-6 (*isol, Nembrotha*)

2-Methoxy-3-methyl-6-(3-methyl-1,3-pentadienyl)-4*H*-pyran-4-one, 9CI M-189
12-Norcycercene B

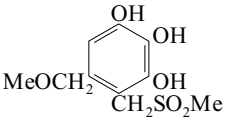


$C_{13}H_{16}O_3$ 220.268

(*E,E*)-*form* [144938-27-2]
Isol. from *Ercolania funerea*.
Vardaro, R.R. *et al., Tetrahedron*, 1992, **48**, 9561 (*isol, struct*)

5-(Methoxymethyl)-4-[(methylsulfonyl)methyl]-1,2,3-benzenetriol M-190

[119188-80-6]



$C_{10}H_{14}O_6S$ 262.283

Constit. of the red alga *Grateloupia filicina*. Exhibits moderate antibacterial activity. Powder. Sol. MeOH, EtOAc. Mp 164.5-166.5°. λ_{max} 280 (ϵ 600) (EtOH) (Derep). λ_{max} 275 (EtOH) (Berdy).

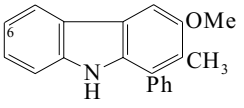
Tri-Ac: [119188-81-7]
Mp 127-129°.

Nozaki, H. *et al., Agric. Biol. Chem.*, 1988, **52**, 3229 (*isol, pmr, cmr, ms*)
Ohira, S. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 2427 (*synth*)

3-Methoxy-2-methyl-1-phenyl-9*H*-carbazole, 9CI M-191

Hyellazole

[74364-11-7]



$C_{20}H_{17}NO$ 287.36

Alkaloid from the blue-green alga *Hyella caespitosa*. Mp 133-134°. λ_{max} 226 (sh) (ϵ 34000); 232 (ϵ 36500); 238 (sh) (ϵ 34500); 250 (sh) (ϵ 20000); 260 (sh) (ϵ 13500); 292 (sh) (ϵ 12500); 304 (ϵ 18500); 338 (ϵ 4500); 352 (ϵ 5000) (EtOH) (Derep).

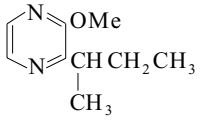
*6-Chloro: 6-Chloro-3-methoxy-2-methyl-1-phenyl-9*H*-carbazole, 9CI.* ***Chlorohyellazole***
[74364-10-6]
$C_{20}H_{16}ClNO$ 321.805
Alkaloid from *Hyella caespitosa*. Mp 163-164°. λ_{max} 220 (ϵ 32600); 235 (ϵ 32600); 242 (ϵ 32700); 255 (sh) (ϵ 20000); 272 (sh) (ϵ 14600); 300 (sh) (ϵ 13200); 310 (ϵ 18000); 348 (ϵ 4400); 360 (ϵ 4200) (EtOH) (Derep).

Cardellina, J.H. *et al., Tet. Lett.*, 1979, 4915 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Kano, S. *et al., Chem. Comm.*, 1980, 1241 (*synth, cmr*)
Takano, S. *et al., Heterocycles*, 1981, **16**, 1479 (*synth*)
Kano, S. *et al., J.O.C.*, 1981, **46**, 3856 (*synth, pmr, ms*)
Bergman, J. *et al., Tetrahedron*, 1988, **44**, 5215 (*synth*)
Kawasaki, T. *et al., Chem. Comm.*, 1989, 43 (*synth*)
Moody, C.J. *et al., J.C.S. Perkin 1*, 1989, 376; 2463 (*synth*)
Kawasaki, T. *et al., J.C.S. Perkin 1*, 1993, 1777 (*synth*)
Beccalli, E.M. *et al., J.C.S. Perkin 1*, 1994, 579 (*synth, Hyellazole, Chlorohyellazole*)
Knölker, H.-J. *et al., Tet. Lett.*, 1995, **36**, 5339 (*synth*)
Choshi, T. *et al., J.O.C.*, 1997, **62**, 2535 (*synth*)
Knoelker, H.-J. *et al., Tetrahedron*, 1999, **55**, 10391-10412 (*synth*)

2-Methoxy-3-(1-methylpropyl)pyrazine, 9CI M-192

*2-*sec*-Butyl-3-methoxypyrazine, 8CI. 2-Methoxy-3-*sec*-butylpyrazine. FEMA 3433*

[24168-70-5]



$C_9H_{14}N_2O$ 166.222

Volatile component of many vegetables, e.g. asparagus, carrot, celery, cucumber, parsnip, bell peppers, *Pisum sativum* (pea). Found in galbanum and petitgrain oils and ginger. Prod. by *Chondromyces crocatus* and a marine *Streptomyces* sp. GWS-BW-H5. Fragrance and flavour ingredient.

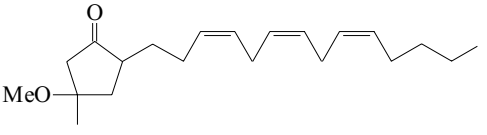
(±)-form

Bp_{10} 78-83°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 842C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 404C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1560D (*ir*)
Bramwell, A.F. *et al., Tet. Lett.*, 1969, 3215
Murray, K.E. *et al., Chem. Ind. (London)*, 1970, 897
Murray, K.E. *et al., J. Sci. Food Agric.*, 1975, **26**, 973
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 459
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1698 (*occur*)
Schulz, S. *et al., Tetrahedron*, 2004, **60**, 3863-3872 (*isol*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 837-865 (*marine isol*)

4-Methoxy-4-methyl-2-(3,6,9-tetradecatrienyl)cyclopentanone M-193

[156992-92-6]



$C_{21}H_{34}O_2$ 318.498

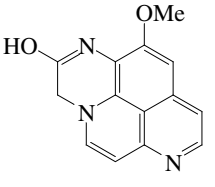
Constit. of the sea pen *Virgularia* sp. Oil. $[\alpha]_D$ +2.8 (c, 0.9 in $CHCl_3$).

Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 55 (*isol, pmr, cmr*)

11-Methoxy-3*H*-naphthridino[6,5,4-*def*]quinoxalin-2-ol M-194

*11-Methoxy-1*H*-naphthridino[6,5,4-*def*]quinoxalin-2(3*H*)-one, 9CI*

[597553-92-9]



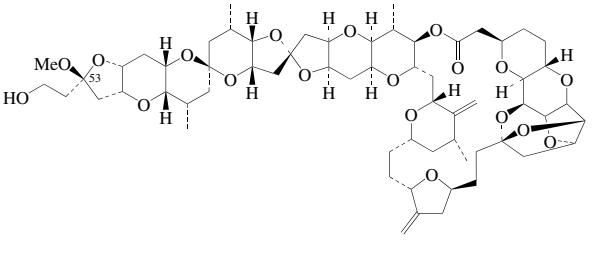
$C_{14}H_{11}N_3O_2$ 253.26

CAS name refers to *NH*-tautomer. Alkaloid from a *Xestospongia* sp. Brown gum. λ_{max} 210 (ϵ 5420); 222 (ϵ 4795); 238 (ϵ 4660); 260 (ϵ 2940); 271 (ϵ 2600); 357 (ϵ 1330); 371 (ϵ 1070) (EtOH).

Calcul, L. *et al., Tetrahedron*, 2003, **59**, 6539-6544 (*isol, pmr, cmr*)

53-Methoxyneoisohomohalichondrin B M-195

[187172-30-1]



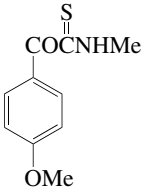
$C_{62}H_{88}O_{19}$ 1137.366

Polyether antibiotic. Isol. from the sponge *Lissodendoryx* sp. Oil.

53-Epimer: ***Epi-53-methoxyneoisohomohalichondrin B***
[187172-32-3]

$C_{62}H_{88}O_{19}$ 1137.366
Isol. from *Lissodendoryx* sp. Oil.
Litaudon, M. *et al., J.O.C.*, 1997, **62**, 1868 (*isol, pmr, cmr*)

(4-Methoxyphenyl)-*N*-methyl-2-oxothioacetamide M-196
4-Methoxy-N-*methyl-α-oxobenzeneethanethioamide*



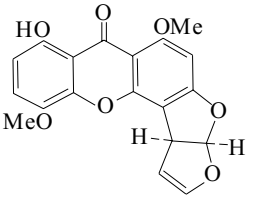
$C_{10}H_{11}NO_2S$ 209.268
Isol. from the ascidian *Polycarpa aurata*. Inhibitor of inosine monophosphate dehydrogenase. Yellow cryst. ($CHCl_3$/MeOH). Probable artifact. Not in CA.

Abas, S.A. *et al., J.O.C.*, 1996, **61**, 2709-2712 (*isol, ir, pmr, cmr, ms, cryst struct*)

***N*-(2-Methoxy-2-propenyl)trimethylammonium(1+)** M-197
(2-Methoxyallyl)trimethylammonium, 8CI
$H_2C{=}C(OMe)CH_2N^{\oplus}Me_3$
$C_7H_{16}NO^{\oplus}$ 130.21
Isol. from the marine sponge *Raspailia* sp. Counterion of natural compd not specified.

Bromide: ***Meprochol, BAN****. Esmodil*
[590-31-8]
$C_7H_{16}BrNO$ 210.114
Muscarinic agonist. Cryst. powder. Sol. H_2O, EtOH. Mp 169°.
▶ BR7167000
Ger. Pat., 1935, 614 462; *CA*, **29**, 5994 (*synth*)
Asakawa, H. *et al., Okayama Igakkai Zasshi*, 1939, **51**, 1020; *CA*, **37**, 682b (*pharmacol*)
Capon, R.J. *et al., Nat. Prod. Res.*, 2004, **18**, 305-309 (*isol, synth, pmr, cmr*)

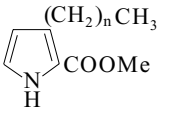
5-Methoxysterigmatocystin M-198
*3a,12c-Dihydro-8-hydroxy-6,11-dimethoxy-7*H-*furo[3′,2′:4,5]furo[2,3-c]xanthen-9-one, 9CI*
[22897-08-1]



Absolute configuration

$C_{19}H_{14}O_7$ 354.315
Formerly assigned the 6-methoxy struct. Metab. of a mutant strain of *Aspergillus versicolor* and the marine-derived *Humicola grisea* Gö 101/26. Mycotoxin. Pale-yellow needles (EtOH). Mp 223° dec. $[\alpha]_D^{20}$ -360 (c, 0.238 in $CHCl_3$).
▶ LV1745000
Ac:
Needles (EtOH). Mp 228°.
Bullock, E. *et al., J.C.S.*, 1963, 829 (*isol, ir, uv*)
Holker, J.S.E. *et al., Chem. Comm.*, 1968, 1574 (*isol, pmr*)
Seto, H. *et al., Tet. Lett.*, 1974, 4491 (*cmr*)
Smith, G.D. *et al., Cryst. Struct. Commun.*, 1975, **4**, 697 (*cryst struct*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

Methyl 3-alkylpyrrole-2-carboxylates M-199



Isol. as a mixt. of n = 18 (29%), n = 19 (24%), n = 20 (40%) and n = 22 (7%). Metab. from the marine sponge *Oscarella lobularis*.

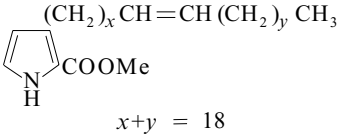
Methyl 3-nonadecyl-1*H*-pyrrole-2-carboxylate [57992-59-3]
$C_{25}H_{45}NO_2$ 391.636
n = 18.

Methyl 3-eicosyl-1*H*-pyrrole-2-carboxylate [57992-60-6]
$C_{26}H_{47}NO_2$ 405.663
n = 19.

Methyl 3-heneicosyl-1*H*-pyrrole-2-carboxylate [57992-61-7]
$C_{27}H_{49}NO_2$ 419.69
n = 20.

Methyl 3-tricosyl-1*H*-pyrrole-2-carboxylate [57992-62-8]
$C_{29}H_{53}NO_2$ 447.743
n = 22.
Cimino, G. *et al., Experientia*, 1975, **31**, 1387 (*isol, uv, ir, pmr, ms, struct*)

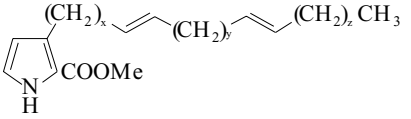
Methyl 3-heneicosenyl-1*H*-pyrrole-2-carboxylate, 9CI M-200
[58018-93-2]



$x+y = 18$

$C_{27}H_{47}NO_2$ 417.674
Isol. in admixture with the homologue having x + y = 20. Metab. from the marine sponge *Oscarella lobularis*.
Cimino, G. *et al., Experientia*, 1975, **31**, 1387 (*isol, pmr, ms*)

Methyl 3-(tricosadienyl)-1*H*-pyrrole-2-carboxylate M-201
*3-(Tricosadienyl)-1*H-*pyrrole-2-carboxylic acid methyl ester*
[58018-98-7]



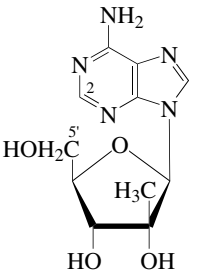
x + y + z = 18

$C_{29}H_{49}NO_2$ 443.712
Metab. from the marine sponge *Oscarella lobularis*.

Dihydro: ***Methyl 3-(tricosenyl)-1*H*-pyrrole-2-carboxylate, 9CI***
[58018-92-1]
$C_{29}H_{51}NO_2$ 445.727
Metab. of *Oscarella lobularis*. Isol. in admixture with its C_{27} lower homologue.
Cimino, G. *et al., Experientia*, 1975, **31**, 1387 (*isol, pmr, ms*)

2′-*C*-Methyladenosine, 9CI, 8CI M-202

*9-(2-*C*-Methyl-β-D-ribofuranosyl)adenine*
[15397-12-3]



$C_{11}H_{15}N_5O_4$ 281.271
Mp 257-258°. $[\alpha]_D$ -21 (c, 0.5 in H_2O). λ_{max} 260 nm (ϵ 15 100) (H_2O).

6N,2′,3′,5′-Tetrabenzoyl:
$C_{39}H_{31}N_5O_8$ 697.703
$[\alpha]_D$ -66 (c, 1.0 in $CHCl_3$).

*2′,3′-*O*-Isopropylidene:*
$C_{14}H_{19}N_5O_4$ 321.335
Mp 291-292°. $[\alpha]_D$ -89 (c, 0.5 in MeOH). λ_{max} 260 (ϵ 15100) (MeOH).

*2-Chloro, 5′-deoxy: 2-Chloro-5′-deoxy-2′-*C*-methyladenosine, 9CI.* ***Kumusine****. Trachycladine A*
[164672-56-4]
$C_{11}H_{14}ClN_5O_3$ 299.716
Isol. from marine sponges *Theonella* sp., *Trachycladus laevispirulifer* and *Theonella cupola*. Cytotoxic and immunosuppressive agent. May have activity against HIV.
Mp 210-213°. $[\alpha]_D$ -19.6 (c, 0.41 in MeOH). Kumusine and Trachycladine A not compared. Mp refers to Kumusine, opt. rotn. to Trachycladine A. λ_{max} 264 (ϵ 14200) (MeOH).

Walton, E. *et al., J.A.C.S.*, 1966, **88**, 4524 (*synth*)
Jenkins, S.R. *et al., J.O.C.*, 1968, **33**, 2490 (*synth, pmr*)
Garrett, E.R. *et al., J.A.C.S.*, 1972, **94**, 8532 (*solvolysis*)
Searle, P.A. *et al., J.O.C.*, 1995, **60**, 4296-4298 (*Trachycladine A*)
Ichiba, T. *et al., Tet. Lett.*, 1995, **36**, 3977-3980 (*Kumusine*)
Higa, T. *et al., ACS Symp. Ser.*, 2000, **745**, 12-21 (*Kumusine, isol, activity*)

Methylamine, 8CI M-203

Methanamine, 9CI. Aminomethane. Carbinamine
[74-89-5]
$MeNH_2$
CH_5N 31.057
Found in fish oils and plants, e.g. *Mercurialis annua, Mercurialis perennis*. Fairly widespread in fungi. Refrigerant, nucleophile in org. synth., solvent. Flammable gas with strong ammoniacal odour. Freq. encountered as strong aq. soln. V. sol. H_2O. d_4^{-10} 0.7. Mp -93.5°. Bp -6.3° Bp_{200} -32.4° Bp_{10} -73.8°. Crit. pt. 156.9°/73.6 atm.
▶ Extremely flammable, fl. p. -18°, autoignition temp. 430°. Eye, skin and respiratory tract irritant (and aq. soln.). OES: long-term 10 ppm. PF6300000

Monohydrate:
Liq. $d^{13.9}$ 0.9.

Trihydrate: Mp -35.8°.

Hydrochloride: [593-51-1]
Used in tanning industry.
Plates (EtOH). Sol. EtOH; insol. Me_2CO, Et_2O, $CHCl_3$. Mp 227-228°. Bp_{15} 225-230°.
▶ PA0603000

N-*Nitro:* See *N*-Nitromethylamine in *The Combined Chemical Dictionary.*

Ac: See *N*-Methylacetamide in *The Combined Chemical Dictionary.*

Di-Ac: Methyldiacetamide
[1113-68-4]
$C_5H_9NO_2$ 115.132
Misc. H_2O; insol. Et_2O. Bp 192°.

N-*(2-Methylpropylidene):* N-*Isobutylidenemethylamine, 8CI*
[6898-70-0]
$C_5H_{11}N$ 85.149
Bp 69.5°.

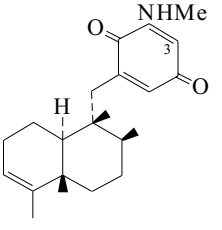
Nitrate: Methylammonium nitrate
[22113-87-7]
$CH_6N_2O_3$ 94.07
Sensitiser for slurry and emulsion explosives containing ammonium nitrate. V. hygroscopic cryst. (EtOH). Mp 110.5-111.5°.
▶ Explosive.

[7436-22-8, 14779-52-3, 14779-55-6, 17000-00-9]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 237B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 279A; 279B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 363D (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 374 (*synth*)
Tiollais, R. *et al., Bull. Soc. Chim. Fr.*, 1947, 708 (*Isobutylidenemethylamine*)
Cottrell, T.L. *et al., J.C.S.*, 1951, 1798-1800 (*nitrate, synth*)
Hesse, G. *et al., Annalen*, 1957, **607**, 24 (*synth*)
von Kamienski, E.S. *et al., CA*, 1958, **52**, 5551,6502 (*occur*)
Suhr, H. *et al., Chem. Ber.*, 1963, **96**, 1720 (*pmr*)
Fr. Pat., 1968, 1 525 149; *CA*, **71**, 80663 (*synth*)
Jayasooriya, U.A. *et al., J. Chem. Soc., Faraday Trans.*, 1992, 1631-1636 (*nitrate, ir, Raman*)
Kurniadi, W. *et al., J.O.C.*, 1994, **59**, 5502-5505 (*nitrate, synth, props*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 2, 1990, 113
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0469
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 825; 826
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MGC250

2-Methylaminoavarone M-204

DB
[83995-06-6]



$C_{22}H_{31}NO_2$ 341.492
Found in the sponge *Dysidea avara*. Inhibitor of cell division in sea urchin eggs. Red cryst. Sol. MeOH, $CHCl_3$; poorly sol. hexane.
Mp 153-155°. Poss. artifact. λ_{max} 288 (ϵ 50029); 486 (ϵ 2088) (MeOH) (Berdy).

Cimino, G. *et al., Experientia*, 1982, **38**, 896 (*isol, uv, ir, pmr, cmr, ms*)

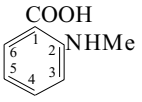
3-Methylaminoavarone M-205

DA
[83995-05-5]
$C_{22}H_{31}NO_2$ 341.492
Isol. from the sponge *Dysidea avara*. Inhibitor of cell division in sea urchin eggs. Red cryst. Sol. MeOH, $CHCl_3$; poorly sol. hexane.
Mp 160-163°. Poss. artifact. λ_{max} 288 (ϵ 5030); 486 (ϵ 2090) (MeOH) (Derep). λ_{max} 289 (ϵ 4688); 485 (ϵ 1065) (MeOH) (Berdy).

Cimino, G. *et al., Experientia*, 1982, **38**, 896 (*isol, uv, ir, pmr, cmr, ms*)
Puliti, R. *et al., Acta Cryst. C*, 1998, **54**, 1954-1957 (*cryst struct*)

2-(Methylamino)benzoic acid, 9CI M-206

N-*Methylanthranilic acid, 8CI*
[119-68-6]



$C_8H_9NO_2$ 151.165
Isol. from grapefruit peel oil. Plates (EtOH or petrol).
Mp 178-179° (175-182°). $Bp_{0.01}$ 80°. pK_{a1} 2; pK_{a2} 5.34 (22°, 0.1*M* KCl). Amphoteric. Sublimes.

▶ Eye irritant. CB3300000

Hydrochloride:
Needles. Mp 141°. No CAS no. found 8-14CI.

Me ester: Methyl N-*methylanthranilate. FEMA 2718*
[85-91-6]
$C_9H_{11}NO_2$ 165.191
Constit. of mandarin peel oil (*Citrus madurensis*), hyacinth oil, petitgrain oil and oil of *Kaempferia ethelae* bulbs. Flavouring agent. Cryst. (petrol) with apple-like flavour at low conc.
Mp 19°. Bp 256° Bp_{15} 130-131°.

▶ CB3500000

Me ester, hydrochloride:
Needles (EtOH). Mp 218°.

Et ester: [35472-56-1]
$C_{10}H_{13}NO_2$ 179.218
Mp 39°. Bp_{45} 172-175°.

Ph ester: [31358-73-3]
$C_{14}H_{13}NO_2$ 227.262
Yellow needles (EtOH aq.). Mp 70-71°.

Amide: 2-(Methylamino)benzamide
[7505-81-9]
$C_8H_{10}N_2O$ 150.18
Alkaloid from the fruit of *Evodia rutaecarpa* and the flowers of *Glycosmis pentaphylla*. Plates (EtOH).
Mp 162-163°.

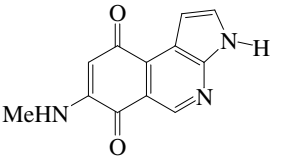
▶ CV5570450

N-*Ac:* [78944-67-9]
$C_{10}H_{11}NO_3$ 193.202
Needles. Mp 192-193°.

N-*(3-Phenylpropanoyl): 2-[Methyl(3-phenylpropanoyl)amino]-benzoic acid*
[207305-65-5]
$C_{17}H_{17}NO_3$ 283.326
Prod. by the marine *Streptomyces* sp. B7747. Antimicroalgal agent. Cryst. (Et_2O).
Mp 107°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 189B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1066C (*nmr*)
Houben, J. *et al., Ber.*, 1906, **39**, 3233-3240; 1909, **42**, 3188-3196 (*synth, Ph ester*)
Cosulich, D.B. *et al., J.A.C.S.*, 1948, **70**, 1922-1926 (*synth*)
Tomita, K. *et al., Yakugaku Zasshi*, 1951, **71**, 1100-1112; *CA*, **46**, 50456 (*synth, esters*)
Freifelder, M. *et al., J. Phys. Chem.*, 1965, **69**, 3645-3648 (*pmr*)
Pant, L.M. *et al., Acta Cryst. B*, 1972, **28**, 647-649 (*cryst struct*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, MGQ250
Sinhababu, A. *et al., Asian J. Chem.*, 1995, **7**, 221-222 (*amide, isol*)
Biabani, M.A.F. *et al., J. Antibiot.*, 1998, **51**, 333-340 (*3-phenylpropanoyl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, MGQ000; MGQ250

7-(Methylamino)-3*H*-pyrrolo[2,3-*c*]isoquinoline-6,9-dione M-207

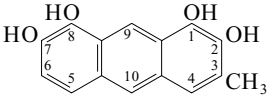


$C_{12}H_9N_3O_2$ 227.222
Prod. by the marine-derived *Streptomyces* sp. B1848. Dark red solid. λ_{max} 233; 287; 295 (sh); 372; 422 (sh); 481 (sh) (MeOH).

Shaaban, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*isol, pmr, cmr, ms*)

3-Methyl-1,2,7,8-anthracenetetrol M-208

1,2,7,8-Tetrahydroxy-3-methylanthracene



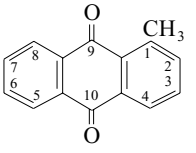
$C_{15}H_{12}O_4$ 256.257

1-Me ether: 2,7,8-Trihydroxy-1-methoxy-3-methylanthracene
$C_{16}H_{14}O_4$ 270.284
Constit. of *Halla parthenopeia* and *Lumbriconereis impatiens*.

Cimino, G. *et al., J. Nat. Prod.*, 1985, **48**, 828-829 (*isol*)

1-Methylanthraquinone M-209

1-Methyl-9,10-anthracenedione, 9CI
[954-07-4]

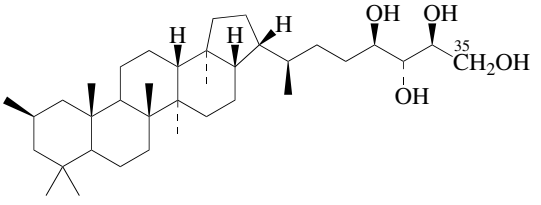


$C_{15}H_{10}O_2$ 222.243
Constit. of the sea cucumber *Holothuria spinifera*. Yellow needles (EtOH or AcOH aq.). V. sol. C_6H_6, sol. AcOH, petrol, spar. sol. Et_2O.
Mp 173-174°. Turns red in air.

Fischer, O. *et al., J. Prakt. Chem.*, 1911, **83**, 204 (*synth*)
Scholl, R. *et al., Ber.*, 1931, **64**, 320
Gudzenko, V. *et al., Zh. Obshch. Khim.*, 1963, **33**, 940 (*synth*)
Stepan, V. *et al., Coll. Czech. Chem. Comm.*, 1971, **36**, 3964 (*synth, ir*)
Torssell, K. *et al., Acta Chem. Scand., Ser. B*, 1976, **30**, 353 (*synth*)
Berger, Y. *et al., Org. Magn. Reson.*, 1981, **15**, 303 (*cmr*)
Baumstark, A.L. *et al., Tet. Lett.*, 1988, **29**, 2143 (*O-17 nmr*)
Nishigaichi, Y. *et al., Chem. Lett.*, 1991, 693 (*synth*)
Gritsan, N.P. *et al., J.A.C.S.*, 1991, **113**, 9615 (*synth*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1993, **32**, 457 (*isol*)

2-Methyl-32,33,34,35-bacteriohopanetetrol M-210

2-Methyl-29-(2,3,4,5-tetrahydroxypentyl)hopane



$C_{36}H_{64}O_4$ 560.899

(2β,32*R*,33*R*,34*S*)-*form* [175669-48-4]
Isol. from *Nostoc* sp. PCC 6720.

35-O-*β*-D-*Galacturonopyranoside:* [179259-90-6]
$C_{42}H_{72}O_{10}$ 737.025
Constit. of *Prochlorothrix hollandica* and *Synechococcus* sp. PCC 6907.

35-O-*α*-D-*Glucuronopyranoside:* [179465-46-4]
$C_{42}H_{72}O_{10}$ 737.025
Constit. of *Synechococcus* sp. PCC 6907.

(2β,32ξ,33ξ,34ξ)-*form*

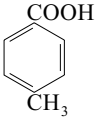
35-O-*α*-D-*Altruronopyranoside:* [185959-16-4]
$C_{42}H_{72}O_{10}$ 737.025
Constit. of *Prochlorothrix hollandica*.

35-O-*(3,6-Anhydro-β-*D-*galacturonopyranoside):* [185959-10-8]
$C_{42}H_{70}O_9$ 719.01
Constit. of *Prochlorothrix hollandica*.

Simonin, P. *et al., Eur. J. Biochem.*, 1996, **241**, 865-871 (*isol, pmr, ms*)
Llopiz, P. *et al., FEMS Microbiol. Lett.*, 1996, **140**, 199-202 (*isol*)
Zhao, N. *et al., Tetrahedron*, 1996, **52**, 2777-2788 (*isol, pmr, cmr*)

4-Methylbenzoic acid, 9CI M-211

p-*Toluic acid. Crithmic acid*
[99-94-5]
[25567-10-6]



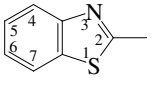
$C_8H_8O_2$ 136.15
Isol. from horseradish. Prod. by the marine-derived *Cladosporium cladosporioides*. Spar. sol. H_2O.
Mp 181°. Bp 274-275°. pK_a 4.37. Sublimes. Steam-volatile.
▶ LD_{50} (rat, orl) 400 mg/kg. XU1575000

[17264-54-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 193B; 294C; 344B; 370C; 381D; 448D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1072C; 1247C; 1248A; 1342A; 1393B; 1412A (*nmr*)
Org. Synth., Coll. Vol., 3, 1955, 822 (*synth*)
Kaiser, E.M. *et al., J.O.C.*, 1970, **36**, 1198 (*synth*)
Takwale, M.G. *et al., Acta Cryst. B*, 1971, **27**, 1152 (*cryst struct*)
Org. Synth., 1971, **51**, 96 (*synth*)
Yamamoto, O. *et al., Anal. Chem.*, 1972, **44**, 1794 (*pmr*)
Brunet, J.J. *et al., J.O.C.*, 1979, **44**, 2199 (*synth*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth, pmr, cmr*)
San-Martin, A. *et al., An. Asoc. Quim. Argent.*, 2005, **93**, 247-251 (*marine, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MPX850; TGU000; TGQ250; TGT750

2-Methylbenzothiazole, 9CI M-212

[120-75-2]



C_8H_7NS 149.216
Prod. by a *Micrococcus* sp. found in *Tedania ignis*. Also known as an aroma constit. of tea leaves.
Mp 14°. Bp 238° Bp_{15} 150-151°. pK_a 2.06 (H_2O). pK_a 8.63 (MeCN).
▶ LD_{50} (mus, ipr) 300 mg/kg. DL5600000
Picrate: Mp 153.5°.

N-*Oxide:* [23808-61-9]
C_8H_7NOS 165.215
Light yellow cryst. + $2H_2O$ (MeCN aq.). Mp 46-48°.

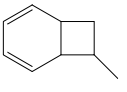
N-*Et: 1-Ethyl-2-methylthiazolium*
[3119-93-5]
$C_{10}H_{12}NS^{\oplus}$ 178.278
Needles (EtOH)(as iodide). Mp 196° (iodide). CAS no. refers to iodide.

N-*Propyl: 2-Methyl-1-propylthiazolium*
[60126-29-6]
$C_{11}H_{14}NS^{\oplus}$ 192.304
Precursor in synth. of carbocyanine dyes. Mp 173-176° (as iodide). CAS no. refers to iodide.

[14933-76-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 699D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 200B; 201B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1511B (*ir*)
Hofmann, A.W. *et al., Ber.*, 1880, **13**, 8-22; 1223-1238 (*synth*)
Mills, W.H. *et al., J.C.S.*, 1922, **121**, 455-466 (*N-Rt*)
Clark, L.M. *et al., J.C.S.*, 1928, 2313-2320 (*synth*)
Brooker, L.G.S. *et al., J.A.C.S.*, 1935, **57**, 2480 (*N-propyl, synth, use*)
Millard, B.J. *et al., Org. Mass Spectrom.*, 1968, **1**, 285 (*ms*)
Schweizer, E.E. *et al., J.O.C.*, 1978, **43**, 2972 (*synth*)
Sawhney, S.N. *et al., J.O.C.*, 1979, **44**, 1136 (*cmr*)
Peyronel, G. *et al., Spectrochim. Acta A*, 1981, **37**, 71 (*ir*)
Bowman, W.R. *et al., Tet. Lett.*, 1982, **23**, 5093 (*synth*)
Wanner, K.T. *et al., Annalen*, 1984, 1100 (*synth*)
Stefaniak, L. *et al., Org. Magn. Reson.*, 1984, **22**, 215 (*N-15 nmr*)
Kolb, B. *et al., J. Agric. Food Chem.*, 1985, **33**, 999 (*isol*)
Alyea, E.C. *et al., J. Het. Chem.*, 1985, **22**, 1325 (*synth*)
Stierle, A.A. *et al., Tet. Lett.*, 1991, **32**, 4847 (*isol*)
Kamila, S. *et al., Heterocycles*, 2005, **65**, 2119-2126 (*synth, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MHI750

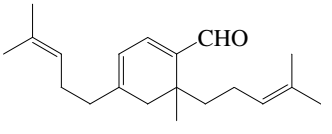
7-Methylbicyclo[4.2.0]octa-2,4-diene M-213



C_9H_{12} 120.194
Constit. of the brown alga *Cutleria multifida*.

Keitel, J. *et al., Helv. Chim. Acta*, 1990, **73**, 2101-2112 (*isol*)

6-Methyl-4,6-bis(4-methyl-3-pentenyl)-1,3-cyclohexadiene-1-carboxaldehyde, 9CI M-214



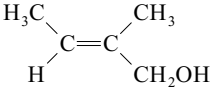
$C_{20}H_{30}O$ 286.456

(±)-*form*
Obt. from *Flustra foliacea*. Probable artifact. λ_{max} 262 (log ε 5.9); 318 (log ε 6.3) (EtOH).

Holst, P.B. *et al., Acta Chem. Scand.*, 1994, **48**, 765-768 (*isol, uv, pmr, cmr, ms*)

2-Methyl-2-buten-1-ol, 9CI M-215

[4675-87-0]



(*E*)-*form*

$C_5H_{10}O$ 86.133
Widespread nat. occurrence, e.g. in *Ochromonas danica*, in *Anthemis nobilis* (as acetate), in fruit juices and animal sources (unspecified stereochem.).

(*E*)-*form*

Tiglic alcohol. Tiglyl alcohol
[497-02-9]
Found in Roman chamomile (*Anthemis nobilis*) (together with esters). Bp 122-127° (135°) Bp_{33} 66°.

O-*β*-D-*Glucopyranoside:*
$C_{11}H_{20}O_6$ 248.275
Constit. of *Foeniculum vulgare*. Needles (MeOH). Mp 55-56°. $[\alpha]_D^{22}$ -15.8 (c, 0.2 in MeOH).

Angeloyl: ***Angeloyl tiglate***
[90358-41-1]
$C_{10}H_{16}O_2$ 168.235
Constit. of the oil of *Anthemis nobilis* (Roman chamomile).

Tigloyl: ***Tiglyl tiglate***
[72845-40-0]
$C_{10}H_{16}O_2$ 168.235
Constit. of the flowers of *Gardenia jasminoides* and *Plectrelminthus caudatus*.

4-Hydroxy-3-methoxy-E-*cinnamoyl:* ***Tiglyl ferulate***. *2-Methyl-2-butenyl ferulate*
$C_{15}H_{18}O_4$ 262.305
Constit. of Uruguayan propolis.

(*Z*)-*form*

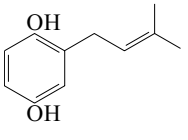
Angelic alcohol. Angelyl alcohol
[19319-26-7] Bp 136-137° Bp_{25} 61-63°. n_D^{20} 1.4410.

Angeloyl: ***Angeloyl angelate***
[217448-58-3]
$C_{10}H_{16}O_2$ 168.235
Constit. of the oil of *Chamaemelum nobile* (Roman chamomile).

Katzenellenbogen, J.A. *et al., J.A.C.S.*, 1976, **98**, 4925 (*synth, ir, pmr*)
Jarolim, V. *et al., Coll. Czech. Chem. Comm.*, 1977, **42**, 3490 (*synth*)
Zaidlewicz, M. *et al., Synthesis*, 1979, 62 (*synth, pmr*)
Depezay, J.-C. *et al., Bull. Soc. Chim. Fr.*, 1981, 306 (*synth, ms, pmr*)
Smith, P.A.S. *et al., J.O.C.*, 1981, **46**, 3970 (*synth, ir, pmr*)
Bury, A. *et al., J.C.S. Perkin 1*, 1982, 645 (*synth, pmr*)
Ono, N. *et al., Tet. Lett.*, 1984, **25**, 5319 (*synth*)
Masami, Y. *et al., Tetrahedron*, 1984, **40**, 3481 (*synth, ir, pmr*)
Ashcroft, M.R. *et al., J. Organomet. Chem.*, 1985, **289**, 403 (*synth*)
Trost, B.M. *et al., J.A.C.S.*, 1985, **107**, 1293 (*synth, pmr*)
Kurth, M.J. *et al., J.O.C.*, 1985, **50**, 5769 (*synth*)
Simon, H. *et al., Angew. Chem., Int. Ed.*, 1987, **26**, 785 (*synth*)
Bicchi, C. *et al., J. Chromatogr.*, 1987, **411**, 237 (*glc, ms*)
Begley, M.J. *et al., J.C.S. Perkin 1*, 1991, 1951 (*synth, ir, pmr*)
Iyer, R.S. *et al., J.O.C.*, 1994, **59**, 6038 (*synth, pmr*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1643-1646 (*glucoside*)
Kumazawa, S. *et al., J. Agric. Food Chem.*, 2002, **50**, 4777-4782 (*Tiglyl ferulate*)

2-(3-Methyl-2-butenyl)-1,4-benzenediol M-216

Prenylhydroquinone
[5919-91-5]



$C_{11}H_{14}O_2$ 178.23

For higher homologues see 2-(3,7-Dimethyl-2,6-octadienyl)-1,4-benzenediol, D-974, Farnesylhydroquinone, F-13 and 2-Polyprenyl-1,4-benzenediol, P-547. Isol. from *Aplidium californicum* and *Phagnalon saxitale*. Cryst. Mp 100-101°.

1-O-*β*-D-*Glucopyranoside:*
$C_{17}H_{24}O_7$ 340.372
Constit. of *Phagnalon rupestre*. Amorph. powder. $[\alpha]_D$ -58 (c, 0.1 in MeOH). λ_{max} 232; 289 (MeOH).

1-O-*[3,4-Dihydroxycinnamoyl-(→4)-β-D-glucopyranoside]:*
$C_{26}H_{30}O_{10}$ 502.517
Constit. of *Phagnalon rupestre*. Amorph. powder. $[\alpha]_D$ -26 (c, 0.1 in MeOH). Config. of cinnamoyl moiety not determined. λ_{max} 242; 331 (MeOH).

4-O-*β*-D-*Glucopyranoside:* ***Nebrodenside A***
$C_{17}H_{24}O_7$ 340.372
Constit. of the aerial parts of *Ephedra nebrodensis*. Amorph. solid. $[\alpha]_D^{25}$ +60 (c, 0.3 in MeOH). λ_{max} 225; 287 (MeOH).

4-Me ether: 4-Methoxy-2-(3-methyl-2-butenyl)phenol. 4-Methoxy-2-prenylphenol
[25974-58-7]
$C_{12}H_{16}O_2$ 192.257
Isol. from basidiomycete *Lactarius fuiginosus* spp.
Mp 56-59°.

4-Me ether, 1-octadecanoyl: [144705-42-0]
$C_{30}H_{50}O_3$ 458.723
Isol. from *Lactarius* spp.
Mp 31-32°.

Quinone: 2-(3-Methyl-2-butenyl)-1,4-benzoquinone. Prenyl-1,4-benzoquinone. Prenylquinone
[5594-02-5]
$C_{11}H_{12}O_2$ 176.215
Isol. from fruit, leaves and stems of *Phagnalon sordidum*; also detected in *Phagnalon atlanticum, Phagnalon rupestre* and *Aplidium californicum*. Yellow cryst.
Mp 30.5°.
▶ Contact allergen.

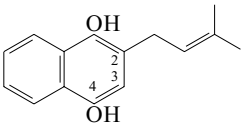
4′-Hydroxy: 2-(4-Hydroxy-3-methyl-2-butenyl)-1,4-benzenediol
$C_{11}H_{14}O_3$ 194.23
Isol. from the mushroom *Piptoporus betulinus*. Pale yellow oil. Possesses *E*-config.

4′-Hydroxy, 1-O-*β*-D-*glucopyranoside:*
$C_{17}H_{24}O_8$ 356.372
Constit. of *Phagnalon rupestre*. Amorph. powder. $[\alpha]_D$ -34 (c, 0.1 in MeOH). Config. of hydroxyprenyl sidechain not determined. λ_{max} 231; 293 (MeOH).

Bohlmann, F. *et al., Chem. Ber.*, 1966, **99**, 885-888 (*isol, struct, pmr, ms*)
Jurd, L. *et al., Tet. Lett.*, 1971, 2275-2278 (*synth*)
Jacobsen, N. *et al., Acta Chem. Scand.*, 1973, **27**, 3211-3216 (*synth*)
Howard, B.M. *et al., Tet. Lett.*, 1979, 4449-4452 (*isol, Aplidium*)
De Bernardi, M. *et al., Tetrahedron*, 1992, **48**, 7331 (*4-Me ether, isol, synth*)
Gongora, L. *et al., J. Nat. Prod.*, 2001, **64**, 1111-1113 (*Phagnalon rupestre glucosides*)
Kawagishi, H. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 2748-2750 (*4′-hydroxy*)
Cottiglia, F. *et al., Nat. Prod. Res.*, 2005, **19**, 117-123 (*Nebrodenside*)

2-(3-Methyl-2-butenyl)-1,4-naphthalenediol M-217

2-(3,3-Dimethylallyl)-1,4-naphthalenediol. 2-Prenylnaphthohydroquinone. 1,4-Dihydroxy-2-prenylnaphthalene



$C_{15}H_{16}O_2$ 228.29

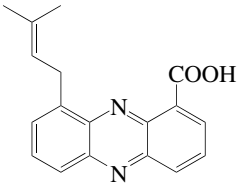
Di-Ac: [17532-55-7]
$C_{19}H_{20}O_4$ 312.365
Needles (EtOH). Mp 74-75°.

Di-Me ether: 1,4-Dimethoxy-2-(3-methyl-2-butenyl)naphthalene. 1,4-Dimethoxy-2-prenylnaphthalene
[137414-53-0]
$C_{17}H_{20}O_2$ 256.344
Constit. of the brown alga *Landsburgia quercifolia*. Pale yellow oil. λ_{max} 245 (ϵ 52500); 300 (ϵ 6920); 330 (ϵ 4070) (hexane) (Derep). λ_{max} 216 (ϵ 58900); 238 (ϵ 77600); 254 (ϵ 17000); 260 (ϵ 13500); 300 (ϵ 11700) (MeOH) (Derep).

Sandermann, W. *et al., Chem. Ber.*, 1963, **96**, 2182 (*synth*)
Inoue, K. *et al., Phytochemistry*, 1984, **23**, 313
Perry, N.B. *et al., J. Nat. Prod.*, 1991, **54**, 978 (*isol*)

9-(3-Methyl-2-butenyl)-1-phenazinecarboxylic acid M-218

9-Prenyl-1-phenazinecarboxylic acid. ***Endophenazine A***



$C_{18}H_{16}N_2O_2$ 292.337

Prod. by various strains of the endosymbiotic *Streptomyces anulatus*. Active against gram-positive bacteria and some fungi. Yellow solid. λ_{max} 255 (log ϵ 4.81); 365 (log ϵ 4.06) (MeOH).

5,10-Dihydro, N^5*-Me: 5,10-Dihydro-5-methyl-9-(3-methyl-2-butenyl)-1-phenazinecarboxylic acid.* ***Endophenazine C***

$C_{19}H_{20}N_2O_2$ 308.379

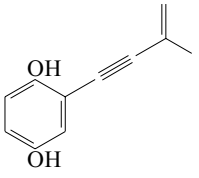
Prod. by *Streptomyces anulatus*. Active against gram-positive bacteria and some fungi. Green solid (probably as a complex with a paramagnetic metal). Orange solid (as Me ester). λ_{max} 254 (log ϵ 4.47); 410 (log ϵ 3.77) (MeOH) (complex). λ_{max} 248 (log ϵ 4.09); 323 (log ϵ 2.6); 432 (log ϵ 3.28) (MeOH) (Me ester).

Gebhardt, K. *et al., J. Antibiot.*, 2002, **55**, 794-800; 801-806 (*isol, pmr, cmr, activity*)

2-(3-Methyl-3-buten-1-ynyl)-1,4-benzenediol, 9CI M-219

4-(2,5-Dihydroxyphenyl)-2-methyl-1-buten-3-yne. ***Siccayne***

[22944-03-2]



$C_{11}H_{10}O_2$ 174.199

Isol. from *Eutypa lata*, *Helminthosporium siccans* and marine basidiomycete *Halocyphina villosa*. Active against gram-positive bacteria and some fungi. Cryst. (C_6H_6). Sol. Me_2CO, C_6H_6, $CHCl_3$, CH_2Cl_2; poorly sol. H_2O.

Mp 115-116°.

Di-Ac: [22944-04-3]

Mp 67-68°.

1-Me ether: 4-Methoxy-3-(3-methyl-3-buten-1-ynyl)phenol. ***Eulatinol***

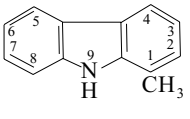
$C_{12}H_{12}O_2$ 188.226

Prod. by *Eutypa lata*. Oil.

Kupka, J. *et al., J. Antibiot.*, 1981, **34**, 298 (*isol*)
Pinault, M. *et al., Synthesis*, 1990, 935 (*synth*)
Defranq, E. *et al., Helv. Chim. Acta*, 1993, **76**, 425 (*synth*)
Molyneux, R.J. *et al., J. Agric. Food Chem.*, 2002, **50**, 1393-1399 (*Eulatinol*)
Smith, L.R. *et al., J. Nat. Prod.*, 2003, **66**, 169-176 (*synth, pmr, cmr*)

1-Methyl-9*H*-carbazole, 9CI M-220

[6510-65-2]



$C_{13}H_{11}N$ 181.237

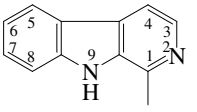
Isol. from the sponge *Tedania ignis*. also from *Ailanthus melabrica*. Toxic to brine shrimp, shows insecticidal props. Plates (petrol). Mp 120.5°. λ_{max} 242 (ϵ 10715); 250 (ϵ 11700); 262 (ϵ 12300); 283 (ϵ 8317); 305 (ϵ 8317); 375 (ϵ 7050) (MeOH) (Berdy).

Campaigne, E. *et al., J.O.C.*, 1959, **24**, 478 (*synth*)
Kuroki, M. *et al., J. Het. Chem.*, 1981, **18**, 709 (*synth, bibl*)
Clancy, M.G. *et al., J.C.S. Perkin 1*, 1984, 429 (*synth*)
Dillman, R.L. *et al., J. Nat. Prod.*, 1991, **54**, 1056 (*isol, pmr, cmr*)

1-Methyl-β-carboline M-221

*1-Methyl-9*H*-pyrido[3,4-*b*]indole, 9CI.* ***Harman****. Loturine. Passiflorine*†*. Zygofabagine. Aribine*

[486-84-0]



$C_{12}H_{10}N_2$ 182.224

Present in tobacco smoke. Alkaloid from *Arariba rubra* (preferred genus name *Simira*) (Rubiaceae), *Passiflora incarnata* (Passifloraceae) and many other *Passiflora* spp., and a wide range of spp. in several families. Prod. by *Nocardia* sp. and *Streptomyces* sp. Also a trace constit. of the fluorescent dinoflagellate *Noctiluca miliaris*. Isol. from *Costaticella hastata*. Cytotoxic intercalating agent. Plant growth and enzyme inhibitor. Sedative. Hallucinogen.

Mp 237-238° (228°). Log P 3.06 (calc).

▶ A comutagen with aromatic amines active towards bacteria. LD_{50} (mus, ipr) 50 mg/kg. UV0280000

Hydrochloride: Mp 292-295°.

Picrate: Mp 250-255°.

N-*Oxide:* ***Harmanine***

[2506-09-4]

$C_{12}H_{10}N_2O$ 198.224

Alkaloid from *Calligonum minimum* and *Ophiorrhiza rosacea*. Needles (EtOAc/MeOH); cryst. (H_2O) (as picrate).

Mp 182-184° subl. Mp 239-248° (picrate).

N^b*-Me:* ***Melinonine F***

[6801-22-5]

$C_{13}H_{13}N_2^{\oplus}$ 197.259

Quaternary alkaloid from *Strychnos melinoniana* and *Strychnos usambaerensis* (Strychnaceae). Antimitotic agent. Poorly sol. hexane.

Mp 288° dec. (as chloride).

*3,4-Dihydro: 4,9-Dihydro-1-methyl-3*H*-pyrido[3,4-*b*]indole.* ***3,4-Dihydro-1-methyl-β-carboline****.* ***Harmalan****. Dihydroharman*

[525-41-7]

$C_{12}H_{12}N_2$ 184.24

Alkaloid from *Flindersia laevicarpa*, *Elaeagnus angustifolia* (Russian olive), *Strychnos dale* and *Burkea africana* (Flindersiaceae, Eleagnaceae, Loganiaceae, Leguminosae). Cream needles (Me_2CO).

Mp 183-185° dec. λ_{max} 237 (log ϵ 3.89); 241 (sh); 319 (log ϵ 3.86); 346 (sh) (log ϵ 3.62) (MeOH).

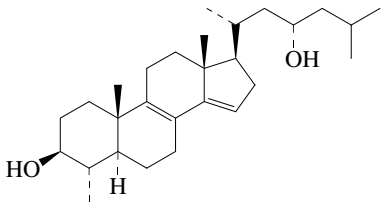
3,4-Dihydro, picrate:

Yellow needles ($CHCl_3$/MeOH). Mp 245° dec. (234-235° dec.).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 682A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 165B (*nmr*)
Manske, R.H.F. *et al., J.C.S.*, 1927, 1-14 (*Harmalan, synth*)
Bächli, E. *et al., Helv. Chim. Acta*, 1957, **40**, 1167-1187 (*Melinonine F, isol, uv, ir*)
Kanaoka, Y. *et al., Chem. Pharm. Bull.*, 1967, **15**, 101-107 (*Harmalan, synth, uv, ir*)
Kametani, T. *et al., J.C.S.(C)*, 1968, 1006-1007 (*synth, pmr*)
Phillipson, J.D. *et al., J. Chromatogr.*, 1975, **105**, 163-178 (*tlc, glc, uv, ms*)
Picker, K. *et al., Aust. J. Chem.*, 1976, **29**, 2023-2036 (*Harmalan, isol, uv, ir, pmr, ms*)
Inoue, S. *et al., Chem. Lett.*, 1980, 297-298 (*isol, dinoflagellate*)
Han, B.H. *et al., Arch. Pharmacal Res.*, 1986, **9**, 21; *CA*, **105**, 57927y (N^a*-Formylharman, isol*)
Yomosa, K. *et al., Agric. Biol. Chem.*, 1987, **51**, 921-922 (*isol, bibl*)
Hardiman, J. *et al., Bioorg. Chem.*, 1987, **15**, 213-223 (*cryst struct*)
Blackman, A.J. *et al., J. Nat. Prod.*, 1987, **50**, 494-496 (*isol, Costaticella*)
Bracher, F. *et al., Annalen*, 1993, 1335-1337 (*synth, pmr, cmr*)
Seki, H. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1169-1172 (*pmr, cmr*)
Rocca, P. *et al., Tetrahedron*, 1993, **49**, 3325-3342 (*synth*)
Dachriyanus, *et al., Aust. J. Chem.*, 2000, **53**, 221-224 (*oxide*)

Kitajima, M. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1410-1412 (*Harmalan, pmr, cmr*)
Nakano, K. *et al., Mutat. Res.*, 2000, **470**, 141-146 (*comutagenicity, pmr*)
Ivanov, I. *et al., Heterocycles*, 2005, **65**, 2483-2492 (*synth, Harmalan, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MPA050

4-Methylcholesta-8,14-diene-3,23-diol M-222



$C_{28}H_{46}O_2$ 414.67

(3β,4α,5α,23*S*)-*form* [119760-84-8]

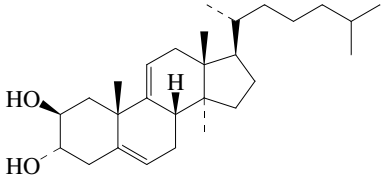
3-O-*[β-D-Galactopyranosyl-(1→2)-β-D-galactopyranoside]:* ***Eryloside A***
[119760-82-6]
$C_{40}H_{66}O_{12}$ 738.954
Constit. of *Erylus lendenfeldi*. Shows antitumour and antifungal props. Amorph. powder. Sol. MeOH.
Mp 168-172° Mp 214-219°. $[\alpha]_D$ +11 (c, 1.5 in $CHCl_3$). λ_{max} 249 (ε 19500) (MeOH).

23-Ketone: 3-Hydroxy-4-methylcholesta-8,14-dien-23-one
$C_{28}H_{44}O_2$ 412.654

23-Ketone, 3-O-*[β-D-galactopyranosyl-(1→2)-β-D-galactopyranoside]:* ***Eryloside L***†
[847613-59-6]
$C_{40}H_{64}O_{12}$ 736.938
Constit. of *Erylus lendenfeldi*. Powder.
Mp 200-204°. $[\alpha]_D$ +10 (c, 0.34 in MeOH). λ_{max} 250 (log ε 4.33) (MeOH).

Carmely, S. *et al., J. Nat. Prod.*, 1989, **52**, 167 (*Eryloside A*)
Sandler, J.S. *et al., Tetrahedron*, 2005, **61**, 1199-1206 (*Eryloside L*)

14-Methylcholesta-5,9(11)-diene-2,3-diol M-223



$C_{28}H_{46}O_2$ 414.67

(2β,3α,14α)-*form*

Disulfate: ***Lembehsterol B***
[452963-39-2]
$C_{28}H_{46}O_8S_2$ 574.799
Constit. of *Petrosia strongylata*.
$[\alpha]_D$ +39 (c, 0.32 in MeOH).

Aoki, S. *et al., Chem. Pharm. Bull.*, 2002, **50**, 827-830 (*isol, pmr, cmr*)

4-Methylcholesta-7,24-dien-3-ol M-224

$C_{28}H_{46}O$ 398.671

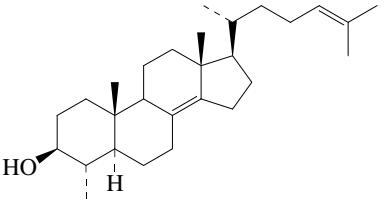
(3β,4α,5α)-*form* [24778-51-6]

Constit. of seeds of *Funtumia latifolia, Holarrhena mitis, Caenorhabditis elegans* , *Asterias rubens*, *Asterias rollentias* and *Claviceps* spp.
Cryst.
Mp 139°.

[92761-52-9]

Charles, G. *et al., C. R. Hebd. Seances Acad. Sci.*, 1969, **268**, 2105-2108 (*Funtumia elastica constit*)
Leboeuf, M. *et al., Ann. Pharm. Fr.*, 1972, **30**, 837-842 (*Holarrhena mitis constit*)
Smith, A.G. *et al., Biochem. J.*, 1973, **135**, 443-455 (*Asterias rubens constit*)
Chitwood, D.J. *et al., Steroids*, 1983, **42**, 311-319 (*Caenorhabditis elegans constit*)
Kren, V. *et al., Biochem. Physiol. Pflanz.*, 1986, **181**, 505-510 (*Claviceps metab*)
Y, Zhan *et al., Zhongguo Yaowu Huaxue Zazhi*, 2005, **15**, 100-102; 115; *CA*, **145**, 79879n (*Asterias ollentias constit*)

4-Methylcholesta-8(14),24-dien-3-ol M-225



$C_{28}H_{46}O$ 398.671

(3β,4α,5α)-*form* [25747-44-8]

Isol. from *Caenorhabditis elegans* and *Panagrellus redivivus*.
Constit. of a zooxanthellae isol. from *Aiptasia pulchella*. Also obt. from *Saccharomyces cerevisiae* and prod. by *Methylococcus capsulatus*.
Mp 131.5-136°. $[\alpha]_D$ +19 (c, 0.5 in $CHCl_3$).

Barton, D.H.R. *et al., J.C.S.(C)*, 1970, 775-785 (*isol*)
Bouvier, P. *et al., Biochem. J.*, 1976, **159**, 267-271 (*isol*)
Withers, N.W. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1982, **79**, 3764-3768 (*isol*)
Chitwood, D.J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1987, **86**, 103-107 (*isol*)

4-Methylcholesta-8,22-dien-3-ol M-226

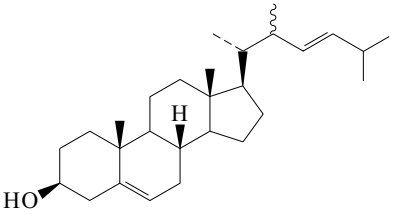
$C_{28}H_{46}O$ 398.671

(3β,4α,5α,22*E*)-*form* [52043-00-2]

Constit. of *Porphyridium cruentum*.

Beastall, G.H. *et al., Eur. J. Biochem.*, 1973, **41**, 301 (*isol, ms, pmr*)

22-Methylcholesta-5,23-dien-3-ol M-227



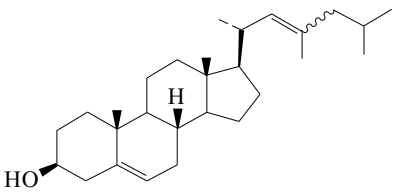
$C_{28}H_{46}O$ 398.671

(3β,22ξ)-*form*

Echifloristerol
Constit. of an *Echinogorgia* sp.
Cryst. (EtOAc).
Mp 136-137°.

Zeng, L. *et al., CA*, 1991, **114**, 98588t (*isol, pmr*)

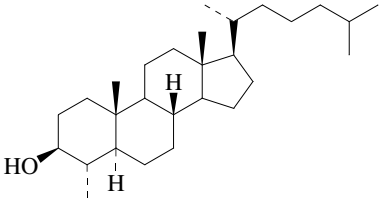
23-Methylcholesta-5,22-dien-3-ol M-228



$C_{28}H_{46}O$ 398.671

(3β,22ξ)-*form* [71932-06-4]
Constit. of *Zoanthus sociatus*.
Cryst.
Mp 141-143°. $[\alpha]_D$ -36 ($CHCl_3$).
Kokke, W.C.M.C. *et al., Tet. Lett.*, 1979, **20**, 3601-3604 (*isol*)
Withers, N.W. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1982, **79**, 3764-3768 (*isol, pmr*)

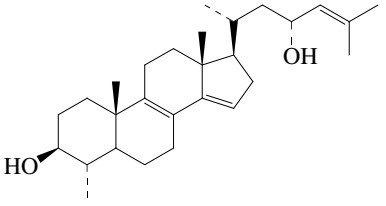
4-Methylcholestan-3-ol M-229



$C_{28}H_{50}O$ 402.702

(3β,4α,5α)-*form*
***Lophenol*†**
[3903-57-9]
Constit. of *Ascidia nigra*, *Plexaura homomalla*, *Holothuria nobilis* and various gorgonians and dinoflagellates.
Cryst.
Mp 161-162° Mp 149-151°.
Ketone: 4-Methylcholestan-3-one. ***Lophanone***
[984-87-2]
$C_{28}H_{48}O$ 400.687
Isol. from *Scrippsiella trochoidea* and other dinoflagellates. Cryst.
Mp 103-105°.
Djerassi, C. *et al., J.A.C.S.*, 1958, **80**, 1005-1006; 6284-6292 (*Lophenol*)
Iida, T. *et al., Steroids*, 1977, **29**, 453-460 (*pmr*)
Iida, T. *et al., Org. Magn. Reson.*, 1982, **19**, 228-229 (*cmr*)
Tam Ha, T.B. *et al., Steroids*, 1982, **40**, 433-453 (*Ascidia nigra constit*)
Dow, W.C. *et al., Steroids*, 1983, **42**, 217-230 (*Pleaxaura homomalla constits*)
Stork, G. *et al., J.A.C.S.*, 1986, **108**, 6826-6828 (*synth*)
Harvey, H.R. *et al., Phytochemistry*, 1988, **27**, 1723-1729 (*Lophanone*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*Holothuria nobilis constit*)

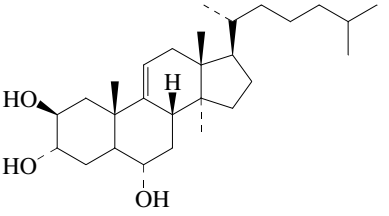
4-Methylcholesta-8,14,24-triene-3,23-diol M-230



$C_{28}H_{44}O_2$ 412.654

(3β,4α,5α,23*R*)-*form*
3-O-*[β-D-Galactopyranosyl-(1→2)-β-D-galactopyranoside]:*
Eryloside K
[781648-13-3]
$C_{40}H_{64}O_{12}$ 736.938
Constit. of *Erylus lendenfeldi*. Amorph. powder.
Mp 208-212°. $[\alpha]_D^{20}$ +6.1 (c, 0.2 in MeOH). $[\alpha]_D$ +10 (c, 0.12 in MeOH). λ_{max} 251 (MeOH).
Fouad, M. *et al., ARKIVOC*, 2004, **xiii**, 17-27 (*isol, pmr, cmr*)
Sandler, J.S. *et al., Tetrahedron*, 2005, **61**, 1199-1206 (*Eryloside K*)

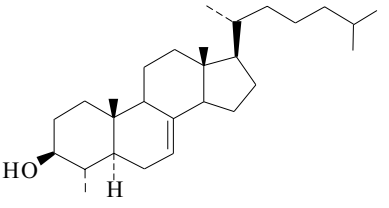
14-Methylcholest-9(11)-ene-2,3,6-triol M-231



$C_{28}H_{48}O_3$ 432.685

(2β,3α,5α,6α,14α)-*form* [452929-64-5]
Trisulfate: ***Lembehsterol A***
[452963-38-1]
$C_{28}H_{48}O_{12}S_3$ 672.878
Constit. of *Petrosia strongylata*.
$[\alpha]_D$ +50.1 (c, 0.41 in MeOH).
Aoki, S. *et al., Chem. Pharm. Bull.*, 2002, **50**, 827-830 (*isol, pmr, cmr*)

4-Methylcholest-7-en-3-ol M-232



$C_{28}H_{48}O$ 400.687

(3β,4α,5α)-*form*
***Lophenol*†**. *Methostenol*
[481-25-4]
Constit. of *Lophocereus schottii*, potato leaves (*Solanum tuberosum*) and *Solanum demissum*. Isol. from *Asterias rubens*, *Caenorhabditis elegans* and the squid *Ommastrephes sloani pacificus*. Also found in mussels and oysters.
Cryst. (MeOH).
Mp 149-151°. $[\alpha]_D$ +5 ($CHCl_3$).
Djerassi, C. *et al., J.A.C.S.*, 1958, **80**, 6284 (*struct*)
Schreiber, K. *et al., Tetrahedron*, 1964, **20**, 2575 (*isol*)
Scallen, T.J. *et al., J. Lipid Res.*, 1968, **9**, 120 (*ir*)
Smith, A.G. *et al., Biochem. J.*, 1973, **135**, 443-455 (*Asterias, isol*)
Sucrow, W. *et al., Chem. Ber.*, 1977, **110**, 1523 (*synth*)
Iida, T. *et al., Steroids*, 1977, **29**, 453 (*pmr*)

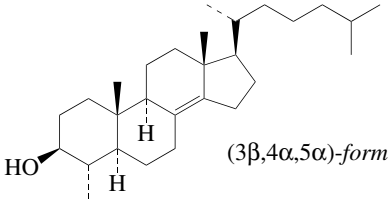
4-Methylcholest-8-en-3-ol M-233

$C_{28}H_{48}O$ 400.687

(3β,4α,5α)-*form* [5241-22-5]
Constit. of *Porphyridium cruentum* and a transplantable preputial tumour. Isol. from the sponge *Agelas flabelliformis*. Shows immunosuppressive activity. Intermediate in cholesterol biosynth.
Cryst.
Mp 136.5-137°. $[\alpha]_D$ +55 (c, 1.85 in $CHCl_3$).
3-Ketone: 4-Methylcholest-8-en-3-one
$C_{28}H_{46}O$ 398.671
Constit. of preputial tumour. Cryst.
Mp 113°. $[\alpha]_D$ +44.

Midgley, J.M. *et al., Chem. Comm.*, 1967, 1297 (*synth*)
Ramsey, R.B. *et al., J. Biol. Chem.*, 1971, **246**, 6393 (*biosynth*)
Beastall, G.H. *et al., Eur. J. Biochem.*, 1974, **41**, 301 (*isol*)
Knapp, F.F. *et al., J.A.C.S.*, 1975, **97**, 3522 (*biosynth*)
Gunasekera, S. *et al., J. Nat. Prod.*, 1989, **52**, 757-760 (*isol, activity*)
König, G.M. *et al., Planta Med.*, 1998, **64**, 443-447 (*isol, pmr, cmr*)

4-Methylcholest-8(14)-en-3-ol M-234



$C_{28}H_{48}O$ 400.687

(3β,4α,5α)-*form* [62014-96-4]
Constit. of the seeds of *Capsicum annuum*. Isol. from the nematodes *Caenorhabditis elegans* and *Turbatrix aceti*. Also from *Amphidinium* spp., *Ascidia nigra* and *Zooxanthella microadriatica*.

Ac: [61973-40-8]
Cryst. Mp 78-78.5°.

Ketone: ***4-Methylcholest-8(14)-en-3-one***
$C_{28}H_{46}O$ 398.671
Constit. of *Scrippsiella trochoidea*.

(3β,4α,5ξ)-*form* [53296-66-5]
Isol. from the oyster (*Crassostrea virginica*), *Nereis diversicolor* and *Scrippsiella trochoidea*.
Teshima, S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1981, **69**, 175-181 (*Crassostrea, isol*)
Kokke, W.C.M.C. *et al., Phytochemistry*, 1981, **20**, 127-134 (*Amphidinium, isol*)
Tam Ha, T.B. *et al., Steroids*, 1982, **40**, 433-453 (*Ascidia nigra, isol*)
Matsumoto, T. *et al., Phytochemistry*, 1983, **22**, 2621-2622 (*isol, pmr, ms*)
Chitwood, D.J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1987, **86**, 103-107 (*nematode, isol*)
Harvey, H.R. *et al., Phytochemistry*, 1988, **27**, 1723-1729 (*Scrippsiella, isol*)

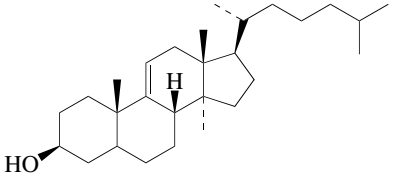
4-Methylcholest-22-en-3-ol M-235

$C_{28}H_{48}O$ 400.687

(3β,4α,5α,22*E*)-*form*
*4α-Methyl-22*E*-dehydrocholestanol*
[73792-93-5]
Constit. of *Zoanthus sociatus* and *Ascidia nigra*.

(3β,4α,5α,22*Z*)-*form* [84924-71-0]
Isol. from *Ascidia nigra*.
Kokke, W.C.M.C. *et al., Tet. Lett.*, 1979, 3601
Lavanchy, A. *et al., Org. Mass Spectrom.*, 1980, **15**, 355 (*ms*)
Tam Ha, T.B. *et al., Steroids*, 1982, **40**, 433 (*isol*)

14-Methylcholest-9(11)-en-3-ol M-236

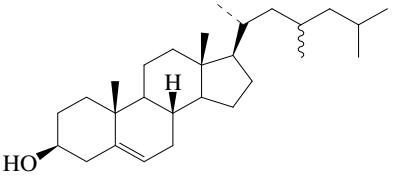


$C_{28}H_{48}O$ 400.687

(3β,5α,14α)-*form* [94773-18-9]
[100017-41-2]
Constit. of *Cucumaria japonica*, *Eupentacta fraudatrix* and other holothurians.

3-O-*Sulfate:* [151890-91-4]
$C_{28}H_{48}O_4S$ 480.751
Constit. of *Eupentacta fraudatrix*.
Kalinovskaya, N.I. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1984, **278**, 630-633; *Dokl. Chem. (Engl. Transl.)*, 1984, **278**, 325 (*Cucumaria japonica constit*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*sulfate*)

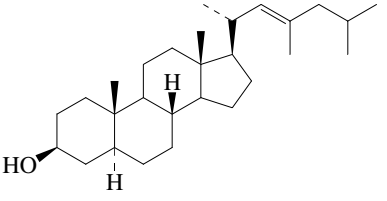
23-Methylcholest-5-en-3-ol M-237



$C_{28}H_{48}O$ 400.687

(3β,23ξ)-*form* [886851-26-9]
Constit. of *Geodia* and *Tedania* spp.
De Rosa, S. *et al., Z. Naturforsch., C*, 2006, **61**, 129-134

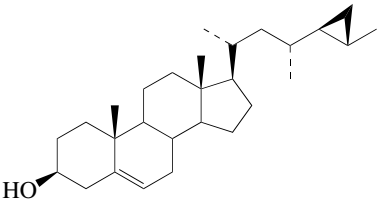
23-Methylcholest-22-en-3-ol M-238



$C_{28}H_{48}O$ 400.687

(3β,5α,22*E*)-*form* [82507-25-3]
Constit. of *Pyrocystis lunula*. Isol. from zooxanthellae in *Melibe pilosa, Oculina diffusa* and *Tridacna gigas*.
Withers, N.W. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1982, **79**, 3764-3768 (*isol*)
Kokke, W.C.M.C. *et al., Steroids*, 1982, **40**, 307-318 (*isol*)

23-Methyl-24,26-cyclocholest-5-en-3-ol M-239

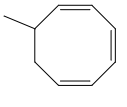


$C_{28}H_{46}O$ 398.671

(3β,23*R*,24*R*,25*S*)-*form*
29-Norhebesterol
[137765-74-3]
Prod. by sponge *Petrosia ficiformis*. Obt. by directed feeding but is a genuine metab. of the sponge.
Silva, C.J. *et al., J.A.C.S.*, 1992, **114**, 295-299 (*synth, pmr, cmr*)

7-Methyl-1,3,5-cyclooctatriene M-240

[99140-88-2]



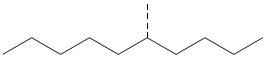
C_9H_{12} 120.194

Constit. of the brown alga *Cutleria multifida*.

Keitel, J. *et al., Helv. Chim. Acta*, 1990, **73**, 2101-2112 (*isol*)

5-Methyldecane M-241

[13151-35-4]



(*R*)-*form*

$C_{11}H_{24}$ 156.311

(R)-form [475575-94-1] $Bp_{8.25}$ 65-67°. $[\alpha]_D^{25}$ -0.25 (c, 4.5 in EtOH).

(ξ)-form

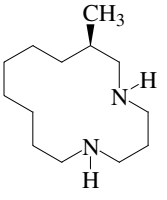
Constit. of the pheromones of *Platynereis dumerilii* and certain ants. Also isol. from *Juncus roemerianus*.

Miles, D.H. *et al., Phytochemistry*, 1973, **12**, 1399 (*isol*)
Zeeck, E. *et al., Tet. Lett.*, 1990, **31**, 5613 (*isol, synth*)
Bagneres, A.G. *et al., Biochem. Syst. Ecol.*, 1991, **19**, 25 (*isol*)
Hedenstroem, E. *et al., Tetrahedron: Asymmetry*, 2002, **13**, 835-844 (*R-form*)

7-Methyl-1,5-diazacyclotetradecane M-242

Haliclorensin

[202747-72-6]



(*R*)-*form*

$C_{13}H_{28}N_2$ 212.378

Struct. revised in 2001.

(R)-form

Oil. $[\alpha]_D$ +20 (c, 2 in MeOH).

(S)-form

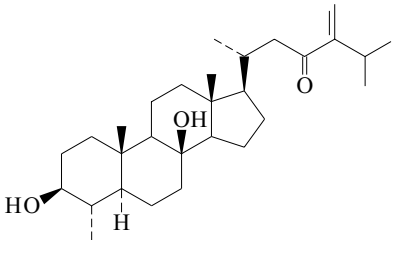
Alkaloid from the marine sponge *Haliclona tulearensis*.

Oil. $[\alpha]_D$ -2.2 (c, 1.3 in MeOH) (natural). $[\alpha]_D$ -18.5 (c, 0.6 in MeOH) (synthetic). Nat. prod. is a partial racemate of 75% o.p.

Koren-Goldshlager, G. *et al., J. Nat. Prod.*, 1998, **61**, 282 (*isol, pmr, cmr, ms*)
Heinrich, M.R. *et al., Tetrahedron*, 2001, **57**, 9973-9978 (*synth, cd, pmr, cmr, struct*)
Zheng, J.-F. *et al., Org. Lett.*, 2004, **6**, 1139-1142 (*synth*)

4-Methyl-3,8-dihydroxyergost-24(28)-en-23-one M-243

3,8-Dihydroxy-4-methyl-24-methylenecholestan-23-one



$C_{29}H_{48}O_3$ 444.696

(3β,4α,5α,8β)-form [65228-14-0]

Constit. of *Litophyton viridis*.

Cryst.

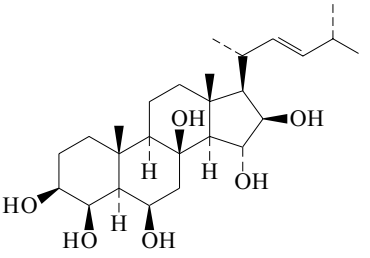
Mp 156-159°. $[\alpha]_D$ +39 (c, 0.35 in MeOH).

Bortolotto, M. *et al., Steroids*, 1977, **30**, 159

24-Methyl-26,27-dinor-22-cholestene-3,4,6,8,15,16,25-heptol M-244

26,27-Dinor-22-ergostene-3,4,6,8,15,16,25-heptol, 9CI

[88191-36-0]



$C_{26}H_{44}O_7$ 468.629

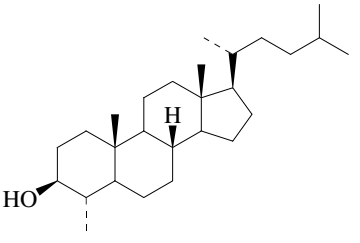
(3β,4β,5α,6β,8β,15α,16β,22E)-form

Constit. of *Hacelia attenuata*.

Minale, L. *et al., J. Nat. Prod.*, 1983, **46**, 736

4-Methyl-26,27-dinorergostan-3-ol M-245

4-Methyl-24-norcholestan-3-ol



$C_{27}H_{48}O$ 388.676

(3β,4α,5α)-form [199611-83-1]

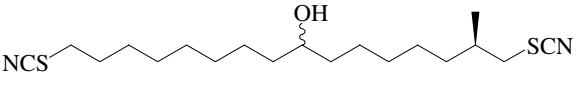
Constit. of *Haliclona cinerea* and *Haliclona flavescens*.

*22,23-Didehydro(*E-*):* ***4-Methyl-26,27-dinorergost-22-en-3-ol***
. 4-Methyl-24-norcholest-22-en-3-ol
[85638-95-5]
$C_{27}H_{46}O$ 386.66
Constit. of *Haliclona cinerea* and *Haliclona flavescens*.

Elenkov, I. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1997, **118**, 155-157 (*isol*)

2-Methyl-1,16-dithiocyanato-8-hexadecanol M-246

Thiocyanatin D_1



$C_{19}H_{34}N_2OS_2$ 370.622

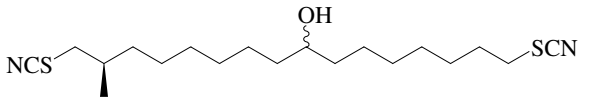
(2R,8ξ)-form [720697-77-8]

Isol. from a marine sponge *Oceanapia* sp. Nematocidal agent. Viscous oil. $[\alpha]_D^{21}$ -3.7 (c, 0.41 in $CHCl_3$). Isol. as a mixt. with 15-Methyl-1,16-dithiocyanato-8-hexadecanol, M-247 to which data applies.

Capon, R.J. *et al., J. Nat. Prod.*, 2004, **67**, 1277-1282 (*isol, pmr, cmr, ms*)

15-Methyl-1,16-dithiocyanato-8-hexadecanol M-247

Thiocyanatin D_2



$C_{19}H_{34}N_2OS_2$ 370.622

(8ξ,15*R*)-*form* [720697-79-0]
Isol. from a marine sponge *Oceanapia* sp. Nematocidal agent. Viscous oil. $[\alpha]_D^{21}$ -3.7 (c, 0.41 in $CHCl_3$). Isol. as a mixt. with 2-Methyl-1,16-dithiocyanato-8-hexadecanol, M-246 to which data applies.
Capon, R.J. *et al., J. Nat. Prod.*, 2004, **67**, 1277-1282 (*isol, pmr, cmr, ms*)

20-Methyl-5,9-docosadienoic acid M-248

$H_3CCH_2CH(CH_3)(CH_2)_9CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$

$C_{23}H_{42}O_2$ 350.584

(*E*,*E*)-*form* [132171-25-6]
Isol. from the sponge *Plakortis halichondroides.*
Carballeira, N.M. *et al., Lipids*, 1990, **25**, 835-840 (*isol, ir, cmr*)

21-Methyl-5,9-docosadienoic acid M-249

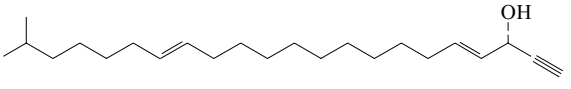
$(H_3C)_2CH(CH_2)_{10}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$

$C_{23}H_{42}O_2$ 350.584

(*E*,*E*)-*form* [132171-24-5]
Isol. from the sponge *Plakortis halichondroides.*
Carballeira, N.M. *et al., Lipids*, 1990, **25**, 835-840 (*isol, ir, cmr*)

21-Methyl-4,15-docosadien-1-yn-3-ol M-250

[139722-83-1]



$C_{23}H_{40}O$ 332.568

(3*S*,4*E*,15*E*)-*form* [129364-97-2]
Isol. from the sponge *Cribrochalina vasculum*.
Oil. $[\alpha]_D$ +17.9 (c, 1.1 in MeOH) (+2.0). λ_{max} 202 (ϵ 1400) (MeOH) (Derep).
Gunasekera, S.P. *et al., J.O.C.*, 1990, **55**, 6223 (*isol, pmr, cmr*)
Kulkarni, B.A. *et al., J.O.C.*, 1993, **58**, 5964 (*synth*)
Hallock, Y.F. *et al., J. Nat. Prod.*, 1995, **58**, 1801 (*isol, abs config*)

21-Methyldocosanoic acid, 9CI M-251

Isotricosanoic acid
[59708-74-6]
$(H_3C)_2CH(CH_2)_{19}COOH$
$C_{23}H_{46}O_2$ 354.615
Constit. of the marine sponge *Microciona prolifera*.
Mp 73.5°.

Et ester:
$C_{25}H_{50}O_2$ 382.669
Mp 55.5°.

Levene, P.A. *et al., J. Biol. Chem.*, 1922, **52**, 227 (*synth*)
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206

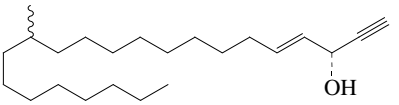
14-Methyl-3-docosen-1-yne M-252

$H_3C(CH_2)_7CH(CH_3)(CH_2)_9CH{=}CHC{\equiv}CH$

$C_{23}H_{42}$ 318.585

(-)-(*Z*)-*form* [184473-40-3]
Isol. from the sponge *Haliclona* sp. Oil. $[\alpha]_D$ -1.
Willliams, D.H. *et al., J. Nat. Prod.*, 1996, **59**, 1099-1101 (*isol, uv, ir, pmr, cmr, ms*)

14-Methyl-4-docosen-1-yn-3-ol M-253



(3*R*,4*E*,14ξ)-*form*

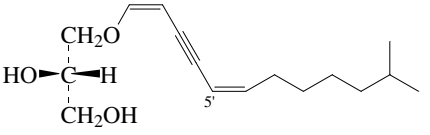
$C_{23}H_{42}O$ 334.584

(3*R*,4*E*,14ξ)-*form* [144259-01-8]
Isol. from the marine sponge *Cribrochalina vasculum*.
$[\alpha]_D$ +1.8 (c, 2.5 in MeOH). λ_{max} 200 (hexane) (Berdy).

(3*S*,4*E*,14ξ)-*form*
Isol. from the sponge *Cribrochalina vasculum*.
Oil. $[\alpha]_D$ +12.4 (c, 0.37 in MeOH).
Aiello, A. *et al., J. Nat. Prod.*, 1992, **55**, 1275 (*isol, pmr, config*)
Hallock, Y.F. *et al., J. Nat. Prod.*, 1995, **58**, 1801-1807

3-(11-Methyl-1,5-dodecadien-3-ynyloxy)-1,2-propanediol M-254

Glycerol 1-(11-methyl-1,5-dodecadien-3-ynyl) ether



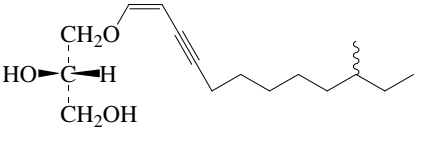
$C_{16}H_{26}O_3$ 266.38

(*S*,*Z*,*Z*)-*form*
Petroraspailyne A_2
[219917-15-4]
Isol. from a *Petrosia* sp.
$[\alpha]_D^{25}$ -3.2 (c, 0.4 in MeOH). λ_{max} 275 (log ϵ 3.82); 291 (log ϵ 3.64) (MeOH).

5′,6′-Dihydro: ***Petroraspailyne B_3***
[219917-19-8]
$C_{16}H_{28}O_3$ 268.395
Isol. from a *Petrosia* sp.
$[\alpha]_D^{25}$ +3.7 (c, 0.3 in MeOH). λ_{max} 238 (log ϵ 3.57) (MeOH).
Seo, Y. *et al., J. Nat. Prod.*, 1999, **62**, 122-126

3-(10-Methyl-1-dodecen-3-ynyloxy)-1,2-propanediol M-255

Glycerol 1-(10-methyl-1-dodecen-3-ynyl) ether



$C_{16}H_{28}O_3$ 268.395

(*S*,1′*Z*,10′ξ)-*form*
Petroraspailyne B_2
[219917-18-7]
Isol. from a *Petrosia* sp.
$[\alpha]_D^{25}$ +5.5 (c, 0.05 in MeOH). λ_{max} 238 (log ϵ 3.51) (MeOH).
Seo, Y. *et al., J. Nat. Prod.*, 1999, **62**, 122-126

2-Methyl-2,6-eicosadienoic acid M-256

$H_3C(CH_2)_{12}CH{=}CHCH_2CH_2CH{=}C(CH_3)COOH$

$C_{21}H_{38}O_2$ 322.53

(2E,6E)-form

(2-Hydroxyethyl)amide: ***Semiplenamide A***
[630100-41-3]
$C_{23}H_{43}NO_2$ 365.598
Alkaloid from *Lyngbya semiplena*. Amorph. solid. λ_{max} 206 (ϵ 5100) (MeOH).

(2-Acetoxyethyl)amide: ***Semiplenamide B***
[630100-42-4]
$C_{25}H_{45}NO_3$ 407.635
Alkaloid from *Lyngbya semiplena*. Oil. λ_{max} 203 (ϵ 5900) (MeOH).

Han, B. *et al., J. Nat. Prod.*, 2003, **66**, 1364-1368 (*isol, pmr, cmr*)

18-Methyl-5,9-eicosadienoic acid M-257

[133530-15-1]
$H_3CCH_2CH(CH_3)(CH_2)_7CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{21}H_{38}O_2$ 322.53
Constit. of the sponge *Erylus formosus*. Isol. as Me ester.

Carballeira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 305 (*isol*)
Kulkarni, B.A. *et al., Nat. Prod. Lett.*, 1993, **3**, 251 (*synth*)

19-Methyl-5,9-eicosadienoic acid M-258

$(H_3C)_2CH(CH_2)_8CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{21}H_{38}O_2$ 322.53

(E,E)-form [132171-20-1]
Constit. of the sponge *Plakortis halichondrioides*.

(Z,Z)-form [133530-16-2]
Constit. of the sponge *Erylus formosus*. Isol. as Me ester.

Carballeira, N.M. *et al., Lipids*, 1990, **25**, 835 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 305 (*isol*)
Kulkarni, B.A. *et al., Nat. Prod. Lett.*, 1993, **3**, 251 (*synth*)

18-Methyleicosanoic acid M-259

[36332-93-1]
$H_3CCH_2CH(CH_3)(CH_2)_{16}COOH$
$C_{21}H_{42}O_2$ 326.562

(±)-form
Cryst. (MeOH aq.). Mp 57-58°.

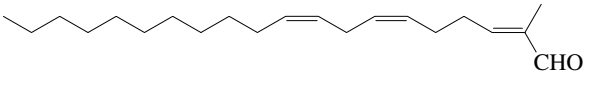
Me ester:
$C_{22}H_{44}O_2$ 340.588
Oil. $Bp_{0.1}$ 150°.

Amide:
$C_{21}H_{43}NO$ 325.577
Cryst. (MeOH). Mp 93-93.5°.

(ξ)-form
Occurs as esters in wool wax and in lipid composition of Caribbean sponge *Calyx podatypa*.

Nunn, J.R. *et al., J.C.S.*, 1951, 1740-1744 (*synth*)
Eur. Pat., 1991, 483 689; *CA*, **117**, 239463z (*synth, pmr, cmr*)
Pat. Coop. Treaty (WIPO), 1998, 98 30 532; *CA*, **129**, 137600x (*isol*)
Cundy, D.J. *et al., Org. Prep. Proced. Int.*, 2000, **32**, 461-468 (*synth, Me ester, pmr, cmr*)

2-Methyl-2,6,9-eicosatrienal M-260

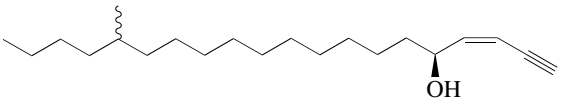


$C_{21}H_{36}O$ 304.515

(2E,6Z,9Z)-form
Isol. from the sponge *Leucetta microraphis*. Exhibits moderate cytotoxic activity. Oil. λ_{max} 230 (log ϵ 4.27) (EtOH).

Watanabe, K. *et al., J. Nat. Prod.*, 2000, **63**, 258-260

16-Methyl-3-eicosen-1-yn-5-ol M-261

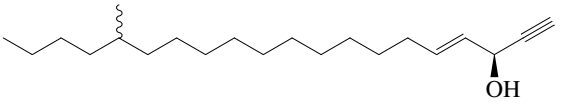


$C_{21}H_{38}O$ 306.531

(3Z,5S,16ξ)-form [173866-88-1]
Isol. from the sponge *Cribrochalina vasculum*.
Oil. $[\alpha]_D$ -23.1 (c, 0.33 in MeOH).

Hallock, Y.F. *et al., J. Nat. Prod.*, 1995, **58**, 1801-1807 (*isol, pmr, cmr, ms, config*)

16-Methyl-4-eicosen-1-yn-3-ol M-262



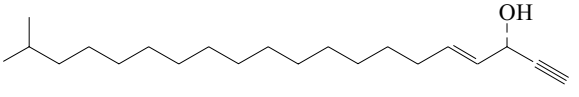
$C_{21}H_{38}O$ 306.531

(3S,4E,16ξ)-form [129364-95-0]
Isol. from the sponge *Cribrochalina vasculum*.
$[\alpha]_D^{25}$ +1.4 (c, 5.6 in MeOH).

Gunasekera, S.P. *et al., J.O.C.*, 1990, **55**, 6223-6225 (*isol, pmr, cmr*)
Hallock, Y.F. *et al., J. Nat. Prod.*, 1995, **58**, 1801-1807 (*isol, pmr, config*)

19-Methyl-4-eicosen-1-yn-3-ol M-263

[139722-82-0]

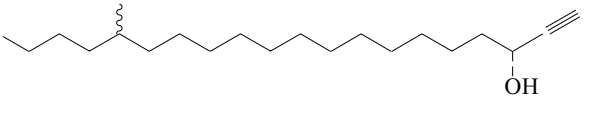


$C_{21}H_{38}O$ 306.531

(3S,4E)-form [129364-96-1]
Isol. from the sponge *Cribrochalina vasculum*.
Solid. $[\alpha]_D$ +22.2 (c, 0.6 in MeOH) (+2.6).

Gunasekera, S.P. *et al., J.O.C.*, 1990, **55**, 6223 (*isol, pmr, cmr*)
Kulkarni, B.A. *et al., J.O.C.*, 1993, **58**, 5964 (*synth*)
Hallock, Y.F. *et al., J. Nat. Prod.*, 1995, **58**, 1801 (*isol, pmr, config*)

16-Methyl-1-eicosyn-3-ol M-264

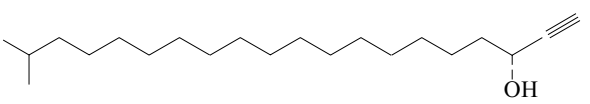


$C_{21}H_{40}O$ 308.546

(3R,16ξ)-form [144259-02-9]
Isol. from the marine sponge *Cribrochalina vasculum*. Toxic to brine shrimp. $[\alpha]_D$ +2.1 (c, 1.7 in MeOH). λ_{max} 200 (hexane) (Berdy).

Aiello, A. *et al., J. Nat. Prod.*, 1992, **55**, 1275

19-Methyl-1-eicosyn-3-ol M-265

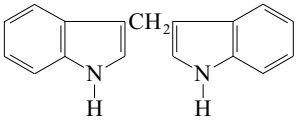


$C_{21}H_{40}O$ 308.546

(R)-form [144259-03-0]
Isol. from the marine sponge *Cribrochalina vasculum*. Toxic to brine shrimp. $[\alpha]_D$ +1.9 (c, 2 in MeOH). λ_{max} 200 (hexane) (Berdy).
Aiello, A. *et al., J. Nat. Prod.*, 1992, **55**, 1275

3,3′-Methylenebisindole, 9CI M-266

3,3′-Methylenediindole. Di-3-indolylmethane. ***Arundine***
[1968-05-4]



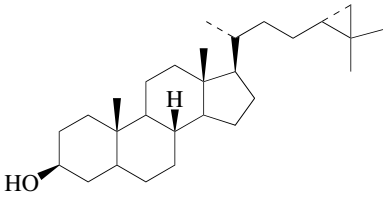
$C_{17}H_{14}N_2$ 246.311
Alkaloid from the roots of *Arundo donax*. Prod by the marine bacterium *Vibrio parahaemolyticus* Bio249. Needles (EtOH aq.). Mp 165-166°.

N-*Me:* ***Ardine***
[174545-80-3]
$C_{18}H_{16}N_2$ 260.338
Alkaloid from *Arundo donax*. Amorph.

N,N′-*Di-Me:*
$C_{19}H_{18}N_2$ 274.365
Plates (EtOH). Mp 110-112°.

Thesing, J. *et al., Chem. Ber.*, 1954, **87**, 692-699 (*synth*)
Jackson, A.H. *et al., J.C.S. Perkin 1*, 1987, 2543-2551 (*synth, pmr*)
Khuzaev, V.U. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1994, **30**, 635; 1995, **31**, 277; 277; 1996, **32**, 190 (*isol, Arundine, Ardine*)
Veluri, R. *et al., J. Nat. Prod.*, 2003, **66**, 1520-1523 (*isol*)

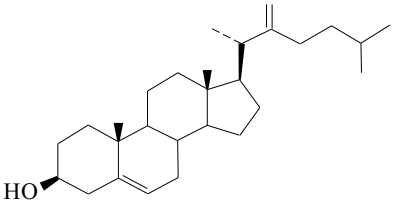
24,25-Methylenecholestan-3-ol M-267



$C_{28}H_{48}O$ 400.687

(3β,24R)-form [182619-60-9]
Constit. of *Rhizochalina incrustata*. Cryst. Mp 113-115°. $[\alpha]_D$ +17 (c, 0.1 in $CHCl_3$).
Makarieva, T.N. *et al., J. Chem. Res., Synop.*, 1996, 468-469 (*isol, pmr*)

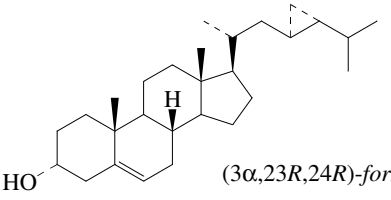
22-Methylenecholest-5-en-3-ol M-268



$C_{28}H_{46}O$ 398.671

3β-form
22-Methylenecholesterol
Constit. of *Halichondria panicea*. Cryst. Mp 114-116°. $[\alpha]_D$ -71 ($CHCl_3$).
Zielinski, J. *et al., Tet. Lett.*, 1981, 2345 (*isol, synth*)

23,24-Methylenecholest-5-en-3-ol M-269



(3α,23*R*,24*R*)-*form*

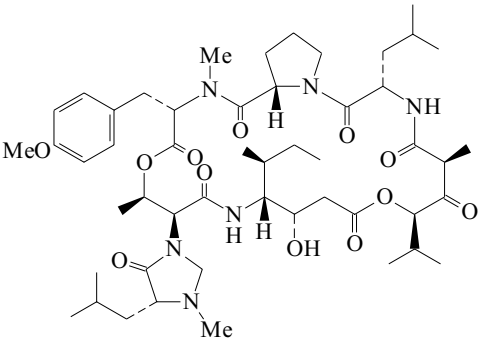
$C_{28}H_{46}O$ 398.671

(3α,23R,24R)-form
5β,6-Dihydro: ***23,24-Methylenecholestan-3-ol***
[123158-93-0]
$C_{28}H_{48}O$ 400.687
Minor sterol from *Calyx nicaeensis*, prob. as endobacterial metab.

(3β,23R,24R)-form
23,24-Methylenecholesterol
[94595-29-6]
Constit. of *Petrosia ficiformis*. Cryst. Mp 95-96°. $[\alpha]_D^{25}$ -22.7 ($CHCl_3$).
5β,6-Dihydro: [123238-28-8]
Minor sterol from sponge *Calyx nicaeensis*, prob. as an endobacterial metab.
Proudfoot, J.R. *et al., Tet. Lett.*, 1984, **25**, 5493-5496 (*synth, struct*)
Ha, T.B.T. *et al., Steroids*, 1989, **53**, 487-499 (*dihydro*)

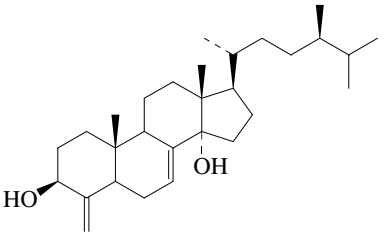
Methylenedidemnin A M-270

[97230-40-5]



$C_{50}H_{78}N_6O_{12}$ 955.199
Depsipeptide antibiotic. Isol. from *Trididemnum solidum*.
Sakai, R. *et al., J.A.C.S.*, 1995, **117**, 3734-3748; 8885 (*isol, uv, ir, pmr, cmr*)

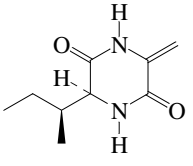
4-Methyleneergost-7-ene-3,14-diol M-271
24-Methyl-4-methylenecholest-7-ene-3,14-diol



$C_{29}H_{48}O_2$ 428.697

(3β,5α,24*R*)-*form*
14-Me ether, 7β,8β-epoxide: 7,8-Epoxy-14-methoxy-4-methylergostan-3-ol
$C_{30}H_{50}O_3$ 458.723
Isol. from *Theonella swinhoei*.
Sugo, Y. *et al., Steroids*, 1995, **60**, 738-742 (*isol, pmr, cmr*)

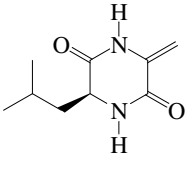
3-Methylene-6-(1-methylpropyl)-2,5-piperazinedione, 9CI M-272
Cyclo(dehydroalanylisoleucyl)



$C_9H_{14}N_2O_2$ 182.222

(*S*,*S*)-*form*
L-form
[160209-95-0]
Prod. by the marine bacterium *Vibrio parahaemolyticus*. No exptl. details given.
Bell, R. *et al., J. Nat. Prod.*, 1994, **57**, 1587-1590

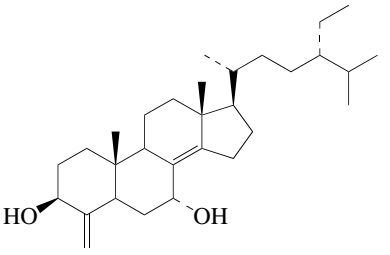
3-Methylene-6-(2-methylpropyl)-2,5-piperazinedione, 9CI M-273
Cyclo(dehydroalanylleucyl)



$C_9H_{14}N_2O_2$ 182.222

(*S*)-*form*
L-form
[65530-38-3]
Prod. by *Penicillium* sp. F70614 and a marine bacterium *Vibrio parahaemolyticus*. Inhibitor of α-glucosidases. Powder.
Mp >290° (synthetic). $[\alpha]_D^{20}$ -91.7 (DMF) (synthetic). λ_{max} 219 (ε 2130); 305 (ε 160) (MeOH).
Izumiya, N. *et al., J.A.C.S.*, 1977, **99**, 8346-8348 (*synth*)
Bell, R. *et al., J. Nat. Prod.*, 1994, **57**, 1587-1590 (*isol*)
Kwon, O.S. *et al., J. Antibiot.*, 2000, **53**, 954-958 (*isol, synth, uv, ir, pmr, cmr*)

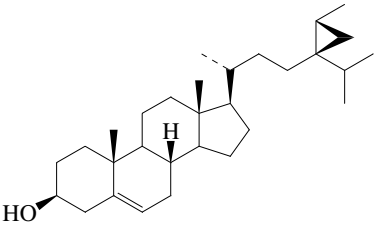
4-Methylenestigmast-8(14)-ene-3,7-diol M-274
24-Ethyl-4-methylenecholest-8(14)-ene-3,7-diol



$C_{30}H_{50}O_2$ 442.724

(3β,7α,24*S*)-*form*
7α-Hydroxytheonellasterol
[273746-39-7]
Constit. of *Theonella swinhoei*.
Oil. $[\alpha]_D$ +19.4 (c, 0.35 in $CHCl_3$). λ_{max} 248 (ε 1560) (MeOH).
7-Me ether: ***Swinhosterol C***
[186313-00-8]
$C_{31}H_{52}O_2$ 456.751
Constit. of *Theonella swinhoei*. Powder. $[\alpha]_D^{25}$ +20 (c, 0.71 in $CHCl_3$).
Umeyama, A. *et al., J. Nat. Prod.*, 1997, **60**, 296-298 (*Swinhosterol C*)
Qureshi, A. *et al., J. Nat. Prod.*, 2000, **63**, 841-842 (*isol, pmr, cmr*)

24,28-Methylenestigmast-5-en-3-ol M-275
23-[2-Methyl-1-(1-methylethyl)cyclopropyl]-24-norchol-5-en-3-ol, 14CI



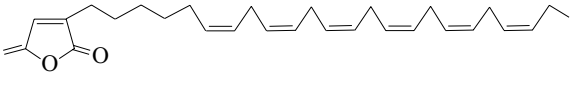
(3β,24*R*,28*R*)-*form*

$C_{30}H_{50}O$ 426.724

(3β,24*R*,28*R*)-*form* [117859-17-3]
Isol. from a marine chrysophyte alga.
Mp 118-121°.

(3β,24*S*,28*S*)-*form* [117859-18-4]
Isol. from the sponge *Petrosia weinbergi* and the pelagophtic alga *Pulvinaria* sp.
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*Chrysophte constit*)
Giner, J.L. *et al., J.O.C.*, 1988, **53**, 5895-5902 (*24S,28S-form, 24R,28R-form, synth, pmr, ms*)
Giner, J.L. *et al., Steroids*, 1999, **64**, 820-824 (*isol, pmr, struct*)

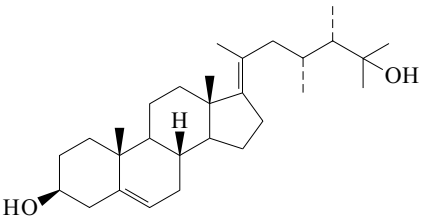
5-Methylene-3-(6,9,12,15,18,21-tetracosahexaenyl)-2(5*H*)-furanone, 9CI M-276
2-(6,9,12,15,18,21-Tetracosahexaenyl)-2,4-pentadien-4-olide



$C_{29}H_{40}O_2$ 420.634

(all-Z)*-*form [81576-09-2]
Isol. from the gorgonian *Plexaura flava*. Incorrectly abstracted as (*all-E*)-form in *CA*. λ_{max} 275 (ε 10500) (hexane) (Derep).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 105 (*isol, ir, pmr, ms*)

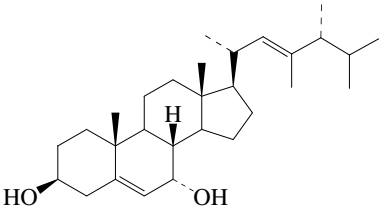
23-Methylergosta-5,17(20)-diene-3,25-diol **M-277**
23,24-Dimethylcholesta-5,17(20)-diene-3,25-diol



$C_{29}H_{48}O_2$ 428.697

(3β,17(20)*E*,23*R*,24*S*)-*form*
25-Hydroxysarcosterol
[153444-87-2]
Constit. of *Sinularia mayi*.
Cryst.
Mp 188-191°. $[\alpha]_D$ -55 (c, 0.36 in $CHCl_3$).
Kobayashi, M. *et al., Steroids*, 1994, **59**, 27-29 (*isol, pmr, cmr*)

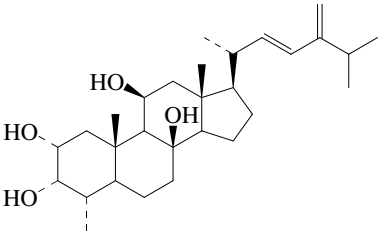
23-Methylergosta-5,22-diene-3,7-diol **M-278**
23,24-Dimethylcholesta-5,22-diene-3,7-diol



$C_{29}H_{48}O_2$ 428.697

(3β,7α,24*R*)-*form* [226716-94-5]
Constit. of *Lobophytum crassum*.
Rao, M.R. *et al., J. Nat. Prod.*, 1999, **62**, 785-786 (*isol, pmr, cmr*)

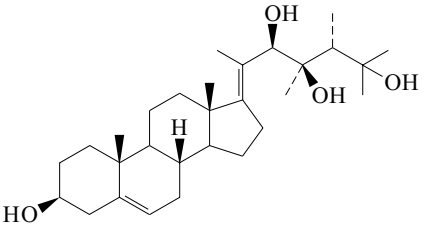
4-Methylergosta-22,24(28)-diene-2,3,8,11-tetrol **M-279**
4-Methyl-24-methylenecholest-22-ene-2,3,8,11-tetrol



$C_{29}H_{48}O_4$ 460.696

(2α,3α,4α,8β,11β,22*E*)-*form*
Hyrtiosterol
[777859-00-4]
Constit. of a *Hyrtios* sp.
Solid. $[\alpha]_D$ -22.5 (c, 0.1 in CH_2Cl_2).
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2004, **67**, 1736-1739 (*isol, pmr, cmr*)

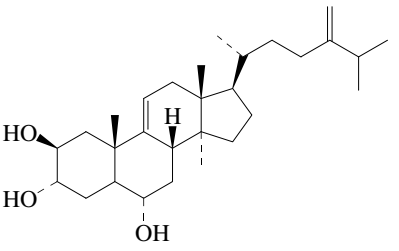
23-Methylergosta-5,17(20)-diene-3,22,23,25-tetrol **M-280**
23,24-Dimethylcholesta-5,17(20)-diene-3,22,23,25-tetrol



$C_{29}H_{48}O_4$ 460.696

(3β,17(20)*E*,22*R*,23*R*,24*R*)-*form* [157459-26-2]
Constit. of *Sinularia mayi*.
Oil. $[\alpha]_D$ -30 (c, 0.54 in $CHCl_3$).
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1994, 44 (*isol, pmr, cmr*)

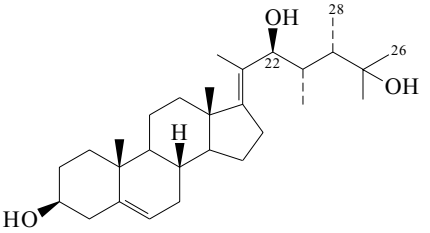
14-Methylergosta-9(11),24(28)-diene-2,3,6-triol **M-281**
14-Methyl-24-methylenecholest-9(11)-ene-2,3,6-triol



$C_{29}H_{48}O_3$ 444.696

(2β,3α,5α,6α)-*form*
Trisulfate: ***Ibisterol sulfate B***
[350228-49-8]
$C_{29}H_{48}O_{12}S_3$ 684.889
Constit. of a *Xestospongia* sp. Powder. $[\alpha]_D$ +50 (c, 0.28 in MeOH). λ_{max} 270 (ε 2160) (MeOH).
Lerch, M.L. *et al., Tetrahedron*, 2001, **57**, 4091-4094 (*isol, pmr, cmr*)

23-Methylergosta-5,17(20)-diene-3,22,25-triol **M-282**
23,24-Dimethylcholesta-5,17(20)-diene-3,22,25-triol



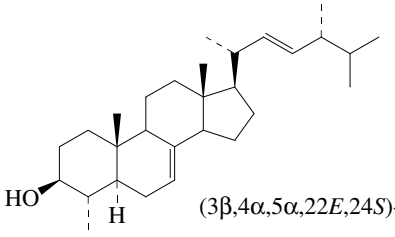
$C_{29}H_{48}O_3$ 444.696

(3β,17(20)*E*,22*S*,23*S*,24*S*)-*form* [157459-25-1]
Constit. of *Sinularia mayi*.
Oil. $[\alpha]_D$ -43 (c, 1.07 in $CHCl_3$).
22-Deoxy, 26-hydroxy: ***23-Methylergosta-5,17(20)-diene-3,25,26-triol***. *23,24-Dimethylcholesta-5,17(20)-diene-3,25,26-triol*
[152833-60-8]
$C_{29}H_{48}O_3$ 444.696
Constit. of *Sinularia mayi*. Cryst.
Mp 184-187°. $[\alpha]_D$ -28 (c, 1.02 in Py). C-25 config. undetd.
22-Deoxy, 28-hydroxy: ***23-Methylergosta-5,17(20)-diene-3,25,28-triol***. *24-Hydroxymethyl-23-methylcholesta-5,17(20)-diene-3,25-diol*

[152833-59-5]
$C_{29}H_{48}O_3$ 444.696
Constit. of *Sinularia mayi*. Cryst.
Mp 189-192°. $[\alpha]_D$ -34 (c, 0.66 in Py).
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1994, 44 (*isol, pmr, cmr*)

4-Methylergosta-7,22-dien-3-ol M-283

4,24-Dimethylcholesta-7,22-dien-3-ol



(3β,4α,5α,22*E*,24*S*)-*form*

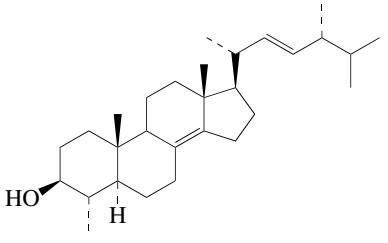
$C_{29}H_{48}O$ 412.698

(3β,4α,5α,22*E*,24*S*)-*form* [63109-18-2]
Isol. from various gorgonians and the amoebae *Naegleria* spp.
Needles (MeOH).
Mp 201-203° (193°). $[\alpha]_D$ -27 (c, 1.1 in $CHCl_3$).
Ac: [63109-19-3]
$C_{31}H_{50}O_2$ 454.735
Cryst. (MeOH). Mp 176-177° (163°). $[\alpha]_D$ +2.3 (c, 1.6 in $CHCl_3$).

(3β,4α,5α,22*E*,24ξ)-*form* [199734-47-9]
Constit. of *Haliclona cinerea* and *Haliclona flavescens*.
[63109-17-1, 108943-00-6]
Odorchai, R. *et al., J.C.S.*, 1964, 1142-1147 (*synth*)
Sucrow, W. *et al., Chem. Ber.*, 1977, **110**, 1523-1531 (*synth, pmr*)
Kokke, W.C.M.C. *et al., Phytochemistry*, 1982, **21**, 881-887 (*isol, pmr, ms*)
Raederstorff, D. *et al., Eur. J. Biochem.*, 1987, **164**, 427-434 (*isol*)
Elenkov, I. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1997, **118**, 155-157 (*Haliclona constit*)

4-Methylergosta-8(14),22-dien-3-ol M-284

4,24-Dimethylcholesta-8(14),22-dien-3-ol



$C_{29}H_{48}O$ 412.698

(3β,4α,5α,22*E*,24*R*)-*form*
Gymnodinosterol
[82660-61-5]
Isol. from various gorgonians and the dinoflagellate *Karenia brevis*.

(3β,4α,5ξ,22*E*,24ξ)-*form* [79295-69-5]
Isol. from *Crassostrea virginica* and *Scrippsiella trochoidea*.
Teshima, S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1981, **69**, 175 (*isol*)
Kokke, W.C.M.C. *et al., Phytochemistry*, 1982, **21**, 881-887 (*isol, pmr, ms*)
Harvey, H.R. *et al., Phytochemistry*, 1988, **27**, 1723-1729 (*isol*)
Giner, J.-L. *et al., J. Phycol.*, 2003, **39**, 315-319 (*Gymnodinosterol*)

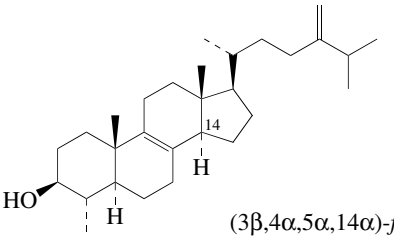
4-Methylergosta-8,22-dien-3-ol M-285

4,24-Dimethylcholesta-8,22-dien-3-ol
$C_{29}H_{48}O$ 412.698

(3β,4α,5α,22*E*,24ξ)-*form* [52043-01-3]
Constit. of *Porphyridium cruentum*.
Beastall, G.H. *et al., Eur. J. Biochem.*, 1973, **41**, 301

4-Methylergosta-8,24(28)-dien-3-ol M-286

4-Methyl-24-methylenecholest-8-en-3-ol



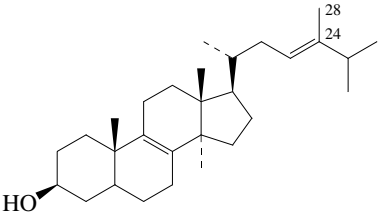
(3β,4α,5α,14α)-*form*

$C_{29}H_{48}O$ 412.698

(3β,4α,5α,14α)-*form*
4α-Methylfecosterol
[17757-07-2]
Minor constit. of yeast and constit. of *Aesculus hippocastanum* seeds and wheat germ oil (*Triticum aestivum*). Also isol. from the Caribbean sponge *Neofibularia nolitangere*.
Cryst. (Me_2CO/MeOH).
Mp 143-145°. $[\alpha]_D^{29}$ +55 (c, 3 in $CHCl_3$).

(3β,4α,5α,14β)-*form*
Triticusterol
[224566-30-7]
Constit. of wheat germ oil (*Triticum aestivum*).
Needles.
Mp 107-109°. $[\alpha]_D^{25}$ +118.6 (c, 0.6 in $CHCl_3$).
Barton, D.H.R. *et al., Chem. Comm.*, 1968, 17 (*isol*)
Barton, D.H.R. *et al., J.C.S.(C)*, 1970, 775 (*biosynth*)
Stanković, S. *et al., Phytochemistry*, 1985, **24**, 2466 (*isol*)
Costantino, V. *et al., Steroids*, 1995, **60**, 768-772 (*isol, sponge*)
Akihisa, T. *et al., J.C.S. Perkin 1*, 1999, 497-500 (*isol, pmr, cmr*)

14-Methylergosta-8,23-dien-3-ol M-287

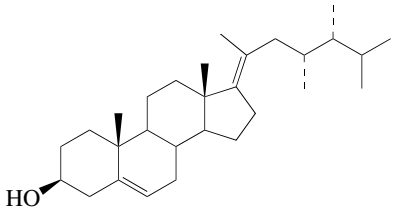


$C_{29}H_{48}O$ 412.698

(3β,23*E*)-*form* [90195-44-1]
Trace constit. of the lipids of a marine unicellular green alga.
$\Delta^{24(28)}$-Isomer: ***14-Methylergosta-8,24(28)dien-3-ol***
[33886-74-7]
$C_{29}H_{48}O$ 412.698
Minor constit. of the lipids of a marine unicellular green alga.
9Z-Octadecenoyl: [122579-36-6]
$C_{47}H_{80}O_2$ 677.148
Isol. from *Saccharomyces cerevisiae*.
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*isol, pmr*)
Fenner, G.P. *et al., Lipids*, 1989, **24**, 625-629 (*octadecenoate*)

23-Methylergosta-5,17(20)-dien-3-ol, 9CI M-288

23,24-Dimethylcholesta-5,17(20)-dien-3-ol



$C_{29}H_{48}O$ 412.698

(3β,17(20*E*),23*R*,24*R*)-*form*

Sarcosterol

[73731-24-5]

Isol. from the soft coral *Sarcophyton glaucum*.

Mp 148-150°. $[\alpha]_D$ -60.

Kobayashi, M. *et al., Steroids*, 1979, **34**, 273; 1994, **59**, 27 (*isol, pmr, cmr, ms, struct*)

Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1994, 44 (*cmr*)

23-Methylergosta-5,22-dien-3-ol M-289

23,24-Dimethylcholesta-5,22-dien-3-ol

$C_{29}H_{48}O$ 412.698

(3β,22*E*,24*R*)-*form* [80925-05-9]

Constit. of *Axinella cannabina*, *Pyrocystis lunula* and *Zooxanthella microadriatica*.

O-*Sulfate:* ***Hymenosulfate***. *Hymenosulphate*

[119108-36-0]

$C_{29}H_{48}O_4S$ 492.762

Constit. of a diatom *Hymenomonas* sp. Calcium release agent.

Cryst. (MeOH) (as Na salt). Sol. C_6H_6, toluene.

Mp 247-250° (Na salt). $[\alpha]_D^{22}$ -23 (c, 0.1 in MeOH) (Na salt). CAS no. refers to Na salt.

(3β,22*E*,24ξ)-*form* [53282-68-1]

Constit. of *Sarcophyton glaucum*, *Sarcophyton elegans* and *Prorocentrum* spp. dinoflagellates.

Cryst.

Mp 156-158.5°. $[\alpha]_D$ -53.7 (c, 1.75 in $CHCl_3$).

Kobayashi, M. *et al., Steroids*, 1979, **34**, 273 (*isol, pmr, ms*)

Bohlin, L. *et al., Phytochemistry*, 1981, **20**, 2397-2401 (*isol*)

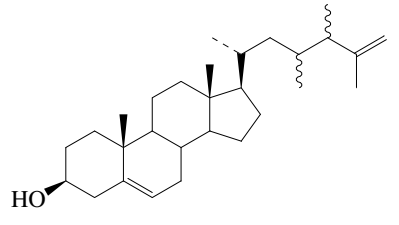
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol*)

Kobayashi, J. *et al., J.C.S. Perkin 1*, 1989, 101-103 (*Hymenosulfate*)

Volkman, J.K. *et al., Phytochemistry*, 1999, **52**, 659-668 (*occur, dinoflagellates*)

23-Methylergosta-5,25-dien-3-ol M-290

23,24-Dimethylcholesta-5,25-dien-3-ol



$C_{29}H_{48}O$ 412.698

(3β,23ξ,24ξ)-*form*

O-*Sulfate:* [211427-01-9]

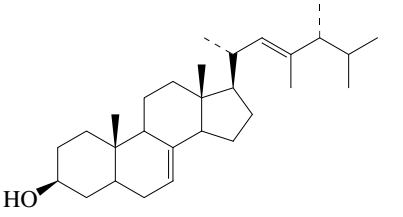
$C_{29}H_{48}O_4S$ 492.762

Constit. of a sea cucumber, *Holothuria* sp.

Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 262-266 (*isol*)

23-Methylergosta-7,22-dien-3-ol M-291

23,24-Dimethylcholesta-7,22-dien-3-ol



$C_{29}H_{48}O$ 412.698

(3β,5α,22*E*,24*R*)-*form* [81275-82-3]

Constit. of *Pseudostichopus trachus* and *Holothuria scabra*.

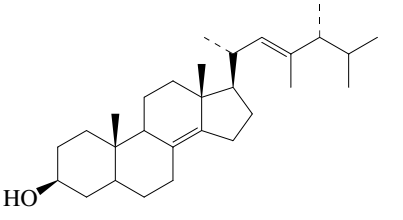
Present in dinoflagellates *Prorocentrum* spp.

Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*isol, pmr*)

Volkman, J.K. *et al., Phytochemistry*, 1999, **52**, 659-668 (*occur, dinoflagellates*)

23-Methylergosta-8(14),22-dien-3-ol M-292

23,24-Dimethylcholest-8(14),22-dien-3-ol



$C_{29}H_{48}O$ 412.698

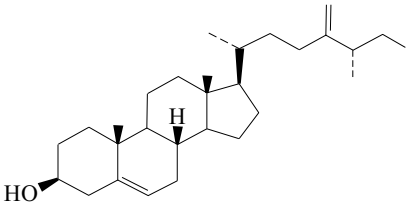
(3β,5α,22*E*,24*R*)-*form* [636599-90-1]

Constit. of *Karenia brevis*.

Giner, J.-L. *et al., J. Phycol.*, 2003, **39**, 315-319 (*isol, pmr, cmr*)

26-Methylergosta-5,24(28)-dien-3-ol M-293

26-Methyl-24-methylenecholest-5-en-3-ol



$C_{29}H_{48}O$ 412.698

(3β,25*S*)-*form*

24(28)-Dehydroaplysterol

[38636-50-9]

Constit. of *Aplysina aerophoba* and other sponges.

Cryst. (MeOH).

Mp 128-130°. $[\alpha]_D$ -37 ($CHCl_3$).

De Luca, P. *et al., J.C.S. Perkin 1*, 1972, 2132 (*isol*)

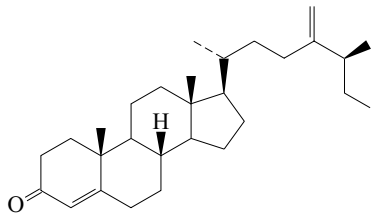
De Luca, P. *et al., Chem. Comm.*, 1973, 825 (*synth*)

Theobald, N. *et al., J.A.C.S.*, 1978, **100**, 7677 (*isol*)

Cho, J.-H. *et al., J.O.C.*, 1988, **53**, 3466 (*biosynth*)

26-Methylergosta-4,24(28)-dien-3-one M-294

25-Ethyl-27-norergosta-4,24(28)-dien-3-one, 9CI. 26-Methyl-24-methylenecholest-4-en-3-one
[91283-91-9]

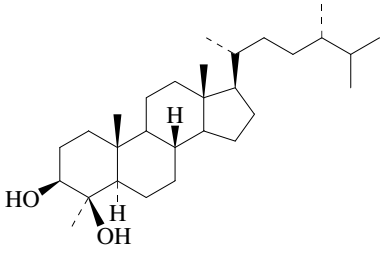


$C_{29}H_{46}O$ 410.682

(25*S*)-*form*
Eydosterone
Metab. of *Neosiphonia supertes* and *Pocillopora eydouxi*.
Cryst. (MeOH).
Mp 98-99°. $[\alpha]_D^{20}$ +42 (c, 1 in $CHCl_3$). Genus name wrongly spelt as Poicillopora.
Rambabu, M. *et al., Indian J. Chem., Sect. B*, 1984, **23**, 173
Oger, J.-M. *et al., J. Nat. Prod.*, 1991, **54**, 273 (*isol, synth, pmr, cmr*)

4-Methylergostane-3,4-diol M-295

4,24-Dimethylcholestane-3,4-diol

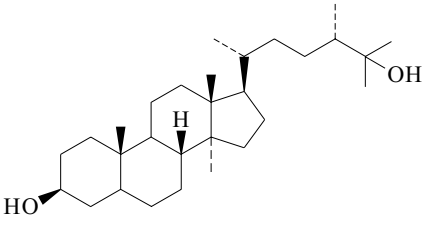


$C_{29}H_{52}O_2$ 432.729

(3β,4β*OH*,5α,24*S*)-*form*
Methylpavlovol
[150994-74-4]
Isol. from *Pavlova gyrans* and *Pavlova lutheri*.
Patterson, G.W. *et al., Lipids*, 1993, **28**, 771-773 (*isol, pmr, cmr*)

14-Methylergostane-3,25-diol M-296

14,24-Dimethylcholestane-3,25-diol

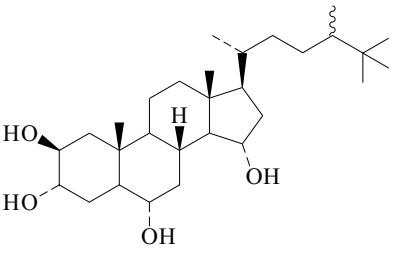


$C_{29}H_{52}O_2$ 432.729

(3β,24*S*)-*form* [160324-92-5]
Constit. of *Nephthea chabroli*.
Anjaneyulu, A.S.R. *et al., J. Indian Chem. Soc.*, 1994, **71**, 523 (*isol, pmr, cmr*)

25-Methylergostane-2,3,6,15-tetrol M-297

24,25-Dimethylcholestane-2,3,6,15-tetrol

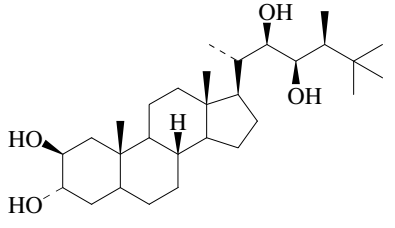


$C_{29}H_{52}O_4$ 464.727

(2β,3α,5α,6α,15α,24ξ)-*form*
2,3,6-Tri-O-*sulfate:* ***Halistanol sulfate E***
[143049-16-5]
$C_{29}H_{52}O_{13}S_3$ 704.92
Constit. of an *Epipolasis* sp. Thrombin inhibitor. $[\alpha]_D^{21}$ +13.3 (c,0.21 in MeOH) (as tri-Na salt).
Kanazawa, S. *et al., Tetrahedron*, 1992, **48**, 5467-5472 (*isol, pmr, cmr*)

25-Methylergostane-2,3,22,23-tetrol M-298

24,25-Dimethylcholestane-2,3,22,23-tetrol

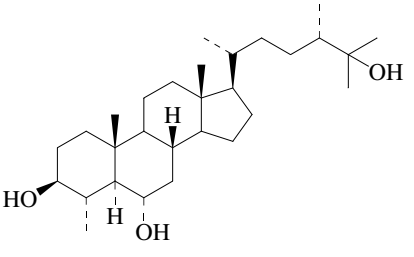


$C_{29}H_{52}O_4$ 464.727

(2β,3α,5α,22*R*,23*R*,24*S*)-*form* [552839-80-2]
2,3-Disulfate: ***Sch 572423***
[552839-79-9]
$C_{29}H_{52}O_{10}S_2$ 624.856
Constit. of a *Topsentia* sp.
Yang, S.-W. *et al., Bioorg. Med. Chem. Lett.*, 2003, **13**, 1791-1794 (*isol, pmr, cmr*)

4-Methylergostane-3,6,25-triol M-299

4,24-Dimethylcholestane-3,6,25-triol

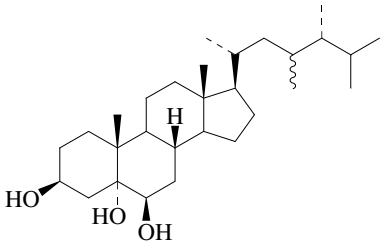


$C_{29}H_{52}O_3$ 448.728

(3β,4α,5α,6α,24*S*)-*form* [794536-92-8]
Constit. of a *Sarcophyton* sp.
Cryst. (Me_2CO/petrol).
Mp 232-234°. $[\alpha]_D^{25}$ +15.2 (c, 0.26 in $CHCl_3$).
Sekhar, V.C. *et al., Asian J. Chem.*, 2004, **16**, 572-576; *CA*, **141**, 422421u (*Sarcophyton constit, isol, pmr*)

23-Methylergostane-3,5,6-triol M-300

23,24-Dimethylcholestane-3,5,6-triol



$C_{29}H_{52}O_3$ 448.728

(3β,5α,6β,23ξ,24*R*)-*form* [872721-84-1]
Constit. of *Sarcophyton tortuosum*.
Lan, W.-J. *et al., Zhongshan Daxue Xuebao Ziran Kexueban*, 2005, **44**, 59-62; *CA*, **144**, 104198d

25-Methylergostane-2,3,6-triol M-301

24,25-Dimethylcholestane-2,3,6-triol

$C_{29}H_{52}O_3$ 448.728

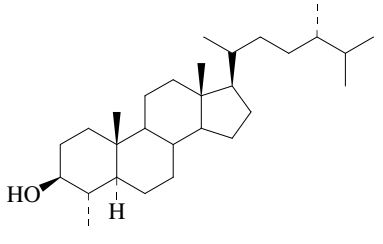
(2β,3α,5α,6α,24*S*)-*form*
Halistanol
[79405-68-8]
[190581-94-3 (imidazolium salt)]
Isol. (as 2-aminoimidazole salt) from a *Topsentia* sp.
Cryst. Mp 248-249°. $[\alpha]_D$ +37.

Tri-O-*sulfate:* ***Halistanol sulfate***
[103065-20-9]
[79405-69-9 (Na salt)]
$C_{29}H_{52}O_{12}S_3$ 688.921
Isol. from *Halichondria moorei*, a *Trachyopsis* sp., *Epipolasis kushimotoensis*, *Haliclona* sp. and a *Topsentia* sp. Haemolytic and ichthyotoxic agent. Adenosine receptor agonist. Starfish fertilisation inhibitor. Thrombin inhibitor. Shows antimicrobial props. Cryst. (as tri-Na salt). Mp 159.5-160.5° (tri-Na salt). $[\alpha]_D$ +17.

Tsukamoto, S. *et al., Fish. Sci.*, 1977, **67**, 310-312 (*isol*)
Fusetani, N. *et al., Tet. Lett.*, 1981, **22**, 1985-1988 (*Halistanol sulfate*)
Kanazawa, S. *et al., Tetrahedron*, 1992, **48**, 5467-5472 (*Halistanol sulfate*)
Sperry, S. *et al., J. Nat. Prod.*, 1997, **60**, 29-32 (*Halistanol sulfate*)

4-Methylergostan-3-ol M-302

4,24-Dimethylcholestan-3-ol



(3β,4α,5α,24*S*)-*form*

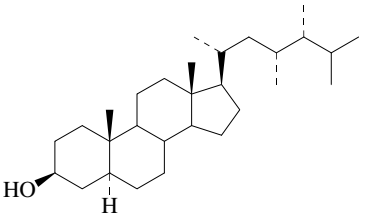
$C_{29}H_{52}O$ 416.729

(3β,4α,5α,24*S*)-*form* [4298-00-4]
Minor sterol from soft coral *Sarcophyton glaucum*.
Mp 192-194° (186-188°). $[\alpha]_D$ +13 ($CHCl_3$).

(3β,4α,5α,24ξ)-*form*
Present in dinoflagellates *Prorocentrum micans* and *Gymnodinium* spp.
Kobayashi, M. *et al., Steroids*, 1982, **40**, 209-221 (*isol, Sarcophyton*)
Volkman, J.K. *et al., Phytochemistry*, 1999, **52**, 659-668 (*isol, dinoflagellates*)

23-Methylergostan-3-ol, 9CI M-303

23,24-Dimethylcholestan-3-ol



(3β,5α,23*R*,24*R*)-*form*

$C_{29}H_{52}O$ 416.729

(3β,5α,23*R*,24*R*)-*form* [85505-68-6]
Isol. from an unidentified sp. of zooxanthellae obt. from *Orbulina universa*.

(3β,5α,23*R*,24*S*)-*form* [86708-37-4]
Cryst. (MeOH). Mp 162-164°. $[\alpha]_D^{20}$ +34.1 (c, 1.15 in $CHCl_3$).

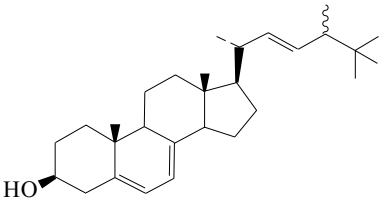
(3β,5α,23*S*,24*R*)-*form* [85505-67-5]
Constit. of *Bugula neritina*.

(3β,5α,23ξ,24ξ)-*form* [70755-56-5]
Isol. from *Gonyaulax polygramma*, *Macoma balthica* and *Prorocentrum micrans*.

(3β,5β,23ξ,24ξ)-*form* [123238-29-9]
Isol. from *Calyx niceensis*, prob. as prod. of endobacterial metab.
Zielinski, J. *et al., J.O.C.*, 1983, **48**, 3471-3477 (*3β,5α,23S,24R-form*)
Volkman, J.K. *et al., Lipids*, 1984, **19**, 456-465 (*isol*)
Kokke, W.C.M.C. *et al., Biochem. Syst. Ecol.*, 1987, **15**, 475-478 (*isol*)
Shu, A.Y.L. *et al., J.C.S. Perkin 1*, 1987, 1291-1305 (*synth*)
Ha, T.B.T. *et al., Steroids*, 1989, **53**, 487-499 (*3β,5β,23ξ,24ξ-form*)
Volkman, J.K. *et al., Phytochemistry*, 1999, **52**, 659-668 (*3β,5α,23ξ,24ξ-form*)

25-Methylergosta-5,7,22-trien-3-ol M-304

24,25-Dimethylcholesta-5,7,22-trien-3-ol



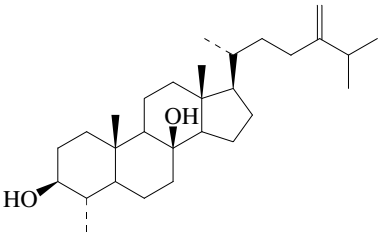
$C_{29}H_{46}O$ 410.682

(3β,22*E*,24ξ)-*form*
Haliclonasterol
[32352-65-1]
Constit. of red algae and *Haliclona longleyi*. Also from green alga *Monostroma nitidum*. Cryst. (Et_2O). Mp 140.5-141°. $[\alpha]_D^{27}$ -41.5 ($CHCl_3$).

Ac: Mp 140-141°. $[\alpha]_D^{27}$ -46 ($CHCl_3$).

Bergman, W. *et al., J.O.C.*, 1949, **14**, 1078-1084; 1951, **16**, 1337-1344 (*isol*)
Tsuda, K. *et al., Chem. Pharm. Bull.*, 1960, **8**, 554-558 (*isol*)
Patterson, G.W. *et al., Lipids*, 1971, **6**, 120-127 (*isol*)

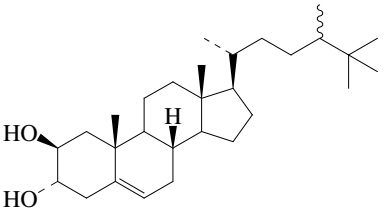
4-Methylergost-24(28)-ene-3,8-diol M-305
4-Methyl-24-methylenecholestane-3,8-diol



$C_{29}H_{50}O_2$ 430.713

(3β,4α,5α)-*form* [250141-64-1]
Constit. of *Nephthea chabroli* and a gorgonian sp.
Cryst.
Mp 120-121°. $[\alpha]_D$ +5.62 (c, 0.2 in $CHCl_3$).
Mehta, G. *et al., J. Chem. Res., Synop.*, 1999, 628-629 (*isol, pmr, cmr, cryst struct*)

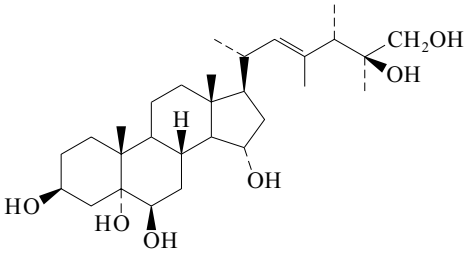
25-Methylergost-5-ene-2,3-diol M-306
24,25-Dimethylcholest-5-ene-2,3-diol



$C_{29}H_{50}O_2$ 430.713

(2β,3α,24ξ)-*form* [97484-54-3]
Mp 257-260°. $[\alpha]_D^{20}$ -32 (c, 0.05 in EtOH).
Di-O-*sulfate:* [97484-53-2]
$C_{29}H_{50}O_8S_2$ 590.841
Isol. from a sponge *Halichondria* sp.
Mp 205-207°. $[\alpha]_D^{20}$ -14.2 (c, 0.12 in Py). Poss. artifact.
Makar'eva, T.N. *et al., Khim. Prir. Soedin.*, 1985, 272-273; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 257-258

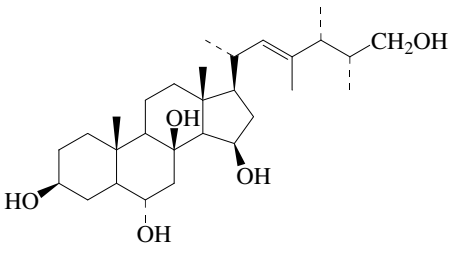
23-Methylergost-22-ene-3,5,6,15,25,26-hexol M-307
23,24-Dimethylcholest-22-ene-3,5,6,15,25,26-hexol



$C_{29}H_{50}O_6$ 494.71

(3β,5α,6β,15α,22*E*,24*S*,25*S*)-*form*
26-Sulfate:
$C_{29}H_{50}O_9S$ 574.775
Constit. of *Styracaster caroli*.
$[\alpha]_D$ +2.7 (MeOH).
Iorizzi, M. *et al., J. Nat. Prod.*, 1994, **57**, 1361 (*isol, pmr, cmr*)

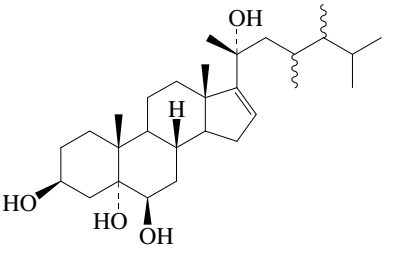
23-Methylergost-22-ene-3,6,8,15,26-pentol M-308
23,24-Dimethylcholest-22-ene-3,6,8,15,26-pentol



$C_{29}H_{50}O_5$ 478.711

(3β,5α,6α,8β,15β,22*E*,24*R*,25*R*)-*form*
Certonardosterol I
[517900-57-1]
Constit. of *Certonardoa semiregularis.*
Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2003, **66**, 384-391 (*isol, pmr, cmr*)

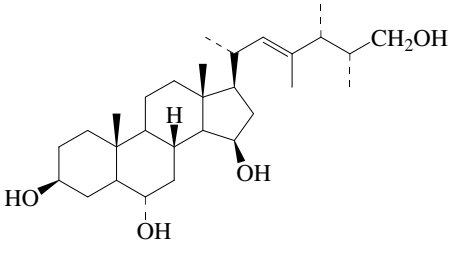
23-Methylergost-16-ene-3,5,6,20-tetrol M-309
23,24-Dimethylcholest-16-ene-3,5,6,20-tetrol



$C_{29}H_{50}O_4$ 462.712

(3β,5α,6β,20*R*,23ξ,24ξ)-*form* [293735-51-0]
Constit. of *Sarcophyton trocheliophorum*.
Amorph. powder. $[\alpha]_D^{20}$ -14.1 (c, 0.16 in EtOH). λ_{max} 225 (log ϵ 0.26) (no solvent reported).
Dong, H. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1087-1089 (*isol, pmr, cmr*)

23-Methylergost-22-ene-3,6,15,26-tetrol M-310
23,24-Dimethylcholest-22-ene-3,6,15,26-tetrol



$C_{29}H_{50}O_4$ 462.712

(3β,5α,6α,15β,22*E*,24*R*,25*R*)-*form*
Certonardosterol J
[517900-58-2]
Constit. of *Certonardoa semiregularis.*
Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2003, **66**, 384-391 (*isol, pmr, cmr*)

4-Methylergost-8(14)-en-3-ol M-311
4,24-Dimethylcholest-8(14)-en-3-ol
$C_{29}H_{50}O$ 414.713

(3β,4α,5α,24*S*)-*form* [78340-85-9]
Constit. of *Glenodinium* sp. and *Scrippsiella trochoidea*.

(3β,4α,5α,24ξ)-*form*
Ketone: ***4-Methylergost-8(14)-en-3-one***. *4,24-Dimethylcholest-8(14)-en-3-one*
[116169-29-0]
$C_{29}H_{48}O$ 412.698
Constit. of *Scrippsiella trochoidea*.

[76758-21-9]

Kho, E. *et al., J.O.C.*, 1981, **46**, 1836 (*synth, pmr, 3β,4β,5α,24R-form*)
Kokke, W.C.M.C. *et al., Phytochemistry*, 1981, **20**, 127 (*isol, 3β,4α,5α,24S-form*)
Harvey, H.R. *et al., Phytochemistry*, 1988, **27**, 1723-1729 (*isol*)

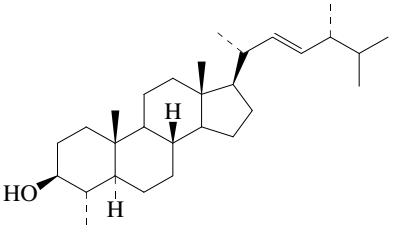
4-Methylergost-14-en-3-ol, 9CI M-312

4,24-Dimethylcholest-14-en-3-ol
$C_{29}H_{50}O$ 414.713

(3β,4α,5α)-*form* [78285-86-6]
Constit. of *Glenodinium* sp.
Kokke, W.C.M.C. *et al., Phytochemistry*, 1981, **20**, 127 (*isol*)

4-Methylergost-22-en-3-ol M-313

4,24-Dimethylcholest-22-en-3-ol



$C_{29}H_{50}O$ 414.713

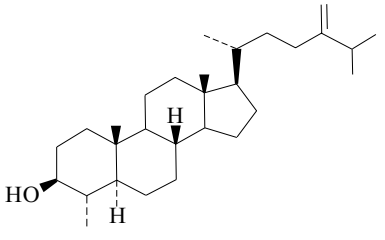
(3β,4α,5α,22*E*,24*R*)-*form* [77982-80-0]
Constit. of *Pachychalina* sp., *Plexaura homomalla*, *Nereis diversicolor* and *Pyrocystis lunula*.
3-Ac: [337379-19-8]
$C_{31}H_{52}O_2$ 456.751
Constit. of *Pseudoplexaura flagellosa*.

(3β,4α,5α,22*E*,24ξ)-*form* [79897-59-9]
Constit. of *Holothuria nobilis* and *Holothuria scabra*.
22,23-Dihydro: ***4-Methylergostan-3-ol***. *4,24-Dimethylcholestan-3-ol*
[76250-37-8]
$C_{29}H_{52}O$ 416.729
Constit. of *Synapta maculata*.

Kokke, W.C.M.C. *et al., Steroids*, 1982, **40**, 307-318 (*isol*)
Ha, T.B.T. *et al., Steroids*, 1982, **40**, 433-453 (*occur*)
Dow, W.C. *et al., Steroids*, 1983, **42**, 217-230 (*synth*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*Holothuria constits*)
Reynolds, W.F. *et al., Magn. Reson. Chem.*, 2001, **39**, 94-97 (*3-Ac*)

4-Methylergost-24(28)-en-3-ol M-314

4,24-Dimethylcholest-24(28)-en-3-ol



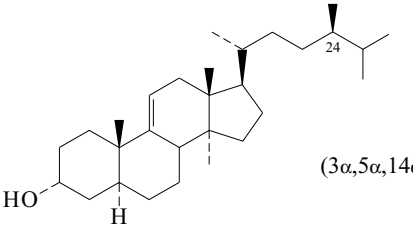
$C_{29}H_{50}O$ 414.713

(4α,5α)-*form*
Zoanthosterol
[77944-03-7]
Constit. of *Zoanthus sociatus*, *Nephthea chabroli*, *Haliclona cinerea* and *Haliclona flavescens*. Component of the lipids of *Prorocentrum* spp. dinoflagellates. Isol. from an unidentified *Lobophytum* sp.
Ac:
Cryst. (MeOH/Et_2O). Mp 130.5-132.5°. $[\alpha]_D$ +27.6 (c, 0.70 in $CHCl_3$).

Kelecom, A. *et al., Bull. Soc. Chim. Belg.*, 1981, **90**, 971-976 (*isol, struct*)
Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 901-903 (*isol*)
Elenkov, I. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1997, **118**, 155-157 (*occur*)
Mehta, G. *et al., J. Chem. Res., Synop.*, 1999, 628-629 (*occur*)
Volkman, J.K. *et al., Phytochemistry*, 1999, **52**, 659-668 (*occur, dinoflagellates*)

14-Methylergost-9(11)-en-3-ol M-315

14,24-Dimethylcholest-9(11)-en-3-ol



(3α,5α,14α,24*R*)−*form*

$C_{29}H_{50}O$ 414.713

(3α,5α,14α,24*R*)-*form* [148839-03-6]
Constit. of *Neolitsea aciculata*.

(3α,5α,14α,24*S*)-*form* [148839-04-7]
Constit. of *Neolitsea aciculata*.

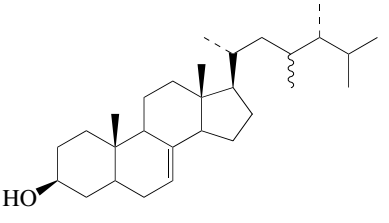
(3β,5α,14α,24*R*)-*form* [122738-87-8]
Constit. of *Gynostemma pentaphyllum*. Isol. from the fern *Gleichenia japonica*.

(3β,5α,14α,24*S*)-*form* [122798-38-3]
Constit. of *Chlorella vulgaris* and *Gynostemma pentaphyllum*. Isol. from *Gleichenia japonica*.
Mp 93-94° (as Ac).

Akihisa, T. *et al., Phytochemistry*, 1989, **28**, 1271-1273 (*Gynostemma, isol*)
Akihisa, T. *et al., Phytochemistry*, 1992, **31**, 1769-1772 (*Chlorella, isol*)
Yano, K. *et al., Phytochemistry*, 1992, **31**, 2902-2904 (*Neolitsea, isol*)
Akihisa, T. *et al., Chem. Pharm. Bull.*, 1993, **41**, 624-626 (*Gleichenia, isol*)

23-Methylergost-7-en-3-ol M-316

23,24-Dimethylcholest-7-en-3-ol



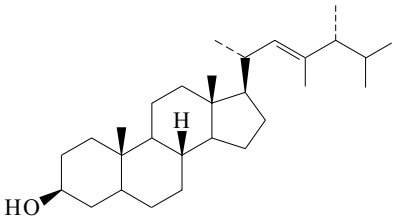
$C_{29}H_{50}O$ 414.713

(3β,5α,23ξ,24*R*)-*form* [214483-19-9]
Constit. of *Trochostoma orientale*.

Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*isol, ms*)

23-Methylergost-22-en-3-ol M-317

23,24-Dimethylcholest-22-en-3-ol



$C_{29}H_{50}O$ 414.713

(3β,5α,22*E*,24*R*)-*form* [80925-06-0]

Constit. of *Gonyaulax monilata*, *Bathyplotes natans* and *Pseudostichopus trachus*. Minor sterol from dinoflagellates *Prorocentrum* spp.

$\Delta^{23,33}$-Isomer: ***23-Methyleneergostan-3-ol****. 24-Methyl-23-methylenecholestan-3-ol*
[80471-68-7]
[85505-66-4]
$C_{29}H_{50}O$ 414.713
Constit. of *Gonyaulax monilata*.

Wengrovitz, P.S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1981, **69**, 535-539 (*isol*)
Gebreyesus, T. *et al., Tet. Lett.*, 1982, **23**, 4427-4430 (*struct*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*isol, pmr*)
Volkman, J.K. *et al., Phytochemistry*, 1999, **52**, 659-668 (*occur, dinoflagellates*)

N-Methylformamide, 9CI, 8CI M-318

Formylmethylamine. NSC 3051
[123-39-7]
HCONHMe
C_2H_5NO 59.068
Isol. from the red alga *Erythrophyllum delesserioides*. Antineoplastic agent. Sol. H_2O, EtOH; insol. Et_2O. d^{19} 1.01.
Mp -3.8°. Bp 180-185°. n_D^{20} 1.4319.

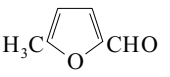
▶ Highly flammable, fl. p.50 (rat, orl) 4000 mg/kg. Exp. reprod. and teratogenic effects. Hepatotoxic. LQ3000000

N-*Bromo:* N-*Bromo*-N-*methylformamide*
C_2H_4BrNO 137.964
Mp 81-83°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 753D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1227C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 778D (*ir*)
Gautier, A. *et al., Annalen*, 1869, **151**, 241 (*synth*)
U.K. Pat., 1926, 252 460; *CA*, **21**, 2273 (*synth*)
Russell, R.A. *et al., Spectrochim. Acta*, 1956, **8**, 138 (*ir*)
Suzuki, I. *et al., Bull. Chem. Soc. Jpn.*, 1962, **35**, 540 (*ir*)
LaPlanche, L.A. *et al., J.A.C.S.*, 1964, **86**, 337 (*pmr*)
Nielsen, E.B. *et al., J. Phys. Chem.*, 1967, **71**, 2297 (*uv*)
Dorman, D.E. *et al., J.O.C.*, 1973, **38**, 1719 (*cmr*)
Warren, J.P. *et al., J. Phys. Chem.*, 1974, **78**, 2507 (*N-15 nmr*)
Izac, R.R. *et al., Phytochemistry*, 1982, **21**, 229 (*isol*)
Ohtaki, H. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 271 (*struct, props, bibl*)
Ettinger, D.S. *et al., Invest. New Drugs*, 1990, **8**, 183-185 (*phase II study, pharmacol*)
McGuire, W.P. *et al., Invest. New Drugs*, 1990, **8**, 191-194; 195-197 (*phase II study, pharmacol*)
Fujisaki, S. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 2426 (*N-bromo*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 2, 1990, 169
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0813
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MKG500

5-Methyl-2-furancarboxaldehyde, 9CI M-319

5-Methylfurfural. 2-Formyl-5-methylfuran. FEMA 2702
[620-02-0]



$C_6H_6O_2$ 110.112
Isol. from brown algae and other plant sources, doubtless as a secondary prod. from saccharides. Oil with sweet spicy odour and caramel-like flavour. d_4^{18} 1.11. Bp 187° Bp_{12} 79-81°. n_D^{20} 1.5263.

▶ LD_{50} (rat, orl) 2200 mg/kg. LT7032500

*Oxime(*E-*):* [57784-58-4]
$C_6H_7NO_2$ 125.127
Prisms (petrol). Mp 51-52°.

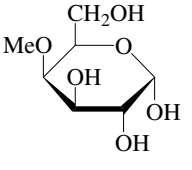
*Oxime(*Z-*):* [57784-53-9]
$C_6H_7NO_2$ 125.127
Needles (petrol). Mp 112°.

Phenylhydrazone: Mp 147-148°.

Thiosemicarbazone: 5-Methyl-2-furancarboxaldehyde thiosemicarbazone
[6823-95-6]
$C_7H_9N_3OS$ 183.234
Used as a 0.4m*M* soln. in EtOH to give colour reaction with Pd (λ_{max} 393 nm, ϵ 44000). Cryst.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 584C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 25B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1458C (*ir*)
Fromherz, K. *et al., Ber.*, 1907, **40**, 404
Reichstein, T. *et al., Helv. Chim. Acta*, 1930, **13**, 346
Org. Synth., 1934, **14**, 62
Grigg, R. *et al., Tetrahedron*, 1965, **21**, 3441 (*ms*)
Mas'ko, L.I. *et al., Zh. Anal. Khim.*, 1975, **30**, 315 (*detn, Pd*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 751 (*rev, tox*)
Comins, D.L. *et al., J.O.C.*, 1987, **52**, 104 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 501
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1761-1762

4-*O*-Methylgalactose, 9CI, 8CI M-320



α-D-Pyranose-*form*

$C_7H_{14}O_6$ 194.184

D-*form* [18404-81-4]
Prisms (AcOH). Mp 218-221°. $[\alpha]_D^{22}$ +61 → +83 (c, 2.2 in H_2O).

α-D-Pyranose-*form* [31505-25-6]

*Me glycoside: Methyl 4-*O*-methyl-α-D-galactopyranoside*
[34698-08-3]
$C_8H_{16}O_6$ 208.211
Cryst. (EtOH). Mp 125-127°. $[\alpha]_D^{25}$ +169.9 (c, 1 in $CHCl_3$).

*Me glycoside, 2,3,6-tri-Ac: Methyl 2,3,6-tri-*O*-acetyl-4-*O*-methyl-α-D-galactopyranoside*
[55697-57-9]
$C_{14}H_{22}O_9$ 334.322
Syrup. $[\alpha]_D^{24}$ +123 (c, 1.4 in $CHCl_3$).

β-D-Pyranose-*form* [25029-37-2]

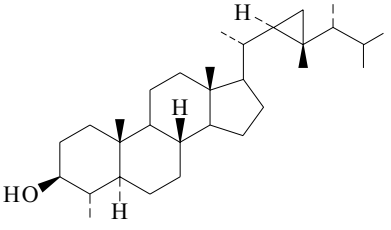
*1,2,3,6-Tetra-Ac: 1,2,3,6-Tetra-*O*-acetyl-4-*O*-methyl-β-D-galactopyranose*
[56809-45-1]
$C_{15}H_{22}O_{10}$ 362.333
Cryst. (diisopropyl ether). Mp 102-105°. $[\alpha]_D$ +32 (c, 0.1 in $CHCl_3$).

*Me glycoside: Methyl 4-*O*-methyl-β-D-galactopyranoside*
[25029-36-1]
$C_8H_{16}O_6$ 208.211
Cryst. (EtOH). Mp 175-176°. $[\alpha]_D^{20}$ -39.9 (c, 1.3 in EtOH).

*Me glycoside, 2,3,6-tribenzoyl: Methyl 2,3,6-tri-*O*-benzoyl-4-*O*-methyl-β-D-galactopyranoside*
[25029-35-0]
$C_{29}H_{28}O_9$ 520.535
Cryst. (EtOH). Mp 135-136°. $[\alpha]_D^{20}$ +29.1 (c, 1.9 in $CHCl_3$).

L-*form*
Residue present in agar from *Gracilaria verrucosa*.
Jeanloz, R.W. *et al., J.A.C.S.*, 1954, **76**, 5684 (*D-form, synth*)
Gros, E.G. *et al., Carbohydr. Res.*, 1969, **10**, 318 (*D-form, β-D-Me pyr, β-D-Me pyr tribenzoyl*)
Rathbone, E.B. *et al., Carbohydr. Res.*, 1971, **20**, 357 (*α/β-D-Me pyr, pmr*)
Flowers, H.M. *et al., Carbohydr. Res.*, 1975, **39**, 245 (*α-D-Me pyr*)
Lee, E.E. *et al., Carbohydr. Res.*, 1975, **41**, 313 (*β-D-pyr tetra-Ac*)
Karamanos, Y. *et al., Carbohydr. Res.*, 1989, **187**, 93 (*occur, L-form*)

4-Methylgorgostan-3-ol M-321



$C_{31}H_{54}O$ 442.767

(3β,4α,5α)-*form* [74036-43-4]
Constit. of *Briareum asbestinum*, *Sarcophyton glaucum*, *Peridinium foliaceum*, *Glenodinium foliaceum* and an unidentified *Lobophytum* sp.
Cryst. (MeOH/$CHCl_3$).
Mp 225.5-226°. $[\alpha]_D$ +10 (c, 0.57 in $CHCl_3$) (+6).
Alam, M. *et al., J.O.C.*, 1979, **44**, 4466-4467 (*Glenodinium foliaceum constit*)
Withers, N.W. *et al., Tet. Lett.*, 1979, 3605
Kobayashi, M. *et al., Steroids*, 1982, **40**, 209-221 (*isol, ms, pmr*)
Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 901-903 (*isol*)

Methylguanidine, 9CI M-322

[471-29-4]
$HN{=}C(NH_2)NHMe$
$C_2H_7N_3$ 73.097
Prod. of putrefaction. Solid. Easily dec. Strong base.
▶ MF3683000

Hydrochloride: [22661-87-6]
V. hygroscopic cryst.

Nitrate: [546-82-7]
Cryst. (EtOH). Mp 151°.

Sulfate salt (2:1): [598-12-9]
Cryst. (H_2O). Mp 239-240°.

Picrate: [1609-02-5]
Yellow plates or needles (H_2O). Mp 200°.

Ac:
$C_4H_9N_3O$ 115.135
Mp 172° (as hydrochloride).

N-*Nitroso:* N-*Methyl*-N-*nitrosoguanidine*
[4262-56-0]
$C_2H_6N_4O$ 102.096
In former use as synth. precursor of Diazomethane.
▶ Exp. carcinogen.

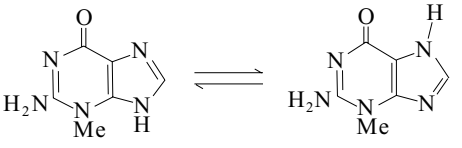
N-*(4-Methoxybenzoyl):* N-*(4-Methoxybenzoyl)*-N′-*methylguanidine*
[387867-99-4]
$C_{10}H_{13}N_3O_2$ 207.232
Isol. from the ascidian *Polycarpa aurata*. Oil. λ_{max} 276 (ε 4754) (MeOH).

[21770-81-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 818D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1328B (*nmr*)
Werner, E.A. *et al., J.C.S.*, 1922, **121**, 1790-1794 (*synth*)
Phillipi, E. *et al., Ber.*, 1927, **60**, 2120-2122 (*synth*)
Davis, T.L. *et al., J.A.C.S.*, 1937, **59**, 2112-2115 (*synth*)
Spasskaya, R.I. *et al., CA*, 1968, **68**, 39059 (*synth*)
Beynon, J.H. *et al., Org. Mass Spectrom.*, 1968, **1**, 169-187 (*ms*)
Wessels, M. *et al., J. Nat. Prod.*, 2001, **64**, 1556-1558 (*4-methoxybenzoyl, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, MKI750

3-Methylguanine, 8CI M-323

*2-Amino-3,7-dihydro-3-methyl-6*H*-purin-6-one, 9CI*
[2958-98-7]



9H–form *7H–form*

$C_6H_7N_5O$ 165.154
Cryst. (H_2O). Mp 375-377°.

7*H*-*form*

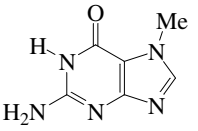
7-Me: 3,7-Dimethylguanine
[19143-67-0]
$C_7H_9N_5O$ 179.181
Isol. from the sponge *Zyzzya fuliginosa*. Cryst. (EtOH aq.).
Mp 327-333° dec.

9*H*-*form*

9-Me: 3,9-Dimethylguanine
[67513-75-1]
$C_7H_9N_5O$ 179.181
Cryst. (H_2O). Mp 326°.
Townsend, L.B. *et al., J.A.C.S.*, 1962, **84**, 3008 (*synth, uv*)
Elion, G.B. *et al., J.O.C.*, 1962, **27**, 2478 (*synth*)
Rice, J.M. *et al., J.A.C.S.*, 1967, **89**, 2719 (*ms*)
Wiley, D.W. *et al., J.O.C.*, 1976, **41**, 1889 (*synth, uv, nmr*)
Abola, J.E. *et al., Tet. Lett.*, 1976, 3483 (*cryst struct*)
Itaya, T. *et al., Chem. Pharm. Bull.*, 1982, **30**, 3392 (*synth, uv, nmr*)
Tasdemir, D. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1628-1630 (*3,7-Dimethylguanine, isol, pmr, cnr, N-15 nmr*)

7-Methylguanine, 9CI M-324

*2-Amino-1,7-dihydro-7-methyl-6*H*-purin-6-one, 9CI. Epiguanine*
[578-76-7]



1*H-form*

$C_6H_7N_5O$ 165.154
Present in biol. systems, prob. as a dec. prod. of 7-Methylguanosine. Urinary marker of exposure to methylating agents.
Needles (H_2O).
Mp 370°.
▶ MF8464000

N^2,N^2-*Di-Me:* **N^2,N^2,7-*Trimethylguanine***
[92333-92-1]
$C_8H_{11}N_5O$ 193.208
Isol. from the ascidian *Lissoclinum notti*. Cryst. (H_2O).
Mp 320° dec. λ_{max} 252 (log ϵ 3.8); 294 (log ϵ 3.6) (MeOH).
Fischer, E. *et al., Ber.*, 1898, **31**, 544 (*synth*)
Gulland, J.M. *et al., J.C.S.*, 1938, 692 (*synth*)
Bredereck, H. *et al., Chem. Biol.*, 1962, **95**, 1812-1819 (N^2,N^2,7-*Trimethylguanine, synth*)
Rice, J.M. *et al., J.A.C.S.*, 1967, **89**, 2719 (*ms*)
Shuker, D.E.G. *et al., Arch. Toxicol.*, Suppl., 1989, **13**, 55 (*use*)
Pearce, A.N. *et al., Nat. Prod. Lett.*, 2001, **15**, 237-241 (N^2,N^2,7-*Trimethylguanine, isol*)

19-Methyl-5,9-heneicosadienoic acid M-325

$H_3CCH_2CH(CH_3)(CH_2)_8CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{22}H_{40}O_2$ 336.557

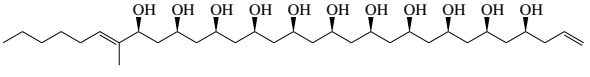
(*E,E*)-*form* [132171-22-3]
Isol. from the sponge *Plakortis halichondroides.*
Carballeira, N.M. *et al., Lipids*, 1990, **25**, 835-840 (*isol, ir, cmr*)

20-Methyl-5,9-heneicosadienoic acid M-326

$(H_3C)_2CH(CH_2)_9CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{22}H_{40}O_2$ 336.557

(*E,E*)-*form* [132171-21-2]
Isol. from the sponge *Plakortis halichondroides.*
Carballeira, N.M. *et al., Lipids*, 1990, **25**, 835-840 (*isol, pmr, cmr*)

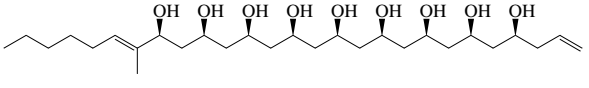
25-Methyl-1,25-hentriacontadiene-4,6,8,10,12,14,16,18,20,22,24-undecol M-327



$C_{32}H_{62}O_{11}$ 622.835

(4*S*,6*S*,8*S*,10*S*,12*S*,14*S*,16*S*,18*S*,20*S*,22*S*,24*S*,25*E*)-*form*
Undeca-Me ether: 4,6,8,10,12,14,16,18,20,22,24-Undecamethoxy-25-methyl-1,25-hentriacontadiene
$C_{43}H_{84}O_{11}$ 777.13
Isol. from the sponge *Myriastra clavosa*. Greenish viscous oil. $[\alpha]_D$ +8 (c, 1 in $CHCl_3$).
Rao, M.R. *et al., J. Nat. Prod.*, 2002, **65**, 1201-1203 (*isol, pmr*)

21-Methyl-1,21-heptacosadiene-4,6,8,10,12,14,16,18,20-nonol M-328



$C_{28}H_{54}O_9$ 534.729

(4*S*,6*S*,8*S*,10*S*,12*S*,14*S*,16*S*,18*S*,20*S*,21*E*)-*form*
Nona-Me ether: 4,6,8,10,12,14,16,18,20-Nonamethoxy-21-methyl-1,21-heptacosadiene
$C_{37}H_{72}O_9$ 660.97
Isol. from the sponge *Myriastra clavosa*. Slightly greenish viscous oil. $[\alpha]_D$ +2.4 (c, 1 in $CHCl_3$).
Rao, M.R. *et al., J. Nat. Prod.*, 2002, **65**, 1201-1203 (*isol, pmr*)

25-Methyl-5,9-heptacosadienoic acid M-329

$H_3CCH_2CH(CH_3)(CH_2)_{14}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{28}H_{52}O_2$ 420.718

(5*Z*,9*Z*,25ξ)-*form* [121981-39-3]
Isol. from the phospholipids of the sponges *Cribrochalina vasculum* and *Ectyoplasia ferox*.
Carballeira, N.M. *et al., Lipids*, 1989, **24**, 371; 1990, **25**, 69 (*isol, struct*)

26-Methyl-5,9-heptacosadienoic acid M-330

$(H_3C)_2CH(CH_2)_{15}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{28}H_{52}O_2$ 420.718

(*Z,Z*)-*form* [121981-40-6]
Isol. from the phospholipids of the sponges *Cribrochalina vasculum* and *Ectyoplasia ferox*.
Carballeira, N.M. *et al., Lipids*, 1989, **24**, 371; 1990, **25**, 69 (*isol, struct*)

19-Methylheptacosanoic acid M-331

[93673-90-6]
$H_3C(CH_2)_7CH(CH_3)(CH_2)_{17}COOH$
$C_{28}H_{56}O_2$ 424.749

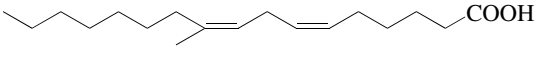
(ξ)-*form*
Isol. from the sponge *Strongylophora durissima*.
Dasgupta, A. *et al., Lipids*, 1984, **19**, 768-776 (*isol*)

19-Methyl-5-heptacosenoic acid M-332

$H_3C(CH_2)_7CH(CH_3)(CH_2)_{12}CH{=}CH(CH_2)_3COOH$
$C_{28}H_{54}O_2$ 422.733

(5*Z*,19ξ)-*form* [93673-87-1]
Isol. from the sponge *Strongylophora durissima*.
Dasgupta, A. *et al., Lipids*, 1984, **19**, 768-776 (*isol*)

10-Methyl-6,9-heptadecadienoic acid M-333



$C_{18}H_{32}O_2$ 280.45

(*Z,Z*)-*form* [163632-71-1]
Isol. from the gorgonian *Leptogorgia piccola.*
Miralles, J. *et al., Lipids*, 1995, **30**, 459 (*isol, struct*)

3-Methylheptadecanoic acid M-334

[60787-51-1]
$H_3C(CH_2)_{13}CH(CH_3)CH_2COOH$
$C_{18}H_{36}O_2$ 284.481
Isol. from the sponge *Desmapsamma anchorata*.

[54934-56-4]

Hwang, Y.-S. *et al., J. Agric. Food Chem.*, 1978, **26**, 557 (*synth*)
Carballeira, N.M. *et al., Lipids*, 1988, **23**, 690 (*isol*)

6-Methyl-1-heptanol, 9CI M-335

Isooctanol
[1653-40-3]
[26952-21-6]

$(H_3C)_2CH(CH_2)_4CH_2OH$
$C_8H_{18}O$ 130.23
Liq. Bp 187.6° Bp_{14} 87-89°.

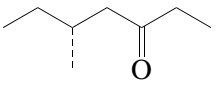
O-*Sulfate:* [309941-87-5]
$C_8H_{18}O_4S$ 210.294
Isol. from the ascidian *Halocynthia papillosa.* Amorph. solid.
Phenylurethane: Mp 81-81.4°.

Levene, P.A. *et al., J. Biol. Chem.*, 1916, **27**, 433-462 (*synth*)
Dorough, G.L. *et al., J.A.C.S.*, 1941, **63**, 3100-3110 (*synth*)
Bestmann, H.J. *et al., Chem. Ber.*, 1976, **109**, 3375-3378 (*synth*)
Aiello, A. *et al., J. Nat. Prod.*, 2000, **63**, 1590-1592 (*isol, sulfate*)
Tai, A. *et al., Bull. Chem. Soc. Jpn.*, 2002, **75**, 111-121 (*synth*)
Chavan, S.P. *et al., Synth. Commun.*, 2004, **34**, 397-404 (*synth, pmr, ms*)

5-Methyl-3-heptanone, 9CI M-336

[541-85-5]

[116003-10-2]



(*R*)-*form*

$C_8H_{16}O$ 128.214

▶ Flammable. Skin and eye irritant. OES: long-term 25 ppm. MJ7350000

(*R*)-*form* [116003-10-2]
Sex pheromone of male *Platynereis dumerilii*. Bp_{40} 100°. $[\alpha]_D^{20}$ +5.31 (c, 4.20 in C_6H_6) (≥98% ee). $[\alpha]_D^{20}$ -8.73 (neat).

(*S*)-*form* [20616-93-7]
Sex pheromone of female *Platynereis dumerilii*. Bp_{16} 54-55°. $[\alpha]_D^{25}$ +8.57 (neat).

2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 66-67°.

(±)-*form* [57968-70-4]
Liq. with minty odour. Bp 161°.

Oxime: [22457-23-4]
$C_8H_{17}NO$ 143.228
Used in perfumery. Liq. with strong leafy odour. Insol. H_2O.
▶ MJ7430000

Semicarbazone: Mp 96°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 409C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 638A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 493B (*ir*)
Brokaw, G.Y. *et al., J.O.C.*, 1948, **13**, 194-199 (*synth*)
Pieroni, O. *et al., J. Polym. Sci., Part C*, 1969, **22**, 993-1007 (*S-form, synth*)
Aglietto, M. *et al., Gazz. Chim. Ital.*, 1975, **105**, 1035-1045 (*S-form, synth*)
Vasi, I.G. *et al., J. Indian Chem. Soc.*, 1975, **52**, 89-90 (*S-form, synth*)
Zeeck, E. *et al., Naturwissenschaften*, 1992, **79**, 182-183 (*isol*)
Ahlbrecht, H. *et al., Eur. J. Org. Chem.*, 1998, 1371-1377 (*R-form, synth, pmr, cmr*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 844
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EGI750

2-Methyl-1,3,5-heptatriene M-337

[928-38-1]

$H_3CCH{=}CHCH{=}CHC(CH_3){=}CH_2$

C_8H_{12} 108.183
Constit. of the brown alga *Fucus evanescens*. Bp_{25} 68-70°.

[17679-94-6, 18304-16-0]

Sorensen, T.S. *et al., Can. J. Chem.*, 1964, **42**, 2781 (*synth*)
van Dongen, J.P.C.M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1967, **86**, 1077 (*synth*)
Spangler, C.W. *et al., J.O.C.*, 1972, **37**, 1020 (*synth*)
Kajiwara, T. *et al., Experientia*, 1981, **37**, 1247 (*isol*)

6-Methyl-5-hepten-2-one, 9CI M-338

Sulcatone. *FEMA 2707*
[110-93-0]
$H_3CCOCH_2CH_2CH{=}C(CH_3)_2$
$C_8H_{14}O$ 126.198
Present in Ceylon citronella oil, lemon-grass oil and palmarosa oil. Prod. by *Endoconidiophora coerulescens* and a marine *Streptomyces* sp. GWS-BW-H5. Isol. from the Australian meat ant, *Iridomyrmex purpureus*. Chemical scent constit. of urine of red fox *Vulpes vulpes*. Intermed. in the manuf. of terpene alcohols. Insecticidal agent. d^{20} 0.86.
Mp -67°. Bp 172-174° (161-162°) Bp_{10} 58.5°.
▶ Fl. p. 57°. MJ9700000

Oxime: [22418-73-1]
$C_8H_{15}NO$ 141.213
Bp_{12} 99°.

2,4-Dinitrophenylhydrazone: [6147-43-9]
Mp 78°.

Semicarbazone: [16769-68-9]
Mp 135° approx.

[409-02-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 415D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 646B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 501B (*ir*)
Birkinshaw, J.H. *et al., Biochem. J.*, 1950, **47**, 55 (*isol*)
Mousseron, M. *et al., Bull. Soc. Chim. Fr.*, 1963, 376 (*synth*)
Saucy, G. *et al., Helv. Chim. Acta*, 1967, **50**, 2091 (*synth*)
Sato, K. *et al., J.O.C.*, 1970, **35**, 565 (*synth*)
Boccara, N. *et al., Bull. Soc. Chim. Fr.*, 1972, 1448 (*synth*)
Ishihara, T. *et al., Agric. Biol. Chem.*, 1974, **38**, 439 (*synth, bibl*)
Dennison, N.R. *et al., Aust. J. Chem.*, 1975, **28**, 1339 (*synth*)
Savoia, D. *et al., J.O.C.*, 1978, **43**, 2907 (*synth*)
Whitten, W.K. *et al., J. Chem. Ecol.*, 1980, **6**, 49
McKenzie, T.C. *et al., Org. Prep. Proced. Int.*, 1987, **19**, 435 (*synth*)
Kim, J.H. *et al., J. Nat. Prod.*, 1989, **52**, 63 (*biosynth*)
Micha, S.H. *et al., Eur. J. Entomol.*, 1993, **90**, 439
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 507
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1771-1772
Mir, N.A. *et al., J. Agric. Food Chem.*, 1999, **47**, 7-11 (*occur*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 837-865 (*marine isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MKK000

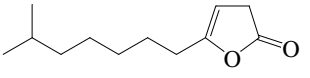
6-Methyl-5-hepten-3-yn-2-one M-339

Taxifolione
[149183-86-8]
$(H_3C)_2C{=}CHC{\equiv}CCOCH_3$
$C_8H_{10}O$ 122.166
Constit. of *Caulerpa taxifolia*. Oil. λ_{max} 275 (ε 12000) (MeOH) (Berdy).

Guerriero, A. *et al., Helv. Chim. Acta*, 1993, **76**, 855 (*isol, pmr, cmr*)

5-(6-Methylheptyl)-2(3*H*)-furanone M-340

10-Methyl-3-undecen-4-olide

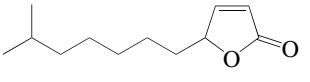


$C_{12}H_{20}O_2$ 196.289

(ξ)-*form*
Prod. by the marine *Streptomyces* sp. strain GWS-BW-H5.
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 837-865 (*isol, synth, pmr, cmr, ms*)

5-(6-Methylheptyl)-2(5*H*)-furanone M-341

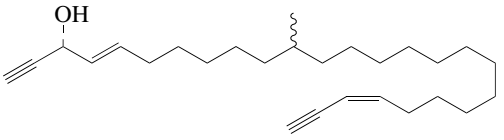
10-Methyl-2-undecen-4-olide



$C_{12}H_{20}O_2$ 196.289

(ξ)-*form*
Prod. by the marine *Streptomyces* sp. strain GWS-BW-H5.
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 837-865 (*isol, synth, pmr, cmr, ms*)

11-Methyl-4,23-hexacosadiene-1,25-diyn-3-ol, 9CI M-342



$C_{27}H_{44}O$ 384.644

(3*R*,4*E*,11ξ,23*Z*)-*form* [184473-39-0]
Isol. from the sponge *Haliclona* sp.
Oil. $[\alpha]_D$ -5.6. λ_{max} 214 (sh); 220; 227 (sh) (MeOH).
Williams, D.H. *et al., J. Nat. Prod.*, 1996, **59**, 1099-1101 (*isol, uv, ir, pmr, cmr, ms*)

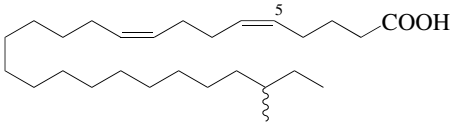
20-Methyl-5,9-hexacosadienoic acid M-343

$H_3C(CH_2)_5CH(CH_3)(CH_2)_9CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{27}H_{50}O_2$ 406.691

(5*Z*,9*Z*,20ξ)-*form* [79605-32-6]
Constit. of the sponge *Aplysina fistularis*.
Walkup, R.D. *et al., Lipids*, 1981, **16**, 631-646 (*isol*)

24-Methyl-5,9-hexacosadienoic acid M-344

[89188-18-1]



$C_{27}H_{50}O_2$ 406.691

(5*Z*,9*Z*,24ξ)-*form* [83474-13-9]
Isol. from various sponges incl. *Jaspis* sp. and *Petrosia* spp.
Carbelleira, N.M. *et al., J.O.C.*, 1986, **51**, 2751 (*isol, biosynth*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 305 (*isol*)

25-Methyl-5,9-hexacosadienoic acid M-345

[89188-17-0]
$(H_3C)_2CH(CH_2)_{14}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{27}H_{50}O_2$ 406.691

(5*Z*,9*Z*)-*form* [83474-12-8]
Isol. from various sponges incl. *Jaspis* sp. and *Petrosia* spp.
Carballeira, N.M. *et al., J.O.C.*, 1986, **51**, 2751 (*isol, biosynth*)
Carbelleira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 305 (*isol*)

18-Methylhexacosanoic acid M-346

$H_3C(CH_2)_7CH(CH_3)(CH_2)_{16}COOH$
$C_{27}H_{54}O_2$ 410.722

(ξ)-*form*
Constit. of the sponge *Cinachyrella alloclada*.
Barnathan, G. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2003, **135**, 297-308 (*isol, ms*)

19-Methylhexacosanoic acid M-347

[93673-89-3]
$H_3C(CH_2)_6CH(CH_3)(CH_2)_{17}COOH$
$C_{27}H_{54}O_2$ 410.722

(ξ)-*form*
Isol. from the sponge *Strongylophora durissima*.
Dasgupta, A. *et al., Lipids*, 1984, **19**, 768-776 (*isol*)

24-Methylhexacosanoic acid M-348

[89838-00-6]
$H_3CCH_2CH(CH_3)(CH_2)_{22}COOH$
$C_{27}H_{54}O_2$ 410.722
Isol. from the phospholipids of the sponge *Petrosia pellasarca*. Also found in the meibomian gland.

Heneicosyl ester: [121877-90-5]
$C_{48}H_{96}O_2$ 705.285
Isol. from the wax of tobacco leaves.

Docosyl ester: [121877-92-7]
$C_{49}H_{98}O_2$ 719.312
Isol. from the wax of tobacco leaves.

Harvey, D.J. *et al., J. Chromatogr.*, 1984, **301**, 173 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1990, **53**, 836 (*isol*)

25-Methylhexacosanoic acid M-349

[128156-70-7]
$(H_3C)_2CH(CH_2)_{23}COOH$
$C_{27}H_{54}O_2$ 410.722
Isol. from the phospholipids of the sponge *Petrosia pellasarca*. Also found in the bacterium *Desulfotomaculum* sp.

Rezanka, T. *et al., FEMS Microbiol. Ecol.*, 1990, **73**, 231 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1990, **53**, 836 (*isol*)

25-Methyl-1-hexacosanol M-350

[75382-95-5]
$(H_3C)_2CH(CH_2)_{23}CH_2OH$
$C_{27}H_{56}O$ 396.739
Isol. from the marine invertebrate *Nereis diversicolor* and from hazelnut oil.

Garcia Olmeda, R. *et al., CA*, 1980, **93**, 20285lj (*isol*)
Bradshaw, S.A. *et al., CA*, 1991, **115**, 1578445v (*isol*)

2-Methyl-17-hexacosenoic acid M-351

[774608-85-4]
$H_3C(CH_2)_7CH{=}CH(CH_2)_{14}CH(CH_3)COOH$
$C_{27}H_{52}O_2$ 408.707

(2ξ,17*Z*)-*form*
Isol. from the marine sponge *Halichondria panicea*.
Imbs, A.B. *et al., Chem. Phys. Lipids*, 2004, **129**, 173-181 (*isol, pmr, ms*)

19-Methyl-5-hexacosenoic acid M-352

$H_3C(CH_2)_6CH(CH_3)(CH_2)_{12}CH{=}CH(CH_2)_3COOH$
$C_{27}H_{52}O_2$ 408.707

(5*Z*,19ξ)-*form* [93673-86-0]
Isol. from the sponge *Strongylophora durissima*.
Dasgupta, A. *et al., Lipids*, 1984, **19**, 768-776 (*isol*)

15-Methyl-5,9-hexadecadienoic acid M-353

$(H_3C)_2CH(CH_2)_4CH{=}CHCH_2CH_2CH{=}CHCH_2CH_2CH_2COOH$
$C_{17}H_{30}O_2$ 266.423

(5*Z*,9*Z*)-*form* [153081-60-8]
Isol. from the sponges *Chondrosia remiformis* and *Myrmekioderma styx*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1993, **56**, 1850 (*isol*)

8-Methyl-2,4-hexadecadiyn-1-ol M-354

Durissimol A
$H_3C(CH_2)_7CH(CH_3)CH_2CH_2C{\equiv}CC{\equiv}CCH_2OH$
$C_{17}H_{28}O$ 248.408

(+)-*form*
Constit. of the sponge *Strongylophora durissima*.

Oil. $[\alpha]_D^{25}$ +23.6 (c, 0.1 in $CHCl_3$). λ_{max} 215 (log ϵ 3.22); 255 (log ϵ 4.13); 268 (log ϵ 3.71); 284 (log ϵ 3.45) (MeOH).

Shen, Y.-C. *et al., J. Nat. Prod.*, 2000, **63**, 1686-1688

3-Methylhexadecanoic acid, 9CI M-355

3-Methylpalmitic acid

[42172-35-0]

$H_3C(CH_2)_{12}CH(CH_3)CH_2COOH$

$C_{17}H_{34}O_2$ 270.454

(±)-*form*

Cryst. (Me_2CO). Mp 42.5-43° (41-42°). $Bp_{0.5}$ 174-176°.

Et ester: [66344-25-0]

$C_{19}H_{38}O_2$ 298.508

Liq. $Bp_{0.7}$ 160-162°.

Amide:

$C_{17}H_{35}NO$ 269.47

Cryst. (EtOAc). Mp 90.5-91°.

(ξ)-*form*

Isol. from the sponge *Erylus formosus*.

[65128-49-6, 91357-11-8]

Weitzel, G. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1951, **287**, 65 (*synth, ester, amide*)
Hwang, Y.S. *et al., J. Agric. Food Chem.*, 1978, **26**, 557 (*synth*)
Dobner, B. *et al., Pharmazie*, 1984, **39**, 69 (*synth*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 305-309 (*isol*)

7-Methylhexadecanoic acid, 9CI M-356

7-Methylpalmitic acid

[56796-91-9]

$H_3C(CH_2)_8CH(CH_3)(CH_2)_5COOH$

$C_{17}H_{34}O_2$ 270.454

(±)-*form*

Cryst. (petrol). Mp 31-31.5°.

Et ester:

$C_{19}H_{38}O_2$ 298.508

Liq. $Bp_{0.4}$ 152°. CAS no. not found 8-14 CI.

Amide:

$C_{17}H_{35}NO$ 269.47

Cryst. (EtOAc). Mp 69-69.5°. CAS no. not found 8-14 CI.

(ξ)-*form*

Major component of fish oils from redfish *Sebastes* sp., menhaden *Brevoortia tyrannus*, salmon *Oncorhynchus nerka*, *Chrysomela vigintipunctata* and *Musa domestica*. CAS no. not found 8-14 CI.

[18720-85-9]

Weitzel, G. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1951, **287**, 65-89; 296-310; **288**, 189-200 (*synth*)
Dobner, B. *et al., Z. Chem.*, 1987, **27**, 63-64 (*synth*)
Ratnayake, W.M.N. *et al., Lipids*, 1989, **24**, 630-637 (*occur, fish*)
Blomquist, G.J. *et al., Insect Biochem.*, 1994, **24**, 803-810 (*occur*)
Nikolova, N. *et al., Z. Naturforsch., C*, 2000, **55**, 661-666 (*occur*)

10-Methylhexadecanoic acid, 9CI M-357

10-Methylpalmitic acid

[17001-26-2]

$H_3C(CH_2)_5CH(CH_3)(CH_2)_8COOH$

$C_{17}H_{34}O_2$ 270.454

Constit. of animal, sponge and bacterial lipids.

(±)-*form*

Cryst. (Me_2CO). Mp 24-24.5°. $Bp_{1.5}$ 189°.

Et ester:

$C_{19}H_{38}O_2$ 298.508

Liq. Bp_1 163°.

Amide:

$C_{17}H_{35}NO$ 269.47

Cryst. (EtOAc). Mp 80.5-81°.

[2490-51-9]

Weitzel, G. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1951, **287**, 65; 296; **288**, 189 (*synth*)
Cason, J. *et al., J. Biol. Chem.*, 1963, **238**, 883 (*isol*)
Ryhage, R. *et al., J. Dairy Res.*, 1967, **34**, 115 (*chromatog, ms*)
Ackman, R.G. *et al., Lipids*, 1972, **7**, 683 (*chromatog*)
Raederstorff, D. *et al., J.O.C.*, 1987, **52**, 2337

11-Methylhexadecanoic acid, 9CI M-358

11-Methylpalmitic acid

[17001-25-1]

$H_3C(CH_2)_4CH(CH_3)(CH_2)_9COOH$

$C_{17}H_{34}O_2$ 270.454

(±)-*form*

Cryst. (Me_2CO). Mp 18.5-19°. $Bp_{0.4}$ 187-188°.

Et ester:

$C_{19}H_{38}O_2$ 298.508

Liq. $Bp_{0.7}$ 160°.

Amide:

$C_{17}H_{35}NO$ 269.47

Cryst. (EtOAc). Mp 71-71.5°.

(ξ)-*form*

Found in butterfat and fish oils.

Weitzel, G. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1951, **287**, 65; **288**, 189 (*synth*)
Ryhage, R. *et al., J. Dairy Res.*, 1967, **34**, 115 (*occur, butter, chromatog, ms*)
Dobner, B. *et al., Z. Chem.*, 1987, **27**, 63 (*synth*)
Ratnayake, W.M.N. *et al., Lipids*, 1989, **24**, 630 (*occur, fish*)

13-Methylhexadecanoic acid, 9CI M-359

13-Methylpalmitic acid

[103386-25-0]

$H_3CCH_2CH_2CH(CH_3)(CH_2)_{11}COOH$

$C_{17}H_{34}O_2$ 270.454

(±)-*form*

Cryst. (Me_2CO). Mp 30-30.5°. $Bp_{0.4}$ 186°.

Et ester:

$C_{19}H_{38}O_2$ 298.508

Liq. Bp_2 172°.

Amide:

$C_{17}H_{35}NO$ 269.47

Cryst. (EtOAc). Mp 78.5-79°.

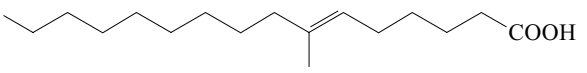
(ξ)-*form*

Isol. from the oils of fish incl. menhaden (*Brevoortia tyrannus*) and sockeye salmon (*Oncorhynchus nerka*).

Weitzel, G. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1951, **287**, 65-91 (*synth, ester, amide*)
Dobner, B. *et al., Z. Chem.*, 1987, **27**, 63-64 (*synth*)
Ratnayake, W.M.N. *et al., Lipids*, 1989, **24**, 630-637 (*occur, gc-ms*)
Finegold, L. *et al., Appl. Environ. Microbiol.*, 1990, **56**, 1191-1194 (*synth*)

7-Methyl-6-hexadecenoic acid, 9CI M-360

[56796-89-5]



$C_{17}H_{32}O_2$ 268.439

(E)*-*form [18689-89-9]

Constit. of *Amphimedon complanata* and from blubber oil of Arctic finwhale (*Balaenoptera physalis*) and sperm whale (*Physeter catodon*).

Sano, Y. *et al., Yukagaku*, 1967, **16**, 605-610; *CA*, **68**, 31327 (*E-form, isol, ir, pmr, ms, occur*)
Pascal, J.L. *et al., Lipids*, 1975, **10**, 478 (*chromatog, pmr, ms*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 315-317 (*isol*)
Kulkarni, B.A. *et al., Synth. Commun.*, 1992, **22**, 2921 (*synth*)

7-Methyl-7-hexadecenoic acid M-361

[40663-81-8]

$H_3C(CH_2)_7CH{=}C(CH_3)(CH_2)_5COOH$

$C_{17}H_{32}O_2$ 268.439

Constit. of liver oil of sunfish *Mola mola* and spadefish *Chaetodipterus faber* and of jellyfish *Physalia physalis*.

Ackman, R.G. *et al., Lipids*, 1973, **8**, 21-24 (*isol, ms, glc*)
Hooper, S.N. *et al., Lipids*, 1973, **8**, 509-516 (*occur*)
Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*occur*)

7-Methyl-8-hexadecenoic acid M-362

[116943-00-1]

$H_3C(CH_2)_6CH{=}CH(CH_3)(CH_2)_5COOH$

$C_{17}H_{32}O_2$ 268.439

Isol. from the sponge *Desmapsamma anchorata*.

[116943-02-3]

Carballeira, N.M. *et al., Lipids*, 1988, **23**, 690-693 (*isol*)

9-Methyl-10-hexadecenoic acid M-363

[202744-04-5]

[226709-89-3]

$H_3C(CH_2)_4CH{=}CHCH(CH_3)(CH_2)_7COOH$

$C_{17}H_{32}O_2$ 268.439

(9ξ,10*E*)-*form* [226709-90-6]

Constit. of *Vibrio alginolyticus* associated with the alga *Cladophora coelothrix*.

[226244-09-3 (*Z-form*,- Me, 226244-11-7 (*E-form*, Me ester)]

Carballeira, N.M. *et al., Lipids*, 1997, **32**, 1271-1275 (*isol*)
Carballeira, N.M. *et al., Chem. Phys. Lipids*, 1999, **97**, 87-91 (*synth, ir, pmr*)

9-Methyl-11-hexadecenoic acid M-364

$H_3C(CH_2)_3CH{=}CHCH_2CH(CH_3)(CH_2)_7COOH$

$C_{17}H_{32}O_2$ 268.439

(*Z*)-*form* [121981-42-8]

Isol. from the sponge *Ectyoplasia ferox*.

Carballeira, N.M. *et al., Lipids*, 1989, **24**, 371 (*isol*)

10-Methyl-6-hexadecenoic acid M-365

$H_3C(CH_2)_5CH(CH_3)CH_2CH_2CH{=}CH(CH_2)_4COOH$

$C_{17}H_{32}O_2$ 268.439

(*Z*)-*form* [163632-68-6]

Isol. from the gorgonian *Leptogorgia piccola*.

Miralles, J. *et al., Lipids*, 1995, **30**, 459 (*isol, struct*)

14-Methyl-6-hexadecenoic acid M-366

$H_3CCH_2CH(CH_3)(CH_2)_6CH{=}CH(CH_2)_4COOH$

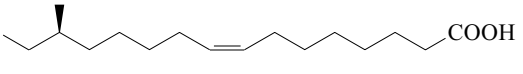
$C_{17}H_{32}O_2$ 268.439

(6*Z*,14ξ)-*form* [123739-74-2]

Isol. from the sponge *Dysidea fragilis*.

Christie, W.W. *et al., Lipids*, 1992, **27**, 640-644 (*isol*)

14-Methyl-8-hexadecenoic acid M-367



(*R*,*Z*)–*form*

$C_{17}H_{32}O_2$ 268.439

(*R*)-(*Z*)-*form* [116943-01-2]

Isol. from the sponge *Cinachyrella* sp.

Me ester: [25227-40-1]

$C_{18}H_{34}O_2$ 282.465

$Bp_{0.1}$ 125-127°. $[\alpha]_D^{25}$ +3.75 (c, 1.975 in $CHCl_3$).

(*S*)-(*Z*)-*form*

Me ester: [51018-59-8]

Sex pheromone for the Khapra beetle *Trogoderma inclusum*. Also weak attractant for *T. granarium*.

(*E*)-*form*

Me ester: [56941-91-4]

Component of the sex pheromone of *T. glabrum*.

Rodin, J.O. *et al., Science (Washington, D.C.)*, 1969, **165**, 904
de Graw, J.I. *et al., J.O.C.*, 1971, **36**, 2902 (*synth*)
Levinson, H.Z. *et al., Naturwissenschaften*, 1974, **61**, 685
Mori, K. *et al., Tetrahedron*, 1974, **30**, 3817 (*synth, ir, pmr, ms*)
Yarger, R.G. *et al., J. Chem. Ecol.*, 1975, **1**, 323
Caballeira, N.M. *et al., Lipids*, 1988, **23**, 690 (*isol*)

15-Methyl-4-hexadecenoic acid M-368

$(H_3C)_2CH(CH_2)_9CH{=}CHCH_2CH_2COOH$

$C_{17}H_{32}O_2$ 268.439

(*Z*)-*form* [211863-36-4]

Isol. from the sponges *Baicalospongia bacilifera* and *Callyspongia fallax*.

Imbs, A.B. *et al., Chem. Phys. Lipids*, 1998, **92**, 117-125 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*isol*)

15-Methyl-5-hexadecenoic acid M-369

$(H_3C)_2CH(CH_2)_8CH{=}CH(CH_2)_3COOH$

$C_{17}H_{32}O_2$ 268.439

(*E*)-*form* [77900-90-4]

Isol. from various bacteria.

(*Z*)-*form* [140220-58-2]

Isol. from the sponge *Callyspongia fallax* and from various bacteria incl. *Thermus aquaticus*.

Patel, B.K.C. *et al., Syst. Appl. Microbiol.*, 1991, **14**, 311-316 (*isol*)
Moss, C.W. *et al., J. Clin. Microbiol.*, 1992, **30**, 2511-2512 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*isol*)

15-Methyl-6-hexadecenoic acid M-370

$(H_3C)_2CH(CH_2)_7CH{=}CH(CH_2)_4COOH$

$C_{17}H_{32}O_2$ 268.439

(*Z*)-*form* [142599-22-2]

Isol. from the sponges *Callyspongia fallax* and *Dysidea fragilis* and the freshwater mussel *Unio tumidus*.

Stefanov, K. *et al., J. Nat. Prod.*, 1992, **55**, 979-981 (*isol*)
Christie, W.W. *et al., Lipids*, 1992, **27**, 640-644 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*isol*)

15-Methyl-7-hexadecenoic acid M-371

[162229-22-3]

$(H_3C)_2CH(CH_2)_6CH{=}CH(CH_2)_5COOH$

$C_{17}H_{32}O_2$ 268.439

(*Z*)-*form* [92661-17-1]

Isol. from the sponge *Callyspongia fallax*.

Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*isol*)

15-Methyl-9-hexadecenoic acid M-372

[62649-56-3]

$(H_3C)_2CH(CH_2)_4CH{=}CH(CH_2)_7COOH$

$C_{17}H_{32}O_2$ 268.439

(*Z*)-*form* [72878-44-5]

Constit. of various bacteria and the phospholipids of sponges.

[65092-92-4]

Boon, J.J. *et al., Lipids*, 1977, **12**, 717-721 (*ms*)
Ayanoglu, E. *et al., Lipids*, 1982, **17**, 617-625 (*isol*)
Christie, W.W. *et al., Lipids*, 1992, **27**, 640-644 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1993, **56**, 1850-1855 (*isol*)

15-Methyl-11-hexadecenoic acid M-373

$(H_3C)_2CHCH_2CH_2CH{=}CH(CH_2)_9COOH$

$C_{17}H_{32}O_2$ 268.439

(*Z*)-*form* [72878-45-6]
Constit. of *Cyamopsis tetragonolobus* and *Myxococcus xanthus* and the sponge *Ectyoplasia ferox*.

[55044-54-7, 109032-23-7]

Gynther, J. *et al., Planta Med.*, 1982, **46**, 60 (*isol*)
Carballeira, N.M. *et al., Lipids*, 1989, **24**, 371 (*isol*)
Reyes, E.D. *et al., Synthesis*, 1996, 693 (*synth, uv, ir, pmr, cmr, ms*)

7-Methyl-7-hexadecenol M-374

[56796-88-4]

$H_3C(CH_2)_7CH{=}C(CH_3)(CH_2)_5CH_2OH$

$C_{17}H_{34}O$ 254.455
Constit. of oil of sperm whale *Physeter catodon*.

Pascal, J.C. *et al., Lipids*, 1975, **10**, 478-482 (*isol, glc, occur*)

15-Methyl-10-hexadecen-2-one M-375

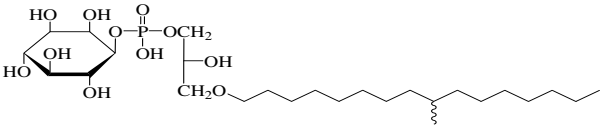
$(H_3C)_2CH(CH_2)_3CH{=}CH(CH_2)_7COCH_3$

$C_{17}H_{32}O$ 252.439

(*Z*)-*form*
Prod. by a marine bacterium.

Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol, synth, pmr, cmr, ms*)

1-(9-Methylhexadecyl)lysoplasmanylinositol M-376



$C_{26}H_{53}O_{11}P$ 572.672
Isol. from the sponge *Theonella swinhoei*. Antimicrobial agent.
Solid. $[\alpha]_D^{20}$ -8.9 (c, 0.03 in MeOH).

Matsunaga, S. *et al., J. Nat. Prod.*, 2001, **64**, 816-818 (*isol, pmr, cmr, ms*)

2-Methyl-3-hexene-2,5-diol M-377

$(H_3C)_2C(OH)CH{=}CHCH(OH)CH_3$

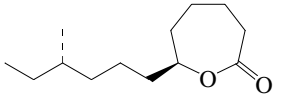
$C_7H_{14}O_2$ 130.186

(3ξ,5ξ)-*form*
Prod. by the marine isolate *Streptomyces* sp. B5525.
Oil.

Maskey, R.P. *et al., Z. Naturforsch., B*, 2002, **57**, 823-829 (*isol, pmr, cmr, ms*)

7-(4-Methylhexyl)-2-oxepanone M-378

10-Methyl-6-dodecanolide



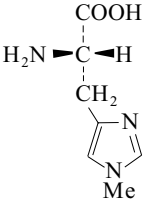
$C_{13}H_{24}O_2$ 212.331

(6*R*,10*S*)-*form*
Prod. by the marine *Streptomyces* sp. B6007.
Oil. $[\alpha]_D^{25}$ -20.1 (c, 2 in Et_2O).

Stritzke, K. *et al., J. Nat. Prod.*, 2004, **67**, 395-401 (*isol, synth, pmr, cmr, ms*)

1-Methylhistidine†, 9CI M-379

2-Amino-3-(1-methyl-4-imidazolyl)propanoic acid. N^{τ}*-Methylhistidine. 3-Methylhistidine*†



$C_7H_{11}N_3O_2$ 169.183
Frequently referred to as 3-methylhistidine in biochemical papers due to the long-standing difference in the numbering of histidine.

(*S*)-*form*
L-form
[332-80-9]
Nonproteinogenic amino acid formed mainly by methylation of histidine residues in muscle actin and myosin. Urinary excretion levels used as an index of muscle protein breakdown.
Plates (DMF aq.).
Mp 248-250° dec. $[\alpha]_D^{20}$ -24.7 (c, 2.8 in H_2O). pK_{a1} 1.92; pK_{a2} 6.56; pK_{a3} 8.73 (25°, 0.1*M* KCl).

Hydrochloride:
Plates (DMF aq.). Mp 251-252° dec. $[\alpha]_D^{22}$ +6.9 (c, 2.0 in H_2O). $[\alpha]_D$ +9.4 (c, 2.0 in *M* HCl).

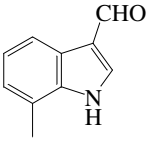
Hydrochloride (1:2): [69614-06-8]
Prisms. Mp 258-259°. $[\alpha]_D^{20}$ +12.9 (c, 2 in *M* HCl).

N^{α}*-Ac:* [84285-33-6]
$C_9H_{13}N_3O_3$ 211.22
Occurs in rat urine and fish tissues.

Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 2763-2764 (*synth*)
Cocks, D.H. *et al., Nature (London)*, 1964, **202**, 184 (*isol*)
Eur. J. Biochem., 1972, **27**, 201-207 (*nomencl*)
Young, V.R. *et al., J. Biol. Chem.*, 1972, **247**, 3592-3600 (*biochem*)
Sasaoka, K. *et al., Arch. Biochem. Biophys.*, 1982, **219**, 454-458 (N^{α}*-Ac, occur*)
Barlos, K. *et al., Annalen*, 1989, 387-388 (*synth*)
Betto, P. *et al., J. Chromatogr.*, 1992, **584**, 256-260 (*detm, hplc, use, bibl*)
Jain, R. *et al., Tetrahedron*, 1996, **52**, 5363-5370 (*synth, pmr*)
Dunnett, M. *et al., J. Chromatogr., B: Biomed. Appl.*, 1997, **688**, 47-55 (*hplc*)
Togashi, M. *et al., Fish. Sci.*, 1998, **64**, 174-175 (N^{α}*-Ac, occur*)
Garlick, P.J. *et al., J. Nutr.*, Suppl. 2, 1998, **128**, 3565-3595 (*rev*)
Colombani, P.C. *et al., Int. J. Sport Nutr.*, 1999, **9**, 181-201 (*biochem*)

7-Methyl-1*H*-indole-3-carboxaldehyde M-380

3-Formyl-7-methylindole
[4771-50-0]



$C_{10}H_9NO$ 159.187
Cryst. (CH_2Cl_2/EtOAc or EtOH). Mp 212-214° (206-208°).

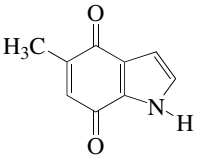
N-*Me: 1,7-Dimethyl-1*H*-indole-3-carboxaldehyde. 3-Formyl-1,7-dimethylindole*
[164353-61-1]
$C_{11}H_{11}NO$ 173.214

Metab. of the marine cyanobacterium *Lyngbya majuscula*.

Boyd, W.J. *et al., Biochem. J.*, 1935, **29**, 555-561 (*synth*)
Belg. Pat., 1964, 628 441; *CA*, **60**, 13226 (*synth*)
Heath-Brown, B. *et al., J.C.S.*, 1965, 7165-7178 (*synth*)
Todd, J.S. *et al., J. Nat. Prod.*, 1995, **58**, 586 (*isol, uv, ir, pmr, cmr, struct, deriv*)

5-Methyl-1*H*-indole-4,7-dione, 9CI M-381

[213040-66-5]



$C_9H_7NO_2$ 161.16

Alkaloid from the muricid gastropod *Drupella fragum*. Antimicrobial agent. Orange prisms.

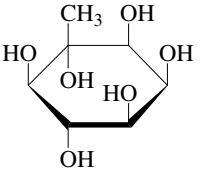
Mp 202-204°. λ_{max} 228 (ϵ 8060); 250 (ϵ 2010); 316 (ϵ 4180); 470 (ϵ 790) (EtOH).

Fukuyama, Y. *et al., Tetrahedron*, 1998, **54**, 10007-10016 (*isol, uv, ir, pmr, cmr*)

4-*C*-Methyl-*myo*-inositol M-382

Laminitol

[472-95-7]



D-*form*

$C_7H_{14}O_6$ 194.184

D-*form* [134680-68-5]

Isol. from red algae, e.g. *Polysiphonia fastigiata* (Ceramiales) and brown alga, e.g. *Laminaria cloustoni*. Osmoregulator, esp. in brown algae freq. exposed to both fresh and salt water. Cryst. (H_2O).

Mp 270-274° (266-269°). $[\alpha]_D^{20}$ -3 (c, 2 in H_2O).

Hexa-Ac: Hexa-O-*acetyl-4*-C-myo-*inositol*
[52795-38-7]
$C_{19}H_{26}O_{12}$ 446.407
Cryst. (EtOH). Mp 151-152°. $[\alpha]_D^{19}$ -19 (c, 2 in $CHCl_3$).

(±)-*form*
Cryst. (H_2O). Mp 262-268°.

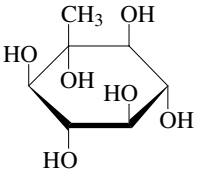
Hexa-Ac:
Cryst. (EtOH). Mp 157-158°.

Lindberg, L. *et al., Acta Chem. Scand.*, 1954, **8**, 1875-1876 (*isol*)
Wickberg, B. *et al., Acta Chem. Scand.*, 1957, **11**, 506-511 (*isol*)
Lindberg, B. *et al., Ark. Kemi*, 1958, **13**, 447-455 (*isol*)
Posternak, T. *et al., Helv. Chim. Acta*, 1960, **43**, 2142-2147; 1961, **44**, 2080-2085 (*synth, config*)
Angyal, S.J. *et al., Aust. J. Chem.*, 1974, **27**, 1075-1086 (*synth, pmr*)
Carless, H.A.J. *et al., Tet. Lett.*, 1991, **32**, 1671-1674 (*synth, pmr*)
Sata, K. *et al., Bull. Chem. Soc. Jpn.*, 1994, **67**, 1633-1640 (*synth*)

1-*C*-Methyl-*scyllo*-inositol M-383

Mytilitol

[564-92-1]



$C_7H_{14}O_6$ 194.184

Isol. from blue mussels *Mytilus edulis*, red alga *Polysiphonia fastigiata* and brown algae. Cryst. (H_2O).

Mp 266-268°.

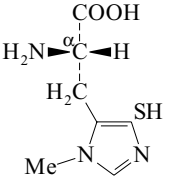
Hexa-Ac:
$C_{19}H_{26}O_{12}$ 446.407
Mp 186-188°.

Posternak, T. *et al., Helv. Chim. Acta*, 1944, **27**, 457-468 (*synth*)
Wickberg, B. *et al., Acta Chem. Scand.*, 1957, **11**, 506-511 (*isol*)
Angyal, S.J. *et al., Aust. J. Chem.*, 1974, **27**, 1075-1086 (*pmr*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1994, **67**, 1633-1640 (*synth*)

1-Methyl-4-mercaptohistidine M-384

5-Mercapto-3-methylhistidine, 9CI. ***Ovothiol A***

[62982-24-5]



$C_7H_{11}N_3O_2S$ 201.249

λ_{max} 235 (ϵ 6000); 278 (sh) (H_2O) (Derep).

(*S*)-*form* [108418-13-9]

[62982-24-5]

Isol. from eggs of the starfish *Evasterias troschelii, Loligo vulgaris* and *Paracentrotus lividus*. Redox-active compd. Egg release pheromone. Oxidoreductase stimulator. Phospholipase A_2 inhibitor. Sol. H_2O.

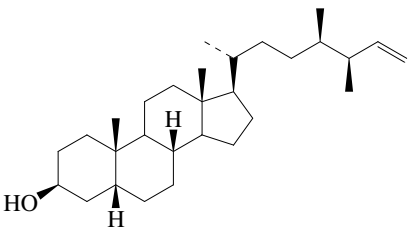
N^{α}-*Me: 5-Mercapto*-N,*3-dimethylhistidine, 9CI.* ***Ovothiol B***
[108418-14-0]
$C_8H_{13}N_3O_2S$ 215.276
Isol. from the scallop *Chlamys hastata*. Oxidoreductase stimulator. Phospholipase A_2 inhibitor. Sol. H_2O. λ_{max} 235 (ϵ 6000); 278 (sh) (H_2O) (Derep).

N^{α},N^{α}-*Di-Me: 5-Mercapto*-N,N,*3-trimethylhistidine, 9CI.* ***Ovothiol C***
[105496-34-2]
$C_9H_{15}N_3O_2S$ 229.302
Isol. from the sea urchin *Strongylocentrotus purpuratus* and *Paracentrotus lividus*. Oxidoreductase stimulator. Sol. H_2O.
λ_{max} 235 (ϵ 6000); 278 (sh) (H_2O) (Derep).

Palumbo, A. *et al., Tet. Lett.*, 1982, **23**, 3207-3208 (*isol*)
Turner, E. *et al., Biochemistry*, 1987, **26**, 4028-4036 (*Ovothiol B, Ovothiol C*)
Holler, T.P. *et al., J.O.C.*, 1987, **52**, 4420-4421; 1989, **54**, 4570-4575 (*synth, bibl*)
Shapiro, B.M. *et al., BioFactors*, 1988, **1**, 85-88 (*rev*)
Steenkamp, D.J. *et al., Eur. J. Biochem.*, 1996, **242**, 557-566 (*biosynth*)
Rōhl, I. *et al., Z. Naturforsch., C*, 1999, **54**, 1145 (*activity*)

24-Methyl-26-methylenecholestan-3-ol **M-385**

25-Ethenyl-27-norergostan-3-ol, 9CI. 24,26-Dimethylcholest-26-en-3-ol. 26-Methyleneergostan-3-ol. 26-Methylergost-26-en-3-ol



$C_{29}H_{50}O$ 414.713

(3β,5β,24*R*,25*R*)-*form* [106518-68-7]

Isol. from sponge *Petrosia ficiformis*, prob. as an endobacterial metab.

Seidel, S.B. *et al., Steroids*, 1986, **47**, 49-62 (*isol, pmr, ms, struct*)

24-Methyl-26-methylenecholest-5-en-3-ol **M-386**

24,26-Dimethylcholesta-5,26-dien-3-ol. 26-Methylergosta-5,26-dien-3-ol. 26-Methyleneergost-5-en-3-ol

$C_{29}H_{48}O$ 412.698

(3β,24*R*)-*form*

26-Methylcampesta-5,26-dien-3-ol

Constit. of *Petrosia ficiformis*.

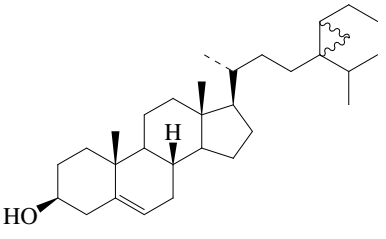
Ac:

Cryst. Mp 111-113°.

Khalil, M.W. *et al., Steroids*, 1980, **35**, 707

29-Methyl-24,28-methylenestigmast-5-en-3-ol **M-387**

24,28-Methylene-24-propylcholest-5-en-3-ol



$C_{31}H_{52}O$ 440.751

No CAS name or number available owing to errors in the paper.

(3β,24ξ,28ξ)-*form*

Constit. of sponge *Pseudaxinyssa* sp.

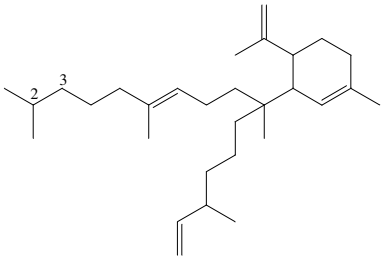
Cryst. (MeOH).

Mp 126-127°.

Tam Ha, T.B. *et al., Tet. Lett.*, 1985, **26**, 4031-4034 (*isol, pmr, ms, struct, synth*)

1-Methyl-4-(1-methylethenyl)-3-[1,5,9-trimethyl-1-(4-methyl-5-hexenyl)-4-decenyl]cyclohexene **M-388**

[652157-36-3]



$C_{30}H_{52}$ 412.741

Constit. of *Rhizosolenia setigera*.

2,3-Didehydro: 1-Methyl-4-(1-methylethenyl)-3-[1,5,9-trimethyl-1-(4-methyl-5-hexenyl)-4,8-decadienyl]cyclohexene

[652157-37-4]

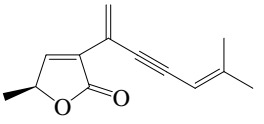
$C_{30}H_{50}$ 410.725

Constit. of *Rhizosolenia setigera*.

Belt, S.T. *et al., Tet. Lett.*, 2003, **44**, 9103-9106 (*isol, pmr, cmr*)

Massé, G. *et al., Phytochemistry*, 2004, **65**, 1101-1106 (*biosynth*)

5-Methyl-3-(5-methyl-1-methylene-4-hexen-2-ynyl)-2(5*H*)-furanone **M-389**



$C_{13}H_{14}O_2$ 202.252

(*S*)-*form* [380629-75-4]

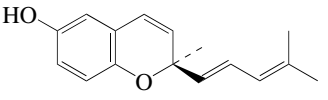
Isol. from the soft coral *Sarcophyton trocheliophorum*.

Pale yellow oil. $[\alpha]_D$ -38.5 (c, 0.12 in EtOH). λ_{max} 204 (log ϵ 4.27); 214 (log ϵ 4.19); 229 (log ϵ 4.15); 263 (log ϵ 3.94); 277 (log ϵ 3.87); 350 (log ϵ 3.24) (EtOH).

Rezanka, T. *et al., Tetrahedron*, 2001, **57**, 8743-8749

2-Methyl-2-(4-methyl-1,3-pentadienyl)-2*H*-1-benzopyran-6-ol, 9CI **M-390**

*6-Hydroxy-2-(4-methyl-1,3-pentadienyl)-2*H*-chromene*



$C_{16}H_{18}O_2$ 242.317

(*R*)-(*E*)-*form* [185839-21-8]

Isol. from the tunicate *Aplidium solidum*.

Yellow oil. $[\alpha]_D$ +32 (c, 1 in $CHCl_3$). λ_{max} 266 (ϵ 17600); 334 (ϵ 10700); 362 (ϵ 6500); 467 (ϵ 1700) (EtOH).

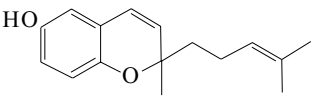
Rochfort, S.J. *et al., Aust. J. Chem.*, 1996, **49**, 1217-1219 (*isol, uv, ir, pmr, cmr, ms*)

2-Methyl-2-(4-methyl-3-pentenyl)-2*H*-1-benzopyran-6-ol, 9CI **M-391**

*6-Hydroxy-2-methyl-2-(4-methyl-3-pentenyl)-2*H*-chromene.*

Cordiachromene A

[63025-48-9]



$C_{16}H_{20}O_2$ 244.333

Constit. of *Cordia alliodora*. Also isol. from the tunicate *Aplidium constellatum*, *Aplidium antillense* and from *Phacelia ixodes*.

Antiinflammatory agent. Light yellow oil. λ_{max} 263 (log ϵ 3.9); 300 (log ϵ 3.66 approximate wavelength); 331 (log ϵ 3.78) (EtOH). λ_{max} 231 (ϵ 6025); 263 (ϵ 7950); 300 (ϵ 4570) (EtOH) (Berdy).

[85611-89-8]

Manners, G.D. *et al., J.C.S. Perkin 1*, 1977, 405

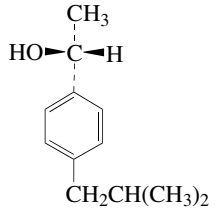
Reynolds, G.W. *et al., Planta Med.*, 1981, **43**, 187 (*isol*)

Targett, N.M. *et al., J. Nat. Prod.*, 1984, **47**, 556 (*isol*)

Benslimane, A.F. *et al., J. Nat. Prod.*, 1988, **51**, 582-583 (*Aplidium antillense constit*)
Kim, I.K. *et al., Magn. Reson. Chem.*, 1993, **31**, 788-789 (*pmr, cmr*)
Kahn, P.H. *et al., Tet. Lett.*, 1999, **40**, 8113-8114 (*synth*)
Bouzbouz, S. *et al., Eur. J. Org. Chem.*, 2000, 3223-3228 (*synth*)

α-Methyl-4-(2-methylpropyl)benzyl alcohol M-392

α-Methyl-4-(2-methylpropyl)benzenemethanol, 9CI. (p-*Isobutylphenyl)methylcarbinol*
[40150-92-3]
[125653-66-9]



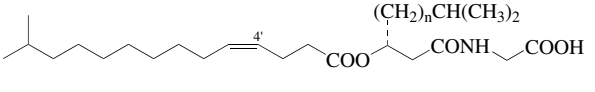
(*R*)-*form*

$C_{12}H_{18}O$ 178.274
Key intermediate in the synth. of Ibuprofen.

(*R*)-*form*
(+)-form
[130007-66-8]
$Bp_{0.1}$ 80°.

(±)-*form* [110773-65-4]
Isol. from the sponge *Phycopsis* sp.
Oil. Bp_{16} 140-141° $Bp_{0.75}$ 100°.
Parrinello, G. *et al., J.A.C.S.*, 1987, **109**, 7122-7127 (*synth, pmr*)
Radhakrishna, A.S. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 373-375 (*synth*)
Eur. Pat., 1990, 398 288; *CA*, **115**, 28891h (*synth*)
Rao, A.V.R. *et al., Tet. Lett.*, 1990, **31**, 2341-2344 (*synth*)
Hsu, S.-H. *et al., Tet. Lett.*, 1990, **31**, 6403-6406 (*resoln*)
Venkateswarlu, Y. *et al., J. Nat. Prod.*, 1995, **58**, 269-270 (*isol*)

N-[15-Methyl-3-(13-methyl-4-tetradecenoyloxy)-hexadecanoyl]glycine M-393



n = 11

$C_{34}H_{63}NO_5$ 565.875

(*R*)-(*Z*)-*form* [193825-66-0]
Prod. by a marine *Cytophaga* sp. N-type calcium channel blocker.
Leaflets (hexane/CH_2Cl_2).
Mp 71-72°. $[\alpha]_D^{25}$ +0.45 (c, 8 in $CHCl_3$).
4′,5′-Dihydro: N-*[15-Methyl-3-(13-methyltetradecanoyloxy)hexadecanoyl]glycine.* ***Topostin B 567****. Cytolipin*
[103196-73-2]
$C_{34}H_{65}NO_5$ 567.891
Prod. by the marine *Cytophaga johnsonae* and *Flexibacter topostinus.* N-type calcium channel blocker. Topoisomerase inhibitor. Leaflets (hexane/CH_2Cl_2). $[\alpha]_D^{22}$ +1.9 (c, 0.2 in $CHCl_3$).

(±)-(*Z*)-*form* [183167-45-5]
Cryst. (hexane/CH_2Cl_2). Mp 84-85°.
Suzuki, K. *et al., J. Antibiot.*, 1990, **43**, 154-157; 158-162 (*Topostin*)
Morishita, T. *et al., J. Antibiot.*, 1997, **50**, 457-468 (*isol, synth, ir, pmr, cmr*)
Nemoto, T. *et al., Tetrahedron*, 1998, **54**, 2683-2690 (*isol, Topostin*)
Shioiri, T. *et al., Tetrahedron*, 1998, **54**, 15701-15710 (*synth*)

N-[14-Methyl-3-(13-methyl-4-tetradecenoyloxy)-pentadecanoyl]glycine M-394

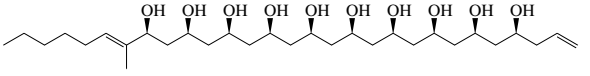
As *N*-[15-Methyl-3-(13-methyl-4-tetradecenoyloxy)hexadecanoyl]glycine, M-393 with
n = 10

$C_{33}H_{61}NO_5$ 551.849

(*R*)-(*Z*)-*form* [193825-67-1]
Prod. by a marine *Cytophaga* sp. N-type calcium channel blocker.
Amorph. solid. $[\alpha]_D^{25}$ -3.4 (c, 0.9 in $CHCl_3$).

(±)-(*Z*)-*form*
Cryst. (hexane/CH_2Cl_2). Mp 74-75°.
Morishita, T. *et al., J. Antibiot.*, 1997, **50**, 457-468 (*isol, synth, ir, pmr, cmr*)

23-Methyl-1,23-nonacosadiene-4,6,8,10,12,14,16,18,20,22-decol M-395



$C_{30}H_{58}O_{10}$ 578.782

(4*S*,6*S*,8*S*,10*S*,12*S*,14*S*,16*S*,18*S*,20*S*,22*S*,23*E*)-*form*
Deca-Me ether: 4,6,8,10,12,14,16,18,20,22-Decamethoxy-23-methyl-1,23-nonacosadiene
$C_{40}H_{78}O_{10}$ 719.05
Isol. from the sponge *Myriastra clavosa*. Slightly greenish viscous oil. $[\alpha]_D$ +6.3 (c, 1 in $CHCl_3$).
Rao, M.R. *et al., J. Nat. Prod.*, 2002, **65**, 1201-1203 (*isol, pmr*)

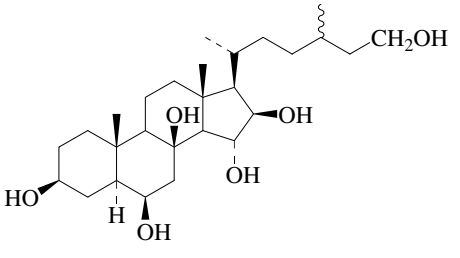
17-Methyl-5,9-nonadecadienoic acid M-396

$H_3CCH_2CH(CH_3)(CH_2)_6CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{20}H_{36}O_2$ 308.503
The claimed isol. of the Me ester as a nat. prod. has been withdrawn.

(5*Z*,9*Z*,17ξ)-*form*
Me ester:
$C_{21}H_{38}O_2$ 322.53
Claimed isol. from the sponge *Plakinastrella* sp. Oil. $[\alpha]_D$ -4 (c, 0.07 in hexane). λ_{max} 221 (ε 4100) (hexane).
Qureshi, A. *et al., J. Nat. Prod.*, 1998, **61**, 1539-1542; 2001, 553-554
Takagi, M. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 2065-2069 (*Me ester, synth*)

24-Methyl-27-nor-3,6,8,15,16,26-cholestanehexol M-397

27-Nor-3,6,8,15,16,26-ergostanehexol, 9CI
[88191-37-1]

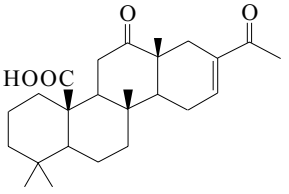


$C_{27}H_{48}O_6$ 468.673

(3β,5α,6β,8β,15α,16β,24ξ)-*form*
Constit. of *Hacelia attenuata*.
4β-Hydroxy: 24-Methyl-27-nor-3,4,6,8,15,16,26-cholestaneheptol
[88191-38-2]
$C_{27}H_{48}O_7$ 484.672
From *Hacelia attenuata*.
Minale, L. *et al., J. Nat. Prod.*, 1983, **46**, 736-741 (*isol*)

24-Methyl-25-nor-12,24-dioxo-16-scalaren-22-oic acid M-398

[107551-76-8]



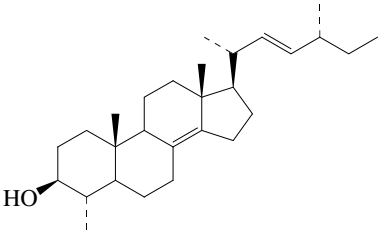
$C_{25}H_{36}O_4$ 400.557

Constit. of a Dictyoceratid sponge and a *Halichondria* spp. Antimicrobial. Amorph. solid. λ_{max} 231 (ϵ 11000) (MeOH) (Derep).

Nakagawa, M. *et al., Tet. Lett.*, 1987, **28**, 431

4-Methyl-27-norergosta-8(14),22-dien-3-ol M-399

4,24-Dimethyl-27-norcholesta-8(14),22-dien-3-ol



$C_{28}H_{46}O$ 398.671

(3β,4α,5α,22*E*,24*R*)-*form*

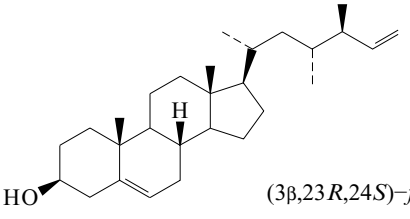
Brevesterol

[500604-71-7]

Constit. of *Karenia brevis.*

Giner, J.-L. *et al., J. Phycol.*, 2003, **39**, 315-319 (*isol, pmr, cmr*)

23-Methyl-27-norergosta-5,25-dien-3-ol M-400



(3β,23*R*,24*S*)–*form*

$C_{28}H_{46}O$ 398.671

(3β,23*R*,24*R*)-*form* [114127-78-5]

Cryst. (CH_2Cl_2/MeOH). Mp 157-158°. $[\alpha]_D^{20}$ -17.2 (c, 1.24 in $CHCl_3$).

(3β,23*R*,24*S*)-*form*

Norficisterol

[114129-12-3]

Isol. from *Petrosia hebes* and *Petrosia ficiformis.*

Cryst. (CH_2Cl_2/MeOH).

Mp 158-161°. $[\alpha]_D^{20}$ -30.7 (c, 3.20 in $CHCl_3$).

(3β,23*S*,24*R*)-*form* [114127-80-9]

Cryst. (MeOH). Mp 154-155°. $[\alpha]_D^{20}$ -23.8 (c, 1.36 in $CHCl_3$).

(3β,23*S*,24*S*)-*form* [114127-79-6]

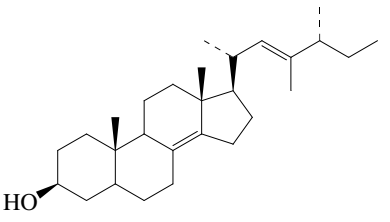
Cryst. (MeOH). Mp 147-150°. $[\alpha]_D^{20}$ -22.3 (c, 0.60 in $CHCl_3$).

Shu, A.Y.L. *et al., J.C.S. Perkin 1*, 1987, 1291 (*synth, struct*)

Cho, J.H. *et al., J.C.S. Perkin 1*, 1987, 1307 (*isol*)

23-Methyl-27-norergosta-8(14),22-dien-3-ol M-401

23,24-Dimethyl-27-norcholesta-8(14),22-dien-3-ol



$C_{28}H_{46}O$ 398.671

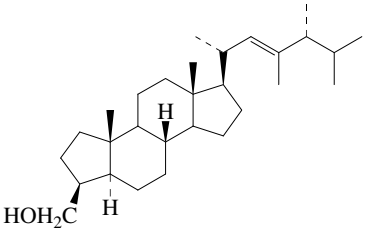
(3β,5α,22*E*,24*R*)-*form* [636599-91-2]

Constit. of *Karenia brevis.*

Giner, J.-L. *et al., J. Phycol.*, 2003, **39**, 315-319 (*isol, pmr, cmr*)

23-Methyl-*A*-norergost-22-ene-3-methanol, 9CI M-402

*3-Hydroxymethyl-23-methyl-*A*-norergost-22-ene*



(3β,5α,22*E*,24*R*)-*form*

$C_{29}H_{50}O$ 414.713

(3β,5α,22*E*,24*R*)-*form*

A-*Nordinosterol*

[83681-81-6]

Isol. from *Homaxinella trachys.*

Mp 168-172°.

(3ξ,5α,22*E*,24*R*)-*form*

Isol. from *Teichaxinella morchella* as acetate.

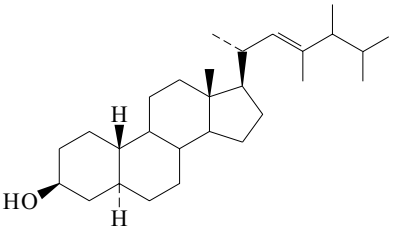
[78285-96-8]

Bohlin, L. *et al., J.C.S. Perkin 1*, 1981, 1023-1028 (*isol*)

Eggersdorfer, M.L. *et al., J.O.C.*, 1982, **47**, 5304-5309 (*isol, pmr, ms*)

23-Methyl-19-norergost-22-en-3-ol M-403

23,24-Dimethyl-19-norcholest-22-en-3-ol



$C_{28}H_{48}O$ 400.687

(3β,5α,22*E*,24*S*)-*form*

23-Methyl-19-norcampest-22-en-3-ol

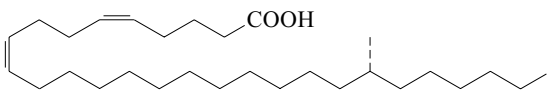
[90038-24-7]

Isol. from *Axinella polypoides.*

Mp 121-123°.

Crist, B.V. *et al., Steroids*, 1983, **42**, 331 (*isol*)

22-Methyl-5,9-octacosadienoic acid M-404



$C_{29}H_{54}O_2$ 434.744

(5*Z*,9*Z*,22*R*)-*form* [108644-87-7]
Isol. from the marine sponge *Aplysina fistularis*.
$[\alpha]_D^{20}$ -0.12 (c, 6.7 in $CHCl_3$).

[79605-33-7]

Walkup, R.D. *et al., Lipids*, 1981, **16**, 631 (*isol*)
Raederstorff, D. *et al., J.O.C.*, 1987, **52**, 2337 (*synth, abs config*)

26-Methyl-5,9-octacosadienoic acid M-405

$H_3CCH_2CH(CH_3)(CH_2)_{15}CH{=}CHCH_2CH_2CH{=}CHCH_2CH_2CH_2COOH$

$C_{29}H_{54}O_2$ 434.744

(5*Z*,9*Z*)-*form* [153081-64-2]
Constit. of the sponges *Chondrosia remiformis* and *Myrmekioderma styx*.

Carballeira, N.M. *et al., J. Nat. Prod.*, 1993, **56**, 1850 (*isol*)

27-Methyl-5,9-octacosadienoic acid M-406

$(H_3C)_2CH(CH_2)_{16}CH{=}CHCH_2CH_2CH{=}CHCH_2CH_2CH_2COOH$

$C_{29}H_{54}O_2$ 434.744

(5*Z*,9*Z*)-*form* [153081-63-1]
Constit. of the sponges *Chondrosia remiformis* and *Myrmekioderma styx*.

Carballeira, N.M. *et al., J. Nat. Prod.*, 1993, **56**, 1850 (*isol*)

20-Methyloctacosanoic acid M-407

[93673-92-8]
$H_3C(CH_2)_7CH(CH_3)(CH_2)_{18}COOH$
$C_{29}H_{58}O_2$ 438.776

(ξ)-*form*
Isol. from the sponge *Strongylophora durissima*.

Dasgupta, A. *et al., Lipids*, 1984, **19**, 768-776 (*isol*)

26-Methyloctacosanoic acid M-408

[94245-50-8]
$H_3CCH_2CH(CH_3)(CH_2)_{24}COOH$
$C_{29}H_{58}O_2$ 438.776
Isol. from the phospholipids of the sponge *Petrosia pellasarca*. Also found in the meibomian gland.

Docosyl ester: [121878-04-4]
$C_{51}H_{102}O_2$ 747.366
Isol. from the wax of tobacco leaves.

Harvey, D.J. *et al., J. Chromatogr.*, 1984, **301**, 173 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1990, **53**, 836 (*isol*)

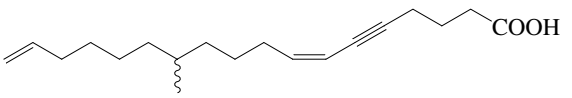
27-Methyloctacosanoic acid M-409

[128174-97-0]
$(H_3C)_2CH(CH_2)_{25}COOH$
$C_{29}H_{58}O_2$ 438.776
Isol. from the phospholipids of the sponge *Petrosia pellasarca*. Also found in the bacterium *Desulfotomaculum* sp.

Rezanka, T. *et al., FEMS Microbiol. Ecol.*, 1990, **73**, 231 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1990, **53**, 836 (*isol*)

12-Methyl-7,17-octadecadien-5-ynoic acid M-410

Stellettic acid C
[502487-43-6]



$C_{19}H_{30}O_2$ 290.445

(7*Z*,12ξ)-*form*
Isol. from the marine sponge *Stelletta* sp.
Pale yellow oil. $[\alpha]_D^{21}$ +6 (c, 0.09 in MeOH).

Zhao, Q. *et al., J. Nat. Prod.*, 2003, **66**, 408-411 (*isol, pmr, cmr, ms*)

11-Methyloctadecanoic acid M-411

11-Methylstearic acid
[79605-28-0]
$H_3C(CH_2)_6CH(CH_3)(CH_2)_9COOH$
$C_{19}H_{38}O_2$ 298.508

(±)-*form* [40811-98-1]
Mp 21°. $Bp_{0.1}$ 174°.

Amide:
$C_{19}H_{39}NO$ 297.523
Mp 73.5-74°.

(ξ)-*form*
Isol. from the sponges *Aplysina fistularis* and *Strongylophora durissima*.

Cason, J. *et al., J.O.C.*, 1950, **15**, 139 (*synth*)
Weitzel, G. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1951, **287**, 310 (*synth*)
Walkup, R.D. *et al., Lipids*, 1981, **16**, 631-646 (*isol*)
Dasgupta, A. *et al., Lipids*, 1984, **19**, 768-776 (*isol*)

16-Methyloctadecanoic acid, 9CI M-412

16-Methylstearic acid. Anteisononadecanoic acid
[17001-28-4]
$H_3CCH_2CH(CH_3)(CH_2)_{14}COOH$
$C_{19}H_{38}O_2$ 298.508

(±)-*form*
Mp 49.9-50.6°.

Me ester: [2490-16-6]
$C_{20}H_{40}O_2$ 312.535
$Bp_{1.2}$ 176°.

Amide:
$C_{19}H_{39}NO$ 297.523
Mp 93.2°.

(ξ)-*form*
Occurs in various woods, butterfat, tobacco and salmon.

Me ester:
Occurs in *Staphylococcus aureus* membrane.

[59992-30-2, 73641-06-2]

Cason, J. *et al., J.A.C.S.*, 1944, **66**, 46
Abrahamsson, S. *et al., Acta Cryst.*, 1958, **11**, 270 (*cryst struct*)
Fischmeister, I. *et al., Ark. Kemi*, 1963, **20**, 353 (*ir*)
Silvius, J.R. *et al., Chem. Phys. Lipids*, 1980, **26**, 67
Jensen, N.J. *et al., Lipids*, 1986, **21**, 362 (*ms*)

17-Methyloctadecanoic acid, 9CI M-413

17-Methylstearic acid. Isononadecanoic acid
[2724-59-6]
$H_3CCH(CH_3)(CH_2)_{15}COOH$
$C_{19}H_{38}O_2$ 298.508

(±)-*form*
Mp 67.3-67.8°. $Bp_{0.3}$ 180°.

Me ester:
$C_{20}H_{40}O_2$ 312.535
Mp 26-27.5°. $Bp_{1.5}$ 171-172° (lit. gives a pressure range).

Amide:
$C_{19}H_{39}NO$ 297.523
Mp 100.2-101.3°.

(ξ)-*form*
Occurs in *Microciona prolifera*, seeds of *Asphodelus tennifolus* and Baltic salmon.
Cason, J. *et al., J.A.C.S.*, 1942, **64**, 1106
Weitzel, G. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1951, **287**, 310 (*synth*)
Golovnya, R.V. *et al., Prikl. Biokhim. Mikrobiol.*, 1978, **14**, 609 (*ms*)

7-Methyl-6-octadecenoic acid M-414

$H_3C(CH_2)_{10}C(CH_3)=CH(CH_2)_4COOH$
$C_{19}H_{36}O_2$ 296.492

(*Z*)-*form* [184176-86-1]
Constit. of *Holothuria mexicana*.
[184176-88-3]
Carballeira, N.M. *et al., J. Nat. Prod.*, 1996, **59**, 1076 (*isol, synth, ir, pmr, cmr*)

10-Methyl-9-octadecenoic acid M-415

$H_3C(CH_2)_7C(CH_3)=CH(CH_2)_7COOH$
$C_{19}H_{36}O_2$ 296.492

(*Z*)-*form* [177602-93-6]
Isol. from the marine fungus *Microsphaeropsis olivacea*.
Oil. λ_{max} 210 (MeOH).
Yu, C.-M. *et al., Can. J. Chem.*, 1996, **74**, 730 (*isol, uv, ir, pmr, cmr, ms*)

11-Methyl-12-octadecenoic acid M-416

[129177-01-1]
$H_3C(CH_2)_4CH=CHCH(CH_3)(CH_2)_9COOH$
$C_{19}H_{36}O_2$ 296.492

(11ξ,12*Z*)-*form* [104061-39-4]
Constit. of *Vibrio alginolyticus* associated with the alga *Cladophora coelothrix*, *Mycobacterium fallax* and the bacteria *Thiobacillus* spp.
Kerger, B.D. *et al., FEMS Microbiol. Ecol.*, 1986, **38**, 67-77 (*isol*)
Courdec, F. *et al., Lipids*, 1995, **30**, 691-699 (*occur*)
Carballeira, N.M. *et al., Lipids*, 1997, **32**, 1271-1275 (*isol*)
Rontani, F. *et al., Lipids*, 2005, **40**, 97-108 (*isol*)

12-Methyl-5-octadecenoic acid M-417

[132171-18-7]
$H_3C(CH_2)_5CH(CH_3)(CH_2)_5CH=CH(CH_2)_3COOH$
$C_{19}H_{36}O_2$ 296.492
Isol. from the sponge *Plakortis halichondroides.*
Carballeira, N.M. *et al., Lipids*, 1990, **25**, 835-840 (*isol, ir, cmr*)

12-Methyl-11-octadecenoic acid M-418

$H_3C(CH_2)_5C(CH_3)=CH(CH_2)_9COOH$
$C_{19}H_{36}O_2$ 296.492

(*E*)-*form*
Prod. by marine-derived *Erythrobacter* spp. and *Roseobacter* spp.
Rontani, F. *et al., Lipids*, 2005, **40**, 97-108 (*isol, ms*)

17-Methyl-6-octadecenoic acid M-419

$(H_3C)_2CH(CH_2)_9CH=CH(CH_2)_4COOH$
$C_{19}H_{36}O_2$ 296.492

(*Z*)-*form* [384817-97-4]
Isol. from the mollusc *Siphonaria denticulata*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 1426-1429 (*isol, synth, pmr, cmr*)

17-Methyl-7-octadecenoic acid M-420

$(H_3C)_2CH(CH_2)_8CH=CH(CH_2)_5COOH$
$C_{19}H_{36}O_2$ 296.492

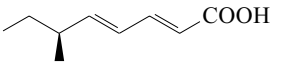
(*Z*)-*form* [384817-98-5]
Isol. from the mollusc *Siphonaria denticulata*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 1426-1429 (*isol, synth, pmr, cmr*)

12-Methyl-17-octadecen-5-ynoic acid M-421

$H_2C=CH(CH_2)_4CH(CH_3)(CH_2)_5C\equiv C(CH_2)_3COOH$
$C_{19}H_{32}O_2$ 292.461

(-)-*form*
Isol. from the sponge *Stelletta* sp.
Gum. $[\alpha]_D$ -1.8 (c, 0.05 in MeOH).
Lee, H.-S. *et al., J. Nat. Prod.*, 2003, **66**, 566-568 (*isol, pmr, cmr*)

6-Methyl-2,4-octadienoic acid, 9CI M-422

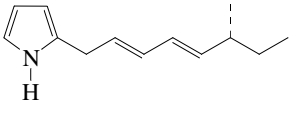


$C_9H_{14}O_2$ 154.208

(2*E*,4*E*,6*S*)-*form*
Dendryphiellic acid A
[121661-45-8]
Metab. of *Dendryphiella salina*.
Oil. $[\alpha]_D^{20}$ +52.2 (c, 0.17 in EtOH aq.).
Me ester: [121702-84-9]
$C_{10}H_{16}O_2$ 168.235
$[\alpha]_D^{20}$ +52.8 (c, 0.3 in $CHCl_3$).
2,3-Dihydroxypropyl ester: ***Glyceryl dendryphiellate A***
[133562-46-6]
$C_{12}H_{20}O_4$ 228.288
Metab. of *Dendryphiella salina*. Oil. $[\alpha]_D^{20}$ +23.6 (c, 0.22 in EtOH).
Guerriero, A. *et al., Helv. Chim. Acta*, 1989, **72**, 438 (*isol, pmr, cmr, synth*)
Guerriero, A. *et al., Helv. Chim. Acta*, 1990, **73**, 2090 (*Glyceryl dendryphiellate A*)
Kim, S. *et al., Bioorg. Med. Chem.*, 1998, **6**, 1975-1982 (*Me ester, synth, pmr*)

2-(6-Methyl-2,4-octadienyl)-1*H*-pyrrole M-423

Axinellamine A†



$C_{13}H_{19}N$ 189.3

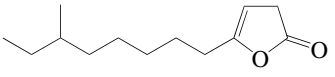
(2′*E*,4′*E*,6*R*)-*form* [213269-06-8]
Alkaloid from the marine sponge *Axinella* sp.
Pale yellow gum. $[\alpha]_D$ -45.4 (c, 0.2 in $CHCl_3$). λ_{max} 227 (ϵ 8000) (MeOH).
Bascombe, K.C. *et al., Heterocycles*, 1998, **48**, 1461-1464 (*isol, uv, ir, pmr, cmr, ms*)
Seki, M. *et al., Eur. J. Org. Chem.*, 2001, 503-506 (*synth, abs config*)

7-Methyl-4-octen-3-one M-424

$(H_3C)_2CHCH_2CH=CHCOCH_2CH_3$
$C_9H_{16}O$ 140.225
Isol. from the marine sponge *Plakortis zygompha*. Sweet-smelling oil. Bp_{30} 92-94°.
[74403-49-9, 77106-71-9]
Faulkner, D.J. *et al., Tet. Lett.*, 1980, 23 (*isol, spectra*)

Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 342 (*synth*)
Durman, J. *et al., Tet. Lett.*, 1983, **24**, 3927 (*synth*)

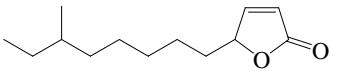
5-(6-Methyloctyl)-2(3*H*)-furanone M-425
10-Methyl-3-dodecen-4-olide



$C_{13}H_{22}O_2$ 210.316

(ξ)-*form*
Prod. by the marine *Streptomyces* sp. strain GWS-BW-H5.
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 837-865 (*isol, synth, pmr, cmr, ms*)

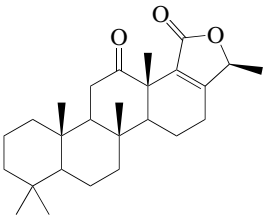
5-(6-Methyloctyl)-2(5*H*)-furanone M-426
10-Methyl-2-dodecen-4-olide



$C_{13}H_{22}O_2$ 210.316

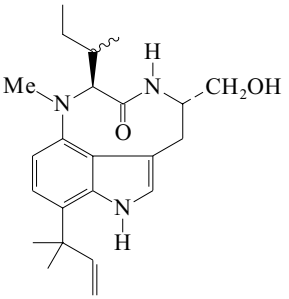
(ξ)-*form*
Prod. by the marine *Streptomyces* sp. strain GWS-BW-H5.
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 837-865 (*isol, synth, pmr, cmr, ms*)

24-Methyl-12-oxo-17-scalaren-25,24-olide M-427
[222960-90-9]



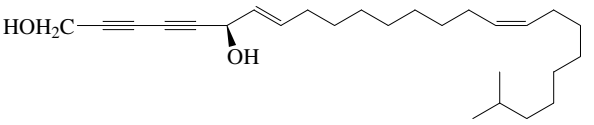
$C_{26}H_{38}O_3$ 398.584
Constit. of *Phyllospongia foliascens*. Amorph. solid. $[\alpha]_D$ +93.8 (c, 0.24 in CH_2Cl_2).
Fu, X. *et al., J. Nat. Prod.*, 1999, **62**, 644-646 (*isol, pmr, cmr*)

16-Methylpendolmycin M-428
[138590-60-0]



$C_{23}H_{33}N_3O_2$ 383.533
Isol. from a *Nocardiopsis* sp. Protein kinase C inhibitor.
Mp 174-178°. $[\alpha]_D$ -76 (c, 0.57 in MeOH). λ_{max} 230 (ε 18000); 289 (ε 6200); 299 (ε 6500) (MeOH) (Berdy).
Sun, H.H. *et al., J. Nat. Prod.*, 1991, **54**, 1440 (*isol, uv, ir, pmr, cmr, cd, struct*)

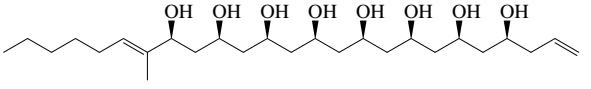
24-Methyl-7,16-pentacosadiene-2,4-diyne-1,6-diol M-429
Strongylodiol I



$C_{26}H_{42}O_2$ 386.617

(6*R*,7*E*,16*Z*)-*form*
Isol. from the sponge *Strongylophora* sp.
Oil. $[\alpha]_D^{22}$ -33.4 (c, 0.13 in $CHCl_3$). Obt. as a partial racemate (97% op). λ_{max} 208 (log ε 3.76) (MeOH).
Watanabe, K. *et al., J. Nat. Prod.*, 2005, **68**, 1001-1005 (*isol, pmr, cmr*)

19-Methyl-1,19-pentacosadiene-4,6,8,10,12,14,16,18-octol M-430



$C_{26}H_{50}O_8$ 490.676

(4*S*,6*S*,8*S*,10*S*,12*S*,14*S*,16*S*,18*S*,19*E*)-*form*
Octa-Me ether: 4,6,8,10,12,14,16,18-Octamethoxy-19-methyl-1,19-pentacosadiene
$C_{34}H_{66}O_8$ 602.891
Isol. from the sponge *Myriastra clavosa*. Slightly greenish viscous oil. $[\alpha]_D$ +4.4 (c, 1 in $CHCl_3$).
Rao, M.R. *et al., J. Nat. Prod.*, 2002, **65**, 1201-1203 (*isol, pmr, cmr*)

23-Methyl-5,9-pentacosadienoic acid M-431
$H_3CCH_2CH(CH_3)(CH_2)_{12}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{26}H_{48}O_2$ 392.664

(*Z*,*Z*)-*form* [126201-34-1]
Isol. from the sponge *Cribrochalina vasculum*.
Carballeira, N.M. *et al., Lipids*, 1990, **25**, 69 (*isol*)

24-Methyl-5,9-pentacosadienoic acid M-432
$(H_3C)_2CH(CH_2)_{13}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{26}H_{48}O_2$ 392.664

(5*Z*,9*Z*)-*form* [83474-17-3]
Isol. from various marine sponges incl. *Dysidea fragilis* and *Petrosia ficiformis*.
Ayanoglu, E. *et al., Lipids*, 1982, **17**, 617-625 (*isol*)
Carballeira, N.M. *et al., J.O.C.*, 1986, **51**, 2751-2756 (*biosynth*)
Reyes, E.D. *et al., Synthesis*, 1997, 1195-1198 (*synth, ir, pmr, cmr, ms*)

18-Methylpentacosanoic acid M-433
$H_3C(CH_2)_6CH(CH_3)(CH_2)_{16}COOH$
$C_{26}H_{52}O_2$ 396.696

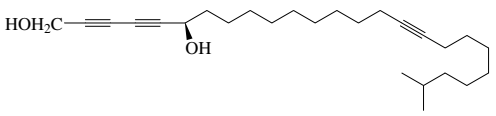
(ξ)-*form*
Constit. of the sponge *Cinachyrella alloclada*.
Barnathan, G. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2003, **135**, 297-308 (*isol, ms*)

19-Methylpentacosanoic acid M-434
[93673-88-2]
$H_3C(CH_2)_5CH(CH_3)(CH_2)_{17}COOH$
$C_{26}H_{52}O_2$ 396.696

(ξ)-*form*
Isol. from the sponge *Strongylophora durissima*.

Dasgupta, A. *et al., Lipids*, 1984, **19**, 768-776 (*isol*)

24-Methyl-2,4,16-pentacosatriyne-1,6-diol M-435
Strongylodiol D



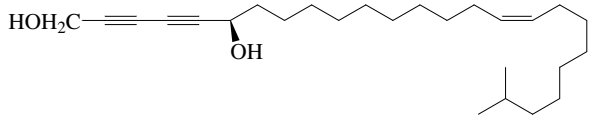
(*R*)-*form*

$C_{26}H_{42}O_2$ 386.617

(*R*)-*form* [334973-93-2]
Isol. from the sponge *Strongylophora* sp.
Amorph. solid. $[\alpha]_D^{25}$ -8 (c, 0.56 in $CHCl_3$). Obt. as a partial racemate, 95% o.p. λ_{max} 231 (log ϵ 2.59); 244 (log ϵ 2.56); 257 (log ϵ 2.35) (EtOH).

(*S*)-*form* [334904-85-7]
Isol. from *Strongylophora* sp.
Watanabe, K. *et al., CA*, 2000, **134**, 308117e (*isol*)
Watanabe, K. *et al., J. Nat. Prod.*, 2005, **68**, 1001-1005 (*isol, pmr, cmr, ms*)

24-Methyl-16-pentacosene-2,4-diyne-1,6-diol M-436
Strongylodiol C



(6*R*,16*Z*)-*form*

$C_{26}H_{44}O_2$ 388.632

(6*R*,16*Z*)-*form* [320717-32-6]
Isol. from the sponge *Strongylophora* sp. Cytotoxic agent. $[\alpha]_D^{22}$ -7.5 (c, 0.09 in $CHCl_3$).

(6*S*,16*Z*)-*form* [320717-35-9]
Isol. from *Strongylophora* sp. Cytotoxic agent. $[\alpha]_D^{22}$ +7.5 (c, 0.03 in $CHCl_3$).
Watanabe, K. *et al., Tet. Lett.*, 2000, **41**, 9271-9276 (*isol, pmr, cmr*)

19-Methyl-5-pentacosenoic acid M-437
$H_3C(CH_2)_5CH(CH_3)(CH_2)_{12}CH{=}CH(CH_2)_3COOH$
$C_{26}H_{50}O_2$ 394.68

(5*Z*,19ξ)-*form* [93673-85-9]
Isol. from the sponge *Strongylophora durissima*.
Dasgupta, A. *et al., Lipids*, 1984, **19**, 768-776 (*isol*)

14-Methyl-5,9-pentadecadienoic acid M-438
$(H_3C)_2CH(CH_2)_3CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{16}H_{28}O_2$ 252.396

(5*Z*,9*Z*)-*form* [189755-31-5]
Isol. from the gorgonian *Eunicea succinea*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1997, **60**, 502-504 (*isol*)
Reyes, E.D. *et al., Synthesis*, 1997, 1195-1198 (*synth, ir, pmr, cmr, ms*)
Carballeira, N.M. *et al., Tet. Lett.*, 2004, **45**, 3761-3763 (*synth*)

3-Methylpentadecanoic acid, 9CI M-439
[35199-78-1]
$H_3C(CH_2)_{11}CH(CH_3)CH_2COOH$
$C_{16}H_{32}O_2$ 256.428
Isol. from the sponges *Callyspongia fallax* and *Erylus formosus*.

(±)-*form*
Cryst. (Me_2CO). Mp 37-38°.

Me ester: [66344-21-6]
$C_{17}H_{34}O_2$ 270.454
Bp_8 170-174°.

[112428-88-3, 112428-89-4]

Cason, J. *et al., J.O.C.*, 1953, **18**, 842-849 (*synth*)
Schulte, K.E. *et al., Chem. Ber.*, 1972, **105**, 24-33 (*synth*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 305-309 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*isol*)

11-Methylpentadecanoic acid M-440
[212377-00-9]
$H_3C(CH_2)_3CH(CH_3)(CH_2)_9COOH$
$C_{16}H_{32}O_2$ 256.428
Isol. from the sponge *Calyx podatypa*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1998, **61**, 1049-1052 (*isol*)

14-Methyl-4-pentadecenoic acid M-441
$(H_3C)_2CH(CH_2)_8CH{=}CHCH_2CH_2COOH$
$C_{16}H_{30}O_2$ 254.412

(*Z*)-*form* [340003-87-4]
Isol. from the sponge *Callyspongia fallax*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623

14-Methyl-5-pentadecenoic acid M-442
$(H_3C)_2CH(CH_2)_7CH{=}CH(CH_2)_3COOH$
$C_{16}H_{30}O_2$ 254.412

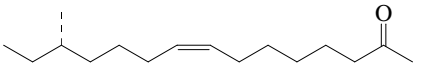
(*E*)-*form* [77900-89-1]
Isol. from gram negative aerobic rods from mangrove swamp.

(*Z*)-*form* [88262-56-0]
Isol. from a *Bacillus* sp. and from the sponge *Callyspongia fallax*.
Gillan, F.T. *et al., Appl. Environ. Microbiol.*, 1981, **41**, 849-856 (*E-form, isol*)
Kaneda, T. *et al., Can. J. Microbiol.*, 1983, **29**, 1634-1641 (*Z-form, isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*Z-form, isol*)

14-Methyl-6-pentadecenoic acid M-443
[127486-79-7]
$(H_3C)_2CH(CH_2)_6CH{=}CH(CH_2)_4COOH$
$C_{16}H_{30}O_2$ 254.412

(*Z*)-*form* [123739-73-1]
Isol. from the freshwater mussel *Unio tumidus* and the sponge *Tethya aurantia*.
Zimmerman, M.P. *et al., Lipids*, 1990, **25**, 383 (*isol*)
Harvey, D.J. *et al., Spectroscopy (Ottawa)*, 1990, **8**, 211 (*ms, struct*)
Stefanov, K. *et al., J. Nat. Prod.*, 1992, **55**, 979 (*isol, struct*)
Hassarajani, S.A. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 429 (*synth, ir, pmr*)

13-Methyl-8-pentadecen-2-one M-444



$C_{16}H_{30}O$ 238.412

(8*Z*,13*S*)-*form*
Prod. by a marine bacterium. $[\alpha]_D$ +7.8 (c, 1.8 in pentane).
8,9-Dihydro: 13-Methyl-2-pentadecanone
$C_{16}H_{32}O$ 240.428
Prod. by a marine bacterium.
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol, synth, pmr, cmr, ms*)

14-Methyl-8-pentadecen-2-one M-445
$(H_3C)_2CH(CH_2)_4CH{=}CH(CH_2)_5COCH_3$
$C_{16}H_{30}O$ 238.412

(Z)-form

Prod. by a marine bacterium.

8,9-Dihydro: 14-Methyl-2-pentadecanone

$C_{16}H_{32}O$ 240.428

Prod. by a marine bacterium.

Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol, synth*)

14-Methyl-10-pentadecen-2-one M-446

$(H_3C)_2CHCH_2CH_2CH{=}CH(CH_2)_7COCH_3$

$C_{16}H_{30}O$ 238.412

(Z)-form

Prod. by a marine bacterium.

Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol, ms*)

4-Methylpentanethioic acid M-447

$(H_3C)_2CHCH_2CH_2COSH \Leftrightarrow (H_3C)_2CHCH_2CH_2C(S)OH$

$C_6H_{12}OS$ 132.226

SH-form

Me ester: S-*Methyl 4-methylpentanethioate. FEMA 3867*

[61122-71-2]

$C_7H_{14}OS$ 146.253

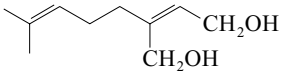
Found in fish oil and hop oil. Pale yellow liq.

Pickett, J.A. *et al., Proc. Anal. Div. Chem. Soc.*, 1976, **13**, 215-217 (*S-Me ester, anal, occur, hop oil*)

Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1160 (*S-Me ester, use*)

2-(4-Methyl-3-pentenyl)-2-butene-1,4-diol M-448

3-Hydroxymethyl-7-methyl-2,6-octadien-1-ol



$C_{10}H_{18}O_2$ 170.251

(Z)-form [76480-92-7]

Constit. of *Chondrococcus hornemanni*. Pale yellow oil.

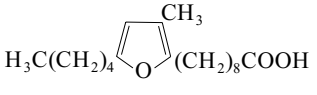
Poulter, C.D. *et al., J.O.C.*, 1981, **46**, 1532 (*synth, pmr*)

Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1983 (*isol, pmr, cmr*)

3-Methyl-5-pentyl-2-furannonanoic acid, 9CI M-449

10,13-Epoxy-11-methyl-10,12-octadecadienoic acid. ***F_2 acid***

[57818-39-0]



$C_{19}H_{32}O_3$ 308.46

Comprises 90% of triacylglycerols of *Hevea brasiliensis* (rubber) latex, a minor component among fish furanoid acids. Component of F acid fraction present in human and beef blood serum.

Glass, R.L. *et al., Lipids*, 1977, **12**, 828 (*occur*)

Hasma, H. *et al., Lipids*, 1978, **13**, 905 (*occur, ms, nmr*)

Lie Ken Jie, M.S.F. *et al., Chem. Phys. Lipids*, 1981, **28**, 99 (*cmr*)

Puchta, V. *et al., Annalen*, 1988, 25 (*occur*)

Batna, A. *et al., Annalen*, 1991, 861 (*biosynth*)

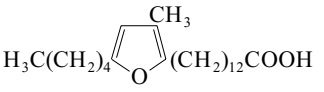
Tsukasa, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 511 (*synth*)

Spiteller, G. *et al., Lipids*, 2005, **40**, 755-771 (*rev, synth, occur*)

3-Methyl-5-pentyl-2-furantridecanoic acid, 9CI M-450

14,17-Epoxy-15-methyl-14,16-docosadienoic acid. ***F_7 acid***

[57818-42-5]



$C_{23}H_{40}O_3$ 364.567

Present in fish oils.

Glass, R.L. *et al., Lipids*, 1974, **9**, 1004; 1975, **10**, 695; 1977, **12**, 828

Gunstone, F.D. *et al., J. Sci. Food Agric.*, 1978, **29**, 539

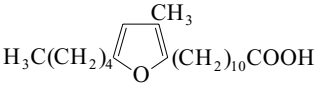
Scheinkönig, J. *et al., Annalen*, 1991, 451 (*biosynth*)

Spiteller, G. *et al., Lipids*, 2005, **40**, 755-771 (*rev, synth, occur*)

3-Methyl-5-pentyl-2-furanundecanoic acid, 9CI M-451

12,15-Epoxy-13-methyl-12,14-eicosadienoic acid. ***F_5 acid***

[57818-37-8]



$C_{21}H_{36}O_3$ 336.514

Constit. of fats of the liver and gonads of fishes, e.g. pike (*Esox lucius*).

Glass, R.L. *et al., Lipids*, 1974, **9**, 1004; 1975, **10**, 695; 1977, **12**, 828

Scheinkönig, J. *et al., Annalen*, 1991, 451 (*biosynth*)

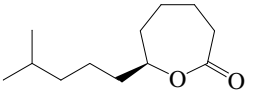
Marson, C.M. *et al., Tet. Lett.*, 1998, **39**, 333-334 (*synth*)

Bach, T. *et al., Eur. J. Org. Chem.*, 1999, 2045-2057 (*synth, pmr, cmr, ms*)

Spiteller, G. *et al., Lipids*, 2005, **40**, 755-771 (*rev, synth, occur*)

7-(4-Methylpentyl)-2-oxepanone M-452

10-Methyl-6-undecanolide



$C_{12}H_{22}O_2$ 198.305

(R)-form

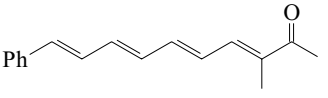
Prod. by the marine *Streptomyces* sp. B6007.

Oil. $[\alpha]_D^{25}$ -1.2 (c, 3.2 in Et_2O).

Stritzke, K. *et al., J. Nat. Prod.*, 2004, **67**, 395-401 (*isol, synth, pmr, cmr, ms*)

3-Methyl-10-phenyl-3,5,7,9-decatetraen-2-one, 9CI M-453

3-Methylnavenone B



$C_{17}H_{18}O$ 238.329

(all-E)-form [73414-54-7]

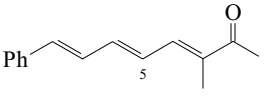
Alarm pheromone of the sea-slug *Navanax inermis.*

Bright yellow cryst.

Mp 113-114°. λ_{max} 355 (ε 58000) (EtOH).

Clelland, J. *et al., Chem. Comm.*, 1983, 1219 (*synth*)

3-Methyl-8-phenyl-3,5,7-octatrien-2-one M-454



(3E,5E,7E)–form

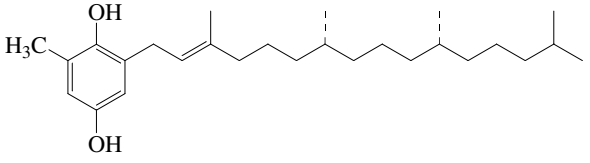
$C_{15}H_{16}O$ 212.291

(3*E*,5*E*,7*E*)-*form*
Lignarenone B
[125010-17-5]
Isol. from *Scaphander lignarius*.

(3*E*,5*Z*,7*E*)-*form*
Lignarenone A
[125010-16-4]
Metab. of *Scaphander lignarius*.
Cimino, G. *et al., Tet. Lett.*, 1989, **30**, 5003-5004 (*isol*)
Borer, B.C. *et al., J. Chem. Res., Synop.*, 1990, 162 (*synth*)
Bell, P.T. *et al., J. Nat. Prod.*, 1992, **55**, 1669 (*synth*)
Alvarez, R. *et al., Nat. Prod. Lett.*, 1995, **6**, 127 (*synth*)

2-Methyl-6-phytylhydroquinone M-455

2-Methyl-6-(3,7,11,15-tetramethyl-2-hexadecenyl)-1,4-benzenediol, 9CI. 6-Phytyltoluquinol
[54432-31-4]



$C_{27}H_{46}O_2$ 402.659
Precursor of tocopherol synth. in spinach chloroplasts.

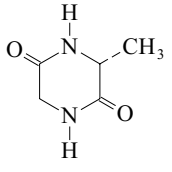
1,4-Quinone: ***2-Methyl-6-phytyl*-p-*benzoquinone***
[34816-26-7]
$C_{27}H_{44}O_2$ 400.643
Constit. of *Taonia atomaria*. Yellow oil. λ_{max} 250 (ϵ 16700); 260 (ϵ 13300) (hexane).

[75513-85-8]

Inoue, S. *et al., J.C.S. Perkin 1*, 1974, 2097 (*synth*)
Soll, J. *et al., Phytochemistry*, 1980, **19**, 215 (*biosynth*)
Marshall, P.S. *et al., Phytochemistry*, 1985, **24**, 1705-1711 (*biosynth, metab*)
Tziveleka, L.-A. *et al., Chem. Biodiversity*, 2005, **2**, 901-909 (*quinone*)

3-Methyl-2,5-piperazinedione, 9CI M-456

3-Methyl-2,5-dioxopiperazine. Glycylalanine anhydride. Methyldiacipiperazine. Cyclo(alanylglycyl). Alanylglycine anhydride



(*R*)–*form*

$C_5H_8N_2O_2$ 128.13

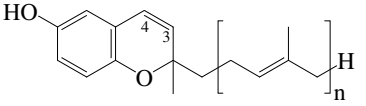
(*R*)-*form*
D-form
[88547-15-3]
Cryst. Mp 247.5-249.5°. $[\alpha]_D^{25}$ +3.56 (H_2O).
1-Benzyl: [132871-09-1]
$C_{12}H_{14}N_2O_2$ 218.255
Solid. Mp 137-139°. $[\alpha]_D^{20}$ +8.56 (c, 1 in $CHCl_3$).

(*S*)-*form*
L-form
[4526-77-6]
Formed during peptide extractions.
Cryst. with a bitter taste.
Mp 247° dec. $[\alpha]_D^{20}$ -5 (H_2O). Sublimes.
1-Benzyl: [132871-10-4]
Solid. Mp 138-139.5°. $[\alpha]_D^{20}$ -8.85 (c, 2 in $CHCl_3$).

(±)-*form* [6062-46-0]
Prod. by a marine-derived *Bacillus* sp.
Needles (EtOH aq.). Sol. H_2O, hot EtOH, spar. sol. Me_2CO.
Mp 244°. Reacts neutral. Tasteless.
Heimrod, G.O. *et al., Ber.*, 1914, **47**, 344 (*synth*)
Abderhalden, E. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1925, **145**, 308 (*synth*)
Birkofer, L. *et al., Annalen*, 1962, **659**, 190 (*synth*)
Pickenhagen, W. *et al., Helv. Chim. Acta*, 1975, **58**, 1078-1086 (*occur*)
Chu, D.T.W. *et al., J. Med. Chem.*, 1991, **34**, 168 (*synth, pmr*)
Zhang, H.-L. *et al., Zhongguo Yaowu Huaxue Zazhi*, 2003, **13**, 294-296; *CA*, **144**, 2926 (*marine, isol*)
Liu, B. *et al., Synth. Commun.*, 2004, **34**, 4111-4118 (*1-benzyl*)

2-Methyl-2-(polyprenylmethyl)-2*H*-1-benzopyran-6-ol M-457

6-Hydroxy-2-methyl-2-(polyprenylmethyl)chromene. 2-Methyl-2-(polyprenylmethyl)-6-chromenol



2-Methyl-2-(prenylmethyl)-2*H*-1-benzopyran-6-ol
$C_{16}H_{20}O_2$ 244.333

3,4-Dihydro: ***2-Methyl-2-(prenylmethyl)-6-chromanol***
[97530-64-8]
$C_{16}H_{22}O_2$ 246.349
Constit. of *Dendrodoris grandiflora*.

2-(Diprenylmethyl)-2-methyl-2*H*-1-benzopyran-6-ol
$C_{21}H_{28}O_2$ 312.451

3,4-Dihydro: ***2-(Diprenylmethyl)-2-methyl-6-chromanol***
$C_{21}H_{30}O_2$ 314.467
Constit. of *Dendrodoris grandiflora*.

2-Methyl-2-(triprenylmethyl)-2*H*-1-benzopyran-6-ol
$C_{26}H_{36}O_2$ 380.569

3,4-Dihydro: ***2-Methyl-2-(triprenylmethyl)-6-chromanol***
[97530-73-9]
$C_{26}H_{38}O_2$ 382.585
Constit. of *Dendrodoris grandiflora*.

2-Methyl-2-(tetraprenylmethyl)-2*H*-1-benzopyran-6-ol
2-Methyl-2-(4,8,12,16-tetramethyl-3,7,11,15-heptadecatetraenyl)-2H-1-benzopyran-6-ol
[170661-41-3]
$C_{31}H_{44}O_2$ 448.687
Isol. from the sponge *Ircinia* sp.

3,4-Dihydro: ***2-Methyl-2-(tetraprenylmethyl)-6-chromanol***
[97530-74-0]
$C_{31}H_{46}O_2$ 450.703
Constit. of *Dendrodoris grandiflora*.

2-Methyl-2-(pentaprenylmethyl)-2*H*-1-benzopyran-6-ol
2-Methyl-2-(4,8,12,16,20-pentamethyl-3,7,11,15,19-heneicosapentaenyl)-2H-1-benzopyran-6-ol. ***Sarcochromenol A***
[839731-97-4]
$C_{36}H_{52}O_2$ 516.806
Isol. from an *Ircinia* sp. and *Ircinia spinosula*. Cryst. (EtOH) (as Ac). Mp 25-26° (Ac). $[\alpha]_{578}$ +39.2 ($CHCl_3$) (Ac).

Sulfate: [170900-07-9]
[144861-46-1, 170900-06-8]
$C_{36}H_{52}O_5S$ 596.87
Isol. from *Ircinia fasciculata* and *Sarcotragus spinulosus*. Na/K-ATPase inhibitor. λ_{max} 251 (ϵ 2300); 266 (ϵ 2700); 285 (ϵ 1100); 318 (ϵ 2000) (MeOH) (Berdy).

3,4-Dihydro: ***2-Methyl-2-(pentaprenylmethyl)-6-chromanol***
[97530-75-1]
$C_{36}H_{54}O_2$ 518.821
Constit. of *Dendrodoris grandiflora*.

2-(Hexaprenylmethyl)-2-methyl-2*H*-1-benzopyran-6-ol
2-(4,8,12,16,20,24-Hexamethyl-3,7,11,15,19,23-pentacosahexae-

*nyl)-2-methyl-2*H*-1-benzopyran-6-ol.* ***Sarcochromenol B***
[159154-50-4]
$C_{41}H_{60}O_2$ 584.924
Isol. from *Ircinia fasciculata* and *Ircinia spinulosa*. Shows activity against gram-positive and -negative bacteria. Oil. $[\alpha]_D$ +3.6 (c, 1 in $CHCl_3$). λ_{max} 243 (ϵ 13800); 264 (ϵ 5100); 330 (ϵ 3800) ($CHCl_3$).

Sulfate: [170900-08-0]
[144861-47-2]
$C_{41}H_{60}O_5S$ 664.988
Isol. from *Dysidea* sp. and *Sarcotragus spinulosus*.

3,4-Dihydro: 2-(Hexaprenylmethyl)-2-methyl-6-chromanol
[97530-76-2]
$C_{41}H_{62}O_2$ 586.94
Isol. from *Ircinia fasciculata*. Oil. $[\alpha]_D$ +8 (c, 0.11 in $CHCl_3$). λ_{max} 242 (ϵ 8500); 298 (ϵ 4300) ($CHCl_3$).

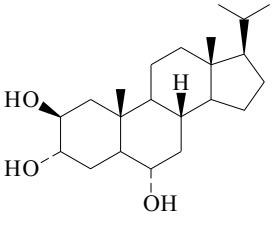
2-(Heptaprenylmethyl)-2-methyl-2*H*-1-benzopyran-6-ol
*2-(4,8,12,16,20,24,28-Heptamethyl-3,7,11,15,19,23,27-nonacosaheptaenyl)-2-methyl-2*H*-1-benzopyran-6-ol, 9CI.*
Sarcochromenol C
[170244-23-2]
$C_{46}H_{68}O_2$ 653.042
Oil (as Ac). $[\alpha]_{578}$ -5 ($CHCl_3$) (Ac).

Sulfate: [144861-48-3]
$C_{46}H_{68}O_5S$ 733.106
Isol. from *Ircinia fasciculata* and *Sarcotragus spinulosus*. CAS no. refers to Na salt.

Cimino, G. *et al., Tetrahedron*, 1985, **41**, 1093-1100 (*Dendrodoris grandiflora constits*)
Stonik, V.A. *et al., J. Nat. Prod.*, 1992, **55**, 1256-1260 (*Sarcochromenol sulfates*)
Venkateswarlu, Y. *et al., J. Nat. Prod.*, 1994, **57**, 1286-1289 (*isol, uv, pmr, cmr, ms*)
Bifulco, G. *et al., J. Nat. Prod.*, 1995, **58**, 1444-1449 (*isol*)
De Rosa, S. *et al., J. Nat. Prod.*, 1995, **58**, 1450-1454 (*isol, uv, ir, pmr, cmr, ms*)
Erdogan, I. *et al., J. Fac. Pharm. Gazi Univ.*, 2000, **17**, 1-7; *CA*, **133**, 249569h (*Sarcochromenol, activity*)
Tziveleka, L.-A. *et al., Chem. Biodiversity*, 2005, **2**, 901-909 (*Ircinia spinosula constit*)

20-Methylpregnane-2,3,6-triol M-458

23,24,25,26,27-Pentanorcholestane-2,3,6-triol



$C_{22}H_{38}O_3$ 350.54

(2β,3α,5α,6α)-*form*
Trisulfate: [163815-29-0]
$C_{22}H_{38}O_{12}S_3$ 590.733
Constit. of *Trachyopsis halichondroides*.

Makarieva, T.N. *et al., Steroids*, 1995, **60**, 316-320 (*isol, pmr, ms*)

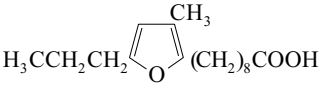
2-Methylpropanoic acid, 9CI M-459

Isobutyric acid, 8CI. FEMA 2222
[79-31-2]
$(H_3C)_2CHCOOH$
$C_4H_8O_2$ 88.106
The free acid and its esters occur in many plants. The acid is a pheromone in the rhesus monkey and the Mediterranean fruit fly. Present in apple, morello cherry, guava fruit, wine grapes, pineapple, crispbread, other breads, cheeses, wines, prawn, scallop, squid and several essential oils, e.g. Roman chamomile. Acid and simple esters used as flavouring agents. Liq. with pungent rancid odour. d_4^{15} 0.95.
Fp -47. Bp 153.5-154.5° Bp_{35} 118-119°. n_D^{20} 1.3930. pK_a 4.79 (4.85).
▶ Fl. p. 56°, autoignition temp. 481°. Corrosive and irritating to skin, eyes and mucous membranes. LD_{50} (rat, orl) 280 mg/kg. NQ4375000

[996-30-5]

Morita, K. *et al., J. Food Sci.*, 2002, **67**, 3456-3462 (*prawn, scallop, squid, gc*)

3-Methyl-5-propyl-2-furannonanoic acid M-460



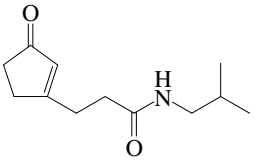
$C_{17}H_{28}O_3$ 280.406

Et ester:
$C_{19}H_{32}O_3$ 308.46
Isol. from the brown alga *Acrocarpia paniculata*. Viscous liq.

Kazlauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 165

N-(2-Methylpropyl)-3-(3-oxo-1-cyclopenten-1-yl)-propanamide M-461

[878633-76-2]

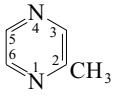


$C_{12}H_{19}NO_2$ 209.288
Prod. by *Streptomyces* sp. GT-20026114 isol. from the mangrove plant *Aegiceras comiculatum*. Amorph. powder. λ_{max} 242 (MeOH).

Lin, W. *et al., J. Antibiot.*, 2005, **58**, 594-598 (*isol, pmr, cmr*)

Methylpyrazine, 9CI, 8CI M-462

FEMA 3309
[109-08-0]



$C_5H_6N_2$ 94.116
Isol. from an arctic marine bacterium. Flavouring agent. Liq. with disagreeable picoline-like odour. Misc. H_2O, EtOH, Et_2O. d_4^{20} 1.03. Bp 136-137°. n_D^{20} 1.4953. pK_{a1} 1.41; pK_{a2} -4.89 (25°, H_2O).
▶ Emits highly toxic fumes when heated to dec. Flammable, fl. p. 50° (oc). UQ3675000

Picrate:
Yellow prisms (EtOH). Mp 133°.

Methiodide: [34260-05-4]
Leaflets and needles (EtOH). V. sol. H_2O. Mp 129-130°.

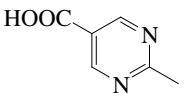
1-Oxide: [31396-35-7]
$C_5H_6N_2O$ 110.115
Mp 93-95°.

4-Oxide: [25594-37-0]
$C_5H_6N_2O$ 110.115
Mp 69-71°.

1,4-Dioxide: [32046-26-7]
$C_5H_6N_2O_2$ 126.115
Cryst. (MeOH). Mp 230-231°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 840A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 397C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1555D (*ir*)
Jones, R.G. *et al., J.A.C.S.*, 1950, **72**, 3539 (*synth*)
Kitchen, L.J. *et al., J.A.C.S.*, 1951, **73**, 1838 (*synth*)
Cox, R.H. *et al., J. Phys. Chem.*, 1968, **72**, 1646 (*pmr*)
Uchimaru, F. *et al., J. Het. Chem.*, 1971, **8**, 99 (*ms*)
Sanyal, N.K. *et al., J. Mol. Spectrosc.*, 1979, **78**, 335 (*uv*)
Matsuo, M. *et al., Org. Magn. Reson.*, 1980, **13**, 172 (*cmr*)
Gumbley, S.J. *et al., J. Het. Chem.*, 1985, **22**, 1143 (*props*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*marine isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MOW750

2-Methyl-5-pyrimidinecarboxylic acid M-463

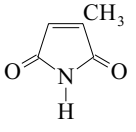


$C_6H_6N_2O_2$ 138.126

Methylamide: N,*2-Dimethyl-5-pyrimidinecarboxamide*
$C_7H_9N_3O$ 151.168
Prod. by an unidentified marine bacterium.
Laatsch, H. *et al., Dissertation*, Univ. of Göttingen, 2005,

3-Methyl-1*H*-pyrrole-2,5-dione, 9CI M-464

3-Methylmaleimide. Citraconimide, 8CI
[1072-87-3]



$C_5H_5NO_2$ 111.1
Prod. of chromic acid oxidation of tetrapyrroles. Cryst. (C_6H_6 or Et_2O/petrol). Mp 103-104° Mp 108° (107°). *N*-substituted derivs. undergo radical homo- and copolym.

5-Oxime: 3-Methylmaleimide 5-oxime
$C_5H_6N_2O_2$ 126.115
Isol. from the sponge *Pseudoceratina purpurea*. Cryst. (MeOH). Mp 170-172°.

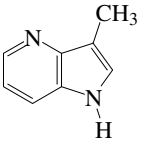
N-*Me: 1,3-Dimethyl-1*H-*pyrrole-2,5-dione, 9CI*
[4050-34-4]
$C_6H_7NO_2$ 125.127
Oil. Bp_{10} 86°. n_D^{26} 1.4970. *N*-Alkylcitraconimides polym. by a radical mechanism to give linear systems with the imide rings intact. Q/e values for radical polym., Q 0.87, e +1.59.

N-*Ph: 3-Methyl-1-phenyl-1*H-*pyrrole-2,5-dione, 9CI*
[3120-04-5]
$C_{11}H_9NO_2$ 187.198
Mp 99°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1454B (*nmr*)
Protopopescu, L. *et al., CA*, 1944, **38**, 3958h (*synth*)
Brown, P.M. *et al., J.C.S.*, 1957, 2882 (*synth*)
Sheremeteva, T.V. *et al., CA*, 1959, **53**, 4127h (*N-Me*)
Kojima, K. *et al., J. Polym. Sci., Part A*, 1966, **4**, 1121 (*synth*)
Sheremeteva, T.V. *et al., J. Polym. Sci., Part C*, 1967, **16**, 1631 (*polym, derivs*)
Ellsworth, R.K. *et al., Arch. Biochem. Biophys.*, 1968, **124**, 358
Chenon, M.T. *et al., J. Het. Chem.*, 1973, **10**, 427 (*cmr*)
Gossauer, A. *et al., Annalen*, 1974, 1496 (*synth*)
Hebenbrock, K.-F. *et al., Annalen*, 1978, 320 (*derivs*)
Earl, R.A. *et al., J. Het. Chem.*, 1978, **15**, 1479 (*synth, pmr, imide*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427 (*Q/e values, deriv*)
Pyriadi, T.M. *et al., J. Polym. Sci., Polym. Chem. Ed.*, 1980, **18**, 2535 (*derivs*)
Martin, J. *et al., Tetrahedron*, 1980, **36**, 3261 (*synth, ms*)
Oishi, T. *et al., Polym. J. (Tokyo)*, 1981, **13**, 65 (*polym, reactivity, derivs*)
Yogo, M. *et al., J.C.S. Perkin 1*, 1984, 2097 (*synth, ir, uv, pmr, imides*)
Bestmann, H.J. *et al., Chem. Ber.*, 1985, **118**, 2640 (*deriv*)
Otsu, T. *et al., Polym. Bull. (Berlin)*, 1990, **24**, 475 (*polym, derivs*)
Gill, G.B. *et al., J.C.S. Perkin 1*, 1993, 2567 (*synth, ir, pmr, cmr*)
Kijjoa, A. *et al., Z. Naturforsch., B*, 2005, **60**, 904-908 (*5-oxime, isol, pmr, cmr*)

3-Methyl-1*H*-pyrrolo[3,2-*b*]pyridine, 9CI M-465

4-Azaskatole
[25796-94-5]

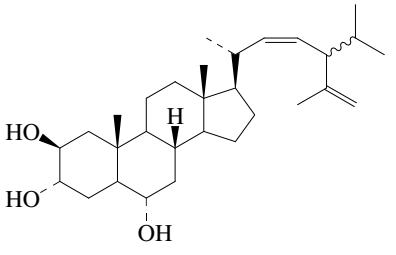


$C_8H_8N_2$ 132.165
Isol. from fish meal tar. Antifungal agent. Cryst. (C_6H_6).
Mp 228-230°. λ_{max} 225 (ϵ 21950); 292 (ϵ 6950) (MeOH) (Berdy).

Kelly, A.H. *et al., J.C.S.(C)*, 1970, 303-307 (*synth*)
Wakabayashi, K. *et al., Yakugaku Zasshi*, 1978, **98**, 898-903 (*isol*)
Fontan, R. *et al., Heterocycles*, 1981, **16**, 1473-1474 (*synth*)

28-Methylstigmasta-22,25-diene-2,3,6-triol M-466

24-Isopropylcholesta-22,25-diene-2,3,6-triol



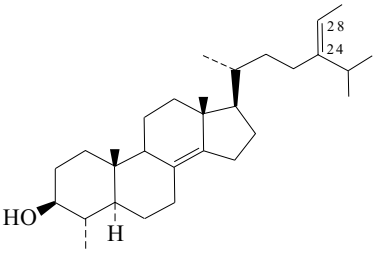
$C_{30}H_{50}O_3$ 458.723

(2β,3α,6α,22*Z*,24ξ)-*form*
Polasterol B
[290353-70-7]
Amorph. powder. Mp 131-141°. $[\alpha]_D^{21}$ -5.82 (c, 0.52 in MeOH).

2,3,6-Trisulfate: ***Polasterol B sulfate***
[290353-69-4]
$C_{30}H_{50}O_{12}S_3$ 698.916
Constit. of a Japanese *Epipolasis* sp. Amorph. powder.
Mp 185-187°. $[\alpha]_D^{21}$ +12.8 (c, 2.7 in MeOH).
Umeyama, A. *et al., J. Nat. Prod.*, 2000, **63**, 1175-1177 (*isol, pmr, cmr*)

4-Methylstigmasta-8(14),24(28)-dien-3-ol, 9CI M-467

24-Ethylidene-4-methylcholest-8(14)-en-3-ol



$C_{30}H_{50}O$ 426.724

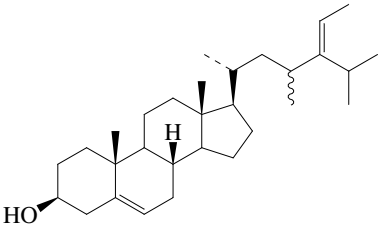
(3β,4α,5α,24*Z*)-*form* [78285-84-4]
Constit. of *Glenodinium* sp. and *Phaseolus vulgaris* (kidney bean).

[123086-81-7]

Kokke, W.C.M.C. *et al., Phytochemistry*, 1981, **20**, 127 (*isol*)
Akihisa, T. *et al., Phytochemistry*, 1989, **28**, 1219 (*isol*)

23-Methylstigmasta-5,24(28)-dien-3-ol M-468

24-Ethylidene-23-methylcholest-5-en-3-ol

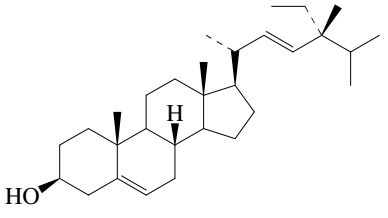


$C_{30}H_{50}O$ 426.724

(3β,23ξ,24(28)*Z*)-*form*
23-Methylisofucosterol
[81826-49-5]
Isol. from *Sinularia ramulosa* from the South China Sea.
Wu, Z. *et al., CA*, 1981, **96**, 214584z

24-Methylstigmasta-5,22-dien-3-ol M-469

24-Ethyl-24-methylcholesta-5,22-dien-3-ol



(3β,22*E*,24*R*)-*form*

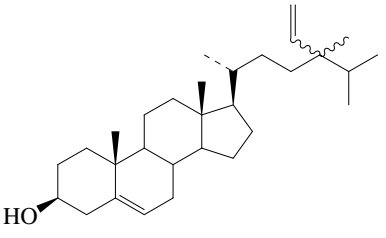
$C_{30}H_{50}O$ 426.724

(3β,22*E*,24*R*)-*form* [102054-46-6]
Constit. of a *Pseudaxinyssa* sp.

(3β,22*E*,24ξ)-*form* [709669-29-4]
Constit. of *Topsentia ophiraphidites.*
Cryst.
Mp 165-166.5°. $[\alpha]_D^{25}$ -45.4 (c, 0.3 in $CHCl_3$).
Tam Ha, T.B. *et al., Steroids*, 1985, **45**, 263-276 (*isol, pmr, ms*)
Calderón, G.J. *et al., Steroids*, 2004, **69**, 93-100 (*isol, pmr, cmr*)

24-Methylstigmasta-5,28-dien-3-ol M-470

24-Ethenyl-24-methylcholest-5-en-3-ol

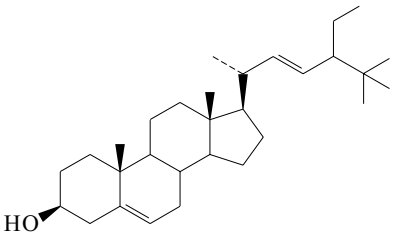


$C_{30}H_{50}O$ 426.724

(3β,24ξ)-*form* [90195-39-4]
Isol. from lipids of a unicellular marine alga.
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*isol, pmr*)

25-Methylstigmasta-5,22-dien-3-ol M-471

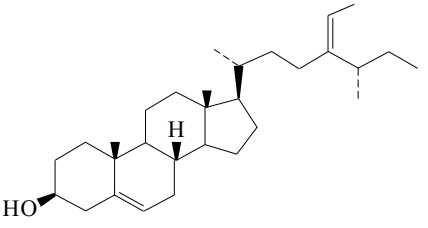
24-Ethyl-25-methylcholesta-5,22-dien-3-ol



$C_{30}H_{50}O$ 426.724

(3β,22*E*,24ξ)-*form* [94451-21-5]
Constit. of *Halichondria* spp. and *Trachyopsis aplysinoides.*
Cryst. (EtOAc).
Mp 166-168°. $[\alpha]_D^{20}$ -52 (c, 0.4 in $CHCl_3$).
Shubina, L.K. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 438-441; 1985, **21**, 676 (*isol*)

26-Methylstigmasta-5,24(28)-dien-3-ol M-472

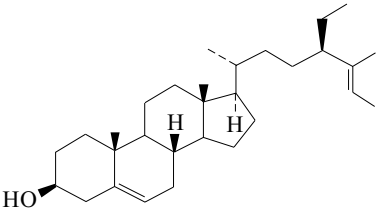


$C_{30}H_{50}O$ 426.724

(3β,24(28)*Z*,25*S*)-*form*
Isostelliferasterol
[69081-88-5]
Constit. of the sponge *Jaspis stellifera*.
Cryst. (MeOH aq.).
Mp 119-120°.
Theobald, N. *et al., J.A.C.S.*, 1978, **100**, 7677

26-Methylstigmasta-5,25-dien-3-ol M-473

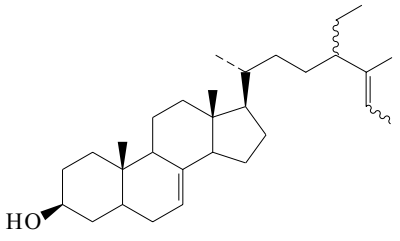
25-Ethylidene-27-norstigmast-5-en-3-ol. 24-Ethyl-26-methylcholesta-5,25-dien-3-ol



$C_{30}H_{50}O$ 426.724

(3β,24*R*,25*E*)-*form*
Stelliferasterol
[69081-87-4]
Constit. of *Jaspis stellifera*.
Cryst. (MeOH).
Mp 121-122°. $[\alpha]_D^{21}$ -37 ($CHCl_3$).
Theobald, N. *et al., J.A.C.S.*, 1978, **100**, 7677
Theobald, N. *et al., Tet. Lett.*, 1978, 4369 (*struct*)

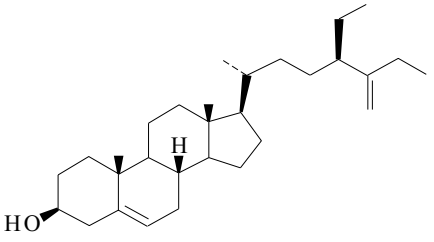
26-Methylstigmasta-7,25-dien-3-ol **M-474**
24-Ethyl-26-methylcholesta-7,25-dien-3-ol



$C_{30}H_{50}O$ 426.724

(3β,24ξ,25ξ)-*form*
Δ⁷-Stelliferasterol
[129620-24-2]
Constit. of a *Xestospongia* sp.
Kerr, R.G. *et al., J.O.C.*, 1991, **56**, 58 (*isol, pmr*)

27-Methylstigmasta-5,25-dien-3-ol **M-475**
25-Ethyl-27-norstigmasta-5,25-dien-3-ol, 9CI. 24-Ethyl-27-methylcholesta-5,25-dien-3-ol



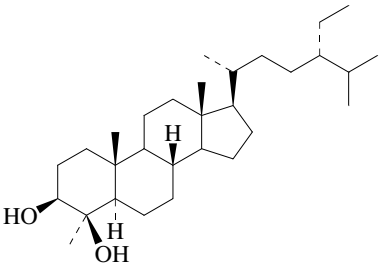
$C_{30}H_{50}O$ 426.724
Mp 112-112.5°.

(3β,24*R*)-*form*
Strongylosterol
[68671-48-7]
Constit. of the sponge *Strongylophora durissima*.
Cryst. (MeOH).
Mp 112-112.5°. $[\alpha]_D$ -43 (c, 0.39 in CH_2Cl_2).
Bartoletto, M. *et al., Bull. Soc. Chim. Belg.*, 1978, **87**, 539-543 (*isol*)
Theobald, N. *et al., Tet. Lett.*, 1978, 4369-4372 (*isol*)
Stoilov, I.L. *et al., J.A.C.S.*, 1986, **108**, 8235-8241 (*biosynth*)

25-Methylstigmasta-5,24(28)-dien-3-ol **M-476**
24-Ethylidene-25-methylcholest-5-en-3-ol
$C_{30}H_{50}O$ 426.724

(3β,24*E*)-*form*
25-Methylfucosterol
[86105-64-8]
Constit. of the sponge *Pseudaxinyssa* sp.
Li, X. *et al., Tet. Lett.*, 1983, **24**, 665-668 (*isol, synth*)

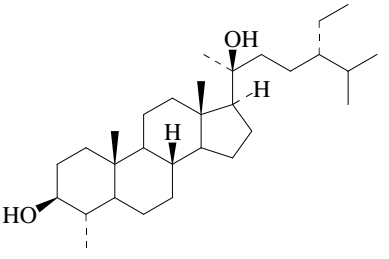
4-Methylstigmastane-3,4-diol **M-477**
24-Ethyl-4-methylcholestane-3,4-diol



$C_{30}H_{54}O_2$ 446.755

(3β,4β*OH*,5α,24*S*)-*form*
Ethylpavlovol
[150994-75-5]
Isol. from *Pavlova gyrans* and *Pavlova lutheri*.
Patterson, G.W. *et al., Lipids*, 1993, **28**, 771-773 (*isol, pmr, cmr*)

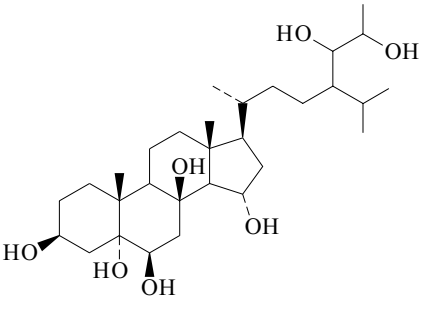
4-Methylstigmastane-3,20-diol **M-478**



$C_{30}H_{54}O_2$ 446.755

(3β,4α,20*S*,24*S*)-*form* [874383-70-7]
Constit. of a *Diacronema* sp.
Cryst.
Mp 221-222°.
Rauter, A.P. *et al., Fitoterapia*, 2005, **76**, 433-438 (*Diacronema constit*)

29-Methylstigmastane-3,5,6,8,15,28,29-heptol **M-479**
24-(1,2-Dihydroxypropyl)cholestane-3,5,6,8,15-pentol

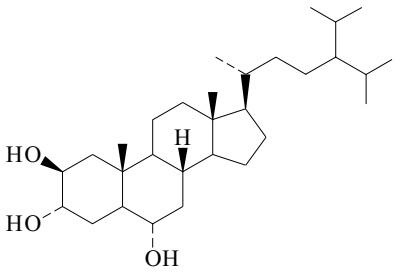


$C_{30}H_{54}O_7$ 526.752

(3β,5α,6β,8β,15α,24ξ,28ξ,29ξ)-*form* [162442-08-2]
Constit. of *Ctenodiscus crispatus*.
Amorph. $[\alpha]_D$ +29.3 (c, 0.5 in MeOH).
Kicha, A.A. *et al., Izv. Akad. Nauk, Ser. Khim.*, 1994, **43**, 1821; *Russ. Chem. Bull. (Engl. Transl.)*, 1994, **43**, 1726 (*isol, pmr, cmr*)

28-Methylstigmastane-2,3,6-triol M-480

24-Isopropylcholestane-2,3,6-triol



$C_{30}H_{54}O_3$ 462.755

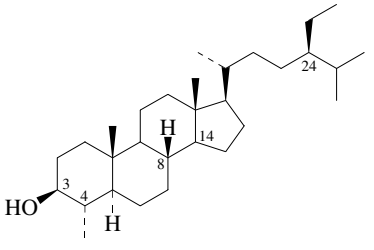
(2β,3α,5α,6α)-*form*

Trisulfate: [163815-34-7]
$C_{30}H_{54}O_{12}S_3$ 702.947
Constit. of *Trachyopsis halichondroides* and *Cymbastela coralliophila*.

Makarieva, T.N. *et al., Steroids*, 1995, **60**, 316-320 (*isol, pmr, ms*)

4-Methylstigmastan-3-ol M-481

24-Ethyl-4-methylcholestan-3-ol



(3β,4α,5α,24*R*-*form*

$C_{30}H_{54}O$ 430.756

(3β,4α,5α,24*R*)-*form*

Citrostanol
[474-39-5]
Isol. from *Glenodinium* sp., *Noctiluca milialis* and *Zooxanthella microadriatica*.
Cryst. (MeOH/petrol).
Mp 186-187°. $[\alpha]_D$ +28 ($CHCl_3$).

8,14-Didehydro: ***4-Methylstigmast-8(14)-en-3-ol***. *24-Ethyl-4-methylcholest-8(14)-en-3-ol*
[31893-35-3]
$C_{30}H_{52}O$ 428.74
Constit. of *Glenodinium* sp.

(3β,4α,5α,24*S*)-*form*

4-Methylporiferastan-3-ol
[80925-07-1]
Constit. of *Muriceopsis flavida*, *Briareum asbestinum* and *Zooxanthella microadriatica*.
Cryst. (MeOH).
Mp 178-181°. $[\alpha]_D$ +19 (c, 0.3 in $CHCl_3$).

8,14-Didehydro: [80925-08-2]
Constit. of *Briareum asbestinum*.

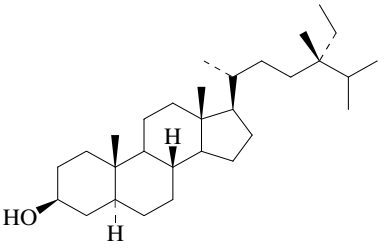
(3β,4α,5α,24ξ)-*form*

Tetrahydro-α_1-sitosterol
[76250-38-9]
[58560-39-7]
Isol. from scallop *Patinopecten yessoensis* and from *Ascidia nigra* and *Glenodinium* sp.

Mazur, Y. *et al., J.A.C.S.*, 1958, **80**, 6293-6296 (*Citrostanol, synth*)
Knapp, F.F *et al., Steroids*, 1975, **26**, 339-357 (*Citrostanol, synth*)
Kobayashi, M. *et al., Steroids*, 1975, **26**, 605 (*Tetrahydro-α_1-sitosterol*)
Kokke, W.C.M.C. *et al., Phytochemistry*, 1981, **20**, 127-134 (*isol, pmr, ms*)
Bohlin, L. *et al., Phytochemistry*, 1981, **20**, 2397-2401 (*Briareum asbestinum constits*)
Tam, H. *et al., Steroids*, 1982, **40**, 433-453 (*isol, Ascidia*)
Stoilov, I. *et al., J.O.C.*, 1993, **58**, 3444-3454 (*Citrostanol, synth, pmr, cmr*)

24-Methylstigmastan-3-ol M-482

24-Ethyl-24-methylcholestan-3-ol. 24-Ethylergostan-3-ol



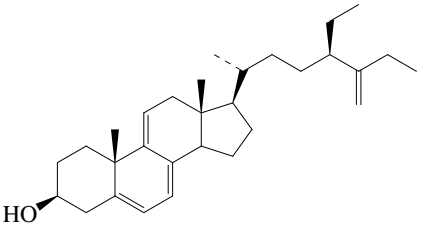
$C_{30}H_{54}O$ 430.756

(3β,5α,24*S*)-*form* [102054-47-7]
Constit. of a *Pseudaxinyssa* sp.

Tam Ha, T.B. *et al., Steroids*, 1985, **45**, 263-276 (*isol, pmr, ms*)
Giner, J.-L. *et al., J.O.C.*, 1988, **53**, 5895-5902 (*synth, pmr, ms*)

27-Methylstigmasta-5,7,9(11),25-tetraen-3-ol M-483

24-Ethyl-27-methylcholesta-5,7,9(11),25-tetraen-3-ol, 9CI



$C_{30}H_{46}O$ 422.693

(3β,24*R*)-*form*

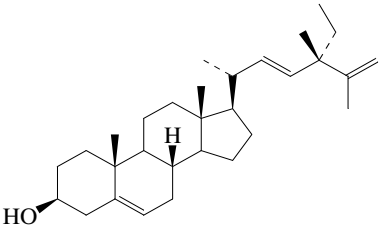
7,8,9,11-Tetradehydrostrongylosterol
[81306-59-4]
Constit. of the sponge *Strongylophora durissima*.

9,11-Dihydro: 24-Ethyl-27-methylcholesta-5,7,25-trien-3-ol, 9CI. 27-Methylstigmasta-5,7,25-trien-3-ol. ***7,8-Didehydrostrongylosterol***
[81306-58-3]
$C_{30}H_{48}O$ 424.709
Constit. of *Strongylophora durissima*.

Li, L.N. *et al., Tet. Lett.*, 1981, **22**, 4639-4642 (*isol*)

24-Methylstigmasta-5,22,25-trien-3-ol M-484

24-Ethyl-24-methylcholesta-5,22,25-trien-3-ol



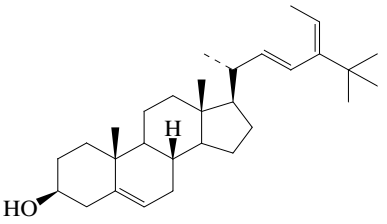
$C_{30}H_{48}O$ 424.709

(3β,22*E*,24*S*)-*form* [102054-48-8]
Constit. of a *Pseudaxinyssa* sp.

Tam Ha, T.B. *et al., Steroids*, 1985, **45**, 263-276 (*isol, pmr, ms*)

25-Methylstigmasta-5,22,24(28)-trien-3-ol M-485

24-Ethylidene-25-methylcholesta-5,22-dien-3-ol

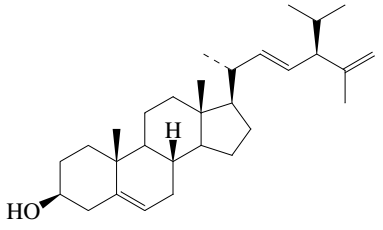


$C_{30}H_{48}O$ 424.709

(3β,22*E*,24*E*)-*form* [102054-49-9]
Constit. of a *Pseudaxinyssa* sp.
Tam Ha, T.B. *et al., Steroids*, 1985, **45**, 263-276 (*isol*)

28-Methylstigmasta-5,22,25-trien-3-ol M-486

24-Isopropylcholesta-5,22,25-trien-3-ol. 24-Isopropenylcholesta-5,22-dien-3-ol



(2β,22*E*,24*R*)-*form*

$C_{30}H_{48}O$ 424.709

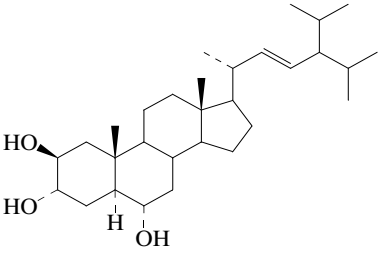
(3β,22*E*,24*R*)-*form* [102130-58-5]
Constit. of *Pseudaxinyssa* sp. and *Topsentia ophiraphidites.*
Plates (MeOH).
Mp 150-152°. $[\alpha]_D^{25}$ -41.7 (c, 2.6 in $CHCl_3$).

(3β,22*E*,24*S*)-*form* [102130-59-6]
Constit. of a *Pseudaxinyssa* sp.
Needles (MeOH).
Mp 174-176°. $[\alpha]_D^{25}$ -46.3 (c, 2.1 in $CHCl_3$).

(3β,22*E*,24ξ)-*form*
Nervisterol
[81262-96-6]
Constit. of *Nervilia purpurea* and *Cordyceps sinensis.*
Needles (MeOH).
Mp 175-177°. $[\alpha]_D^{24}$ -47.9 (c, 0.19 in $CHCl_3$).
Ac:
Cryst. Mp 187-189°. $[\alpha]_D$ -55.2 ($CHCl_3$).
Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1982, **30**, 370; 1985, **33**, 2235-2242 (*Nervisterol*)
Tam Ha, T.B. *et al., Steroids*, 1985, **45**, 263-265 (*Pseudaxinyssa constits*)
Echigo, S. *et al., Chem. Pharm. Bull.*, 2006, **54**, 1473-1477 (*synth, pmr, cmr*)

28-Methylstigmast-22-ene-2,3,6-triol M-487

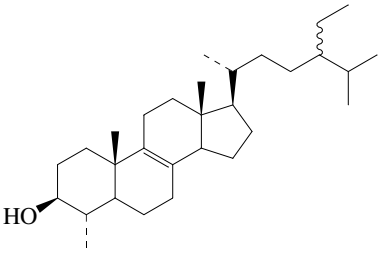
24-Isopropylcholest-22-ene-2,3,6-triol



$C_{30}H_{52}O_3$ 460.739

(2β,3α,5α,6α,22*E*)-*form*
Trisulfate: [109023-42-9]
$C_{30}H_{52}O_{12}S_3$ 700.932
Constit. of *Trachyopsis halichondroides.*
Makarieva, T.N. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 93-96 (*isol, struct*)

4-Methylstigmast-8-en-3-ol M-488

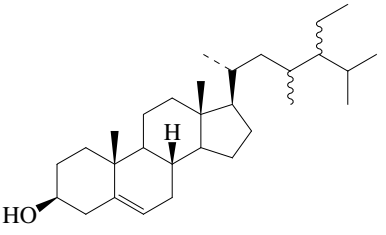


$C_{30}H_{52}O$ 428.74

(3β,4α,24ξ)-*form* [117142-14-0]
Constit. of *Agelas dispar.*
Carballeira, N.M. *et al., Biochem. Syst. Ecol.*, 1988, **16**, 421-424 (*isol, pmr*)

23-Methylstigmast-5-en-3-ol M-489

24-Ethyl-23-methylcholest-5-en-3-ol

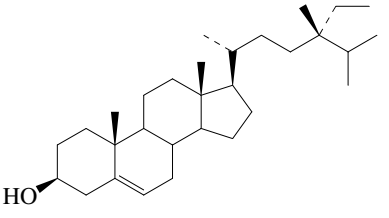


$C_{30}H_{52}O$ 428.74

(3β,23ξ,24ξ)-*form* [254441-51-5]
Minor sterol from dinoflagellate *Prorocentrum micans.*
5α,6-Dihydro: ***23-Methylstigmastan-3-ol****. 24-Ethyl-23-methylcholestan-3-ol*
[254441-52-6]
$C_{30}H_{54}O$ 430.756
Minor sterol from *Prorocentrum micans.*
Volkman, J.K. *et al., Phytochemistry*, 1999, **52**, 659-668

24-Methylstigmast-5-en-3-ol M-490

24-Ethylergost-5-en-3-ol. 24-Ethyl-24-methylcholest-5-en-3-ol



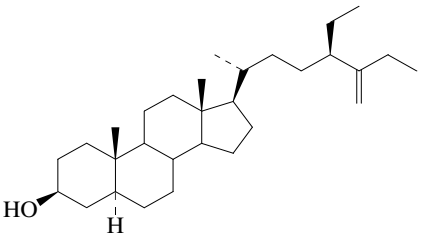
(3β,24*S*)-*form*

$C_{30}H_{52}O$ 428.74

(3β,24*S*)-*form*
24-Ethyl-24-methylcholesterol
[86105-65-9]
Constit. of sponge *Pseudaxinyssa* sp.
Li, X. *et al., Tet. Lett.*, 1983, **24**, 665-668 (*isol, synth, pmr*)
Tam Ha, T.B. *et al., Steroids*, 1985, **45**, 263-276 (*isol*)

27-Methylstigmast-25-en-3-ol M-491

24-Ethyl-27-methylcholest-25-en-3-ol, 9CI



$C_{30}H_{52}O$ 428.74

(3β,5α,24*R*)-*form*

Strongylostanol

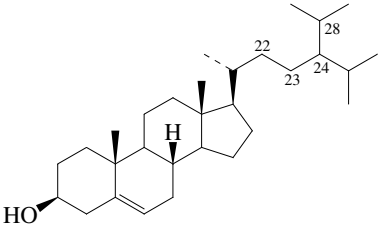
[81306-60-7]

Constit. of the sponge *Strongylophora durissima*.

Li, L.N. *et al., Tet. Lett.*, 1981, **22**, 4639-4642 (*isol*)

28-Methylstigmast-5-en-3-ol M-492

24-Isopropylcholest-5-en-3-ol



$C_{30}H_{52}O$ 428.74

3β-*form*

24-Isopropylcholesterol

[71885-20-6]

Constit. of *Pseudaxinyssa* sp.

Cryst. (MeOH).

Mp 135-136°. $[\alpha]_D^{19}$ -41 (c, 0.17 in $CHCl_3$).

*22,23-Didehydro (*E-*): 24-Isopropylcholesta-5,22-dien-3-ol*

[71497-03-5]

$C_{30}H_{50}O$ 426.724

Constit. of *Pseudaxinyssa* sp. Gum; cryst. (EtOAc)(as Ac).

Mp 123-125° (Ac). $[\alpha]_D^{20}$ -62 (c, 0.5 in $CHCl_3$) (Ac).

*22,23-Didehydro (*Z-*):*

$C_{30}H_{50}O$ 426.724

Metab. of a *Halichondria* sp.

24,28-Didehydro: ***24-Isopropylidenecholest-5-en-3-ol***

$C_{30}H_{50}O$ 426.724

Constit. of *Verongia cauliformis*. Cryst. (MeOH).

Mp 123-124°.

*28,29-Didehydro (24*S-*): 24-Isopropenylcholest-5-en-3-ol.* ***24-Isopropenylcholesterol***

$C_{30}H_{50}O$ 426.724

Constit. of *Nervilia purpurea*. Cryst. (MeOH).

Mp 135-135.3°. $[\alpha]_D$ -39.8 (c, 0.44 in $CHCl_3$).

*28,29-Didehydro (24*R-*):*

$C_{30}H_{50}O$ 426.724

Occurs in *Verongia cauliformis*. Cryst. (MeOH).

Mp 141-142°. $[\alpha]_D$ -38.8 (c, 0.4 in $CHCl_3$). Isol. as epimeric mixt. with 24*S*-form.

Hofheinz, W. *et al., Helv. Chim. Acta*, 1979, **62**, 1307 (*isol*)

Kokke, W.C.M.C. *et al., Helv. Chim. Acta*, 1979, **62**, 1310 (*isol, synth*)

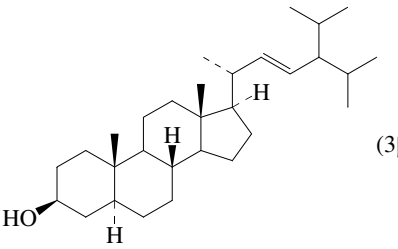
Shubina, L.K. *et al., Khim. Prir. Soedin.*, 1985, **21**, 232; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 217 (*isol*)

Kikuchi, T. *et al., Tet. Lett.*, 1985, **26**, 3817 (*synth*)

Kadota, S. *et al., Chem. Pharm. Bull.*, 1987, **35**, 200 (*isol, abs config*)

28-Methylstigmast-22-en-3-ol M-493

24-Isopropylcholest-22-en-3-ol



(3β,5α,22*E*)-*form*

$C_{30}H_{52}O$ 428.74

(3β,5α,22*E*)-*form* [76836-17-4]

Constit. of *Porifera* spp.

(3β,5α,22*Z*)-*form* [128657-74-9]

[97510582- A-c]

Metab. of a *Halichondria* sp.

Cryst. (EtOAc)(as Ac).

Mp 153-155° (Ac). $[\alpha]_D^{20}$ -20 (c, 0.2 in $CHCl_3$) (Ac).

22,23-Dihydro: 28-Methylstigmastan-3-ol. 24-Isopropylcholestan-3-ol

[102054-45-5]

$C_{30}H_{54}O$ 430.756

Constit. of a *Pseudaxinyssa* sp.

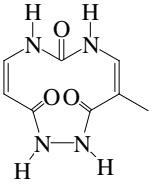
Bergquist, P.R. *et al., Biochem. Syst. Ecol.*, 1980, **8**, 423-435 (*22E-form, occur*)

Shubina, L.K. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 217-223 (*22Z-form, isol*)

Tam Ha, T.B. *et al., Steroids*, 1985, **45**, 263-276 (*isol, Pseudaxinyssa*)

4-Methyl-1,2,6,8-tetraazacycloundeca-4,9-diene-3,7,11-trione, 9CI M-494

[246167-60-2]



$C_8H_{10}N_4O_3$ 210.192

Isol. from the marine brown alga *Sargassum vachellianum*. Cryst. (MeOH).

Mp 228-230°.

Xu, S.H. *et al., Chin. Chem. Lett.*, 1999, **10**, 401-402

22-Methyl-5,9-tetracosadienoic acid M-495

$H_3CCH_2CH(CH_3)(CH_2)_{11}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$

$C_{25}H_{46}O_2$ 378.637

(5*Z*,9*Z*,22ξ)-*form*

Isol. from the sponge *Geodinella robusta*. Cytotoxic.

Makarieva, T.N. *et al., Lipids*, 2002, **37**, 75-80 (*isol, pmr, cmr, ms*)

23-Methyl-5,9-tetracosadienoic acid M-496

$(H_3C)_2CH(CH_2)_{12}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$

$C_{25}H_{46}O_2$ 378.637

(*Z*,*Z*)-*form* [140245-76-7]

Isol. from the sponges *Geodinella robusta*, *Pseudaxinella lunaecharta*, *Cinachyrella schulzei*, *Dysidea fragilis* and *Ircinia* spp.

Carballeira, N.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **100**, 489-492 (*isol*)

Makarieva, T.N. *et al., Lipids*, 2002, **37**, 75-80 (*isol*)

17-Methyltetracosanoic acid M-497

$H_3C(CH_2)_6CH(CH_3)(CH_2)_{15}COOH$

$C_{25}H_{50}O_2$ 382.669

(ξ)-*form*

Isol. from sponge *Cinachyrella kükenthali*.

Barnathan, G. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2003, **135**, 297-308 (*isol, ms*)

18-Methyltetracosanoic acid M-498

$H_3C(CH_2)_5CH(CH_3)(CH_2)_{16}COOH$

$C_{25}H_{50}O_2$ 382.669

(ξ)-*form*

Constit. of the sponge *Cinachyrella alloclada*.

Barnathan, G. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 2003, **135**, 297-308 (*isol, ms*)

19-Methyltetracosanoic acid M-499

[93673-91-7]

$H_3C(CH_2)_4CH(CH_3)(CH_2)_{17}COOH$

$C_{25}H_{50}O_2$ 382.669

(ξ)-*form*

Isol. from sponge *Strongylophora durissima*.

Dasgupta, A. *et al., Lipids*, 1984, **19**, 768-776 (*isol*)

2-Methyl-17-tetracosenoic acid M-500

[774608-84-3]

$H_3C(CH_2)_5CH{=}CH(CH_2)_{14}CH(CH_3)COOH$

$C_{25}H_{48}O_2$ 380.653

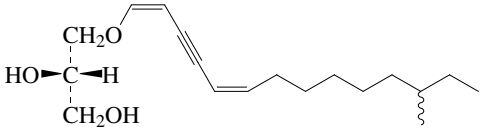
(2ξ,17*Z*)-*form*

Isol. from the marine sponge *Halichondria panicea*.

Imbs, A.B. *et al., Chem. Phys. Lipids*, 2004, **129**, 173-181 (*isol, pmr, ms*)

3-(12-Methyl-1,5-tetradecadien-3-ynyloxy)-1,2-propanediol M-501

Glycerol 1-(12-methyl-1,5-tetradecadien-3-ynyl) ether



$C_{18}H_{30}O_3$ 294.433

(*S*,1′*Z*,5′*Z*,12′ξ)-*form*

Petroraspailyne A₃

[219917-16-5]

Isol. from a *Petrosia* sp.

$[\alpha]_D^{28}$ +2.6 (c, 0.05 in MeOH). λ_{max} 276 (log ϵ 3.92); 290 (log ϵ 3.74) (MeOH).

Seo, Y. *et al., J. Nat. Prod.*, 1999, **62**, 122-126

7-Methyltetradecane M-502

[6165-39-5]

[55194-68-8]

$H_3C(CH_2)_6CH(CH_3)(CH_2)_5CH_3$

$C_{15}H_{32}$ 212.418

Constit. of *Lilium lancifolium* and *Zoanthus* sp. Also found in the Dufour gland of the ant *Pogonomyrmex salinus*. (*S*)-enantiomer has been synthesised.

(±)-*form*

Bp_{10} 130°.

Petrov, A.A. *et al., CA*, 1960, **54**, 1257d (*synth*)
Schlenk, K. *et al., Annalen*, 1973, 1179 (*synth*)
Kameoka, H. *et al., Dev. Food Sci.*, 1988, **18**, 469 (*isol*)
Nascimento, R.R. *et al., J. Chem. Ecol.*, 1993, **19**, 1993 (*isol*)
Babu, U.V. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 627 (*isol*)

11-Methyltetradecanoic acid M-503

[17001-20-6]

$H_3CCH_2CH_2CH(CH_3)(CH_2)_9COOH$

$C_{15}H_{30}O_2$ 242.401

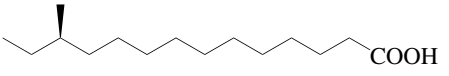
Isol. from the fish oils of *Brevoortia tyrannus* and *Oncorhynchus nerka*.

Ratnayake, W.M.N. *et al., Lipids*, 1989, **24**, 630 (*isol*)

12-Methyltetradecanoic acid M-504

Anteisopentadecanoic acid. ***Sarcinic acid***. *Aseanostatin P5*

[5502-94-3]



(*R*)-*form*

$C_{15}H_{30}O_2$ 242.401

(*R*)-*form* [73711-59-8]

Mp 24.2°. $[\alpha]_D^{22}$ -5.8 (c, 2 in $CHCl_3$).

Me ester: [162610-53-9]

$C_{16}H_{32}O_2$ 256.428

Bp_4 128°. $[\alpha]_D^{22}$ -5.6 (c, 2 in $CHCl_3$).

(*S*)-*form* [5746-58-7]

Isol. from *Bacillus* sp., *Sarcina* phospholipids and other microbial lipids. β-Lactamase inhibitor. Liq.

Mp 23.7°. $[\alpha]_D^{21}$ +5.4 (c, 0.9 in $CHCl_3$).

Me ester: [62691-05-8]

Bp_3 130°. $[\alpha]_D^{21}$ +5.1 (c, 2 in $CHCl_3$).

(±)-*form* [73679-18-2]

Liq. Mp 24-26°. n_D^{20} 1.4580.

(ξ)-*form*

Found in fish oils.

[135096-46-7]

Akashi, S. *et al., J. Biochem. (Tokyo)*, 1960, **47**, 222 (*isol*)
Song, Y. *et al., J. Antibiot.*, 1981, **34**, 980 (*isol, props, bibl*)
Omura, S. *et al., J. Antibiot.*, 1986, **39**, 1180 (*Aggreceride A*)
Carballeira, N. *et al., J.O.C.*, 1986, **51**, 2751 (*synth*)
Ishida-Okawara, A. *et al., J. Antibiot.*, 1991, **44**, 524 (*Aseanostatin*)
Kitahara, T. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 78 (*synth, ir, pmr, cmr, abs config*)
Biermann, U. *et al., J.A.C.S.*, 2004, **126**, 10319-10330 (*synth, pmr, cmr*)

13-Methyltetradecanoic acid, 9CI M-505

Subtilopentadecanoic acid. Aseanostatin P6

[2485-71-4]

$(H_3C)_2CH(CH_2)_{11}COOH$

$C_{15}H_{30}O_2$ 242.401

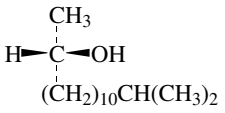
Occurs widely in nature esp. bacteria. Myeloperoxydase release inhibitor. Cryst. (Me_2CO).

Mp 52.5-53°.

[5129-59-9, 64317-63-1]

Saito, K. *et al., J. Biochem. (Tokyo)*, 1960, **47**, 710 (*isol*)
Klein, R.A. *et al., Lipids*, 1980, **15**, 572 (*synth, use*)
Ratnayake, W.M.N. *et al., Lipids*, 1989, **24**, 630-637 (*occur, fish*)
Ishida-Okawara, A. *et al., J. Antibiot.*, 1991, **44**, 524-532 (*Aseanostatin P6*)
Grzeszczyk, B. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1992, **66**, 1627-1632 (*synth*)
Foglia, T.A. *et al., Org. Prep. Proced. Int.*, 1993, **25**, 209 (*synth*)
Shiori, T. *et al., Tetrahedron*, 1998, **54**, 15701-15710 (*synth*)

13-Methyl-2-tetradecanol M-506



$C_{15}H_{32}O$ 228.417

(*S*)-*form*
Prod. by a marine bacterium.
$[\alpha]_D^{27}$ +4.8 (c, 3 in pentane).
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol, synth, pmr, cmr, ms*)

12-Methyl-2-tetradecanone M-507

$H_3CCH_2CH(CH_3)(CH_2)_9COCH_3$
$C_{15}H_{30}O$ 226.401

(ξ)-*form*
Prod. by a marine bacterium.
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol*)

12-Methyl-3-tetradecanone M-508

$H_3CCH_2CH(CH_3)(CH_2)_8COCH_2CH_3$
$C_{15}H_{30}O$ 226.401

(ξ)-*form*
Prod. by a marine bacterium.
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol*)

5-Methyl-4-tetradecenoic acid M-509

[56796-90-8]
$H_3C(CH_2)_8C(CH_3)=CHCH_2CH_2COOH$
$C_{15}H_{28}O_2$ 240.385
Constit. of oil of sperm whale *Physeter catodon* and lipids of *Oncorhynchus nerka* f. *adonis* and *Acanthodiaptomus pacificus.*
Pascal, J.C. *et al., Lipids*, 1975, **10**, 478-482 (*isol, glc, ms, occur*)
Ota, T. *et al., CA*, 1982, **98**, 70513 (*occur*)

13-Methyl-4-tetradecenoic acid M-510

$(H_3C)_2CH(CH_2)_7CH=CHCH_2CH_2COOH$
$C_{15}H_{28}O_2$ 240.385

(*Z*)-*form* [136194-85-9]
Isol. from *Flavobacterium* spp. and Halomonadaceae. Also from *Callyspongia fallax*.
Skerratt, J.H. *et al., Syst. Appl. Microbiol.*, 1991, **14**, 8 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*isol*)

13-Methyl-7-tetradecenoic acid M-511

$(H_3C)_2CH(CH_2)_4CH=CH(CH_2)_5COOH$
$C_{15}H_{28}O_2$ 240.385

(*Z*)-*form* [88505-44-6]
Isol. from the sponge *Callyspongia fallax*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623

13-Methyl-9-tetradecenoic acid M-512

$(H_3C)_2CHCH_2CH_2CH=CH(CH_2)_7COOH$
$C_{15}H_{28}O_2$ 240.385

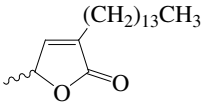
(*Z*)-*form* [104364-12-7]
Isol. from the sponge *Callyspongia fallax*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623

13-Methyl-8-tetradecen-2-one M-513

$(H_3C)_2CH(CH_2)_3CH=CH(CH_2)_5COCH_3$
$C_{15}H_{28}O$ 224.386

(*Z*)-*form*
Prod. by a marine bacterium.
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol, synth, pmr, cmr, ms*)

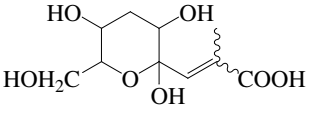
5-Methyl-3-tetradecyl-2(5*H*)-furanone M-514
Hateramine



$C_{19}H_{34}O_2$ 294.476

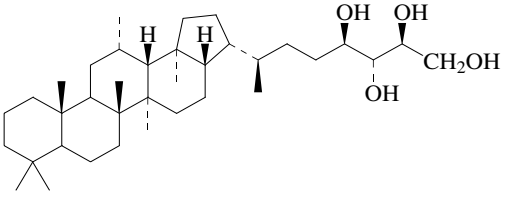
(ξ)-*form* [157611-53-5]
Isol. from an unidentified sponge. Biofilm formation accelerator.
Yamada, A. *et al., CA*, 1996, **124**, 225716s

2-Methyl-3-(tetrahydro-2,3,5-trihydroxy-6-hydroxymethyl-2*H*-pyran-2-yl)-2-propenoic acid M-515



$C_{10}H_{16}O_7$ 248.232
Isol. from *Mycale mytilorum*. Needles (EtOAc/MeOH).
Mp 191-193°. $[\alpha]_D^{28}$ +26.3 (c, 0.3 in MeOH). λ_{max} 219 (ε 9500) (EtOH).
Reddy, G.B.S. *et al., Bioorg. Med. Chem.*, 2000, **8**, 27-36

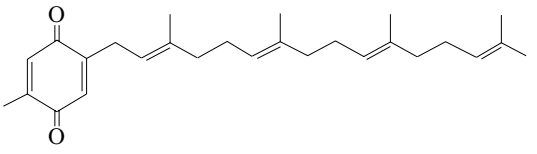
12-Methyl-29-(2,3,4,5-tetrahydroxypentyl)hopane M-516
12-Methylbacteriohopanetriol



$C_{36}H_{64}O_4$ 560.899

(12α,32*R*,33*R*,34*S*)-*form* [287203-63-8]
Constit. of *Plakortis simplex*.
Powder. $[\alpha]_D$ +7 (c, 0.5 in $CHCl_3$).
Costantino, V. *et al., Tetrahedron*, 2000, **56**, 3781-3784 (*isol, pmr, cmr*)

5-Methyl-2-(3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)-1,4-benzoquinone M-517
2-Geranylgeranyl-5-methyl-1,4-benzoquinone. 5-Methyl-2-tetraprenyl-p-*benzoquinone. Tetraprenyl*-p-*toluquinone*
[81010-86-8]



$C_{27}H_{38}O_2$ 394.596

Found in the gorgonian *Plexaura flava*, and a *Nephthea* sp. of soft coral. Yellow oil. λ_{max} 267 (ϵ 19500) (hexane) (Derep). λ_{max} 265 (ϵ 19000) (MeOH) (Derep).

Hydroquinone: 5-Methyl-2-(3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)-1,4-benzenediol. 2-Geranylgeranyl-5-methylhydroquinone
$C_{27}H_{40}O_2$ 396.612
Constit. of a *Nephthea* sp. Oil.

Hydroquinone, 4-O-β-D-arabinopyranoside: ***Nephthoside***
[172998-31-1]
$C_{32}H_{48}O_6$ 528.728
Constit. of a *Nephthea* sp. Oil. $[\alpha]_D$ -114.3 (c, 3.3 in $CHCl_3$).

Hydroquinone, 4-O-(4-O-acetyl-β-D-arabinopyranoside):
4″-O-Acetylnephthoside
[172923-10-3]
$C_{34}H_{50}O_7$ 570.765
Constit. of a *Nephthea* sp. Oil. $[\alpha]_D$ -83.3 (c, 1.2 in $CHCl_3$).

Bowden, B.F. *et al., Aust. J. Chem.*, 1981, **34**, 2677 (*isol, struct*)
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 105 (*isol, struct*)
Koren-Goldshlager, G. *et al., J. Nat. Prod.*, 1996, **59**, 262 (*Nephthoside, Acetylnephthoside*)

3-(Methylthio)propanoic acid, 9CI M-518

[646-01-5]

$MeSCH_2CH_2COOH$

$C_4H_8O_2S$ 120.172

Prod. by *Enterobacter intermedium* 60-2G, *Xanthomonas campestris* and marine bacterium strain He159b. Antifungal agent. Phytotoxin. Pale yellow oil or flaky solid (hexane).
Mp 20.5-21.5°. Bp_{13} 131-133°.

S,S-*Dioxide: 3-(Methylsulfonyl)propanoic acid, 9CI*
[645-83-0]
$C_4H_8O_4S$ 152.171
Cryst. ($CHCl_3$/Me_2CO). Mp 102-105°.

▶ UA2474200

Me ester: FEMA 2720
[13532-18-8]
$C_5H_{10}O_2S$ 134.199
Isol. from pineapple (*Ananas comosus*), melon and naranjila fruit (*Solanum quitoense*). Flavouring ingredient. Oil with sweet pineapple flavour at high dilutions. Bp 170-180° Bp_{100} 106-108°.

Me ester, S,S-*dioxide:* [89211-37-0]
$C_5H_{10}O_4S$ 166.198
Cryst. (EtOH aq.). Mp 94-94.6°.

Et ester: FEMA 3343
[13327-56-5]
$C_6H_{12}O_2S$ 148.226
Isol. from pineapple (*Ananas comosus*), melon, passion fruit and other fruits. Flavouring ingredient. Oil. Bp_{18} 88°.

Et ester, S-*oxide, (±)-:* [52754-04-8]
$C_6H_{12}O_3S$ 164.225
Liq.

Et ester, S,S-*dioxide:* [118675-14-2]
$C_6H_{12}O_4S$ 180.224
Cryst. (EtOH). Mp 68-69°.

[14090-35-8, 71922-81-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 670C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1064C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 729C (*ir*)
Haagen-Smit, A.J. *et al., J.A.C.S.*, 1945, **67**, 1646-1650; 1651-1652 (*isol, synth*)
Adlerová, E. *et al., Coll. Czech. Chem. Comm.*, 1959, **24**, 1208 (*synth*)
Gundermann, K.D. *et al., Chem. Ber.*, 1962, **95**, 2191-2194 (*dioxide, synth*)
Connell, D.W. *et al., Aust. J. Chem.*, 1964, **17**, 130-140 (*occur*)
Rodin, J.O. *et al., J. Food Sci.*, 1966, **31**, 721-725; *CA*, **65**, 19225d (*isol*)
Langler, R.F. *et al., Can. J. Chem.*, 1979, **57**, 3193-3199 (*Me ester, ir, pmr, ms*)
Perraux, D. *et al., Physiol. Plant Pathol.*, 1982, **20**, 313-319 (*isol*)
Doi, J.T. *et al., J.O.C.*, 1986, **51**, 1026-1029 (*synth, pmr*)
Cadamuro, S. *et al., Synthesis*, 1986, 1070-1073 (*synth*)
Hwu, J.R. *et al., J.C.S. Perkin 1*, 1991, 3199-3206 (*dioxide esters, synth, ir, pmr, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1018; 1801 (*esters, use, occur*)
Kim, Y.C. *et al., J. Antibiot.*, 2003, **56**, 177-180 (*isol, pmr, cmr, ms*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)

3-(Methylthio)propylamine, 8CI M-519

3-(Methylthio)propanamine, 9CI. 3-Methylmercaptopropylamine. 3-Aminopropyl methyl sulfide
[4104-45-4]
$H_2NCH_2CH_2CH_2SMe$

$C_4H_{11}NS$ 105.204
Formed by *Streptomyces* from Methionine. Constit. of *Iberis amara* and from the brown alga *Desmarestia aculeata*. Steam-volatile liq. Misc. H_2O, EtOH, Et_2O. Bp 170° Bp_{14} 66-67°.

Hydrochloride: [2419-62-7]
Hygroscopic needles (Me_2CO). Mp 144°.

▶ UI4100000

Picrate:
Cryst. Mp 126-127°.

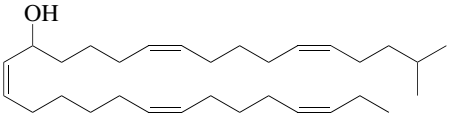
S-*Oxide: 3-(Methylsulfinyl)propylamine*
$C_4H_{11}NOS$ 121.203
Cryst. Mp 27°. $Bp_{0.04}$ 90-91°.

S,S-*Dioxide: 3-(Methylsulfonyl)propylamine*
$C_4H_{11}NO_2S$ 137.202
Hygroscopic cryst. Mp 44°. Bp_6 165-168°.

Schneider, W. *et al., Annalen*, 1910, **375**, 207 (*synth*)
Karrer, P. *et al., Helv. Chim. Acta*, 1950, **33**, 1237 (*synth*)
Dose, K. *et al., Chem. Ber.*, 1957, **90**, 1251 (*synth*)
Suyama, T. *et al., Yakugaku Zasshi*, 1964, **84**, 1012; *CA*, **62**, 6552 (*synth*)
Pesch, R. *et al., Org. Mass Spectrom.*, 1974, **9**, 861 (*ms*)

2-Methyl-5,10,16,22,27-triacontapentaen-15-ol M-520

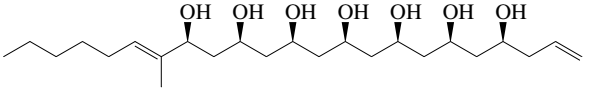
[134283-14-0]



$C_{31}H_{54}O$ 442.767
Constit. of the red alga *Gracilaria foliifera*.

Hayee-Memon, A. *et al., Bot. Mar.*, 1991, **34**, 107 (*isol, cmr*)

17-Methyl-1,17-tricosadiene-4,6,8,10,12,14,16-heptol M-521



$C_{24}H_{46}O_7$ 446.623

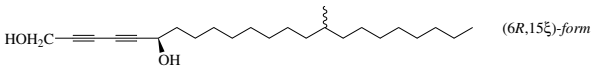
(4*S*,6*S*,8*S*,10*S*,12*S*,14*S*,16*S*,17*E*)-*form*

Hepta-Me ether: 4,6,8,10,12,14,16-Heptamethoxy-17-methyl-1,17-tricosadiene
$C_{31}H_{60}O_7$ 544.811
Isol. from the sponge *Myriastra clavosa*. Viscous greenish oil. $[\alpha]_D$ +3.2 (c, 0.3 in $CHCl_3$).

Rao, M.R. *et al., J. Nat. Prod.*, 2002, **65**, 1201-1203 (*isol, pmr*)

15-Methyl-2,4-tricosadiyne-1,6-diol M-522

Strongylodiol G



$C_{24}H_{42}O_2$ 362.595

(6*R*,15ξ)-*form* [334973-96-5]
Isol. from *Strongylophora* sp.
Amorph. solid. $[\alpha]_D^{22}$ -3.9 (c, 0.55 in $CHCl_3$). λ_{max} 229 (log ϵ 2.78); 243 (log ϵ 2.72); 257 (log ϵ 2.52) (EtOH).

(6*S*,15ξ)-*form* [334973-97-6]
Isol. from *Strongylophora* sp.
Watanabe, K. *et al., CA*, 2000, **134**, 308117e (*isol*)
Watanabe, K. *et al., J. Nat. Prod.*, 2005, **68**, 1001-1005 (*isol, pmr, cmr*)

12-Methyltridecanoic acid, 9CI M-523

Isomyristic acid. Aseonostatin P1. Aseanostatin P1
[2724-57-4]
$(H_3C)_2CH(CH_2)_{10}COOH$
$C_{14}H_{28}O_2$ 228.374
Occurs in several natural sources including wool wax, pine resin, Baltic salmon and sperm whale. Also prod. by various bacteria. Has bactericidal activity.
Mp 53°. Bp_2 158°.

Et ester:
$C_{16}H_{32}O_2$ 256.428
Bp_5 140-142°.

Amide:
$C_{14}H_{29}NO$ 227.389
Mp 107°.

Fordyce, C.R. *et al., J.A.C.S.*, 1933, **55**, 3371 (*synth*)
Tyrrell, D. *et al., Lipids*, 1968, **3**, 368 (*ir, ms*)
Goodrich, B. *et al., Aust. J. Chem.*, 1971, **24**, 153
Carballeira, N. *et al., J.O.C.*, 1986, **51**, 2751 (*synth*)
Ratanayake, W.M.N. *et al., Lipids*, 1989, **24**, 630-637 (*occur, fish oil*)
Ishida-Okawara, A. *et al., J. Antibiot.*, 1991, **44**, 524 (*Aseonostatin*)
Biermann, U. *et al., J.A.C.S.*, 2004, **126**, 10319-10330 (*synth*)

11-Methyl-2-tridecanone M-524

$H_3CCH_2CH(CH_3)(CH_2)_8COCH_3$
$C_{14}H_{28}O$ 212.375

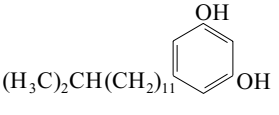
(ξ)-*form*
Prod. by a *Streptomyces* sp. GWS-H5 isol. from the North sea, and from an Arctic bacterium.
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*Arctic bacteria isolate, synth, pmr, cmr, ms*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 837-865 (*Streptomyces isolate*)

12-Methyl-2-tridecanone M-525

$(H_3C)_2CH(CH_2)_9COCH_3$
$C_{14}H_{28}O$ 212.375
Prod. by a marine bacterium.
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol, synth, pmr, cmr, ms*)

5-(12-Methyltridecyl)-1,3-benzenediol M-526

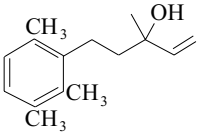
[138168-62-4]



$C_{20}H_{34}O_2$ 306.487
Constit. of the sponge *Haliclona* sp. Oil. Darkens in air.
Barrow, R.A. *et al., Aust. J. Chem.*, 1991, **44**, 1393 (*isol, uv, ir, pmr, cmr, ms*)

3-Methyl-5-(2,3,6-trimethoxyphenyl)-1-penten-3-ol M-527

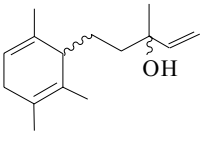
α-Ethenyl-α,2,3,6-tetramethylbenzenepropanol, 9CI. 2-(3-Hydroxy-3-methyl-4-pentenyl)-1,3,4-trimethylbenzene
[51148-40-4]



$C_{15}H_{22}O$ 218.338
Possible metab. of *Laurencia nidifica*. Oil.
Sun, H.H. *et al., Tet. Lett.*, 1976, 585

3-Methyl-5-(2,3,6-trimethyl-2,5-cyclohexadienyl)-1-penten-3-ol M-528

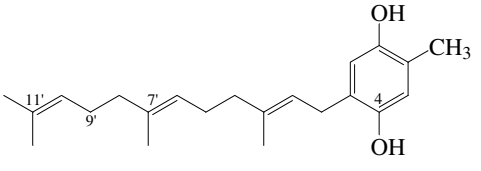
α-Ethenyl-α,2,3,6-tetramethyl-2,5-cyclohexadiene-1-propanol, 9CI. 3-(3-Hydroxy-3-methyl-4-pentenyl)-1,2,4-trimethyl-1,4-cyclohexadiene
[59700-20-8]



$C_{15}H_{24}O$ 220.354
Sesquiterpenoid from the marine alga *Laurencia nidifica*. Oil.
Sun, H.H. *et al., Tet. Lett.*, 1976, 585 (*isol, ir, pmr, cmr, struct*)

2-Methyl-5-(3,7,11-trimethyl-2,6,10-dodecatrienyl)-1,4-benzenediol M-529

2-Farnesyl-5-methylhydroquinone. Isogrifolin



$C_{22}H_{32}O_2$ 328.494

(2′*E*,6′*E*)-*form* [439856-45-8]
Isol. from a marine-derived *Penicillium* sp. Potent radical scavenger.
Amorph. solid. λ_{max} 206 (ϵ 12000); 294 (ϵ 2000) (MeOH).

4-Me ether: **O-*Methylisogrifolin***
[64997-54-2]
$C_{23}H_{34}O_2$ 342.52
Constit. of *Scleronephthya* sp.

4-O-*(3,6-Di*-O-*acetyl-β-*D*-galactopyranoside):* ***Euplexide G***
[364594-71-8]
$C_{32}H_{46}O_9$ 574.71
Constit. of *Euplexaura anastromosans*. Gum. $[\alpha]_D^{25}$ -21.6 (c, 0.12 in MeOH). λ_{max} 210 (log ϵ 4.52); 287 (log ϵ 3.55) (MeOH).

4-O-*(4,6-Di*-O-*acetyl-β-*D*-galactopyranoside):* ***Euplexide F***
[364594-70-7]
$C_{32}H_{46}O_9$ 574.71
Constit. of *Euplexaura anastromosans*. Gum. $[\alpha]_D^{25}$ -15.1 (c, 0.07 in MeOH). λ_{max} 210 (log ϵ 4.32); 288 (log ϵ 3.05) (MeOH).

4-O-*(3,4,6-Tri*-O-*acetyl-β-*D*-galactopyranoside):* ***Euplexide C***
[223385-02-2]
$C_{34}H_{48}O_{10}$ 616.747
Constit. of *Euplexaura anastromosans*. Gum. $[\alpha]_D^{25}$ -11.9 (c, 0.2 in

$CHCl_3$). λ_{max} 210 (log ϵ 4.27); 288 (log ϵ 3.22) (MeOH).

9′-Oxo, 10′,11′-dihydro: ***12-(2,5-Dihydroxy-4-methylphenyl)-2,6,10-trimethyl-6,10-dodecadien-4-one****. 2-Methyl-5-(3,7,11-trimethyl-9-oxo-2,6-dodecadienyl)-1,4-benzenediol*
[369368-16-1]
$C_{22}H_{32}O_3$ 344.493
Isol. from *Leminda millecra*. Orange oil. λ_{max} 295 (log ϵ 3.27) (MeOH).

*9′-Oxo, 10′,11′-dihydro, 4-*O*-(3,4,6-tri-*O*-acetyl-β-D-galactopyranoside):* ***Euplexide D***
[223385-06-6]
$C_{34}H_{48}O_{11}$ 632.747
Constit. of *Euplexaura anastromosans*. Gum. $[\alpha]_D^{25}$ -13.1 (c, 0.3 in $CHCl_3$). λ_{max} 212 (log ϵ 4.15); 287 (log ϵ 3.43) (MeOH).

*9′*R*-Hydroxy, 4-*O*-(3,4,6-tri-*O*-acetyl-β-D-galactopyranoside):* ***Euplexide A***
[223384-82-5]
$C_{34}H_{48}O_{11}$ 632.747
Constit. of *Euplexaura anastromosans*. Solid.
Mp 92-93°. $[\alpha]_D^{25}$ -2.5 (c, 0.2 in $CHCl_3$). λ_{max} 210 (log ϵ 4.15); 285 (log ϵ 3.49). (MeOH).

*9′*R*-Hydroxy, 4-*O*-(tetra-*O*-acetyl-β-D-galactopyranoside):* ***Euplexide B***
[223384-83-6]
$C_{36}H_{50}O_{12}$ 674.784
Constit. of *Euplexaura anastromosans*. Solid.
Mp 170-180°. $[\alpha]_D^{25}$ -7.9 (c, 0.2 in $CHCl_3$). λ_{max} 212 (log ϵ 4.23); 287 (log ϵ 3.59) (MeOH).

*9′ξ-Hydroxy, 4-*O*-(3,4,6-tri-*O*-acetyl-α-D-altropyranoside):* ***Moritoside***
[100665-52-9]
$C_{34}H_{48}O_{11}$ 632.747
Constit. of a gorgonian *Euplexaura* sp. Inhibits development of starfish embryo. Toxic to brine shrimp. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{23}$ +22.6 (c, 0.1 in $CHCl_3$). λ_{max} 280 (ϵ 3580) (MeOH) (Berdy).

9′ξ-Hydroxy, 10′,11′-dihydro: ***2-(9-Hydroxy-3,7,11-trimethyl-2,6-dodecadienyl)-1,4-benzenediol***
[369380-53-0]
$C_{22}H_{34}O_3$ 346.509
Isol. from *Leminda millecra*. Orange oil. λ_{max} 294 (log ϵ 3.24) (MeOH).

*$\Delta^{7',8'}$-Isomer(*Z*-), 9′-oxo, 10′,11′-dihydro:* ***12-(2,5-Dihydroxy-4-methylphenyl)-2,6,10-trimethyl-5,10-dodecadien-4-one, 9CI****. 2-Methyl-5-(3,7,11-trimethyl-9-oxo-2,7-dodecadienyl)-1,4-benzenediol*
[369368-17-2]
$C_{22}H_{32}O_3$ 344.493
Isol. from *Leminda millecra*. Orange oil. λ_{max} 232 (log ϵ 4.31); 294 (log ϵ 3.19) (MeOH).

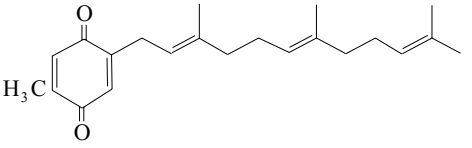
*$\Delta^{7',8'}$-Isomer(*Z*-), 9′-oxo, 10′,11′-dihydro, 4-Ac:* [369368-20-7]
$C_{24}H_{34}O_4$ 386.53
Isol. from *Leminda millecra*. Yellow oil. λ_{max} 242 (log ϵ 4.11); 281 (log ϵ 3.52) (MeOH).

*$\Delta^{9',10'}$-Isomer(*E*-), 11′-methoxy, 4-*O*-(3,4,6-tri-*O*-acetyl-β-D-galactopyranoside):* ***Euplexide E***
[223385-20-4]
$C_{35}H_{50}O_{11}$ 646.773
Constit. of *Euplexaura anastromosans*. Gum. $[\alpha]_D^{25}$ -12.6 (c, 0.2 in $CHCl_3$). λ_{max} 211 (log ϵ 4.24); 287 (log ϵ 3.48) (MeOH).

Fusetani, N. *et al., Tet. Lett.*, 1985, **26**, 6449 (*Moritoside*)
Shin, J. *et al., J.O.C.*, 1999, **64**, 1853-1858 (*Euplexides A-E*)
McPhail, K.L. *et al., J. Nat. Prod.*, 2001, **64**, 1183-1190 (*Leminda millecra constits*)
Seo, Y. *et al., Nat. Prod. Lett.*, 2001, **15**, 81-87 (*Euplexides F,G*)
Son, B.W. *et al., Arch. Pharmacal Res.*, 2002, **25**, 77-79 (*isol, pmr, cmr, ms*)
Yan, X.-H. *et al., Youji Huaxue*, 2004, **24**, 1233-1238; *CA*, **142**, 71702 (*Isogrifolin, Methylisogrifolin*)

2-Methyl-5-(3,7,11-trimethyl-2,6,10-dodecatrienyl)-1,4-benzoquinone M-530

2-Farnesyl-5-methyl-1,4-benzoquinone
[57402-26-3]



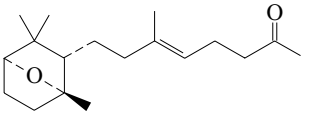
$C_{22}H_{30}O_2$ 326.478
Constit. of *Seseli* spp. Metab. of the fungus *Phellinus pini*. Yellow oil.

9′-Oxo, 10′,11′-dihydro: 2-Methyl-5-(3,7,11-trimethyl-9-oxo-2,6-dodecadienyl)-1,4-benzoquinone
[369368-10-5]
$C_{22}H_{30}O_3$ 342.477
Isol. from *Leminda millecra*. Bright yellow oil. λ_{max} 252 (log ϵ 3.76) (MeOH).

*$\Delta^{7',8'}$-Isomer(*Z*-), 9′-oxo, 10′,11′-dihydro: 2-Methyl-5-(3,7,11-trimethyl-9-oxo-2,7-dodecadienyl)-1,4-benzoquinone*
[369368-13-8]
$C_{22}H_{30}O_3$ 342.477
Isol. from *Leminda millecra*. Bright yellow oil. λ_{max} 250 (log ϵ 3.45) (MeOH).

Bohlmann, F. *et al., Chem. Ber.*, 1975, **108**, 2818 (*isol, pmr*)
Ayer, W.A. *et al., Phytochemistry*, 1996, **42**, 1321-1324 (*isol, pmr, cmr*)
McPhail, K.L. *et al., J. Nat. Prod.*, 2001, **64**, 1183-1190 (*Leminda derivs*)

6-Methyl-8-(2,2,6-trimethyl-3,6-epoxycyclohexyl)-5-octen-2-one M-531

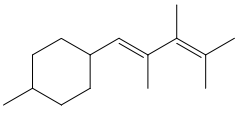


$C_{18}H_{30}O_2$ 278.434

(E)-form
Isol. from *Cystophora moniliformis*.
Oil. $[\alpha]_D^{22}$ +30 (c, 1.1 in CH_2Cl_2).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 171

1-Methyl-4-(2,3,4-trimethyl-1,3-pentadienyl)cyclohexane M-532

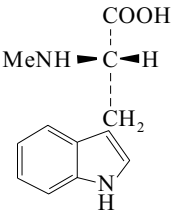
[119979-82-7]



$C_{15}H_{26}$ 206.37
Unusual carbon skeleton. Constit. of *Purpura pansa*.
Perez G., R.M. *et al., Herba Pol.*, 1988, **34**, 81-84; *CA*, **110**, 170443d

N-Methyltryptophan, 9CI M-533

3-(2-Indolyl)-2-methylaminopropanoic acid. ***Abrine***



(*S*)–*form*

$C_{12}H_{14}N_2O_2$ 218.255

Antiinflammatory, antiophthalmic agent. Log P -0.81 (uncertain value) (calc).

(*S*)-*form*

L-form

[526-31-8]

Isol. from seeds of *Abrus precatorius* and *Desmodium tiliaefolium* (Leguminosae).

Prisms (H_2O). Sol. H_2O, EtOH; insol. Et_2O. $[\alpha]_D^{21}$ +47 (c, 2.01 in 0.5*M* HCl). Dec. at 295° (275-90° dec.).

Hydrochloride:

Needles. Mp 221.5°.

Picrate:

Red prisms (H_2O, EtOH or AcOH). Mp 185-186° dec.

Me ester: **N-*Methyltryptophan methyl ester***

[32164-04-8]

[169547-59-5]

$C_{13}H_{16}N_2O_2$ 232.282

Alkaloid from *Aotus subglauca, Sida cordifolia* and *Gastrolobium callistachys* (Leguminosae, Malvaceae). Noncryst.; cryst. (as hydrochloride).

Mp 171-172° (hydrochloride). $[\alpha]_D^{23}$ +47.2 (c, 2 in MeOH) (hydrochloride).

▶Strong allergen.

Me ester, picrate: Mp 151-153°.

(±)-*form* [26988-72-7]

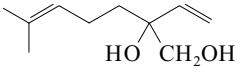
Needles (EtOH aq.). Mp 297° dec. (darkens at 280°).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 672B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 144C (*nmr*)
Hoshino, T. *et al., Annalen*, 1935, **520**, 31-34 (*isol, struct*)
Cahill, W.M. *et al., J. Biol. Chem.*, 1938, **126**, 29-36 (*isol, config*)
Miller, E.J. *et al., J.C.S.*, 1938, 1910-1912 (*synth*)
Peter, H. *et al., Helv. Chim. Acta*, 1963, **46**, 577-586 (*synth, ir*)
Johns, S.R. *et al., Aust. J. Chem.*, 1971, **24**, 439-449 (*Me ester*)
Waelders, S.F. *et al., Biopolymers*, 1977, **16**, 623-620 (*pmr*)
Seetharaman, J. *et al., J. Crystallogr. Spectrosc. Res.*, 1993, **23**, 167-170 (*cryst struct*)

6-Methyl-2-vinyl-5-heptene-1,2-diol M-534

3-Hydroxymethyl-7-methyl-1,6-octadien-3-ol

[73510-11-9]



$C_{10}H_{18}O_2$ 170.251

Constit. of *Chondrococcus hornemanni*. Oil.

1-O-*β*-*D*-*Glucopyranoside:* ***Unshuoside A***

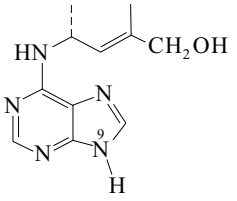
$C_{16}H_{28}O_7$ 332.393

Constit. of *Citrus unshiu* (satsuma mandarin). Amorph. powder. $[\alpha]_D$ -5 (c, 0.45 in MeOH).

Ishida, T. *et al., J. Pharm. Sci.*, 1981, **70**, 406
Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1983 (*isol, pmr, cmr*)
Yoshikawa, K. *et al., Nat. Med. (Tokyo)*, 1996, **50**, 176; *CA*, **125**, 81942h (*Unshuoside A*)

1′-Methylzeatin M-535

*2-Methyl-4-(1*H*-purin-6-ylamino)-2-penten-1-ol, 9CI. 6-(4-Hydroxy-1,3-dimethyl-2-butenylamino)purine*



$C_{11}H_{15}N_5O$ 233.272

λ_{max} 275 (ϵ 17400) (pH 1 H_2O) (Derep). λ_{max} 275 (ϵ 18200) (pH 13 H_2O) (Derep). λ_{max} 270 (ϵ 18500) (95% EtOH) (Derep).

(*R*)-*form* [101512-26-9]

Isol. from the culture filtrate of *Pseudomonas syringae* p.v. *savastanoi*. Sol. H_2O.

Mp 201-202°. $[\alpha]_D^{26}$ -109 (c, 0.153 in EtOH) (-52.6). λ_{max} 270 (ϵ 11359) (EtOH) (Berdy). λ_{max} 269 (ϵ 11842) (H_2O) (Berdy). λ_{max} 272 (ϵ 17900); 275 (ϵ 11912) (pH 10 buffer) (Berdy). λ_{max} 275 (ϵ 17400) (pH 1 buffer) (Berdy).

9-β-D-Ribofuranosyl: [98211-30-4]

$C_{16}H_{23}N_5O_5$ 365.388

Isol. from *Pseudomonas syringae* p.v. *savastanoi*. Cytokinin. Cryst. + ½H_2O. Sol. MeOH.

Mp 130-132°. $[\alpha]_D^{14}$ -117 (c, 0.102). λ_{max} 265 (ϵ 19200) (pH 1 H_2O) (Derep). λ_{max} 269 (ϵ 19400) (pH 13 H_2O) (Derep). λ_{max} 270 (ϵ 18400) (95% EtOH) (Derep). λ_{max} 269 (ϵ 19200) (H_2O) (Berdy). λ_{max} 270 (ϵ 15200) (EtOH) (Berdy). λ_{max} 265 (ϵ 19600) (HCl) (Berdy). λ_{max} 269 (ϵ 19800) (NaOH) (Berdy).

2-Hydroxy: ***2-Hydroxy-1′-methylzeatin***

[137592-13-3]

$C_{11}H_{15}N_5O_2$ 249.272

Prod. by *Alternaria brassicae* and isol. from marine green algae (NIO-143). Shows cytokinin activity. Plant growth stimulator. Sol. MeOH.

Mp 300°. $[\alpha]_D^{19}$ +41.6 (c, 0.288 in MeOH). Darkens at 275°. Probable abs. config. λ_{max} 232; 242; 262; 282 (MeOH) (Berdy). λ_{max} 256; 288 (MeOH/HCl) (Berdy). λ_{max} 257; 288 (MeOH/NaOH) (Berdy).

(±)-*form* [127516-55-6]

Prisms (H_2O). Mp 175.5-176.5°.

Surico, G. *et al., Phytochemistry*, 1985, **24**, 1499-1502 (*isol, pmr, cmr, ms, uv*)
Evidente, A. *et al., Phytochemistry*, 1986, **25**, 525-526 (*isol, pmr, cmr, uv, ms*)
Itaya, T. *et al., Tet. Lett.*, 1986, **27**, 6349 (*synth, cd, abs config*)
Fujii, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 3119-3121; 1990, **38**, 2702-2706 (*synth, uv, pmr, cmr*)
Ohba, M. *et al., Heterocycles*, 1990, **31**, 599-602 (*cmr*)
Farooqi, A.H.A. *et al., Phytochemistry*, 1990, **29**, 2061-2063 (*isol, 2-hydroxy*)
Dahiya, J.S. *et al., Phytochemistry*, 1991, **30**, 2825-2828 (*isol, 2-hydroxy*)
Fujii, T. *et al., Heterocycles*, 1992, **34**, 21-24 (*2-hydroxy, synth, abs config*)
Fujii, T. *et al., Heterocycles*, 1997, **46**, 659-671 (*rev*)

Metridin M-536

[110685-18-2]

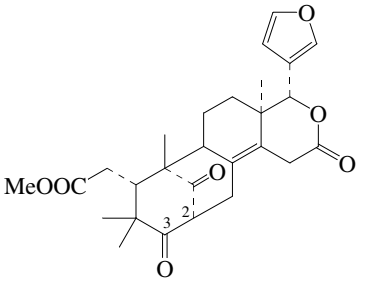
H-Asp-Ser-Asp-Cys-Lys-Asp-Lys-Leu-Pro-Ala-Cys-Gly-Glu-Tyr-Arg-Gly-Ser-Phe-Cys-Lys-Leu-Glu-Lys-Val-Lys-Ser-Asn-Cys-Glu-Lys-Thr-Cys-Gly-Val-Lys-Cys-OH

Isol. from the sea anemone *Metridium senile*. Haemolytic agent.

Krebs, H.C. *et al., Naturwissenschaften*, 1987, **74**, 395 (*isol, struct*)

Mexicanolide M-537

Cedrela odorata *Substance B*
[1915-67-9]



$C_{27}H_{32}O_7$ 468.546
Constit. of *Carapa mexicana, Carapa odorata* and *Xylocarpus moluccensis*. Also from *Carapa procera* and *Khaya grandifoliola*. Cryst.
Mp 222-227°. $[\alpha]_D^{25}$ -100 ($CHCl_3$).

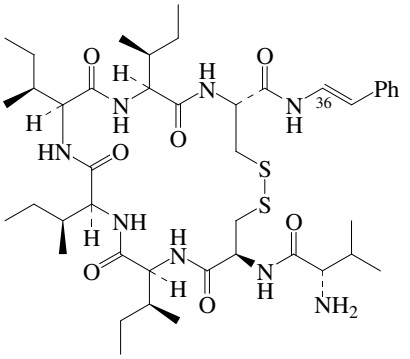
2α-Hydroxy: ***2-Hydroxymexicanolide***
[200352-17-6]
$C_{27}H_{32}O_8$ 484.545
Constit. of *Khaya senegalensis*. Cryst.
Mp 212°. $[\alpha]_D$ -64 (c, 0.5 in MeOH). λ_{max} 230 (log ϵ 3.27); 280 (log ϵ 2.62) (MeOH).

2α-Hydroxy, 3β-alcohol: ***3-Deoxo-2,3-dihydroxymexicanolide***.
2,3-Dihydroxy-3-deoxymexicanolide
[209866-05-7]
$C_{27}H_{34}O_8$ 486.561
Constit. of *Khaya senegalensis*. Cryst.
Mp 120°. $[\alpha]_D$ +79.5 (c, 0.088 in MeOH). λ_{max} 224 (log ϵ 3.07); 280 (log ϵ 2.82) (MeOH).

*6*R*-Hydroxy:* ***6-Hydroxymexicanolide***
[18664-04-5]
$C_{27}H_{32}O_8$ 484.545
Constit. of *Lansium domesticum*. Cryst.
Mp 264-265°.

Adeoye, S.A. *et al., Chem. Comm.*, 1965, 301 (*cryst struct*)
Connolly, J.D. *et al., Tetrahedron*, 1968, **24**, 1489; 1497 (*pmr, isol*)
Connolly, J.D. *et al., J.C.S. Perkin 1*, 1973, 2407 (*synth*)
Govindachari, T.R. *et al., Phytochemistry*, 1998, **47**, 1423-1425 (*derivs*)
Chantrapromma, K. *et al., Acta Cryst. E*, 2004, **60**, o312-o314 (*6-Hydroxymexicanolide, cryst struct*)

Microcionamide A M-538



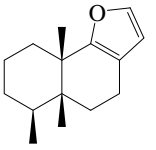
Absolute Configuration

$C_{43}H_{70}N_8O_7S_2$ 875.207
Isol. from the sponge *Clathria* (*Thalysias*) *abietina*. Cytotoxic. Glass (TFA salt). $[\alpha]_D$ -36.5 (c, 0.27 in MeOH) (TFA salt). λ_{max} 206 (sh) (ϵ 20000); 220 (sh) (ϵ 12000); 284 (ϵ 16000) (MeOH).

36Z-Isomer: ***Microcionamide B***
$C_{43}H_{70}N_8O_7S_2$ 875.207
Isol. from *Clathria abietina*. Cytotoxic. Glass (TFA salt).
$[\alpha]_D$ -40.3 (c, 0.32 in MeOH) (TFA salt). λ_{max} 208 (sh) (ϵ 23000); 222 (sh) (ϵ 15000); 274 (ϵ 14000) (MeOH).
Davis, R.A. *et al., J.O.C.*, 2004, **69**, 4170-4176 (*isol, pmr, cmr*)

Microcionin 1 M-539

[59805-75-3]



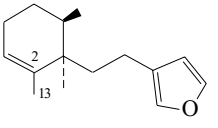
Absolute Configuration

$C_{15}H_{22}O$ 218.338
Constit. of *Fasciospongia cavernosa* and *Dendrodoris grandiflora*. Oil. $[\alpha]_D$ +7. *F. cavernosa* originally misidentified as *Microciona toxystila*.

Cimino, G. *et al., Tetrahedron*, 1985, **41**, 1093-1100 (*isol, struct*)
Gaspar, H. *et al., Tetrahedron*, 2005, **61**, 11032-11037 (*struct*)

Microcionin 2 M-540

[59805-78-6]



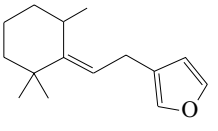
$C_{15}H_{22}O$ 218.338
Constit. of *Microciona toxystila* and molluscs *Cadlina luteomarginata* and *Dendrodoris grandiflora*. Oil. $[\alpha]_D$ -58.3.

$\Delta^{2,13}$-Isomer: ***Microcionin 4***
[59805-80-0]
$C_{15}H_{22}O$ 218.338
Constit. of *Microciona toxystila* and *Dendrodoris grandiflora*. Oil. Stereochem. undefined.

Cimino, G. *et al., Tet. Lett.*, 1975, 3723
Hellou, J. *et al., Tetrahedron*, 1982, **38**, 1875
Cimino, G. *et al., Tetrahedron*, 1985, **41**, 1093
Potvin, S. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 2821 (*synth*)

Microcionin 3 M-541

[59805-79-7]

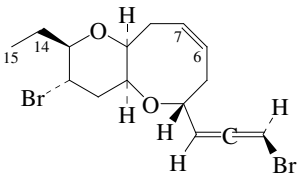


$C_{15}H_{22}O$ 218.338
Constit. of *Microciona toxystila*, *Halichondria panicea* and *Dendrodoris grandiflora*. Oil. Sol. MeOH; poorly sol. H_2O. $[\alpha]_D$ +36.5. λ_{max} 208 (ϵ 9700) (MeOH) (Berdy).

Cimino, G. *et al., Tet. Lett.*, 1975, 3723
Cimino, G. *et al., Tetrahedron*, 1985, **41**, 1093

Microcladallene A M-542

3-Bromo-6-(3-bromo-1,2-propadienyl)-2-ethyl-2,3,4,4a,6,7,10,10a-octahydropyrano[3,4-b]oxocin, 9CI. 1,12-Dibromo-4,10:9,13-diepoxy-1,2,6-pentadecatriene
[90468-75-0]



Absolute Configuration

$C_{15}H_{20}Br_2O_2$ 392.13
Isol. from *Laurencia microcladia* and an Okinawan *Laurencia* sp. Cryst.
Mp 91°. $[\alpha]_D^{24}$ +109 (c, 0.72 in $CHCl_3$). $[\alpha]_D^{20}$ +114 (c, 0.5 in Me_2CO).

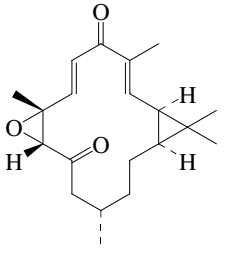
14,15-Didehydro: ***Microcladallene B***
[90468-74-9]
$C_{15}H_{18}Br_2O_2$ 390.114
Isol. from *Laurencia microcladia*. Plates.
Mp 83°. $[\alpha]_D^{20}$ +96 (c, 0.5 in Me_2CO).

14,15-Didehydro, 6,7-dihydro, 6β,7β-dichloro: ***Microcladallene C***
[90468-73-8]
$C_{15}H_{20}Br_2Cl_2O_2$ 463.035
Isol. from *Laurencia microcladia*. Viscous oil. $[\alpha]_D^{20}$ +116.7 (c, 0.5 in Me_2CO).

Kennedy, D.J. *et al., Chem. Comm.*, 1984, 153-155 (*isol, pmr, cmr, cryst struct*)
Suzuki, M. *et al., J. Nat. Prod.*, 2002, **65**, 801-804 (*isol, pmr, cmr*)

Microclavatin M-543

[860639-16-3]

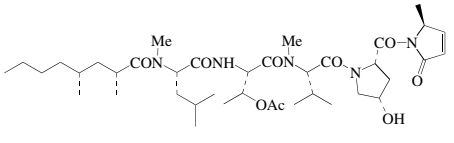


$C_{20}H_{28}O_3$ 316.439
Constit. of *Sinularia microclavata*. Cryst. (EtOAc/petrol).
Mp 145-146°. $[\alpha]_D^{20}$ -15.7 (c, 0.07 in $CHCl_3$). λ_{max} 242 (log ε 3.89); 282 (log ε 4.04) ($CHCl_3$).

Zhang, C.-X. *et al., J. Nat. Prod.*, 2005, **68**, 1087-1089 (*cryst struct*)

Microcolin A M-544

[141205-31-4]



Absolute Configuration

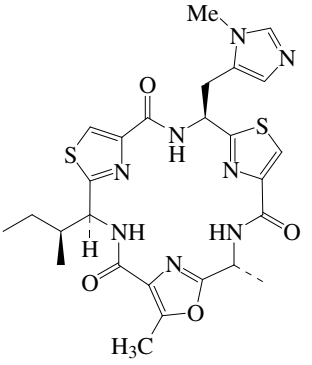
$C_{39}H_{65}N_5O_9$ 747.971
Isol. from the blue-green alga *Lyngbya majuscula*. Immunosuppressant. Glass. Sol. MeOH, EtOAc. $[\alpha]_D^{25}$ -145.3 (c, 0.003 in EtOH). λ_{max} 205 (ε 31300); 233 (sh) (EtOH) (Derep). λ_{max} 205 (ε 31300) (MeOH) (Berdy).

Deoxy: ***Microcolin B***
[141205-32-5]
$C_{39}H_{65}N_5O_8$ 731.971
Isol. from *Lyngbya majuscula*. Immunosuppressant. Glass. Sol. MeOH, EtOAc. $[\alpha]_D^{25}$ -174 (c, 0.005 in EtOH). λ_{max} 205 (ε 31300); 233 (sh) (EtOH) (Derep). λ_{max} (MeOH) (Berdy).

Koehn, F.E. *et al., J. Nat. Prod.*, 1992, **55**, 613-619 (*Microcolins A and B*)
Koehn, F.E. *et al., J. Med. Chem.*, 1994, **37**, 3181 (*synth, analogues*)
Decicco, C.P. *et al., J.O.C.*, 1996, **61**, 3534 (*synth, abs config*)
Andrus, M.B. *et al., J.O.C.*, 1997, **62**, 5542 (*synth, Microcolin B*)

Microcyclamide M-545

[297730-40-6]

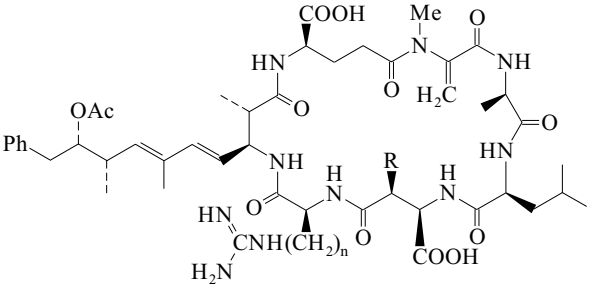


Absolute Configuration

$C_{26}H_{30}N_8O_4S_2$ 582.706
Abs. config. revised in 2002. Isol. from *Microcystis aeruginosa*. Moderate cytotoxic agent. Amorph. solid. $[\alpha]_D^{23}$ -46.3 (c, 0.1 in MeOH). λ_{max} 231 (ε 26500) (MeOH).

Ishida, K. *et al., J. Nat. Prod.*, 2000, **63**, 1315-1317 (*isol, pmr, cmr*)
Fujii, K. *et al., Tetrahedron*, 2002, **58**, 6873-6879 (*isol, pmr, abs config*)

(*ADMAdda*^{5})Microcystins M-546



(ADMAdda ^{5})MLR R = CH_3, n = 3
(ADMAdda ^{5})MLHar R = CH_3, n = 4
(D−Asp^3,ADMAdda ^{5})MLR R = H, n = 3

Cyclic peptide antibiotics. Prod. by the cyanobacterium *Nostoc* sp. strain 152. Hepatotoxin.

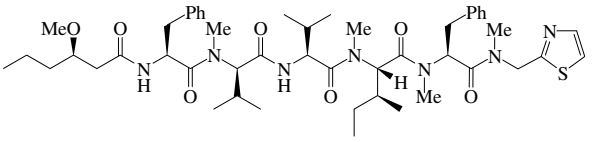
(*ADMAdda*^{5})Microcystin LR [129707-51-3]
$C_{50}H_{74}N_{10}O_{13}$ 1023.194

(*ADMAdda*^{5})Microcystin LHar [129707-52-4]
$C_{51}H_{76}N_{10}O_{13}$ 1037.221

(D-*Asp,ADMAdda*^{5})Microcystin LR [129678-93-9]
$C_{49}H_{72}N_{10}O_{13}$ 1009.167

Sivonen, K. *et al., Appl. Environ. Microbiol.*, 1990, **56**, 2650 (*isol, ms, pmr*)
Namikoshi, M. *et al., J.O.C.*, 1990, **55**, 6135-6139; 1992, **57**, 866 (*pmr, cmr, ms*)

Micromide M-547



$C_{49}H_{73}N_7O_7S$ 904.224

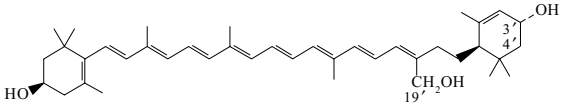
Isol. from a *Symploca* sp. Cytotoxic. Amorph. powder. $[\alpha]_D^{21}$ -28 (c, 0.5 in MeOH). λ_{max} 201 (log ϵ 4.4); 225 (log ϵ 3.8); 274 (log ϵ 2.4) (MeOH).

Williams, P.G. *et al., J. Nat. Prod.*, 2004, **67**, 49-53 (*isol, pmr, cmr*)

Micromonol M-548

7′,8′-Dihydro-β,ϵ-carotene-3,3′,19′-triol, 9CI

[169217-36-1]



$C_{40}H_{58}O_3$ 586.896

Constit. of *Micromonas pusilla*.

19′-Aldehyde: ***Micromonal***

[169221-37-8]

$C_{40}H_{56}O_3$ 584.881

Constit. of *Micromonas pusilla*, *Bathycoccus prasinos* and *Mantoniella squamata*.

3′-Deoxy, 3′,4′-didehydro: ***Anhydromicromonol***

[168781-47-3]

$C_{40}H_{56}O_2$ 568.881

Constit. of *Mantoniella squamata*. MF incorrectly assigned in the lit.

19′-Aldehyde, 3′-deoxy, 3′,4′-didehydro: ***Anhydromicromonal***

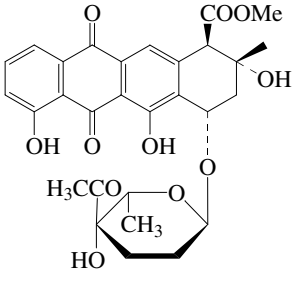
[168781-46-2]

$C_{40}H_{54}O_2$ 566.865

Constit. of *Mantoniella squamata*. MF incorrectly assigned in the lit.

Egeland, E.S. *et al., Phytochemistry*, 1995, **40**, 515 (*isol, pmr, cmr*)

Micromonomycin M-549

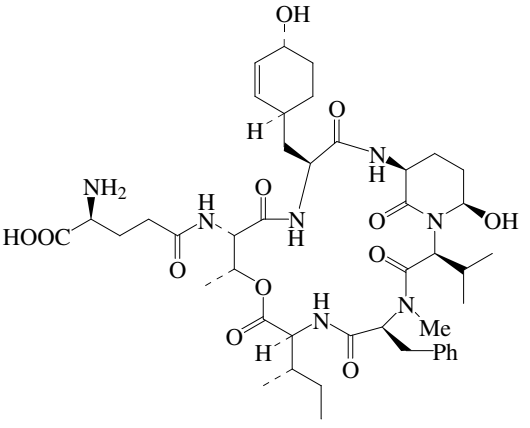


$C_{29}H_{30}O_{11}$ 554.549

Anthracycline antibiotic. Related to Auramycin A, A-745. Prod. by *Micromonospora* sp. Antibacterial agent.

Yang, S.-W. *et al., J. Antibiot.*, 2004, **57**, 601-604 (*isol, pmr, cmr*)

Micropeptin 88A M-550

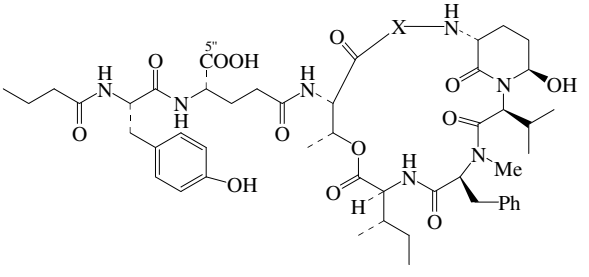


$C_{44}H_{65}N_7O_{12}$ 884.037

Depsipeptide antibiotic. Prod. by *Microcystis aeruginosa* NIES-88. Chymotrypsin and elastase inhibitor. Amorph. powder. $[\alpha]_D^{23}$ -46.7 (c, 0.1 in MeOH). λ_{max} 278 (ϵ 1170) (MeOH).

Ishida, K. *et al., Tetrahedron*, 1998, **54**, 5545-5556 (*isol, pmr, cmr*)

Micropeptin 88B M-551



X = Glu

$C_{53}H_{74}N_8O_{16}$ 1079.212

Depsipeptide antibiotic. Prod. by *Microcystis aeruginosa* NIES-88. Chymotrypsin inhibitor. Amorph. powder. $[\alpha]_D^{23}$ -17.2 (c, 0.5 in MeOH). λ_{max} 278 (ϵ 1100) (MeOH).

Ishida, K. *et al., Tetrahedron*, 1998, **54**, 5545-5556 (*isol, pmr, cmr*)

Micropeptin 88C M-552

As Micropeptin 88B, M-551 with

X = Tyr

$C_{57}H_{76}N_8O_{15}$ 1113.272

Depsipeptide antibiotic. Prod. by *Microcystis aeruginosa* NIES-88. Chymotrypsin inhibitor. Amorph. powder. $[\alpha]_D^{23}$ -47.4 (c, 0.1 in MeOH). λ_{max} 278 (ϵ 3000) (MeOH).

5″-Me ester: ***Micropeptin 88F***

$C_{58}H_{78}N_8O_{15}$ 1127.299

Prod. by *Microcystis aeruginosa* NIES-88. Chymotrypsin inhibitor. Amorph. powder. $[\alpha]_D^{23}$ -27.2 (c, 0.05 in MeOH). λ_{max} 278 (ϵ 2700) (MeOH).

Ishida, K. *et al., Tetrahedron*, 1998, **54**, 5545-5556 (*isol, pmr, cmr*)

Micropeptin 88D M-553

As Micropeptin 88B, M-551 with

X = 3-(4-Hydroxy-2-cyclohexen-1-yl)-L-alanine (1*S*,4*R*)

$C_{57}H_{80}N_8O_{15}$ 1117.304

Depsipeptide antibiotic. Prod. by *Microcystis aeruginosa* NIES-88. Chymotrypsin inhibitor. Amorph. powder. $[\alpha]_D^{23}$ -29.2 (c, 0.1

in MeOH). λ_{max} 278 (ϵ 1600) (MeOH).

Ishida, K. *et al., Tetrahedron*, 1998, **54**, 5545-5556 (*isol, pmr, cmr*)

Micropeptin 88E **M-554**

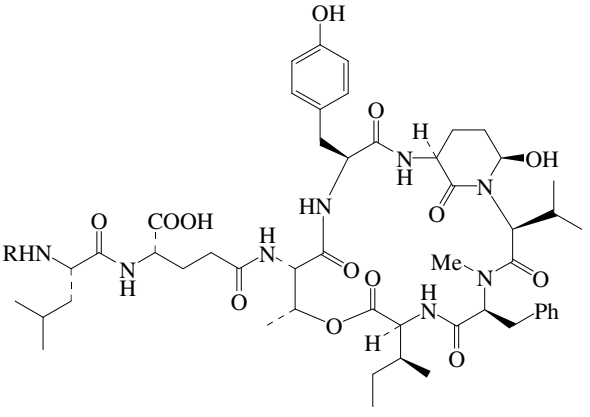
As Micropeptin 88B, M-551 with
X = Leu

$C_{54}H_{78}N_8O_{14}$ 1063.255

Depsipeptide antibiotic. Prod. by *Microcystis aeruginosa* NIES-88. Chymotrypsin inhibitor. Amorph. powder. $[\alpha]_D^{23}$ -64 (c, 0.1 in MeOH). λ_{max} 278 (ϵ 1830) (MeOH).

Ishida, K. *et al., Tetrahedron*, 1998, **54**, 5545-5556 (*isol, pmr, cmr*)

Micropeptin 88N **M-555**



R = -$COCH_2CH_2CH_3$

$C_{54}H_{78}N_8O_{14}$ 1063.255

Depsipeptide antibiotic. Prod. by *Microcystis aeruginosa* NIES-88. Chymotrypsin inhibitor. Amorph. solid. $[\alpha]_D^{22}$ -57 (c, 0.05 in MeOH). λ_{max} 278 (log ϵ 3.08) (MeOH).

Yamaki, H. *et al., J. Nat. Prod.*, 2005, **68**, 14-18 (*isol, pmr, cmr*)

Micropeptin 88Y **M-556**

As Micropeptin 88N, M-555 with
R = -$COCH_3$

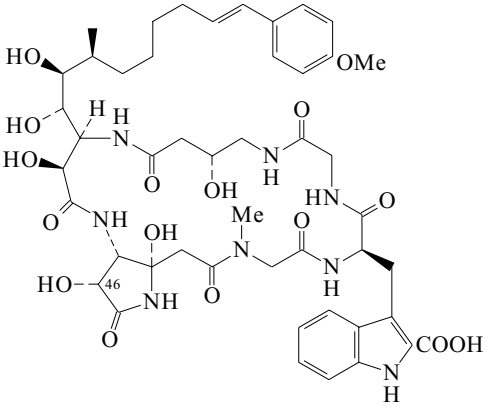
$C_{52}H_{74}N_8O_{14}$ 1035.202

Depsipeptide antibiotic. Prod. by *Microcystis aeruginosa* NIES-88. Chymotrypsin inhibitor. Amorph. solid. $[\alpha]_D^{22}$ -52 (c, 0.05 in MeOH). λ_{max} 278 (log ϵ 3.35) (MeOH).

Yamaki, H. *et al., J. Nat. Prod.*, 2005, **68**, 14-18 (*isol, pmr, cmr*)

Microsclerodermin A **M-557**

[157171-93-2]



$C_{47}H_{62}N_8O_{16}$ 995.051

Cyclic hexapeptide antibiotic. Isol. from the lithistid sponge *Microscleroderma* sp. Antifungal agent. Powder. $[\alpha]_D$ -113 (c, 0.5 in 0.1*M* NH_4HCO_3, pH 7.0). λ_{max} 208 (ϵ 7600); 260 (ϵ 2500); 290 (ϵ 1900) (MeOH) (Berdy).

46-Deoxy: ***Microsclerodermin B***

[157171-94-3]

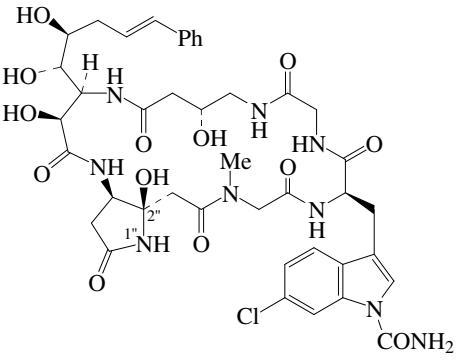
$C_{47}H_{62}N_8O_{15}$ 979.051

From *Microscleroderma* sp. Antifungal agent. Powder. $[\alpha]_D$ -64 (c, 0.2 in 0.1*M* NH_4HCO_3, pH 7.0). λ_{max} 204 (ϵ 6100); 260 (ϵ 2100); 290 (ϵ 1700) (MeOH) (Berdy).

Bewley, C.A. *et al., J.A.C.S.*, 1994, **116**, 7631 (*isol, uv, ir, pmr, cmr, ms*)

Microsclerodermin C **M-558**

[206535-29-7]



$C_{41}H_{50}ClN_9O_{13}$ 912.351

Isol. from the sponge *Theonella* sp. Powder. $[\alpha]_D$ -24 (c, 0.06 in MeOH/DMSO). λ_{max} 202 (ϵ 46500); 239 (ϵ 28000); 250 (ϵ 27100); 256 (ϵ 28000) (MeOH).

N-*De(aminocarbonyl):* ***Microsclerodermin D***

[206535-30-0]

$C_{40}H_{49}ClN_8O_{12}$ 869.326

Isol. from the sponges *Microscleroderma* sp. and *Theonella* sp. Powder. $[\alpha]_D$ -56 (c, 0.07 in MeOH/DMSO). λ_{max} 202 (ϵ 56000); 224 (ϵ 34000); 242 (ϵ 16100); 269 (ϵ 9600); 277 (ϵ 9000) (MeOH).

2″-Deoxy, 1″,2″-didehydro: ***Dehydromicrosclerodermin C***

[294210-38-1]

$C_{41}H_{48}ClN_9O_{12}$ 894.336

Isol. from *Theonella cupola*.

2″-Deoxy, 1″,2″-didehydro, N-*de(aminocarbonyl):* ***Dehydromicrosclerodermin D***

[294210-39-2]

$C_{40}H_{47}ClN_8O_{11}$ 851.311

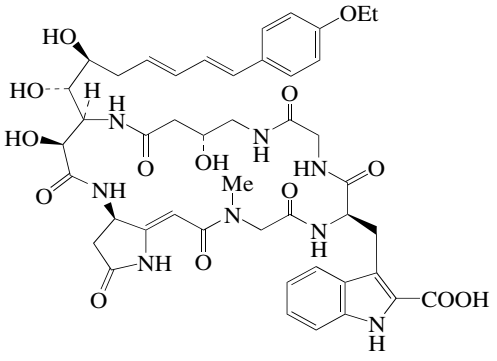
Isol. from *Theonella cupola*.

Schmidt, E.W. *et al., Tetrahedron*, 1998, **54**, 3043-3056 (*isol, uv, ir, pmr, cmr*)

Erdogan, I. *et al., CA*, 2000, **133**, 235401k (*Dehydromicrosclerodermins*)

Microsclerodermin E M-559

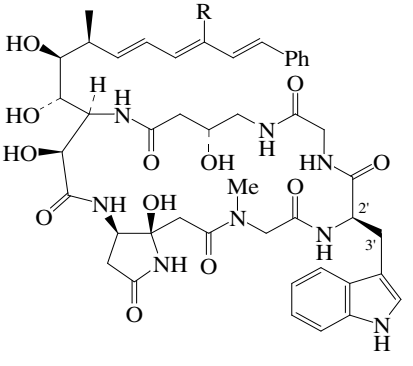
[206535-31-1]



$C_{45}H_{54}N_8O_{14}$ 930.967
Isol. from the sponge *Microscleroderma* sp. Powder. $[\alpha]_D$ -24 (c, 0.2 in MeOH/0.1*M* NH_4HCO_3). λ_{max} 203 (ϵ 33100); 206 (ϵ 34700); 218 (ϵ 33000); 284 (ϵ 37200) (MeOH). λ_{max} 203 (ϵ 33100); 206 (ϵ 34700); 218 (ϵ 33000); 284 (ϵ 37200) (MeOH) (Berdy).

Schmidt, E.W. *et al., Tetrahedron*, 1998, **54**, 3043-3056 (*isol, uv, ir, pmr, cmr*)
Zhu, J. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 5348-5351 (*synth*)

Microsclerodermin F M-560



R = H

$C_{45}H_{56}N_8O_{12}$ 900.984
Isol. from the lithistid sponge *Microscleroderma* sp. Antifungal agent. Powder. $[\alpha]_D$ -19 (c, 0.62 in MeOH aq.). λ_{max} 317 (ϵ 30400); 332 (ϵ 23000) (MeOH aq.).

2′,3′-Didehydro(Z-): ***Microsclerodermin G***
$C_{45}H_{54}N_8O_{12}$ 898.968
Isol. from *Microscleroderma* sp. Antifungal agent. Powder. $[\alpha]_D$ -20 (c, 0.31 in MeOH aq.). λ_{max} 317 (ϵ 43100); 332 (ϵ 36600) (MeOH aq.).

Qureshi, A. *et al., Tetrahedron*, 2000, **56**, 3679-3685

Microsclerodermin H M-561

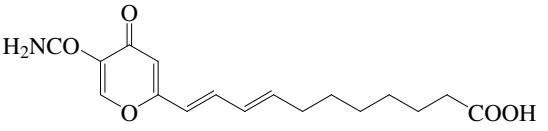
As Microsclerodermin F, M-560 with
R = CH_3

$C_{46}H_{58}N_8O_{12}$ 915.011
Isol. from the lithistid sponge *Microscleroderma* sp. Antifungal agent. Powder. $[\alpha]_D$ -13 (c, 0.95 in MeOH aq.). λ_{max} 319 (ϵ 51800); 334 (ϵ 38000) (MeOH aq.).

2′,3′-Didehydro(Z-): ***Microsclerodermin I***
$C_{46}H_{56}N_8O_{12}$ 912.995
Isol. from *Microscleroderma* sp. Antifungal agent. Powder. $[\alpha]_D$ -35 (c, 0.08 in MeOH aq.). λ_{max} 319 (ϵ 30200); 334 (ϵ 25000) (MeOH aq.).

Qureshi, A. *et al., Tetrahedron*, 2000, **56**, 3679-3685

Microsphaerone B M-562

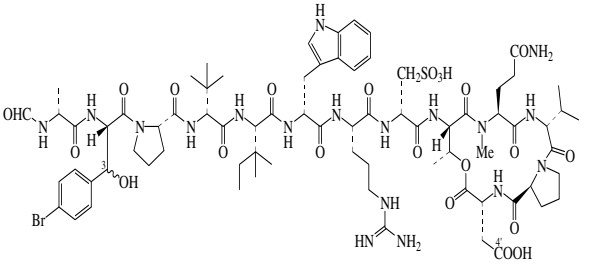


$C_{17}H_{21}NO_5$ 319.357
Prod. by the fungus *Microsphaeropsis* sp. isol. from the sponge *Aplysina aerophoba*. Yellow powder (MeOH). λ_{max} 211 (log ϵ 3.65); 231 (log ϵ 3.63); 313 (log ϵ 3.71) (MeOH).

N-*(3*S*-Carboxybutanoyl):* ***Microsphaerone A***
$C_{22}H_{27}NO_8$ 433.457
Prod. by a *Microsphaeropsis* sp. from *Aplysina aerophoba*. Yellow powder (MeOH). $[\alpha]_D^{20}$ -8.9 (c, 0.56 in MeOH). λ_{max} 229 (log ϵ 3.77); 312 (log ϵ 3.63) (MeOH).

Wang, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 772-775 (*isol, pmr, cmr, ms*)

Microspinosamide M-563

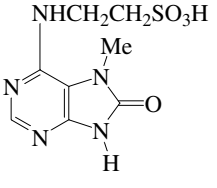


$C_{75}H_{109}BrN_{18}O_{22}S$ 1726.764
Isol. from the sponge *Sidonops microspinosa*. Amorph. powder. $[\alpha]_D$ +2.4 (c, 0.5 in MeOH). λ_{max} 211 (log ϵ 4.51); 218 (log ϵ 4.49); 278 (log ϵ 3.52); 289 (log ϵ 3.45) (EtOH).

3-Deoxy, 4′-amide: ***Polydiscamide A***
[138877-62-0]
$C_{75}H_{110}BrN_{19}O_{20}S$ 1709.779
Isol. from the sponge *Discodermia* sp. Powder (as Na salt). Mp 212-216° (Na salt). $[\alpha]_D^{24}$ -1.1 (c, 1.89 in MeOH).

Gulavita, N.K. *et al., J.O.C.*, 1992, **57**, 1767 (*Polydiscamide A*)
Rashid, M.A. *et al., J. Nat. Prod.*, 2001, **64**, 117-121 (*isol, pmr, cmr, abs config*)

Microxine M-564

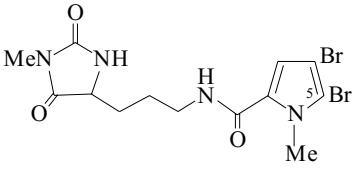


$C_8H_{11}N_5O_4S$ 273.272
Isol. from the sponge *Microxina* sp. Weak cdc2 kinase inhibitor. Amorph. solid. λ_{max} 210 (ϵ 12890); 274 (ϵ 8410) (H_2O).

Killday, K.B. *et al., J. Nat. Prod.*, 2001, **64**, 525-526 (*isol*)

Midpacamide M-565

4,5-Dibromo-1-methyl-N-*[3-(1-methyl-2,5-dioxo-4-imidazolidinyl)propyl]-1*H*-pyrrole-2-carboxamide, 9CI*
[66067-05-8]



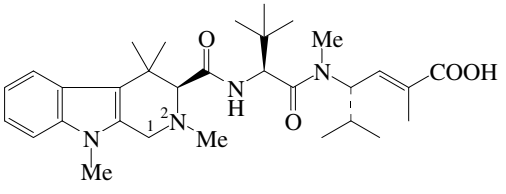
$C_{13}H_{16}Br_2N_4O_3$ 436.102
Isol. from an unidentified marine sponge and from the sponge *Agelas mauritiana*. Cryst. (MeCN).
Mp 93-95°. λ_{max} 206 (ϵ 5010); 239 (ϵ 7940); 276 (ϵ 11200) (MeOH) (Derep).

5-Debromo: ***5-Debromomidpacamide***
[114216-89-6]
$C_{13}H_{17}BrN_4O_3$ 357.206
Isol. from the marine sponge *Agelas mauritiana*.
Mp 116-119°.

Chevolot, L. *et al., Heterocycles*, 1977, **7**, 891 (*isol, pmr, cmr, struct*)
Fathi-Afshar, R. *et al., Can. J. Chem.*, 1988, **66**, 45 (*isol, ir, pmr, cmr, ms, deriv*)
Lindel, T. *et al., Liebigs Ann./Recl.*, 1997, 1525-1528 (*synth, pmr, cmr, ms*)
Fresneda, P.M. *et al., Tet. Lett.*, 2001, **42**, 851-854 (*synth*)

Milnamide A M-566

[156430-97-6]



$C_{31}H_{46}N_4O_4$ 538.729
Peptide antibiotic. Alkaloid from Papua New Guinean collections of the marine sponge *Auletta* cf. *constricta*. Cytotoxic agent, microtubule formation inhibitor. Amorph. solid. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{27}$ +28.8 (c, 0.5 in CH_2Cl_2). λ_{max} 223 (ϵ 14700); 285 (ϵ 2810); 294 (ϵ 3070); 304 (ϵ 3030); 380 (ϵ 1260) (MeOH).

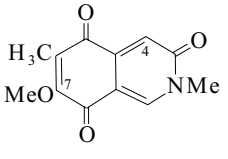
*1(2*N*)-Dehydro:* ***Milnamide D***
$C_{31}H_{45}N_4O_4^{\oplus}$ 537.721
Quaternary alkaloid from a *Cymbastela* sp. Cytotoxic agent. CAS No. not found 8-14CI.

1-Oxo: ***Milnamide C***
[675875-88-4]
$C_{31}H_{44}N_4O_5$ 552.712
Alkaloid from an *Auletta* sp. Cytotoxic. Yellow solid.

Crews, P. *et al., J.O.C.*, 1994, **59**, 2932-2934 (*isol, uv, ir, pmr, cmr*)
Chevallier, C. *et al., Org. Lett.*, 2003, **5**, 3737-3739 (*Milnamide D*)
Liu, C. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 5951-5954 (*synth*)
Sonnenschein, R.N. *et al., Org. Lett.*, 2004, **6**, 779-782 (*Milnamide C*)

Mimosamycin M-568

*7-Methoxy-2,6-dimethyl-3,5,8(2*H*)-isoquinolinetrione, 9CI*
[59493-94-6]



$C_{12}H_{11}NO_4$ 233.223
Benzoquinone-type antibiotic. Isol. from *Streptomyces lavendulae* and from the sponges *Reniera*, *Xestospongia* and *Petrosia* spp.; also from *Oceanapia* sp. Mainly active against mycobacteria. Also exhibits antifungal activity. Yellow prisms (MeOH). Mp 227-231° (219-221°). $[\alpha]_D^{24}$ -1.8 (c, 1 in $CHCl_3$). λ_{max} 230 (sh) (ϵ 14500); 317 (ϵ 14500); 396 (ϵ 3630) (MeOH) (Derep).

▶ NX5123400
O^7*-De-Me,* O^7*-Et: 7-Ethoxy-2,6-dimethyl-3,5,8(2*H*)-isoquinolinetrione, 9CI.* ***Cribrostatin 2***
[144279-36-7]
$C_{13}H_{13}NO_4$ 247.25
Alkaloid from the blue sponge *Cribrochalina* sp. Shows activity against P388 lymphocytic leukaemia. Shows broad spectrum antibacterial activity. Golden-yellow solid.
Mp 194-195°.

4-Hydroxy: ***4-Hydroxymimosamycin***
[224558-89-8]
$C_{12}H_{11}NO_5$ 249.223
Isol. from the sponge *Haliclona cribricutis*. Orange-red cryst.
Mp 225°. λ_{max} 227 (log ϵ 4.05); 485 (log ϵ 3.58) (MeOH).

1,4-Dihydroxy: ***1,4-Dihydroxymimosamycin***
[224558-92-3]
$C_{12}H_{11}NO_6$ 265.222
Isol. from the sponge *Haliclona cribricutis*. λ_{max} 220 (log ϵ 4.11); 255 (log ϵ 3.75); 500 (log ϵ 3.58) (MeOH).

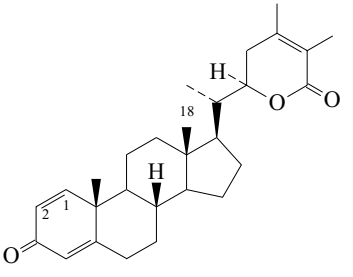
4-Amino: ***4-Aminomimosamycin***
[157227-53-7]
$C_{12}H_{12}N_2O_4$ 248.238
Isol. from the Indian Sea sponge, *Petrosia* sp. cAMP inhibitor. Deep red needles.
Mp 250-251°. λ_{max} 350 (ϵ 2187); 483 (ϵ 3800) (MeOH) (Berdy).

7-Demethoxy, 7-amino: ***7-Amino-7-demethoxymimosamycin***
[157227-54-8]
$C_{11}H_{10}N_2O_3$ 218.212
Isol. from the sponge *Petrosia* sp. cAMP inhibitor. Light brown solid.
Mp 300°. λ_{max} 250 (ϵ 3715); 327 (ϵ 4677); 434 (ϵ 812) (MeOH) (Berdy).

Arai, T. *et al., J. Antibiot.*, 1976, **29**, 398-407 (*isol, uv, ir, pmr*)
Mishima, H. *et al., Heterocycles*, 1977, **6**, 1652-1657 (*synth*)
Hata, T. *et al., Acta Cryst. B*, 1978, **34**, 2899-2901 (*cryst struct*)
Mishima, H. *et al., Chem. Pharm. Bull.*, 1978, **26**, 2175-2180 (*synth*)
Fukumi, H. *et al., J. Antibiot.*, 1978, **31**, 847-849 (*isol, pmr, cmr, ms*)
Frincke, J.M. *et al., J.A.C.S.*, 1982, **104**, 265-269 (*isol*)
Thomson, R.H. *et al., Naturally Occurring Quinones III, Recent Advances*, Chapman and Hall, 1987, 634 (*synth*)
Parker, K.A. *et al., J.O.C.*, 1988, **53**, 2847-2850 (*synth*)
Pettit, G.R. *et al., Can. J. Chem.*, 1992, **70**, 1170-1175 (*Cribrostatin 2*)
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1994, 282-283 (*Petrosia constits*)
Edrada, R.A. *et al., J. Nat. Prod.*, 1996, **59**, 973-976 (*isol, props*)
Parameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 1258-1263 (*1,4-Dihydroxymimosamycin, 4-Hydroxymimosamycin*)
Pettit, G.R. *et al., J. Nat. Prod.*, 2000, **63**, 793-798 (*Cribrostatin 2, activity*)
Kesteleyn, B. *et al., J.O.C.*, 2000, **65**, 635-639 (*synth*)
Fontana, A. *et al., Tetrahedron*, 2000, **56**, 7305-7308 (*isol*)

Minabeolide 1 M-569

*3-Oxo-22*R*-witha-1,4,24-trienolide*
[114820-24-5]



$C_{28}H_{38}O_3$ 422.606

Constit. of *Minabea* sp. Oil. λ_{max} 240 (ϵ 16200) (EtOH) (Derep).

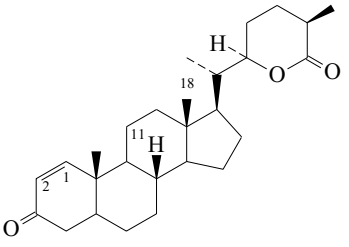
1,2-Dihydro: ***Minabeolide 3***
[114820-25-6]
$C_{28}H_{40}O_3$ 424.622
Constit. of *Minabea* sp. Oil. λ_{max} 240 (ϵ 16200) (EtOH) (Derep).

18-Acetoxy: ***Minabeolide 2***
[114836-87-2]
$C_{30}H_{40}O_5$ 480.643
Constit. of *Minabea* sp. Oil. λ_{max} 240 (ϵ 16200) (EtOH) (Derep).

Ksebati, M.B. *et al., J.O.C.*, 1988, **53**, 3926 (*isol, pmr, cmr*)
Tsubuki, M. *et al., J.O.C.*, 1992, **57**, 2930 (*synth*)

Minabeolide 4 M-570

[114820-26-7]



$C_{27}H_{40}O_3$ 412.611
Constit. of *Minabea* sp. Oil. λ_{max} 240 (ϵ 16200) (EtOH) (Derep).

18-Acetoxy: ***Minabeolide 5***
[114820-27-8]
$C_{29}H_{42}O_5$ 470.648
Constit. of *Minabea* sp. Oil. λ_{max} 240 (ϵ 16200) (EtOH) (Derep).

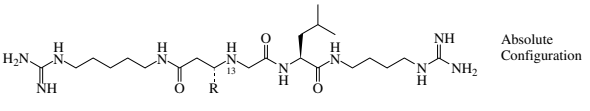
1,2-Dihydro: ***Minabeolide 6***
[114820-28-9]
$C_{27}H_{42}O_3$ 414.627
Constit. of *Minabea* sp. Oil. λ_{max} 240 (ϵ 16200) (EtOH) (Derep).

18-Acetoxy, 1,2-dihydro: ***Minabeolide 7***
[114820-29-0]
$C_{29}H_{44}O_5$ 472.664
Constit. of *Minabea* sp. Oil. λ_{max} 240 (ϵ 16200) (EtOH) (Derep).

11α-Acetoxy, 1,2-dihydro: ***Minabeolide 8***
[114820-30-3]
$C_{29}H_{44}O_5$ 472.664
Constit. of *Minabea* sp. Oil. λ_{max} 240 (ϵ 16200) (EtOH) (Derep).

Ksebati, M.B. *et al., J.O.C.*, 1988, **53**, 3926 (*isol, pmr, cmr*)

Minalemines M-571



Absolute Configuration

Minalemine A R = $-(CH_2)_6CH_3$
Minalemine B R = $-(CH_2)_7CH_3$
Minalemine C R = $-(CH_2)_8CH_3$

Isol. from the marine tunicate *Didemnum rodriguesi*.

Minalemine A [210828-85-6]
$C_{29}H_{60}N_{10}O_3$ 596.858
$[\alpha]_D$ -22.8 (c, 0.002 in MeOH). λ_{max} 222 (MeOH).

N^{13}-*Sulfate:* ***Minalemine D***
[210828-88-9]
$C_{29}H_{60}N_{10}O_6S$ 676.922
λ_{max} 272 (EtOH).

Minalemine B [210828-86-7]
$C_{30}H_{62}N_{10}O_3$ 610.885
$[\alpha]_D$ -21.2 (c, 0.001 in MeOH). λ_{max} 222 (MeOH).

N^{13}-*Sulfate:* ***Minalemine E***
[210828-89-0]
$C_{30}H_{62}N_{10}O_6S$ 690.949
λ_{max} 272 (EtOH).

Minalemine C [210828-87-8]
$C_{31}H_{64}N_{10}O_3$ 624.912
$[\alpha]_D$ -23.3 (c, 0.001 in MeOH). λ_{max} 222 (MeOH).

N^{13}-*Sulfate:* ***Minalemine F***
[210828-90-3]
$C_{31}H_{64}N_{10}O_6S$ 704.976
λ_{max} 272 (EtOH).

Exposito, M.A. *et al., Tetrahedron*, 1998, **54**, 7539-7550 (*isol, uv, pmr, cmr, ms*)
Exposito, M.A. *et al., J.O.C.*, 2001, **66**, 4206-4213 (*synth, uv, cd, abs config*)

Aplysia MIP-related peptides M-572

AMRP
Gly-Ala-Pro-Arg-Phe-Ile-NH_2
Peptides related to *Mytilus* inhibiting peptide; struct. of GAPRFI amide shown. Isol. from the CNS of the mollusc *Aplysia kurodai*.

GAPRFI amide [233610-59-8]
$C_{31}H_{50}N_{10}O_6$ 658.799

GPPRFI amide [255366-16-6]
$C_{33}H_{52}N_{10}O_6$ 684.837

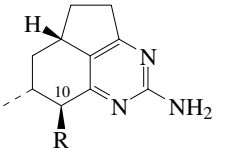
GSPRFF amide [255366-10-0]
$C_{34}H_{48}N_{10}O_7$ 708.816

GSPHFI amide [255366-13-3]
$C_{31}H_{45}N_9O_7$ 655.753

Fujisawa, Y. *et al., J. Neurosci.*, 1999, **19**, 9618-9634 (*isol*)

Mirabilin B M-574

[182266-75-7]



Relative Configuration

R = $-CH_2CH_2CH_2CH_3$

$C_{15}H_{23}N_3$ 245.367
Alkaloid from the sponges *Arenochalina mirabilis*, *Batzella* sp. and *Monanchora unguifera*. Antifungal agent. Cryst. $[\alpha]_D$ +41.6 (c, 0.48 in MeOH). λ_{max} 236; 302; 375 (MeOH).

N-*Ac:*
Pale yellow oil. $[\alpha]_D$ +89 (c, 0.40 in $CHCl_3$). λ_{max} 244 (ϵ 11800); 275 (ϵ 400) (MeOH).

Barrow, R.A. *et al., Aust. J. Chem.*, 1996, **49**, 767-773 (*isol, pmr, cmr, ms*)
Patil, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 704-707 (*isol, pmr, cmr*)
Hua, H.-M. *et al., Bioorg. Med. Chem.*, 2004, **12**, 6461-6464 (*isol*)

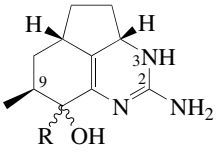
Mirabilin C M-575

[182266-76-8]
As Mirabilin B, M-574 with
R = $-CH_2CH{=}CHCH_2CH_2CH_3$ (*Z*)
$C_{17}H_{25}N_3$ 271.405
Alkaloid from the Australian marine sponge *Arenochalina mirabilis*. Pale yellow oil (as *N*-Ac). $[\alpha]_D$ +153 (c, 0.57 in $CHCl_3$) (*N*-Ac). Isol. and characterised as the monoacetate. λ_{max} 244 (ϵ 12400); 274 (ϵ 4500) (MeOH) (*N*-Ac) (Berdy).

10-Epimer: ***Mirabilin A***
[182145-37-5]
$C_{17}H_{25}N_3$ 271.405
From *Arenochalina mirabilis.* Pale yellow oil (as *N*-Ac). $[\alpha]_D$ +12.8 (c, 0.74 in $CHCl_3$) (*N*-Ac). λ_{max} 206 (ϵ 5500); 244 (ϵ 1300); 275 (ϵ 4400) (MeOH) (*N*-Ac) (Berdy).
Barrow, R.A. *et al., Aust. J. Chem.*, 1996, **49**, 767 (*isol, uv, ir, pmr, cmr, ms, struct*)

Mirabilin D M-576

[182145-57-9]



Relative Configuration

R = $-CH_2CH{=}CHCH_2CH_2CH_3$ (*Z*-)

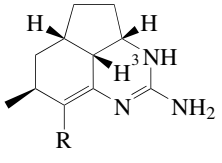
$C_{17}H_{27}N_3O$ 289.42
Alkaloid from the Australian marine sponge *Arenochalina mirabilis.* Pale yellow oil (as di-Ac). $[\alpha]_D$ +285 (c, 0.3 in $CHCl_3$) (di-Ac). λ_{max} 204 (ϵ 4600); 246 (ϵ 3600); 287 (ϵ 3750) (MeOH) (di-Ac) (Berdy). λ_{max} 246 (ϵ 3600); 287 (ϵ 3750) (EtOH) (di-Ac).
Barrow, R.A. *et al., Aust. J. Chem.*, 1996, **49**, 767 (*isol, uv, ir, pmr, cmr, ms, struct*)

Mirabilin E M-577

[182145-71-7]
As Mirabilin D, M-576 with
R = $-CH_2CH_2CH_2CH_3$
$C_{15}H_{25}N_3O$ 263.382
Alkaloid from the Australian marine sponge *Arenochalina mirabilis.* Pale yellow oil (as di-Ac). $[\alpha]_D$ +332 (c, 0.05 in $CHCl_3$) (di-Ac). Relative stereochem. about C9 not detd. λ_{max} 202 (ϵ 2100); 241 (ϵ 1650); 285 (ϵ 1250) (EtOH) (di-Ac).
Barrow, R.A. *et al., Aust. J. Chem.*, 1996, **49**, 767 (*isol, uv, ir, pmr, cmr, ms, struct*)

Mirabilin F M-578

[182145-74-0]



Relative Configuration

R = $-CH{=}CHCH_2CH_3$(*E*-)

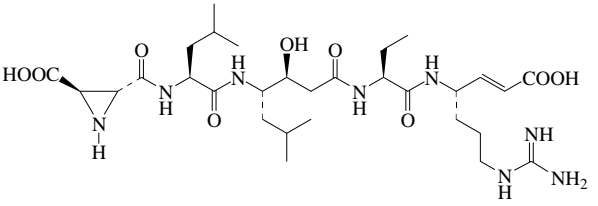
$C_{15}H_{23}N_3$ 245.367
Appears to be a didehydro deriv. of Ptilocaulin, P-696 shown with different tautomerism of the cyclic guanidine system. Alkaloid from the Australian marine sponge *Arenochalina mirabilis.* Pale yellow oil (as *N*-Ac). $[\alpha]_D$ +384 (c, 0.2 in $CHCl_3$) (*N*-Ac). λ_{max} 241 (ϵ 5278); 295 (ϵ 3150) (EtOH) (*N*-Ac).
Barrow, R.A. *et al., Aust. J. Chem.*, 1996, **49**, 767-773 (*isol, uv, ir, pmr, cmr, ms, struct*)

Mirabilin G M-579

As Mirabilin F, M-578 with
R = $-CH{=}CH(CH_2)_3CH_3$(*E*-)
$C_{17}H_{27}N_3$ 273.42
Alkaloid from the Australian marine sponge *Clathria* sp. Pale yellow oil. $[\alpha]_D$ +49 (c, 0.1 in $CHCl_3$). λ_{max} 241 (log ϵ 3.7); 295 (log ϵ 3.4) (EtOH).
Capon, R.J. *et al., J. Nat. Prod.*, 2001, **64**, 643-644 (*isol, uv, pmr, cmr, ms*)

Miraziridine A M-580

[312322-94-4]

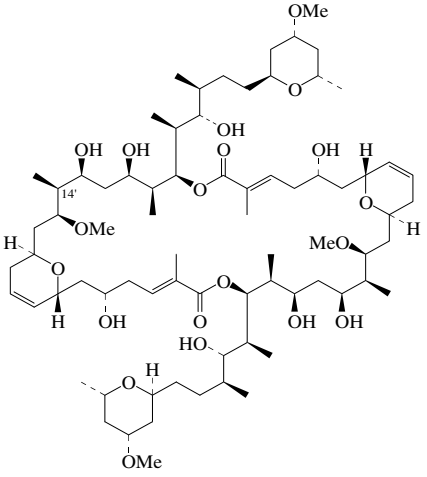


Absolute Configuration

$C_{30}H_{52}N_8O_9$ 668.789
Isol. from the marine sponge *Theonella* aff. *mirabilis.* Cysteine protease inhibitor. Also amino-proteinase and serine-proteinase inhibitor. $[\alpha]_D^{20}$ -74 (c, 0.085 in MeOH). λ_{max} 205 (ϵ 14000) (MeOH).
Nakao, Y. *et al., J.A.C.S.*, 2000, **122**, 10462-10463 (*isol, cmr, pmr*)
Schaschke, N. *et al., Bioorg. Med. Chem. Lett.*, 2004, **14**, 855-857 (*pharmacol*)

Misakinolide A M-581

Bistheonellide A
[105304-96-9]



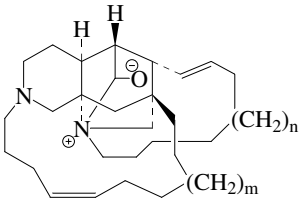
Absolute Configuration

$C_{74}H_{128}O_{20}$ 1337.813
Macrolide antibiotic. Related to Swinholide A, S-548. Constit. of sponge *Theonella* sp. Antitumour and antifungal agent. Shows actin-capping activity. Oil. $[\alpha]_D^{20}$ -21.4 (c, 5.6 in $CHCl_3$). λ_{max} 225 (ϵ 12000) (MeOH) (Derep).

14′-Demethyl: ***Bistheonellide B***
[112692-66-7]
$C_{73}H_{126}O_{20}$ 1323.786
Constit. of sponge *Theonella* sp. Cytotoxic agent. λ_{max} 225 (ϵ 12000) (MeOH) (Derep).
Sakai, R. *et al., Chem. Lett.*, 1986, 1499 (*isol*)
Kato, Y. *et al., Tet. Lett.*, 1987, **28**, 6225 (*struct*)
Tanaka, J. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2967-2970 (*abs config*)
Higa, T. *et al., ACS Symp. Ser.*, 2000, **745**, 12-21 (*activity*)

Misenine M-582

[202075-41-0]



m + n = 6

$C_{33}H_{54}N_2O$ 494.802

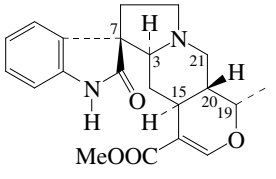
Alkaloid from the sponge *Reniera* sp. Oil. $[\alpha]_D$ +6.4 (c, 2.2 in $CHCl_3$).

Guo, Y. *et al., Tetrahedron*, 1998, **54**, 541-550 (*isol, ir, pmr, cmr*)

Mitraphylline M-583

Ajmalicine oxindole B. Rubradinine

[509-80-8]



Absolute Configuration

$C_{21}H_{24}N_2O_4$ 368.432

Alkaloid from *Mitragyna hirsuta*, some other *Mitragyna* spp. and some *Uncaria* spp. (Naucleaceae). Hypotensive agent, general depressant.

Mp 275-276° (265-266°). $[\alpha]_D$ -7 ($CHCl_3$) (-3). $[\alpha]_D$ -10 (EtOH). $[\alpha]_D$ +11 (Py). $[\alpha]_D^{24}$ -3 (c, 1.3 in $CHCl_3$). λ_{max} 243 (log ϵ 4.22); 280 (sh) (log ϵ 3.18) (EtOH).

7,20-Diepimer: ***Uncarine E****. Isopteropodine*

[5171-37-9]

$C_{21}H_{24}N_2O_4$ 368.432

Alkaloid from *Mitragyna parvifolia* and *Uncaria* spp. (Naucleaceae). Also isol. from the marine mollusc *Nerita albicilla*. Needles (C_6H_6 or MeOH).

Mp 209-211°. $[\alpha]_D$ -111 ($CHCl_3$).

Chan, K.C. *et al., J.C.S.(C)*, 1966, 2245-2249 (*Pteropodine, Isopteropodine, isol, pmr, ir*)

Beecham, A.F. *et al., Aust. J. Chem.*, 1968, **21**, 491-504 (*Uncarines A-F, stereochem*)

Martin, G.E. *et al., J. Nat. Prod.*, 1986, **49**, 406-411 (*Isopteropodine, isol, pmr, cmr*)

García, R. *et al., Z. Naturforsch., C*, 2005, **60**, 385-388 (*Uncarine E, cmr, ms*)

Mitrocomin M-584

Halistaurin

[152618-86-5]

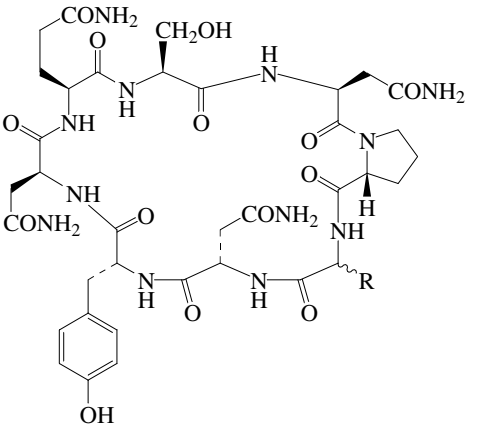
Peptide containing 190 amino acid units with 3 $Ca^{2\oplus}$-binding sites and a Tyr residue at the C-terminus. Isol. from the luminescent jellyfish *Mitrocoma celluraria*. $Ca^{2\oplus}$-activated photoprotein.

Shimomura, O. *et al., J. Cell. Comp. Physiol.*, 1963, **62**, 9-15 (*isol*)

Shimomura, O. *et al., Biochem. J.*, 1985, **228**, 745-749 (*isol*)

Fagan, T.F. *et al., FEBS Lett.*, 1993, **333**, 301-305 (*isol, struct*)

Mixirin A M-585



R = $-(CH_2)_{11}CH_3$

$C_{48}H_{74}N_{12}O_{14}$ 1043.185

Cyclic peptide antibiotic. Prod. by a marine *Bacillus* sp. (culture MIX-62). Cytotoxic. Amorph. powder.

Mp 285-286°. $[\alpha]_D^{22}$ -18.2 (c, 0.16 in MeOH).

Zhang, H.L. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1029-1030 (*isol, pmr, cmr*)

Mixirin B M-586

As Mixirin A, M-585 with

R = $-(CH_2)_8CH_3$

$C_{45}H_{68}N_{12}O_{14}$ 1001.104

Cyclic peptide antibiotic. Prod. by a marine *Bacillus* sp. (culture MIX-62). Cytotoxic.

Zhang, H.L. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1029-1030 (*isol*)

Mixirin C M-587

As Mixirin A, M-585 with

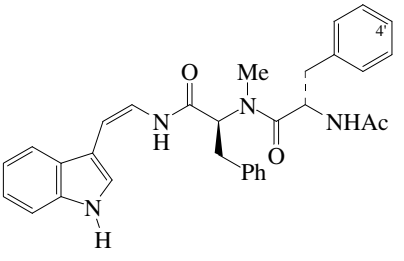
R = $-(CH_2)_7CH(CH_3)CH_2CH_3$

$C_{47}H_{72}N_{12}O_{14}$ 1029.158

Cyclic peptide antibiotic. Prod. by a marine *Bacillus* sp. (culture MIX-62). Cytotoxic.

Zhang, H.L. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1029-1030 (*isol*)

Miyakamide A_1 M-588



$C_{31}H_{32}N_4O_3$ 508.619

Peptide antibiotic. Similar to Terpeptin. Prod. by *Aspergillus flavus* var. *columnaris* FKI-0739. Cytotoxic. Pale yellow powder.

Mp 92-94° dec. $[\alpha]_D^{25}$ -34.9 (c, 0.23 in MeOH). λ_{max} 212 (sh) (ϵ 8600); 228 (ϵ 13600); 284 (sh) (ϵ 8200); 288 (sh) (ϵ 9000); 300 (ϵ 10400) (MeOH).

4′-Hydroxy: ***Miyakamide B_1***

$C_{31}H_{32}N_4O_4$ 524.618

Prod. by *Aspergillus flavus* var. *columnaris* FKI-0739 and the marine-derived *Aspergillus flavus* Gö 100/4. Pale yellow powder.

Mp 103-106° dec. $[\alpha]_D^{25}$ -24.2 (c, 0.15 in MeOH). λ_{max} 204 (ϵ 37700); 225 (ϵ 29300); 288 (ϵ 15200); 301 (sh) (ϵ 14150) (MeOH).

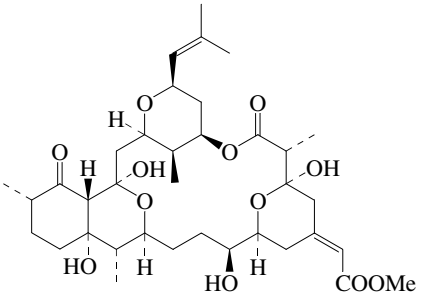
E-*Isomer:* ***Miyakamide A$_2$***
$C_{31}H_{32}N_4O_3$ 508.619
Prod. by *Aspergillus flavus* var. *columnaris* FKI-0739 and the marine-derived *Aspergillus flavus* Gö 100/4. Pale yellow powder. Mp 98-100° dec. $[\alpha]_D^{25}$ -27.1 (c, 0.24 in MeOH). λ_{max} 204 (ϵ 25900); 258 (ϵ 5800); 280 (ϵ 6100); 306 (ϵ 6400) (MeOH).

E-*Isomer, 4′-hydroxy:* ***Miyakamide B$_2$***
$C_{31}H_{32}N_4O_4$ 524.618
Prod. by *Aspergillus flavus* var. *columnaris* FKI-0739. Pale yellow powder.
Mp 107-111° dec. $[\alpha]_D^{25}$ -34.1 (c, 0.29 in MeOH). λ_{max} 202 (ϵ 26700); 225 (ϵ 18860); 280 (sh) (ϵ 10500); 307 (ϵ 13100) (MeOH).

Shiomi, K. *et al., J. Antibiot.*, 2002, **55**, 952-961 (*isol, uv, ir, pmr, cmr, ms*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

Miyakolide M-589

[143346-97-8]



Absolute Configuration

$C_{36}H_{54}O_{12}$ 678.815
Constit. of a *Polyfibrospongia* sponge. Cryst. (CH_2Cl_2/MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 197-199°. $[\alpha]_D^{24}$ -24 (c, 1.05 in $CHCl_3$). λ_{max} 225 (ϵ 21000) (MeOH) (Derep). λ_{max} 225 (ϵ 21000) (MeOH) (Berdy).

Higa, T. *et al., J.A.C.S.*, 1992, **114**, 7587 (*isol, pmr, cmr, cryst struct*)
Evans, D.A. *et al., J.A.C.S.*, 1999, **121**, 6816-6826 (*synth, abs config*)

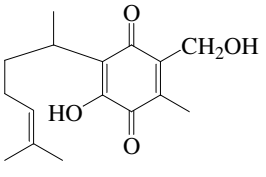
Mnemiopsin M-590

Protein. Isol. from the ctenophore *Mnemiopsis leidyi*. $Ca^{2\oplus}$-activated photoprotein.

Ward, W.W. *et al., Biochemistry*, 1974, **13**, 1500-1510 (*isol*)
Girsch, S.J. *et al., Mol. Cell. Biochem.*, 1978, **19**, 113-124 (*isol, props*)

Mochiquinone M-591

[309957-97-9]

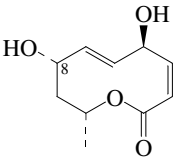


$C_{16}H_{22}O_4$ 278.347
Constit. of *Pseudopterogorgia rigida*. Yellow oil.

D'Armas, H.T. *et al., J. Nat. Prod.*, 2000, **63**, 1593-1595 (*isol, pmr, cmr*)

Modiolide A M-592

*5,8,9,10-Tetrahydro-5,8-dihydroxy-10-methyl-2*H*-oxecin-2-one*



Absolute Configuration

$C_{10}H_{14}O_4$ 198.218
Isol. from the fungus *Paraphaeosphaeria* sp. (N-119) obt. from the mussel *Modiolus auriculatus*. Also from the endophytic fungus *Periconia siamensis* (CMUGE015). Oil. $[\alpha]_D^{18}$ +42 (c, 0.25 in MeOH). λ_{max} 204 (ϵ 6400) (MeOH).

*8-Deoxy: 5,8,9,10-Tetrahydro-5-hydroxy-10-methyl-2*H*-oxecin-2-one.* ***Modiolide B***
$C_{10}H_{14}O_3$ 182.219
Isol. from the fungus *Paraphaeosphaeria* sp. (N-119) obt. from the mussel *Modiolus auriculatus*. Oil. λ_{max} 204 (ϵ 6400) (MeOH).

8,10-Diepimer: ***Fusanolide B***
$C_{10}H_{14}O_4$ 198.218
Prod. by a *Fusarium* sp. Needles (EtOAc).
Mp 180-182°. $[\alpha]_D^{20}$ +25 (c, 0.2 in MeOH). Only relative config. was determined. λ_{max} 208 (log ϵ 3.33) (EtOH).

Shimada, A. *et al., Z. Naturforsch., B*, 2002, **57**, 239-242 (*Fusanolide B*)
Tsuda, M. *et al., J. Nat. Prod.*, 2003, **66**, 412-415 (*isol, pmr, cmr*)
Fun, H.-K. *et al., Acta Cryst. E*, 2006, **62**, 2478-2480 (*isol, cryst struct*)

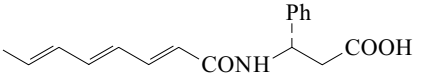
Modiolin M-593

Modiolus modiolus *Lectin*
Glycoprotein consisting of 3 subunits and existing as aggregates. Isol. from the haemolymph of the horse mussel *Modiolus modiolus*. Sialic acid-binding lectin with antibacterial activity. Can be fractionated into molecular entities with distinct specificities towards human and/or horse erythrocytes (modulin H and/or E activity, respectively).

Tunkijjanuki, J.S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1997, **112**, 273-286 (*isol*)
Tunkijjanuki, J.S. *et al., Dev. Comp. Immunol.*, 1998, **22**, 139-150 (*isol*)

Moiramide A M-594

[124731-96-0]

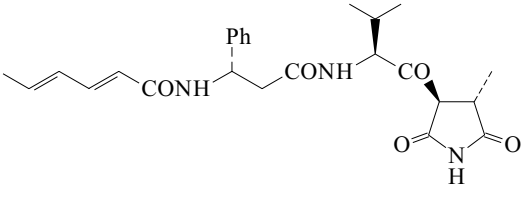


$C_{17}H_{19}NO_3$ 285.342
Metab. of a marine *Pseudomonas fluorescens*. Amorph. solid. Sol. MeOH, EtOAc. λ_{max} 294 (ϵ 27421) (MeOH). λ_{max} 293 (ϵ 27421) (MeOH) (Berdy).

Needham, J. *et al., J.O.C.*, 1994, **59**, 2059-2063 (*Moiramide A*)

Moiramide B M-595

[155233-31-1]

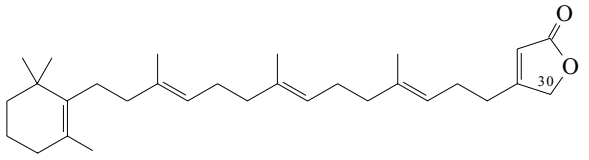


$C_{25}H_{31}N_3O_5$ 453.537
Metab. of a marine *Pseudomonas fluorescens*. Amorph. solid. Similar to Andrimid, A-492.

Needham, J. *et al., J.O.C.*, 1994, **59**, 2059-2063 (*Moiramide B*)
Davies, S.G. *et al., J.C.S. Perkin 1*, 1998, 2635-2643 (*synth*)

Mokupalide M-596

[65717-88-6]



$C_{30}H_{46}O_2$ 438.692
Constit. of a marine sponge *Megalopastas* sp. Oil.

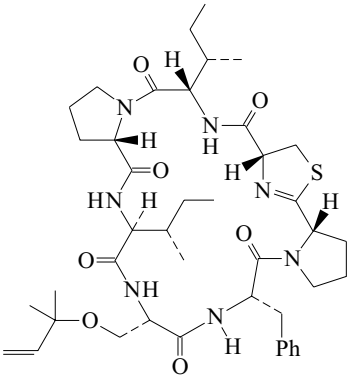
30-Hydroxy: ***Hydroxymokupalide***
[65717-89-7]
$C_{30}H_{46}O_3$ 454.692
Constit. of a *Megalopastas* sp. Syrup. λ_{max} 210 (ϵ 18000); 251 (ϵ 4800) (MeOH/NaOH) (Derep). λ_{max} 211 (ϵ 17300) (MeOH) (Derep).

30-Acetoxy: ***Acetoxymokupalide***
[65717-90-0]
$C_{32}H_{48}O_4$ 496.729
Constit. of a *Megalopastas* sp. Oil. λ_{max} 210 (ϵ 18000); 251 (ϵ 4800) (MeOH/NaOH) (Derep). λ_{max} 211 (ϵ 17300) (MeOH) (Derep).

Yunker, M.B. *et al., J.A.C.S.*, 1978, **100**, 307-309 (*isol*)
Kobayashi, M. *et al., J.O.C.*, 1980, **45**, 5223-5225 (*synth*)
Sum, F.W. *et al., Tetrahedron*, 1981, **37**, 303-317 (*synth*)

Mollamide M-597

[154037-66-8]

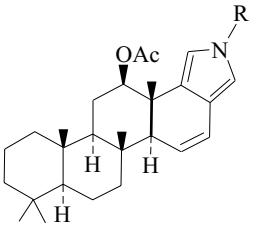


$C_{42}H_{61}N_7O_7S$ 808.053
Cyclic heptapeptide antibiotic. Constit. of the ascidian *Didemnum molle*. Cytotoxic agent. RNA biosynthesis inhibitor. Prisms (CH_2Cl_2/petrol).
Mp 154-156°. $[\alpha]_D$ -2.75 (c, 0.08 in $CHCl_3$). λ_{max} 222 (ϵ 30100); 245 (ϵ 16140) (EtOH).

Carroll, A.R. *et al., Aust. J. Chem.*, 1994, **47**, 61-69 (*isol, uv, ir, pmr, cmr, cryst struct*)
McKeever, B. *et al., Tetrahedron*, 2003, **59**, 2701-2712 (*synth*)

Molliorin A M-598

[63693-18-5]



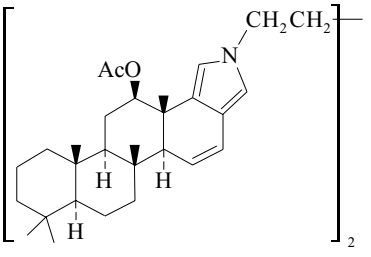
R = $CH_2CH(CH_3)CH_2CH_3$

$C_{32}H_{49}NO_2$ 479.745
Constit. of the marine sponge *Cacospongia mollior*.
Mp 102-105°. $[\alpha]_D$ +51.7 (c, 1 in $CHCl_3$).

Cafieri, F. *et al., Tet. Lett.*, 1977, 477 (*isol, ir, pmr, uv, ms, struct*)

Molliorin B M-599

[64421-20-1]



$C_{58}H_{84}N_2O_4$ 873.313
Constit. of the marine sponge *Cacospongia mollior*. Cryst. (petrol).
Mp 173-174°. $[\alpha]_D$ +14.6 (c, 1.2 in $CHCl_3$).

Cafieri, F. *et al., Experientia*, 1977, **33**, 994 (*isol, uv, synth, struct*)

Molliorin C M-600

[66648-53-1]
As Molliorin A, M-598 with
R = $-CH_2CH(CH_3)_2$
$C_{31}H_{47}NO_2$ 465.718
Minor alkaloid from the marine sponge *Cacospongia mollior*.
Amorph. solid. $[\alpha]_D$ -46.9 (c, 0.9 in $CHCl_3$). λ_{max} 257 (ϵ 11900) (EtOH).

Cafieri, F. *et al., Experientia*, 1978, **34**, 300 (*isol, ms, pmr, synth*)

Molliorin D M-601

[70022-71-8]
As Molliorin A, M-598 with
R = $-CH_2CH_2Ph$
$C_{35}H_{47}NO_2$ 513.762
Minor alkaloid from the marine sponge *Cacospongia mollior*.
$[\alpha]_D$ +11.6. λ_{max} 262 (ϵ 11760) (EtOH).

Cafieri, F. *et al., Experientia*, 1979, **35**, 157 (*isol, struct, ir, pmr, ms, synth*)

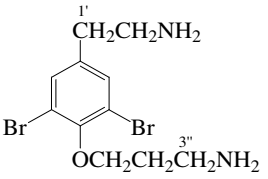
Molliorin E M-602

[69819-82-5]
As Molliorin A, M-598 with
R = Me
$C_{28}H_{41}NO_2$ 423.637
Minor alkaloid from the marine sponge *Cacospongia mollior*.
$[\alpha]_D$ +6.5. λ_{max} 263 (ϵ 11900) (EtOH).

Cafieri, F. *et al., Experientia*, 1979, **35**, 157 (*isol, struct, ir, pmr, ms, synth*)

Molokaiamine M-603

4-(3-Aminopropoxy)-3,5-dibromobenzeneethanamine, 9CI
[151345-09-4]



$C_{11}H_{16}Br_2N_2O$ 352.068
Metab. from the marine sponge *Pseudoceratina purpurea*, also from *Psammaplysilla* sp. and *Aplysinella* sp. Cytotoxic. Off-white powder (MeOH) (as dihydrochloride). λ_{max} 206 (ϵ 28000); 284 (ϵ 600) (MeOH).

$N^{3''}$-*(Cyanoformyl):* ***Ceratinamine****. Pseudoceramine*
[175993-07-4]
$C_{13}H_{15}Br_2N_3O_2$ 405.088
Metab. from *Pseudoceratina purpurea* and *Aplysinella* sp. Cytotoxic against P388 murine leukaemia cells. Antifouling substance. Solid (presumably as hydrochloride). Sol. MeOH. First report of a cyanoformamide nat. prod. λ_{max} 207 (ϵ 37800); 276 (ϵ 850) (MeOH) (Berdy).

$N^{2'}$-*Me:* **N′-*Methylmolokaiamine***
$C_{12}H_{18}Br_2N_2O$ 366.095
Isol. from a *Hexadella* sp. Powder. λ_{max} 277 (ϵ 340); 284 (ϵ 330) (MeOH).

$N^{2'}$-*Me,* $N^{3''}$-*(cyanoformyl):* **N-*Methylceratinamine***
[256448-59-6]
$C_{14}H_{17}Br_2N_3O_2$ 419.115
Metab. of an undescribed Verongid sponge. λ_{max} 278 (log ϵ 3.76); 285 (log ϵ 3.77) (MeOH).

$N^{3''}$-*Me,* $N^{2'}$-*methoxycarbonyl:*
$C_{14}H_{20}Br_2N_2O_3$ 424.132
Alkaloid from *Psammaplysilla purpurea*. Brown semisolid. λ_{max} 250 (ϵ 2210) (MeOH).

$N^{3''}$,$N^{3''}$-*Di-Me:* ***Purpurealidin E***
[260437-59-0]
$C_{13}H_{20}Br_2N_2O$ 380.122
Metab. of the sponge *Psammaplysilla purpurea*. Oil.
Mp 148° (as 2′-Ac, hydrochloride). Not indexed in CA **141**. λ_{max} 223 (ϵ 5770); 275 (ϵ 950); 280 (ϵ 944) (MeOH) (2′-Ac, hydrochloride).

$N^{3''}$,$N^{3''}$-*Di-Me,* $N^{2'}$-*Ac:* [215942-07-7]
$C_{15}H_{22}Br_2N_2O_2$ 422.159
Isol. from *Psammaplysilla purpurea*.

$N^{3''}$,$N^{3''}$-*Di-Me,* $N^{2'}$-*methoxycarbonyl: Methyl 3,5-dibromo-4-[[3-(dimethylamino)propoxy]phenylethyl]carbamate*
$C_{15}H_{22}Br_2N_2O_3$ 438.158
Alkaloid from *Psammaplysilla purpurea*. Brown solid. Mp 160-162°. Also isol. as the monohydrochloride, Mp 170-173°. Not indexed in CA **141**.

$N^{2'}$,$N^{2'}$,$N^{3''}$-*Tri-Me:* ***Purealidin F***
[145205-29-4]
$C_{14}H_{22}Br_2N_2O$ 394.149
Alkaloid from the Okinawan sponge *Psammaplysilla purpurea*. Inhibitor of Na/K-ATPase. Oil (as dihydrochloride). Sol. MeOH. CAS no. refers to hydrochloride. λ_{max} 218 (ϵ 12000); 274 (ϵ 800); 285 (ϵ 1000) (MeOH) (hydrochloride). λ_{max} 218 (ϵ 12000); 274 (ϵ 800); 285 (ϵ 1000) (MeOH) (Berdy).

$N^{2'}$,$N^{3''}$,$N^{3''}$-*Tri-Me:* ***Purealidin G***
[145196-30-1]
$C_{14}H_{22}Br_2N_2O$ 394.149
Alkaloid from *Psammaplysilla purpurea*. Na/K-ATPase inhibitor. Sol. MeOH. CAS no. refers to dihydrochloride. λ_{max} 214 (ϵ 14000); 276 (ϵ 800); 288 (ϵ 1100) (MeOH) (hydrochloride).

$N^{2'}$,$N^{2'}$,$N^{3''}$,$N^{3''}$-*Tetra-Me:* ***Aplysamine 1***
[159026-30-9]
[125547-38-8]
$C_{15}H_{24}Br_2N_2O$ 408.175
Metab. of an Australian marine sponge *Aplysina* sp. Pale yellow semicryst. solid (as hydrochloride).
Mp 122-123° (hydrochloride). Biol. inactive against several test bacteria and fungi.

$N^{2'}$-*Cyano,* $N^{2'}$-*Me:* **N′-*Cyano*-N′-*methylmolokaiamine***
$C_{13}H_{17}Br_2N_3O$ 391.105
Isol. from a *Hexadella* sp. Amorph. solid. λ_{max} 277 (ϵ 440); 284 (ϵ 440) (MeOH).

1″-Hydroxy, $N^{3''}$-*(cyanocarbonyl):* ***7-Hydroxyceratinamine***
[230295-94-0]
$C_{13}H_{15}Br_2N_3O_3$ 421.088
Isol. from *Aplysinella* sp. Amorph. solid. $[\alpha]_D$ +3 (c, 0.8 in MeOH).

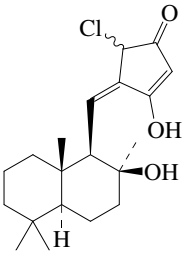
1′ξ-Hydroxy, $N^{3''}$,$N^{3''}$-*di-Me:* ***Purpurealidin F***
[799246-90-5]
$C_{13}H_{20}Br_2N_2O_2$ 396.121
Isol. from *Psammaplysilla purpurea*. Oil. λ_{max} 277 (ϵ 925); 282 (ϵ 950) (MeOH).

1′ξ-Hydroxy, $N^{3''}$,$N^{3''}$-*di-Me,* $N^{2'}$-*propanoyl:* ***Purpurealidin G***
[799246-91-6]
$C_{16}H_{24}Br_2N_2O_3$ 452.185
Isol. from *Psammaplysilla purpurea*. Oil. λ_{max} 277 (ϵ 925); 282 (ϵ 950) (MeOH).

Xynas, R. *et al., Aust. J. Chem.*, 1989, **42**, 1427-1433 (*Aplysamine 1*)
Tsuda, M. *et al., J. Nat. Prod.*, 1992, **55**, 1325-1327 (*Purealidins*)
Hamann, M.T. *et al., J.O.C.*, 1993, **58**, 6565-6569 (*isol, uv, ir, pmr, cmr, ms, struct, N-Methylceratinamine*)
Tsukamoto, S. *et al., J.O.C.*, 1996, **61**, 2936-2937 (*Ceratinamine*)
Tsukamoto, S. *et al., Tetrahedron*, 1996, **52**, 8181-8186 (*isol, props*)
Venkateswarlu, Y. *et al., J. Nat. Prod.*, 1998, **61**, 1388-1389; 1999, **62**, 893-894 (*Psammaplysilla purpurea constits*)
Schoenfeld, R.C. *et al., Tet. Lett.*, 1998, **39**, 4147-4150 (*synth*)
Rao, M.R. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 1301-1303 (*N-di-Me-N$^{2'}$-Ac*)
Fu, X. *et al., J. Nat. Prod.*, 1999, **62**, 1072-1073 (*7-Hydroxyceratinamine*)
Lacy, C. *et al., J. Nat. Prod.*, 2000, **63**, 119-121 (*N-Methylceratinamine*)
Schoenfeld, R.C. *et al., Bioorg. Med. Chem. Lett.*, 2002, **12**, 823-825 (*synth*)
Tilvi, S. *et al., Tetrahedron*, 2004, **60**, 10207-10215 (*Purpurealidins*)
Ravinder, K. *et al., ARKIVOC*, 2005, **iii**, 51-55 (*N-Me N′-methoxycarbonyl*)
Matsunaga, S. *et al., J.O.C.*, 2005, **70**, 1893-1896 (*N′-Methylmolokaiamine, N′-Cyano-N′-methylmolokaiamine*)

Molokinenone M-604

[169217-37-2]



$C_{20}H_{29}ClO_3$ 352.9
Isol. from a sponge, *Hyrtios* spp. Tan glass. $[\alpha]_D$ -400 (c, 0.012 in MeOH). λ_{max} 204 (ϵ 6096); 214 (ϵ 5522); 284 (ϵ 12367) (MeOH).

Nasu, S.S. *et al., J.O.C.*, 1995, **60**, 7290-7292 (*isol, uv, ir, pmr, cmr, ms*)
Urban, S. *et al., J. Nat. Prod.*, 1996, **59**, 900-901 (*config*)

Mololipids M-605

A series of fatty acid lipids with a core containing Molokaiamine, M-603. Isol. from a Hawaiian sponge of the order Verongidae. Active against HIV-1. Waxy solid. λ_{max} 240 (ϵ 1900); 277 (ϵ 650); 284 (ϵ 620) (MeOH).

Ross, S.A. *et al., J. Nat. Prod.*, 2000, **63**, 501-503 (*isol*)

Molt-inhibiting hormones M-606

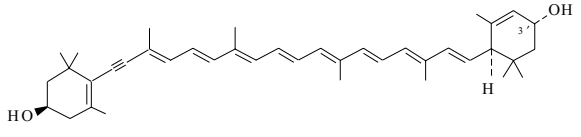
Crustacean molt-inhibiting hormones
[131571-33-0]
Peptides, members of the crustacean hyperglycemic hormone family. Struct. consists of a chain of 71-78 amino acid residues including 6 cysteines. Isol. from sinus of crustaceans, e.g. lobsters (*Homarus americanus*, *Jasus lalandii*), crabs (*Carcinus maenas*, *Cancer pagarus*), crayfish (*Procambarus clarkii*, *Procambarus bouvieri*), prawn (*Penaeus japonicus*). Reduces molting by inhibiting the secretion of ecdysteroids.

[175389-63-6, 175864-06-9, 177646-66-1, 316198-35-3, 319427-15-1, 368957-29-3]

Chang, E.S. *et al., Biochem. Biophys. Res. Commun.*, 1990, **171**, 818-826 (*Homarus americanus, isol, struct*)
Webster, S.G. *et al., Proc. R. Soc. London*, 1991, **244**, 247-252 (*Carcinus maenas*)
Nagasawa, H. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 554-556 (*Procambarus clarkii*)
Chung, J.-S. *et al., Neuropeptides (Edinburgh)*, 1996, **30**, 95-101 (*Cancer pagarus*)
Yang, Y.T. *et al., Peptides (N.Y.)*, 1996, **17**, 197-202 (*Penaeus japonicus*)
Agular, M.B. *et al., Peptides (N.Y.)*, 1996, **17**, 367-374 (*Procambarus bouvieri*)
Kawakami, T. *et al., J. Biochem. (Tokyo)*, 2000, **128**, 455-461 (*Procambarus clarkii*)
Marco, H.G. *et al., Peptides (N.Y.)*, 2000, **21**, 1313-1321 (*Jasus lalandii*)
Chang, E.S. *et al., Am. Zool.*, 2001, **41**, 380-382 (*rev*)
Katayama, H. *et al., J. Biol. Chem.*, 2003, **278**, 9620-9623 (*Penaeus japonicus, soln struct*)

Monadoxanthin M-607

7,8-Didehydro-β,ϵ-carotene-3,3′-diol
[27085-16-1]

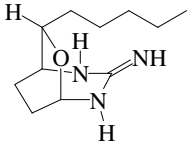


$C_{40}H_{54}O_2$ 566.865
Constit. of *Rhodomonas*, *Chroomonas* and *Cryptomonas* spp.
Cryst. (Me_2CO/petrol).
Mp 165°. λ_{max} 422; 445; 475 (hexane).

3′-Deoxy: ***Crocoxanthin***. *7,8-Didehydro-β,ϵ-caroten-3-ol. α-Crocoxanthin*
[21284-10-6]
$C_{40}H_{54}O$ 550.866
Isol. from *Cryptomonas ovata, Rhodomonas* sp. and *Hemiselmis virescens.* Large plates (C_6H_6/MeOH).
Mp 163-165°. λ_{max} 422; 445; 475 (hexane).

Chapman, D.J. *et al., Phytochemistry*, 1966, **5**, 1331 (*isol*)
Mallams, A.K. *et al., Chem. Comm.*, 1967, 301 (*struct*)
Pennington, F.C. *et al., Biochem. Syst. Ecol.*, 1985, **13**, 215 (*isol, abs config*)

Monanchorin M-608



$C_{11}H_{21}N_3O$ 211.306
Isol. from the sponge *Monanchora unguiculata*. Light yellow oil.
$[\alpha]_D^{25}$ +39 (c, 3.9 in MeOH).

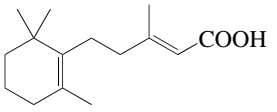
Meragelman, K.M. *et al., J. Nat. Prod.*, 2004, **67**, 1165-1167 (*isol, pmr, cmr*)

Monastatin M-609

Glycoprotein. Isol. from *Alteromonas* B-10-31 isol. from near-shore seawater of Japan. Alkaline and thiol protease inhibitor.

Imada, C. *et al., Can. J. Microbiol.*, 1985, **31**, 1089-1094 (*isol*)

Monocyclofarnesoic acid M-610



$C_{15}H_{24}O_2$ 236.353

Me ester:
$C_{16}H_{26}O_2$ 250.38
Isol. from the sponge *Halichondria panicea*. Oil.

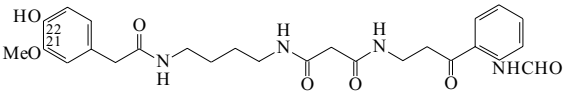
*(1-Acetoxy-3-hydroxy-2-propyl) ester (*S-*):* ***Tanyolide B***
[170312-91-1]
$C_{20}H_{32}O_5$ 352.47
Constit. of *Sclerodoris tanya*. Ichthyotoxin, feeding deterrent. Oil. $[\alpha]_D$ -3 (c, 0.1 in $CHCl_3$). λ_{max} 241 (ϵ 7140) (MeOH) (Berdy).

(1,3-Diacetoxy-2-propyl) ester: ***Tanyolide A***
[170312-92-2]
$C_{22}H_{34}O_6$ 394.507
Constit. of *Sclerodoris tanya*. Ichthyotoxin, feeding deterrent. Oil. λ_{max} 241 (ϵ 7370) (MeOH) (Berdy).

Cimino, G. *et al., Experientia*, 1973, **29**, 1063-1064 (*Me ester, isol*)
Negishi, E. *et al., J.O.C.*, 1980, **45**, 2526-2528 (*synth*)
Schmidt, C. *et al., Synthesis*, 1982, 391-393 (*synth*)
Krug, P.J. *et al., Tetrahedron*, 1995, **51**, 11063-11074 (*isol, pmr, cmr, synth*)
Graziani, E.I. *et al., Tetrahedron*, 1996, **52**, 6869-6878 (*biosynth*)

Monodontamide B M-611

[152273-62-6]



$C_{26}H_{32}N_4O_7$ 512.561
Alkaloid from the marine gastropod mollusc *Monodonta labio*. Serine protease inhibitor. Amorph. solid. λ_{max} 231 (ϵ 26600); 259 (ϵ 9830); 318 (ϵ 3930) (MeOH) (Berdy).

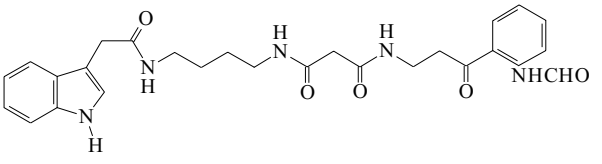
Deformyl: ***Monodontamide C***
[152273-63-7]
$C_{25}H_{32}N_4O_6$ 484.551
From *Monodonta labio*. Serine protease inhibitor. Amorph. solid. λ_{max} 226 (ϵ 32300); 256 (ϵ 6990); 281 (ϵ 3720); 365 (ϵ 6000) (MeOH) (Berdy).

21-Demethoxy, 22-deoxy: ***Monodontamide A***
[152273-61-5]
$C_{25}H_{30}N_4O_5$ 466.536
Alkaloid from *Monodonta labio*. Serine protease inhibitor. Amorph. solid. λ_{max} 229 (ϵ 15300); 258 (ϵ 6020); 318 (ϵ 2900) (MeOH) (Berdy).

Niwa, H. *et al., Tetrahedron*, 1994, **50**, 6805-6818 (*isol, uv, ir, pmr, cmr, struct, synth*)

Monodontamide D M-612

[156401-06-8]



$C_{27}H_{31}N_5O_5$ 505.572

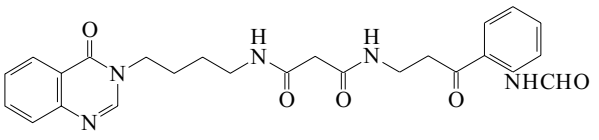
Alkaloid from the marine gastropod mollusc *Monodonta labio*. Amorph. solid.

Deformyl: ***Monodontamide E***
[156401-05-7]
$C_{26}H_{31}N_5O_4$ 477.562
From *Monodonta labio*. Amorph. solid.

Niwa, H. *et al., Tetrahedron*, 1994, **50**, 6805-6818 (*isol, uv, ir, pmr, cmr, struct, synth*)

Monodontamide F M-613

[156401-04-6]



$C_{25}H_{27}N_5O_5$ 477.519
Alkaloid from the marine gastropod mollusc *Monodonta labio*. Plates (MeOH).
Mp 129-132°.

Niwa, H. *et al., Tetrahedron*, 1994, **50**, 6805-6818 (*isol, uv, ir, pmr, cmr, struct, synth*)

Monohexyl sulfate M-614

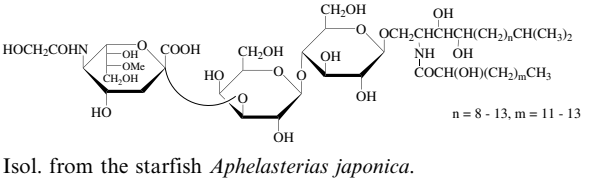
Sulfuric acid monohexyl ester, 9CI
[3233-49-6]
$H_3C(CH_2)_5OSO_3H$
$C_6H_{14}O_4S$ 182.24
Isol. from the tunicate *Sidnyum turbinatum*.

Na salt: [2207-98-9] Surfactant.
Cryst.

S-*Benzylthiouronium salt:* [34036-71-0]
Cryst. (EtOH aq.). Mp 83-84.5°.

Bair, R.K. *et al., J.A.C.S.*, 1942, **64**, 1978 (*synth*)
Musaki, M. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 3174-3179 (*synth*)
Okabayashi, H. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 1075-1077 (*Na salt, synth, Raman*)
Aiello, A. *et al., J. Nat. Prod.*, 2001, **64**, 219-221 (*isol*)

Aphelasterias japonica Monosialoganglioside M-615

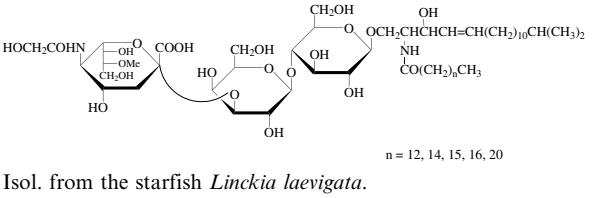


Isol. from the starfish *Aphelasterias japonica*.

[110183-18-1]

Smirnova, G.P. *et al., Biochim. Biophys. Acta*, 1987, **920**, 47-55 (*isol, struct*)

Linckia laevigata Monosialoganglioside M-616



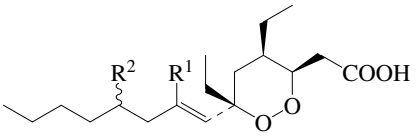
Isol. from the starfish *Linckia laevigata*.

[110183-18-1]

Smirnova, G.P. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2000, **49**, 165-168 (*isol, struct*)

Monotriajaponide B M-617

4,6-Diethyl-6-(4-methyl-1-octenyl)-1,2-dioxane-3-acetic acid



R^1 = H, R^2 = CH_3

$C_{19}H_{34}O_4$ 326.475
Isol. from the sponge *Monotria japonica*. Selectively lyses starfish oocytes. Viscous oil. $[\alpha]_D^{25}$ +127 (c, 0.52 in $CHCl_3$).

Yanai, M. *et al., Bioorg. Med. Chem.*, 2003, **11**, 1715-1721 (*isol, cd, pmr, cmr*)

Monotriajaponide C M-618

As Monotriajaponide B, M-617 with
R^1 = R^2 = CH_3

$C_{20}H_{36}O_4$ 340.502
Isol. from the sponge *Monotria japonica*. Selectively lyses starfish oocytes. Viscous oil. $[\alpha]_D^{25}$ +64 (c, 0.6 in $CHCl_3$).

Yanai, M. *et al., Bioorg. Med. Chem.*, 2003, **11**, 1715-1721 (*isol, cd, pmr, cmr*)

Monotriajaponide D M-619

As Monotriajaponide B, M-617 with
R^1 = CH_3, R^2 = CH_2CH_3

$C_{21}H_{38}O_4$ 354.529
Isol. from the sponge *Monotria japonica*. Selectively lyses starfish oocytes. Viscous oil. $[\alpha]_D^{25}$ +108 (c, 0.9 in $CHCl_3$).

Yanai, M. *et al., Bioorg. Med. Chem.*, 2003, **11**, 1715-1721 (*isol, cd, pmr, cmr*)

Montiporic acid A M-620

(2,4-Dodecadiynyloxy)acetic acid, 9CI
[179600-04-5]
$H_3C(CH_2)_6C{\equiv}CC{\equiv}CCH_2OCH_2COOH$
$C_{14}H_{20}O_3$ 236.31
Isol. from the eggs of the coral *Montipora digitata*. Exhibits antibacterial and cytotoxic activities. Feeding attractant for *Drupella cornus*. Oil. λ_{max} 255 (ϵ 1059); 273 (ϵ 799) (MeOH).

Me ester: ***Methyl montiporate A***
[362677-44-9]
$C_{15}H_{22}O_3$ 250.337
Isol. from *Montipora* sp. Cytotoxic. Yellow oil.

11′,12′-Didehydro: (11-Dodecene-2,4-diynyloxy)acetic acid. ***Montiporic acid C***
[363136-46-3]
[362677-46-1]
$C_{14}H_{18}O_3$ 234.294
Isol. from *Montipora* sp. Cytotoxic. Light yellow solid (as Na salt).

11′,12′-Didehydro, Me ester: ***Methyl montiporate C***
$C_{15}H_{20}O_3$ 248.321
Isol. from *Montipora* sp. Cytotoxic. Light yellow oil. λ_{max} 226 (log ϵ 3.76); 286 (log ϵ 3.4) (MeOH).

Fusetani, N. *et al., J. Nat. Prod.*, 1996, **59**, 796-797 (*isol, uv, ir, pmr, cmr*)
Stefani, H.A. *et al., Tet. Lett.*, 1999, **40**, 9215-9217 (*synth*)
Alam, N. *et al., J. Nat. Prod.*, 2001, **64**, 1059-1063 (*Me ester, Montiporic acid C*)
Alam, N. *et al., Chem. Pharm. Bull.*, 2002, **50**, 661-662 (*Methyl montiporate C*)
Kita, M. *et al., Tet. Lett.*, 2005, **46**, 8583-8585 (*isol, activity*)

Montiporic acid B M-621

(13-Tetradecene-2,4-diynyloxy)acetic acid, 9CI
[179600-05-6]
$H_2C{=}CH(CH_2)_7C{\equiv}CC{\equiv}CCH_2OCH_2COOH$

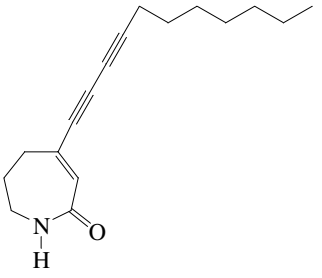
$C_{16}H_{22}O_3$ 262.348
Isol. from the eggs of the coral *Montipora digitata*. Exhibits antibacterial and cytotoxic activities. Oil. λ_{max} 256 (ϵ 861); 273 (ϵ 668) (MeOH).

Me ester: ***Methyl montiporate B***
$C_{17}H_{24}O_3$ 276.375
Isol. from *Montipora* sp. Cytotoxic. Yellow oil.

Fusetani, N. *et al., J. Nat. Prod.*, 1996, **59**, 796-797 (*isol, uv, ir, pmr, cmr*)
Stefani, H.A. *et al., Tet. Lett.*, 1999, **40**, 9215-9217 (*synth*)
Alam, N. *et al., J. Nat. Prod.*, 2001, **64**, 1059-1063 (*Me ester*)

Montiporyne E M-622

*1,5,6,7-Tetrahydro-4-(1,3-undecadiynyl)-2*H*-azepin-2-one*

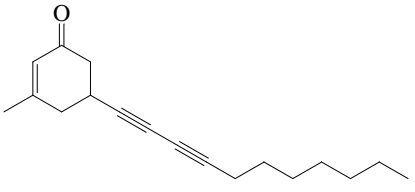


$C_{17}H_{23}NO$ 257.375
Isol. from the stony coral *Montipora* sp. Cytotoxic agent. Pale yellow gum.

Bae, B.H. *et al., J. Nat. Prod.*, 2000, **63**, 1511-1514

Montiporyne F M-623

3-Methyl-5-(1,3-undecadiynyl)-2-cyclohexen-1-one

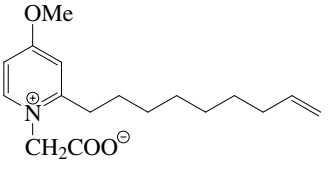


$C_{18}H_{24}O$ 256.387
Isol. from the stony coral *Montipora* sp. Cytotoxic agent. Pale yellow gum.

Bae, B.H. *et al., J. Nat. Prod.*, 2000, **63**, 1511-1514

Montipyridine M-624

1-Carboxymethyl-4-methoxy-2-(8-nonenyl)pyridinium
[352230-21-8]



$C_{17}H_{25}NO_3$ 291.389
Alkaloid from the stony coral *Montipora* sp. Light brown solid.

Alam, N. *et al., J. Nat. Prod.*, 2001, **64**, 956-957 (*isol, pmr, cmr*)
Fürstner, A. *et al., J.A.C.S.*, 2002, **124**, 13856-13863 (*synth*)

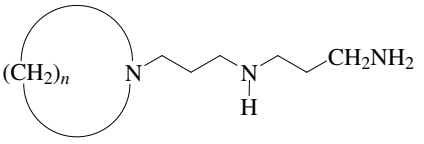
Morulin Pm M-625

Modified polypeptide containing 6-Bromotryptophan and 2-Amino-3-(3,4,5-trihydroxyphenyl)propanoic acid, A-422. MW *ca.* 3825. Isol. from the morula cells of the ascidian *Phallusia mammillata*.

Taylor, S.W. *et al., Arch. Biochem. Biophys.*, 1997, **348**, 278-288 (*isol, pmr, cmr*)

Motuporamine A M-626

N-*(3-Azacyclotridec-1-ylpropyl)-1,3-propanediamine, 9CI*
[211566-77-7]



n = 12

$C_{18}H_{39}N_3$ 297.526
Alkaloid from the sponge *Xestospongia exigua*. Cytotoxic agent. Oil (as di-Ac).

Goldring, W.P.D. *et al., Org. Lett.*, 1999, **1**, 1471-1473 (*synth, struct*)
Baldwin, J.E. *et al., Tet. Lett.*, 1999, **40**, 5401-5404 (*synth*)
Williams, D.E *et al., J.O.C.*, 2002, **67**, 245-258 (*isol, pmr, cmr, activity*)

Motuporamine B M-627

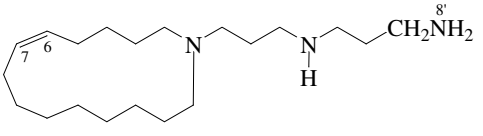
[211566-78-8]
As Motuporamine A, M-626 with
n = 13
$C_{19}H_{41}N_3$ 311.553
Alkaloid from the sponge *Xestospongia exigua*. Cytotoxic agent. Oil (as di-Ac).

5Z,6-Didehydro: N-*[3-(Azacyclotetradec-5-en-1-yl)propyl]-1,3-propanediamine.* ***Motuporamine D***
[398144-67-7]
$C_{19}H_{39}N_3$ 309.537
Alkaloid from *Xestospongia exigua*. Oil.

Williams, D.E. *et al., J.O.C.*, 1998, **63**, 4838-4841; 2002, **67**, 245-258 (*Motuporamines B,D, isol, pmr, cmr, activity*)
Goldring, W.P.D. *et al., Org. Lett.*, 1999, **1**, 1471-1473 (*synth, struct*)
Baldwin, J.E. *et al., Tet. Lett.*, 1999, **40**, 5401-5404 (*synth*)

Motuporamine C M-628

[211569-34-5]



$C_{20}H_{41}N_3$ 323.564
Alkaloid from the sponge *Xestospongia exigua*. Cytotoxic agent. Oil (as di-Ac).

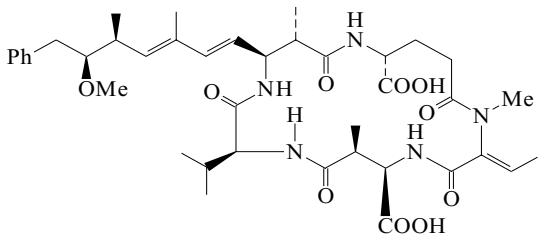
$N^{8'}$*-Formyl:* ***Motuporamine F***
[398144-69-9]
$C_{21}H_{41}N_3O$ 351.574
Alkaloid from *Xestospongia exigua*. Oil (as di-Ac).

9Z,10-Didehydro: ***Motuporamine E***
[398144-68-8]
$C_{20}H_{39}N_3$ 321.548
Alkaloid from *Xestospongia exigua*. Oil.

Williams, D.E. *et al., J.O.C.*, 1998, **63**, 4838-4841; 2002, **67**, 245-258 (*Motuporamines C,E,F, isol, pmr, cmr, activity*)
Goldring, W.P.D. *et al., Org. Lett.*, 1999, **1**, 1471-1473 (*synth, struct*)
Fuerstner, A. *et al., J.O.C.*, 2000, **65**, 2608-2611 (*synth*)

Motuporin M-629

Nodularin 5. [Val^2]nodularin
[141672-08-4]



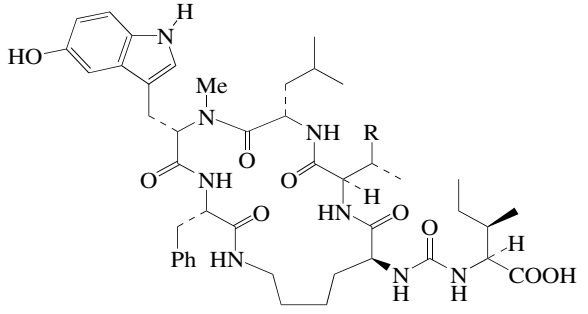
$C_{40}H_{57}N_5O_{10}$ 767.918

Cyclic pentapeptide antibiotic. Isol. from the sponge *Theonella swinhoei*. Protein phosphatase inhibitor. Cytotoxic and hepatotoxic agent. Glass. $[\alpha]_D$ -83.8. λ_{max} 238 (ϵ 30000) (MeOH) (Derep).

de Silva, E.D. *et al., Tet. Lett.*, 1992, **33**, 1561-1564 (*isol, pmr, cmr, struct*)
Bauer, S.M. *et al., J.A.C.S.*, 1999, **121**, 6355-6366 (*synth*)
Samy, R. *et al., J.O.C.*, 1999, **64**, 2711-2727 (*synth, pmr*)
Hu, T. *et al., J.A.C.S.*, 2002, **124**, 11368-11378 (*synth*)

Mozamide A M-630

[193064-60-7]



R = CH_3

$C_{45}H_{64}N_8O_9$ 861.049

Cyclic peptide. Isol. from a Theonellid sponge. Powder. $[\alpha]_D$ -66 (c, 0.02 in MeOH). λ_{max} 208 (ϵ 19600); 268 (ϵ 2600) (MeOH).

Schmidt, E.W. *et al., J. Nat. Prod.*, 1997, **60**, 779-782 (*isol, uv, ir, pmr, cmr*)

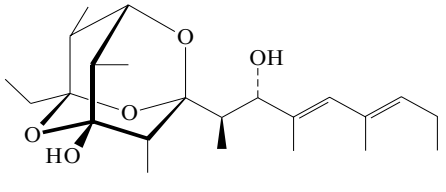
Mozamide B M-631

[193064-61-8]
As Mozamide A, M-630 with
R = CH_2CH_3
$C_{46}H_{66}N_8O_9$ 875.076
Isol. from a Theonellid sponge. Powder. $[\alpha]_D$ -33 (c, 0.02 in MeOH). λ_{max} 208 (ϵ 19600); 268 (ϵ 2600) (MeOH).

Schmidt, E.W. *et al., J. Nat. Prod.*, 1997, **60**, 779-782 (*isol, uv, ir, pmr, cmr*)

Muamvatin M-632

[104013-99-2]



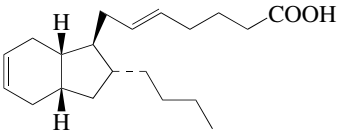
$C_{23}H_{38}O_5$ 394.55

Isol. from the Fijian mollusc *Siphonaria normalis*. Oil. $[\alpha]_D^{25}$ +61.1 (c, 0.175 in CH_2Cl_2). λ_{max} 236 (ϵ 10200) (CH_2Cl_2) (Derep).

Roll, D.M. *et al., J.A.C.S.*, 1986, **108**, 6680-6682 (*occur, pmr, cmr, ir, uv*)
Paterson, I. *et al., J.A.C.S.*, 1993, **115**, 1608 (*synth*)
Hoffmann, R.W. *et al., Tet. Lett.*, 1993, **34**, 1115-1118 (*abs config*)
Dahmann, G. *et al., Annalen*, 1994, 837 (*abs config*)

Mucosin M-633

[191480-35-0]



$C_{20}H_{32}O_2$ 304.472
Isol. from the sponge *Reniera mucosa*.
$[\alpha]_D$ -35.5 (c, 0.8 in hexane) (as Me ester).

Casapullo, A. *et al., Tet. Lett.*, 1997, **38**, 3643-3646 (*isol, pmr, cmr*)

Mugiline β M-634

[53240-94-1]

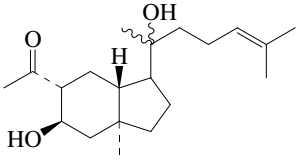
H-Pro-[Arg]$_4$-Glu-Thr-Ser-Arg-Pro-Ile-[Arg]$_5$-Ala-Arg-Arg-Ala-Pro-Ile-[Arg]$_5$-Val-Val-[Arg]$_4$-OH
Polypeptide complex consisting of at least 7 components, M1 → M7. Struct. of M6 shown. Isol. from the mature sperm nuclei of the Formosan grey mullet, *Mugil japonicus*.

[110734-13-9, 110734-14-0, 110734-15-1, 110734-16-2]

Okamoto, Y. *et al., J. Biochem. (Tokyo)*, 1987, **101**, 1017 (*struct*)

Mugipolasol M-635

[215440-73-6]



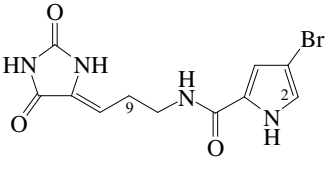
$C_{20}H_{34}O_3$ 322.487

An abeo-sphenolobane. Constit. of an *Epipolasis* sp. Oil. $[\alpha]_D^{25}$ +31.7 (c, 1.7 in $CHCl_3$).

Umeyama, A. *et al., J. Nat. Prod.*, 1998, **61**, 1435-1436 (*isol, pmr, cmr*)

Mukanadin B M-636

[250782-32-2]



$C_{11}H_{11}BrN_4O_3$ 327.137

Similar to Midpacamide, M-565. Isol. from the sponges *Agelas nakamurai* and *Axinella verrucosa*. Amorph. solid. λ_{max} 274 (ϵ 6700) (MeOH).

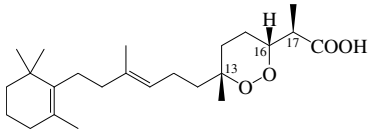
9-Hydroxy: ***9-Hydroxymukanadin B***
$C_{11}H_{11}BrN_4O_4$ 343.136
Isol. from *Axinella verrucosa*.

2-Bromo: ***Mukanadin D***
[193619-42-0]
$C_{11}H_{10}Br_2N_4O_3$ 406.033
Isol. from the sponge *Didiscus oxeata*.

Lindel, T. *et al., Liebigs Ann./Recl.*, 1997, 1525-1528 (*synth*)
Uemoto, H. *et al., J. Nat. Prod.*, 1999, **62**, 1581-1583 (*isol, pmr, cmr*)
Hu, J.-F. *et al., J. Chem. Res., Synop.*, 2005, 427-428 (*Mukanadin D*)
Aiello, A. *et al., Bioorg. Med. Chem.*, 2006, **14**, 17-24 (*9-Hydroxymukanadin B*)

Muqubilin M-637

Prianicin A



(13*R*,16*R*,17*R*)-*form*

$C_{24}H_{40}O_4$ 392.578

Terpene antibiotic.

(13*R*,16*R*,17*R*)-*form*

Epimuqubilin A

Constit. of *Diacarnus* cf. *spinopoculum*.
Yellow oil. $[\alpha]_D$ +61.7 (c, 0.7 in $CHCl_3$).

(13*R*,16*S*,17*R*)-*form*

Muqubilin A. ent-*Muqubilin*
Prod. by *Diacarnus* cf. *spinopoculum*.
Yellow oil. $[\alpha]_D$ -35.6 (c, 9.8 in $CHCl_3$).

(13*S*,16*R*,17*S*)-*form* [72154-33-7]

Constit. of *Prianos* sp. Active against streptococci, fungi and yeasts, inhibits the cell division of sea urchin eggs. Yellow oil. $[\alpha]_D$ +31.6 (c, 0.18 in $CHCl_3$).

Benzyl ester: [211239-41-7]
$C_{31}H_{46}O_4$ 482.702
Constit. of *Diacarnus levii*.
$[\alpha]_D^{25}$ -24.8 (c, 0.33 in $CHCl_3$).

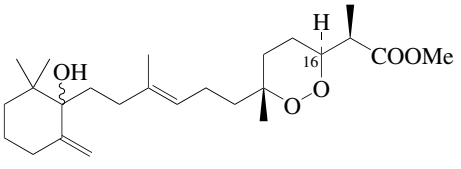
(13*S*,16*S*,17*S*)-*form*

Prod. by an unidentified sponge.
Oil (as Me ester). $[\alpha]_D^{25}$ -59.2 (c, 5.75 in $CHCl_3$) (Me ester).

Kashman, Y. *et al., Tet. Lett.*, 1979, 1707-1708 (*isol*)
Sokoloff, S. *et al., Experientia*, 1982, **38**, 337-338 (*isol*)
Manes, L.V. *et al., Tet. Lett.*, 1984, **25**, 931-934 (*isol*)
Capon, R.J. *et al., Tetrahedron*, 1985, **41**, 3391-3404 (*abs config*)
D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1998, **81**, 1285-1292 (*benzyl ester*)
Sperry, S. *et al., J. Nat. Prod.*, 1998, **61**, 241-247 (*Muqubilin A, Epimuqubilin A*)

Muqubilin B M-638

[204500-42-5]



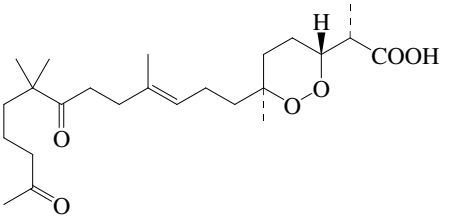
$C_{25}H_{42}O_5$ 422.604
Constit. of *Diacarnus* cf. *spinopoculum*. Oil. $[\alpha]_D$ -15.5 (c, 0.54 in $CHCl_3$).

16-Epimer: ***Epimuqubilin B***
[204500-43-6]
$C_{25}H_{42}O_5$ 422.604
Constit. of *Diacarnus* cf. *spinopoculum*. Oil.

Sperry, S. *et al., J. Nat. Prod.*, 1998, **61**, 241-247 (*isol, pmr, cmr*)

Muqubilone M-639

Aikupikoxide A
[340156-50-5]

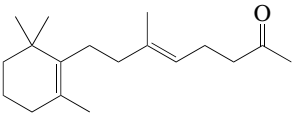


$C_{24}H_{40}O_6$ 424.576
Constit. of a red sponge *Diacarnus erythraeanus*. Oil. $[\alpha]_D^{25}$ +48 (c, 0.1 in $CHCl_3$). $[\alpha]_D$ +81 (c, 0.8 in CH_2Cl_2). Related to Muqubilin, M-637. λ_{max} 229 (log ϵ 2.72); 257 (log ϵ 2.41) (MeOH).

El Sayed, K.A. *et al., J. Nat. Prod.*, 2001, **64**, 522-524 (*isol, pmr, cmr*)
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2001, **64**, 1332-1335 (*isol, pmr, cmr*)

Muquketone M-640

10,15-Cyclo-1,2-dinor-6,10-phytadien-3-one
[1150-17-0]

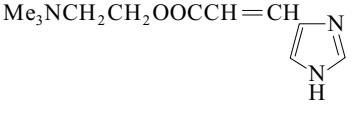


$C_{18}H_{30}O$ 262.434
Constit. of sponge *Diacarnus* cf. *spinopoculum*. Oil.

Sperry, S. *et al., J. Nat. Prod.*, 1998, **61**, 241-247 (*isol, pmr, cmr*)

Murexine M-641

*2-[[3-(1*H*-Imidazol-4-yl)-1-oxo-2-propenyl]oxy]*-N,N,N-*trimethylethanaminium(1+), 9CI. Choline imidazole-4-acrylate. Choline urocanate*
[20284-40-6]



$C_{11}H_{18}N_3O_2^{\oplus}$ 224.282
Found in large amts. in the hypobranchial glands of molluscs, esp. *Murex* spp., and also *Concholepas concholepas* and *Tritonalia erinacea*. Muscle relaxant with strong curariform action. Cholinesterase inhibitor. Sol. H_2O. pK_a 4.6. λ_{max} 285 (ϵ 16700) (pH 4.5 buffer) (Berdy).

Chloride: [6209-43-4]
$C_{11}H_{18}ClN_3O_2$ 259.735
Hygroscopic cryst. + $1H_2O$. Unstable, instantly hydrol. by H_2O.

Chloride; hydrochloride:
Microcryst. powder + ½ H_2O. Mp 219-221° dec. Hygroscopic.

Dipicrate:
Yellow needles (H_2O). Mp 221-222° dec.

N-*Me:* **N-*Methylmurexine***
$C_{12}H_{20}N_3O_2^{\oplus}$ 238.309
Reported to occur in the marine gastropod mollusc *Nucella emarginata*. Struct. assignment prob. incorrect. A recent unambiguous synth. of the two possible *N*-Me derivs. of Murexine indicates that the natural compd. is neither of these.

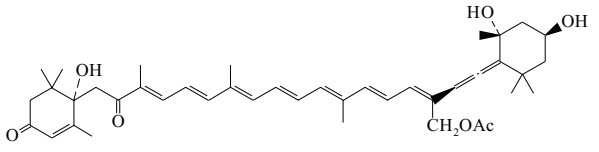
1-Me, iodide:
Synthetic. Cryst. (MeOH). Mp 224-225°.

3-Me, iodide:
Synthetic. Mp 224°.

Erspamer, V. *et al., Arch. Int. Pharmacodyn. Ther.*, 1947, **74**, 263; *CA*, **43**, 1491b (*isol*)
Pasini, C. *et al., Annalen*, 1952, **578**, 6 (*synth, uv*)
Roseghini, M. *et al., Eur. J. Biochem.*, 1970, **12**, 468 (*isol*)
Bender, J.A. *et al., Comp. Gen. Pharmacol.*, 1974, **5**, 191 (*deriv*)
Duke, C.C. *et al., Tet. Lett.*, 1978, 5047 (*synth, pmr*)

Muricellaxanthin M-642

19-Acetoxy-6,7-didehydro-5,6,7′,8′-tetrahydro-3,5,6′-trihydroxy-β,ϵ-carotene-3′,8′-dione. 19′-Acetoxy-4,5,6′,7′-tetrahydro-5,5′,6,6′,7,8-hexahydro-3′,5′,6-trihydroxy-3,8-dioxo-β,β-carotene
[178460-53-2]

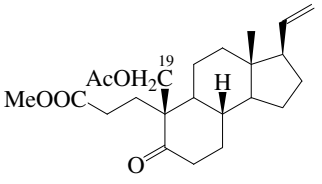


$C_{42}H_{56}O_7$ 672.9
Constit. of a *Muricella* sp. Amorph. red solid.
Mp 86-87°. $[\alpha]_D$ -8.9 (c, 0.3 in MeOH).

Rho, J.-R. *et al., Bull. Korean Chem. Soc.*, 1996, **17**, 529-531; *CA*, **125**, 82261x (*isol, pmr, cmr*)

Muricenone A M-643

[479197-79-0]



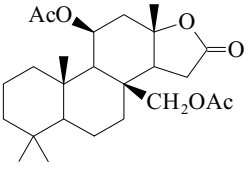
$C_{23}H_{34}O_5$ 390.519
Constit. of a *Muricea* sp. Oil. $[\alpha]_D^{25}$ +24 (c, 0.1 in $CHCl_3$).

19-Deacetoxy: ***Muricenone B***
[479197-80-3]
$C_{21}H_{32}O_3$ 332.482
Constit. of a *Muricea* sp. Oil. $[\alpha]_D^{25}$ +15 (c, 0.1 in $CHCl_3$).

Ortega, M.J. *et al., Eur. J. Org. Chem.*, 2002, 3250-3253 (*isol, pmr, cmr*)

Murrayanolide M-644

[173994-03-1]

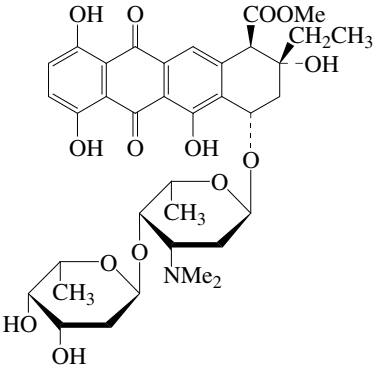


$C_{25}H_{38}O_6$ 434.572
Constit. of *Dendrobeania murrayana*. Collagenase Iv inhibitor. Powder.
Mp 185-187°. $[\alpha]_D^{25}$ -16.6 (c, 0.75 in $CHCl_3$).

Yu, C.-M. *et al., J. Nat. Prod.*, 1995, **58**, 1978 (*isol, pmr, cmr*)

Musettamycin M-645

MA 144S_2. Antibiotic MA 144S_2. Aclacinomycin S_2. Pyrrocycline A
[63710-09-8]



Absolute Configuration

$C_{36}H_{45}NO_{14}$ 715.75
Anthracycline antibiotic. Isol. from *Actinosporangium* spp., *Streptomyces galilaeus* and marine *Streptomyces* sp. B8904. Antitumour agent. Dark red plates.
Mp 162-163°.
▶ QI9283000

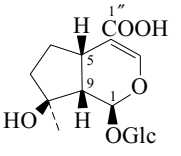
N-*De-Me:* ***Schaunardimycin***
[93423-02-0]
$C_{35}H_{43}NO_{14}$ 701.723
Prod. by *Actinosporangium bohemicum*. Shows antitumour activity. Dark red amorph. solid.

1-Epimer: ***Collinemycin***
[72598-49-3]
$C_{36}H_{45}NO_{14}$ 715.75
From *Actinosporangium bohemicum* . Active against gram-positive bacteria and tumours. Red solid + H_2O.
Mp 139-141° dec. Possible artifact. λ_{max} 257 (ϵ 22600); 288 (ϵ 9300); 296 (ϵ 9090); 484 (ϵ 13800); 494 (ϵ 14700); 514 (ϵ 11200); 528 (ϵ 9600) (MeOH) (Berdy).
▶ QI9281700

Nettleton, D.E. *et al., J. Antibiot.*, 1977, **30**, 525 (*isol, struct, ir, uv, nmr, ms*)
Oki, T. *et al., J. Antibiot.*, 1979, **32**, 791; 801 (*isol, props*)
Doyle, T.W. *et al., J.A.C.S.*, 1979, **101**, 7041 (*cmr, struct*)
Nettletton, D.E. *et al., J. Nat. Prod.*, 1980, **43**, 242; 1984, **47**, 698 (*isol, struct, ir, uv, pmr, ms, derivs*)
Matsuzawa, T. *et al., J. Antibiot.*, 1981, **34**, 1596 (*props*)
Monneret, C. *et al., J. Carbohydr. Chem.*, 1988, **7**, 417-434 (*partial synth*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, APV000

Mussaenosidic acid M-646

[82451-22-7]



$C_{16}H_{24}O_{10}$ 376.36
Constit. of *Melampyrum cristatum*. Foam. $[\alpha]_D^{20}$ -118 (c, 0.7 in MeOH).

2′-Cinnamoyl: ***2′-Cinnamoylmussaenosidic acid***
[97857-25-5]
$C_{25}H_{30}O_{11}$ 506.505
Constit. of *Avicennia germinans, Avicennia officinalis* and *Avicennia marina*. Syrup.

*8-Cinnamoyl(*E-*): 8*-O-*Cinnamoylmussaenosidic acid*
[176226-56-5]
$C_{25}H_{30}O_{11}$ 506.505
Constit. of *Avicennia officinalis*.
$[\alpha]_D^{25}$ -8.5 (c, 0.5 in $CHCl_3$) (tetra-Ac).

2′-O-*(4-Hydroxy*-E-*cinnamoyl):* [194234-73-6]
$C_{25}H_{30}O_{12}$ 522.505
Constit. of *Avicennia germinans*. Syrup.

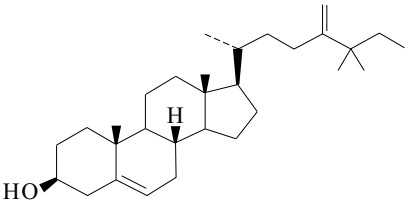
2′-O-*(4-Hydroxy*-Z-*cinnamoyl):* ***2′-Coumaroylmussaenosidic acid***
[273410-51-8]
$C_{25}H_{30}O_{12}$ 522.505
Constit. of *Avicennia germinans*.

2′-O-*(3,4-Dihydroxy*-E-*cinnamoyl):* ***2′-Caffeoylmussaenosidic acid***
[163496-26-2]
$C_{25}H_{30}O_{13}$ 538.504
Constit. of *Avicennia germinans*. Syrup.

König, G. *et al., Phytochemistry*, 1985, **24**, 1245-1248 (*Avicennia marina constit*)
König, G. *et al., Phytochemistry*, 1987, **26**, 423-427 (*2′-Cinnamoylmussaenosidic acid*)
Fauvel, M.-T. *et al., Phytochemistry*, 1995, **38**, 893-894 (*Avicennia germinans constits*)
Sharma, M. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 459 (*8-cinnamoyl*)
Fauvel, M. *et al., Nat. Prod. Lett.*, 1997, **10**, 139-142; 1999, **14**, 99-106 (*2′-caffeoyl, 2′-coumaroyl*)

Mutasterol M-647

25-Ethylergosta-5,24(28)-dien-3β-ol, 9CI. 25-Ethyl-24-methylene-cholest-5-en-3β-ol. 25,26-Dimethyl-24-methylenecholest-5-en-3-ol. 25,26-Dimethylergosta-5,24(28)-dien-3-ol
[75886-12-3]

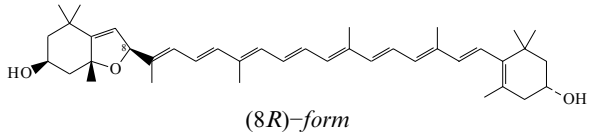


$C_{30}H_{50}O$ 426.724
Constit. of *Xestospongia muta*. Cryst. (MeOH).
Mp 146-148°. $[\alpha]_D^{25}$ -26 (c, 0.29 in $CHCl_3$).

Li, L.N. *et al., J.A.C.S.*, 1981, **103**, 115
Kerr, R.G. *et al., J.O.C.*, 1991, **56**, 63 (*biosynth*)

Mutatoxanthin M-648

5,8-Epoxy-5,8-dihydro-β,β-carotene-3,3′-diol. Cryptoxanthin 5,8-epoxide
[31661-06-0]



(8*R*)–*form*

$C_{40}H_{56}O_3$ 584.881
Poss. isol. from *Prunus persica* (peach), *Diospyros kaki* (persimmon), *Medicago* spp. and *Averrhoa carambola*. Leaves (C_6H_6/petrol).
Mp 171°. Natural occurrence poorly documented, poss. artifact.

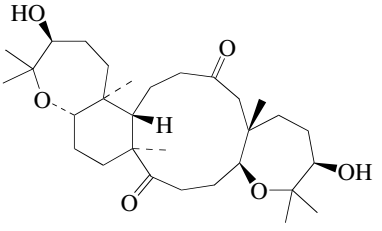
(8*R*)-*form* [85201-99-6]
Constit. of *Corallina* spp. and ripe rose hips. Post-mortem artifact from the red alga *Erythrotrichia carnea*.

(8*S*)-*form* [85202-00-2]
Constit. of *Corallina* spp., rose hips and *Erythrotrichia carnea*.
Light orange cryst.
Mp 213°.

Karrer, P. *et al., Helv. Chim. Acta*, 1946, **29**, 229 (*synth*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1982, **65**, 2198; 1983, **66**, 494 (*isol, pmr*)
Bjrnland, T. *et al., Phytochemistry*, 1984, **23**, 1711 (*isol*)
Palermo, J.A. *et al., Phytochemistry*, 1991, **30**, 2983 (*isol, pmr, cmr*)

Muzitone M-649

[233607-65-3]

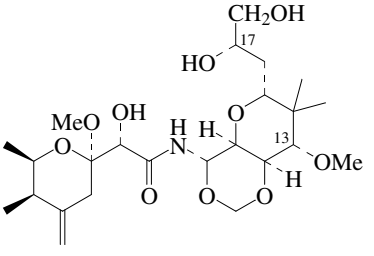


$C_{30}H_{50}O_6$ 506.721
Constit. of *Ptilocaulis spiculifer*. Oil. $[\alpha]_D$ -14.2 (c, 0.1 in MeOH). Possibly derived from Abudinol B.

Rudi, A. *et al., Tetrahedron*, 1999, **55**, 5555-5566 (*isol, pmr, cmr*)

Mycalamide A M-650

[115185-92-7]



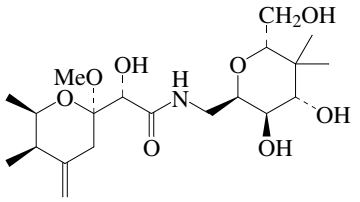
$C_{24}H_{41}NO_{10}$ 503.589
Polyether-type antibiotic. Isol. from the sponge *Mycale* sp. Antiviral and antitumour agent. Undergoing preclinical trials at U.S. Natl. Cancer Inst. (1994). Oil. $[\alpha]_{365}$ +110 (c, 0.2 in $CHCl_3$). Related to Pederin and Onnamide A, O-107.

17-Me ether: ***Mycalamide B***
[124512-46-5]
$C_{25}H_{43}NO_{10}$ 517.615
Isol. from *Mycale* sp. Antiviral and antitumour agent. Oil.
$[\alpha]_D$ +39 (c, 0.2 in $CHCl_3$).

13-O-*De-Me:* ***Mycalamide D***
$C_{23}H_{39}NO_{10}$ 489.562
Isol. from a *Mycale* sp. and a *Stylinos* sp. Cytotoxic agent. Oil.
$[\alpha]_D^{20}$ +41 (c, 0.3 in $CHCl_3$).

Perry, N.B. *et al., J.O.C.*, 1990, **55**, 223 (*isol, pmr, conformn, struct*)
Hong, C.Y. *et al., J.O.C.*, 1990, **55**, 4242 (*synth, abs config*)
Thompson, A.M. *et al., J.C.S. Perkin 1*, 1992, 1335 (*derivs, props*)
Kocienski, P. *et al., J.O.C.*, 1996, **61**, 1797 (*synth*)
Simpson, J.S. *et al., J. Nat. Prod.*, 2000, **63**, 704-706 (*Mycalamide D*)
West, L.M. *et al., J. Nat. Prod.*, 2000, **63**, 707-709 (*Mycalamide D*)
Kocienski, P. *et al., J.C.S. Perkin 1*, 2000, 2357-2384 (*Mycalamide B, synth*)
Roush, W.R. *et al., Org. Lett.*, 2000, **2**, 858-862 (*synth*)
Hood, K.A. *et al., Apoptosis*, 2001, **6**, 207-219 (*Mycalamide A, activity*)
Trost, B.M. *et al., J.A.C.S.*, 2004, **126**, 48-49 (*synth*)
Sohn, J.-H. *et al., J.A.C.S.*, 2005, **127**, 7290-7291 (*synth*)
Kagawa, N. *et al., J.O.C.*, 2006, **71**, 6796-6805 (*synth*)

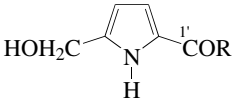
Mycalamide C M-651



$C_{20}H_{35}NO_8$ 417.498
Isol. from a sponge *Stylinos* sp. Cytotoxic agent.

Simpson, J.S. *et al., J. Nat. Prod.*, 2000, **63**, 704-706

Mycalazoles M-652



Mycalazole	R
1	$(CH_2)_5(CH{=}CHCH_2)_6CH_3$
2	$(CH_2)_{10}(CH{=}CHCH_2)_3CH_3$
3	$(CH_2)_9(CH{=}CHCH_2)_4CH_3$
4	$(CH_2)_{12}(CH{=}CH(CH_2)_3CH_3$
7	$(CH_2)_{14}CH(CH_3)_2$
10	$(CH_2)_{12}CH{=}CH(CH_2)_5CH_3$

All double bonds have *Z*-config. Metabs. from the sponge *Mycale micracanthoxea*. Cytotoxic agents.

Mycalazole 1
*1-[5-(Hydroxymethyl)-1*H*-pyrrol-2-yl]-7,10,13,16,19,22-pentacosahexaen-1-one, 9CI*
[185387-05-7]
$C_{30}H_{43}NO_2$ 449.675
Oil. λ_{max} 201 (ϵ 4170); 247 (ϵ 1581); 294 (ϵ 7656) (MeOH).

*7′,8′-Dihydro: 1-[5-(Hydroxymethyl)-1*H*-pyrrol-2-yl]-10,13,16,19,22-pentacosapentaen-1-one, 9CI.* ***Mycalazole 5***
[185389-23-5]
$C_{30}H_{45}NO_2$ 451.691
Oil. λ_{max} 204 (ϵ 11230); 250 (ϵ 2122); 296 (ϵ 10003) (MeOH).

*7′,8′,10′,11′-Tetrahydro: 1-[5-(Hydroxymethyl)-1*H*-pyrrol-2-yl]-13,16,19,22-pentacosatetraen-1-one, 9CI.* ***Mycalazole 9***
[185389-50-8]
$C_{30}H_{47}NO_2$ 453.707
Oil. λ_{max} 203 (ϵ 10145); 251 (ϵ 1580); 293 (ϵ 13110) (MeOH).

Mycalazole 2
*1-[5-(Hydroxymethyl)-1*H*-pyrrol-2-yl]-12,15,18-heneicosatrien-1-one, 9CI*
[185387-07-9]
$C_{26}H_{41}NO_2$ 399.615
Oil. λ_{max} 202 (ϵ 8490); 238 (ϵ 6912); 296 (ϵ 16584) (MeOH).

*18′,19′-Dihydro: 1-[5-(Hydroxymethyl)-1*H*-pyrrol-2-yl]-12,15-heneicosadien-1-one, 9CI.* ***Mycalazole 6***
[185389-27-9]
$C_{26}H_{43}NO_2$ 401.631
Oil. λ_{max} 204 (ϵ 7452); 294 (ϵ 9470) (MeOH).

Mycalazole 3
*1-[5-(Hydroxymethyl)-1*H*-pyrrol-2-yl]-11,14,17,20-tricosatetraen-1-one, 9CI*
[185388-42-5]
$C_{28}H_{43}NO_2$ 425.653
Oil. λ_{max} 206 (ϵ 11045); 246 (ϵ 2332); 295 (ϵ 10106) (MeOH).

*11′,12′-Dihydro: 1-[5-(Hydroxymethyl)-1*H*-pyrrol-2-yl]-14,17,20-tricosatrien-1-one, 9CI.* ***Mycalazole 8***
[185389-47-3]
$C_{28}H_{45}NO_2$ 427.669
Oil. λ_{max} 201 (ϵ 9128); 240 (ϵ 4312); 295 (ϵ 16348) (MeOH).

*11′,12′,20′,21′-Tetrahydro: 1-[5-(Hydroxymethyl)-1*H*-pyrrol-2-yl]-14,17-tricosadien-1-one, 9CI.* ***Mycalazole 12***
[185389-63-3]
$C_{28}H_{47}NO_2$ 429.685
Oil. λ_{max} 203 (ϵ 7852); 295 (ϵ 8864) (MeOH).

Mycalazole 4
*1-[5-(Hydroxymethyl)-1*H*-pyrrol-2-yl]-14-nonadecen-1-one, 9CI*
[185389-09-7]
$C_{24}H_{41}NO_2$ 375.593
Cryst. (MeOH). Mp 68-70°. λ_{max} 206 (ϵ 10492); 252 (ϵ 1106); 292 (ϵ 13105) (MeOH).

*14′,15′-Dihydro: 1-[5-(Hydroxymethyl)-1*H*-pyrrol-2-yl]-1-nonadecanone, 9CI.* ***Mycalazole 11***
[185389-61-1]
$C_{24}H_{43}NO_2$ 377.609
Amorph. powder. λ_{max} 204 (ϵ 7452); 294 (ϵ 9470) (MeOH).

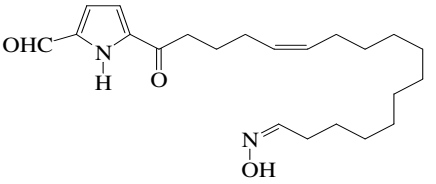
Mycalazole 7
*1-[5-(Hydroxymethyl)-1*H*-pyrrol-2-yl]-16-methyl-1-heptadecanone, 9CI*
[185389-45-1]
$C_{23}H_{41}NO_2$ 363.582
Oil. λ_{max} 204 (ϵ 7452); 294 (ϵ 9470) (MeOH).

Mycalazole 10
*1-[5-(Hydroxymethyl)-1*H*-pyrrol-2-yl]-14-heneicosen-1-one, 9CI*
[185389-60-0]
$C_{26}H_{45}NO_2$ 403.647
Cryst. (MeOH). Mp 74-76°. λ_{max} 204 (ϵ 10978); 252 (ϵ 925); 296 (ϵ 12940) (MeOH).

Ortega, M.J. *et al., Tetrahedron*, 1997, **53**, 331-340 (*isol, uv, ir, pmr, cmr, ms, struct*)
Nabbs, B.K. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 505-508 (*Mycalazole 11, synth*)
Hansen, T.V. *et al., Tet. Lett.*, 2004, **45**, 2809-2811 (*Mycalazole 5, synth*)

Mycaleoxime M-653

[290825-58-0]

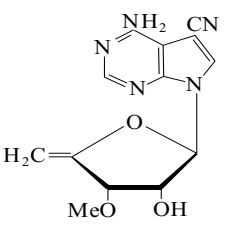


$C_{22}H_{34}N_2O_3$ 374.522
Isol. from the sponge *Mycale tenuispiculata*. Viscous liq. λ_{max} 232 (ϵ 8228); 304 (ϵ 19640) (MeCN).

Venketesham, U. *et al., J. Nat. Prod.*, 2000, **63**, 1318-1320 (*isol, ir, uv, pmr, cmr, ms*)

Mycalisine A M-654

[98890-73-4]



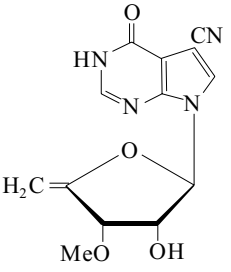
$C_{13}H_{13}N_5O_3$ 287.277

Nucleoside antibiotic. Related to Sangivamycic acid, S-20. Found in the sponge *Mycale* sp., prob. prod. by symbiotic microorganisms. Inhibits cell division in starfish eggs. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{21}$ -88 (c, 0.05 in EtOH). Unstable at r.t. λ_{max} 207 (ϵ 17000); 233 (sh) (ϵ 15000); 279 (ϵ 11000) (pH 2 EtOH) (Derep). λ_{max} 279 (EtOH at pH 12) (Derep). λ_{max} 207 (ϵ 30000); 233 (sh) (ϵ 8900); 279 (ϵ 14000) (pH 7 EtOH) (Derep).

Kato, Y. *et al., Tet. Lett.*, 1985, **26**, 3483-3486 (*isol, struct*)

Mycalisine B M-655

*5-Cyano-7-(3-*O*-methyl-5-deoxy-β-D-*erythro*-pent-4-enofuranosyl)pyrrolo[2,3-*d*]pyrimidin-4-one*
[98890-72-3]

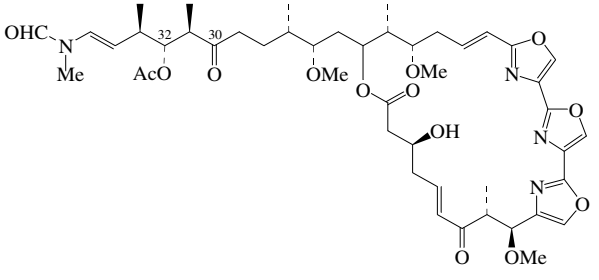


$C_{13}H_{12}N_4O_4$ 288.262
Isol. from *Mycale* sp., Japanese marine sponge. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{21}$ -75.9 (c, 0.26 in EtOH). Unstable at r.t. λ_{max} 214 (ϵ 3000); 265 (ϵ 3000) (pH 2 EtOH) (Derep). λ_{max} 265 (sh) (pH 12 EtOH) (Derep). λ_{max} 210 (ϵ 6000); 265 (ϵ 3000) (pH 7 EtOH) (Derep).

Kato, Y. *et al., Tet. Lett.*, 1985, **26**, 3483 (*isol, ir, pmr, cmr, uv*)

Mycalolide A M-656

[121038-36-6]



$C_{47}H_{64}N_4O_{14}$ 909.041
Isol. from the sponge *Mycale* sp. Cytotoxic and antifungal agent. Yellowish gum. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D$ -60.3 (c, 0.5 in $CHCl_3$). λ_{max} 230 (ϵ 30000) (MeOH) (Derep).

O-*De-Ac:* ***32-Hydroxymycalolide A***
[216770-61-5]
$C_{45}H_{62}N_4O_{13}$ 867.004
Isol. from *Mycale magellanica*. Cytotoxic agent. $[\alpha]_D^{27}$ -90 (c, 0.1 in MeOH). Misleading synonym. λ_{max} 230 (ϵ 26000) (MeOH).

*30*R-*Alcohol:* ***30-Hydroxymycalolide A***
[216770-57-9]
$C_{47}H_{66}N_4O_{14}$ 911.057
Isol. from *Mycale magellanica*. Cytotoxic agent. $[\alpha]_D^{27}$ -86.9 (c, 0.1 in MeOH). Misleading synonym. λ_{max} 230 (ϵ 27000) (MeOH).

*30*R-*Alcohol, 30-*O-*(2*R*,3-dimethoxypropanoyl):* ***Mycalolide B***
[122752-21-0]
$C_{52}H_{74}N_4O_{17}$ 1027.173
Isol. from the sponge *Mycale* sp. Cytotoxic and antifungal agent. Yellowish gum. $[\alpha]_D$ -53.4 (c, 1.3 in $CHCl_3$). λ_{max} 230 (ϵ 31000) (MeOH).

*30*R-*Alcohol, 30-*O-*(3*R*-hydroxy-2-methoxypropanoyl):* ***38-Hydroxymycalolide B***
[216770-65-9]
$C_{51}H_{72}N_4O_{17}$ 1013.146
Isol. from the sponge *Mycale magellanica*. Cytotoxic agent. $[\alpha]_D^{27}$ -80.9 (c, 0.1 in MeOH). Misleading synonym. λ_{max} 230 (ϵ 25000) (MeOH).

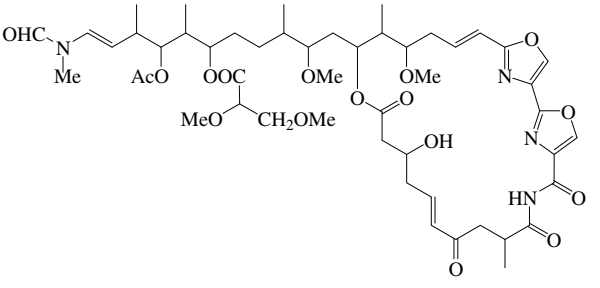
*30*R-*Alcohol, 30-*O-*(2*R*-methoxypropanoyl):* ***Mycalolide C***
[122752-20-9]
$C_{51}H_{72}N_4O_{16}$ 997.147
Isol. from the sponge *Mycale* sp. and from the stony coral *Tubastrea faulkneri*. Cytotoxic and antifungal agent. Yellowish gum. $[\alpha]_D$ -62.1 (c, 3.7 in $CHCl_3$). λ_{max} 230 (ϵ 31000) (MeOH).

*30*R-*Alcohol,* O-*de-Ac:* ***30,32-Dihydroxymycalolide A***
[442690-43-9]
$C_{45}H_{64}N_4O_{13}$ 869.02
Isol. from *Mycale izuensis*.
$[\alpha]_D^{22}$ -68.7 (c, 0.1 in MeOH). λ_{max} 231 (ϵ 33055) (MeOH).

Fusetani, N. *et al., Tet. Lett.*, 1989, **30**, 2809-2812 (*isol, uv, ir, pmr, cmr, struct*)
Rashid, M.A. *et al., J. Nat. Prod.*, 1995, **58**, 1120-1125 (*Mycalolides C-E, isol*)
Matsunaga, S. *et al., J. Nat. Prod.*, 1998, **61**, 1164-1167 (*Mycale magellanica constits*)
Matsunaga, S. *et al., J.A.C.S.*, 1999, **121**, 5605-5606; 8969 (*abs config*)
Liu, P. *et al., J.A.C.S.*, 2000, **122**, 1235-1236 (*synth*)
Phuwapraisirisan, P. *et al., J. Nat. Prod.*, 2002, **65**, 942-943 (*30,32-Dihydroxymycalolide A*)

Mycalolide D M-657

[168301-18-6]

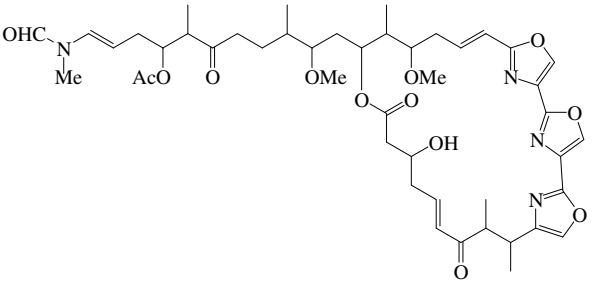


$C_{50}H_{72}N_4O_{17}$ 1001.135
Isol. from the stony coral *Tubastrea faulkneri*. Cytotoxic. Gum. $[\alpha]_D$ -19.5 (c, 0.5 in $CHCl_3$). λ_{max} 228 (ϵ 47700); 260 (MeOH) (Berdy).

Rashid, M.A. *et al., J. Nat. Prod.*, 1995, **58**, 1120 (*isol, uv, ir, pmr, cmr, struct*)

Mycalolide E M-658

[168301-19-7]

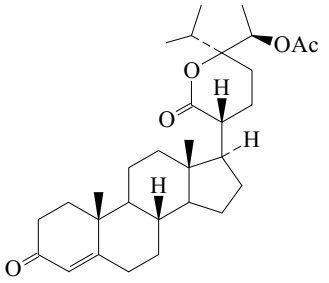


$C_{46}H_{62}N_4O_{13}$ 879.015
Minor constit. of the stony coral *Tubastrea faulkneri*. Cytotoxic. Gum. $[\alpha]_D$ -39 (c, 0.1 in $CHCl_3$). λ_{max} 231 (ϵ 33200); 254 (ϵ 30800) (MeOH) (Berdy).

Rashid, M.A. *et al., J. Nat. Prod.*, 1995, **58**, 1120 (*isol, uv, ir, pmr, struct*)

Mycalone M-659

[181363-35-9]

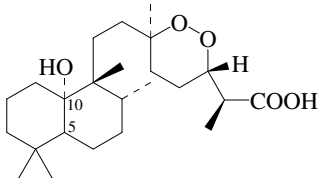


$C_{31}H_{46}O_5$ 498.701
Constit. of a *Mycale* sp. Needles (MeCN/petrol).
Mp 196-196.5°. $[\alpha]_D$ +53.4 (c, 0.4 in $CHCl_3$).

Rochfort, S.J. *et al., Aust. J. Chem.*, 1996, **49**, 715-718 (*isol, pmr, cmr, cryst struct*)

Mycaperoxide A M-660

[149260-79-7]



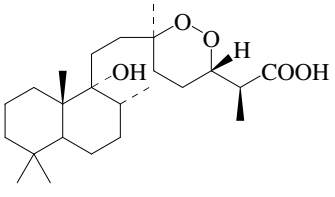
$C_{24}H_{42}O_5$ 410.593
Constit. of a *Mycale* sp. Shows antibacterial and antiviral activities. Cryst. (Me_2CO).
Mp 158-159.5°. $[\alpha]_D^{30}$ -41 (c, 1.28 in Me_2CO).

10-Deoxy, 5-hydroxy: [133530-25-3]
$C_{24}H_{42}O_5$ 410.593
Oil (as Me ester). $[\alpha]_D$ -22.6 (c, 3.1 in $CHCl_3$) (Me ester).
Stereochem. not defined.

Capon, R.J. *et al., J. Nat. Prod.*, 1991, **54**, 190-195 (*10-deoxy-5-hydroxy*)
Tanaka, J. *et al., J.O.C.*, 1993, **58**, 2999 (*isol, pmr, cmr, cryst struct, activity*)
Singh, M. *et al., Planta Med.*, 1999, **65**, 2-8 (*rev*)

Mycaperoxide B M-661

[149260-80-0]

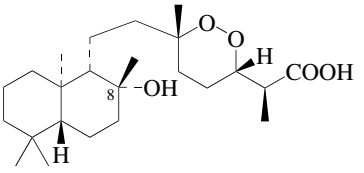


$C_{24}H_{42}O_5$ 410.593
Constit. of a *Mycale* sp. Shows antibacterial and antiviral activity.
Gum. $[\alpha]_D^{30}$ -41.3 (c, 1.27 in Me_2CO).

Tanaka, J. *et al., J.O.C.*, 1993, **58**, 2999 (*isol, pmr, cmr, activity*)
Singh, M. *et al., Planta Med.*, 1999, **65**, 2-8 (*rev*)

Mycaperoxide C M-662

[199012-85-6]



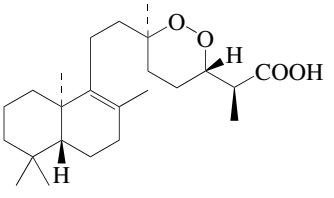
$C_{24}H_{42}O_5$ 410.593
Constit. of a *Mycale* sp. Oil (as Me ester). $[\alpha]_D$ -71 (c, 1.1 in $CHCl_3$) (Me ester).

8-Epimer: ***Mycaperoxide D***
[199012-86-7]
$C_{24}H_{42}O_5$ 410.593
Constit. of a *Mycale* sp. Oil (as Me ester). $[\alpha]_D^0$ -52 (c, 0.3 in $CHCl_3$) (Me ester).

8-Deoxy, 5-hydroxy: [133530-24-2]
$C_{24}H_{42}O_5$ 410.593
Constit. of *Mycale spongiosa*. Oil (as Me ester). $[\alpha]_D$ -22.6 (c, 3.1 in $CHCl_3$) (Me ester). Stereochem. not defined.

Capon, R.J. *et al., J. Nat. Prod.*, 1991, **54**, 190-195; 1997, **60**, 1261-1264 (*isol, pmr, cmr*)

Mycaperoxide G M-663



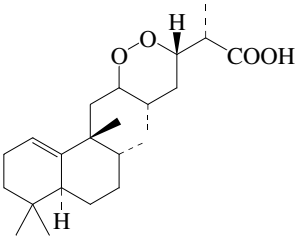
$C_{24}H_{40}O_4$ 392.578

Me ester: [205382-23-6]
$C_{25}H_{42}O_4$ 406.604
Constit. of a *Mycale* sp. Oil. $[\alpha]_D$ -55.5 (c, 0.23 in $CHCl_3$).

Capon, R.J. *et al., J. Nat. Prod.*, 1998, **61**, 525-528 (*isol, pmr, cmr*)

Mycaperoxide H M-664

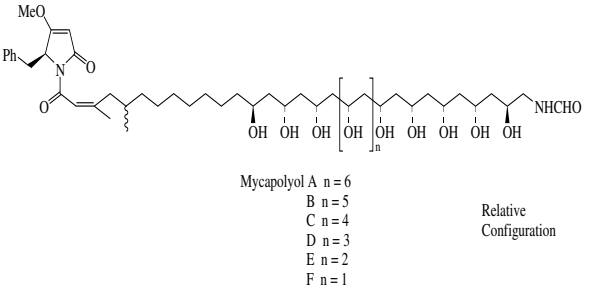
[498572-90-0]



$C_{24}H_{40}O_4$ 392.578
Constit. of a *Mycale* sp.
$[\alpha]_D^{25}$ -142.9 (c, 0.1 in Me_2CO).

Phuwapraisirisan, P. *et al., J. Nat. Prod.*, 2003, **66**, 289-291 (*isol, pmr, cmr*)

Mycapolyols M-665



Isol. from the marine sponge *Mycale izuensis*. Cytotoxic.

Mycapolyol A

$C_{55}H_{94}N_2O_{18}$ 1071.35
Powder. $[\alpha]_D^{21}$ +101.1 (c, 0.34 in MeOH aq.). λ_{max} 259 (log ϵ 4.15) (MeOH aq.).

Mycapolyol B

$C_{53}H_{90}N_2O_{17}$ 1027.297
Powder. $[\alpha]_D^{27}$ +104.7 (c, 0.22 in MeOH aq.). λ_{max} 259 (log ϵ 4.6) (MeOH aq.).

Mycapolyol C

$C_{51}H_{86}N_2O_{16}$ 983.244
Powder. $[\alpha]_D^{27}$ +105.7 (c, 0.32 in MeOH aq.). λ_{max} 259 (log ϵ 4.09) (MeOH aq.).

Mycapolyol D

$C_{49}H_{82}N_2O_{15}$ 939.191
Powder. $[\alpha]_D^{27}$ +100.6 (c, 0.25 in MeOH aq.). λ_{max} 259 (log ϵ 4.18) (MeOH aq.).

Mycapolyol E

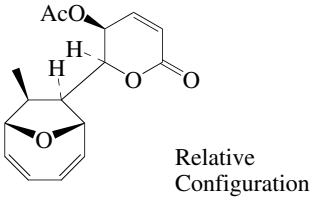
$C_{47}H_{78}N_2O_{14}$ 895.138
Powder. $[\alpha]_D^{21}$ +117.7 (c, 0.27 in MeOH aq.). λ_{max} 258 (log ϵ 4.15) (MeOH aq.).

Mycapolyol F

$C_{45}H_{74}N_2O_{13}$ 851.085
Powder. $[\alpha]_D^{21}$ +120.1 (c, 0.2 in MeOH aq.). λ_{max} 257 (log ϵ 4) (MeOH aq.).

Phuwapraisirisan, P. *et al., Org. Lett.*, 2005, **7**, 2233-2236 (*isol, pmr, cmr, ms*)

Mycoepoxydiene M-666



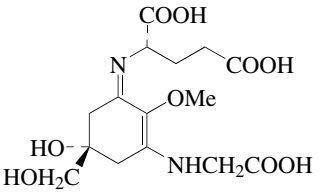
$C_{16}H_{18}O_5$ 290.315

Related to Antibiotic 1893B, A-533. Prod. by a fungal culture (OS-F66617) and a marine *Diaporthe* sp. Needles (MeOH). $[\alpha]_D$ +210 (c, 0.11 in MeOH). λ_{max} 256 (MeOH).

Cai, P. *et al., Tet. Lett.*, 1999, **40**, 1479-1482 (*isol, uv, pmr, cmr, cryst struct*)
Takao, K. *et al., J.O.C.*, 2004, **69**, 8789-8795 (*synth*)
Lin, X. *et al., FEMS Microbiol. Lett.*, 2005, **251**, 53-58 (*isol, cryst struct*)
Chen, G. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2006, **42**, 138-141 (*isol, pmr, cmr*)

Mycosporin-Glu-Gly M-667

[186599-00-8]

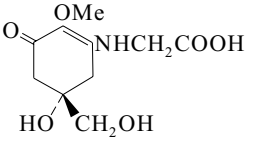


$C_{15}H_{22}N_2O_9$ 374.347
Isol. from the sponge *Dysidea herbacea*. λ_{max} 330 (ϵ 43900) (no solvent reported).

Bandaranayake, W.M. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1996, **115**, 281-286 (*isol, uv, struct*)

Mycosporin-Gly M-668

N-*[5-Hydroxy-5-(hydroxymethyl)-2-methoxy-3-oxo-1-cyclohexen-1-yl]glycine, 9CI*



$C_{10}H_{15}NO_6$ 245.232

(S)-form [65318-21-0]
Constit. of the zoanthid *Palythoa tuberculosa*.
Pale yellow amorph. powder. λ_{max} 311 (ϵ 20900) (H_2O) (Derep).

Me ester: [65318-51-6]
Mp 121-122°. $[\alpha]_D$ -12 (c, 0.4 in H_2O).

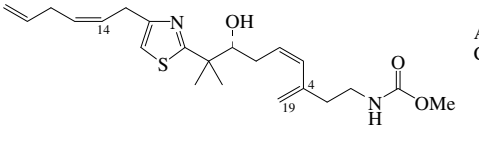
N-*De(carboxymethyl),* N-*(2-sulfoethyl):* ***Mycosporin-taurine***
[152833-55-1]
$C_{10}H_{17}NO_7S$ 295.313
Isol. from *Anthopleura elegantissima*. λ_{max} 310 (no solvent reported).

Imide: See Palythine, P-73

Ito, S. *et al., Tet. Lett.*, 1977, 2429 (*isol, uv, ir, pmr, cmr, struct*)
Stochaj, W.R. *et al., Mar. Biol. (Berlin)*, 1994, **118**, 149-156 (*Mycosporin-taurine*)
White, J.D. *et al., J.O.C.*, 1995, **60**, (*synth, ir, pmr, cmr, abs config*)

Mycothiazole M-669

[114582-75-1]



$C_{22}H_{32}N_2O_3S$ 404.572
Isol. from the marine sponge *Cacospongia mycofijiensis* and the sea slug *Chromodoris lochi*. Exhibits anthelminthic activity (*in vitro*). Highly toxic to mice. Viscous oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{20}$ -3.8 (c, 2.9 in $CHCl_3$). $[\alpha]_D^{27}$ -13.7 (c, 0.6 in MeOH). C-14 config. revised in 2006. λ_{max} 235 (ϵ 5270); 290 (ϵ 1780) (MeOH) (Berdy).

4,19-Dihydro, 4ξ,19-dihydroxy: ***Mycothiazole-4,19-diol***
$C_{22}H_{34}N_2O_5S$ 438.587
Isol. from *Cacospongia mycofijiensis*. Powder. $[\alpha]_D^{27}$ -2.5 (c, 0.04 in MeOH).

Crews, P. *et al., J.A.C.S.*, 1988, **110**, 4365-4368 (*isol, uv, ir, pmr, cmr, ms, struct*)
Sugiyama, H. *et al., Tetrahedron*, 2003, **59**, 6579-6593 (*synth, abs config*)
Le Flohic, A. *et al., Org. Lett.*, 2005, **7**, 339-342 (*synth*)

Sonnenschein, R.N. *et al., J. Nat. Prod.*, 2006, **69**, 145-147 (*Mycothiazole-4,19-diol*)

Perinereis vancaurica Myomodulin M-670

Alanylmethionylglycylmethionylleucylarginylmethionamide
[157203-83-3]
H-Ala-Met-Gly-Met-Leu-Arg-Met-NH_2
$C_{32}H_{61}N_{11}O_7S_3$ 808.101
Isol. from the annelid *Perinereis vancaurica*. Morphogenesis inducer.

Takahashi, T. *et al., Pept. Chem.*, 1993, **31**, 169 (*isol*)
Takahashi, T. *et al., Zool. Sci.*, 1994, **11**, 33 (*isol, struct, props*)

Aplysia californica Myomodulins M-671

[157243-32-8]
H-Pro-Met-Ser-Met-Leu-Arg-Leu-NH_2
Struct. of Myomodulin A shown. Isol. from motor neurons of *Aplysia californica*. Potentiates ARC neuromuscular activity.

Myomodulin A [110570-93-9]

Myomodulin B [137362-30-2]

Myomodulin C [153982-87-7]

Myomodulin D [147741-10-4]

Myomodulin E [153982-88-8]

Myomodulin F [147741-13-7]

Myomodulin G [147741-08-0]

Myomodulin H [147741-11-5]

Myomodulin I [147741-09-1]

Cropper, E.C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1987, **84**, 5483-5486 (*Myomodulin A*)
Cropper, E.C. *et al., Peptides (N.Y.)*, 1991, **12**, 683-690 (*Myomodulin B*)
Brezina, V. *et al., J. Neurophysiol.*, 1995, **74**, 54-72 (*Myomodulins C-I*)

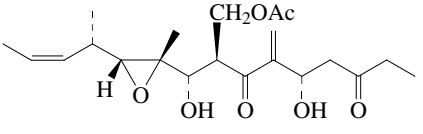
Myonin M-672

Myosin-linked regulatory protein of *ca.* 230 kDa. Isol. from Hokki clam (*Pseudocardium sachalinensis*) adductor muscles.

Yazawa, Y. *et al., Mol. Cell. Biochem.*, 1999, **190**, 63-66 (*isol*)

Myriaporone 1 M-673

Antibiotic MT 381. MT 381
[177481-42-4]



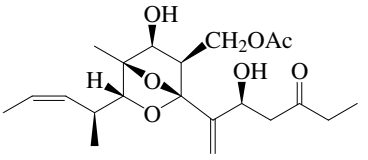
Absolute Configuration

$C_{21}H_{32}O_7$ 396.48
Isol. from the bryozoan *Myriapora truncata*.
$[\alpha]_D^{26}$ +71.7 (c, 0.24 in MeOH). λ_{max} 217 (ϵ 16200); 261 (ϵ 2400) (MeOH).

U.S. Pat., 1996, 5 514 708; *CA*, **125**, 5896f (*isol*)
Pérez, M. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 1724-1727 (*synth, abs config*)
Fleming, K.N. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 1728-1730 (*synth, abs config*)

Myriaporone 2 M-674

Antibiotic MT 381B. MT 381B
[177481-43-5]



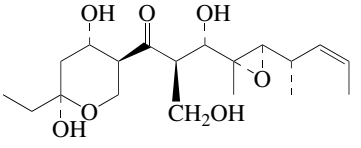
Absolute Configuration

$C_{21}H_{32}O_7$ 396.48
Isol. from the bryozoan *Myriapora truncata*.
$[\alpha]_D^{26}$ -66.6 (c, 0.13 in MeOH).

U.S. Pat., 1996, 5 514 708; *CA*, **125**, 5896f (*isol*)
Pérez, M. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 1724-1727 (*synth, abs config*)
Fleming, K.N. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 1728-1730 (*synth, abs config*)

Myriaporone 3 M-675

MT 332. Antibiotic MT 332
[177481-40-2]

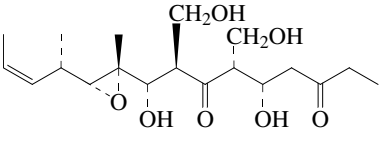


$C_{19}H_{32}O_7$ 372.458
Isol. from the bryozoan *Myriapora truncata*. Cytotoxic agent.

U.S. Pat., 1996, 5 514 708; *CA*, **125**, 5896f (*isol*)
Pérez, M. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 1724-1727 (*synth, config*)
Fleming, K.N. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 1728-1730 (*synth, config*)

Myriaporone 4 M-676

[177481-41-3]

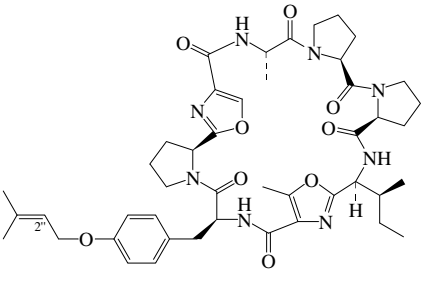


Absolute Configuration

$C_{19}H_{32}O_7$ 372.458
Isol. from the bryozoan *Myriapora truncata*. Cytotoxic agent.

U.S. Pat., 1996, 5 514 708; *CA*, **125**, 5896f
Pérez, M. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 1724-1727 (*synth, abs config*)
Fleming, K.N. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 2728-2730 (*synth, abs config*)

Myriastramide A M-677



Absolute Configuration

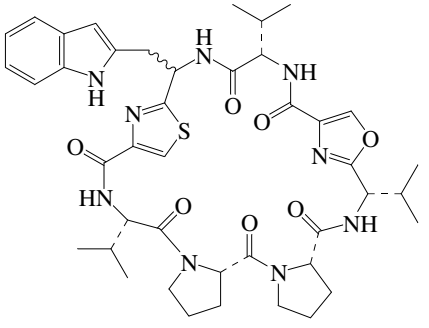
$C_{45}H_{58}N_8O_9$ 855.001

Isol. from the sponge *Myriastra clavosa*.
$[\alpha]_D$ -115.4 (c, 0.13 in MeOH). λ_{max} 210 (ϵ 33990); 222 (sh) (ϵ 28660); 275 (ϵ 14700) (MeOH).

Δ³′′-Isomer, 2′′ξ-chloro: ***Myriastramide B***
$C_{45}H_{57}ClN_8O_9$ 889.446
Isol. from the sponge *Myriastra clavosa*.
$[\alpha]_D$ -90 (c, 0.03 in MeOH). λ_{max} 220 (ϵ 21510); 227 (ϵ 1320) (MeOH).

Erickson, K.L. *et al., Tetrahedron*, 2003, **59**, 10231-10238 (*isol, pmr, cmr*)

Myriastramide C M-678

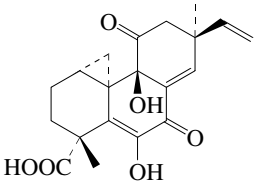


$C_{42}H_{53}N_9O_7S$ 828.003
Isol. from the sponge *Myriastra clavosa*.
$[\alpha]_D$ -136.5 (c, 0.26 in MeOH). λ_{max} 210 (ϵ 47140); 282 (ϵ 5095); 289 (ϵ 4275) (MeOH).

Erickson, K.L. *et al., Tetrahedron*, 2003, **59**, 10231-10238 (*isol, pmr, cmr*)

Myrocin A M-679

[723302-27-0]



$C_{20}H_{22}O_6$ 358.39
Metab. of a marine-derived *Apiospora montagnei*. Solid. $[\alpha]_D^{22}$ -418.6 (c, 0.36 in MeOH). λ_{max} 204 (log ϵ 4.1); 254 (log ϵ 3.76) (MeOH).

Klemke, C. *et al., J. Nat. Prod.*, 2004, **67**, 1058-1063 (*isol, pmr, cmr*)

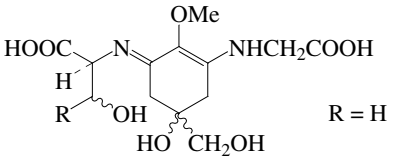
Myticin M-680

Peptide containing 40 amino acid residues crosslinked by 4 disulfide bridges; 2 isoforms are known. Isol. from haemocytes of the mussel *Mytilus galloprovincialis*. Shows antimicrobial activity.

Mitta, G. *et al., Eur. J. Biochem.*, 1999, **265**, 71-78 (*isol, struct*)

Mytilin A M-681

N-*[3-[(Carboxymethyl)amino]-5-hydroxy-5-(hydroxymethyl)-2-methoxy-2-cyclohexen-1-ylidene]serine, 9CI. Shinorine. Substance Y. Mycosporin-Gly-Ser*
[73112-73-9]
[73522-56-2, 97170-22-4]



$C_{13}H_{20}N_2O_8$ 332.31
Isol. from *Strongylocentrotus droebachiensis* from the edible mussel *Mytilus galloprovincialis* (as a 3:1 insep. mixt. with Mytilin B, M-682), from the red algae *Chondrus yendoi* and *Trichocarpus crinitus*, from brine shrimp *Artemia* and from a *Lissoclinum/Prochloron* symbiont. Uv protectant. Cryst.
Mp 154-156° dec. $[\alpha]_D^{19}$ -3.47. λ_{max} 334 (H_2O).

Chioccara, F. *et al., Tet. Lett.*, 1979, 3181-3182 (*uv, pmr, cmr, ms*)
Tsujino, I. *et al., Bot. Mar.*, 1980, **23**, 65-67; *CA*, **92**, 124955j (*isol*)
Yabe, K. *et al., CA*, 1981, **95**, 21251j (*isol*)
Grant, P.T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 755-759 (*occur*)
Chioccara, F. *et al., Gazz. Chim. Ital.*, 1985, **115**, 643-647 (*isol*)
Dionisio-See, M.L. *et al., Mar. Biol. (Berlin)*, 1997, **128**, 455-461 (*isol*)
Bandaranayake, W.M. *et al., Nat. Prod. Rep.*, 1998, **15**, 159-172 (*rev*)

Mytilin B M-682

Porphyra 334. Mycosporin-Thr
[70579-26-9]
As Mytilin A, M-681 with
R = CH_3

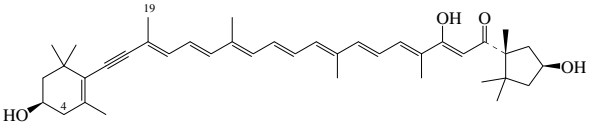
$C_{14}H_{23}N_2O_8^{\oplus}$ 347.344
Isol. from the edible mussel *Mytilus galloprovincialis* as a 1:3 inseparable mixt. with Mytilin A, M-681. Also from *Porphyra tenera* and *Halocynthia roretzi*. Powder. λ_{max} 334 (ϵ 42300) (H_2O).

[73495-42-8 (Na salt), 79980-53-3]

Takano, S. *et al., Chem. Lett.*, 1979, 419-420 (*isol, uv*)
Chioccara, F. *et al., Tet. Lett.*, 1979, 3181 (*uv, pmr, cmr, ms, struct*)
Kobayashi, J. *et al., Tet. Lett.*, 1981, **22**, 3001-3002 (*isol*)
Grant, P.T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 755 (*isol*)

Mytiloxanthin M-683

7,8-Didehydro-3,3′,8′-trihydroxy-β,κ-caroten-6′-one
[50906-61-1]



$C_{40}H_{54}O_4$ 598.864
Isol. from the mussels *Mytilus edulis*. Reddish needles.
Mp 147°.

3′-Ketone: ***Mytiloxanthinone****. 7,8-Didehydro-3,8′-dihydroxy-β,κ-carotene-3′,6′-dione*
[83746-66-1]
$C_{40}H_{52}O_4$ 596.848
Constit. of sea squirt *Halocynthia roretzi*. Reddish needles.
Mp 226-228°.

4S-Hydroxy: 7,8-Didehydro-3,3′,4,8′-tetrahydroxy-β,κ-caroten-6′-one. ***4-Hydroxymytiloxanthin***
[124392-06-9]
$C_{40}H_{54}O_5$ 614.864
Isol. from *Asterina amurensis* and *Asterina pectinifera*.

4-Oxo: 7,8-Didehydro-3,3′,8′-trihydroxy-β,κ-carotene-4,6′-dione. ***4-Oxomytiloxanthin***
[84537-00-8]
$C_{40}H_{52}O_5$ 612.848
Isol. from the carotenoprotein Asteriarubin from *Asterias rubens*. Struct. assignment is considered tentative by the authors. λ_{max} 447; 473; 502 (no solvent reported).

19-Butanoyloxy: ***19-Butanoyloxymytiloxanthin***

[179818-35-0]
$C_{44}H_{60}O_6$ 684.954
Constit. of *Phakellia stelliderma*. Red powder. λ_{max} 480 (ϵ 85000) (C_6H_6). λ_{max} 475 (ϵ 94000) (Me_2CO).

19-Hexanoyloxy: ***19-Hexanoyloxymytiloxanthin***
[179818-34-9]
$C_{46}H_{64}O_6$ 713.008
Constit. of *Phakellia stelliderma*. Red powder. λ_{max} 480 (ϵ 66900) (C_6H_6). λ_{max} 470 (ϵ 72900) (Me_2CO).

Khare, A. *et al., Tet. Lett.*, 1973, 3921-3924 (*isol*)
Bernhard, K. *et al., Helv. Chim. Acta*, 1982, **65**, 2224-2229 (*4-Oxomytiloxanthin*)
Matsuno, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 4309-4315 (*isol, uv, ms, pmr*)
Matsuno, T. *et al., J. Nat. Prod.*, 1985, **48**, 606-613 (*biosynth*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 419
Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495-503 (*isol, pmr, uv, ms*)
Chopra, A.K. *et al., J.C.S. Perkin 1*, 1988, 1383-1388 (*struct, synth*)
Maoka, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **93**, 829-834 (*4-Hydroxymytiloxanthin*)
Higa, T. *et al., Pure Appl. Chem.*, 1994, **66**, 2227-2230 (*19-acyloxy derivs*)
Kitamura, A. *et al., J. Nat. Toxins*, 1996, **5**, 219-224 (*19-acyloxy derivs*)
Tode, C. *et al., J.C.S. Perkin 1*, 2002, 1581-1587 (*synth*)

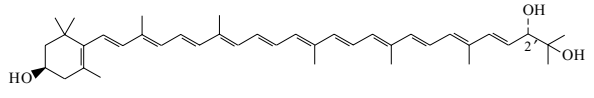
Mytimycin M-684

A 6.2 kDa peptide containing 12 cysteines; struct. only partially elucidated. Isol. from blood of *Mytilus edulis*. Shows antimicrobial activity.

Charlet, M. *et al., J. Biol. Chem.*, 1996, **271**, 21808-21813 (*isol*)

Myxol M-685

1′,2′-Dihydro-β,ψ-carotene-1′,2′,3-triol. 3-Hydroxyplectaniaxanthin
[31894-69-6]



$C_{40}H_{56}O_3$ 584.881
Isol. from *Flexibacter* spp. and from a *Flavobacterium* sp. associated with a marine sponge *Homaxinella* sp. Antioxidant. λ_{max} 462; 488; 522 (MeOH) (Berdy).

2′-O-(3-O-Methyl-α-L-fucoside): [103881-48-7]
$C_{47}H_{68}O_7$ 745.05
Isol. from *Oscillatoria limosa* and *Oscillatoria bornetii* f. *tenuis*. λ_{max} 445; 470; 501 (MeOH).

2′-O-6-Deoxy-α-L-glucoside: ***Myxoxanthophyll***. *Myxol 2′-quinovoside*
[11004-68-5]
$C_{46}H_{66}O_7$ 731.023
Isol. from *Oscillatoria rubescens*, *Oscillatoria agardhii*, *Arthrospira* spp. *Anabaena flos-aquae*, *Phormidium faveolarum* and *Phormidium luridum*. The characteristic carotenoid of blue-green algae. Violet cryst.
Mp 172°. Struct. revised in 1986. Usually isol. as a mixt. of glycosides of which the quinovoside is the major component. λ_{max} 471; 502 (no solvent reported).

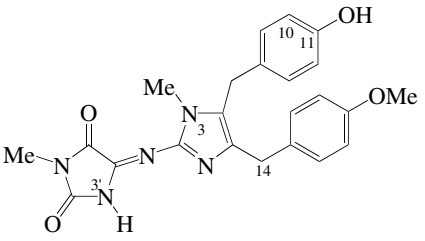
2′-O-Glucopyranoside: Myxol 2′-glucoside
$C_{46}H_{66}O_8$ 747.023
Minor congener of Myxoxanthophyll.

3-Ketone, 2′-O-α-L-rhamnopyranoside: ***4-Ketomyxoxanthophyll***. *4-Ketomyxol 2′-methylpentoside. P 483*
[35408-90-3]
$C_{46}H_{64}O_7$ 729.007
Isol. from the blue-green algae *Oscillatoria limosa* and *Phormidium faveolarum*. Needles (petrol) (as tetraacetate). Struct. not certain. Thought to have 2′*S*,3*S* config.

Hertzberg, S. *et al., Phytochemistry*, 1966, **5**, 557-563; 1969, **8**, 1259-1280; 1971, **10**, 3121-3127 (*Myxoxanthophyll, isol, struct*)
Francis, G.W. *et al., Phytochemistry*, 1970, **9**, 629-635 (*Oscillatoria limosa constits*)
Aguilar-Martinez, M. *et al., Acta Chem. Scand.*, 1972, **26**, 2528-2530 (*isol*)
Watts, C.D. *et al., Org. Mass Spectrom.*, 1975, **10**, 1102-1110 (*ms*)
Fiksdahl, A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **76**, 599-601 (*occur*)
Rønneberg, H. *et al., Phytochemistry*, 1985, **24**, 309-319 (*cd, abs config*)
Foss, P. *et al., Phytochemistry*, 1986, **25**, 1127-1132 (*Myxoxanthophyll, struct, bibl, 3-O-methylfucoside*)
Yokoyama, A. *et al., Fish. Sci.*, 1995, **61**, 684-686 (*Flavobacterium constit*)

Naamidine A N-1

[110189-06-5]



$C_{23}H_{23}N_5O_4$ 433.466

Extensive tautomerism possible in all Naamidines. Alkaloid from the Red Sea sponge *Leucetta chagosensis* and from *Notodoris citrina*. Antagonist of the epidermal growth factor receptor. Yellow foaming oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 240 (ϵ 1160); 281 (ϵ 4330); 366 (ϵ 10500); 392 (ϵ 13500); 416 (ϵ 10700) ($CHCl_3$) (Derep). λ_{max} 225 (ϵ 21400); 276 (ϵ 4800); 384 (ϵ 10060) (MeOH) (Berdy).

Zn complex: ***Bis(naamidinato A)zinc(II)***
[171114-02-6]
$C_{46}H_{44}N_{10}O_8Zn$ 930.306
From *Leucetta* sp. Yellow amorph. solid. MF erroneously given as $C_{46}H_{44}N_{10}O_{10}Zn$ in CA.

$N^{3'}$*-Me:* ***Naamidine C***
[121819-69-0]
$C_{24}H_{25}N_5O_4$ 447.493
Alkaloid from *Leucetta chagosensis*. Exists as $\Delta^{4'(N)}$-isomer.

O^{11}*-Me:* ***Naamidine G***
[171784-01-3]
$C_{24}H_{25}N_5O_4$ 447.493
From *Leucetta* sp. Yellow solid (EtOAc).
Mp 94°.

O^{11}*-Me, Zn complex:* ***Bis(naamidinato G)zinc(II)***
[171114-03-7]
$C_{48}H_{48}N_{10}O_8Zn$ 958.359
From *Leucetta* sp. Yellow amorph. solid. MF erroneously given as $C_{48}H_{48}N_{10}O_{10}Zn$ in CA.

O^{11}*-Me,* N^3*-De-Me:* ***Naamidine D***
[121819-71-4]
$C_{23}H_{23}N_5O_4$ 433.466
Trace alkaloid from *Leucetta chagosensis*. λ_{max} 240 (ϵ 8800); 268 (ϵ 305); 386 (ϵ 6500) ($CHCl_3$/MeOH) (Derep). λ_{max} 240 (ϵ 8800); 268 (ϵ 3050); 386 (ϵ 6500) (MeOH-$CHCl_3$) (Berdy).

10-Hydroxy, O^{11}*-Me:* ***Naamidine B***
[121819-68-9]
$C_{24}H_{25}N_5O_5$ 463.492
Alkaloid from *Leucetta chagosensis*.

14-Hydroxy, O^{11}*-Me:* ***14-Hydroxynaamidine G***
[171114-06-0]
$C_{24}H_{25}N_5O_5$ 463.492
From *Leucetta* sp.
$[\alpha]_D^{25}$ -8 (c, 0.2 in MeOH).

14-Hydroxy: ***14-Hydroxynaamidine A***
[171114-05-9]
$C_{23}H_{23}N_5O_5$ 449.465
Alkaloid from a calcareous sponge, *Leucetta* sp., of the Coral Sea.
$[\alpha]_D^{25}$ +6 (c, 0.3 in MeOH).

14-Methoxy: ***14-Methoxynaamidine A***
[171114-07-1]
$C_{24}H_{25}N_5O_5$ 463.492
From *Leucetta* sp. Isol. as a 12:88 mixt. with Naamidine A.

14-Methoxy, O^{11}*-Me:* ***14-Methoxynaamidine G***
[171114-08-2]
$C_{25}H_{27}N_5O_5$ 477.519
From *Leucetta* sp.
$[\alpha]_D^{25}$ +4 (c, 0.3 in MeOH).

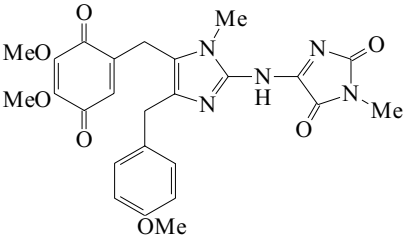
14-Oxo, O^{11}*-Me:* ***14-Oxonaamidine G***
[171114-09-3]
$C_{24}H_{23}N_5O_5$ 461.476
From *Leucetta* sp.

O^{11}*-Me, Zn complex with naamidine A:* ***(Naamidinato A)(naamidinato G)zinc(II)***
[171114-04-8]
$C_{47}H_{46}N_{10}O_8Zn$ 944.333
From *Leucetta* sp. Yellow amorph. solid. First naturally occurring mixed-ligand metal complex. MF erroneously given as $C_{47}H_{46}N_{10}O_{10}Zn$ in CA.

Carmely, S. *et al., Tetrahedron*, 1989, **45**, 2193-2200 (*isol, uv, ir, pmr, cmr, ms, struct*)
Mancini, I. *et al., Helv. Chim. Acta*, 1995, **78**, 1178 (*derivs*)
Copp, B.R. *et al., J. Med. Chem.*, 1998, **41**, 3909-3911 (*isol, use*)
Ohta, S. *et al., Heterocycles*, 2000, **53**, 1939-1955 (*synth*)
Aberle, N.S. *et al., Org. Lett.*, 2006, **8**, 419-421 (*synth*)

Naamidine F N-2

[152273-85-3]

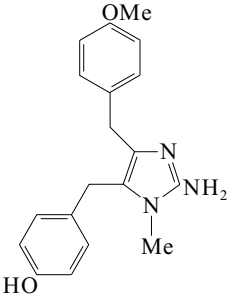


$C_{25}H_{25}N_5O_7$ 507.502
Alkaloid from the sponge *Leucetta* sp. Weakly cytotoxic. Yellow needles.
Mp 172-174°.

Carroll, A.R. *et al., Aust. J. Chem.*, 1993, **46**, 1229 (*isol, uv, ir, pmr, cmr, ms, struct*)

Naamine A N-3

*4-[[2-Amino-4-[(4-methoxyphenyl)methyl]-1-methyl-1*H*-imidazol-5-yl]methyl]phenol, 9CI. 2-Amino-5-(*p*-hydroxybenzyl)-4-(*p*-methoxybenzyl)-1-methylimidazole*
[110189-03-2]

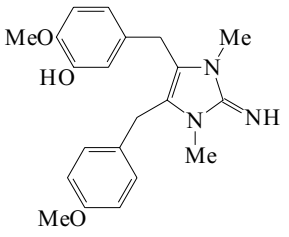


$C_{19}H_{21}N_3O_2$ 323.394
Alkaloid from the Red Sea sponge *Leucetta chagosensis* and from *Notodoris citrina*. Also obt. by acid treatment of Naamidine A, N-1. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 185-187.5° (as picrate). λ_{max} 226 (ϵ 17000); 260 (ϵ 11600); 282 (ϵ 6000); 290 (ϵ 5500); 302 (ϵ 4700) (dioxan) (Derep).

Carmely, S. *et al., Tetrahedron*, 1989, **45**, 2193 (*isol, uv, ir, pmr, cmr, ms, struct*)
Ohta, S. *et al., Heterocycles*, 2000, **53**, 1939-1955 (*synth*)

Naamine B N-4

[121849-79-4]

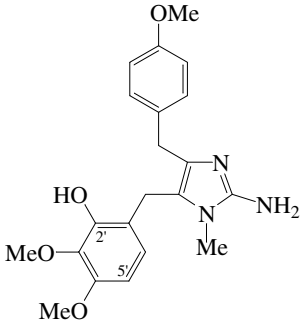


$C_{21}H_{25}N_3O_3$ 367.447
Alkaloid from the Red Sea sponge *Leucetta chagosensis* with *Notodoris citrina*.

Carmely, S. *et al., Tetrahedron*, 1989, **45**, 2193 (*isol, ir, pmr, cmr, ms, struct*)
Kawasaki, I. *et al., J.C.S. Perkin 1*, 2001, 3095-3099 (*synth*)

Naamine C N-5

[189825-81-8]



$C_{21}H_{25}N_3O_4$ 383.446
Alkaloid from the Micronesian sponge *Leucetta chagosensis*. Yellow powder. λ_{max} 228; 276; 368 (MeOH).

2′-Deoxy, 5′-hydroxy, 3′-O-*de-Me:* ***Naamine E***
[454472-13-0]
$C_{20}H_{23}N_3O_4$ 369.419
Alkaloid from *Leucetta* cf. *chagosensis*. Amorph. yellow solid. λ_{max} 233 (ϵ 21600); 277 (ϵ 6090) (MeOH).

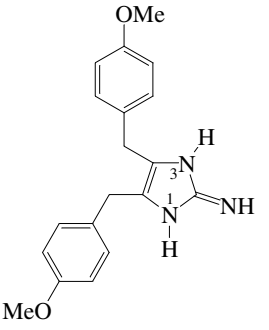
5′-Methoxy, 2′-deoxy, 4′-O-*de-Me:* ***Naamine G***
[700813-14-5]
$C_{21}H_{25}N_3O_4$ 383.446
Alkaloid from *Leucetta chagosensis*. Antifungal agent. Yellow-brown oil. λ_{max} 230; 276 (MeOH).

2′-Deoxy, 4′-O-*de-Me:* ***Naamine F***
$C_{20}H_{23}N_3O_3$ 353.42
Alkaloid from *Leucetta chagosensis*. Dark brown solid. CAS No. not found 8-14CI. λ_{max} 226; 279 (MeOH).

Fu, X. *et al., J. Nat. Prod.*, 1997, **60**, 497-498 (*Naamine C*)
Gross, H. *et al., J. Nat. Prod.*, 2002, **65**, 1190-1193 (*Naamine E*)
Nakamura, S. *et al., J.C.S. Perkin 1*, 2002, 1061-1066 (*synth, pmr*)
Hassan, W. *et al., J. Nat. Prod.*, 2004, **67**, 817-822 (*Naamines F,G*)

Naamine D N-6

*4,5-Bis[(4-methoxyphenyl)methyl]-1*H-*imidazol-2-amine, 9CI*
[316814-71-8]

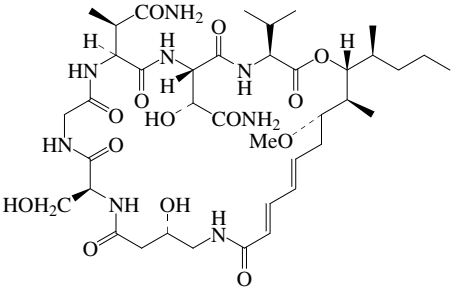


$C_{19}H_{21}N_3O_2$ 323.394
Alkaloid from the sponge *Leucetta* cf. *chagosensis*. Antifungal and nitric oxide synthase inhibitory agent. Amorph. powder. λ_{max} 230 (ϵ 15400); 262 (ϵ 1290); 299 (ϵ 3300) ($CHCl_3$).

N^1,N^3*-Di-Me:* ***N^1,N^3-Dimethylnaamine D***
[496954-15-5]
$C_{21}H_{25}N_3O_2$ 351.447
Alkaloid from a *Leucetta* sp. Amorph. amber solid. λ_{max} 205 (log ϵ 4.25); 281 (log ϵ 3.75); 312 (log ϵ 3.58) (MeOH).

Dunbar, D.C. *et al., Tetrahedron*, 2000, **56**, 8795-8798 (*isol, pmr, cmr, ir, uv*)
Crews, P. *et al., J. Nat. Prod.*, 2003, **66**, 177-182 (*N,N-Dimethylnaamine D*)

Nagahamide A N-7



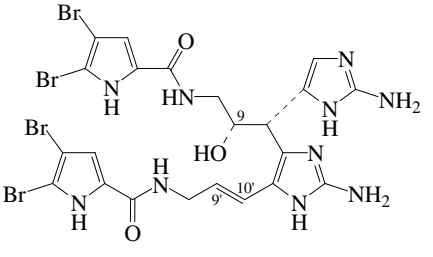
Absolute Configuration

$C_{39}H_{64}N_8O_{14}$ 868.98
Isol. from the sponge *Theonella swinhoei*. Powder. $[\alpha]_D$ +26.6 (c, 0.1 in 1-propanol aq.). λ_{max} 260 (ϵ 7800) (1-propanol aq.).

Okada, Y. *et al., Org. Lett.*, 2002, **4**, 3039-3042 (*isol, pmr, cmr, abs config*)

Nagelamide B N-8

[690627-55-5]



Relative Configuration

$C_{22}H_{22}Br_4N_{10}O_3$ 794.097
Alkaloid from the sponge *Agelas* sp. Antibacterial agent. Amorph. solid. λ_{max} 202 (ϵ 19200); 282 (ϵ 16000) (MeOH).

9-Deoxy: ***Nagelamide A***
[690627-54-4]
$C_{22}H_{22}Br_4N_{10}O_2$ 778.098
Alkaloid from an *Agelas* sp. Antibacterial agent. Amorph. solid. λ_{max} 202 (ϵ 29800); 279 (ϵ 27800) (MeOH).

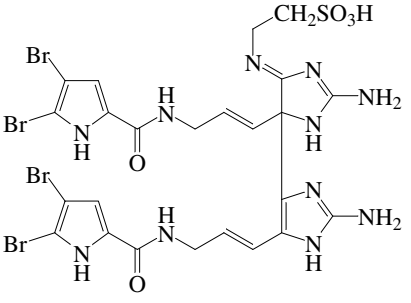
*9-Deoxy, 9,10-didehydro(*E-*):* ***Nagelamide C***
[690627-56-6]
$C_{22}H_{20}Br_4N_{10}O_2$ 776.082
Alkaloid from an *Agelas* sp. Antibacterial agent. Amorph. solid. λ_{max} 202 (ϵ 21200); 280 (ϵ 19700) (MeOH).

9-Deoxy, 9′,10′-dihydro: ***Nagelamide D***
[690627-57-7]
$C_{22}H_{24}Br_4N_{10}O_2$ 780.113
Alkaloid from an *Agelas* sp. Antibacterial agent. Amorph. solid. λ_{max} 202 (ϵ 16500); 280 (ϵ 14900) (MeOH).

Endo, T. *et al., J. Nat. Prod.*, 2004, **67**, 1262-1267 (*isol, pmr, cmr*)

Nagelamide H N-9

[690627-61-3]

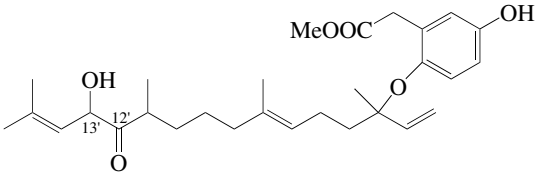


$C_{24}H_{25}Br_4N_{11}O_5S$ 899.214
Related to Mauritiamine, M-121. Alkaloid from the sponge *Agelas* sp. Amorph. solid. λ_{max} 221 (ϵ 34900); 279 (ϵ 28300) (MeOH).

Endo, T. *et al., J. Nat. Prod.*, 2004, **67**, 1262-1267 (*isol, pmr, cmr*)

Nahocol A N-10

[160262-42-0]



$C_{29}H_{42}O_6$ 486.647
Constit. of *Sargassum autumnale.* Oil. $[\alpha]_D^{25}$ -168.7 (c, 0.99 in EtOH). λ_{max} 205 (log ϵ 4.3); 225 (log ϵ 3.8); 293 (log ϵ 3.3) (EtOH).

12′-Alcohol: ***Nahocol C***
[160262-44-2]
$C_{29}H_{44}O_6$ 488.663
Constit. of *Sargassum autumnale.* Oil. $[\alpha]_D^{25}$ +6.3 (c, 0.71 in EtOH). λ_{max} 206 (log ϵ 4.2); 229 (log ϵ 3.8); 293 (log ϵ 3.3) (EtOH).

13′-Deoxy: ***Nahocol B***
[160262-43-1]
$C_{29}H_{42}O_5$ 470.648
Constit. of *Sargassum autumnale.* Oil. $[\alpha]_D^{25}$ -9.7 (c, 0.96 in EtOH). λ_{max} 204 (log ϵ 4.4); 228 (log ϵ 3.9); 293 (log ϵ 3.4) (EtOH).

*10′,11′-Didehydro(*E-*), 12′-alcohol:* ***Nahocol D₁***
[160335-93-3]
$C_{29}H_{42}O_6$ 486.647
Constit. of *Sargassum autumnale.* Oil. $[\alpha]_D^{25}$ +2.6 (c, 0.76 in EtOH). λ_{max} 206 (log ϵ 4.5); 228 (log ϵ 3.9); 293 (log ϵ 3.5) (EtOH).

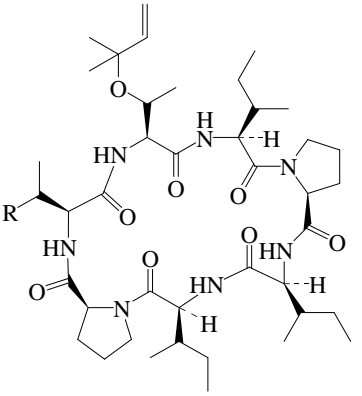
Diastereoisomer: ***Nahocol A₁***
[160262-45-3]
$C_{29}H_{42}O_6$ 486.647
Constit. of *Sargassum autumnale.* Oil. $[\alpha]_D^{25}$ +10.5 (c, 0.78 in EtOH). λ_{max} 207 (log ϵ 4.5); 293 (log ϵ 3.3) (EtOH). λ_{max} 207 (ϵ 31650); 293 (ϵ 1950) (MeOH) (Berdy).

*10′,11′-Didehydro(*E-*),12′-alcohol, diastereoisomer:* ***Nahocol D₂***
[160262-46-4]
$C_{29}H_{42}O_6$ 486.647
Constit. of *Sargassum autumnale.* Oil. $[\alpha]_D^{25}$ +4.5 (c, 0.95 in EtOH). λ_{max} 206 (log ϵ 4.4); 229 (log ϵ 3.9); 293 (log ϵ 3.4) (EtOH).

Tsuchiya, N. *et al., Phytochemistry*, 1998, **48**, 1003-1011 (*isol, pmr, cmr*)

Nairaiamide A N-11

[149380-60-9]



R = CH_3

$C_{42}H_{71}N_7O_8$ 802.065
Isol. from the ascidian *Lissoclinum bistratum*. Clear glass. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{25}$ -116 (c, 2.15 in CH_2Cl_2). λ_{max} 230 (ϵ 2060) (CH_2Cl_2).

Foster, M.P. *et al., Tet. Lett.*, 1993, **34**, 2871-2873 (*isol, uv, ir, pmr, cmr, ms*)

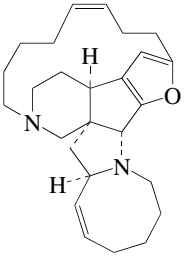
Nairaiamide B N-12

[149380-61-0]
As Nairaiamide A, N-11 with
R = CH_2CH_3
$C_{43}H_{73}N_7O_8$ 816.092
Isol. from a Fijian *Lissoclinum bistratum*. Clear glass. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{25}$ -140 (c, 2.06 in CH_2Cl_2). λ_{max} 230 (ϵ 2580) (CH_2Cl_2).

Foster, M.P. *et al., Tet. Lett.*, 1993, **34**, 2871-2873 (*isol, uv, ir, pmr, cmr, ms*)

Nakadomarin A N-13

[199483-01-7]



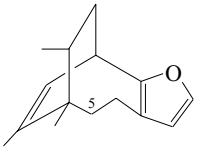
Relative Configuration

$C_{26}H_{36}N_2O$ 392.583
Alkaloid from the sponge *Amphimedon* sp. Cyclin-dependent kinase inhibitor. Amorph. solid. $[\alpha]_D^{25}$ -16 (c, 0.1 in MeOH). λ_{max} 206 (ϵ 11000); 228 (ϵ 10000) (MeOH).

Kobayashi, J. *et al., J.O.C.*, 1997, **62**, 9236-9239 (*isol, uv, ir, pmr, cmr*)
Nagata, T. *et al., J.A.C.S.*, 2003, **125**, 7484-7485; 13618 (*synth*)
Ono, K. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 2020-2023 (*synth*)

Nakafuran 8 N-14

[76844-25-2]



$C_{15}H_{20}O$ 216.322
Constit. of sponge *Dysidea fragilis* and molluscs *Chromodoris maridadulis*, *Hypselodoris godeffroyana*, *Hypselodoris capensis*, *Hypselodoris californiensis* and *Hypselodoris ghiselini*. Shows antifeedant props. Oil. Sol. MeOH, $CHCl_3$, C_6H_6; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D^{25}$ +24.2 (c, 2.65 in $CHCl_3$). λ_{max} 228 (ϵ 6100) (hexane) (Derep).

5α-Hydroxy: ***5-Hydroxynakafuran 8***
$C_{15}H_{20}O_2$ 232.322
Constit. of *Dysidea etheria*. Antifeedant and insecticide. Toxic to brine shrimp. Oil. $[\alpha]_D$ -65.3 (c, 2.07 in $CHCl_3$).

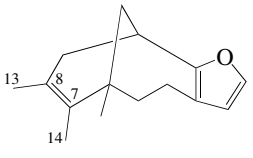
5α-Acetoxy: ***5-Acetoxynakafuran 8***
$C_{17}H_{22}O_3$ 274.359
Constit. of *Dysidea etheria*. Oil. $[\alpha]_D$ -31.1 (c, 3.06 in $CHCl_3$).

5-Oxo: ***5-Ketonakafuran 8***
$C_{15}H_{18}O_2$ 230.306
Constit. of *Dysidea etheria*. Insecticide. Toxic to brine shrimp. Oil. $[\alpha]_D$ +35.1 (c, 1.51 in $CHCl_3$).

Schulte, G. *et al., Helv. Chim. Acta*, 1980, **63**, 2159
Hochlowski, J.E. *et al., J.O.C.*, 1982, **47**, 88
Cardellina, J.H. *et al., J.O.C.*, 1988, **53**, 882 (*isol, pmr, cmr*)
Uyehara, T. *et al., J.C.S. Perkin 1*, 1992, 1785 (*synth*)

Nakafuran 9 N-15

[76844-26-3]



$C_{15}H_{20}O$ 216.322
Constit. of sponge *Dysidea fragilis* and of molluscs *Hypselodoris ghisleni*, *Hypselodoris godeffoyana*, *Chromodoris maridadilus* and *Chromodoris capensis*. Shows antifeedant props. Oil. Sol. MeOH, C_6H_6, $CHCl_3$; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D^{25}$ -106 (c, 0.33 in $CHCl_3$). λ_{max} 219 (ϵ 4290) (hexane) (Derep).

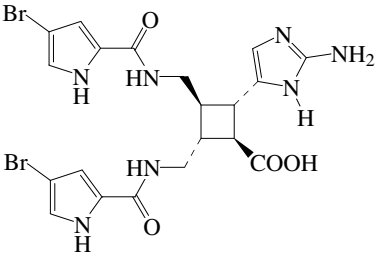
$\Delta^{8(13)}$-Isomer: ***Isonakafuran 9***
[147732-33-0]
$C_{15}H_{20}O$ 216.322
Constit. of *Hypselodoris* spp.

$\Delta^{7(14)}$-Isomer: ***$\Delta^{7(14)}$-Isonakafuran 9***
$C_{15}H_{20}O$ 216.322
Constit. of a *Dysidea* sp.
$[\alpha]_D^{25}$ +53.7 (c, 0.13 in $CHCl_3$). λ_{max} 222 (ϵ 10776) (hexane).

Schulte, G.R. *et al., Helv. Chim. Acta*, 1980, **63**, 2159-2167 (*isol*)
Hochlowski, J.E. *et al., J.O.C.*, 1982, **47**, 88 (*isol*)
Fontana, A. *et al., J. Chem. Ecol.*, 1993, **19**, 339 (*Isonakafuran 9*)
Flowers, A.E. *et al., Aust. J. Chem.*, 1998, **51**, 195-200 (*7(14)-isomer*)

Nakamuric acid N-16

[247145-39-7]



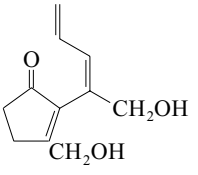
$C_{20}H_{21}Br_2N_7O_4$ 583.238
Isol. from the sponge *Agelas nakamurai*. Antibacterial agent. Amorph. brown solid. $[\alpha]_D$ -9.9 (c, 0.26 in MeOH). Incorr. MF in ref. λ_{max} 213 (log ϵ 4.02); 269 (log ϵ 4.08) (MeOH).

Me ester: [247113-88-8]
$C_{21}H_{23}Br_2N_7O_4$ 597.265
Isol. from *Agelas nakamurai*. Amorph. brown solid. $[\alpha]_D$ -4.1 (c, 0.3 in MeOH). Possible artifact. λ_{max} 213 (log ϵ 4.04); 269 (log ϵ 4.09) (MeOH).

Eder, C. *et al., J. Nat. Prod.*, 1999, **62**, 1295-1297 (*isol, pmr, cmr, uv*)

Nakienone A N-17

3-(Hydroxymethyl)-2-[1-(hydroxymethyl)-1,3-butadienyl]-2-cyclopenten-1-one
[161407-85-8]

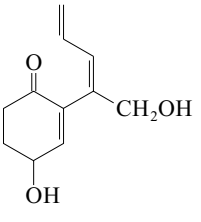


$C_{11}H_{14}O_3$ 194.23
Metab. of a cyanobacterial (*Synechocystis* sp.) growth on the coral *Acropora* sp. Cytotoxic agent. λ_{max} 234 (log ϵ 4.7) (EtOH). λ_{max} 234 (ϵ 50100) (MeOH) (Berdy).

Nagle, D.G. *et al., Tet. Lett.*, 1995, **36**, 849 (*isol, uv, ir, pmr, cmr*)
Pour, M. *et al., Tet. Lett.*, 1997, **38**, 525 (*synth*)

Nakienone B N-18

4-Hydroxy-2-[1-(hydroxymethyl)-1,3-butadienyl]-2-cyclohexen-1-one, 9CI
[161407-87-0]



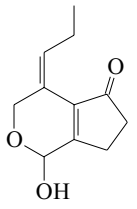
$C_{11}H_{14}O_3$ 194.23
Metab. of a cyanobacterial (*Synechocystis* sp.) growth on the coral *Acropora* sp. Cytotoxic agent. $[\alpha]_D^{25}$ +123 (c, 0.1 in MeOH) (as di-Ac).

Nagle, D.G. *et al., Tet. Lett.*, 1995, **36**, 849 (*isol, pmr, cmr*)
Pour, M. *et al., Tet. Lett.*, 1996, **37**, 4679-4682; 1997, **38**, 525-528 (*synth*)

Nakienone C N-19

3,4,6,7-Tetrahydro-1-hydroxy-4-propylidenecyclopenta[c]pyran-5(1H)-one, 9CI

[161407-88-1]



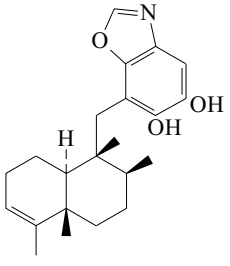
$C_{11}H_{14}O_3$ 194.23

Metab. of a cyanobacterial (*Synechocystis* sp.) growth on the coral *Acropora* sp. Cytotoxic agent. Rearrangement prod. of Nakienone A, N-17. Poss. artifact. λ_{max} 262 (log ϵ 4.2) (MeOH).

Nagle, D.G. *et al., Tet. Lett.*, 1995, **36**, 849 (*isol, pmr, cmr*)

Nakijinol N-20

[166990-20-1]



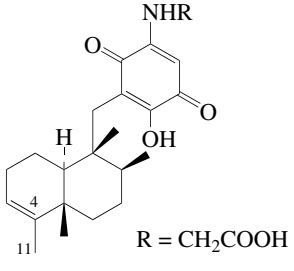
$C_{22}H_{29}NO_3$ 355.476

Constit. of an Okinawan sponge of the family Spongiidae. Amorph. powder. $[\alpha]_D^{20}$ -172 (c, 0.03 in MeOH). λ_{max} 300 (ϵ 3600); 332 (ϵ 2000) (MeOH) (Berdy).

Kobayashi, J. *et al., Tet. Lett.*, 1995, **36**, 5589 (*isol, pmr, cmr, uv, ir*)

Nakijiquinone A N-21

[157207-60-8]



$C_{23}H_{31}NO_5$ 401.502

Constit. of an Okinawan marine sponge. Protein -tyrosine kinase inhibitor. Red solid.

Mp 156-158°. $[\alpha]_D^{20}$ -71.7 (c, 1 in MeOH). Related to Avarol, A-766. λ_{max} 317 (ϵ 11800); 488 (ϵ 860) (MeOH) (Berdy).

Shigemori, H. *et al., Tetrahedron*, 1994, **50**, 8347 (*isol, pmr, cmr*)
Stahl, P. *et al., J.A.C.S.*, 2001, **123**, 11586-11593 (*synth*)

Nakijiquinone B N-22

[157232-59-2]

As Nakijiquinone A, N-21 with

R = CH(COOH)CH(CH_3)$_2$(*S*-)

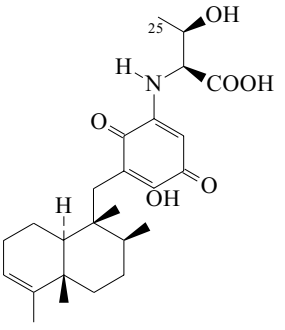
$C_{26}H_{37}NO_5$ 443.582

Constit. of an Okinawan marine sponge. Protein-tyrosine kinase inhibitor. Red solid. $[\alpha]_D^{20}$ -282.3 (c, 0.13 in $CHCl_3$). λ_{max} 320 (ϵ 12000); 492 (ϵ 910) (MeOH) (Berdy).

Shigemori, H. *et al., Tetrahedron*, 1994, **50**, 8347 (*isol, pmr, cmr*)
Stahl, P. *et al., J.A.C.S.*, 2001, **123**, 11586-11593 (*synth*)

Nakijiquinone D N-23

[169438-44-2]



$C_{25}H_{35}NO_6$ 445.555

Constit. of a marine sponge. Protein-tyrosine kinase inhibitor. Red amorph. solid. $[\alpha]_D^{20}$ -172 (c, 0.2 in EtOH). λ_{max} 317 (ϵ 12600); 490 (ϵ 1000) (MeOH) (Berdy).

25-Demethyl: ***Nakijiquinone C***

[169438-43-1]

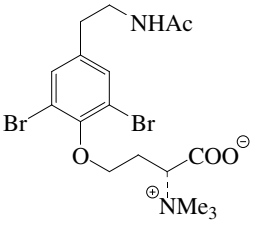
$C_{24}H_{33}NO_6$ 431.528

Constit. of a marine sponge. Protein-tyrosine kinase inhibitor. Red amorph. solid. $[\alpha]_D^{20}$ -73 (c, 0.03 in EtOH). λ_{max} 321 (ϵ 12100); 498 (ϵ 920) (MeOH) (Berdy).

Kobayashi, J. *et al., Tetrahedron*, 1995, **51**, 10867 (*isol, pmr, cmr*)
Stahl, P. *et al., J.A.C.S.*, 2001, **123**, 11586-11593 (*synth*)

Nakirodine A N-24

[473304-17-5]



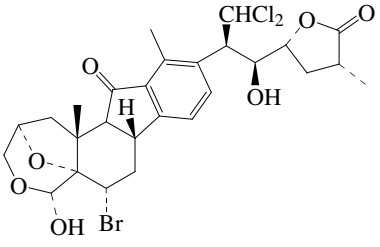
$C_{17}H_{24}Br_2N_2O_4$ 480.196

Isol. from a Verongid sponge. Oil. $[\alpha]_D^{25}$ +35 (c, 0.1 in MeOH). λ_{max} 283 (ϵ 880) (MeOH).

Tsuda, M. *et al., J. Nat. Prod.*, 2002, **65**, 1670-1671 (*isol, pmr, cmr, ms*)

Nakiterpiosin N-25

[571176-94-8]



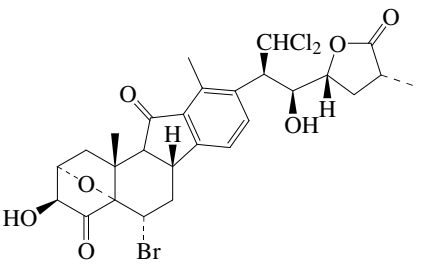
$C_{27}H_{31}BrCl_2O_7$ 618.347

Constit. of *Terpios hoshinota*.

Teruya, T. *et al., Tetrahedron*, 2004, **60**, 6989-6993 (*isol, pmr, cmr*)

Nakiterpiosinone N-26

[757976-67-3]

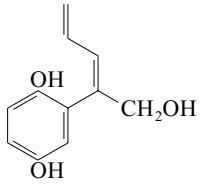


$C_{27}H_{29}BrCl_2O_7$ 616.331
Constit. of *Terpios hoshinota*.

Teruya, T. *et al., Tetrahedron*, 2004, **60**, 6989-6993 (*isol, pmr, cmr*)

Nakitriol N-27

2-[1-(Hydroxymethyl)-1,3-butadienyl]-1,4-benzenediol. 2-(2,5-Dihydroxyphenyl)-2,4-hexadien-1-ol
[161407-86-9]

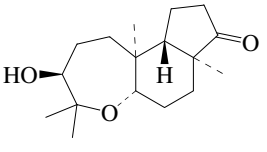


$C_{11}H_{12}O_3$ 192.214
Metab. of a cyanobacterial (*Synechocystis* sp.) growth on the coral *Acropora* sp. Cytotoxic. λ_{max} 228 (log ϵ 3.6); 302 (log ϵ 4.3) (MeOH).

Nagle, D.G. *et al., Tet. Lett.*, 1995, **36**, 849 (*isol, uv, pmr, cmr*)

Nakorone N-28

[233607-66-4]

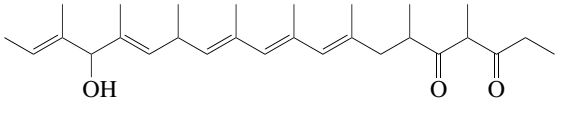


$C_{17}H_{28}O_3$ 280.406
Constit. of *Ptilocaulis spiculifer*. Oil. $[\alpha]_D$ -210 (c, 0.2 in MeOH). Probably derived from Abudinol, A-28.

Rudi, A. *et al., Tetrahedron*, 1999, **55**, 5555-5566 (*isol, pmr, cmr*)

Nalodionol N-29

17-Hydroxy-4,6,8,10,12,14,16,18-octamethyl-8,10,12,15,18-eicosapentaene-3,5-dione, 9CI
[179118-59-3]

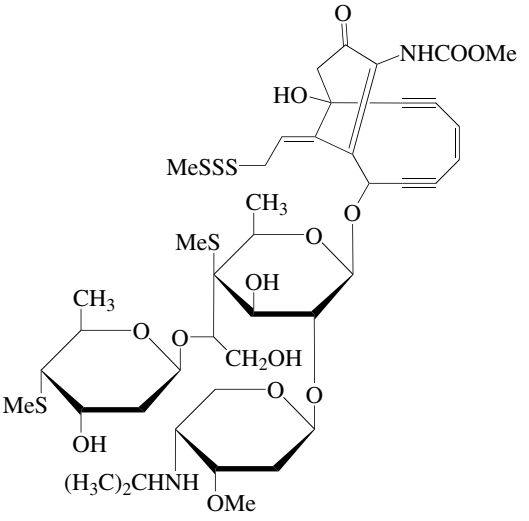


$C_{28}H_{44}O_3$ 428.654
Isol. from the mollusc *Smaragdinella calyculata*. Cytotoxic agent. Amorph. solid. $[\alpha]_D$ +19 (c, 1.2 in MeOH). λ_{max} 207 (ϵ 1100); 267 (ϵ 9500) (MeOH).

Szabo, C.M. *et al., Tetrahedron*, 1996, **52**, 9681-9686 (*isol, uv, ir, pmr, cmr*)

Namenamicin N-30

[184349-17-5]

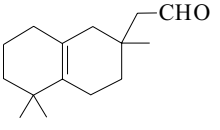


$C_{43}H_{62}N_2O_{14}S_5$ 991.298
Isol. from the marine ascidian *Polysyncraton lithostrotum*. Antitumour agent. Related to Calicheamicins.

McDonald, L.A. *et al., J.A.C.S.*, 1996, **118**, 10898 (*isol*)
Weinstein, D.S. *et al., J.C.S. Perkin 1*, 1999, 545-557 (*synth*)

Nanaimoal N-31

1,2,3,4,5,6,7,8-Octahydro-2,5,5-trimethyl-2-naphthaleneacetaldehyde, 9CI
[89320-84-3]

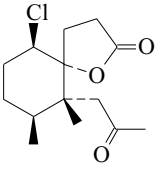


$C_{15}H_{24}O$ 220.354
Constit. of nudibranch *Acanthodoris nanaimoensis*.

Ayer, S.W. *et al., Tet. Lett.*, 1984, **25**, 141-144 (*isol, synth*)
Yamada, T. *et al., Chem. Lett.*, 1993, 29 (*synth*)
Omadani, T. *et al., Chem. Comm.*, 1994, 2781 (*synth*)
Graziani, E.I. *et al., J.A.C.S.*, 1996, **118**, 4701 (*biosynth*)
Engler, T.A. *et al., J.O.C.*, 1996, **61**, 8456 (*synth*)

Napalilactone N-32

[145458-38-4]

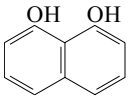


$C_{14}H_{21}ClO_3$ 272.771
Constit. of *Lemnalia africana*. Oil. $[\alpha]_D$ +7.2 (c, 0.63 in MeOH).

Carney, J.R. *et al., Tet. Lett.*, 1992, **33**, 7115 (*isol, pmr, cmr*)

1,8-Naphthalenediol, 9CI, 8CI N-33

1,8-Dihydroxynaphthalene
[569-42-6]



$C_{10}H_8O_2$ 160.172
Found in ascomycete fungi. Used in photometric detn. of Ti. Intermed. in biosynth. of fungal melanin pigments by oxidative polym. Leaflets (H_2O). Sol. hot H_2O. Mp 140°.

O-α-D-Glucopyranoside: [22427-32-3]
$C_{16}H_{18}O_7$ 322.314
Prod. by *Xylaria mellisii* BCC 1005. Active against herpes simplex virus-type 1. Cytotoxic. Brown amorph. solid.
Mp 205-207° dec. $[\alpha]_D^{31}$ +127 (c, 0.32 in EtOH). λ_{max} 226 (log ϵ 4.89); 302 (log ϵ 4.09); 317 (log ϵ 4.04); 332 (log ϵ 4.01) (EtOH).

Di-Ac: [6566-25-2]
$C_{14}H_{12}O_4$ 244.246
Mp 147-148°.

Mono-Me ether: 8-Methoxy-1-naphthol
[3588-75-8]
$C_{11}H_{10}O_2$ 174.199
Isol. from a strain of *Daldinia concentrica* and occurs in *Hypoxylon macrocarpum*. Nematocide. Melanin biosynthesis inhibitor. Cryst. (petrol or EtOH). Mp 55-56° (47°).

Di-Me ether: 1,8-Dimethoxynaphthalene
[10075-66-8]
$C_{12}H_{12}O_2$ 188.226
Produced by *Daldinia concentrica*. Nematocide. Melanin biosynthesis inhibitor. Leaflets (Et_2O or EtOH aq.).
Mp 158-161°.

Mono-Et ether: 8-Ethoxy-1-naphthol
[104422-22-2]
$C_{12}H_{12}O_2$ 188.226
$Bp_{0.2}$ 72°.

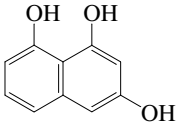
Di-Et ether: 1,8-Diethoxynaphthalene
[104422-23-3]
$C_{14}H_{16}O_2$ 216.279
Cryst. (EtOH).

Mono(trifluoromethyl) ether: [403646-58-2]
$C_{11}H_7F_3O_2$ 228.17
Mp 48-49°.

Buu-Hoï, N.P. *et al., J.C.S.*, 1956, 2412 (*synth*)
Allport, D.C. *et al., J.C.S.*, 1960, 654 (*isol, derivs*)
Lurie, A.P. *et al., J.A.C.S.*, 1961, **83**, 5015-5019 (*synth*)
v. Gemert, J.T. *et al., Aust. J. Chem.*, 1968, **21**, 2203 (*ir*)
Ashworth, P. *et al., J.C.S. Perkin 2*, 1974, 739 (*epr*)
Granger, P. *et al., J. Magn. Reson.*, 1976, **22**, 405 (*cmr, pmr*)
Eremenko, M.V. *et al., Zh. Anal. Khim.*, 1978, **33**, 1955 (*detn, Ti*)
Snieckus, V. *et al., J.O.C.*, 1986, **57**, 271 (*deriv*)
Ragot, J.P. *et al., J.C.S. Perkin 1*, 1999, 1073-1082 (*synth, ir, pmr, cmr*)
Schlosser, M. *et al., Eur. J. Org. Chem.*, 2001, 3991-3997 (*monotrifluoromethyl ether*)
Barrett, A.G.M. *et al., J.O.C.*, 2002, **67**, 2735-2750 (*synth*)
Muhlbauer, A. *et al., Mycol. Prog.*, 2002, **1**, 235-248 (*mono-Me ether, occur*)
Pittayakhajonwut, P. *et al., Tet. Lett.*, 2005, **46**, 1341-1344 (*α-D-glucoside*)

1,3,8-Naphthalenetriol, 9CI, 8CI N-34

1,3,8-Trihydroxynaphthalene
[7124-49-4]



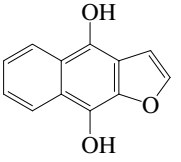
$C_{10}H_8O_3$ 176.171
Metab. of *Lachnellula* sp. and *Verticillium dahliae*. Also prod. by the marine-derived *Alternaria* sp. Stamm 6588. Biosynth. intermediate of melanin. Mp 194-196° (darkening). Unstable in air.

Tri-Ac: [7288-20-2]
$C_{16}H_{14}O_6$ 302.283
Cryst. (petrol). Mp 120-121.5°.

Aldridge, D.C. *et al., J.C.S. Perkin 1*, 1974, 1540-1541 (*synth, ir, pmr*)
Cameron, D.W. *et al., Aust. J. Chem.*, 1976, **29**, 1865-1867 (*struct, synth*)
Viviani, F. *et al., J.C.S. Perkin 1*, 1990, 1255-1259 (*synth, uv, ir, pmr*)
Semar, M. *et al., Z. Naturforsch., C*, 1996, **51**, 500 (*isol, uv, ir, pmr*)
Simpson, T.J. *et al., J.C.S. Perkin 1*, 2000, 2771-2775 (*synth, pmr, cmr, ms*)
Ichinose, K. *et al., Chem. Pharm. Bull.*, 2001, **49**, 192-196 (*synth*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

Naphtho[2,3-*b*]furan-4,9-diol N-35

*4,9-Dihydroxynaphtho[2,3-*b*]furan*. ***Di-O-demethylavicenol B***



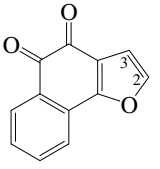
$C_{12}H_8O_3$ 200.193
Constit. of *Tabebuia heptaphylla*.

*Di-Me ether: 4,9-Dimethoxynaphtho[2,3-*b*]furan*. ***Avicenol B***
[189763-01-7]
$C_{14}H_{12}O_3$ 228.247
Constit. of the stem bark of *Avicennia alba*. Oil. λ_{max} 212; 246; 331; 345 (MeOH).

Ito, C. *et al., Chem. Pharm. Bull.*, 2000, **48**, 339-343 (*Avicenol B*)
Schmeda-Hirschmann, G. *et al., Z. Naturforsch., C*, 2003, **58**, 495-501, (*isol, pmr, ms*)

Naphtho[1,2-*b*]furan-4,5-dione, 9CI N-36

[32358-83-1]



$C_{12}H_6O_3$ 198.178
Produced by *Avicennia marina* in response to a fungal (Phytophthora) infection. Phytoalexin. Dark reddish-orange needles (EtOH). Mp 215-216° (209.5-210°). λ_{max} 243; 275 (EtOH) (Berdy).

2,3-Dihydro: [32013-77-7]
$C_{12}H_8O_3$ 200.193
Present in the spines of sea urchins. Orange felted needles (Me_2CO). Mp 227-228°.

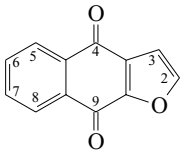
*3-Hydroxy: 3-Hydroxynaphtho[1,2-*b*]furan-4,5-dione, 9CI*
[100675-95-4]
$C_{12}H_6O_4$ 214.177
Prod. by *Avicennia marina* infected with *Phytophthora* sp. Phytoalexin. Tentative identification. λ_{max} 264; 301 (EtOH) (Berdy).

Scholl, R. *et al., Ber.*, 1919, **52**, 1142 (*synth*)
Hooker, S.C. *et al., J.A.C.S.*, 1936, **58**, 1202 (*synth*)
Oliver, R.W.A. *et al., J.C.S.(B)*, 1971, 341 (*ms*)
Sutton, D.C. *et al., Phytochemistry*, 1985, **24**, 2877-2879 (*isol, pmr, ms*)
Rosenkranz, H.S. *et al., Carcinogenesis (London)*, 1990, **11**, 349 (*tox*)
Gupta, R.B. *et al., Synlett*, 1990, 335 (*synth, ir, uv, pmr, dihydro*)
Lee, Y.R. *et al., Synth. Commun.*, 2002, **32**, 3099-3105 (*synth, ir, pmr*)

Naphtho[2,3-*b*]furan-4,9-dione N-37

2,3-Phthalyfuran. ***Avicequinone B***

[5656-82-6]



$C_{12}H_6O_3$ 198.178

Constit. of the stem bark of *Avicennia alba*. Exhibits strong inhibitory activity against Epstein-Barr virus. Derivs. occur naturally and show various biological activities. Yellow needles (EtOH aq.).

Mp 225-225.5° (220-221°). λ_{max} 244; 248; 286; 336 (MeOH).

2,3-Dihydro: [32013-78-8]

$C_{12}H_8O_3$ 200.193

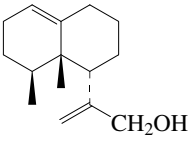
Present in sea urchins. Yellow rods (EtOH aq.).

Mp 218.5-219°.

Mathieson, J.W. *et al., J.C.S.(C)*, 1971, 153 (*synth, ir, uv, pmr, occur, deriv*)
Rivalle, C. *et al., Tetrahedron*, 1974, **30**, 3193 (*synth, ir, pmr*)
Konoshima, T. *et al., J. Nat. Prod.*, 1989, **52**, 987 (*activity, synth, ir, uv, ms, pmr*)
Koyanagi, J. *et al., J. Het. Chem.*, 1994, **31**, 1303; 1995, **32**, 1289 (*synth, ir, pmr*)
Starling, S.M. *et al., Synth. Commun.*, 1998, **28**, 3567-3578 (*synth, pmr*)
Ito, C. *et al., Chem. Pharm. Bull.*, 2000, **48**, 339-343 (*isol, pmr, cmr*)
Lee, Y.R. *et al., Synth. Commun.*, 2002, **32**, 3099-3105 (*synth, ir, pmr*)

1(10),11(13)-Nardosinadien-12-ol N-38

[168781-82-6]

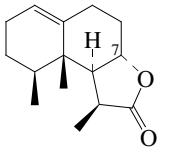


$C_{15}H_{24}O$ 220.354

Constit. of *Phyllogorgia dilatata*.

Fernandes, L. *et al., Ann. Acad. Bras. Cienc.*, 1995, **67**, 171-173; *CA*, **123**, 251818a (*isol, pmr, cmr*)

1(10)-Nardosinen-12,7-olide N-39



(7α,11β)-*form*

$C_{15}H_{22}O_2$ 234.338

(7α,11β)-*form*

7-Epilemnalactone

[72541-01-6]

Constit. of *Paralemnalia digitiformis*.

Cryst.

Mp 30°. $[\alpha]_D$ -84 (c, 0.6 in $CHCl_3$).

(7β,11β)-*form*

Lemnalactone

[63043-49-2]

Constit. of *Paralemnalia digitiformis*.

Cryst.

Mp 105-106°. $[\alpha]_D$ -240 (c, 0.3 in $CHCl_3$).

Ahond, A. *et al., Bull. Soc. Chim. Belg.*, 1979, 313 (*isol*)
Ahond, A. *et al., Tet. Lett.*, 1979, **20**, 1879-1880 (*struct*)
Dischmann, M. *et al., Annalen*, 1989, 727 (*synth*)

Anguilla japonica Natriuretic factor N-40

[135493-52-6]

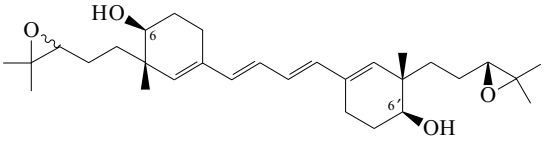
H-Lys-Ser-Phe-Asn-Ser-Cys-Phe-Gly-Thr-Arg-Met-Asp-Arg-Ile-Gly-Ser-Trp-Ser-Gly-Leu-Gly-Cys-Asn-Ser-Leu-Lys-Asn-Gly-Thr-Lys-Lys-Lys-Ile-Phe-Gly-Asn-OH

Isol. from the cardiac ventricles of *Anguilla japonica*. Natriuretic agent.

Takei, Y. *et al., FEBS Lett.*, 1991, **282**, 317

Naurol A N-41

[130246-98-9]



$C_{30}H_{46}O_4$ 470.691

The proposed struct. has been shown to be incorrect by synth.

Constit. of an unidentified sponge, prob.*Rhaphisia* sp. Shows cytotoxic activity. Solid.

Mp 97°. $[\alpha]_D$ +6.21 (c, 2.64 in MeOH). λ_{max} 286 (ϵ 49130) (MeOH) (Berdy).

6,6′-Diepimer: ***Naurol B***

[130322-42-8]

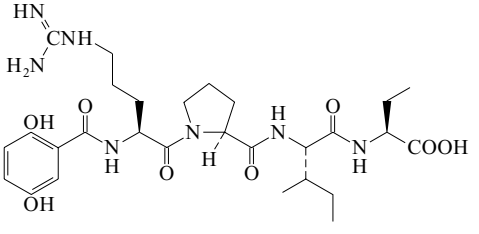
$C_{30}H_{46}O_4$ 470.691

Constit. of an unidentified sponge, prob. *Rhaphisia* sp. Solid. $[\alpha]_D$ +12.63 (c, 0.19 in MeOH). λ_{max} 292 (ϵ 44240) (MeOH) (Berdy).

De Guzman, F.S. *et al., J.O.C.*, 1991, **56**, 55-58 (*isol, pmr, cmr*)
Nozawa, D. *et al., J.C.S. Perkin 1*, 2000, 2043-2046 (*synth, activity*)

Nazumamide A N-42

[138949-86-7]

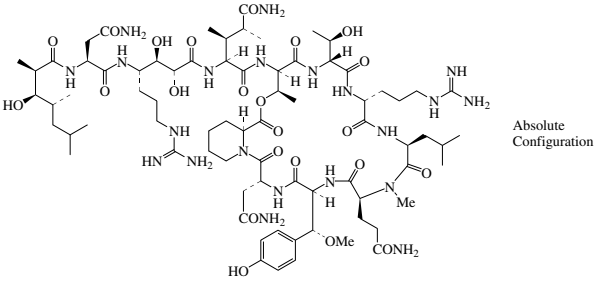


$C_{28}H_{43}N_7O_8$ 605.69

Isol. from the sponge *Theonella* sp. Thrombin inhibitor. Amorph. powder. Sol. MeOH, butanol. $[\alpha]_D^{23}$ +87.1 (c, 0.075 in MeOH). λ_{max} 212 (ϵ 36000); 240 (ϵ 11300); 325 (ϵ 4400) (MeOH).

Fusetani, N. *et al., Tet. Lett.*, 1991, **32**, 7073-7074 (*isol, struct*)
Nienaber, V.L. *et al., J.A.C.S.*, 1996, **118**, 6807-6810 (*cryst struct*)

Neamphamide A N-43



Absolute Configuration

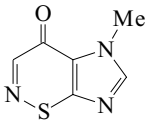
$C_{75}H_{125}N_{21}O_{23}$ 1688.939

Isol. from the sponge *Neamphius huxleyi*. Exhibits potent cytoprotection against HIV-1. Amorph. solid. $[\alpha]_D^{21}$ -0.6 (c, 0.2 in MeOH). λ_{max} 276 (ϵ 1900) (MeOH).

Oku, N. *et al., J. Nat. Prod.*, 2004, **67**, 1407-1411 (*isol, pmr, cmr*)
Oku, N. *et al., J.O.C.*, 2005, **70**, 6842-6847 (*abs config*)

Neamphine N-44

5-Methylimidazo[4,5-e]-1,2-thiazin-4(5H)-one, 9CI
[135384-35-9]



$C_6H_5N_3OS$ 167.191
Metab. of the marine sponge *Neamphius huxleyi*. Cytotoxic. Needles (hexane/$CHCl_3$).

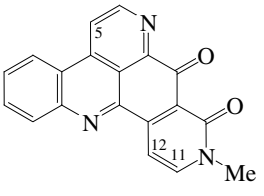
de Silva, E.D. *et al., Tet. Lett.*, 1991, **32**, 2707 (*isol, cryst struct*)

Negimoctin N-45

[112099-21-5]
Struct. unknown. Isol. from *Sargassum segamianum*. Inhibitor of lipid peroxide formn; used to decrease blood level of lipid peroxides. Sol. MeOH, DMSO, $CHCl_3$, DMF; poorly sol. hexane, H_2O. λ_{max} 288 (ϵ 3370) (MeOH) (Berdy).
Japan. Pat., 1987, 62 155 219; *CA*, **108**, 26950h (*isol*)

Neoamphimedine N-46

10-Methyl-8H-benzo[b]pyrido[4,3,2-de][1,8]phenanthroline-8,9(10H)-dione, 9CI
[221456-55-9]

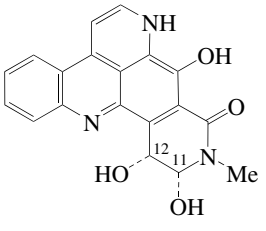


$C_{19}H_{11}N_3O_2$ 313.315
Alkaloid from *Xestospongia* cf. *carbonaria* and *Xestospongia* cf. *exigua*. Topoisomerase II inhibitor which catenates DNA. Yellow solid.
Mp >300°. λ_{max} 205 (ϵ 26370); 226 (ϵ 23740); 278 (ϵ 16870); 371 (ϵ 10190) (EtOH).

5-Methoxy: ***5-Methoxyneoamphimedine***
[485817-61-6]
$C_{20}H_{13}N_3O_3$ 343.341
Alkaloid from *Xestospongia* cf. *carbonaria* and *Xestospongia* cf. *exigua*. Yellow solid.
De Guzman, F.S. *et al., J.O.C.*, 1999, **64**, 1400-1402 (*Neoamphimedine*)
Thale, Z. *et al., J.O.C.*, 2002, **67**, 9384-9391 (*5-Methoxyneoamphimedine*)

Neoamphimedine Y N-47

[486992-27-2]

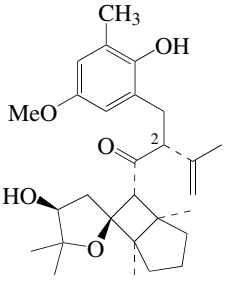


$C_{19}H_{15}N_3O_4$ 349.345
Alkaloid from *Xestospongia* cf. *carbonaria*. Purple solid. Turns brown on standing.

11,12-Di-Me ether: ***Neoamphimedine Z***
[486992-28-3]
$C_{21}H_{19}N_3O_4$ 377.399
Alkaloid from *Xestospongia* cf. *carbonaria*. Purple solid. Turns brown on standing.
Thale, Z. *et al., J.O.C.*, 2002, **67**, 9384-9391 (*isol, pmr, cmr*)

Neobalearone N-48

[124990-66-5]



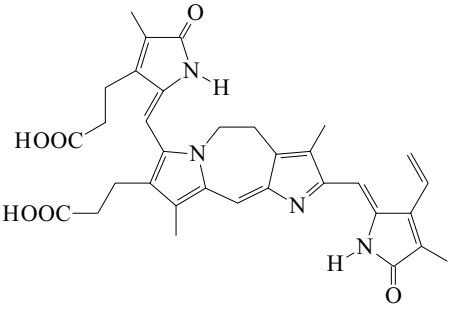
$C_{28}H_{40}O_5$ 456.621
Metab. of *Cystoseira stricta*. Oil. $[\alpha]_D^{25}$ +120 (c, 1.6 in EtOH).

2-Epimer: ***Epineobalearone***
[124898-14-2]
$C_{28}H_{40}O_5$ 456.621
Metab. of *Cystoseira stricta*. Oil. $[\alpha]_D^{25}$ -77.1 (c, 1.86 in EtOH).

2,12-Diepimer: ***2,12-Diepineobalearone***
[194550-99-7]
$C_{28}H_{40}O_5$ 456.621
Metab. of *Cytoseira amentacea* var. *stricta*. Oil. $[\alpha]_D^{25}$ -109.8 (c, 1.3 in EtOH). C-12 is the spiro centre.
Amico, V. *et al., J. Nat. Prod.*, 1989, **52**, 962; 1997, **60**, 1088-1093 (*isol, pmr, cmr, abs config*)
Mesguiche, V. *et al., Phytochemistry*, 1997, **45**, 1489-1494 (*2,12-Diepineobalearone*)

Neobiliverdin IXδ N-49

[61477-99-4]

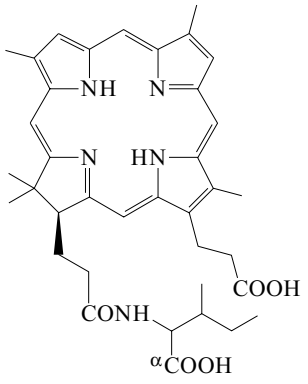


$C_{33}H_{34}N_4O_6$ 582.655
Isol. from the ovary of *Turbo cornutus*. Deep blue pigment.

Bois-Choussy, M. *et al., Helv. Chim. Acta*, 1980, **63**, 1098 (*synth, pmr, struct*)
Petrier, C. *et al., Org. Magn. Reson.*, 1983, **21**, 221 (*cmr*)
Benedikt, E. *et al., Eur. J. Biochem.*, 1988, **175**, 643 (*isol*)
Iturraspe, J.B. *et al., J.A.C.S.*, 1989, **111**, 1525 (*synth*)

Neobonellin N-50

[69257-05-2]



$C_{37}H_{45}N_5O_5$ 639.793

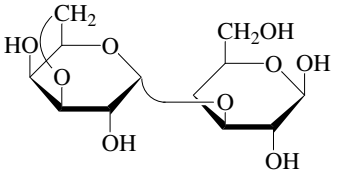
Pigment of the skin of *Bonellia viridis*. Embryotoxic agent. λ_{max} 391; 491; 521; 536 (sh); 588; 613; 640 ($CHCl_3$) (Derep).

α-Me ester: [75074-84-9]
$C_{38}H_{47}N_5O_5$ 653.82
Constit. of *Bonellia viridis*.

Cariello, L. *et al., Experientia*, 1978, **34**, 1427-1429 (*isol*)
Ballantine, J.A. *et al., J.C.S. Perkin 1*, 1980, 1080 (*deriv*)

Neocarrabiose N-51

3-O-*(3,6-Anhydro-α-D-galactopyranosyl)-D-galactose*
[70456-76-7]



β-Pyranose-*form*

$C_{12}H_{20}O_{10}$ 324.284

Repeating unit of carrageenans. Constit. of Mediterranean red alga *Rissoella verruculosa*.

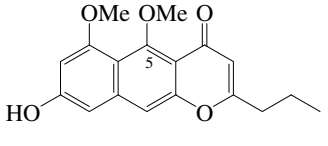
β-Pyranose-*form* [79297-08-8]
Cryst. (2-propanol aq.). Mp 164-166°. $[\alpha]_D^{24}$ +96 → +110 (c, 1.0 in H_2O).

[150571-82-7]

Combaut, G. *et al., Phytochemistry*, 1985, **24**, 1597 (*occur*)
Lamba, D. *et al., Carbohydr. Res.*, 1990, **208**, 215 (*cryst struct*)
Ueda, K. *et al., Biopolymers*, 1996, **38**, 461 (*conformn*)
Stortz, C.A. *et al., J. Carbohydr. Chem.*, 2000, **19**, 1115-1130 (*conformn*)

Neocomantherin N-52

*8-Hydroxy-5,6-dimethoxy-2-propyl-4*H-*naphtho[2,3-*b*]pyran-4-one*
[31665-32-4]



$C_{18}H_{18}O_5$ 314.337
Constit. of *Comantheria perplexa* and *Comantheria briareus*.
Yellow cryst. (EtOAc).
Mp 237° dec.

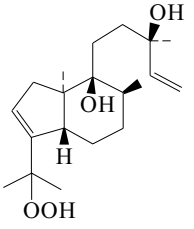
8-O-*Sulfate:* [72241-32-8]
$C_{18}H_{18}O_8S$ 394.401
Isol. from *Comantheria perplexa*.

5-O-*De-Me: 5,8-Dihydroxy-6-methoxy-2-propyl-4*H-*naphtho[2,3-*b*]pyran-4-one*
[77165-78-7]
$C_{17}H_{16}O_5$ 300.31
Isol. from *Comantheria briareus*. Cryst. (MeOH).
Mp 205-207°. λ_{max} 224 (log ε 4.27); 250 (log ε 4.24); 275 (log ε 4.4); 324 (log ε 3.42); 405 (log ε 3.6) (EtOH).

Kent, R.A. *et al., Aust. J. Chem.*, 1970, **23**, 2325-2335 (*isol, pmr*)
Francesconi, K.A. *et al., Aust. J. Chem.*, 1980, **33**, 2781-2784 (*5-demethyl, isol, pmr, ms*)

Neoconcinndiol hydroperoxide N-53

[64504-60-5]

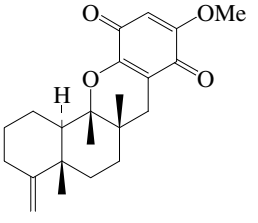


$C_{20}H_{34}O_4$ 338.486
Constit. of *Laurencia snyderae*. Cryst.
Mp 158-159°. $[\alpha]_D^{22}$ -35 (c, 0.8 in MeOH).

Howard, B.M. *et al., J.A.C.S.*, 1977, **99**, 6440

Neodactyloquinone N-54

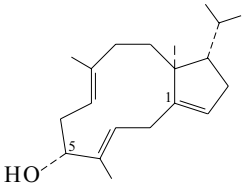
[487016-14-8]



$C_{22}H_{28}O_4$ 356.461
Constit. of *Dactylospongia elegans*. Pale yellow amorph. solid.
$[\alpha]_D^{27}$ +28.6 (c, 0.4 in $CHCl_3$). λ_{max} 291 (log ε 4.2) (EtOH).

Mitome, H. *et al., J. Nat. Prod.*, 2003, **66**, 46-50 (*isol, pmr, cmr*)

1(14),3,7-Neodolabellatrien-5-ol N-55



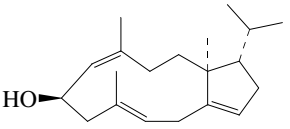
(3*E*,5α,7*E*)–*form*

$C_{20}H_{32}O$ 288.472

(3E,5α,7E)-form
Neodolabellenol
[69010-14-6]
Constit. of soft corals *Clavularia koellikeri* and *Clavularia inflata*. Needles.
Mp 158-160°.

(3*E*,5β,7*E*)-*form* [68978-05-2]
Constit. of soft corals.
Cryst. (MeCN).
Mp 108-109°. $[\alpha]_D$ +65.7 (c, 0.4 in $CHCl_3$).
Bowden, B.F. *et al., Aust. J. Chem.*, 1978, **31**, 2039; 1980, **33**, 927 (*isol, cryst struct*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 2306 (*isol*)
Williams, D.R. *et al., Tet. Lett.*, 1995, **36**, 35 (*synth*)

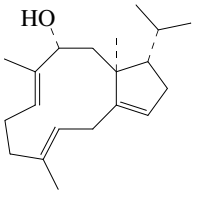
1(14),3,7-Neodolabellatrien-6-ol N-56



$C_{20}H_{32}O$ 288.472

(3*E*,6β,7*Z*)-*form*
Hydroclathrol
[368867-33-8]
Constit. of the alga *Hydroclathrus tenuis.*
Needles.
Mp 124-125°.
Xu, X.H. *et al., Chin. Chem. Lett.*, 2001, **12**, 709-712 (*isol, pmr, cmr*)

1(14),3,7-Neodolabellatrien-9-ol N-57

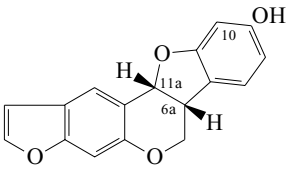


$C_{20}H_{32}O$ 288.472

9α-*form* [680210-19-9]
Constit. of *Clavularia koellikeri*.
Cryst. $[\alpha]_D^{25}$ +131 (c, 0.43 in $CHCl_3$).
9-Ketone: ***1(14),3,7-Neodolabellatrien-9-one***
[680210-18-8]
$C_{20}H_{30}O$ 286.456
Constit. of *Clavularia koellikeri*. Cryst. $[\alpha]_D^{25}$ +153 (c, 0.18 in $CHCl_3$). λ_{max} 234 (ε 5600) (EtOH).
Iguchi, K. *et al., J. Nat. Prod.*, 2004, **67**, 577-583 (*isol, pmr, cmr, cryst struct*)

Neodunol N-58

*6*a,*11*a-*Dihydro-6*H-*benzofuro[3,2-*c*]furo[3,2-*g*][1]benzopyran-9-ol, 9CI*
[53766-53-3]



$C_{17}H_{12}O_4$ 280.279
Pterocarpan numbering shown. Isol. from *Neorautanenia edulis*, also from *Neorautanenia amboensis* and *Pachyrrhizus erosus* (yam bean). Cryst. (C_6H_6/hexane).
Mp 170.5-171.5°. $[\alpha]_D^{22}$ -284.9 (c, 0.8 in $CHCl_3$). λ_{max} 246 (ε 27000) (MeOH) (Berdy). λ_{max} 213; 241; 248; 255; 294 (EtOH) (Berdy). λ_{max} 216; 248; 255; 301 (EtOH-NaOH) (Berdy).

Me ether: ***9-O-Methylneodunol***
[53833-80-0]
$C_{18}H_{14}O_4$ 294.306
Isol. from the marine coral *Echinopora lamellosa*.
Mp 175°. $[\alpha]_D^{25}$ -217 (c, 0.415 in $CHCl_3$). Rare animal source of a flavonoid.

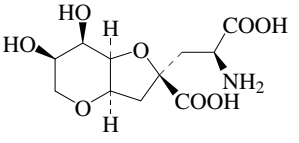
Me ether, 10-methoxy: ***Ambonane***
[76165-15-6]
$C_{19}H_{16}O_5$ 324.332
Isol. from *Neorautanenia amboensis* root bark. Light-yellow needles (Et_2O/hexane).
Mp 125-127°. $[\alpha]_D$ -214 (c, 0.01 in $CHCl_3$).

*6*a,*11*a-*Didehydro:* ***Neorauteen***. *6*H-*Benzofuro[3,2-*c*]furo[3,2-*g*][1]benzopyran-9-ol, 9CI*
[53766-54-4]
$C_{17}H_{10}O_4$ 278.264
Isol. from *Neorautanenia edulis* root bark. Plates (MeOH).
Mp 202.5-204°.

*6*a,*11*a-*Didehydro, Ac:*
Needles. Mp 197.5-199°.

Brink, A.J. *et al., Phytochemistry*, 1972, **16**, 273 (*isol*)
Brink, A.J. *et al., Phytochemistry*, 1974, **13**, 1581 (*Neorauteen*)
Chalmers, A.A. *et al., Tetrahedron*, 1977, **33**, 1735-1737 (*cmr*)
Ingham, J.L. *et al., Z. Naturforsch., C*, 1979, **34**, 683 (*isol*)
Breytenbach, J.C. *et al., J.C.S. Perkin 1*, 1980, 1804 (*Ambonane*)
Sanduja, R. *et al., J. Het. Chem.*, 1984, **21**, 845 (*isol, deriv, cryst struct, abs config*)

Neodysiherbaine A N-59



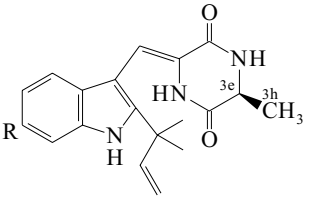
Absolute Configuration

$C_{11}H_{17}NO_8$ 291.257
Isol. from *Dysidea herbacea*. Neurotoxin. Pale yellow solid. $[\alpha]_D^{23}$ -6.5 (c, 0.75 in H_2O).

Sakai, R. *et al., Org. Lett.*, 2001, **3**, 1479-1482 (*isol, synth, cd, pmr, cmr*)
Lygo, B. *et al., Tet. Lett.*, 2005, **46**, 6629-6632 (*synth*)
Takahashi, K. *et al., J.O.C.*, 2006, **71**, 4227-4231 (*synth*)
Shoji, M. *et al., J.O.C.*, 2006, **71**, 5208-5220 (*synth*)

Neoechinulin A N-60

*3-[[2-(1,1-Dimethyl-2-propenyl)-1*H-*indol-3-yl]methylene]-6-methyl-2,5-piperazinedione, 9CI*
[51551-29-2]



R = H

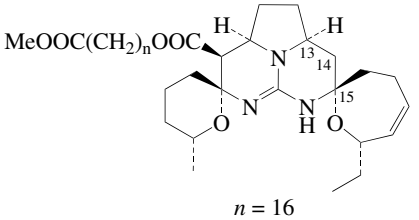
$C_{19}H_{21}N_3O_2$ 323.394
Isol. from *Aspergillus amstelodami*, *Aspergillus repens* and *Aspergillus ruber*. Potential food preservative. Shows high antioxidative activity. Ivory cryst. (MeOH).
Mp 264-265°. λ_{max} 283 (ε 8300); 338 (ε 9300) (EtOH).

*3*e,*3*h-*Didehydro:* ***Neoechinulin B***. *Alkaloid E10*
[55179-53-8]
$C_{19}H_{19}N_3O_2$ 321.378
Isol. from *Aspergillus amstelodami*. Yellow cryst. (MeOH).
Mp 234-236°.
Marchelli, M. *et al., J.C.S. Perkin 1*, 1977, 713-717 (*isol, uv, ir, pmr*)

Nagasawa, H. *et al., Agric. Biol. Chem.*, 1979, **43**, 1759-1763 (*cmr, struct*)
Nakatsuka, S. *et al., Tet. Lett.*, 1980, 2817-2820 (*synth, uv, ir, pmr*)
Yagi, R. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 932-933 (*isol, pmr, cmr, activity*)
Li, Y. *et al., Chem. Pharm. Bull.*, 2004, **52**, 375-376 (*isol, pmr, cmr*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 469; 471

Neofolitispate 1 N-61

[229160-50-3]



Absolute Configuration

n = 16

$C_{40}H_{67}N_3O_6$ 685.986

Related to Ptilomycalin A, P-698. Alkaloid from the sponge *Neofolitispa dianchora*. Antiviral agent.

Lower homologue (n = 14): ***Neofolitispate 3***
[229160-52-5]
$C_{38}H_{63}N_3O_6$ 657.932
Alkaloid from *Neofolitispa dianchora*. Antiviral agent.

Lower homologue (n = 15): ***Neofolitispate 2***. *Crambescidin 657 methyl ester*
[229160-51-4]
$C_{39}H_{65}N_3O_6$ 671.959
Alkaloid from *Neofolitispa dianchora*. Antiviral agent. Oil. $[\alpha]_D$ -18 (c, 1 in $CHCl_3$).

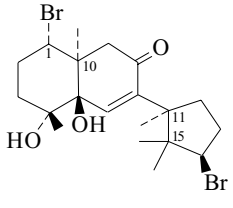
Lower homologue (n = 15), parent acid: ***Crambescidin 657***
[214215-58-4]
$C_{38}H_{63}N_3O_6$ 657.932
Alkaloid from *Crambe crambe*. Cytotoxic agent. Zwitterionic.

Lower homologue (n = 15), 13,14,15-triepimer, parent acid: ***Isocrambescidin 657***
[214215-60-8]
$C_{38}H_{63}N_3O_6$ 657.932
Alkaloid from *Crambe crambe*. Zwitterionic.

Venkateswarlu, Y. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 254-256 (*isol*)
Coffey, D.S. *et al., J.A.C.S.*, 2000, **122**, 4893-4903; 4904-4914 (*synth*)

Neoirienone N-62

[84297-62-1]



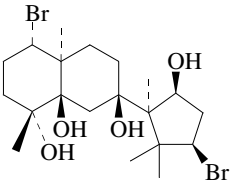
$C_{20}H_{30}Br_2O_3$ 478.263

Constit. of red marine alga *Laurencia irieii*. Viscous oil. $[\alpha]_D^{20}$ +1 (c, 1.5 in $CHCl_3$).

Howard, B.M. *et al., Tet. Lett.*, 1982, **23**, 3847 (*cryst struct*)

Neoirietetrol N-63

[410071-72-6]



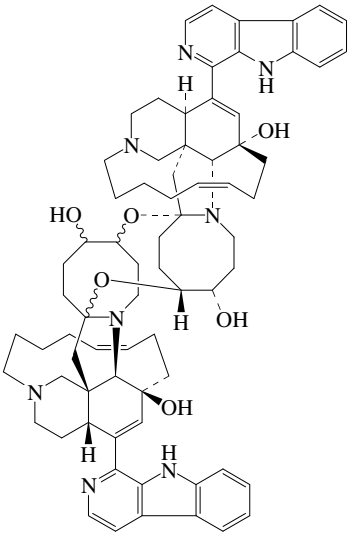
$C_{20}H_{34}Br_2O_4$ 498.294

Metab. of *Laurencia yonaguniensis*. Cryst.
Mp 126-128°. $[\alpha]_D^{28}$ -43 (c, 0.53 in $CHCl_3$).

Takahashi, Y. *et al., J. Nat. Prod.*, 2002, **65**, 395-398 (*isol, pmr, cmr*)

Neokauluamine N-64

[334491-54-2]



Relative Configuration

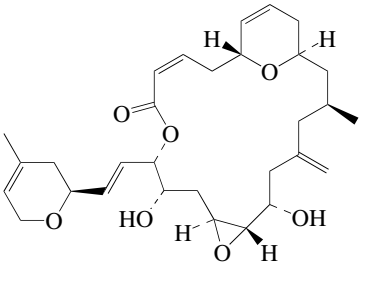
$C_{72}H_{88}N_8O_6$ 1161.537

Alkaloid from an undescribed sponge of the Petrosiidae. Cytotoxic. Needles (EtOH).
Mp 184°. $[\alpha]_D^{25}$ +94.6 (c, 0.1 in $CHCl_3$). λ_{max} 252 (log ϵ 4.2); 357 (log ϵ 3.85) (MeOH).

El Sayed, K.A. *et al., J.A.C.S.*, 2001, **123**, 1804-1808 (*isol, pmr, cmr*)

Neolaulimalide N-65

[175992-98-0]

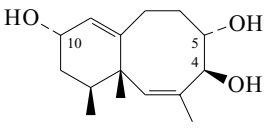


$C_{30}H_{42}O_7$ 514.658

Macrolide antibiotic. Isol. from the sponge *Fasciospongia rimosa*. Cytotoxic agent. $[\alpha]_D^{26}$ -57 (c, 0.09 in $CHCl_3$).

Tanaka, J. *et al., Chem. Lett.*, 1996, 255 (*isol, ir, pmr, cmr*)

2,8-Neolemnadiene-4,5,10-triol N-66



$C_{15}H_{24}O_3$ 252.353

(4β,5α,10α)-form

4-Ac: [143705-33-3]
$C_{17}H_{26}O_4$ 294.39
Constit. of *Parerythropodium fulvum fulvum*.
$[\alpha]_D$ +17 (c, 0.8 in CCl_4).

4,10-Di-Ac: [143705-34-4]
$C_{19}H_{28}O_5$ 336.427
Constit. of *Parerythropodium fulvum fulvum*.

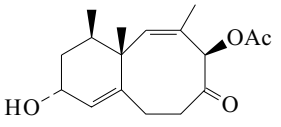
5,10-Diketone: 4-Hydroxy-2,8-neolemnadiene-5,10-dione
$C_{15}H_{20}O_3$ 248.321

5,10-Diketone, 4-Ac: ***Laevinone A***
[874384-43-7]
$C_{17}H_{22}O_4$ 290.358
Constit. of *Lemnalia laevis*.
$[\alpha]_D^{25}$ +165 (c, 0.4 in $CHCl_3$). λ_{max} 232 (log ϵ 3.2) (no solvent reported).

Green, D. *et al., J. Nat. Prod.*, 1992, **55**, 1186 (*Paraerythropodium constits*)
El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 1749-1753 (*Laevinone A*)

Neolemnane N-67

[133812-11-0]



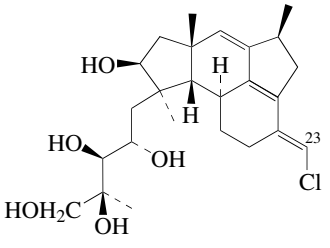
$C_{17}H_{24}O_4$ 292.374
Constit. of *Lemnalia africana*. Cryst. (C_6H_6/2,3,3-trimethylpentane).
Mp 111-112°. $[\alpha]_D$ +440 (c, 1.16 in $CHCl_3$).

Ac: ***Neolemnanyl acetate***
[107242-60-4]
$C_{19}H_{26}O_5$ 334.411
Constit. of *Lemnalia africana*. Oil. $[\alpha]_D$ +222 (c, 1.1 in $CHCl_3$).

Izac, R.R. *et al., Tetrahedron*, 1981, **37**, 2569 (*isol, cryst struct*)
Majetich, G. *et al., J.O.C.*, 1991, **56**, 3988 (*synth*)

Neomangicol A N-68

[217478-72-3]



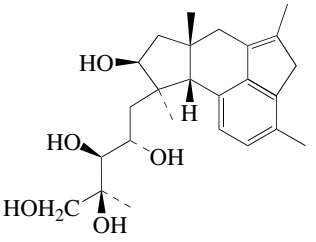
$C_{25}H_{37}ClO_5$ 453.017
Metab. of a marine *Fusarium* sp. Amorph. solid. $[\alpha]_D$ -96 (c, 0.39 in MeOH). λ_{max} 274 (ϵ 9400); 284 (ϵ 12200); 295 (ϵ 10100) (MeOH).

Dechloro, 23-bromo: ***Neomangicol B***
[217478-73-4]
$C_{25}H_{37}BrO_5$ 497.468
Metab. of a marine *Fusarium* sp. Amorph. solid. $[\alpha]_D$ -106 (c, 0.2 in MeOH). Has same *E*-config. at C-23 as Neomangicol A.
λ_{max} 276 (ϵ 8100); 286 (ϵ 10200); 298 (ϵ 8900) (MeOH).

Renner, M.K. *et al., J.O.C.*, 1998, **63**, 8346-8354 (*isol, pmr, cmr*)

Neomangicol C N-69

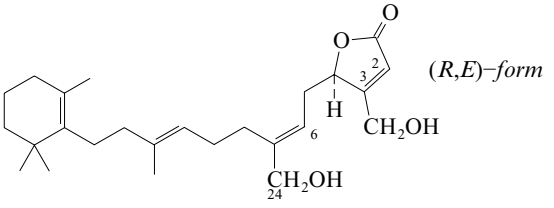
[217478-74-5]



$C_{25}H_{36}O_5$ 416.556
Constit. of a marine *Fusarium* sp. Oil. $[\alpha]_D$ +57 (c, 0.4 in MeOH). λ_{max} 216 (ϵ 26000); 260 (ϵ 15000) (MeOH). λ_{max} 216 (ϵ 26000); 260 (ϵ 15000); 298 (ϵ 8900) (MeOH) (Berdy).

Renner, M.K. *et al., J.O.C.*, 1998, **63**, 8346-8354 (*isol, pmr, cmr*)

Neomanoalide N-70



(R,E)–form

$C_{25}H_{38}O_4$ 402.573

(4R,6E,10E)-form [80388-49-4]
Constit. of *Luffariella variabilis* and *Hyrtios erecta*. Antibacterial, antipsoriatic agent. Ornithine decarboxylase inhibitor. Glass. Poorly sol. hexane. $[\alpha]_D$ -25.9 (c, 0.54 in CH_2Cl_2). λ_{max} 221 (ϵ 6500) (MeOH) (Derep).

Di-Ac: [798557-99-0]
$C_{29}H_{42}O_6$ 486.647
Constit. of a *Brachiaster* sp. Oil. $[\alpha]_D$ -32.9 (c, 0.023 in MeOH). λ_{max} 224 (log ϵ 3.72) (MeOH).

24-Aldehyde: ***Neomanoalid-24-al***
$C_{25}H_{36}O_4$ 400.557
Constit. of a *Luffariella* sp. Molluscicide. Oil. $[\alpha]_D^{25}$ -10.6 (c, 0.18 in $CHCl_3$). λ_{max} 214 (EtOH) (Berdy).

(4R,6Z,10E)-form [80433-15-4]
Isol. from *Luffariella variabilis* and *Hyrtios erecta*. Antibacterial, antipsoriatic agent. Ornithine decarboxylase inhibitor. Glass. Poorly sol. hexane. $[\alpha]_D$ -27.8 (c, 0.79 in CH_2Cl_2). λ_{max} 221 (ϵ 6500) (MeOH) (Derep).

24-Ac: ***24-Acetylneomanoalide***
$C_{27}H_{40}O_5$ 444.61
Constit. of a *Luffariella* sp. Molluscicide. Oil. $[\alpha]_D^{25}$ -16.4 (c, 0.14 in $CHCl_3$). λ_{max} 212 (ϵ 13900) (EtOH) (Berdy).

Di-Ac: [690259-45-1]
Isol. from a *Luffariella* sp.

2,3-Dihydro: ***2,3-Dihydroneomanoalide***
$C_{25}H_{40}O_4$ 404.589
Isol. from a *Luffariella* sp. Molluscicide. Oil. $[\alpha]_D^{25}$ +2.5 (c, 0.44 in $CHCl_3$).

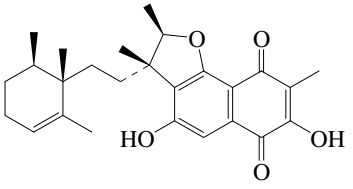
2,3-Dihydro, 24-Ac: ***24-Acetyl-2,3-dihydroneomanoalide***
$C_{27}H_{42}O_5$ 446.626
Isol. from a *Luffariella* sp. Molluscicide. Oil. $[\alpha]_D^{25}$ +11 (c, 0.1 in $CHCl_3$).

De Silva, E.D. *et al., Tet. Lett.*, 1981, **22**, 3147

Katsumura, S. *et al., Tet. Lett.*, 1987, **28**, 1191 (*synth*)
Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705 (*abs config*)
König, G.M. *et al., J. Nat. Prod.*, 1992, **55**, 174 (*isol, pmr, cmr*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 265 (*abs config, pmr, cmr*)
Jefford, C.W. *et al., Helv. Chim. Acta*, 1994, **77**, 661 (*synth*)
Namikoshi, M. *et al., Fish. Sci.*, 2004, **70**, 152-158; *CA*, **140**, 420871w (*di-Ac*)
Wonganuchitmeta, S.-N. *et al., J. Nat. Prod.*, 2004, **67**, 1767-1770 (*Brachiaster constit*)

Neomarinone N-71

[272458-31-8]



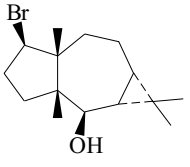
$C_{26}H_{32}O_5$ 424.536

Struct. revised in 2003. Prod. by a marine actinomycete (strain CNH-099). Moderate cytotoxic agent. $[\alpha]_D^{25}$ +86 (c, 0.5 in MeOH). λ_{max} 213 (ϵ 19800); 259 (sh) (ϵ 13500); 263 (ϵ 13900); 312 (ϵ 7800); 398 (ϵ 2700) (MeOH).

Hardt, I.H. *et al., Tet. Lett.*, 2000, **41**, 2073-2076 (*isol, pmr, cmr*)
Kalaitzis, J.A. *et al., Org. Lett.*, 2003, **5**, 4449-4452 (*struct, pmr, cmr, biosynth*)

Neomeranol N-72

[120637-78-7]



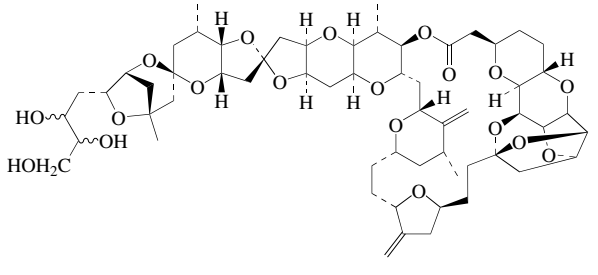
$C_{15}H_{25}BrO$ 301.266

Constit. of *Neomeris annulata*. Oil. $[\alpha]_D$ -27.3 (c, 1.65 in $CHCl_3$).

Barnekow, D.E. *et al., J.A.C.S.*, 1989, **111**, 3511-3517 (*isol, pmr, cmr*)

Neonorhalichondrin B N-73

[156742-02-8]



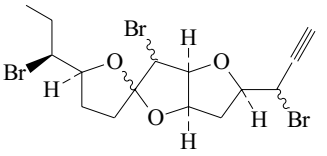
$C_{59}H_{84}O_{19}$ 1097.301

Polyether antibiotic. Isol. from the sponge *Lissodendoryx* sp. Oil.

Litaudon, M. *et al., J.O.C.*, 1997, **62**, 1868 (*isol, pmr, cmr*)

Neoobtusin N-74

[103955-75-5]



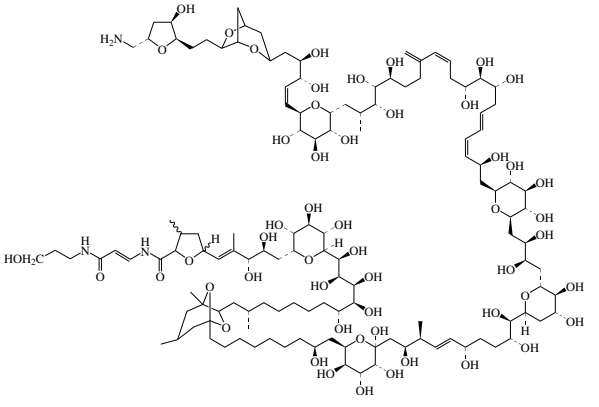
$C_{15}H_{19}Br_3O_3$ 487.025

Constit. of *Laurencia obtusa*. Cryst. (hexane/C_6H_6). Mp 107-108°.

Caccamese, S. *et al., Gazz. Chim. Ital.*, 1986, **116**, 177 (*isol*)

Neopalytoxin N-75

[96411-44-8]



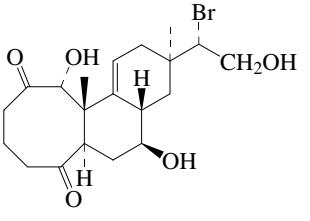
$C_{129}H_{221}N_3O_{53}$ 2662.153

Related to Palytoxin, P-76. Prod. by *Palythoa tuberculosa*. λ_{max} 233; 263 (H_2O).

Uemura, D. *et al., Tetrahedron*, 1985, **41**, 1007-1017 (*struct*)

Neoparguerolidione N-76

[539824-87-8]



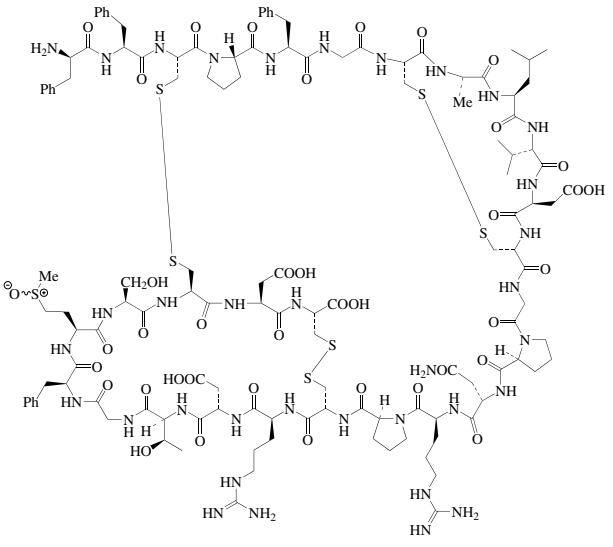
Relative Configuration

$C_{20}H_{29}BrO_5$ 429.35

Isol. from the sea hare *Aplysia punctata*. Gummy solid. $[\alpha]_D$ +2.5 (c, 0.002 in Me_2CO).

Findlay, J.A. *et al., Can. J. Chem.*, 2002, **80**, 1697-1707 (*isol, pmr, cmr, ms*)

Neopetrosiamide A N-77

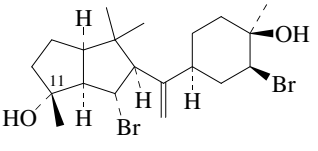


$C_{129}H_{183}N_{35}O_{39}S_7$ 3072.538
Constit. of the sponge *Neopetrosia* sp. Inhibits amoeboid invasion of human tumour cells. Glass. $[\alpha]_D$ -65.2 (c, 4.2 in MeOH).

S-*Epimer:* ***Neopetrosiamide B***
$C_{129}H_{183}N_{35}O_{39}S_7$ 3072.538
Constit. of a *Neopetrosia* sp. Glass.
Williams, D.E. *et al., Org. Lett.*, 2005, **7**, 4173-4176 (*isol, pmr, cmr*)

Neorogioldiol N-78

[321847-12-5]

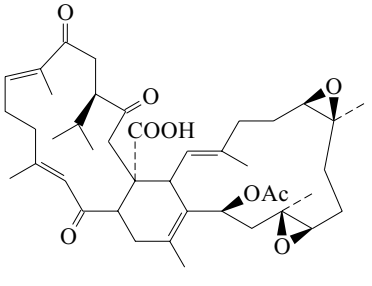


Absolute Configuration

$C_{20}H_{32}Br_2O_2$ 464.28
Constit. of *Laurencia microcladia*.
$[\alpha]_D^{20}$ -57 (c, 0.1 in CCl_4).

11-Epimer: ***Neorogioldiol B***
[615285-33-1]
$C_{20}H_{32}Br_2O_2$ 464.28
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ -39.28 (c, 0.14 in $CHCl_3$). λ_{max} 202 (log ϵ 3.84) (hexane).
Guella, G. *et al., Helv. Chim. Acta*, 2000, **83**, 2946-2952 (*Neorogioldiol*)
Iliopoulou, D. *et al., J.O.C.*, 2003, **68**, 7667-7674 (*Neorogioldiol B*)

Neosartortuic acid N-79

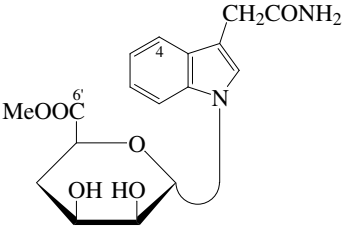


$C_{42}H_{58}O_9$ 706.915

Me ester: Methyl neosartortuate
[149182-64-9]
$C_{43}H_{60}O_9$ 720.942
Constit. of *Sarcophyton tortuosum*. Oil. $[\alpha]_D$ +142 (c, 1 in CCl_4).
Leone, P.A. *et al., J. Nat. Prod.*, 1993, **56**, 521 (*isol, pmr, cmr*)

Neosidomycin N-80

[72033-44-4]



$C_{17}H_{20}N_2O_6$ 348.355
Nucleoside-type antibiotic. Metab. from *Streptomyces hygroscopicus*. Weakly active against gram-negative bacteria. Amorph. powder + $\frac{1}{2}H_2O$. Sol. MeOH, butanol.
Mp 93-103°. $[\alpha]_D^{26}$ +51 (c, 0.48 in MeOH). Similar to Antibiotic SF 2140. λ_{max} 270 (ϵ 8130); 279 (ϵ 7760); 283 (sh) (ϵ 7410); 298 (ϵ 5750) (MeOH) (Derep).

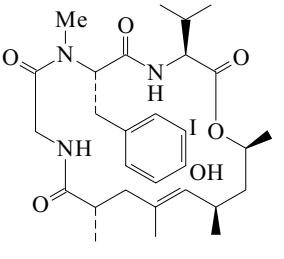
Di-O-*Ac:* Mp 78-80°.

4-Methoxy: 4-Methoxyneosidomycin. ***Kahakamide A***
[362051-29-4]
$C_{18}H_{22}N_2O_7$ 378.381
Prod. by the marine *Nocardiopsis dassonvillei*. Stereochem. not confirmed. λ_{max} 222; 266; 286; 295 (no solvent reported).

4-Methoxy, 6′-parent acid, 6′-amide: ***Kahakamide B***
[362051-30-7]
$C_{17}H_{21}N_3O_6$ 363.369
Prod. by the marine *Nocardiopsis dassonvillei*. Stereochem. not confirmed.
Furuta, R. *et al., Tet. Lett.*, 1979, 1701-1704 (*isol, uv, ir, pmr, ms*)
Isono, K. *et al., J. Antibiot.*, 1988, **41**, 1711-1739 (*rev*)
Buchanan, J.G. *et al., J.C.S. Perkin 1*, 1994, 1417-1426 (*synth*)
Schumacher, R.W. *et al., Tet. Lett.*, 2001, **42**, 5133-5135 (*Kahakamides*)

Neosiphoniamolide A N-81

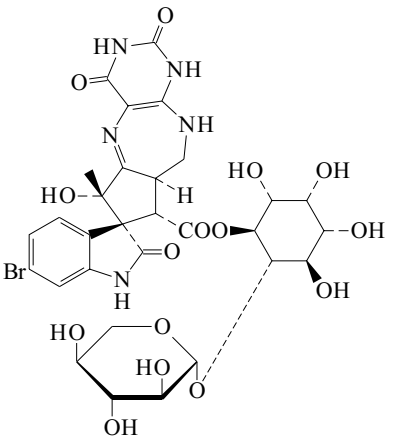
[165198-54-9]



$C_{29}H_{42}IN_3O_6$ 655.572
Depsipeptide antibiotic. Isol. from the sponge *Neosiphonia superstes*. Antifungal agent. Amorph. solid. $[\alpha]_D$ +5.2. Related to Geodiamolide TA, G-52 and Geodiamolide D, G-46. λ_{max} 219 (ϵ 13270); 284 (ϵ 4000); 292 (ϵ 3000) (MeOH) (Berdy).
D'Auria, M.V. *et al., J. Nat. Prod.*, 1995, **58**, 121 (*isol, uv, pmr, cmr*)

Neosurugatoxin N-82

[80680-43-9]



$C_{30}H_{34}BrN_5O_{15}$ 784.527

Toxin from the mid-gut gland of *Babylonia japonica* (Japanese ivory shell) of dietary origin and from *Corynebacterium* sp. Shows powerful antimydriatic activity. Insecticide, nematocide. Prisms + $1H_2O$ (H_2O). Sol. H_2O-MeOH.

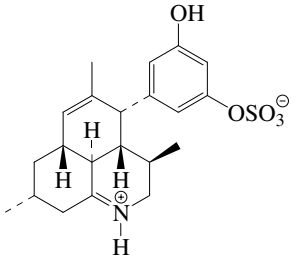
Mp 331-335° dec. Extremely unstable in alkaline medium and fairly heat-labile. λ_{max} 220 (ϵ 44700); 282 (ϵ 15100); 310 (sh) (ϵ 9120); 325 (sh) (ϵ 6310) (H_2O) (Derep).

5′-O-*Dexylosyl:* ***Prosurugatoxin***
[99102-40-6]
$C_{25}H_{26}BrN_5O_{11}$ 652.411

Isol. from *Babylonia japonica*. Ganglion blocking agent, phycotoxin, mydriatic agent. λ_{max} 220 (ϵ 44700); 282 (ϵ 15100); 310 (sh) (ϵ 9120); 325 (sh) (ϵ 6310) (H_2O) (Derep).

Kosuge, T. *et al., Tet. Lett.*, 1981, **22**, 3417-3420 (*cryst struct*)
Kosuge, T. *et al., Chem. Pharm. Bull.*, 1982, **30**, 3255-3259; 1985, **33**, 2890-2895; 3059-3061 (*isol, Prosurgatoxin*)
Inoue, S. *et al., CA*, 1983, **100**, 191639 (*synth*)
Hayashi, E. *et al., J. Neurochem.*, 1984, **42**, 1491 (*props*)
Inoue, S. *et al., Tet. Lett.*, 1986, **27**, 5225 (*synth*)
Inoue, S. *et al., Yakugaku Zasshi*, 1987, **107**, 645 (*rev, synth*)
Wada, A. *et al., Methods Neurosci.*, 1992, **8**, 311 (*rev, props*)
Inoue, S. *et al., Tetrahedron*, 1994, **50**, 2753 (*synth*)

Neosymbioimine N-83



Absolute Configuration

$C_{21}H_{27}NO_5S$ 405.514

Alkaloid from the marine dinoflagellate *Symbiodinium* sp. Oil. $[\alpha]_D^{23}$ +149 (c, 0.1 in MeOH).

Kita, M. *et al., Bioorg. Med. Chem.*, 2005, **13**, 5253-5258 (*isol, pmr, cmr*)

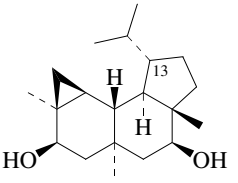
Neovastat N-84

AE 941

Shark cartilage extract. Antiangiogenic agent. Phase I/II clinical trials against lung and prostate cancers (1999). Phase III clin. trial (2001) for lung cancer and metastatic renal cell carcinoma. Phase I/II clin. trial for treatment of plaque psoriasis (2002)

Dupont, E. *et al., J. Cutan. Med. Surg.*, 1998, **2**, 146-152 (*activity*)
Wojtowicz-Praga, S. *et al., Drugs RD*, 1999, **1**, 117-129; 135-136 (*rev*)
Falardeau, P. *et al., Semin. Oncol.*, 2001, **28**, 620-625 (*rev*)
Beliveau, R. *et al., Clin. Cancer Res.*, 2002, **8**, 1242-1250 (*pharmacol*)
Sauder, D.N. *et al., J. Am. Acad. Dermatol.*, 2002, **47**, 535-541 (*clin trial*)
Dredge, K. *et al., Curr. Opin. Invest. Drugs*, 2004, **5**, 668-677 (*rev*)

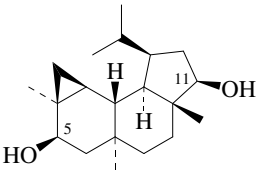
5,9-Neoverrucosanediol N-85



$C_{20}H_{34}O_2$ 306.487

(5β,9β,13α)-*form* [562100-20-3]
Constit. of *Saprospira grandis.*
Oil. $[\alpha]_D$ -2.39 (c, 0.795 in $CHCl_3$).
Spyere, A. *et al., J. Nat. Prod.*, 2003, **66**, 818-822 (*isol, pmr, cmr*)

5,11-Neoverrucosanediol N-86



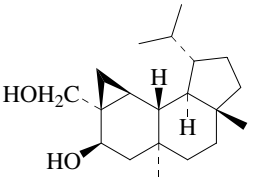
$C_{20}H_{34}O_2$ 306.487

(5β,11β,13β)-*form*

11-Sulfate: [864668-52-0]
$C_{20}H_{34}O_5S$ 386.552
Constit. of *Axinyssa tethyoides.*
$[\alpha]_D^{22}$ +18.4 (c, 0.19 in MeOH).

5-Ac, 11-sulfate: [864668-53-1]
$C_{22}H_{36}O_6S$ 428.589
Constit. of *Axinyssa tethyoides.*
$[\alpha]_D^{22}$ +14.7 (c, 0.23 in MeOH).
Shimogawa, H. *et al., Bull. Chem. Soc. Jpn.*, 2005, **78**, 1345-1347 (*Axinyssa tethyoides constits*)

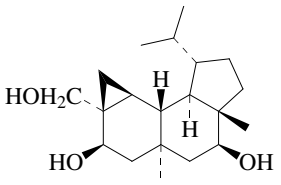
5,18-Neoverrucosanediol N-87



$C_{20}H_{34}O_2$ 306.487

(5β,13α)-*form* [562100-22-5]
Constit. of *Saprospira grandis.*
Oil. $[\alpha]_D$ -11.5 (c, 0.175 in $CHCl_3$).
Spyere, A. *et al., J. Nat. Prod.*, 2003, **66**, 818-822 (*isol, pmr, cmr*)

5,9,18-Neoverrucosanetriol N-88

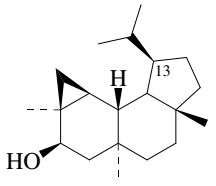


$C_{20}H_{34}O_3$ 322.487

(5β,9β,13α)-*form* [562100-25-8]
Constit. of *Saprospira grandis.*
Oil. $[\alpha]_D$ -18.4 (c, 0.16 in $CHCl_3$).

18-Aldehyde: 5,9-Dihydroxy-18-neoverrucosanal
[562100-27-0]
$C_{20}H_{32}O_3$ 320.471
Constit. of *Saprospira grandis.* Oil. $[\alpha]_D$ -101.3 (c, 0.15 in $CHCl_3$).
λ_{max} 241 (log ϵ 2.16) ($CHCl_3$).
Spyere, A. *et al., J. Nat. Prod.*, 2003, **66**, 818-822 (*isol, pmr, cmr*)

5-Neoverrucosanol N-89



(5β,13α*H*)-*form*

$C_{20}H_{34}O$ 290.488

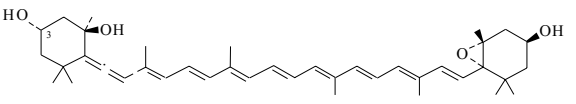
(5β,13α*H*)-*form*
13-Epi-5β-neoverrucosanol
[116502-06-8]
Constit. of *Schistochila nobilis* and *Plagiochila stephensoniana*.
Cryst. (hexane).
Mp 151-153.5°. $[\alpha]_D$ +45.5 (c, 0.8 in $CHCl_3$).

5-Ketone: 5-Neoverrucosanone. ***13-Epi-5-neoverrucosanone****. 5-Oxoepineoverrucosane*
$C_{20}H_{32}O$ 288.472
Constit. of *Fossombronia alaskana*. Cryst. (hexane).
Mp 92°. $[\alpha]_D^{20}$ +177.2 (c, 0.2 in $CHCl_3$).

(5β,13β*H*)-*form*
Neoverrucosanol
[76235-09-1]
Constit. of *Axinyssa aplysinoides*, *Schistochila rigidula*, *Epipolasis kushimotoensis* and *Mylia verrucosa*.
Cryst.
Mp 174-175° Mp 138-140°. $[\alpha]_D$ -10. $[\alpha]_D$ +2.6 (c, 2.8 in $CHCl_3$).
Matsuo, A. *et al., Chem. Comm.*, 1980, 822 (*isol*)
Wu, C.-L. *et al., J. Hattori Bot. Lab.*, 1988, **64**, 151 (*isol*)
Fukuyama, Y. *et al., Phytochemistry*, 1988, **27**, 1797-1799 (*13-Epi-5β-neoverrucosanol, isol, cryst struct*)
Asakawa, Y. *et al., Phytochemistry*, 1988, **27**, 3509-3511 (*13-Epi-5β-neoverrucosanol, isol*)
Compagnone, R.S. *et al., J. Nat. Prod.*, 1995, **58**, 145-148 (*isol*)
Tanaka, J. *et al., Chem. Lett.*, 1997, 489-490 (*isol, pmr, cmr*)
Grammes, C. *et al., Phytochemistry*, 1997, **44**, 1495 (*ketone, pmr, cmr, cryst struct*)
Piers, E. *et al., Tet. Lett.*, 1997, **38**, 8815-8818 (*synth*)

Neoxanthin N-90

6,7-Didehydro-5′,6′-epoxy-5,5′,6,6′-tetrahydro-β,β-carotene-3,3′,5-triol. Foliaxanthin. Trollixanthin. Trolliflor
[30743-41-0]



$C_{40}H_{56}O_4$ 600.88
Constit. of paprika, lucerne, maple, Valencia orange and *Trollius europaeus.* Minor carotenoid of marine Chrysophyte algae. Also in green algae. Light brown-orange cryst. (C_6H_6/Et_2O).
Mp 200° (136-139°, 142-145°). $[\alpha]_D^{20}$ +32 ($CHCl_3$). Undergoes thermal isom. into a mixt. of neochromes upon melting. Related to Vaucheriaxanthin, V-20. λ_{max} 434; 464 (MeOH). λ_{max} 437; 466 (heptane). λ_{max} 463; 493 (CS_2).

3-Ac: ***Dinoxanthin****. Neoxanthin 3-acetate*
[54369-12-9]
$C_{42}H_{58}O_5$ 642.917
Constit. of the Dinophyceae.

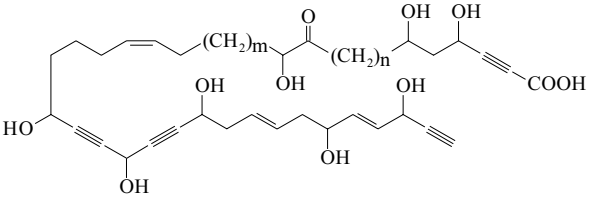
(9′Z)-form
9′-cis-*Neoxanthin*
[14660-91-4]
Constit. of numerous plant spp.

[52949-72-1, 52949-73-2, 142204-43-1]

Schimmer, B.P. *et al., Biochemistry*, 1966, **5**, 1814; 3649 (*struct*)
de Ville, T.E. *et al., Chem. Comm.*, 1969, 754; 1311 (*struct*)
Cholnoky, L. *et al., J.C.S.(C)*, 1969, 1256 (*isol*)
Nitsche, H. *et al., Z. Naturforsch., C*, 1973, **28**, 641 (*Vaucheriaxanthin*)
Johansen, J.E. *et al., Phytochemistry*, 1974, **13**, 2261; 1980, **19**, 441 (*Dinoxanthin*)
Nitsche, H. *et al., Z. Naturforsch., C*, 1974, **29**, 657 (*synth*)
Buchecker, R. *et al., Phytochemistry*, 1975, **14**, 797 (*struct*)
Swift, I.E. *et al., Phytochemistry*, 1982, **21**, 2859 (*biosynth*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 234 (*bibl*)
Bjoernland, T. *et al., Tet. Lett.*, 1989, **30**, 2577 (*pmr, struct*)
Maerki-Fischer, E. *et al., Helv. Chim. Acta*, 1990, **73**, 1637 (*pmr*)
Baumeler, A. *et al., Helv. Chim. Acta*, 1992, **75**, 773; 1994, **77**, 909 (*synth*)
Strand, A. *et al., J.C.S. Perkin 1*, 2000, 595-598 (*synth*)

Nepheliosyne A N-91

[159250-30-3]



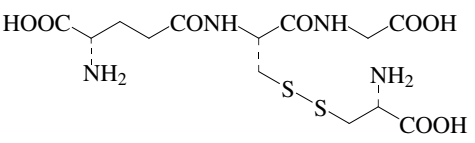
$m + n = 16$

$C_{47}H_{70}O_{11}$ 811.063
Constit. of the sponge *Xestospongia* sp. Weak cytotoxic agent.
Amorph. solid. $[\alpha]_D^{22}$ +7 (c, 0.3 in MeOH).

Kobayashi, J. *et al., J. Nat. Prod.*, 1994, **57**, 1300 (*isol, pmr, cmr*)

Nereithione N-92

Cysteine-glutathione disulfide
[13081-14-6]

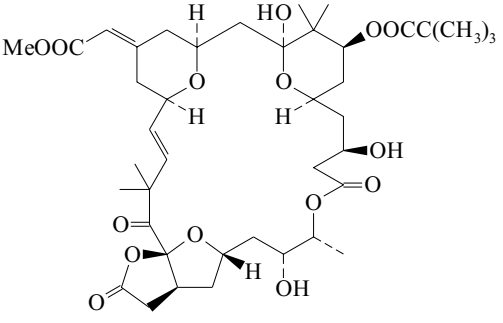


$C_{13}H_{22}N_4O_8S_2$ 426.471
Spawning pheromone of the marine polychaete *Nereis succinea*. Mp 234°. $[\alpha]_D^{25}$ -110 (c, 0.25 in 1*M* HCl).

Hart, T.W. *et al., Tet. Lett.*, 1985, **26**, 3879-3882 (*synth, cmr*)
Zeeck, E. *et al., Chemoecology*, 1998, **8**, 33-38 (*isol*)
Hardege, J.D. *et al., Peptides (N.Y.)*, 2004, **25**, 1517-1522 (*rev*)

Neristatin I N-93

[135004-30-7]



$C_{41}H_{60}O_{15}$ 792.916
Macrocyclic antibiotic. Isol. from the bryozoan *Bugula neritina*. Antineoplastic agent. Binds to Protein Kinase C. Powder. Mp 214-216°. $[\alpha]_D$ +98 (c, 0.26 in CH_2Cl_2). λ_{max} 228 (ϵ 18300) (MeOH) (Derep).

Pettit, G.R. *et al., J.A.C.S.*, 1991, **113**, 6693-6695 (*isol, pmr, cmr*)

Cardisoma carnifex Neuropeptide I, 9CI N-94

[111411-06-4]
As *Cardisoma carnifex* Neuropeptide C, N-96 with
Y = -Ser-Leu-Leu-Thr-Ser-Leu-OH
$C_{73}H_{122}N_{22}O_{25}S$ 1739.965
Isol. from sinus gland of *Cardisoma carnifex*. No phys. props. reported.

Newcomb, R.W. *et al., J. Neurochem.*, 1987, **49**, 574 (*isol, struct*)

Oncorhynchus mykiss Neuropeptide γ N-95

Trout neuropeptide γ
[152343-99-2]
Ser-Ser-Ala-Asn-Pro[5]-Gln-Ile-Thr-Arg[9]-Lys-Arg-His[12]-Lys-Ile-Asn-Ser-Phe-Val-Gly-Leu-Met-NH_2
$C_{103}H_{175}N_{35}O_{28}S$ 2383.799
Isol. from intestine of the rainbow trout *Oncorhynchus mykiss*. Neuropeptide.

5-Arginine, 9-glycine, 12-glutamic acid analogue: [251443-74-0]
$C_{99}H_{172}N_{34}O_{29}S$ 2334.724
Isol. from brain of the sturgeon *Scaphirhynchus albus*. Neuropeptide.

Jensen, J. *et al., Am. J. Physiol.*, 1993, **265**, R804-810 (*isol trout*)
Wang, Y. *et al., Gen. Comp. Endocrinol.*, 1999, **116**, 21-30 (*isol, sturgeon*)

Cardisoma carnifex Neuropeptide C N-96

[111461-47-3]

H–Arg–Ser–Ala–Asp–Gly–Phe–Gly–Arg–Met–Glu–Y

Y = H

$C_{45}H_{72}N_{16}O_{16}S$ 1125.227
Isol. from sinus gland of *Cardisoma carnifex*. No phys. props. reported.

Newcomb, R.W. *et al., J. Neurochem.*, 1987, **49**, 574 (*isol, struct*)

Macrocallista nimbosa Neuropeptide C N-97

Phenylalanylmethionylarginylphenylalaninamide, 9CI. Neuropeptide C. Molluscan cardioexcitatory peptide. FMRF amide
[64190-70-1]
H-Phe-Met-Arg-Phe-NH_2
Isol. from *Macrocallista nimbosa*.
Cardiac stimulant. Mp 87-88°. $[\alpha]_D^{25}$ -8.8 (c, 0.4 in 1*M* AcOH).

Hydrochloride (1:2): [67872-50-8]
Hygroscopic solid. $[\alpha]_D^{24}$ -4.4 (c, 0.25 in MeOH).

N-tert-*Butyloxycarbonyl, monoacetate:* [67845-02-7]
Amorph. $[\alpha]_D^{24}$ -14.1 (c, 1 in MeOH).

Price, D. *et al., Science (Washington, D.C.)*, 1977, **197**, 670 (*isol, struct*)
Freidinger, R.M. *et al., J.O.C.*, 1978, **43**, 4800 (*synth*)
Sakina, K. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4345 (*synth*)
Cottrell, G.A. *et al., Comp. Biochem. Physiol., A: Comp. Physiol.*, 1989, **93**, 41 (*rev*)

Cardisoma carnifex Neuropeptide D N-98

[111461-48-4]
H-Gly-Ser-Ala-Glu-Ser-Pro-Ala-Ala-Leu-Gly-Glu-Ala-Ser-Ala-Ala-His-Pro-Leu-Glu-OH
$C_{74}H_{117}N_{21}O_{29}$ 1764.862
Isol. from sinus gland of *Cardisoma carnifex*. No phys. props. reported.

Newcomb, R.W. *et al., J. Neurochem.*, 1987, **49**, 574 (*isol, struct*)

Cardisoma carnifex Neuropeptide F, 9CI N-99

[111411-05-3]
H-Leu-Leu-Thr-Ser-Leu-Arg-Gly-Ser-Ala-Glu-Ser-Pro-Ala-Ala-Leu-Gly-Glu-Ala-Ser-Ala-Ala-His-Pro-Leu-Glu-OH
$C_{105}H_{174}N_{30}O_{37}$ 2448.708
Isol. from sinus gland of *Cardisoma carnifex*. No phys. props. reported.

Newcomb, R.W. *et al., J. Neurochem.*, 1987, **49**, 574 (*isol, struct*)

Cardisoma carnifex Neuropeptide H N-100

[111518-00-4]
H-Arg-Ser-Ala-Asp-Gly-Phe-Gly-Arg-Met-Glu-Ser-Leu-Leu-Thr-Ser-Leu-Arg-Gly-Ser-Ala-Glu-Ser-Pro-Ala-Ala-Leu-Gly-Glu-Ala-Ser-Ala-Ala-His-Pro-Leu-Glu-OH
$C_{153}H_{249}N_{47}O_{54}S$ 3642.999
Isol. from sinus gland of *Cardisoma carnifex*. No phys. props. reported.

Newcomb, R.W. *et al., J. Neurochem.*, 1987, **49**, 574 (*isol, struct*)

Asterias Neuropeptide S1 N-101

[134439-73-9]
H-Gly-Phe-Asn-Ser-Ala-Leu-Met-Phe-NH_2
$C_{41}H_{60}N_{10}O_{10}S$ 885.052
Neuropeptide isol. from the starfish *Asterias forbesi* and *Asterias rubens*.

Elphick, M.R. *et al., Peptides (N.Y.)*, 1991, **12**, 455 (*isol, props*)
Elphick, M.R. *et al., Proc. R. Soc. London, B*, 1991, **243**, 121 (*isol, struct*)

Asterias Neuropeptide S2 N-102

[134439-74-0]

H-Ser-Gly-Pro-Tyr-Ser-Phe-Asn-Ser-Gly-Leu-Thr-Phe-NH_2

$C_{59}H_{82}N_{14}O_{18}$ 1275.38

Neuropeptide isol. from the starfish *Asterias forbesi* and *Asterias rubens*.

Elphick, M.R. *et al., Proc. R. Soc. London, B*, 1991, **243**, 121 (*isol, struct*)

Limulus polyphemus Neuropeptides N-103

H-Asp-Glu-Gly-His-Lys-Met-Leu-Tyr-Phe-NH_2

Isol. from the brain of the horseshoe crab *Limulus polyphemus*. FMRF amide-related neuropeptides.

DEGHKMLYF amide [150502-84-4]

$C_{52}H_{75}N_{13}O_{14}S$ 1138.309

GHSLLHF amide [150502-85-5]

$C_{38}H_{56}N_{12}O_8$ 808.936

PDHHMMYF amide [150502-86-6]

$C_{49}H_{65}N_{13}O_{11}S_2$ 1076.265

DHGNMLYF amide [150502-87-7]

$C_{45}H_{62}N_{12}O_{12}S$ 995.124

GGRSPSLRLRF amide [150502-83-3]

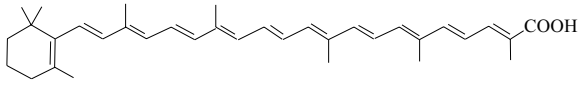
$C_{54}H_{93}N_{21}O_{13}$ 1244.462

Gaus, G. *et al., Biol. Bull. (Woods Hole, Mass.)*, 1993, **184**, 322-329 (*isol, struct*)
Gaus, G. *et al., J. Comp. Physiol., B*, 1994, **164**, 191-194 (*isol, struct*)

Neurosporaxanthin N-104

4′-Apo-β,ψ-caroten-4′-oic acid. 4′-Apo-β-caroten-4′-oic acid

[2468-88-4]



$C_{35}H_{46}O_2$ 498.747

Produced by *Neurospora crassa* and *Neurospora sitophila*. Also from *Fusarium aquaeductuum*, *Rhizophlyctis rosea, Arthrobotrys oligospora* and others. Dark green-purple plates (hexane).
Mp 193°.

β-D-Glucopyranosyl ester: [474519-26-1]
$C_{41}H_{56}O_7$ 660.889
Constit. of a marine-derived *Fusarium* sp. λ_{max} 475 (Et_2O).

Me ester:
$C_{36}H_{48}O_2$ 512.774
Produced by *Verticillium agaricinum*.

Barber, M.S. *et al., Proc. Chem. Soc., London*, 1960, 2870 (*pmr*)
Aasen, A.J. *et al., Acta Chem. Scand.*, 1965, **19**, 1843 (*struct*)
Enzell, C.R. *et al., Acta Chem. Scand.*, 1969, **23**, 727 (*ms*)
Valadon, L.R.G. *et al., Phytochemistry*, 1977, **16**, 613 (*isol, ester*)
Sakaki, H. *et al., J. Nat. Prod.*, 2002, **65**, 1683-1684 (*glucosyl ester*)

Stichodactyla helianthus Neurotoxin I N-105

Peptide. Struct. comprises 48 amino acid residues. Isol. from the Caribbean sea anemone *Stichodactyla helianthus*.

Foch, R.F. *et al., Biochemistry*, 1989, **28**, 1826 (*struct*)
Kem, W.R. *et al., Biochemistry*, 1989, **28**, 3483 (*isol*)
Pennington, M.W. *et al., Int. J. Pept. Protein Res.*, 1990, **36**, 335 (*synth*)

Neurotoxin B-IV N-106

Peptide containing 55 amino acid residues and 4 disulfide bonds. Isol. from the marine worm *Cerebratulus lacteus*. Crustacean-selective neurotoxin.

Kem, W.R. *et al., J. Biol. Chem.*, 1976, **251**, 4184-4192 (*isol*)
Blumenthal, K.M. *et al., J. Biol. Chem.*, 1976, **251**, 6025-6029; 1977, **252**, 3328-3331; 1981, **256**, 9063-9067 (*struct*)
Kem, W.R. *et al., J. Protein Chem.*, 1990, **9**, 433-443 (*cd, Raman*)
Hansen, P.E. *et al., Eur. J. Biochem.*, 1992, **210**, 231-240 (*pmr, struct*)
Barnham, K.J. *et al., J. Mol. Biol.*, 1997, **268**, 886-902 (*struct*)

Anemonia erythraea Neurotoxins N-107

AETX

Three peptides; AETX-I contains 47 amino acid residues and 3 disulfide bonds; AETX-II and -III are highly homologous and contain 59 amino acid residues and 5 disulfide bonds. Isol. from the sea anemone *Anemonia eyrthraea*. Neurotoxins; lethal to crabs.

[189020-93-7]

Shiomi, K. *et al., Biochim. Biophys. Acta*, 1997, **1335**, 191-198 (*isol, struct*)

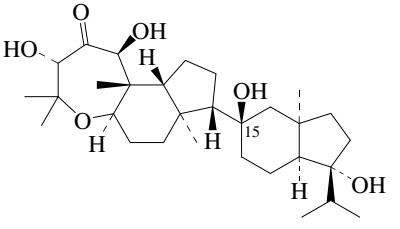
Radianthus macrodactylus Neurotoxins RTX N-108

Five peptides (RTX I-V) containing 47-48 amino acid residues and 3 disulfide bonds. Isol. from the sea anemone *Radianthus macrodactylus*. Cytolysins.

Zykova, T.A. *et al., Bioorg. Khim.*, 1988, **14**, 878-882; 1489-1494; 1989, **15**, 1301-1306 (*isol*)

Neviotine A N-109

[100244-36-8]



$C_{30}H_{50}O_6$ 506.721
Constit. of *Siphonochalina siphonella*. Cryst. (Me_2CO/C_6H_6).
Mp 231-233°. $[\alpha]_D$ -50 (c, 4 in $CHCl_3$).

15-Epimer: ***Neviotine B***
[329197-89-9]
$C_{30}H_{50}O_6$ 506.721
Constit. of *Siphonochalina siphonella*. Oil. $[\alpha]_D$ -53 (c, 1.6 in $CHCl_3$).

Carmely, S. *et al., J.O.C.*, 1986, **51**, 784-788 (*Neviotine A*)
Kashman, Y. *et al., J. Nat. Prod.*, 2001, **64**, 175-180 (*Neviotine B*)

NGIWY amide N-110

[212968-78-0]

Asn-Gly-Ile-Trp-Tyr-NH_2

$C_{32}H_{42}N_8O_7$ 650.733

Isol. from the body wall of the sea cucumber *Stichopus japonicus*. Controls the stiffness of the dermis.

Birenheide, R. *et al., Biol. Bull. (Woods Hole, Mass.)*, 1998, **194**, 253-259 (*isol*)

Nicaeensin N-111

N-*[4-[[[(Aminoiminomethyl)amino]carbonyl]amino]butyl]*-N-*methylacetamide, 9CI. 1-(3-Amidinoureido)-4-(*N*-methylacetamido)butane*

[131669-98-2]
[131669-99-3 (picrate)]

$HN{=}C(NH_2)NHCONH(CH_2)_4NMeAc$

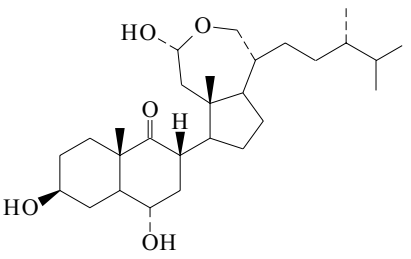
$C_9H_{19}N_5O_2$ 229.281

Isol. from the red alga *Schottera nicaeensis*. Powder; yellow cryst. (EtOH aq.) (as picrate).
Mp 171-173° (picrate).

Chillemi, R. *et al., J. Nat. Prod.*, 1990, **53**, 1220 (*isol, pmr, cmr, ms, struct*)

Nicobarsterol N-112

11,21-Epoxy-3,6,11-trihydroxy-9,11-secoergostan-9-one
[133883-22-4]

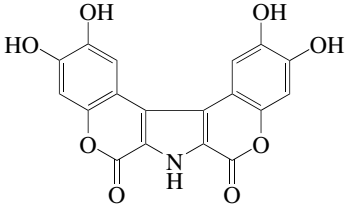


$C_{28}H_{48}O_5$ 464.684
Constit. of a *Sclerophytum* sp. Cryst.
Mp 193-194°. $[\alpha]_D^{29}$ -43 (c, 1.36 in Py).

Kobayashi, M. *et al., J.C.S. Perkin 1*, 1991, 493 (*isol, pmr, cmr*)

Ningalin A N-113

[188111-67-3]

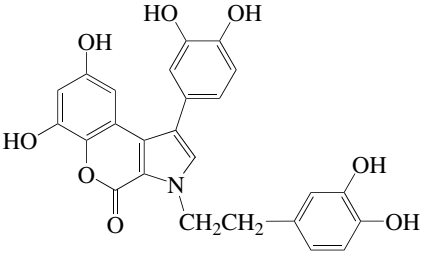


$C_{18}H_9NO_8$ 367.271
Alkaloid from the ascidian *Didemnum* sp. Amorph. yellow solid. λ_{max} 262 (ϵ 8650); 303 (ϵ 8450); 325 (sh); 370 (ϵ 2160) (DMSO/MeOH).

Kang, H. *et al., J.O.C.*, 1997, **62**, 3254 (*isol, uv, ir, pmr, cmr*)
Boger, D.L. *et al., J.A.C.S.*, 1999, **121**, 54-62 (*synth*)

Ningalin B N-114

[188111-68-4]

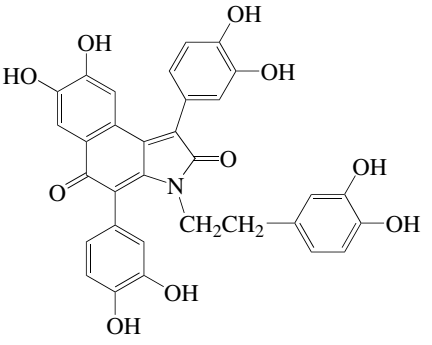


$C_{25}H_{19}NO_8$ 461.427
Alkaloid from the ascidian *Didemnum* sp. Multidrug-resistant reversal agent. Dark yellow solid. λ_{max} 204 (ϵ 46000); 236; 289 (ϵ 10000); 332 (ϵ 8700) (MeOH).

Kang, H. *et al., J.O.C.*, 1997, **62**, 3254-3262 (*isol, uv, ir, pmr, cmr*)
Boger, D.L. *et al., J.O.C.*, 2000, **65**, 2479-2483 (*synth*)
Bullington, J.L. *et al., J.O.C.*, 2002, **67**, 9439-9442 (*synth*)
Iwao, M. *et al., Tet. Lett.*, 2003, **44**, 4443-4446 (*synth*)
Gupton, J.T. *et al., Tetrahedron*, 2003, **59**, 207-215 (*synth*)

Ningalin C N-115

[188111-69-5]

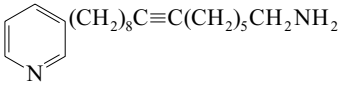


$C_{32}H_{23}NO_{10}$ 581.534
Alkaloid from the ascidian *Didemnum* sp. Amorph. red solid. λ_{max} 204 (ϵ 34000); 289 (ϵ 9400); 301 (sh); 355 (ϵ 5800); 450 (sh) (MeOH).

Kang, H. *et al., J.O.C.*, 1997, **62**, 3254 (*isol, uv, ir, pmr, cmr*)
Peschko, C. *et al., Tet. Lett.*, 2000, **41**, 9477-9481 (*synth*)
Namsa-aid, A. *et al., Org. Lett.*, 2002, **4**, 2633-2635 (*synth*)

Niphatesine B N-116

16-(3-Pyridinyl)-7-hexadecyn-1-amine, 9CI. 3-(16-Amino-9-hexadecynyl)pyridine
[132923-11-6]

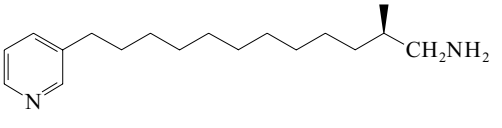


$C_{21}H_{34}N_2$ 314.513
Alkaloid from the marine sponge *Niphates* sp. Antineoplastic. Oil. λ_{max} 206 (ϵ 7800); 228 (ϵ 3300); 257 (ϵ 3100); 264 (ϵ 3400); 269 (ϵ 2500); 313 (ϵ 300) (MeOH) (Berdy).

Kobayashi, J. *et al., J.C.S. Perkin 1*, 1990, 3301 (*isol, uv, ir, ms, pmr, cmr, struct*)
Rao, A.V.R. *et al., Tet. Lett.*, 1993, **34**, 8329 (*synth*)

Niphatesine C N-117

β-Methyl-3-pyridinedodecanamine, 9CI. 2-Methyl-12-(3-pyridinyl)dodecylamine. 3-(12-Amino-11-methyldodecyl)pyridine



(*R*)–*form*

$C_{18}H_{32}N_2$ 276.464

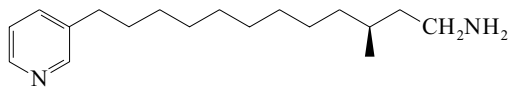
(R)-form [170716-95-7] Synthetic. $[\alpha]_D^{20}$ -3.2 (c, 3.2 in MeOH).

(S)-form [132923-12-7]
Alkaloid from the marine sponge *Niphates* sp. Antineoplastic. Oil. $[\alpha]_D^{25}$ +9.4 (c, 0.053 in MeOH). $[\alpha]_D^{20}$ +2.4 (c, 0.5 in MeOH) (synthetic). λ_{max} 206 (ϵ 2600); 258 (ϵ 2400); 264 (ϵ 2700); 269 (ϵ 2200) (MeOH) (Berdy).

Kobayashi, J. *et al., J.C.S. Perkin 1*, 1990, 3301 (*isol, uv, ir, ms, pmr, cmr, struct*)
Rao, A.V.R. *et al., Tet. Lett.*, 1993, **34**, 8329 (*synth, abs config*)
Bracher, F. *et al., J.C.S. Perkin 1*, 1995, 2323 (*synth, abs config*)
Wang, Y. *et al., J.O.C.*, 2003, **68**, 3090-3098 (*synth*)
Krauss, J. *et al., Arch. Pharm. (Weinheim, Ger.)*, 2004, **337**, 371-375 (*synth*)

Niphatesine D **N-118**

γ-Methyl-3-pyridinedodecanamine, 9CI. 3-Methyl-12-(3-pyridinyl)dodecylamine. 3-(12-Amino-10-methyldodecyl)pyridine
[132923-13-8]



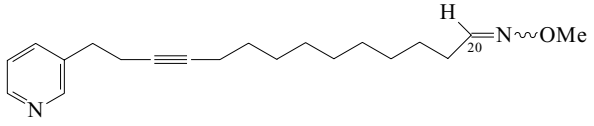
$C_{18}H_{32}N_2$ 276.464

The assignment of the configuration has been shown to be unreliable (2004). Alkaloid from the marine sponge *Niphates* sp. Antineoplastic. Oil. $[\alpha]_D^{25}$ +4.4 (c, 0.045 in MeOH). λ_{max} 207 (ϵ 4300); 259 (ϵ 2800); 264 (ϵ 3200); 270 (ϵ 2400) (MeOH) (Berdy).

Kobayashi, J. *et al., J.C.S. Perkin 1*, 1990, 3301 (*isol, uv, ir, ms, pmr, cmr, struct*)
Rao, A.V.R. *et al., Tet. Lett.*, 1993, **34**, 8329 (*synth, abs config*)
Romeril, S.P. *et al., Tet. Lett.*, 2004, **45**, 3273-3277 (*config*)

Niphatesine E **N-119**

14-(3-Pyridinyl)-11-tetradecynal O-*methyloxime*
[143052-05-5]



$C_{20}H_{30}N_2O$ 314.47

Isol. as a *ca*. 1.4:1 mixt. of *E* and *Z* isomers. Alkaloid from the Okinawan marine sponge *Niphates* sp. Exhibits cytotoxicity against murine leukaemia L1210 cells and human epidermoid carcinoma KB cells *in vitro*. Also shows antimicrobial activity against some fungi and gram-positive bacteria. Oil. λ_{max} 262 (ϵ 19000) (MeOH) (Berdy).

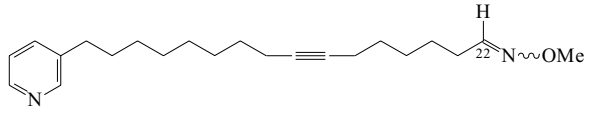
*20,*N-*Dihydro:* ***Niphatesine H***. N-*Methoxy-14-(3-pyridinyl)-11-tetradecyn-1-amine, 9CI*
[143052-08-8]
$C_{20}H_{32}N_2O$ 316.486
Alkaloid from *Niphates* sp. Exhibits cytotoxic and antimicrobial activities. Oil. λ_{max} 262 (ϵ 2500) (MeOH) (Berdy).

[143052-09-9]

Kobayashi, J. *et al., J.C.S. Perkin 1*, 1992, 1291-1294 (*Niphatesines E,H, struct*)

Niphatesine F **N-120**

16-(3-Pyridinyl)-7-hexadecynal O-*methyloxime, 9CI*
[143052-06-6]



$C_{22}H_{34}N_2O$ 342.523

Isol. as a 1.7:1 mixt. of *E* and *Z* isomers. Alkaloid from the Okinawan marine sponge *Niphates* sp. Exhibits cytotoxicity against murine leukaemia L1210 cells and human epidermoid KB cells *in vitro*. Also shows antimicrobial activity against some fungi and gram-positive bacteria. Oil. λ_{max} 263 (ϵ 3100) (MeOH) (Berdy).

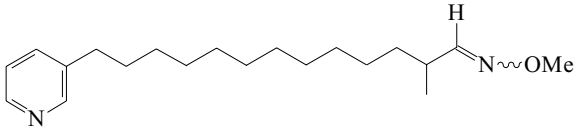
*22,*N-*Dihydro:* See Niphatyne A, N-125

[143052-10-2]

Kobayashi, J. *et al., J.C.S. Perkin 1*, 1992, 1291 (*isol, uv, ir, pmr, cmr, ms, struct*)

Niphatesine G **N-121**

α-Methyl-3-pyridinetridecanal O-*methyloxime, 9CI*
[143052-07-7]



$C_{20}H_{34}N_2O$ 318.501

Isol. as a 3.2:1 mixt. of *E* and *Z* isomers. Alkaloid from the Okinawan marine sponge *Niphates* sp. Exhibits cytotoxicity against murine leukaemia L1210 cells and human epidermoid carcinoma KB cells *in vitro*. Also shows antimicrobial activity against some fungi and gram-positive bacteria. Oil. λ_{max} 263 (ϵ 1500) (MeOH) (Berdy).

[143120-50-7]

Kobayashi, J. *et al., J.C.S. Perkin 1*, 1992, 1291 (*isol, uv, ir, pmr, ms, struct*)

Niphatevirin **N-122**

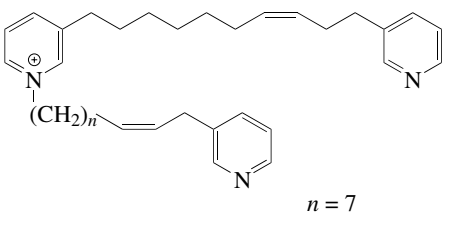
[191617-96-6]

Glycoprotein of *ca*. 19 kDa. Isol. from the marine sponge *Niphates erecta*. HIV-1 inhibitor.

O'Keefe, B.R. *et al., Eur. J. Biochem.*, 1997, **245**, 47-53 (*isol, activity*)

Niphatoxin A **N-123**

3-[10-(3-Pyridinyl)-7-decenyl]-1-[11-(3-pyridinyl)-8-decenyl]pyridinium(1+), 9CI
[142808-48-8]



$C_{35}H_{48}N_3^{\oplus}$ 510.784

Incorrect struct. given in ref. Alkaloid from the Red Sea sponge *Niphates* sp. Ichthyotoxic and cytotoxic.

Talpir, R. *et al., Tet. Lett.*, 1992, **33**, 3033 (*isol, pmr, cmr, struct*)

Niphatoxin B **N-124**

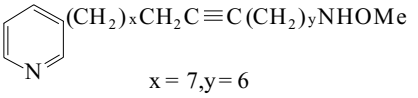
3-[10-(3-Pyridinyl)-7-decenyl]-1-[11-(3-pyridinyl)-9-undecenyl]-pyridinium(1+), 9CI
[142808-49-9]
As Niphatoxin A, N-123 with
$n = 8$
$C_{36}H_{50}N_3^{\oplus}$ 524.811

Incorrect struct. given in 1992 ref. Alkaloid from the Red Sea sponge *Niphates* sp. Ichthyotoxic and cytotoxic.

Talpir, R. *et al., Tet. Lett.*, 1992, **33**, 3033 (*isol, pmr, cmr, struct*)
Kaiser, A. *et al., J.O.C.*, 1999, **64**, 3778-3782 (*synth, ir, pmr, cmr*)

Niphatyne A **N-125**

N-*Methoxy-16-(3-pyridinyl)-7-hexadecyn-1-amine, 9CI*
[109741-36-8]



$C_{22}H_{36}N_2O$ 344.539

Isol. from the sponge *Niphates* sp. Cytotoxic agent. Sol. MeOH, $CHCl_3$. λ_{max} 260 (ϵ 2500); 265 (ϵ 3100); 270 (ϵ 2000) (MeOH) (Derep).

Quiñoà, E. *et al., Tet. Lett.*, 1987, **28**, 2467 (*isol, uv, ir, pmr, cmr, ms, struct*)

Niphatyne B N-126

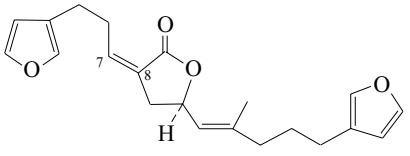
N-*Methoxy-16-(3-pyridinyl)-5-hexadecyn-1-amine, 9CI*
[109741-37-9]
As Niphatyne A, N-125 with
x = 9, y = 4

$C_{22}H_{36}N_2O$ 344.539
Isol. from the marine sponge, *Niphates* sp. Cytotoxic agent. Sol. MeOH, $CHCl_3$. Obt. contaminated with Niphatyne A, N-125. λ_{max} 260 (ϵ 2500); 265 (ϵ 3100); 270 (ϵ 2000) (MeOH) (Derep).

Quiñoà, E. *et al., Tet. Lett.*, 1987, **28**, 2468 (*isol, uv, ir, pmr, cmr, ms, struct*)

Nitenin† N-127

[33762-13-9]



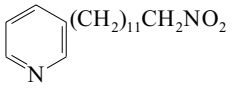
$C_{21}H_{24}O_4$ 340.418
Constit. of *Spongia nitens*.
$[\alpha]_D$ -45.4 (c, 2 in $CHCl_3$). λ_{max} 221 (ϵ 14000) (cyclohexane) (Berdy).

7,8α-Dihydro: ***Dihydronitenin***
[33762-14-0]
$C_{21}H_{26}O_4$ 342.434
From *Spongia nitens*. Oil. $[\alpha]_D$ -25.2 (c, 1.4 in $CHCl_3$).

Fattorusso, E. *et al., Tetrahedron*, 1971, **27**, 3909
Fontana, A. *et al., J. Nat. Prod.*, 1996, **59**, 869 (*abs config, pmr, cmr*)

3-(12-Nitrododecyl)pyridine N-128

1-Nitro-12-(3-pyridinyl)dodecane. ***Untenine B***
[174624-22-7]

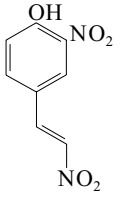


$C_{17}H_{28}N_2O_2$ 292.42
Alkaloid from the Okinawan marine sponge *Callyspongia* sp. Exhibits potent anti-microfouling activity.

Wang, G.-Y.-S. *et al., Tet. Lett.*, 1996, **37**, 1813 (*isol, pmr, cmr, struct*)

2-Nitro-4-(2-nitroethenyl)phenol, 9CI N-129

2-Nitro-4-(2-nitrovinyl)phenol
[2084-92-6]

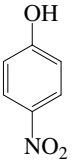


$C_8H_6N_2O_5$ 210.146
Isol. from the leaves of *Sonneratia acida*. Prod. by the marine-derived *Flavobacterium* sp. T436. Yellow needles (AcOH/MeOH). Mp 152° (synthetic).

Japan. Pat., 1964, 64 26 960; *CA*, **62**, 14569e (*synth*)
Bose, A.K. *et al., Oceanogr. Indian Ocean*, 1992, 407; *CA*, **120**, 212589 (*isol, struct*)
Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

4-Nitrophenol N-130

[100-02-7]
[25154-55-6]



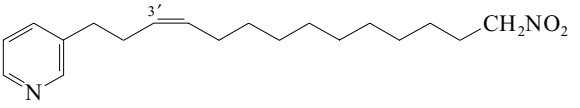
$C_6H_5NO_3$ 139.11
Isol. from the marine-derived *Flavobacterium* sp. T436. Reagent used in peptide synth. Used as EtOH soln. as an acid-base indicator (orange → yellow).
Mp 114°. pK_a 7.15 (25°). pK_a -9.18 (H_2SO_4 aq.). Dimorphous. The metastable α-form is obt. as cryst. from toluene >63° and is light-stable. The β-form is obt. as yellow prisms from toluene
▶ Reacts violently with Diethyl phosphonate in absence of solvent. Deflagrates with (solid) KOH. Inhalation or skin absorption may cause methaemoglobinaemia leading to cyanosis. LD_{50} (mus, orl) 380 mg/kg. SM2275000

[1124-30-7, 1124-31-8, 1124-32-9, 14609-74-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1340D; 1341B; **2**, 313C; 313D; 314A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 696A; 696B; 696C; 1290B; 1290C; 1291A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1192B; 1192C; 1192D; 1381B; 1381C (*ir*)
Hart, R.S. *et al., J.A.C.S.*, 1910, **32**, 1105 (*synth*)
Fujio, M. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2127 (*pmr*)
Karasek, F.W. *et al., Anal. Chem.*, 1976, **48**, 1133 (*ms*)
Le Goaller, R. *et al., Tetrahedron*, 1980, **36**, 237-243 (*K salt*)
O'Connor, C.J. *et al., Aust. J. Chem.*, 1987, **40**, 677 (*cmr, pmr*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 3751-3752 (*use*)
Krapcho, A.P. *et al., Synth. Commun.*, 1998, **28**, 3415-3422 (*synth, pmr*)
Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2131
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 917
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ABS750; NID000; NIF000; NER500

3-(14-Nitro-3-tetradecenyl)pyridine N-131

1-Nitro-14-(3-pyridinyl)-11-tetradecene



$C_{19}H_{30}N_2O_2$ 318.458

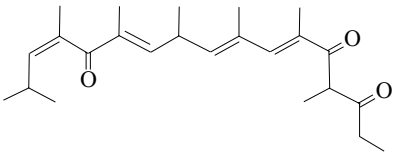
(Z)-form
Untenine A
[174756-37-7]
Alkaloid from the Okinawan marine sponge *Callyspongia* sp. Exhibits potent anti-microfouling activity.

3′,4′-Didehydro: 3-(14-Nitro-3-tetradecynyl)pyridine. 1-Nitro-14-(3-pyridinyl)-11-tetradecyne. ***Untenine C***
[174756-38-8]
$C_{19}H_{28}N_2O_2$ 316.442
From *Callyspongia* sp. Exhibits potent anti-microfouling activity.

Wang, G.-Y.-S. *et al., Tet. Lett.*, 1996, **37**, 1813 (*isol, pmr, cmr, synth, struct*)

Niuhinone A N-132

4,6,8,10,12,14,16-Heptamethyl-6,8,11,14-heptadecatetraene-3,5,13-trione
[99624-10-9]

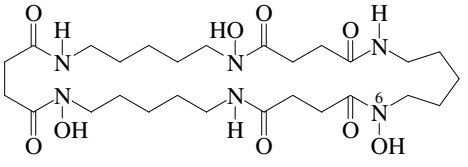


$C_{24}H_{36}O_3$ 372.547
Metab. of mollusc *Philinopsis speciosa*. Toxic to brine shrimp. Oil. $[\alpha]_D$ +55 (c, 0.68 in hexane). λ_{max} 238 (ϵ); 312 (ϵ) (EtOH/NaOH) (Derep). λ_{max} 238 (ϵ 10500); 285 (ϵ 10400) (EtOH) (Derep).

Coval, S.J. *et al., Tet. Lett.*, 1985, **26**, 5359-5362 (*isol*)

Nocardamine N-133

1,12,23-Trihydroxy-1,6,12,17,23,28-hexaazacyclotritriacontane-2,5,13,16,24,27-hexone, 9CI, 8CI. Deferrioxamine E. Desferrioxamine E. Proferrioxamine E
[26605-16-3]



$C_{27}H_{48}N_6O_9$ 600.711
Isol. from a *Nocardia* sp., *Pseudomonas stutzeri*, *Streptomyces hygroscopicus geldanus* and a marine-derived *Streptomyces* sp. strain M1087. Active against mycobacteria. Induces morphological changes in insect cells. Siderophore. Needles (MeOH).
Sol. hot H_2O, MeOH, bases.
Mp 192-195°. pK_{a1} 8.65; pK_{a2} 9.42; pK_{a3} 9.89 (20°, 0.1*M* $NaNO_3$).
Related to the ferrichrome antibiotics. λ_{max} 435 (MeOH) (Berdy).

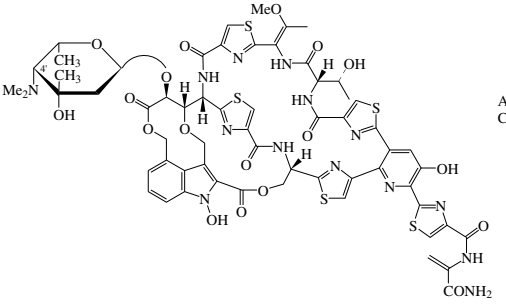
Fe complex: See Ferrioxamine E in *The Combined Chemical Dictionary.*

N^6-*Deoxy: Deoxynocardamine.* ***Terragine E***
$C_{27}H_{48}N_6O_8$ 584.712
Prod. by *Streptomyces lividans* recombinant 436-s4-5b1 and a marine-derived *Streptomyces* sp. strain M1087. Siderophore. Amorph. solid.
Mp 179-182° (dec).

Keller-Schierlein, W. *et al., Helv. Chim. Acta*, 1961, **44**, 1981 (*synth, ir, struct*)
De Boer, C. *et al., J. Antibiot.*, 1976, **29**, 1182 (*isol*)
Maehr, H. *et al., Z. Naturforsch., B*, 1977, **32**, 937 (*pmr, cmr, ms*)
Meyer, J.M. *et al., J. Gen. Microbiol.*, 1980, **118**, 125 (*isol*)
Hossain, M.B. *et al., Acta Cryst. B*, 1983, **39**, 258 (*cryst struct*)
Bergeron, R.J. *et al., Tetrahedron*, 1990, **46**, 5881 (*synth*)
Matsubara, K. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 2049-2051 (*activity*)
Wang, G.-Y.-S. *et al., Org. Lett.*, 2000, **2**, 2401-2404 (*isol, pmr, cmr, Terragine E*)
Lee, H.-S. *et al., J. Nat. Prod.*, 2005, **68**, 623-625 (*Terragine E*)

Nocathiacin I N-134

MJ 347-81F4-A. Antibiotic MJ 347-81F4-A
[214044-52-7]



$C_{61}H_{60}N_{14}O_{18}S_5$ 1437.558
Cyclic thiazole-peptide antibiotic. Prod. by *Amycolatopsis* sp. MJ347-81F4 and *Nocardia* sp. WW-12651. Active against gram-positive bacteria. Pale yellow amorph. solid. λ_{max} 222 (log ϵ 4.89); 290 (log ϵ 4.52); 364 (log ϵ 4.17) (MeOH).

4′-N-*De-Me: Antibiotic MJ 347-81F4-B. MJ 347-81F4-B*
[214044-53-8]
$C_{60}H_{58}N_{14}O_{18}S_5$ 1423.531
Prod. by *Amycolatopsis* sp. MJ347-81F4. Active against gram-positive bacteria.

N-*Deoxy:* ***Nocathiacin II***
[256230-46-3]
$C_{61}H_{60}N_{14}O_{17}S_5$ 1421.559
Prod. by *Nocardia* sp. WW-12651. Pale yellow solid. λ_{max} 220 (log ϵ 5.01); 295 (log ϵ 4.67); 364 (log ϵ 4.36) (MeOH).

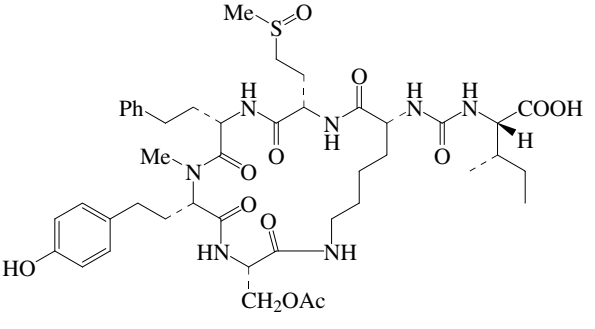
De-O-*glycosyl:* ***Nocathiacin III***
[256230-47-4]
$C_{52}H_{43}N_{13}O_{16}S_5$ 1266.319
Prod. by *Nocardia* sp. WW-12651. Buff-coloured solid. λ_{max} 224 (log ϵ 4.85); 290 (log ϵ 4.52); 364 (log ϵ 4.11) (MeOH).

N-*De(aminocarbonylethenyl): Nocathiacin IV*
$C_{58}H_{57}N_{13}O_{17}S_5$ 1368.495
Semisynthetic.

Sasaki, T. *et al., J. Antibiot.*, 1998, **51**, 715-721 (*isol, activity*)
Pat. Coop. Treaty (WIPO), 2000, 03 722; *CA*, **132**, 121531b (*isol, pmr, cmr, struct*)
Constantine, K.L. *et al., J.A.C.S.*, 2002, **124**, 7284-7285 (*synth, abs config*)
Regueiro-Ren, A. *et al., J.O.C.*, 2002, **67**, 8699-8702 (*semisynth*)
Leet, J.E. *et al., J. Antibiot.*, 2003, **56**, 226-231; 232-242 (*isol, pmr, cmr, ms*)

Nodulapeptin B N-135

[184682-37-9]



$C_{44}H_{63}N_7O_{12}S$ 914.087
Isol. from the marine cyanobacterium *Nodularia spumigena* AV1. Phycotoxin, hepatotoxin. Amorph. $[\alpha]_D^{26}$ -44.7 (c, 0.03 in MeOH).

S-*Oxide:* ***Nodulapeptin A***
[184682-36-8]
$C_{44}H_{63}N_7O_{13}S$ 930.087

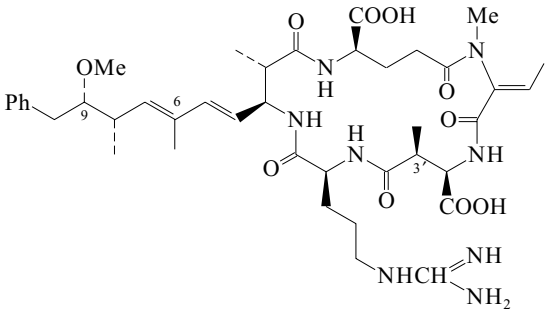
Isol. from the marine cyanobacterium *Nodularia spumigena* AV1. Phycotoxin, hepatotoxin. Amorph. Sol. MeOH. $[\alpha]_D^{26}$ -43.5 (c, 0.03 in MeOH).

Fujii, K. *et al., Tet. Lett.*, 1997, **38**, 5525-5528 (*isol, pmr, ms*)

Nodularin N-136

Nodularin 1

[118399-22-7]



$C_{41}H_{60}N_8O_{10}$ 824.973

Cyclic pentapeptide antibiotic. Similar to Cyanoginosins. From strains of *Nodularia spumigena* isol. from marine brackish water. Phycotoxin. Hepatotoxin. Tumour promoter and protein phosphatase inhibitor. λ_{max} 238 (ϵ 33200) (MeOH) (Derep).

▶ LD_{50} (mus, ipr) 0.06 mg/kg.

9-O-De-Me: ***Nodularin 2***. *[DMAdda³]Nodularin*

[159410-67-0]

$C_{40}H_{58}N_8O_{10}$ 810.946

From *Nodularia spumigena* isol. from brackish water. Phycotoxin. Hepatotoxin. $[\alpha]_D^{23}$ -53 (c, 0.01 in MeOH).

▶ LD_{50} (mus, ipr) 0.15 mg/kg.

6Z-Isomer: ***Nodularin 3***. *[(6Z)-Adda³]nodularin*

[159516-66-2]

$C_{41}H_{60}N_8O_{10}$ 824.973

From *Nodularia spumigena* isol. from brackish water. $[\alpha]_D^{23}$ -63.8 (c, 0.01 in MeOH).

▶ LD_{50} (mus, ipr) 2 mg/kg.

Homoarginine analogue: 2-Homoargininenodularin. ***[L-Har²]Nodularin***. *Nodularin-Har*

[286477-88-1]

$C_{42}H_{62}N_8O_{10}$ 838.999

isol. from a freshwater *Nodularia* sp. PCC 7804. Phycotoxin. Hepatotoxin. Cryst. $[\alpha]_D^{27}$ -81.9 (c, 0.12 in MeOH). λ_{max} 236 (MeCN aq.).

3′-Demethyl: ***Nodularin 4***. *[D-Asp¹]nodularin*

[159410-68-1]

$C_{40}H_{58}N_8O_{10}$ 810.946

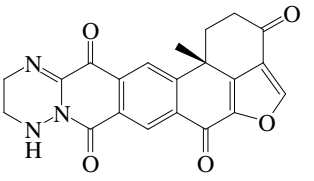
Isol. from cultured cells (strain L-575) of *Nodularia spumigena*. Phycotoxin. Hepatotoxin. $[\alpha]_D^{25}$ -87.6 (c, 0.01 in MeOH).

▶ LD_{50} (mus, ipr) 0.075 mg/kg.

Rinehart, K.L. *et al., J.A.C.S.*, 1988, **110**, 8557-8558 (*isol, struct*)
Sivonen, K. *et al., Appl. Environ. Microbiol.*, 1989, **55**, 1990-1995 (*occur, bibl*)
Namikoshi, M. *et al., J.O.C.*, 1994, **59**, 2349-2357 (*isol, pmr, cmr, ms*)
Moroder, L. *et al., Stud. Nat. Prod. Chem.*, 1998, **20**, 887-920 (*rev*)
Beattie, K.A. *et al., Phytochemistry*, 2000, **54**, 57-61 (*Homargininenodularin*)
Saito, K. *et al., J. Nat. Prod.*, 2001, **64**, 139-141 (*Har-Nodularin*)
Karjalainen, M. *et al., Mar. Biol. (Berlin)*, 2006, **148**, 683-691 (*occur*)

Noelaquinone N-137

[220503-29-7]



$C_{21}H_{15}N_3O_5$ 389.367

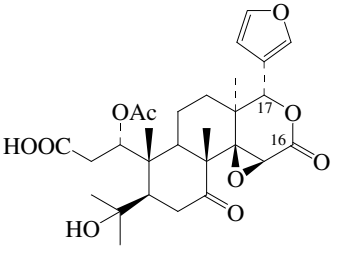
Alkaloid from a sponge *Xestospongia* sp. Yellow solid. $[\alpha]_D^{23}$ +53.6 (c, 0.25 in MeOH). Slow dec. >300°. λ_{max} 206 (ϵ 45000); 215 (ϵ 16660); 254 (ϵ 10620) (MeOH).

Zhu, Y. *et al., Heterocycles*, 1998, **49**, 355-360

Nomilinic acid N-138

1-Acetoxy-1,2-dihydroobacunoic acid

[35930-20-2]



$C_{28}H_{36}O_{10}$ 532.586

Constit. of grapefruit seeds. Noncryst.; cryst. (Et_2O/hexane) (as Me ester).

Mp 108-110° (Me ester).

Lactone, 7α-acetoxy, 7-deoxo: ***7-Acetoxydihydronomilin***. *Cneorin G*

[66879-86-5]

$C_{30}H_{38}O_{10}$ 558.624

Constit. of *Xylocarpus granatum*. Cryst. (MeOH).

Mp 265-266°.

Dreyer, D.L. *et al., Phytochemistry*, 1966, **5**, 367 (*rev*)
Ahmed, F.R. *et al., Can. J. Chem.*, 1978, **56**, 1020 (*7-Acetoxydihydronomilin*)

1,20-Nonacosadiene N-139

[28914-19-4]

$H_3C(CH_2)_7CH{=}CH(CH_2)_{17}CH{=}CH_2$

$C_{29}H_{56}$ 404.761

(E)-form [104899-46-9]

Isol. from the alga *Botryococcus braunii*.

(Z)-form [104899-41-4]

Isol. from *Botryococcus braunii*.

Metzger, P. *et al., Phytochemistry*, 1986, **25**, 1869; 1993, **33**, 1125 (*isol, pmr, cmr*)

5,9-Nonacosadienoic acid N-140

$H_3C(CH_2)_{18}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$

$C_{29}H_{54}O_2$ 434.744

(5Z,9Z)-form [120903-53-9]

Constit. of *Amphimedon complanata*, *Aplysina archari*, *Erylus formosus* and *Verongula gigantea*.

Carballeira, N.M. *et al., Lipids*, 1989, **24**, 229-232 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 305-309; 315-317 (*isol*)

1-Nonacosanol N-141

[6624-76-6]

$H_3C(CH_2)_{27}CH_2OH$

$C_{29}H_{60}O$ 424.792

Constit. of *Agave sisalana*, *Citrullus colocynthis* and *Rhizophora apiculata*. Cryst. (C_6H_6).

Mp 85°.

3,4-Dihydroxy-E-*cinnamoyl: Nonacosyl caffeate*

$C_{38}H_{66}O_4$ 586.937

Constit. of *Hypericum laricifolium*. λ_{max} 220; 244; 299; 330 (MeOH).

Piper, S.H. *et al., Biochem. J.*, 1934, **28**, 2175 (*synth*)
Razafindrazaka, J. *et al., Bull. Soc. Chim. Fr.*, 1963, 1633 (*isol*)
Rao, S.J. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 208 (*synth*)
Kokpol, U. *et al., Phytochemistry*, 1993, **33**, 1129 (*isol*)
Manorajani, M. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 1148-1150 (*isol, pmr, ms*)
El-Seedi, H.R. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1439-1440 (*caffeate*)

1,20,22-Nonacosatriene N-142

[104899-47-0]

$H_3C(CH_2)_5CH{=}CHCH{=}CH(CH_2)_{17}CH{=}CH_2$

$C_{29}H_{54}$ 402.746

(20Z,22Z)-form [108074-27-7]

Isol. from the green alga *Botryococcus braunii*.

(20ξ,22ξ)-form

Isol. from *Botryococcus braunii*. An (*E,Z*)-isomer.

Metzger, P. *et al., Phytochemistry*, 1986, **25**, 1869-1872; 1997, **44**, 1071-1075 (*isol, pmr, cmr*)

5,9,23-Nonacosatrienoic acid N-143

[79605-30-4]

$H_3C(CH_2)_4CH{=}CH(CH_2)_{12}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$

$C_{29}H_{52}O_2$ 432.729

Isol. from the phospholipids of various sponges incl. *Aplysina fistularis* and *Amphimedon compressa*.

[152336-69-1]

Walkup, R.D. *et al., Lipids*, 1981, **16**, 631 (*isol*)
Carballeira, N.M. *et al., Lipids*, 1989, **24**, 89 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1993, **56**, 1850 (*isol*)

1-Nonacosene N-144

[18835-35-3]

$H_3C(CH_2)_{26}CH{=}CH_2$

$C_{29}H_{58}$ 406.777

Isol. from *Balsamorhiza sagittata* and the alga *Botryococcus braunii*. Oil.

Driesbach, R.R. *et al., Adv. Chem. Ser.*, 1959, **22**, 1 (*props*)
Bohlmann, F. *et al., Phytochemistry*, 1985, **24**, 2029-2036 (*isol, pmr, ms*)
Metzger, P. *et al., Phytochemistry*, 1997, **44**, 1071 (*isol, pmr, cmr*)

28-Nonacosene-9,10-diol N-145

$H_2C{=}CH(CH_2)_{17}CH(OH)CH(OH)(CH_2)_7CH_3$

$C_{29}H_{58}O_2$ 438.776

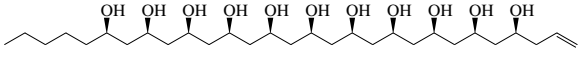
9-(9-Octadecenoyl)(Z-): [168981-90-6]

$C_{47}H_{90}O_3$ 703.226

Constit. of *Botryococcus braunii*.

Metzger, P. *et al., Phytochemistry*, 1995, **40**, 543-554 (*isol, pmr, cmr, ms*)

1-Nonacosene-4,6,8,10,12,14,16,18,20,22,24-undecol N-146



$C_{29}H_{58}O_{11}$ 582.771

(4S,6S,8S,10S,12S,14R,16R,18R,20R,22R,24R)-form

Undeca-Me ether: 4,6,8,10,12,14,16,18,20,22,24-Undecamethoxy-1-nonacosene

[265649-28-3]

$C_{40}H_{80}O_{11}$ 737.065

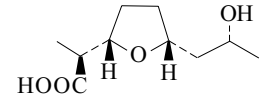
Isol. from the cyanobacterium *Aphanizomenon ovalisporum*.

Banker, R. *et al., J. Nat. Prod.*, 2000, **63**, 387-389

Nonactic acid N-147

Tetrahydro-5-(2-hydroxypropyl)-α-methyl-2-furanacetic acid, 9CI. Nonactinic acid

[60761-12-8]



(+)–*form*

$C_{10}H_{18}O_4$ 202.25

Hydrol. prod. of Nonactin, N-149 and other *Streptomyces* metabolites.

(+)-form

Me ester:

$C_{11}H_{20}O_4$ 216.277

$[\alpha]_D^{20}$ +19.2 (c, 0.93 in $CHCl_3$) (97% ee).

(-)-form

Me ester:

$Bp_{0.03}$ 80°. $[\alpha]_D^{20}$ -19.2 (c, 1.02 in $CHCl_3$) (97% ee).

(±)-form [55220-86-5]

$Bp_{0.01}$ 120°.

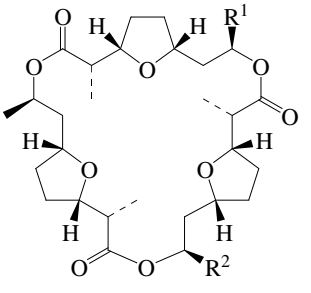
Me ester: [74892-41-4]

$Bp_{0.01}$ 85°.

[16221-10-6, 16221-11-7, 54594-22-8, 54594-23-9, 55221-38-0, 55221-40-4, 56761-10-5, 58769-09-8, 74892-42-5, 74957-68-9, 74957-69-0, 74983-78-1]

Bech, J. *et al., Helv. Chim. Acta*, 1962, **45**, 620 (*synth, nmr, ir, isol*)
Gerlach, H. *et al., Annalen*, 1963, **669**, 121 (*config*)
Beck, G. *et al., Chem. Ber.*, 1971, **104**, 21 (*synth*)
Gerlach, H. *et al., Helv. Chim. Acta*, 1974, **57**, 2306 (*synth, ir, uv, nmr*)
Schmidt, U. *et al., Chem. Ber.*, 1976, **109**, 2628 (*synth, nmr, ir, uv, ms*)
Arco, M.J. *et al., J.O.C.*, 1976, **41**, 2075 (*synth, ir, nmr, ms*)
Baldwin, S.W. *et al., J.O.C.*, 1987, **52**, 320 (*synth, bibl*)
Wang, Y. *et al., Tetrahedron: Asymmetry*, 2000, **11**, 3995-3999 (*Me ester, resoln*)
Fraser, B. *et al., J.C.S. Perkin 1*, 2002, 2896-2899 (*synth, Me ester, pmr*)

Nonactic acid trimer N-148



Absolute Configuration

$R^1 = R^2 = CH_3$

$C_{30}H_{48}O_9$ 552.704

Struct. proposed shown to be unlikely by Wu *et al* in 2006. Prod. by a strain of *Streptomyces globisporus* and the marine -derived *Streptomyces* sp. KORDI-3238. Pale yellow oil. $[\alpha]_D^{25}$ +14.5 (c, 0.09 in EtOH).

Homologue ($R^1 = CH_3$, $R^2 = CH_2CH_3$):

$C_{31}H_{50}O_9$ 566.731

Prod. by a strain of *Streptomyces globisporus*. Pale brown oil. $[\alpha]_D^{25}$ +9.8 (c, 0.16 in EtOH).

Homologue ($R^1 = R^2 = CH_2CH_3$):

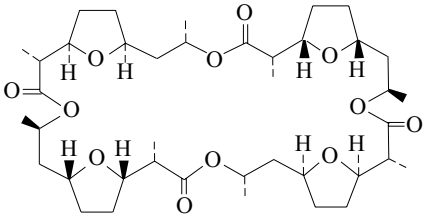
$C_{32}H_{52}O_9$ 580.757

Prod. by a strain of *Streptomyces globisporus*. Pale yellow oil. $[\alpha]_D^{25}$ +19 (c, 0.15 in EtOH).

Rezanka, T. *et al., Tetrahedron*, 2004, **60**, 4781-4787 (*isol, pmr, cmr*)
Jeong, S.-Y. *et al., J. Antibiot.*, 2006, **59**, 234-240 (*marine, isol*)
Wu, Y. *et al., Org. Lett.*, 2006, **8**, 2831-2834 (*struct*)

Nonactin N-149

*Werramycin. FH 3582*A. *NSC 52141. AKD 1A. Antibiotic AKD 1A*
[6833-84-7]



$C_{40}H_{64}O_{12}$ 736.938

Polyether macrotetrolide antibiotic. Prod. by *Streptomyces* spp. incl. *Streptomyces griseus* ssp. *griseus* and the marine-derived *Streptomyces* sp. KORDI-3238. Active against gram-positive bacteria. Needles (MeOH).

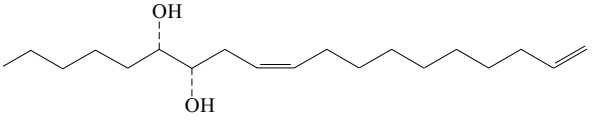
Mp 149-150°. $[\alpha]_D^{20}$ 0 (c, 2.0 in $CHCl_3$). Effectively coordinates to a variety of metal cations.

▶ LD_{50} (mus, ivn) 246 mg/kg. RH1685000

KNCS complex: Mp 251-254°.

Dominguez, J. *et al., Helv. Chim. Acta*, 1962, **45**, 129 (*isol*)
Dobler, M. *et al., Helv. Chim. Acta*, 1969, **52**, 2573; 1972, **55**, 1371 (*cryst struct*)
Gerlach, H. *et al., Helv. Chim. Acta*, 1975, **58**, 2036 (*synth, nmr, ms, ir*)
Schmidt, U. *et al., Chem. Ber.*, 1976, **109**, 2628 (*synth, pmr, cmr, ms, ir*)
Anteunis, M.J.O. *et al., Bull. Soc. Chim. Belg.*, 1977, **86**, 445 (*conformn, pmr*)
Ashworth, D.M. *et al., Chem. Comm.*, 1982, 491 (*biosynth, cmr*)
Nawata, Y. *et al., Tetrahedron*, 1983, **39**, 1133 (*conformn, cryst struct*)
Bartlett, P. *et al., J.A.C.S.*, 1984, **106**, 5304 (*synth*)
Bulman Page, P.C. *et al., Chem. Comm.*, 1985, 822 (*synth*)
Batmangherlich, S. *et al., Chem. Comm.*, 1985, 1399 (*synth*)
Clark, C.A. *et al., Chem. Comm.*, 1985, 1568 (*nmr, biosynth*)
Lee, J.Y. *et al., Tetrahedron*, 1996, **52**, 571 (*synth*)
Fleming, I. *et al., J.C.S. Perkin 1*, 1998, 2733-2747 (*synth*)
Jeong, S.-Y. *et al., J. Antibiot.*, 2006, **59**, 234-240 (*marine, isol*)
Wu, Y. *et al., Org. Lett.*, 2006, **8**, 2831-2834 (*synth, bibl*)

9,18-Nonadecadiene-6,7-diol, 9CI N-150



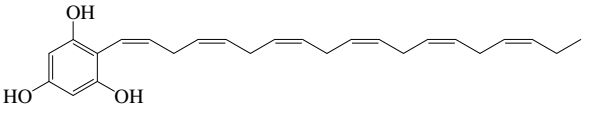
$C_{19}H_{36}O_2$ 296.492

(6*S*,7*S*,9*Z*)-*form* [129436-89-1]
Isol. from the brown alga *Notheia anomala*.
Unstable oil. $[\alpha]_D$ -7.5 (c, 0.3 in $CHCl_3$).

[129436-90-4]

Barrow, R.A. *et al., Aust. J. Chem.*, 1990, **43**, 895 (*isol, ms, pmr, cmr*)

2-(1,4,7,10,13,16-Nonadecahexaenyl)-1,3,5-benzenetriol N-151



$C_{25}H_{32}O_3$ 380.526

(all-Z)-form
Schimperiol
Constit. of the brown alga *Stypopodium schimperi*.
Unstable yellow oil. λ_{max} 236 (MeOH) (as tri-Ac).

Sampli, P. *et al., Nat. Prod. Lett.*, 2000, **14**, 365-372

Nonadecanoic acid N-152

[646-30-0]
$H_3C(CH_2)_{17}COOH$
$C_{19}H_{38}O_2$ 298.508
Isol. from wood of *Ulex europaeus* and *Shorea maranti* and other plant sources. Present in lipids of *Physalia physalis* (Portuguese-man-of-war). Cryst. (EtOH).
Mp 68.7°. Bp_{100} 297-298° Bp_{10} 227-230°.

Me ester: [1731-94-8]
$C_{20}H_{40}O_2$ 312.535
Mp 38.9°.

Heptadecyl ester:
$C_{36}H_{72}O_2$ 536.964
Constit. of the seeds of *Centratherum anthelminticum*. Cryst. (EtOAc).
Mp 115-116°.

Tetratriacontanyl ester: Tetratriacontanyl nonadecanoate
[94410-18-1]
$C_{53}H_{106}O_2$ 775.419
Isol. from seeds of *Cassia spectabilis* (Leguminosae). Cryst. (C_6H_6).
Mp 65°.

2,3-Dihydroxypropyl ester: [62927-07-5]
$C_{22}H_{44}O_4$ 372.587
Constit. of the roots of *Rumex patientia* (patience dock).

Nitrile: 1-Cyanooctadecane
[28623-46-3]
$C_{19}H_{37}N$ 279.508
Cryst. (Me_2CO). Mp 42.5-43.5°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 485D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 757C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 631D (*ir*)
Shirley, D.A. *et al., J.O.C.*, 1953, **18**, 1591 (*nitrile*)
Jones, R.N. *et al., Can. J. Chem.*, 1962, **40**, 321 (*ir*)
Ames, D.E. *et al., J.C.S.*, 1963, 775 (*synth*)
Cocker, W. *et al., Perfum. Essent. Oil Res.*, 1963, **54**, 235; 1964, **55**, 442 (*isol*)
Matucha, M. *et al., J. Chromatogr.*, 1972, **65**, 371 (*glc*)
Marosi, L.S. *et al., Annalen*, 1973, 584 (*cryst struct*)
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206 (*isol*)
Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*Physalia physalis constit*)
Singh, M. *et al., Z. Naturforsch., B*, 1984, **39**, 1425 (*Tetratriacontanyl nonadecanoate*)
Yuan, Y. *et al., CA*, 2001, **135**, 270046m (*2,3-dihydroxypropyl ester*)
Verma, M. *et al., Indian J. Chem., Sect. B*, 2004, **43**, 442-446 (*heptadecyl ester*)

2-Nonadecanone N-153

[629-66-3]
$H_3C(CH_2)_{16}COCH_3$
$C_{19}H_{38}O$ 282.509
Constit. of the marine sponge *Spheciospongia vagabunda*. Cryst. (EtOH).
Mp 55-56°. Bp_{110} 266.5°.

Oxime:
$C_{19}H_{39}NO$ 297.523
Cryst. (EtOH). Mp 76°.

Semicarbazone: Mp 125.5-126° (119°).

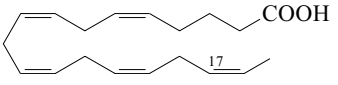
Thoms, H. *et al., Annalen*, 1907, **357**, 161
Bailey, A.V. *et al., J. Chem. Eng. Data*, 1970, **15**, 542 (*cryst struct*)
Golemba, F.J. *et al., Macromolecules*, 1972, **5**, 63
Middleditch, B.S. *et al., Org. Mass Spectrom.*, 1972, **6**, 179 (*ms*)
Simoneit, B.R. *et al., Adv. Org. Geochem., Proc. Int. Meet., 6th*, 1974, 191 (*isol*)
Ghirinhelli, D. *et al., Synthesis*, 1982, 580-582 (*synth*)
Xiao, D. *et al., Fenxi Huaxue*, 2004, **32**, 1621-1623; *CA*, **143**, 23210 (*Spheciospongia vagabunda constit*)

3,6,9,12,15-Nonadecapentaene, 9CI N-154

$H_3CCH_2(CH{=}CHCH_2)_5CH_2CH_3$
$C_{19}H_{30}$ 258.446

(all-Z)-form [33426-21-0]
Found in marine benthic algae.
Youngblood, W.W. *et al., Mar. Biol. (Berlin)*, 1971, **8**, 190 (*isol, struct, ir, ms*)

5,8,11,14,17-Nonadecapentaenoic acid N-155



$C_{19}H_{28}O_2$ 288.429

(all-Z)-form [170515-90-9]
Prod. by the fungus *Saprolegnia* sp., the cause of cotton-wool fungus disease in freshwater fish.

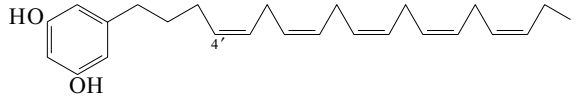
17,18-Dihydro: ***5,8,11,14-Nonadecatetraenoic acid***
[20088-29-3]
[3036-89-3]
$C_{19}H_{30}O_2$ 290.445
Prod. by *Saprolegnia* sp. and *Mortierella alpina*.

17,18-Dihydro, Et ester:
$C_{21}H_{34}O_2$ 318.498
Isol. from *Nephthea hainansis*. Oil.

[20088-68-0]

Beerthuis, R.K. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1968, **87**, 461-480 (*synth, deriv*)
Inami, K. *et al., Tet. Lett.*, 1990, **31**, 4033-4036 (*synth, deriv*)
Shimizu, S. *et al., J. Am. Oil Chem. Soc.*, 1991, **68**, 254-258 (*isol*)
Shirasaka, N. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1963-1965 (*isol, struct*)
Li, G.Q. *et al., Chin. Chem. Lett.*, 2005, **16**, 494-496 (*Nephthea hainansis ester*)

5-(4,7,10,13,16-Nonadecapentaenyl)-1,3-benzenediol N-156



$C_{25}H_{34}O_2$ 366.542

(all-Z)-form [138168-60-2]
Constit. of the sponge *Haliclona* sp.
Oil. Darkens in air.

4′,5′-Dihydro: 5-(7,10,13,16-Nonadecatetraenyl)-1,3-benzenediol
[138168-59-9]
$C_{25}H_{36}O_2$ 368.558
Constit. of *Haliclona* sp. Oil. Darkens in air.
Barrow, R.A. *et al., Aust. J. Chem.*, 1991, **44**, 1393 (*isol, uv, ir, pmr, cmr, ms*)

1,10,13,16-Nonadecatetraene, 9CI N-157

3,6,9,18-Nonadecatetraene (incorr.)
$H_2C{=}CH(CH_2)_7CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH_3$
$C_{19}H_{32}$ 260.462

(all-Z)-form [129436-92-6]
Isol. from the brown alga *Notheia anomala*.
Unstable oil. Not obt. pure.

10S,11R:13S,14R-Diepoxide: 10,11:13,14-Diepoxy-1,17-nonadecadiene
[129451-32-7]
Constit. of *Notheia anomala*.
Unstable oil. $[\alpha]_D$ +19.6 (c, 1.1 in $CHCl_3$).

16,17-Dihydro: 1,10,13-Nonadecatriene, 9CI. 6,9,18-Nonadecatriene (incorr.)
[106799-43-3]
$C_{19}H_{34}$ 262.478
Isol. from *Notheia anomala*. Unstable oil.

16,17-Dihydro,10S,11R:13S,14R-diepoxide: 10,11:13,14-Diepoxy-1-nonadecene
[129436-85-7]
$C_{19}H_{34}O_2$ 294.476
Isol. from *Notheia anomala*. Unstable oil. $[\alpha]_D$ +20.6 (c, 0.7 in $CHCl_3$).

Bestmann, H.J. *et al., Annalen*, 1987, 417 (*synth*)
Barrow, R.A. *et al., Aust. J. Chem.*, 1990, **43**, 895 (*isol, pmr, cmr, ms*)

8-Nonadecene N-158

[103963-42-4]
[76402-64-7 (*E*-form)]

$H_3C(CH_2)_9CH{=}CH(CH_2)_6CH_3$
$C_{19}H_{38}$ 266.509
Constit. of larvae of Khapra beetles *Trogoderma granarium* and glands of honey bee *Bombus terrestris*.

(Z)-form [76402-65-8]
Constit. of gizzard shad *Clupanodon punctatus* and sardine *Sardinops melanosticta*.
Hoshita, N. *et al., Lipids*, 1982, **17**, 390-392 (*Z-form, isol, synth*)
Malinski, E. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **84**, 211-215 (*occur*)
Sojak, L. *et al., J. Chromatogr., A*, 1992, **609**, 283-288 (*gc*)
Hefetz, A. *et al., Z. Naturforsch., C*, 1996, **51**, 409-422 (*occur*)

3-Nonadecene-1,8,10,18-tetrayne N-159

Aikupikanyne A
$HC{\equiv}C(CH_2)_6C{\equiv}CC{\equiv}C(CH_2)_3CH{=}CHC{\equiv}CH$
$C_{19}H_{22}$ 250.383

(Z)-form
Isol. from a *Callyspongia* sp.
Oil.
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2000, **63**, 1406-1410

6-Nonadecenoic acid N-160

$H_3C(CH_2)_{11}CH{=}CH(CH_2)_4COOH$
$C_{19}H_{36}O_2$ 296.492

(Z)-form [134381-22-9]
Isol. from the sponge *Geodia gibberosa*.
Carballeira, N.M. *et al., Lipids*, 1991, **26**, 324 (*isol*)

11-Nonadecenoic acid N-161

[71997-08-5]
$H_3C(CH_2)_7CH{=}CH(CH_2)_9COOH$
$C_{19}H_{36}O_2$ 296.492

(Z)-form [80648-66-4]
Constit. of various crustaceans, molluscs and sponges. Also isol. from lichens and slime moulds.

Christie, W.W. *et al., Lipids*, 1992, **27**, 640-644 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1993, **56**, 1850-1855 (*isol*)

2,6-Nonadienal, 9CI N-162

[26370-28-5]

$H_3CCH_2CH{=}CHCH_2CH_2CH{=}CHCHO$

$C_9H_{14}O$ 138.209

(2E,6E)-form

FEMA 3766

[17587-33-6]

Present in fruits, e.g. mango, and fish. Flavouring agent. Bp_{11} 88-89°. n_D^{20} 1.4420.

Di-Et acetal: 1,1-Diethoxy-2,6-nonadiene. FEMA 3378

[106950-34-9]

$C_{13}H_{24}O_2$ 212.331

$Bp_{0.2}$ 67-70°. n_D^{20} 1.4439.

(2E,6Z)-form

Violet-leaf aldehyde. Cucumber aldehyde. FEMA 3377

[557-48-2]

Constit. of violet leaf oil, cherry, melon, peas, and other plant sources, also fish, oyster, clam. Used in perfumery.

Liq. with cucumber odour. d 0.87. Bp 187° Bp_{11} 94-98°. n_D^{20} 1.4460.

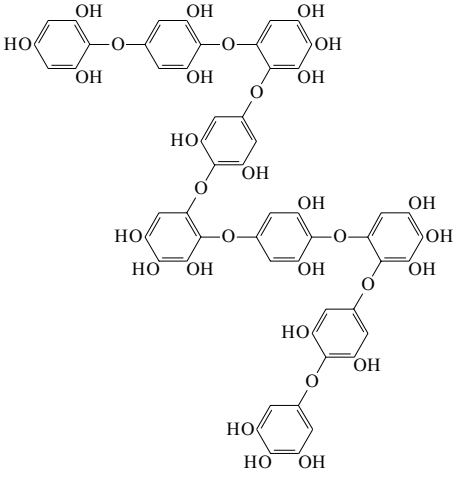
▶ Skin irritant. LD_{50} (rat, orl) > 5000 mg/kg. RA5391800

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 743C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 565D (*ir*)
Ruzicka, L. *et al., Helv. Chim. Acta*, 1942, **25**, 760; 1944, **27**, 1561 (*isol, synth*)
Seifert, R.M. *et al., J. Agric. Food Chem.*, 1968, **16**, 880 (*synth*)
Hariel, J. *et al., Soap, Perfum. Cosmet.*, 1969, **42**, 571 (*use*)
Meyers, A.I. *et al., J.O.C.*, 1973, **38**, 36 (*synth*)
Kajiwara, T. *et al., Agric. Biol. Chem.*, 1975, **39**, 1617 (*synth, ir*)
Tadema, G. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1976, **95**, 66 (*synth*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 769 (*rev, tox*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, NMV760; NMV775
Shieberle, P. *et al., J. Food Sci.*, 1990, **55**, 193-195 (*isol*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1991, 567 (*synth, ir, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 595-596 (*di-Et acetal*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1966-1968 (*di-Et acetal, occur, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NMV760

Nonafuhalol A N-163

Nonafuhalol

[83903-58-6]

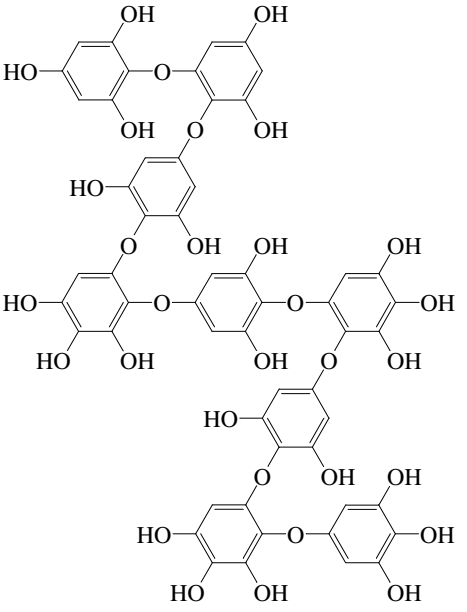


$C_{54}H_{38}O_{31}$ 1182.876

Constit. of brown algae *Sargassum muticum*, *Sargassum spinuligerum*, *Carpophyllum maschalocarpum* and *Carpophyllum angustifolium*.

Glombitza, K.-W. *et al., Bot. Mar.*, 1982, **25**, 449-453 (*isol, pmr*)
Glombitza, K.-W. *et al., Phytochemistry*, 1991, **30**, 2741; 1995, **38**, 987-995 (*isol*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

Nonafuhalol B N-164



$C_{54}H_{38}O_{31}$ 1182.876

Isol. from *Sargassum spinuligerum*.

Keusgen, M. *et al., Phytochemistry*, 1995, **38**, 975-985

2-Nonen-1-ol N-165

FEMA 3379

[22104-79-6]

$H_3C(CH_2)_5CH{=}CHCH_2OH$

$C_9H_{18}O$ 142.241

Present in melon, cucumber, brown algae, nectarine and prickly pear (*Opuntia ficus-indica*). Used in food flavouring.

(E)-form [31502-14-4]

d_4^{19} 0.85. $Bp_{0.6}$ 68-73°. n_D^{25} 1.4418.

3,5-Dinitrobenzoyl:

Solid (EtOH). Mp 61-62°.

(Z)-form [41453-56-9] Bp_{20} 106°.

3,5-Dinitrobenzoyl:

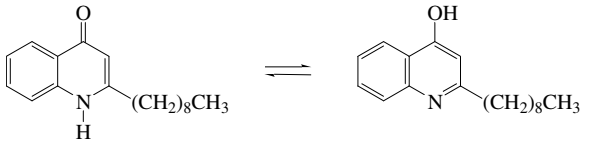
Solid (EtOH). Mp 44-45°.

[22104-79-6]

Zolvist, F. *et al., Helv. Chim. Acta*, 1952, **35**, 2380 (*deriv, E-form*)
Jacobson, M. *et al., J. Med. Chem.*, 1971, **14**, 236 (*synth, E-form*)
Kitching, W. *et al., J.O.C.*, 1989, **54**, 3893 (*pmr, cmr, ms, E-form*)
Daeuble, J.F. *et al., Tet. Lett.*, 1990, **31**, 2397 (*synth, Z-form*)
Subbaraman, A.S. *et al., Indian J. Chem., Sect. B*, 1991, **30**, 511 (*synth, ir, pmr, Z-form*)
Sakoda, Y. *et al., Z. Naturforsch., C*, 1995, **50**, 757-765 (*synth, ir, pmr, cmr, ms*)
Zhang, Z.-B. *et al., J.C.S. Perkin 1*, 2000, 53-57 (*E-form, synth*)

2-Nonyl-4(1*H*)-quinolinone N-166

2-Nonyl-4-quinolinol. 4-Hydroxy-2-nonylquinoline. Pyo Ic. Pseudane IX
[55396-45-7]



$C_{18}H_{25}NO$ 271.402
Isol. from *Pseudomonas aeruginosa*. Also prod.by a bacterium isol. from the sponge *Suberea creba*. Antibacterial agent. Cryst. Sol. MeOH, Et_2O; poorly sol. H_2O, acids.
Mp 138.8-139.2°. λ_{max} 213 (ϵ 23500); 236 (ϵ 26900); 316 (ϵ 10400); 327 (ϵ 10000) (MeOH) (Berdy). λ_{max} 236 (E1%/1cm 1050); 316 (E1%/1cm 431); 328 (E1%/1cm 415) (EtOH) (Berdy).

Oxalate: Mp 158-159°.

N-*Oxide:* [316-66-5]
$C_{18}H_{25}NO_2$ 287.401
Leaflets (EtOH). Mp 148-149°.

*1′,2′-Didehydro (*E-*): 2-(1-Nonenyl)-4(1*H*)-quinolinone. 4-Hydroxy-2-(1-nonenyl)quinoline. 2-(1-Nonenyl)-4-quinolinol. Δ[1]-Pseudene IX. Pyo III*
[60783-01-9]
[1033-24-5]
$C_{18}H_{23}NO$ 269.386
Isol. from *Pseudomonas aeruginosa*. Also prod. by a bacterium isol. from the sponge *Suberea creba*. Moderately active against gram-positive bacteria. Cryst. Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 152.8-153.5°. λ_{max} 258 (ϵ 39000); 267 (ϵ 38000); 308 (ϵ 8700); 330 (ϵ 11000) (MeOH) (Berdy). λ_{max} 258 (E1%/1cm 1460); 266 (E1%/1cm 1376); 307 (E1%/1cm 340); 338 (E1%/1cm 434) (EtOH) (Berdy).

3′,4′,6′,7′-Tetradehydro: ***2-(3,6-Nonadienyl)-4(1*H*)-quinolinone.*** *4-Hydroxy-2-(3,6-nonadienyl)quinoline. 2-(3,6-Nonadienyl)-4-quinolinol*
[29479-51-4]
$C_{18}H_{21}NO$ 267.37
Alkaloid from *Vepris ampody* (Rutaceae).
Mp 103°. Config. of double bonds unknown.

9′-Hydroxy: ***2-(9-Hydroxynonyl)-4(1*H*)-quinolinone***
[29479-52-5]
$C_{18}H_{25}NO_2$ 287.401
Alkaloid from leaves of *Vepris ampody* (Rutaceae). Cryst. (Me_2CO).
Mp 50°.

*8′-Oxo: 2-(8-Oxononyl)-4(1*H*)-quinolinone*
$C_{18}H_{23}NO_2$ 285.385
Alkaloid from *Ruta montana*. λ_{max} 216 (log ϵ 4.5); 236 (log ϵ 4.2); 320 (log ϵ 3.8); 332 (log ϵ 3.8) (MeOH).

8′-Oxo, N-*Me: 1-Methyl-2-(8-oxononyl)-4(1*H*)-quinolinone*
$C_{19}H_{25}NO_2$ 299.412
Alkaloid from *Ruta montana*. λ_{max} 220 (log ϵ 4.2); 235 (log ϵ 4.5); 320 (log ϵ 3.8); 332 (log ϵ 3.8) (MeOH).

NH-form

N-*Me:* ***1-Methyl-2-nonyl-4(1*H*)-quinolinone***
[68353-24-2]
$C_{19}H_{27}NO$ 285.428
Alkaloid from *Ruta graveolens* (rue) and the ripe fruit of *Evodia rutaecarpa* (Rutaceae). Plates (C_6H_6/cyclohexane).
Mp 71-75°.

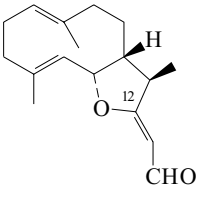
N-*Acetoxymethyl:* ***1-Acetoxymethyl-2-nonyl-4(1*H*)-quinolinone***
$C_{21}H_{29}NO_3$ 343.465
Alkaloid from aerial parts of *Boronia bowmanii* (Rutaceae). Amorph. solid.
Mp 79°.

OH-form

8′-Oxo, Me ether: ***4-Methoxy-2-(8-oxononyl)quinoline.*** *9-(4-Methoxy-2-quinolinyl)-2-nonanone*
$C_{19}H_{25}NO_2$ 299.412
Alkaloid from *Ruta montana*. λ_{max} 228 (log ϵ 4.5); 300 (log ϵ 2.9); 314 (log ϵ 2.8) (MeOH).

Hays, E.E. *et al., J. Biol. Chem.*, 1945, **159**, 725 (*isol, uv*)
Wells, I.C. *et al., J. Biol. Chem.*, 1952, **196**, 331 (*isol, struct, synth*)
Kan-Fan, C. *et al., Phytochemistry*, 1970, **9**, 1283 (*9′-hydroxy, 3′,4′,6′,7′-tetradehydro*)
Ritter, C. *et al., Eur. J. Biochem.*, 1971, **18**, 391 (*biosynth*)
Wratten, S.J. *et al., Antimicrob. Agents Chemother.*, 1977, **11**, 411
Kamikado, T. *et al., Agric. Biol. Chem.*, 1978, **42**, 1515 (*deriv*)
Budzikiewicz, H. *et al., Monatsh. Chem.*, 1979, **110**, 947 (*isol, uv*)
Grundon, M.F. *et al., Phytochemistry*, 1979, **18**, 1768 (*deriv*)
Somanathan, R. *et al., J. Het. Chem.*, 1981, **18**, 1077 (*synth, uv, ir, pmr*)
Ahsan, M. *et al., J. Nat. Prod.*, 1994, **57**, 670 (*1-Acetoxymethyl-2-nonyl-4(1H)-quinolinone*)
Debitus, C. *et al., J. Mar. Biotechnol.*, 1998, **6**, 136-141 (*isol*)
Touati, D. *et al., Phytochemistry*, 2000, **53**, 277-279 (*8′-oxo derivs*)
Biavatti, M.W. *et al., J. Braz. Chem. Soc.*, 2002, **13**, 66-70 (*isol, pmr, cmr*)

Norasperenal A N-167

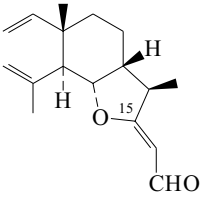


$C_{17}H_{24}O_2$ 260.375
Metabolite of gorgonian *Eunicea* sp. Solid.
Mp 101.5-102.5°. $[\alpha]_D$ +131 (c, 1.2 in MeOH).

*12*E-*isomer:* ***Norasperenal C***
$C_{17}H_{24}O_2$ 260.375
Metabolite of *Eunicea* sp. Unstable oil.

Shin, J. *et al., Tet. Lett.*, 1989, **30**, 6821

Norasperenal B N-168



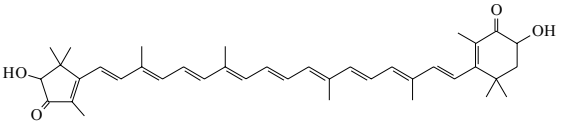
$C_{17}H_{24}O_2$ 260.375
Metabolite of gorgonian *Eunicea* sp. Solid.
Mp 123-124.5°. $[\alpha]_D$ -23 (c, 0.5 in MeOH).

*15*E-*Isomer:* ***Norasperenal D***
$C_{17}H_{24}O_2$ 260.375
Metab. of *Eunicea* sp. Unstable oil.

Shin, J. *et al., Tet. Lett.*, 1989, **30**, 6821

2-Norastaxanthin N-169

3,3′-Dihydroxy-2-nor-β,β-carotene-4,4′-dione
[76548-17-9]



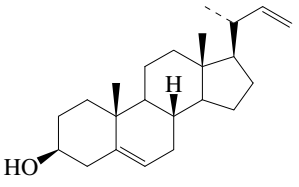
$C_{39}H_{50}O_4$ 582.822

Poorly characterised at present. Isol. from *Euchaeta russelli*; present as monoacyl esters and from *Actinia equina* as diacyl esters (Ester X). λ_{max} 483; 515 (hexane). λ_{max} 492 (Me_2CO) (monoacyl esters). λ_{max} 490 (Me_2CO) (diacyl esters).

Hertzberg, S. *et al., Acta Chem. Scand.*, 1969, **23**, 3290 (*isol*)
Francis, G.W. *et al., Acta Chem. Scand.*, 1972, **26**, 1097
Jacobs, P.B. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **72**, 157
Bandaranayake, W.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **72**, 409

24-Norchola-5,22-dien-3-ol N-170

24,25,26,27-Tetranorcholesta-5,22-dien-3-ol. 20-Ethenylpregn-5-en-3-ol

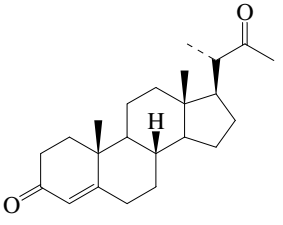


$C_{23}H_{36}O$ 328.537

3β-*form* [57597-07-6]
Constit. of *Cystoseira crinita*.
Kamenarska, Z. *et al., Z. Naturforsch., C*, 2002, **57**, 584-590 (*isol*)

24-Norchol-4-ene-3,22-dione N-171

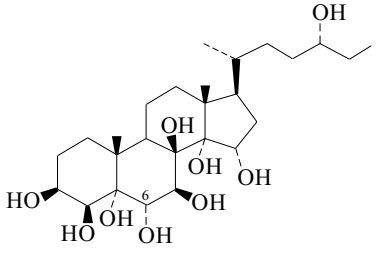
20-Acetylpregn-4-en-3-one
[80981-37-9]



$C_{23}H_{34}O_2$ 342.52
Constit. of *Aldisa smaragdina*. Cryst. (Et_2O/petrol).
Mp 203-204°. $[\alpha]_D$ +34 (c, 0.12 in $CHCl_3$). λ_{max} 238 (log ϵ 3.48) (MeOH).

Gavagnin, M. *et al., Eur. J. Org. Chem.*, 2002, 1500-1504 (*isol, pmr, cmr, synth*)

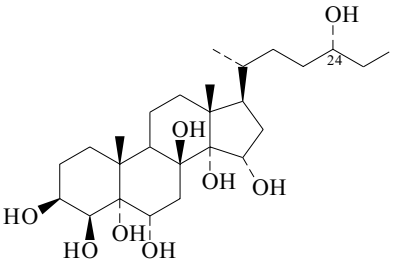
27-Norcholestane-3,4,5,6,7,8,14,15,24-nonol N-172



$C_{26}H_{46}O_9$ 502.644

(3β,4β,5α,6α,7β,15α,24*R*)-*form* [102988-63-6]
Constit. of *Archaster typicus*.
Cryst.
Mp 288-290°. $[\alpha]_D$ +37.6 (c, 0.8 in MeOH).
6-Sulfate: [102988-64-7]
$C_{26}H_{46}O_{12}S$ 582.708
From *Archaster typicus*.
6-Sulfate, Na salt: $[\alpha]_D$ +52 (c, 1 in MeOH).
Riccio, R. *et al., J.C.S. Perkin 1*, 1986, 665-670 (*isol, 6-sulfate*)
Mattia, C.A. *et al., Acta Cryst. C*, 1988, **44**, 2170-2173 (*cryst struct*)

27-Norcholestane-3,4,5,6,8,14,15,24-octol N-173



$C_{26}H_{46}O_8$ 486.645

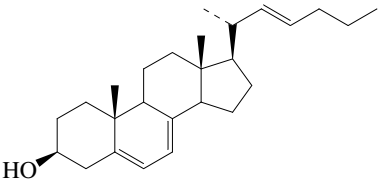
(3β,4β,5α,6α,15α,24*R*)-*form* [102988-65-8]
Constit. of *Archaster typicus*.
Cryst.
Mp 294°. $[\alpha]_D$ +43.4 (c, 0.8 in MeOH).
24-Ketone: 3,4,5,6,8,14,15-Heptahydroxy-27-norcholestan-24-one [102988-66-9]
$C_{26}H_{44}O_8$ 484.629
From *Archaster typicus*.
$[\alpha]_D$ +40 (c, 0.5 in MeOH).
Riccio, R. *et al., J.C.S. Perkin 1*, 1986, 665-670 (*isol, pmr, cmr, 24-ketone*)

19-Norcholestan-3-ol N-174

$C_{26}H_{46}O$ 374.649

(3β,5α)-*form* [54602-15-2]
Constit. of *Axinella polypoides*.
*22,23*E*-Didehydro: **19-Norcholest-22-en-3-ol***
$C_{26}H_{44}O$ 372.633
From *Axinella polypoides*.
22,23-Didehydro, Ac: [54602-07-2]
Cryst. (MeOH). Mp 103-105°. $[\alpha]_D$ +15.8 (c, 0.4 in $CHCl_3$).
Minale, L. *et al., J.C.S. Perkin 1*, 1974, 1888

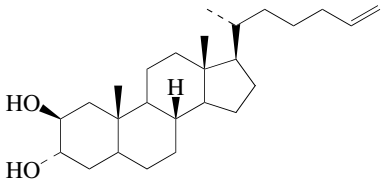
27-Norcholesta-5,7,22-trien-3-ol N-175



$C_{26}H_{40}O$ 368.601

(3β,22*E*)-*form* [85733-75-1]
Constit. of the sponge *Axinella cannabina*. λ_{max} 262; 271; 281; 293 (EtOH).
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol, pmr, ms*)

27-Norcholest-25-ene-2,3-diol N-176



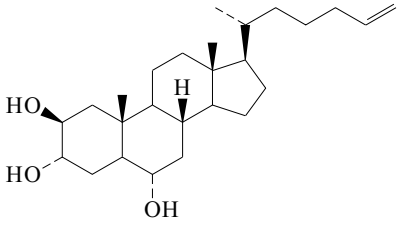
$C_{26}H_{44}O_2$ 388.632

(2β,3α,5α)-*form*

Di-O-*sulfate:* ***Halistanol disulfate B***
[176666-83-4]
$C_{26}H_{44}O_8S_2$ 548.761
Constit. of a *Pachastrella* sp. Powder. $[\alpha]_D^{22}$ +20.1 (c, 1.43 in MeOH).

Patil, A.D. *et al., J. Nat. Prod.*, 1996, **59**, 606-608 (*isol, pmr, cmr*)

27-Norcholest-25-ene-2,3,6-triol N-177



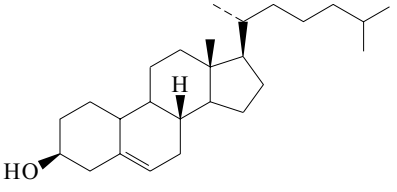
$C_{26}H_{44}O_3$ 404.632

(2β,3α,5α,6α)-*form*

Tri-O-*sulfate:* ***Halistanol sulfate B***
[143049-13-2]
$C_{26}H_{44}O_{12}S_3$ 644.824
Constit. of an *Epipolasis* sp. Thrombin inhibitor. $[\alpha]_D^{21}$ +11.4 (c, 1 in MeOH).

Kanazawa, S. *et al., Tetrahedron*, 1992, **48**, 5467-5472 (*isol, pmr, cmr*)
Makarieva, T.N. *et al., Steroids*, 1995, **60**, 316-320 (*isol, pmr, cmr, ms*)

19-Norcholest-5-en-3-ol N-178



$C_{26}H_{44}O$ 372.633

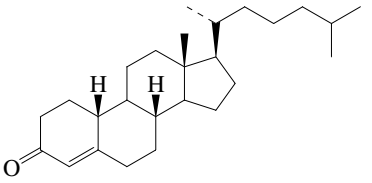
3β-*form*

19-Norcholesterol
[2137-16-8]
Constit. of *Pseudoplexaura porosa*.

Popov, S. *et al., Tet. Lett.*, 1976, 3491

19-Norcholest-4-en-3-one N-179

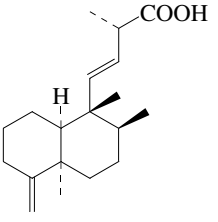
[3404-22-6]



$C_{26}H_{42}O$ 370.617
Isol. from the gorgonian *Muricea californica*.
$[\alpha]_D^{26}$ +44.2 (c, 1.05 in $CHCl_3$). λ_{max} 240 (ϵ 14000) (MeOH).

Akhtar, M. *et al., J.A.C.S.*, 1962, **84**, 1496 (*synth*)
Popov, S. *et al., Steroids*, 1983, **41**, 537-548 (*isol*)

15-Nor-4(18),11-clerodadien-14-oic acid N-180



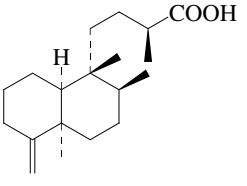
$C_{19}H_{30}O_2$ 290.445

(5α,11*E*,13*S*)-*form*

Sigmosceptrin B
[204980-40-5]
Isol. from the marine sponge *Sigmosceptrella* sp.
Cryst. (as Me ester).
Mp 72-74° (Me ester). $[\alpha]_D$ -1.7 (c, 2.4 in $CHCl_3$) (Me ester). λ_{max} 245 (ϵ 52000) ($CHCl_3$) (Me ester).

Bassett, S. *et al., Aust. J. Chem.*, 1997, **50**, 1137-1143 (*isol, pmr, cmr, ms, cryst struct*)

15-Nor-4(18)-cleroden-14-oic acid N-181



$C_{19}H_{32}O_2$ 292.461

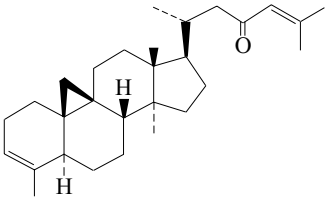
(5α,13*S*)-*form*

Sigmosceptrin C
[204921-12-0]
Isol. from the marine sponge *Sigmosceptrella* sp.
Yellow oil (as Me ester). $[\alpha]_D$ +9.5 (c, 0.5 in $CHCl_3$) (Me ester).
λ_{max} 235 (ϵ 3255); 270 (ϵ 26040) ($CHCl_3$) (Me ester).

Bassett, S. *et al., Aust. J. Chem.*, 1997, **50**, 1137-1143 (*isol, pmr, cmr*)

29-Norcycloarta-3,24-dien-23-one N-182

[84323-27-3]



$C_{29}H_{44}O$ 408.666
Constit. of green alga *Tydemania expeditionitis*.
$[\alpha]_D$ +5.6 (c, 1.0 in $CHCl_3$).

24,25-Dihydro: ***29-Norcycloart-3-en-23-one***
[84323-28-4]
$C_{29}H_{46}O$ 410.682
Constit. of *Tydemania expeditionitis*.
$[\alpha]_D$ +16.1 (c, 1.4 in $CHCl_3$).

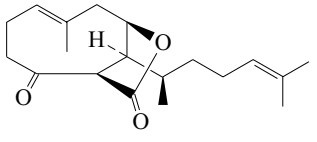
24,25-Dihydro, 23ξ-alcohol: ***29-Norcycloart-3-en-23-ol***
$C_{29}H_{48}O$ 412.698
Isol. from *Tydemania expeditionitis*.

Tetrahydro: ***29-Norcycloart-3-en-23-ol***
[84323-29-5]
$C_{29}H_{48}O$ 412.698
Constit. of *Tydemania expeditionitis*.
$[\alpha]_D$ +12.6 (c, 1.7 in $CHCl_3$).

Paul, V.J. *et al., Tet. Lett.*, 1982, **23**, 3459 (*isol, cryst struct*)
Wright, A.D. *et al., J. Nat. Prod.*, 1990, **53**, 845-861 (*isol*)

Nordictyotalide N-183

[116406-18-9]

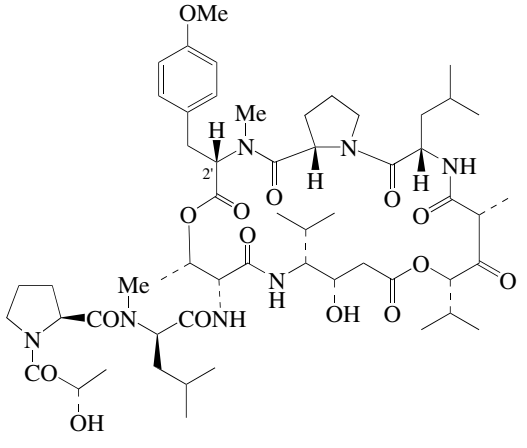


$C_{19}H_{28}O_3$ 304.428
Constit. of *Dictyota dichotoma*. Oil. Sol. MeOH, hexane; poorly sol. H_2O. $[\alpha]_D$ -31 (c, 0.43 in $CHCl_3$).

Ishitsuki, M.O. *et al., J.O.C.*, 1988, **53**, 5010 (*isol, pmr, cmr*)

Nordidemnin B N-184

[117710-03-9]



$C_{56}H_{87}N_7O_{15}$ 1098.341

C-Demethyl analogue of Didemnin B, D-399. Constit. of the sea tunicates *Tridemnum cyanophorum* and *Tridemnum solidum*. Cytotoxic. Cryst. (Et_2O/hexane). λ_{max} 225 (ϵ 6600); 277 (ϵ 2190); 283 (ϵ 1900) (MeOH).

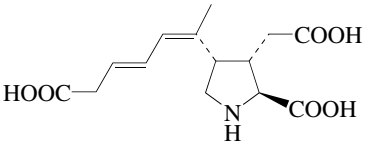
$N^{2'}$,O-*Di-de-Me:* ***Nordidemnin N***
[155608-53-0]
$C_{54}H_{83}N_7O_{15}$ 1070.288
Isol. from *Tridemnum solidum*. Powder.
Mp 154-156°. $[\alpha]_D^{24}$ -49 (c, 1.6 in $CHCl_3$). λ_{max} 224 (sh) (ϵ 10960); 277 (ϵ 1590) (MeOH).

N-*De(lactylprolyl):* ***Nordidemnin A***
[141344-11-8]
$C_{48}H_{76}N_6O_{12}$ 929.161
Isol. from *Tridemnum solidum*.

Jouin, P. *et al., J.O.C.*, 1989, **54**, 617 (*synth*)
McKee, T.C. *et al., Tet. Lett.*, 1989, **30**, 3053-3056 (*isol, struct*)
Sakai, R. *et al., J.A.C.S.*, 1995, **117**, 3734-3748; 8885 (*Nordidemnin N, Nordidemnin A*)

Nordomoic acid N-185

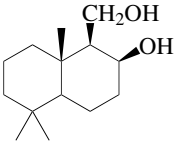
2-Carboxy-4-(5-carboxy-1-methyl-1,3-pentadienyl)pyrrolidineacetic acid, 9CI
[101899-43-8]



$C_{14}H_{19}NO_6$ 297.307
Constit. of the red alga *Chondria armata*. Insecticidal agent.

Maeda, M. *et al., CA*, 1986, **104**, 183260t (*isol*)

12-Nor-8,11-drimanediol N-186



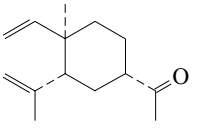
$C_{14}H_{26}O_2$ 226.358

8β-*form*
Di-Ac: [198423-25-5]
$C_{18}H_{30}O_4$ 310.433
Constit. of a *Dysidea* sp. Solid.
Mp 84-85°. $[\alpha]_D^{25}$ +36 (c, 0.2 in MeOH).

Paul, V.J. *et al., J. Nat. Prod.*, 1997, **60**, 1115-1120 (*isol, pmr, cmr*)

13-Nor-1,3-elemadien-11-one N-187

Lobocalone
[147731-93-9]

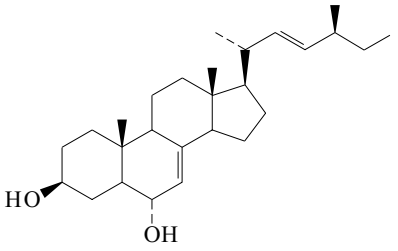


$C_{14}H_{22}O$ 206.327
Constit. of *Lobophytum* spp. Oil. $[\alpha]_D$ +16 (c, 0.5 in $CHCl_3$).

Su, J.-Y. *et al., J. Nat. Prod.*, 1993, **56**, 279 (*isol, pmr, cmr*)
Raju, B.L. *et al., J. Nat. Prod.*, 1993, **56**, 961 (*isol, pmr, cmr*)

27-Norergosta-7,22-diene-3,6-diol N-188

24-Methyl-27-norcholesta-7,22-diene-3,6-diol

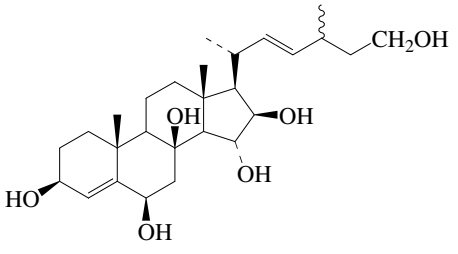


$C_{27}H_{44}O_2$ 400.643

(3β,5α,6α,22*E*24*S*)-*form*

Constit. of *Spongionella gracilis*.
Cryst. (MeOH/petrol).
Mp 185-187°.
Madaio, A. *et al., J. Nat. Prod.*, 1989, **52**, 952 (*isol, pmr*)

27-Norergosta-4,22-diene-3,6,8,15,16,26-hexol N-189

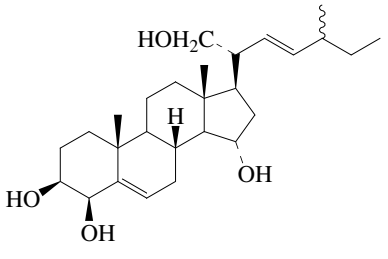


$C_{27}H_{44}O_6$ 464.641

(3β,6β,8β,15α,16β,22*E*,24ξ)-*form*

3-O-*(2,3-Di*-O-*methyl-β-*D*-xylopyranoside)*: ***Leviusculoside J***
[876726-96-4]
$C_{34}H_{56}O_{10}$ 624.81
Constit. of *Henricia leviuscula*. Amorph. powder. $[\alpha]_D$ -12 (c, 0.1 in MeOH).
Ivanchina, N.V. *et al., J. Nat. Prod.*, 2006, **69**, 224-228 (*Leviusculoside J*)

27-Norergosta-5,22-diene-3,4,15,21-tetrol N-190



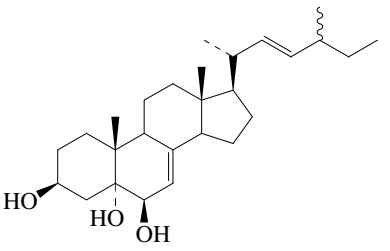
$C_{27}H_{44}O_4$ 432.642

(3β,4β,15α,22*E*)-*form*

3-O-*[β-*D*-Galactopyranosyl-(1→2)-α-*L*-arabinopyranosyl-(1→3)-[β-*D*-galactopyranosyl-(1→4)]-β-*D*-glucopyranoside]*: ***Mycaloside B***
[593280-51-4]
$C_{50}H_{82}O_{23}$ 1051.184
Constit. of *Mycale laxissima*. Solid.
Mp 218-222°. $[\alpha]_D^{25}$ -27.8 (c, 0.8 in MeOH).
Antonov, A.S. *et al., J. Nat. Prod.*, 2003, **66**, 1082-1088 (*isol, pmr, cmr*)

27-Norergosta-7,22-diene-3,5,6-triol N-191

24-Methyl-27-norcholesta-7,22-diene-3,5,6-triol



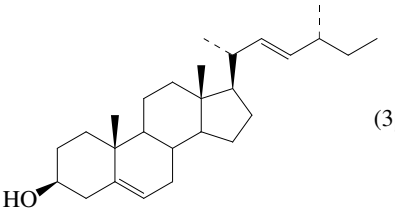
$C_{27}H_{44}O_3$ 416.643

(3β,5α,6β,22*E*,24ξ)-*form* [112058-03-4]

Constit. of *Heliometra gracialis maxima* and the sponge *Spongionella gracilis*.
Cryst. (MeOH).
Mp 235-237°.
Piccialli, V. *et al., J. Nat. Prod.*, 1987, **50**, 915-920 (*isol, pmr*)
Shubina, L.K. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **119**, 505-511 (*isol*)

27-Norergosta-5,22-dien-3-ol N-192

24-Methyl-27-norcholesta-5,22-dien-3-ol



(3β,22*E*,24*R*)-*form*

$C_{27}H_{44}O$ 384.644

(3β,22*E*,24*R*)-*form*

24-Epioccelasterol
[64783-84-2]
Constit. of a dinoflagellate symbiont of *Orbulina universa*.

(3β,22*E*,24*S*)-*form*

Occelasterol
[54278-89-6]
Constit. of *Pseudopotamilla occelata*, *Patinopecten yessoensis*, *Bugula neritina*, *Esperiopsis edwardii*, *Lephogorgia subcomressa*, *Mactra chinensis*, *Aulacomya ater*, *Pseudostichopus trachus* and many other marine organisms.
Cryst.
Mp 128.5-129.5°. $[\alpha]_D$ -43.

3-O-*Sulfate:* [140245-74-5]
[152005-12-4]
$C_{27}H_{44}O_4S$ 464.708
Constit. of *Gymnocrinus richeri*, *Eupentacta fraudatrix* and *Ophioderma longicaudum*.

Ac:
Cryst. (MeOH). Mp 138-141°. $[\alpha]_D$ -47 (c, 0.32).

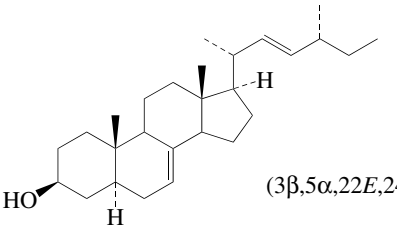
Me ether: 3-Methoxy-27-norergosta-5,22-diene. 3-Methoxy-24-methyl-27-norcholesta-5,22-diene
[139765-27-8]
$C_{28}H_{46}O$ 398.671
Constit. of *Jereicopsis graphidiophora*.

Kobayashi, M. *et al., Steroids*, 1974, **24**, 399-410; 1975, **26**, 605 (*Occelasterol, isol*)
Romero, M.S. *et al., J. Nat. Prod.*, 1983, **46**, 588-590 (*occur*)
Romero, M.S. *et al., Lipids*, 1983, **18**, 510-590 (*occur*)
Rovirosa, J. *et al., Lipids*, 1983, **18**, 570-572 (*occur*)
Riccio, R. *et al., Tetrahedron*, 1985, **41**, 6041-6046 (*occur, sulfate*)
Kokke, W.C.M.C. *et al., Biochem. Syst. Ecol.*, 1987, **15**, 475-478, (*24-Epioccelasterol*)

Seldes, A.M. *et al., Tetrahedron*, 1988, **44**, 1359-1362 (*occur*)
De Riccardis, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **100**, 647-651 (*sulfate, occur*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*Me ether*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*occur*)
Kerr, R.G. *et al., J. Nat. Prod.*, 1999, **62**, 468-470 (*Bugula neritina constit*)

27-Norergosta-7,22-dien-3-ol N-193

24-Methyl-27-norcholesta-7,22-dien-3-ol. 27-Norcampesta-7,22-dien-3-ol



(3β,5α,22*E*,24*R*)-*form*

$C_{27}H_{44}O$ 384.644

(3β,5α,22*E*,24*R*)-*form* [69977-27-1]
Constit. of *Holothuria nobilis* and *Agelas schmidt*.
3-O-*Sulfate:* [151891-05-3]
$C_{27}H_{44}O_4S$ 464.708
Constit. of *Eupentacta fraudatrix*.
3-O-*β-D-Xylopyranoside:* [151890-87-8]
$C_{32}H_{52}O_5$ 516.76
Constit. of *Eupentacta fraudatrix*.

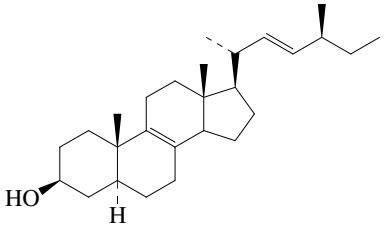
(3β,5α,22*E*,24*S*)-*form*
Amuresterol
[54848-29-2]
Constit. of *Asterias amurensis, Axinella cannabina* and other sponges.
Cryst. (MeOH).
Mp 151-152°. $[\alpha]_D$ +4 (c, 1.2 in $CHCl_3$).

[81275-81-2, 96149-83-6, 102778-12-1]

Kobayashi, M. *et al., Tetrahedron*, 1974, **30**, 2147-2150 (*isol*)
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol*)
Bergquist, P.R. *et al., Biochem. Syst. Ecol.*, 1986, **14**, 105 (*isol*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Duque, C. *et al., CA*, 1995, **122**, 235561 (*24ξ-form, isol*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*3β,5α,22E,24ξ-form, occur*)

27-Norergosta-8,22-dien-3-ol N-194

24-Methyl-27-norcholesta-8,22-dien-3-ol

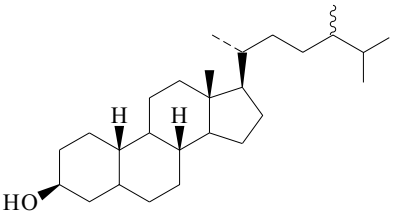


$C_{27}H_{44}O$ 384.644

(3β,5α,22*E*,24*S*)-*form* [85733-79-5]
Constit. of the sponge *Axinella cannabina*.
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol, pmr, ms*)

19-Norergostan-3-ol N-195

24-Methyl-19-norcholestan-3-ol



$C_{27}H_{48}O$ 388.676

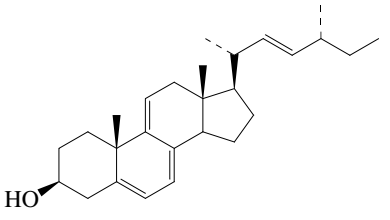
(3β,5α,24ξ)-*form* [54602-16-3]
Constit. of *Axinella polypoides*.
Ac: [54602-11-8]
Cryst. (MeOH). Mp 89-90°.

[54656-23-4]

Minale, L. *et al., J.C.S. Perkin 1*, 1974, 1888

27-Norergosta-5,7,9(11),22-tetraen-3-ol N-196

24-Methyl-27-norcholesta-5,7,9(11),22-tetraen-3-ol



(3β,22*E*,24*R*)-*form*

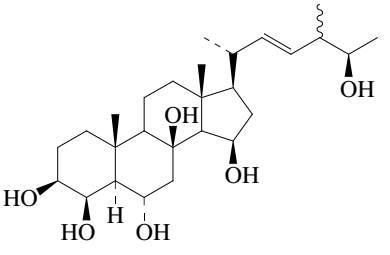
$C_{27}H_{40}O$ 380.612

(3β,22*E*,24*R*)-*form* [85761-57-5]
Constit. of the sponge *Axinella cannabina*.
9,11-Dihydro: 27-Norergosta-5,7,22-trien-3-ol. 24-Methyl-27-norcholesta-5,7,22-trien-3-ol
[85761-60-0]
$C_{27}H_{42}O$ 382.628
Constit. of *Axinella cannabina*.

(3β,22*E*,24*S*)-*form* [85733-69-3]
Constit. of *Axinella cannabina*. λ_{max} 312; 324; 338 (EtOH).
9,11-Dihydro: [85733-76-2]
Constit. of *Axinella cannabina*. λ_{max} 262; 271; 281; 293 (EtOH).
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol, pmr, ms*)

27-Norergost-22-ene-3,4,6,8,15,25-hexol N-197

24-Methyl-27-norcholest-22-ene-3,4,6,8,15,25-hexol

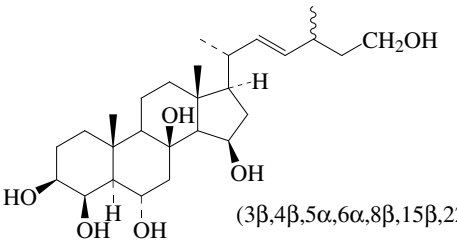


$C_{27}H_{46}O_6$ 466.657

(3β,4β,5α,6α,8β,15β,22*E*,24ξ,25*R*)-*form*
Certonardosterol A₄
[781646-86-4]
Constit. of *Certonardoa semiregularis*. Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 1654-1660 (*isol, pmr, cmr*)

27-Norergost-22-ene-3,4,6,8,15,26-hexol N-198

24-Methyl-27-norcholest-22-ene-3,4,6,8,15,26-hexol



(3β,4β,5α,6α,8β,15β,22*E*,24ξ)-*form*

$C_{27}H_{46}O_6$ 466.657

(3β,4β,5α,6α,8β,15β,22*E*,24ξ)-*form*

26-O-[2-O-Methyl-β-D-xylopyranosyl-(1→2)-β-D-xylopyranoside]: ***Placentoside A***

[112058-00-1]

$C_{38}H_{64}O_{14}$ 744.915

Constit. of *Sphaerodiscus placenta*. $[\alpha]_D$ -3 (c, 0.3 in MeOH).

(3β,4ξ,5α,6α,8β,15β,22*E*,24ξ)-*form*

Certonardosterol K

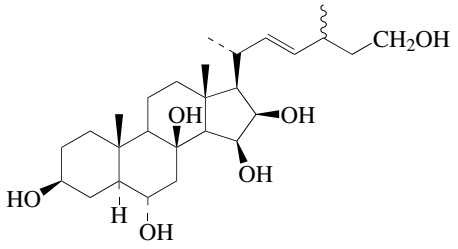
[517900-59-3]

Constit. of *Certonardoa semiregularis.*

Zollo, F. *et al., J. Nat. Prod.*, 1987, **50**, 794-799 (*Placentoside A*)
Wang, W. *et al., J. Nat. Prod.*, 2003, **66**, 384-391 (*Certonardosterol K*)

27-Norergost-22-ene-3,6,8,15,16,26-hexol N-199

24-Methyl-27-norcholest-22-ene-3,6,8,15,16,26-hexol



$C_{27}H_{46}O_6$ 466.657

(3β,5α,6α,15β,16β,22*E*,24ξ)-*form*

26-O-(4-O-Sulfo-β-D-glucopyranoside): ***Coscinasteroside D***

[105377-95-5 (Na salt)]

$C_{33}H_{56}O_{14}S$ 708.863

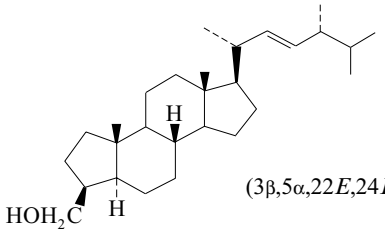
Constit. of *Coscinasterias tenuispina.*

$[\alpha]_D$ +11.6 (MeOH) (as Na salt).

Riccio, R. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 869-893 (*isol, pmr, cmr, ms*)

A-Norergost-22-ene-3-methanol, 9CI N-200

3-Hydroxymethyl-24-methyl-A-norcholest-22-ene. 3-Hydroxymethyl-A-norergost-22-ene



(3β,5α,22*E*,24*R*)–*form*

$C_{28}H_{48}O$ 400.687

(3β,5α,22*E*,24*R*)-*form* [55081-41-9]

[55081475- A-c]

Constit. of sponges *Axinella verrucosa* and *Hymeniacidon aldis.*

Cryst. (MeOH) (as Ac).

Mp 104-105° (Ac). $[\alpha]_D^{17}$ +33 (c, 0.1 in $CHCl_3$) (Ac).

(3β,5α,22*E*,24*S*)-*form* [83709-56-2]

Constit. of the sponges *Acanthella aurantiaca* and *Homaxinella trachys.*

(3β,5α,22*Z*,24*R*)-*form*

Constit. of *Pseudaxinyssa cantharella*.

Cryst. ($CHCl_3$).

Mp 156-158°. $[\alpha]_D^{20}$ +3.1 (c, 0.32 in $CHCl_3$).

(3β,5α,22*Z*,24*S*)-*form*

3β-Hydroxymethyl-A-nor-5α-campest-22Z-ene

[100992-91-4]

Constit. of sponge *Pseudaxinyssa cantharella*.

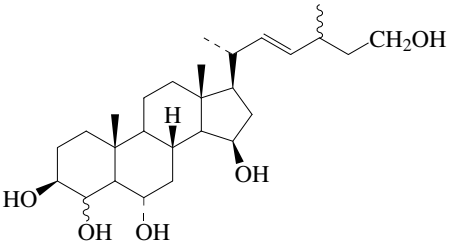
Cryst. ($CHCl_3$).

Mp 152-154°. $[\alpha]_D^{20}$ +25 (c, 0.12 in $CHCl_3$).

[100992-90-3]

Minale, L. *et al., J.C.S. Perkin 1*, 1974, 2380 (*isol*)
Eggersdorfer, M.L. *et al., J.O.C.*, 1982, **47**, 5304-5309 (*isol*)
Bohlin, L. *et al., J.O.C.*, 1982, **47**, 5309-5314 (*isol*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2321 (*isol*)
De Nanteuil, G. *et al., Tetrahedron*, 1985, **41**, 6035 (*isol*)

27-Norergost-22-ene-3,4,6,15,26-pentol N-201



$C_{27}H_{46}O_5$ 450.657

(3β,4ξ,5α,6α,15β,22*E*,24ξ)-*form*

Certonardosterol L

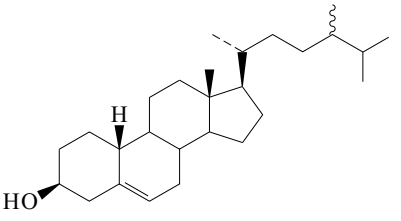
[517900-60-6]

Constit. of *Certonardoa semiregularis.*

Wang, W. *et al., J. Nat. Prod.*, 2003, **66**, 384-391 (*isol, pmr, cmr*)

19-Norergost-5-en-3-ol N-202

24-Methyl-19-norcholest-5-en-3-ol



$C_{27}H_{46}O$ 386.66

(3β,24ξ)-*form*

24-Methyl-19-norcholesterol

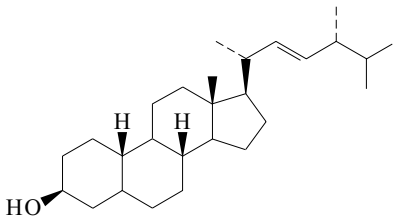
[61843-79-6]

Constit. of *Pseudoplexaura porosa*.

Popov, S. *et al., Tet. Lett.*, 1976, 3491

19-Norergost-22-en-3-ol N-203

24-Methyl-19-norcholest-22-en-3-ol



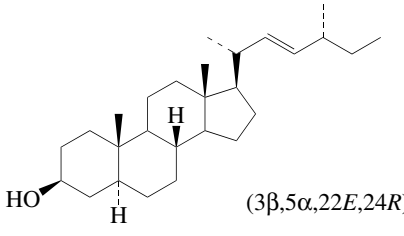
$C_{27}H_{46}O$ 386.66

(3β,5α,22*E*)-*form* [54602-14-1]
Constit. of *Axinella polypoides*.
Ac: [54602-04-9]
Cryst. (MeOH). Mp 112-113°. $[\alpha]_D$ +16.3 (c, 1.2 in $CHCl_3$).

(3β,5α,22*E*,24*S*)-*form*
19-Norcampest-22-en-3-ol
[90081-28-0]
From *Axinella polypoides*.
Minale, L. *et al., J.C.S. Perkin 1*, 1974, 1888 (*isol*)
Crist, B.V. *et al., Steroids*, 1983, **42**, 331 (*isol*)

27-Norergost-22-en-3-ol N-204

24-Methyl-27-norcholest-22-en-3-ol. 27-Norcampest-22-en-3-ol



(3β,5α,22*E*,24*R*)-*form*

$C_{27}H_{46}O$ 386.66

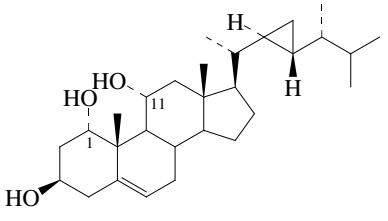
(3β,5α,22*E*,24*R*)-*form*
3-O-*Sulfate:* [151891-00-8]
$C_{27}H_{46}O_4S$ 466.724
Constit. of *Eupentacta fraudatrix*.

(3β,5α,22*E*,24*S*)-*form*
Patinosterol
[58514-32-2]
Constit. of *Patinopecten yessoensis*. Cryst. Mp 132-133°.

(3β,5α,22*E*,24ξ)-*form* [65908-46-5]
Constit. of *Bathyplotes natans* and *Holothuria nobilis*.
Kobayashi, M. *et al., Steroids*, 1975, **26**, 605-624; 1977, **29**, 823-826 (*isol, struct, synth*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*sulfate*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*3β,5α,22E,24ξ-form, occur*)

33-Norgorgost-5-ene-1,3,11-triol N-205

23-Demethylgorgost-5-ene-1,3,11-triol

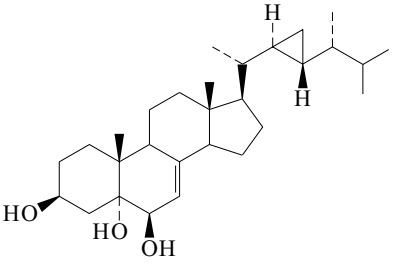


$C_{29}H_{48}O_3$ 444.696

(1α,3β,11α)-*form*
1,11-Dihydroxy-23-demethylgorgosterol
[95513-64-7]
From *Sinularia dissecta*.
5β,6β-Epoxide, 1-ketone, 11-Ac: ***11-Acetoxy-5,6-epoxy-3,11-dihydroxy-23-norgorgostan-1-one***
[180001-22-3]
$C_{31}H_{48}O_5$ 500.717
Constit. of *Clavularia viridis*. Viscous oil. $[\alpha]_D$ -87.3 (c, 0.055 in $CHCl_3$).
Jagodzinska, B.M. *et al., J.O.C.*, 1985, **50**, 1435 (*isol, ms, pmr*)
Watanabe, K. *et al., Steroids*, 1996, **61**, 439 (*deriv*)

33-Norgorgost-7-ene-3,5,6-triol N-206

23-Demethylgorgost-7-ene-3,5,6-triol

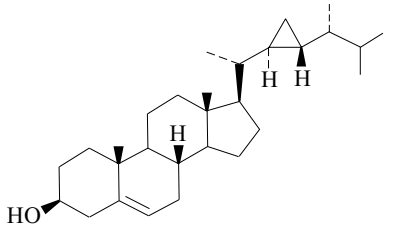


$C_{29}H_{48}O_3$ 444.696

(3β,5α,6β,22*R*,23*R*,24*R*)-*form* [147170-08-9]
Constit. of *Sinularia* sp.
Needles.
Mp 229-232°. $[\alpha]_D$ -45 (c, 2.18 in Py).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1993, **41**, 87 (*isol, pmr, cmr*)

33-Norgorgost-5-en-3-ol N-207

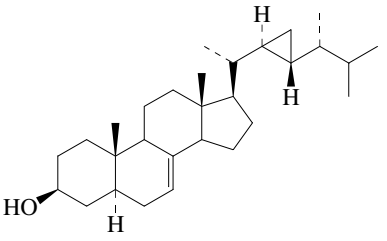
24-Methyl-22,23-methylenecholest-5-en-ol. 23-Demethylgorgosterol
[29939-97-7]



$C_{29}H_{48}O$ 412.698
Constit. of *Gorgonia flabellum*, *Gorgonia ventalina*, *Tridacna gigas* and other marine organisms. Synth. by an aposymbiotic dinoflagellate. Cryst.
Mp 162-163°. $[\alpha]_D^{21}$ -34.5 ($CHCl_3$).
Schmitz, F.J. *et al., J.A.C.S.*, 1970, **92**, 6073 (*isol*)
Hsu, I.-N. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1973, **92**, 1134 (*cryst struct*)
Anderson, G.D. *et al., J.A.C.S.*, 1975, **97**, 388 (*synth*)
Popov, S. *et al., Steroids*, 1976, **28**, 699 (*isol*)
Kobayashi, M. *et al., Steroids*, 1979, **34**, 273 (*isol*)
Blanc, P.A. *et al., J.A.C.S.*, 1980, **102**, 7113 (*isol, pmr*)
Sato, S. *et al., Chem. Pharm. Bull.*, 1981, **29**, 406 (*synth*)
Withers, N.W. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1982, **79**, 3764 (*isol, synth*)

33-Norgorgost-7-en-3-ol N-208

23-Demethylgorgost-7-en-3-ol. 22,23-Methyleneergost-7-en-3-ol. 24-Methyl-22,23-methylenecholest-7-en-3-ol

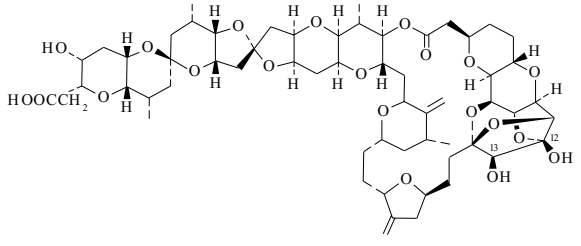


$C_{29}H_{48}O$ 412.698

(3β,5α,24*R*)-*form*
23-Demethylacanthasterol
[75479-11-7]
Constit. of *Acanthaster planci*.
Sato, S. *et al., Steroids*, 1980, **36**, 65-71 (*isol, synth, ms*)

Norhalichondrin A N-209

[97316-00-2]



$C_{59}H_{82}O_{21}$ 1127.284
Polyether-macrolide antibiotic. Isol. from marine sponge *Halichondria okadai*. Antitumour agent. Sol. MeOH, EtOH; poorly sol. H_2O. $[\alpha]_D$ -47.8 (c, 1.13 in MeOH).

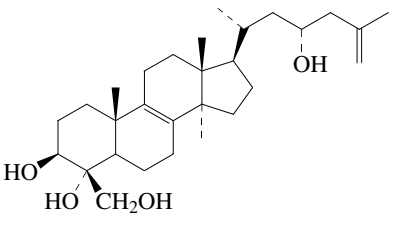
p-*Bromophenacyl ester:*
Cryst. (Me_2CO/MeOH). Mp 173.5-175°.

12,13-Dideoxy: ***Norhalichondrin B***
[101365-29-1]
$C_{59}H_{82}O_{19}$ 1095.285
Isol. from *Halichondria okadai*. Sol. MeOH, Py, butanol; poorly sol. H_2O.

13-Deoxy: ***Norhalichondrin C***
[101365-28-0]
$C_{59}H_{82}O_{20}$ 1111.285
Isol. from *Halichondria okadai*. Sol. MeOH, Py, butanol; poorly sol. H_2O.

Uemura, D. *et al., J.A.C.S.*, 1985, **107**, 4796 (*isol, cryst struct*)
Hirata, Y. *et al., Pure Appl. Chem.*, 1986, **58**, 701 (*isol*)
Aicher, T.D. *et al., J.A.C.S.*, 1992, **114**, 3162 (*synth*)

28-Norlanosta-8,25-diene-3,4,23,29-tetrol N-210



$C_{29}H_{48}O_4$ 460.696

(3β,4α,5α,23*R*)-*form* [346577-15-9]
Oil. $[\alpha]_D^{25}$ -4 (c, 0.01 in MeOH).

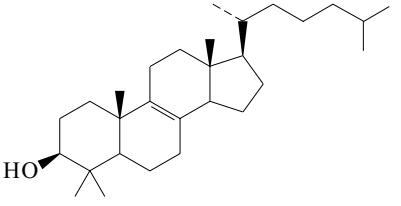
3-O-[α-L-Rhamnopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→3)-α-L-rhamnopyranosyl-(1→2)]-β-D-glucopyranoside]: ***Feroxoside A***
[346597-25-9]
$C_{53}H_{88}O_{22}$ 1077.265
Constit. of *Ectyoplasia ferox*. Amorph. solid. $[\alpha]_D^{25}$ -16 (c, 0.05 in MeOH).

25,26-Dihydro: 28-Norlanost-8-ene-3,4,23,29-tetrol
$C_{29}H_{50}O_4$ 462.712

25,26-Dihydro, 3-O-[α-L-rhamnopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→3)-α-L-rhamnopyranosyl-(1→2)]-β-D-glucopyranoside]: ***Feroxoside B***
[346596-80-3]
$C_{53}H_{90}O_{22}$ 1079.281
Constit. of *Ectyoplasia ferox*. Amorph. solid. $[\alpha]_D^{25}$ -25 (c, 0.02 in MeOH).

Campagnuolo, C. *et al., Tetrahedron*, 2001, **57**, 4049-4055 (*isol, pmr, cmr*)

30-Norlanost-8-en-3-ol N-211

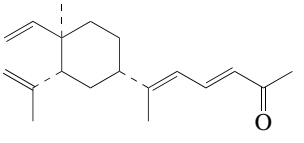


$C_{29}H_{50}O$ 414.713

3β-*form* [5241-24-7]
Constit. of *Pseudoceratina crassa*.
$[\alpha]_D^{25}$ +31.7 (MeOH).
Albrizio, S. *et al., Tetrahedron*, 1994, **50**, 783 (*isol, pmr, cmr*)

19-Norloba-8,10,13(15),16-tetraen-18-one N-212

[185223-45-4]

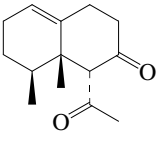


$C_{19}H_{28}O$ 272.43
Constit. of *Lobophytum microlobulatum*. Oil. $[\alpha]_D^{25}$ +12.6 (c, 1.3 in $CHCl_3$).

Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 1294-1303 (*isol, uv, ir, pmr, cmr*)

13-Nor-1(10)-nardosinene-7,11-dione N-213

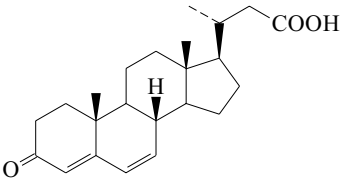
Paralemnolin B
[870152-41-3]



$C_{14}H_{20}O_2$ 220.311
Constit. of *Paralemnalia thyrsoides*. Powder.
Mp 47-49°. $[\alpha]_D^{25}$ -600 (c, 1.46 in $CHCl_3$).

Huang, H.-C. *et al., Tet. Lett.*, 2005, **46**, 7711-7714 (*Paralemnolin B*)

24-Nor-3-oxochola-4,6-dien-23-oic acid N-214



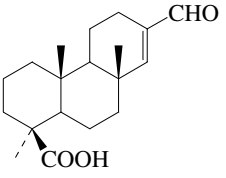
$C_{23}H_{32}O_3$ 356.504
Constit. of *Deltocyathus magnificus*.

Me ester: [180603-65-0]
$[\alpha]_D^{20}$ -10 (c, 0.06 in EtOH).

Guirriero, A. *et al., Helv. Chim. Acta*, 1996, **79**, 982-988 (*isol, pmr, cmr*)

15-Nor-16-oxo-13-isocopalen-19-oic acid N-215

[263746-87-8]

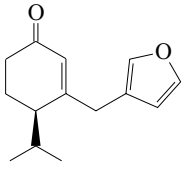


$C_{19}H_{28}O_3$ 304.428
Constit. of *Coscinoderma mathewsi*. Oil. $[\alpha]_D$ -41 (c, 0.029 in MeOH/$CHCl_3$).

Hyosus, M. *et al., J. Nat. Prod.*, 2000, **63**, 422-423 (*isol, pmr, cmr*)

Noroxopenlanfuran N-216

3-(3-Furanylmethyl)-4-(1-methylethyl)-2-cyclohexen-1-one, 9CI



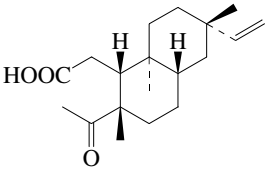
$C_{14}H_{18}O_2$ 218.295

(*R*)-*form* [95653-79-5]
Constit. of *Dysidea fragilis*.
Oil. $[\alpha]_D^{20}$ -91 (c, 0.79 in $CHCl_3$). λ_{max} 236 (ϵ 8200) (MeOH).

Guella, G. *et al., Helv. Chim. Acta*, 1985, **68**, 39-48 (*isol, uv, pmr, cmr, struct*)
Kato, M. *et al., Chem. Comm.*, 1990, 1706 (*synth*)

3-Nor-4-oxo-2,3-seco-15-erythroxylen-2-oic acid N-217

3-Nor-4-oxo-2,3-seco-15-dolabren-2-oic acid



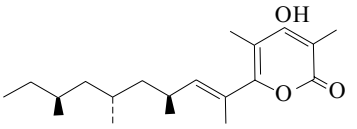
$C_{19}H_{30}O_3$ 306.444

(*ent*-5α)-*form*
Tagalsin H
[862588-86-1]
Constit. of the mangrove *Ceriops tagal*.
Powder.
Mp 101-102°.

Zhang, Y. *et al., Phytochemistry*, 2005, **66**, 1465-1471 (*Tagalsin H*)

Norpectinatone N-218

[90220-12-5]

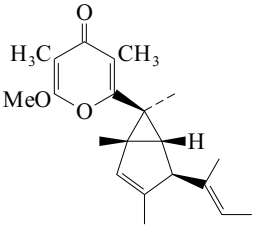


$C_{20}H_{32}O_3$ 320.471
Compd. with the assigned structure has been synthesized and is different from natural norpectinatone. Metab. of *Siphonaria lessoni*. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ +49.2 (c, 2.5 in $CHCl_3$). λ_{max} 232 (ϵ 13100); 300 (ϵ 7600) (EtOH) (Berdy).

Capon, R.J. *et al., J.O.C.*, 1984, **49**, 2506-2508 (*isol*)
Oppolzer, W. *et al., Tet. Lett.*, 1986, **27**, 4713

15-Norphotodeoxytridachione N-219

[153736-12-0]

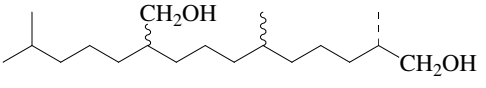


$C_{21}H_{28}O_3$ 328.45
Isol. from the mollusc *Elysia timida*. Ichthyotoxin. $[\alpha]_D^{25}$ +26.5 (c, 0.5 in $CHCl_3$). Similar to Crispatene, C-917. λ_{max} 254 (ϵ 15500) (MeOH) (Berdy).

Gavagnin, M. *et al., J. Nat. Prod.*, 1994, **57**, 298 (*isol, pmr, cmr*)

1-Nor-2,19-phytanediol N-220

2,6-Dimethyl-10-(4-methylpentyl)-1,11-undecanediol



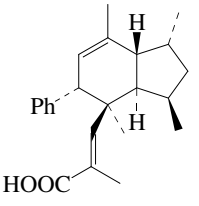
$C_{19}H_{40}O_2$ 300.524

(3*S*,7ξ,11ξ)-*form* [329039-35-2]
Di-O-*sulfate:* [329039-34-1]
$C_{19}H_{40}O_8S_2$ 460.652
Constit. of *Sidnyum turbinatum* and *Ascidia mentula*. Amorph. solid. $[\alpha]_D^{25}$ +5 (c, 0.004 in MeOH).

Aiello, A. *et al., Tetrahedron*, 1997, **53**, 5877-5882 (*Ascidia mentula constit*)
Aiello, A. *et al., J. Nat. Prod.*, 2001, **64**, 219-221 (*Sidnyum turbinatum constit*)

Norplakotenin N-221

[246245-16-9]



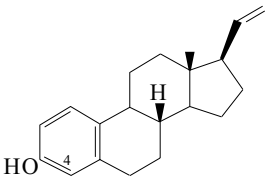
$C_{23}H_{30}O_2$ 338.489

Constit. of *Plakortis lita*. Solid (as Na salt). $[\alpha]_D$ +101 (c, 0.08 in MeOH) (Na salt). λ_{max} 217 (ϵ 14900) (MeOH) (Na salt).

Qureshi, A. *et al., J. Nat. Prod.*, 1999, **62**, 1205-1207 (*isol, pmr, cmr*)

19-Norpregna-1,3,5(10),20-tetraen-3-ol N-222

[97560-70-8]



$C_{20}H_{26}O$ 282.425
Constit. of a *Capnella* sp. Cryst. (petrol).
Mp 115-117°. $[\alpha]_D^{21}$ +126 ($CHCl_3$).

3-O-β-D-Arabinopyranoside: [220428-89-7]
$C_{25}H_{34}O_5$ 414.541
Constit. of *Scleronephthya pallida*. Amorph. solid. $[\alpha]_D^{25}$ +68 (c, 0.18 in MeOH). λ_{max} 207 (log ϵ 4.22); 274 (log ϵ 3.42); 282 (log ϵ 3.22) (MeOH).

3-O-α-L-Fucopyranoside: [220428-87-5]
$C_{26}H_{36}O_5$ 428.567
Constit. of *Scleronephthya pallida*. Amorph. solid. $[\alpha]_D^{25}$ +47 (c, 0.26 in MeOH). λ_{max} 202 (log ϵ 4.2); 274 (log ϵ 3.23); 281 (log ϵ 3.13) (MeOH).

O-*(4-O-Acetyl-β-D-fucopyranoside):* [250144-48-0]
$C_{28}H_{38}O_6$ 470.605
Constit. of *Alcyonium gracillimum*.
$[\alpha]_D^{22}$ -96.5 (c, 0.055 in $CHCl_3$). λ_{max} 215 (ϵ 19000); 222 (ϵ 15000); 229 (ϵ 11000); 274 (ϵ 2100); 283 (ϵ 1500) (MeOH).

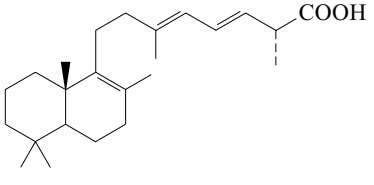
Me ether: ***3-Methoxy-19-norpregna-1,3,5(10),20-tetraene***
[21321-95-9]
$C_{21}H_{28}O$ 296.452
Constit. of *Alcyonium gracillimum*.
$[\alpha]_D^{22}$ +19.9 (c, 0.2 in $CHCl_3$). λ_{max} 222 (ϵ 12000); 278 (ϵ 1700); 287 (ϵ 1500) (MeOH).

4-Hydroxy, 3-Me ether: 3-Methoxy-19-norpregna-1,3,5(10), 20-tetraen-4-ol
$C_{21}H_{28}O_2$ 312.451
Constit. of a *Capnella* sp. Cryst. (petrol).
Mp 130-132°. $[\alpha]_D^{21}$ +57.5 ($CHCl_3$).

Blackman, A.J. *et al., Aust. J. Chem.*, 1985, **38**, 565
Kittakoop, P. *et al., J. Nat. Prod.*, 1999, **62**, 318-320 (*glycosides*)
Tomono, Y. *et al., J. Nat. Prod.*, 1999, **62**, 1538-1541 (*Alcyonium gracillimum constits*)

19-Nor-15-prenyl-8,13,15-labdatrien-18-oic acid N-223

[133883-13-3]



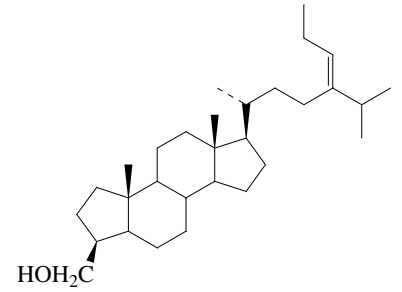
$C_{24}H_{38}O_2$ 358.563
Constit. of *Latrunculia brevis*. Unstable pale yellow oil. $[\alpha]_D$ +14.6 (c, 0.06 in $CHCl_3$).

Me ester: [133883-15-5]
$C_{25}H_{40}O_2$ 372.59
Constit. of *Latrunculia brevis*. Unstable pale yellow oil. $[\alpha]_D$ +13.3 (c, 2.55 in $CHCl_3$).

Butler, M.S. *et al., Aust. J. Chem.*, 1991, **44**, 77 (*isol, pmr, cmr*)

A-Nor-24-propylidenecholestane-3-methanol N-224

*29-Methyl-*A*-norstigmast-24(28)-ene-3-methanol. 3-Hydroxymethyl-*A*-nor-24-propylidenecholestane*



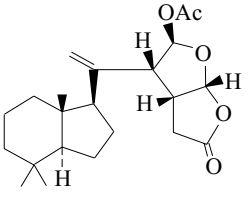
$C_{30}H_{52}O$ 428.74
Tentative identification.

(3β,5α,24*E*)-*form* [90996-23-9]
Isol. from sponge *Acanthella cristagalli*.

Teshima, S. *et al., Nippon Suisan Gakkaishi*, 1984, **50**, 702-712; *CA*, **101**, 52053

Norrisolide N-225

[85066-78-0]



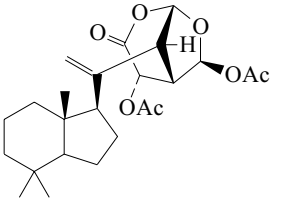
Relative configuration

$C_{22}H_{32}O_5$ 376.492
Constit. of *Chromodoris norrisi*, *Chelonaplysilla violacea*, *Dendrilla* sp., and *Dysidea* spp. Phospholipase A inhibitor. Antiinflammatory and ichtyotoxic agent. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 144.5-146°. $[\alpha]_D$ +1 (c, 1 in $CHCl_3$).

Hochlowski, J.E. *et al., J.O.C.*, 1983, **48**, 1141 (*isol, cryst struct*)
Bobzin, S.C. *et al., J.O.C.*, 1989, **54**, 3902 (*isol*)
Rudi, A. *et al., Tetrahedron*, 1990, **46**, 4019 (*isol*)
Bergquist, P.R. *et al., Aust. J. Chem.*, 1993, **46**, 623 (*isol, pmr, cmr*)
Brady, T.P. *et al., Chem. Eur. J.*, 2005, **11**, 7175-7190 (*synth*)

Norrlandin N-226

[129350-18-1]

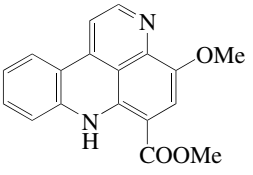


$C_{24}H_{34}O_7$ 434.528
Rearranged spongiane. Constit. of *Dysidea* sp. Oil. $[\alpha]_D$ -5.4 (c, 0.3 in $CHCl_3$).

Rudi, A. *et al., Tetrahedron*, 1990, **46**, 4019 (*isol, struct*)

Norsegoline N-227

[117694-98-1]



$C_{18}H_{14}N_2O_3$ 306.32

Alkaloid from the Red Sea tunicate *Eudistoma* sp. λ_{max} 225 (ϵ 18900); 264 (ϵ 12000); 295 (ϵ 10900); 366 (ϵ 1500); 385 (ϵ 2300); 402 (ϵ 2300); 515 (ϵ 850) (MeOH/HCl) (Derep). λ_{max} 225 (ϵ 17300); 264 (ϵ 12700); 340 (ϵ 3000); 367 (ϵ 1500); 400 (ϵ 2800); 440 (ϵ 1200) (MeOH) (Derep).

Rudi, A. *et al., J.O.C.*, 1989, **54**, 5331 (*isol, uv, ir, pmr, cmr, struct*)
Dunn, S.H. *et al., J.C.S. Perkin 1*, 1993, 879 (*synth*)
Kitahara, Y. *et al., Nat. Prod. Lett.*, 1993, **2**, 159 (*synth*)
Nakahara, S. *et al., Heterocycles*, 2005, **65**, 1925-1929 (*synth*)

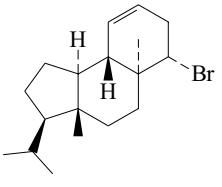
sym-Norspermidine synthase N-228

E.C. 2.5.1.23. S-*Adenosylmethioninamine:1,3-propanediamine 3-aminopropyltransferase*

Enzyme. Isol. from *Euglena gracilis*. Catalyses the reaction of *S*-adenosylmethioninamine with 1,3-propanediamine to give 5′-methylthioadenosine and bis(3-aminopropyl)amine.

Aleksijevic, A. *et al., Biochim. Biophys. Acta*, 1979, **565**, 199-207

Norsphaerol N-229



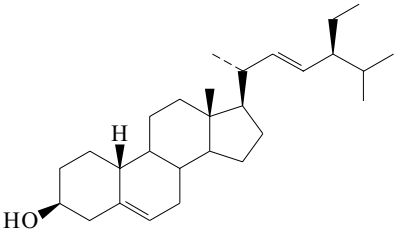
$C_{18}H_{29}Br$ 325.331

Constit. of *Sphaerococcus coronopifolius*. Cryst. Mp 107-109°. $[\alpha]_D$ -39 (c, 0.8 in $CHCl_3$).

Bavaso, A. *et al., Gazz. Chim. Ital.*, 1987, **117**, 87 (*isol, pmr, cmr, cryst struct*)

19-Norstigmasta-5,22-dien-3-ol N-230

24-Ethyl-19-norcholesta-5,22-dien-3-ol. 24-Ethyl-22-dehydro-19-norcholesterol



$C_{28}H_{46}O$ 398.671

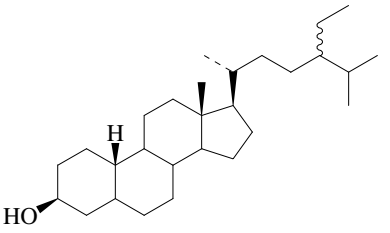
(3β,22*E*,24*S*)-*form* [61843-80-9]

Constit. of *Pseudoplexaura porosa*.

Popov, S. *et al., Tet. Lett.*, 1976, 3491

19-Norstigmastan-3-ol N-231

24-Ethyl-19-norcholestan-3-ol



$C_{28}H_{50}O$ 402.702

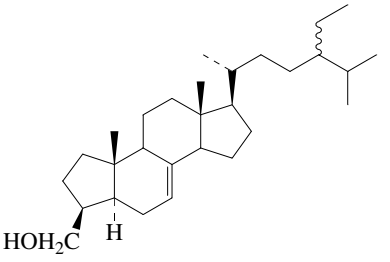
(3β,5α,24ξ)-*form* [54602-17-4]

Constit. of *Axinella polypoides*.

Minale, L. *et al., J.C.S. Perkin 1*, 1974, 1888

A-Norstigmast-7-ene-3-methanol N-232

24-Ethyl-A-*norcholest-7-ene-3-methanol. 3-Hydroxymethyl-24-ethyl*-A-*norcholest-7-ene*



$C_{29}H_{50}O$ 414.713

Tentative identification.

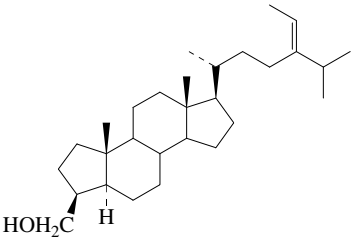
(3β,5α,24ξ)-*form* [90996-24-0]

Isol. from sponge *Acanthella cristagalli*.

Teshima, S. *et al., Nippon Suisan Gakkaishi*, 1984, **50**, 707-712; *CA*, **101**, 52053

A-Norstigmast-24(28)-ene-3-methanol N-233

3-Hydroxymethyl-24-ethylidene-A-*norcholestane*



(3β,5α,24(28)*E*)-*form*

$C_{29}H_{50}O$ 414.713

Tentative identification, not certain that the two isomers here described were both isol.

3β,5α,24(28)*E*-*form* [90996-22-8]

Isol. from sponge *Acanthella cristagalli*.

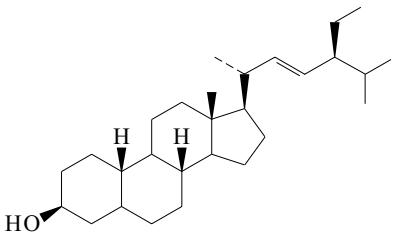
(3β,5α,24(28)*Z*)-*form* [90735-43-6]

Isol. from *Acanthella cristagalli*.

Teshima, S. *et al., Nippon Suisan Gakkaishi*, 1984, **50**, 545; 707-712; *CA*, **101**, 36267; 52053

19-Norstigmast-22-en-3-ol, 9CI N-234

24-Ethyl-19-norcholest-22-en-3-ol



$C_{28}H_{48}O$ 400.687

(3β,22ξ)-*form* [54602-19-6]

Constit. of *Axinella polypoides*.

Ac: [54602-08-3]

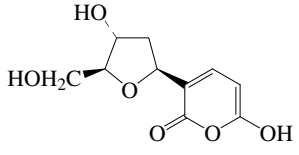
Cryst. (MeOH). Mp 116-117°. $[\alpha]_D$ +7.5 (c, 0.4 in $CHCl_3$).

Minale, L. *et al., J.C.S. Perkin 1*, 1974, 1888

Nortetillapyrone N-235

*3-(2-Deoxy-β-*erythro*-pentofuranosyl)-6-hydroxy-2*H*-pyran-2-one, 9CI*

[363136-44-1]



Relative Configuration

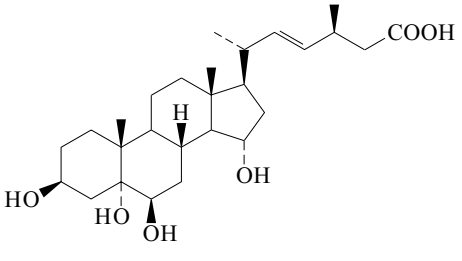
$C_{10}H_{12}O_6$ 228.201

Like Tetillapyrone, T-71, exists as ionic enolate in the solid state, but appears to protonate on C-6 in soln. to give an isomeric struct. Isol. from the sponge *Tetilla japonica*. Gum. $[\alpha]_D^{20}$ +8.6 (c, 0.35 in Me_2CO). λ_{max} 205 (log ϵ 3.5); 262 (log ϵ 3.36) (MeOH).

Watanadilok, R. *et al., J. Nat. Prod.*, 2001, **64**, 1056-1058

27-Nor-3,5,6,15-tetrahydroxyergost-22-en-26-oic acid N-236

24-Methyl-27-nor-3,5,6,15-tetrahydroxycholest-22-en-26-oic acid



$C_{27}H_{44}O_6$ 464.641

(3β,5α,6β,15α,22*E*,24*S*)-*form* [130799-37-0]

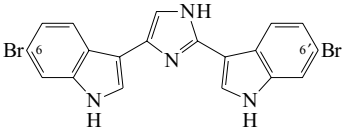
Constit. of *Myxoderma platyacanthum*. $[\alpha]_D$ +18.5 (MeOH).

Finamore, E. *et al., J.O.C.*, 1991, **56**, 1146-1153 (*isol, pmr, cmr*)

Nortopsentin A N-237

*3,3′-(1*H*-Imidazole-2,4-diyl)bis[6-bromo-1*H*-indole], 9CI. 2,4-Bis(6-bromo-3-indolyl)imidazole*

[134029-43-9]



$C_{19}H_{12}Br_2N_4$ 456.139

Alkaloid from the marine sponges *Spongosorites ruetzleri* and *Halichondria* sp. Exhibits cytotoxic and antifungal activities. Oil. λ_{max} 207 (ϵ 50300); 236 (ϵ 42300); 277 (ϵ 26400); 310 (sh) (MeOH) (Derep).

6-Debromo: ***Nortopsentin B***

[134029-44-0]

$C_{19}H_{13}BrN_4$ 377.242

Alkaloid from *Spongosorites ruetzleri* and *Halichondria* sp. Exhibits cytotoxic and antifungal activities. Plates (EtOAc/$CHCl_3$). Dec. at 250-270°. λ_{max} 206 (ϵ 50700); 232 (ϵ 45200); 278 (ϵ 25600); 310 (sh) (MeOH) (Derep).

6′-Debromo: ***Nortopsentin C***

[134029-45-1]

$C_{19}H_{13}BrN_4$ 377.242

Alkaloid from *Spongosorites ruetzleri* and *Halichondria* sp. Exhibits cytotoxic and antifungal activities. Oil. λ_{max} 206 (ϵ 50700); 232 (ϵ 45200); 278 (ϵ 25600); 310 (sh) (MeOH) (Derep). λ_{max} 207 (ϵ 50300); 280 (MeOH) (Berdy).

*6,6′-Bisdebromo: 3,3′-(1*H*-Imidazole-2,4-diyl)bis-1*H*-indole, 9CI.* ***Nortopsentin D***†

[134779-34-3]

$C_{19}H_{14}N_4$ 298.346

Prod. by *Halichondria* sp. λ_{max} 207 (ϵ 50300); 280 (MeOH) (Berdy).

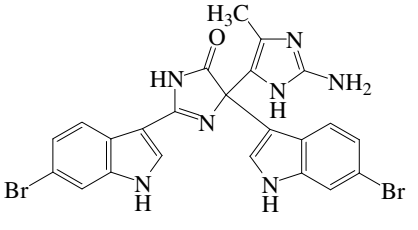
Sun, H.H. *et al., CA*, 1991, **115**, 35701z

Sakemi, S. *et al., J.O.C.*, 1991, **56**, 4304 (*isol, uv, ir, pmr, cmr, ms, struct*)

Kawasaki, I. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1831 (*synth*)

Miyake, F.Y. *et al., Org. Lett.*, 2000, **2**, 2121-2123 (*synth*)

Nortopsentin D† N-238



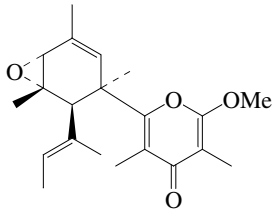
$C_{23}H_{17}Br_2N_7O$ 567.242

Alkaloid from the sponge *Dragmacidon* sp. Amorph. solid. Not to be confused with, 6,6′-Bisdebromo. λ_{max} 276 (ϵ 28000); 294 (ϵ 22000); 360 (ϵ 15400) (MeOH). λ_{max} 276 (ϵ 2800); 334 (ϵ 210000) (MeOH/HCl) (Berdy). λ_{max} 283 (ϵ 28000); 352 (ϵ 6000) (MeOH/NaOH) (Berdy).

Mancini, I. *et al., Helv. Chim. Acta*, 1996, **79**, 2075-2082

15-Nortridachione N-239

[95399-75-0]



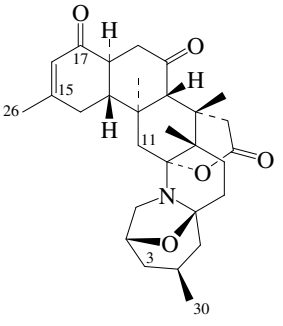
$C_{21}H_{28}O_4$ 344.45
Constit. of *Tridachiella diomedea*.

9,10-Deepoxy, 9,10-didehydro: 9,10-Deoxy-15-nortridachione
[95410-41-6]
$C_{21}H_{28}O_3$ 328.45
Constit. of *Tridachiella diomedea*.

Kay, P.S. *et al., Bol. Soc. Chil. Quim.*, 1984, **29**, 329-332 (*isol, pmr*)

Norzoanthamine N-240

[164991-65-5]



$C_{29}H_{39}NO_5$ 481.631
Alkaloid from the colonial zoanthid *Zoanthus* sp. Cytotoxic agent. Active against osteoporosis. Cryst.
Mp 282-285°. $[\alpha]_D$ +1.6 (c, 1 in $CHCl_3$).

3β-Hydroxy: ***3-Hydroxynorzoanthamine***
$C_{29}H_{39}NO_6$ 497.63
Alkaloid from a zoanthid. Amorph. solid. $[\alpha]_D^{25}$ +12 (c, 0.075 in Et_2O).

11ξ-Hydroxy: ***11-Hydroxynorzoanthamine***
$C_{29}H_{39}NO_6$ 497.63
Alkaloid from a zoanthid. Amorph. solid. $[\alpha]_D^{25}$ -11.5 (c, 0.13 in Et_2O).

11-Oxo: ***Norzoanthaminone***
[164991-66-6]
$C_{29}H_{37}NO_6$ 495.614
Alkaloid from the zoanthid *Zoanthus* sp. Interleukin-6 inhibitor, osteoporosis inhibitor.

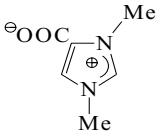
30-Hydroxy: ***30-Hydroxynorzoanthamine***
$C_{29}H_{39}NO_6$ 497.63
Alkaloid from a zoanthid. Amorph. solid. $[\alpha]_D^{25}$ -1.1 (c, 0.27 in $CHCl_3$).

*$\Delta^{15,26}$-Isomer, 17*S*-alcohol:* ***Epinorzoanthamine***
[159509-37-2]
$C_{29}H_{41}NO_5$ 483.647
Alkaloid from *Zoanthus* sp. Misleading name.

Fukuzawa, S. *et al., Heterocycl. Commun.*, 1995, **1**, 207-214 (*isol*)
Kuramoto, M. *et al., Tet. Lett.*, 1997, **38**, 5683-5686 (*pmr, abs config*)
Kuramoto, M. *et al., Bull. Chem. Soc. Jpn.*, 1998, **71**, 771-779 (*isol, deriv*)
Daranas, A.H. *et al., Tetrahedron*, 1999, **55**, 5539-5546 (*Hydroxyzoanthamines*)
Miyashita, M. *et al., Science (Washington, D.C.)*, 2004, **305**, 495-499 (*rev, synth*)

Norzooanemonin N-241

*4-Carboxy-1,3-dimethyl-1*H*-imidazolium hydroxide inner salt, 9CI. 1,3-Dimethyl-4-imidazolecarboxylic acid betaine*
[51800-34-1]



$C_6H_8N_2O_2$ 140.141
Isol. from the sponges *Axinyssa* sp. and *Niphates* sp.; also from the Caribbean gorgonian *Pseudopterogorgia americana* and the hydroid *Tubularia larynx*. Also from *Cacospongia scalaris* and *Astrosclera willeyana*. Cryst. (MeOH/Me_2CO).
Mp 260-263° (250-251°). λ_{max} 212 (ϵ 2005) (MeOH).

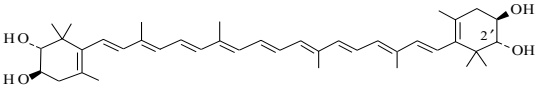
Hydrochloride:
Cryst. (MeOH). Mp 216-219° (213-217°).

Me ester:
$C_7H_{11}N_2O_2^{\oplus}$ 155.176
Isol. from various sponges incl. *Axinyssa* sp., *Axinella* sp., *Echinodictyum* sp. and *Niphates* sp. Counterion not specified.
λ_{max} 264 (MeOH).

Weinheimer, A.J. *et al., Tetrahedron*, 1973, **29**, 3135-3136 (*isol, synth, ir, pmr, ms*)
Gupta, K.C. *et al., Experientia*, 1977, **33**, 1556 (*isol, cryst struct*)
Jahn, T. *et al., Tet. Lett.*, 1997, **38**, 3883-3884 (*isol, pmr, cmr*)
Capon, R.J. *et al., Org. Biomol. Chem.*, 2005, **3**, 118-122 (*Me ester*)

Nostoxanthin N-242

β,β-Carotene-2,2′,3,3′-tetrol
[29307-44-6]
[62837-46-1, 72001-59-3]



$C_{40}H_{56}O_4$ 600.88
Constit. of *Nostoc* spp., *Anacystis nidulans* and *Rhizobium lupini*.

3-O-*Sulfate:* [184849-35-2]
$C_{40}H_{56}O_7S$ 680.944
Isol. from a marine *Flavobacterium* sp. Isol. as Na salt. λ_{max} 458 (ϵ 102500) ($CHCl_3$/MeOH).

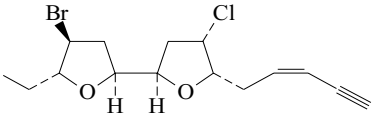
2′-Deoxy: β,β-Carotene-2,3,3′-triol. ***Caloxanthin***
[29267-88-7]
$C_{40}H_{56}O_3$ 584.881
Isol. from *Calothrix* spp. and *Anacystis nidulans*.

2′-Deoxy, 3′-sulfate: ***Caloxanthin 3′-sulfate***
[137813-38-8]
$C_{40}H_{56}O_6S$ 664.945
Isol. from *Erythrobacter longus*. Yellow solid. λ_{max} 344; 450; 475 (MeOH/NH_4OH).

Smallidge, R.L. *et al., Phytochemistry*, 1973, **12**, 2481 (*isol*)
Buchecker, R. *et al., Phytochemistry*, 1976, **15**, 1015
Kleinig, H. *et al., Helv. Chim. Acta*, 1977, **60**, 254 (*isol*)
Takaichi, S. *et al., Phytochemistry*, 1991, **30**, 3411-3415 (*Caloxanthin 3′-sulfate*)
Yokoyama, A. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 1877 (*sulfate*)

Notoryne N-243

[135730-57-3]



$C_{15}H_{20}BrClO_2$ 347.678

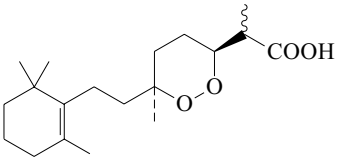
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D$ +40.3 (c, 1.03 in $CHCl_3$).

Kikuchi, H. *et al., Bull. Chem. Soc. Jpn.*, 1991, **64**, 1763,

Nuapapuin A N-244

10,15-Cyclo-4,7-epoxy-1-nor-10-phyten-2-oic acid. Nuapapuanoic acid

[91297-07-3]



$C_{19}H_{32}O_4$ 324.459

The name Nuapapuanoic acid is not used by the authors but they propose the name Nuapapuane for the carbon skeleton. Constit. of a *Sigmosceptrella* sponge.

Me ester: ***Nuapapuin A methyl ester****. Methyl nuapapuanoate*

[90375-60-3]

$C_{20}H_{34}O_4$ 338.486

Constit. of a sponge, *Prianos* sp. Oil. $[\alpha]_D$ +61.7 (c, 0.78 in $CHCl_3$). MF incorr. given as $C_{19}H_{34}O_4$.

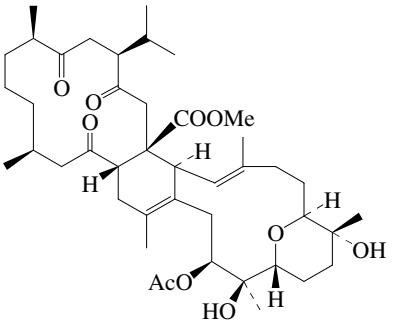
Manes, L.V. *et al., Tet. Lett.*, 1984, **25**, 931

Sperry, S. *et al., J. Nat. Prod.*, 1998, **61**, 241-247 (*cmr*)

Ovenden, S.P.B. *et al., J. Nat. Prod.*, 1999, **62**, 214-218 (*isol, pmr, cmr*)

Nyalolide N-245

[757954-40-8]



$C_{43}H_{66}O_{10}$ 742.988

Constit. of *Sarcophyton glaucum*. Cryst. $[\alpha]_D^{25}$ +98 (c, 0.08 in $CHCl_3$).

Feller, M. *et al., J. Nat. Prod.*, 2004, **67**, 1303-1308 (*isol, pmr, cmr, cryst struct*)

Obelin O-1

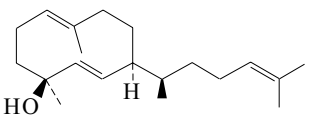
[162572-16-9]

Single chain protein. Isol. from the hydroid *Obelia geniculata*. $Ca^{2\oplus}$-activated photoprotein.

Campbell, A.K. *et al., Biochem. J.*, 1974, **143**, 411-418 (*isol*)
Vysotski, E.S. *et al., Acta Cryst. D*, 1999, **55**, 1965-1966; 2001, **57**, 1919-1921 (*cryst struct*)
Vysotski, E.S. *et al., Acc. Chem. Res.*, 2004, **37**, 405-415 (*rev*)
Liu, Z.-J. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2006, **103**, 2570-2575 (*cryst struct*)

Obscuronatin O-2

[74176-06-0]



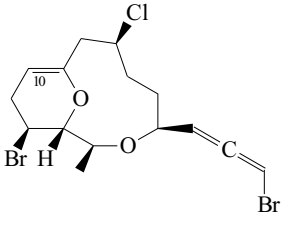
Absolute configuration

$C_{20}H_{34}O$ 290.488
Constit. of coral *Xenia obscuronata* and brown alga *Pachydictyon coriaceum*. Oil. $[\alpha]_D$ -112 (c, 0.49 in $CHCl_3$).

Kashman, Y. *et al., J.O.C.*, 1980, **45**, 3814 (*struct*)
Kodama, M. *et al., Tet. Lett.*, 1984, **25**, 5781 (*synth, rel config*)
Ishitsuka, M. *et al., Tet. Lett.*, 1986, **27**, 2639 (*abs config*)

Obtusallene I O-3

[81920-18-5]



Relative configuration

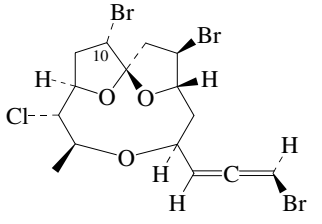
$C_{15}H_{17}Br_2ClO_2$ 424.559
Constit. of *Laurencia obtusa*. Cryst. (Et_2O/petrol).
Mp 165-167°. $[\alpha]_D^{17}$ -257.6 (c, 0.53 in $CHCl_3$).

10-Bromo: ***10-Bromoobtusallene I***
[133883-63-3]
$C_{15}H_{16}Br_3ClO_2$ 503.455
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ -240 (c, 0.19 in $CHCl_3$).

Cox, P.J. *et al., Acta Cryst. B*, 1982, **38**, 1386-1387 (*abs config*)
Cox, P.J. *et al., Tet. Lett.*, 1982, **23**, 579-580 (*cryst struct*)
Oztunc, A. *et al., Tetrahedron*, 1991, **47**, 2273-2276 (*10-Bromoobtusallene I*)

Obtusallene V O-4

1,7,10-Tribromo-13-chloro-4,14:6,9:9,12-triepoxy-1,2-pentadecadiene
[265652-99-1]



Relative Configuration

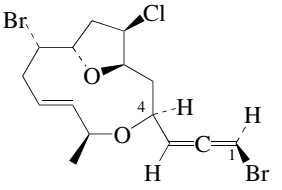
$C_{15}H_{18}Br_3ClO_3$ 521.47
Isol. from *Laurencia obtusa*.
$[\alpha]_D^{20}$ -76 (c, 0.4 in EtOH). λ_{max} 203 (ϵ 14700) (EtOH).

10-Debromo: ***Obtusallene VI***
[265653-05-2]
$C_{15}H_{19}Br_2ClO_3$ 442.574
Isol. from *Laurencia obtusa*.
$[\alpha]_D^{20}$ -80 (c, 0.42 in EtOH). λ_{max} 203 (ϵ 15100) (EtOH).

Guella, G. *et al., Helv. Chim. Acta*, 2000, **83**, 336-348 (*isol, cd, pmr, cmr, ms*)

Obtusallene II O-5

[133485-41-3]



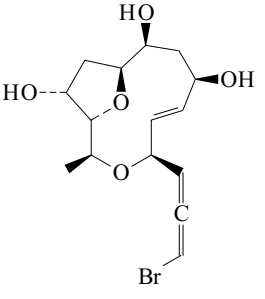
$C_{15}H_{19}Br_2ClO_2$ 426.575
Metab. of *Laurencia obtusa*. Cryst. (hexane/C_6H_6).
Mp 147-149°. $[\alpha]_D^{23}$ -272 (c, 0.35 in $CHCl_3$).

1,4-Diepimer: Dactylallene. ***Obtusallene IV***
$C_{15}H_{19}Br_2ClO_2$ 426.575
Isol. from the mollusc *Aplysia dactylomela* and from *Laurencia obtusa*. Pale yellow cryst. (hexane).
Mp 82-84°. $[\alpha]_D^{20}$ +247 (c, 0.23 in MeOH). λ_{max} 204 (ϵ 21000) (MeOH).

Öztunç, A. *et al., Phytochemistry*, 1991, **30**, 255-257 (*isol, pmr, cmr, ms, cryst struct*)
Guella, G. *et al., Chem. Eur. J.*, 1997, **3**, 1223-1231 (*isol, cd, pmr, cmr, ms*)
Ciavatta, M.L. *et al., Tetrahedron*, 1997, **53**, 17343-17350 (*Dactylallene*)

Obtusallene III O-6

[133462-32-5]

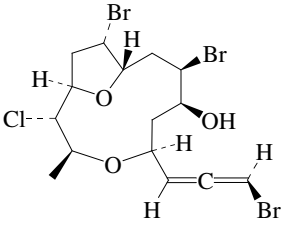


$C_{15}H_{21}BrO_5$ 361.232
Metab. of *Laurencia obtusa*. Cryst. ($CHCl_3$).
Mp 78-80° dec. $[\alpha]_D^{24}$ -141.5 (c, 0.245 in Me_2CO). λ_{max} 204 (ϵ 19600) (MeOH).

Öztunç, A. *et al., Phytochemistry*, 1991, **30**, 255-257 (*isol, pmr, cmr, ms, cryst struct*)
Guella, G. *et al., Chem. Eur. J.*, 1997, **3**, 1223-1231 (*isol, cd, pmr, cmr*)

Obtusallene VII O-7

1,7,10-Tribromo-13-chloro-4,14:9,12-diepoxy-1,2-pentadecadien-6-ol
[265653-10-9]



Relative Configuration

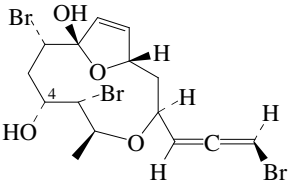
$C_{15}H_{20}Br_3ClO_3$ 523.486

Isol. from *Laurencia obtusa*.
$[\alpha]_D^{20}$ -119 (c, 0.68 in $CHCl_3$).

Guella, G. *et al., Helv. Chim. Acta*, 2000, **83**, 336-348 (*isol, pmr, cmr, ms*)

Obtusallene VIII O-8

3,6,15-Tribromo-2,12:7,10-diepoxy-8,13,14-pentadecatriene-4,7-diol
[265653-18-7]



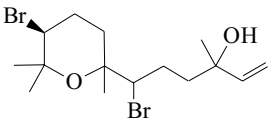
$C_{15}H_{19}Br_3O_4$ 503.025
Isol. from *Laurencia obtusa*.
$[\alpha]_D^{20}$ -11.3 (c, 0.33 in $CHCl_3$).

4-Ac: ***Obtusallene IX***
[265653-22-3]
$C_{17}H_{21}Br_3O_5$ 545.062
Isol. from *Laurencia obtusa*.
$[\alpha]_D^{20}$ -24 (c, 0.12 in $CHCl_3$). Unstable. λ_{max} 205 (ϵ 13100) (MeCN).

Guella, G. *et al., Helv. Chim. Acta*, 2000, **83**, 336-348 (*isol, cd, pmr, cmr, ms*)

Obtusenol O-9

[79406-07-8]

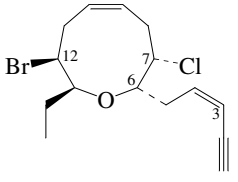


$C_{15}H_{26}Br_2O_2$ 398.177
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D^{16}$ -50.2 (c, 1.7 in $CHCl_3$).

Imre, S. *et al., Phytochemistry*, 1981, **20**, 833-835 (*isol*)
Gonzalez, A.G. *et al., Tet. Lett.*, 1981, **22**, 5071 (*synth*)
Aydogmuş, Z. *et al., Nat. Prod. Res.*, 2004, **18**, 43-49 (*isol, pmr, cmr*)

Obtusenyne O-10

3-Bromo-8-chloro-2-ethyl-2,3,4,7,8,9-hexahydro-9-(2-penten-4-ynyl)oxonin, 9CI. 12-Bromo-7-chloro-6,13-epoxy-13-ethyl-3-pentadecen-1-yne
[71939-43-0]



$C_{15}H_{20}BrClO$ 331.679
Constit. of *Laurencia* spp. Oil. $[\alpha]_D^{20}$ +111.4 (c, 2.8 in $CHCl_3$).

12-Epimer: ***12-Epiobtusenyne***
[79433-82-2]
$C_{15}H_{20}BrClO$ 331.679
Constit. of the sea hare *Aplysia dactylomela*. Liq. $[\alpha]_D$ +73.5 (c, 1.3 in $CHCl_3$).

*12-Epimer, 3*E*-isomer:* **trans-*12-Epiobtusenyne***
[79433-81-1]
$C_{15}H_{20}BrClO$ 331.679
Constit. of *Aplysia dactylomela*. Cryst. (hexane).
Mp 72-73°. $[\alpha]_D$ +7.3 (c, 1.3 in $CHCl_3$).

6,7-Diepimer: ***6,7-Diepiobtusenyne***
[860791-78-2]
$C_{15}H_{20}BrClO$ 331.679
Constit. of *Aplysia dactylomela*. Pale yellow oil. $[\alpha]_D$ +10 (c, 0.2 in $CHCl_3$).

*6,7-Diepimer, 3*E*-isomer:* **trans-*6,7-Diepiobtusenyne***
[860791-77-1]
$C_{15}H_{20}BrClO$ 331.679
Constit. of *Aplysia dactylomela*. Pale yellow oil. $[\alpha]_D$ +18 (c, 0.17 in $CHCl_3$).

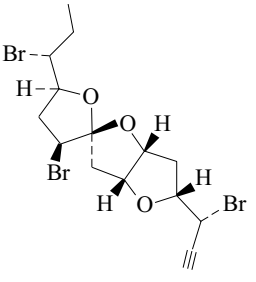
12,13-Diepimer: ***12,13-Diepiobtusenyne***
[236109-73-2]
$C_{15}H_{20}BrClO$ 331.679
Constit. of *Laurencia pinnatifida*. Oil. $[\alpha]_D^{25}$ -15.4 (c, 0.31 in $CHCl_3$). λ_{max} 222 (ϵ 12500) (EtOH).

*12,13-Diepimer, 3*E*-isomer:* **trans-*12,13-Diepiobtusenyne***
[236109-74-3]
$C_{15}H_{20}BrClO$ 331.679
Constit. of *Laurencia pinnatifida*. Powder. $[\alpha]_D^{25}$ -39.7 (c, 0.8 in $CHCl_3$). λ_{max} 223 (ϵ 12800) (EtOH).

King, T.J. *et al., Tet. Lett.*, 1979, **20**, 1453-1454 (*cryst struct*)
Howard, B.M. *et al., Tetrahedron*, 1980, **36**, 1747-1751 (*isol*)
Gopichand, Y. *et al., J.O.C.*, 1981, **46**, 5192-5197 (*12-Epiobtusenynes*)
Norte, M. *et al., Tetrahedron*, 1991, **47**, 9411-9418 (*12,13-Diepiobtusenynes*)
Awakura, D. *et al., Chem. Lett.*, 1999, 461-462 (*synth, abs config*)
Fujiwara, K. *et al., J.O.C.*, 1999, **64**, 2616-2617 (*12,13-Diepiobtusenynes, synth*)
Crimmins, M.T. *et al., J.A.C.S.*, 2003, **125**, 7592-7595 (*synth*)
Manzo, E. *et al., Tetrahedron*, 2005, **61**, 7456-7460 (*6,7-Diepiobtusenynes*)

Obtusin† O-11

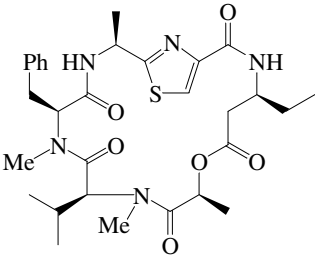
[73618-74-3]



$C_{15}H_{19}Br_3O_3$ 487.025
Constit. of *Laurencia obtusa*. Cryst. (hexane).
Mp 93-95°. $[\alpha]_D$ -107 (c, 0.84 in $CHCl_3$).

Howard, B.M. *et al., Tet. Lett.*, 1979, 2841 (*cryst struct, abs config*)
González, A.G. *et al., Tet. Lett.*, 1983, **24**, 4143 (*cryst struct*)

Obyanamide O-12



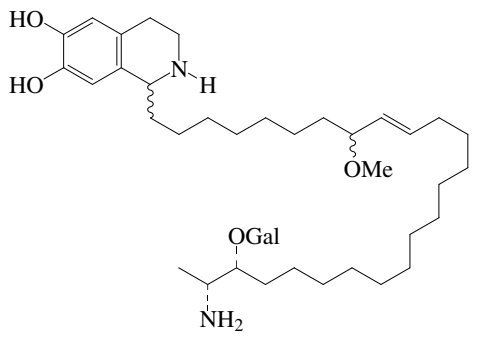
Absolute Configuration

$C_{30}H_{41}N_5O_6S$ 599.75

Depsipeptide antibiotic. Synthesis in 2006 indicates that the structure might need revision. Isol. from *Lyngbya confervoides*. Cytotoxic. Powder. $[\alpha]_D^{27}$ +20 (c, 0.04 in MeOH). λ_{max} 210 (log ϵ 5.2); 222 (log ϵ 4.32) (MeOH).

Williams, P.G. *et al., J. Nat. Prod.*, 2002, **65**, 29-31 (*isol, pmr, cmr*)
Zhang, W. *et al., Chin. Chem. Lett.*, 2006, **17**, 285-288 (*synth*)

Oceanalin A O-13

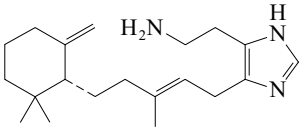


$C_{41}H_{72}N_2O_9$ 737.028
Isol. from the sponge *Oceanapia* sp. Antifungal agent. Amorph. solid. $[\alpha]_D$ -5.7 (c, 0.14 in EtOH). λ_{max} 238 (ϵ 7600); 288 (ϵ 7850) (MeOH).

Makarieva, T.N. *et al., Org. Lett.*, 2005, **7**, 2897-2900 (*isol, pmr, cmr*)

Oceanapamine O-14

[162857-98-9]

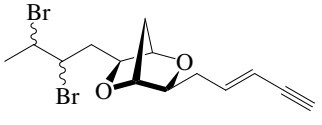


$C_{20}H_{33}N_3$ 315.501
Alkaloid from the Philippine sponge *Oceanapia* sp. Shows antimicrobial activity. Oil (as trifluoroacetate). $[\alpha]_D^{22}$ -6.4 (c, 3.1 in MeOH) (as trifluoroacetate). λ_{max} 202 (ϵ 14290); 220 (ϵ 6690) (MeOH) (Berdy).

Boyd, K.G. *et al., J. Nat. Prod.*, 1995, **58**, 302 (*isol, uv, ir, pmr, cmr, struct*)

Ocellenyne O-15

3-(2,3-Dibromopentyl)-6-(2-pentyl-4-ynyl)-2,5-dioxabicyclo[2.2.1]heptane, 9CI
[79435-29-3]



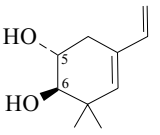
$C_{15}H_{20}Br_2O_2$ 392.13

(*E*)-*form* [78370-97-5]
Constit. of *Aplysia oculifera*.
Oil. $[\alpha]_D^{25}$ +3.21 (c, 0.53 in $CHCl_3$).

(*Z*)-*form* [78419-35-9]
Constit. of *Aplysia oculifera*.
Solid. $[\alpha]_D^{25}$ +2.22 (c, 0.27 in $CHCl_3$).
Schulte, G.R. *et al., J.O.C.*, 1981, **46**, 3870-3873 (*isol*)

1,3(8)-Ochtodadiene-5,6-diol O-16

5-Ethenyl-3,3-dimethyl-4-cyclohexene-1,2-diol, 9CI. 3,3-Dimethyl-5-vinyl-4-cyclohexene-1,2-diol



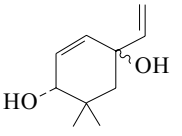
$C_{10}H_{16}O_2$ 168.235

(5*R,6*R**)-*form*** [73872-83-0]
Constit. of *Ochtodes crockeri*.
Oil. $[\alpha]_D^{20}$ 0 (c, 1.2 in $CHCl_3$).

(5ξ,6*S)-*form*** [73872-84-1]
Constit. of *Ochtodes crockeri*.
Oil. $[\alpha]_D^{20}$ 0 (c, 1 in $CHCl_3$).
Paul, V.J. *et al., J.O.C.*, 1980, **45**, 3401 (*isol, struct*)
Zegarski, J. *et al., Tet. Lett.*, 1985, **26**, 1363 (*synth*)

1,4-Ochtodadiene-3,6-diol O-17

1-Ethenyl-5,5-dimethyl-2-cyclohexene-1,4-diol, 9CI. 5,5-Dimethyl-1-vinyl-2-cyclohexene-1,4-diol
[73872-85-2]

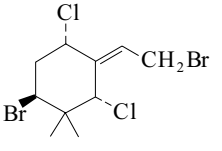


$C_{10}H_{16}O_2$ 168.235
Constit. of *Ochtodes crockeri*. Oil. $[\alpha]_D^{20}$ -14.8 (c, 0.5 in $CHCl_3$).

Paul, V.J. *et al., J.O.C.*, 1980, **45**, 3401 (*isol, struct*)
Zegarski, J. *et al., Tet. Lett.*, 1985, **26**, 1363 (*synth*)

Ochtodene O-18

1-Bromo-4-(2-bromoethylidene)-3,5-dichloro-2,2-dimethylcyclohexane, 9CI. 1,6-Dibromo-4,8-dichloro-2-ochtodene
[67237-02-9]

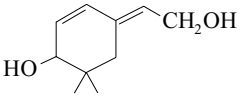


$C_{10}H_{14}Br_2Cl_2$ 364.934
Constit. of *Ochtodes secundiramea*.
Mp 60-62°. $[\alpha]_D^{22}$ +179 (c, 12 in $CHCl_3$).

McConnell, O.J. *et al., J.O.C.*, 1978, **43**, 4238-4241 (*Ochtodene*)

2,4-Ochtodiene-1,6-diol O-19

4-(2-Hydroxyethylidene)-6,6-dimethyl-2-cyclohexen-1-ol, 9CI



(*E*)–*form*

$C_{10}H_{16}O_2$ 168.235

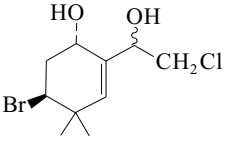
(*E*)-*form* [73891-29-9]
Constit. of *Ochtodes crockeri*.
Oil. $[\alpha]_D^{20}$ +4.3 (c, 2 in $CHCl_3$).

(*Z*)-*form*
Constit. of *Ochtodes crockeri*.
Oil. $[\alpha]_D^{20}$ 0 (c, 2 in $CHCl_3$).

Paul, V.J. *et al., J.O.C.*, 1980, **45**, 3401 (*isol, struct*)
Masaki, Y. *et al., Tet. Lett.*, 1982, **23**, 1481 (*synth*)
Zegarski, J. *et al., Tet. Lett.*, 1985, **26**, 1363 (*synth*)

Ochtodiol O-20

4-Bromo-α-(chloromethyl)-6-hydroxy-3,3-dimethyl-1-cyclohexene-1-methanol, 9CI. 6-Bromo-1-chloro-3(8)-ochtodene-2,4-diol
[67237-01-8]

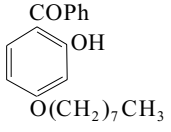


$C_{10}H_{16}BrClO_2$ 283.592
Constit. of *Ochtodes secundiramea*. Oil (as di-Ac). $[\alpha]_D^{23}$ -37 (c, 0.3 in $CHCl_3$) (di-Ac).

McConnell, O.J. *et al., J.O.C.*, 1978, **43**, 4238

Octabenzone, INN, USAN O-21

[2-Hydroxy-4-(octyloxy)phenyl]phenylmethanone, 9CI. 2-Hydroxy-4-(octyloxy)benzophenone, 8CI. Aduvex 248. Advastab 46. Benzon 00. Carstab 700. Chimassorb 81. Cyasorb UV 531. Ongrostab HOB. Spectra-Sorb UV 531. Viosorb 130
[1843-05-6]



$C_{21}H_{26}O_3$ 326.435
Reported from *Desmarestia menziesii* and *Pinus sibirica* (suspect isol. due to its presence in many polymers). UV screen, light stabiliser for polymers.
Mp 45-46°. Log P 7.28 (uncertain value) (calc).

▶ DJ1595000

Larin, N.A. *et al., Zh. Obshch. Khim.*, 1960, **30**, 2377; *CA*, **55**, 8348 (*synth*)
Patel, Y.M. *et al., Food Cosmet. Toxicol.*, 1968, **6**, 199 (*metab, toxicol*)
Gurvich, Y. *et al., Zh. Org. Khim.*, 1969, **5**, 1658 (*synth*)
Carrick, A. *et al., Org. Mass Spectrom.*, 1974, **8**, 229 (*ms*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 9311
Rivera, L. *et al., Bol. Soc. Chil. Quim.*, 1990, **35**, 397-399 (*isol*)
Brito, I. *et al., Acta Cryst. C*, 1992, **48**, 934 (*cryst struct*)
Khamidullina, E.A. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 101-102 (*isol, pmr, cmr*)

17,21-Octacosadienoic acid O-22

$H_3C(CH_2)_5CH{=}CHCH_2CH_2CH{=}CH(CH_2)_{15}COOH$
$C_{28}H_{52}O_2$ 420.718

(*Z,Z*)-*form* [187657-34-7]
Isol. from the sponge *Haliclona cinerea*.
Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*isol, ms*)

19,23-Octacosadienoic acid O-23

$H_3C(CH_2)_3CH{=}CHCH_2CH_2CH{=}CH(CH_2)_{17}COOH$
$C_{28}H_{52}O_2$ 420.718

(*Z,Z*)-*form* [174480-43-4]
Constit. of the sponge *Pseudaxinella* cf. *lunaecharta*.
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol, ms*)

4,7,10,13,16,19,22,25-Octacosaoctaenoic acid O-24

$H_3C[CH_2CH{=}CH]_8CH_2CH_2COOH$
$C_{28}H_{40}O_2$ 408.623

(*all-Z*)-*form* [222851-33-4]
Isol. from various marine dinoflagellate spp. Also in fish oils.
25,26-Dihydro: 4,7,10,13,16,19,22-Octacosaheptaenoic acid
[130048-62-3]
$C_{28}H_{42}O_2$ 410.639
Isol. from various marine dinoflagellate spp.
Van Pelt, C.K. *et al., J. Lipid Res.*, 1999, **40**, 1501-1505 (*isol, ms*)
Mansour, M.P. *et al., Phytochemistry*, 1999, **50**, 541-548 (*isol, ms*)

5,9,19-Octacosatrienoic acid O-25

$H_3C(CH_2)_7CH{=}CH(CH_2)_8CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{28}H_{50}O_2$ 418.702

(*all-Z*)-*form* [66274-42-8]
Isol. from the sponges *Suberites domuncula* and *Xestospongia halichondroides*.
Litchfield, C. *et al., Lipids*, 1978, **13**, 199-202 (*isol*)
Dembitskii, V.M. *et al., Bioorg. Khim.*, 1980, **6**, 1542-1548 (*isol*)

5-Octacosenoic acid O-26

$H_3C(CH_2)_{21}CH{=}CH(CH_2)_3COOH$
$C_{28}H_{54}O_2$ 422.733

(*Z*)-*form* [156181-09-8]
Isol. from the sponge *Cinachyrella* aff. *schulzei*.
Barnathan, G. *et al., Lipids*, 1994, **29**, 297 (*isol*)

11-Octacosenoic acid O-27

$H_3C(CH_2)_{15}CH{=}CH(CH_2)_9COOH$
$C_{28}H_{54}O_2$ 422.733

(*Z*)-*form* [173866-85-8]
Constit. of the sponge *Pseudaxinella* cf. *lunaecharta*.
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol, ms*)

21-Octacosenoic acid O-28

$H_3C(CH_2)_5CH{=}CH(CH_2)_{19}COOH$
$C_{28}H_{54}O_2$ 422.733

(*Z*)-*form* [140163-41-3]
Constit. of the sponge *Amphimedon compressa*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1992, **55**, 333

5,9-Octadecadienoic acid O-29

$H_3C(CH_2)_7CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{18}H_{32}O_2$ 280.45
Isol. from Gymnospermae seed lipids.

(5*Z*,9*E*)-*form* [7049-91-4]
Metabolic prod. of (*E*)-9-Octadecenoic acid.

(5*Z*,9*Z*)-*form* [26549-54-2]
Occurs in *Larix leptolepis* and *Taxus baccata* and other seed oils.
Isol. from various sponges.

(5*E*,9*Z*)-*form*
Isol. from seed oil of *Thalictrum venulosum*.
Bhatty, M.K. *et al., Can. J. Biochem.*, 1966, **44**, 311 (*isol*)
Guo, L.S.S. *et al., Nutr. Metab.*, 1974, **16**, 51
Lam, C.H. *et al., J. Chromatogr.*, 1975, **115**, 559; 1976, **117**, 365; **121**, 303 (*synth, glc*)
Plattner, R.D. *et al., Lipids*, 1975, **10**, 413 (*occur*)
Madrigal, R.V. *et al., Lipids*, 1975, **10**, 502 (*occur*)
Takagi, T. *et al., Lipids*, 1982, **17**, 716 (*occur, glc, cmr*)
Gillan, F.T. *et al., Lipids*, 1988, **23**, 1139-1145 (*isol*)

5,11-Octadecadienoic acid O-30

[62528-83-0]
$H_3C(CH_2)_5CH{=}CH(CH_2)_4CH{=}CH(CH_2)_3COOH$

$C_{18}H_{32}O_2$ 280.45

(all-Z)-form [71541-85-0]
Obt. from the seaweed *Cladophora rupestris.*
Ratnayake, W.N. *et al., Lipids*, 1979, **14**, 580

6,11-Octadecadienoic acid O-31

[61628-30-6]
$H_3C(CH_2)_5CH{=}CH(CH_2)_3CH{=}CH(CH_2)_4COOH$
$C_{18}H_{32}O_2$ 280.45

(E,E)-form
Mp 27-27.5°.

(6E,11Z)-form [88216-90-4]
Formed by *Eubacterium lentum*.

(Z,Z)-form
Cilienic acid
[50381-82-3]
Found in the ciliated protozoan *Tetrahymena pyriformis* and related spp. Occurs in the sponge *Eurayspongia rosea*.

Me ester: [26181-68-0]
$C_{19}H_{34}O_2$ 294.476
Bp_{20} 80-82°.

[26181-77-1]

Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1969, **3**, 297; 1970, **4**, 1; 1977, **18**, 115 (*cmr, pmr, synth*)
Lie Ken Jie, M.S.F. *et al., J. Chromatogr.*, 1975, **109**, 81 (*synth, glc*)
Koroly, M.J. *et al., J. Biol. Chem.*, 1976, **251**, 7588
Schick, B.P. *et al., Biochim. Biophys. Acta*, 1979, **575**, 475 (*metab*)
Watanabe, T. *et al., Biochim. Biophys. Acta*, 1980, **620**, 133; 1981, **665**, 66; **666**, 36 (*isol*)
Janssen, G. *et al., Biomed. Mass Spectrom.*, 1985, **12**, 134 (*synth*)
Carballeira, N.M. *et al., Lipids*, 1989, **24**, 665 (*isol, ms*)
Kulkarni, B.A. *et al., Molecules*, 1997, **2**, 3-6; 99 (*synth*)

7,11-Octadecadienoic acid O-32

$H_3C(CH_2)_5CH{=}CHCH_2CH_2CH{=}CH(CH_2)_5COOH$
$C_{18}H_{32}O_2$ 280.45

(7Z,11Z)-form [115956-84-8]
Isol. from the sponge *Haliclona cinerea.*
Low-melting solid.

Tetrabromide: 7,8,11,12-Tetrabromooctadecanoic acid
$C_{18}H_{32}Br_4O_2$ 600.066
Mp 120-122°.

Gunstone, F.D. *et al., J.C.S.*, 1962, 3055 (*synth*)
Lam, C.H. *et al., J. Chromatogr.*, 1975, **115**, 559; 1976, **117**, 365; **121**, 303 (*synth, glc*)
Howarth, O.W. *et al., J.C.S. Perkin 2*, 1995, 2307-2310 (*cmr*)
Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*isol, ms*)

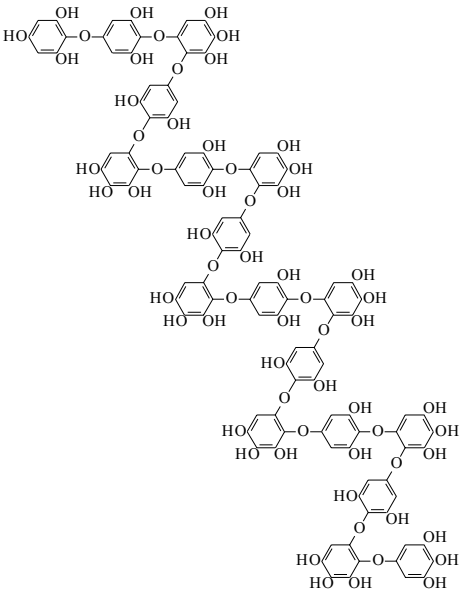
2,5-Octadecadiynoic acid, 8CI O-33

[18202-14-7]
$H_3C(CH_2)_{11}C{\equiv}CCH_2C{\equiv}CCOOH$
$C_{18}H_{28}O_2$ 276.418
Metab. of the mollusc *Mytilus edulis* (blue mussel).
Mp 53-54°.

Christie, W.W. *et al., Chem. Phys. Lipids*, 1967, **1**, 407 (*synth*)
Sprecher, H. *et al., Prog. Chem. Fats Other Lipids*, 1978, **15**, 219
Cho, Y.J. *et al., Nat. Prod. Sci.*, 1995, **1**, 5; *CA*, **124**, 256071g (*isol*)

Octadecafuhalol A O-34

[164176-35-6]



$C_{108}H_{74}O_{63}$ 2379.735
Constit. of the brown alga *Sargassum spinuligerum.*

Glombitza, K.-W. *et al., Phytochemistry*, 1995, **38**, 987-995 (*isol, pmr, cmr, ms*)

1,12-Octadecanediol, 9CI O-35

Ioxanol
[2726-73-0]
$H_3C(CH_2)_5CH(OH)(CH_2)_{10}CH_2OH$
$C_{18}H_{38}O_2$ 286.497

1-Sulfate:
$C_{18}H_{38}O_5S$ 366.561
Isol. from a marine tunicate. Matrix metalloproteinase 2 inhibitor (Na salt). Powder (as Na salt). $[\alpha]_D^{24}$ -1 (c, 0.1 in MeOH) (Na salt). Partial racemate.

(±)-form
Mp 78.1°.

Tassignon, P.S.G. *et al., Tetrahedron*, 1995, **51**, 11863 (*synth, pmr, cmr, ms, purifn*)
Fujita, M. *et al., J. Nat. Prod.*, 2002, **65**, 1936-1938 (*1-sulfate, isol, synth, pmr, cmr*)

Octadecanoic acid, 9CI O-36

Stearic acid. Bassinic acid. Lactaric acid. Stearophanic acid. Talgic acid. FEMA 3035
[57-11-4]
$H_3C(CH_2)_{16}COOH$
$C_{18}H_{36}O_2$ 284.481
Manuf. by hydrolysis of fats and oils. Constit. of most vegetable and animal fats, including the lipids of *Physalia physalis* (Portuguese-man-of-war). Acid and derivatives widely used as additives to industrial preparations. Used as EtOH soln. for nephelometric detn. of Ca. Used (with heptadecanoic acid) for amino acid sequencing in peptides. Used for surfactants, soaps and plasticisers. Pharmaceutical excipient (tablet lubricant; Ca and Mg salts are used similarly). Leaflets. Sol. EtOH, C_6H_6, $CHCl_3$; sl. sol. H_2O.
Mp 69.7°. Bp 386° Bp_5 213°. Polymorphic, at least 4 cryst. forms are known.
▶ Skin irritant. Fl. p. 196°, autoignition temp. 395°. WI2800000
Tetradecyl ester: Tetradecyl octadecanoate. Tetradecyl stearate
[17661-50-6]
$C_{32}H_{64}O_2$ 480.856

Constit. of *Cereus peruvianus* and the soft coral *Sarcophyton trocheliophorum*.
Mp 50.1°.

Amide: Octadecanamide. Stearamide. Amide C-18. Hidorin M7. Kemamide S
[124-26-5]
$C_{18}H_{37}NO$ 283.496
Alkaloid from *Zostera marina* (Zosteraceae) and *Rhizoclonium hieroglyphicum*. Cryst. (EtOH).
Mp 109°. Bp_{12} 250-251°.
▶RG0182000

[593-29-3, 4568-28-9]

Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*Physalia physalis constit*)
Kawasaki, W. *et al., Phytochemistry*, 1998, **47**, 27-29 (*amide*)
Dong, H. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1087-1089 (*tetradecyl ester*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, BSL600; MJW000; OAR000; ZMS000; SLK000; CAX350; SLL500; SJV500

2-Octadecanone O-37

[7373-13-9]
$H_3C(CH_2)_{15}COCH_3$
$C_{18}H_{36}O$ 268.482
Constit. of the leaves of *Euonymus latifolius* and the sponge *Spheciospongia vagabunda*.
Mp 52°. Bp_{100} 251-252°.

Semicarbazone: Mp 125.5-126°.

Morgan, G.T. *et al., Chem. Ind. (London)*, 1925, **44**, 108
Ulubelen, A. *et al., Phytochemistry*, 1973, **12**, 1824 (*Euonymus latifolius constit*)
Brown, N.M.D. *et al., J.C.S. Perkin 2*, 1976, 1769-1773 (*synth*)
Bergbreiter, D.E. *et al., J.O.C.*, 1976, **41**, 2750-2753 (*synth*)
Gawronski, J. *et al., Tet. Lett.*, 1976, 3845-3846 (*cd*)
Xiao, D. *et al., Fenxi Huaxue*, 2004, **32**, 1621-1623; *CA*, **143**, 23210 (*Spheciospongia vagabunda constit*)

3,6,9,12,15-Octadecapentaenoic acid O-38

[56683-48-8]
$H_3C(CH_2CH{=}CH)_5CH_2COOH$
$C_{18}H_{26}O_2$ 274.402

(all-Z)-form [51592-59-7]
Found in photosynthetic dinoflagellates and in zooxanthellae (*Gymnodinium microadriaticum*) isol. from clam tissue.

Joseph, J.D. *et al., Lipids*, 1975, **10**, 395 (*ir, config, bibl*)
Bishop, D.G. *et al., Aust. J. Plant Physiol.*, 1976, **3**, 33 (*occur*)
Kuklev, D.V. *et al., Phytochemistry*, 1992, **31**, 2401 (*isol, pmr, synth*)

1,6,9,12,15-Octadecapentaen-3-one O-39

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH_2COCH{=}CH_2$
$C_{18}H_{26}O$ 258.403

(all-Z)-form [192383-82-7]
Constit. of the Australian sponge *Callyspongia* sp.

Urban, S. *et al., Lipids*, 1997, **32**, 675-677 (*isol, struct*)

4,8,12,15-Octadecatetraenoic acid, 9CI O-40

[67329-10-6]
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH_2CH{=}CHCH_2CH_2CH{=}CHCH_2CH_2COOH$
$C_{18}H_{28}O_2$ 276.418
Isol. from sardine oil, from seeds of *Lithospermum officinale* and from *Salpa thomsoni*.

[81275-46-9, 106440-10-2]

Toyama, Y. *et al., Bull. Chem. Soc. Jpn.*, 1935, **10**, 232 (*isol*)
Hörhammer, L. *et al., Arzneim.-Forsch.*, 1964, **14**, 34 (*isol*)
Mimura, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4562 (*isol*)

6,9,12,15-Octadecatetraenoic acid O-41

[2091-28-3]
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_4COOH$
$C_{18}H_{28}O_2$ 276.418

(6Z,9Z,12Z,15Z)-form
Stearidonic acid
[20290-75-9]
Isol. from *Lithospermum officinale, Onosmodium occidentale*, and from herring and other fish oils. Also isol. from the green alga *Ulva fasciata*.
Pale yellow oil.
Mp *ca.*-57°. n_D^{16} 1.4888.

[73097-00-4, 81275-46-9]

Klenk, E. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1957, **307**, 272 (*isol*)
Craig, B.M. *et al., J. Am. Oil Chem. Soc.*, 1964, **41**, 209 (*isol*)
De Gomez Dumm, I.N.T. *et al., J. Lipid Res.*, 1975, **16**, 264
De Gomez Dumm, I.N.T. *et al., Lipids*, 1975, **10**, 315
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1991, **59**, 83 (*cmr*)
Griffiths, G. *et al., Phytochemistry*, 1996, **43**, 381 (*isol, biosynth*)
Alamsjah, M.A. *et al., Biosci., Biotechnol., Biochem.*, 2005, **69**, 2186-2192 (*isol, pmr, cmr*)

6,12,14-Octadecatrienoic acid, 9CI O-42

$H_3CCH_2CH_2CH{=}CHCH{=}CH(CH_2)_4CH{=}CH(CH_2)_4COOH$
$C_{18}H_{30}O_2$ 278.434

(6Z,12Z,14Z)-form [129722-95-8]
Isol. from the diatom *Navicula gracilis*.

Manivasaham, S. *et al., Planta Med.*, 1991, **57**, A85 (*isol*)

7,9,12-Octadecatrien-5-ynoic acid O-43

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CHCH{=}CHC{\equiv}C(CH_2)_3COOH$
$C_{18}H_{26}O_2$ 274.402

(all-Z)-form
Liagoric acid
[76152-32-4]
Isol. from the red marine alga *Liagora farinosa*. Inhibitor of prostaglandin biosynth. Sol. $CHCl_3$, hexane; poorly sol. H_2O.

[76152-33-5]

Paul, V.J. *et al., Tet. Lett.*, 1980, **21**, 3327 (*isol, pmr, cmr*)

6-Octadecenoic acid O-44

$H_3C(CH_2)_{10}CH{=}CH(CH_2)_4COOH$
$C_{18}H_{34}O_2$ 282.465
Isol. from volatiles of *Coriandrum sativum* (coriander), *Anethum sowa* (dill), *Cuminum cyminum* (cumin), *Daucus carota* (carrot), *Nigella sativa* (black cumin), *Apium graveolens* (celery), *Pimpinella anisum* (anise) and *Petroselinum sativum* (parsley).

(E)-form
Petroselaidic acid. Tarelaidinic acid
[593-40-8]
Minor constit. of plant oils. Constit. of milk fat and from porcine parasites *Oesophagostomum dentatum* and *Oesophagostomum quadrispinulatum*.
Cryst. ($CHCl_3$ or MeOH).
Mp 52.7-53.4° Mp 54-59°.

Me ester: [14620-36-1]
$C_{19}H_{36}O_2$ 296.492
Bp_{10} 208-210° Bp_4 185-186°.

Chloride:
$C_{18}H_{33}ClO$ 300.911
Bp_2 144-146°.

(Z)-form
Petroselinic acid
[593-39-5]

Found in umbelliferous and other seed oils e.g. major constit. of oils of parsley, ivy, fennel, celery, *Seseli indicum*, *Daucus carota* (carrot), *Coriandrum sativum* (coriander), ripe berries of *Aralia spinosa*, seed oil of *Gevuina avellana* (Chilean hazelnut) and others. Also isol. from the tunicate *Salpa thompsoni* and the marine sponge *Phyllospongia papyracea*.
Cryst. (MeOH or EtOH aq.).
Mp 33°. $Bp_{2.5}$ 215-217° (lit. gives a pressure range) $Bp_{0.15}$ 148-152°.

Lumb, P.B. *et al., J.C.S.*, 1952, 5032-5035 (*synth, config*)
Baker, B.W. *et al., J.C.S.*, 1954, 1804-1808 (*synth*)
Swern, D. *et al., J. Am. Oil Chem. Soc.*, 1955, **32**, 539-540 (*cryst struct*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311-323 (*synth*)
Batchelor, J.G. *et al., J.O.C.*, 1974, **39**, 1698-1705 (*cmr*)
Parodi, P.W. *et al., J. Dairy Sci.*, 1976, **59**, 1870-1873 (*synth, glc*)
Saito, Y. *et al., Biochim. Biophys. Acta*, 1978, **529**, 224-229 (*occur*)
Conacher, H.B.S. *et al., J. Assoc. Off. Anal. Chem.*, 1978, **61**, 702-708 (*glc*)
Mimura, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4562-4568 (*Z-form, occur*)
Mallet, J.F. *et al., J. Am. Oil Chem. Soc.*, 1990, **67**, 607-610 (*Z-form, detn, occur, gc, cmr*)
Kaneko, F. *et al., Acta Cryst. C*, 1992, **48**, 1054-1057; 1057-1060 (*cryst struct*)
Goto, R. *et al., Biofouling*, 1992, **6**, 61-68 (*Z-form, occur*)
Cahoon, E.B. *et al., Prog. Lipid Res.*, 1994, **33**, 155-163 (*rev, biosynth*)
Joachim, A. *et al., CA*, 2000, **133**, 307888 (*E-form, occur*)
Guiet, S. *et al., Phytochemistry*, 2003, **64**, 227-233 (*biosynth*)

7-Octadecenoic acid O-45

[14122-42-0]

$H_3C(CH_2)_9CH{=}CH(CH_2)_5COOH$

$C_{18}H_{34}O_2$ 282.465

Isol. from volatiles of *Coriandrum sativum* (coriander), *Anethum sowa* (dill), *Cuminum cyminum* (cumin), *Daucus carota* (carrot), *Nigella sativa* (black cumin), *Apium graveolens* (celery), *Pimpinella anisum* (anise) and *Petroselinum sativum* (parsley).

(*E*)-*form* [13126-32-4]
Found in partially hydrogenated fats, e.g. human and bovine milk. Also isol. from Portuguese Man of war, *Physalia physalis.*
Mp 44.2-44.5°.

(*Z*)-*form* [13126-31-3]
Found in partially hydrogenated fats, e.g. herring oil, sesame seed oil. Constit. of spot prawn *Pandalus platyceros*, salmon *Oncorhynchus nerka* and *Oncorhynchus keta*, Atlantic halibut *Hippoglossus hippoglossus*, fresh water sponge *Lubomirskia baicalensis* and lichens *Acholeplasma laidlawii* and *Cladonia* spp.
Mp 11.8-12.5° Mp 12.5-13.1°.

Huber, W.F. *et al., J.A.C.S.*, 1951, **73**, 2730-2733 (*synth*)
Swern, D. *et al., J. Am. Oil Chem. Soc.*, 1955, **32**, 539-540 (*cryst struct*)
Kartha, A.R.S. *et al., Chem. Ind. (London)*, 1969, 1869-1870 (*occur*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311-323 (*synth*)
Stepaneko, G.A. *et al., Khim. Prir. Soedin.*, 1972, **8**, 709-715; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 694-698 (*occur*)
Schwartz, D.P. *et al., Anal. Biochem.*, 1976, **74**, 320-328 (*detn*)
Stillway, L.W. *et al., Comp. Biochem. Physiol.*, 1976, **538**, 535-537 (*occur*)
Parodi, P.W. *et al., J. Dairy Sci.*, 1976, **59**, 1870-1873 (*glc, occur*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1977, **18**, 115-129 (*cmr*)
Saito, Y. *et al., Biochim. Biophys. Acta*, 1978, **529**, 224-229 (*occur*)
Whyte, J.N.C *et al., Can. J. Fish. Aquat. Sci.*, 1991, **48**, 382-390 (*Z-form, occur*)
Dembitskii, V.M. *et al., Phytochemistry*, 1991, **30**, 4015-4018 (*Z-form, occur*)
Chen, Z.-Y. *et al., Lipids*, 1995, **30**, 15-21 (*E-form, occur*)

8-Octadecenoic acid O-46

$H_3C(CH_2)_8CH{=}CH(CH_2)_6COOH$

$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [5684-81-1]
Found in partially hydrogenated fat as glyceride. Constit. of milk fat, Kangaroo fat, olive oil, rape seed oil, *Thunbergia alata* seed oil and human milk. Isol. from Portuguese man of war *Physalia physalis.*
Mp 51.5-52.3° Mp 52-52.6°.

(*Z*)-*form* [5684-71-9]
Found in partially hydrogenated fat as a glyceride. Isol. from milk fat, soybean oil and rape seed oil.
Mp 22.7-23.8°.

Huber, W.F. *et al., J.A.C.S.*, 1951, **73**, 2730-2733 (*synth*)
Swern, D. *et al., J. Am. Oil Chem. Soc.*, 1955, **32**, 539-540 (*cryst struct*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311-323 (*synth*)
Spencer, G.F. *et al., Lipids*, 1971, **6**, 712-714 (*E-form, occur*)
Davies, J.E.D. *et al., J.C.S. Perkin 2*, 1972, 1557-1561 (*ir, Raman*)
Stepanenko, G.A. *et al., Khim. Prir. Soedin.*, 1972, **8**, 709-715; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 694-698 (*occur*)
Stillway, L.W. *et al., Comp. Biochem. Physiol.*, 1976, **53B**, 535-537 (*occur*)
Parodi, P.W. *et al., J. Dairy Sci.*, 1976, **59**, 1870-1873 (*glc, occur*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1977, **18**, 115-129 (*cmr*)
Saito, Y. *et al., Biochim. Biophys. Acta*, 1978, **529**, 224-229 (*occur*)
Fogerty, A.C. *et al., Nutr. Rep. Int.*, 1983, **28**, 375-380 (*occur*)
Boskou, D. *et al., Fette, Seifen, Anstrichm.*, 1986, **88**, 13-15 (*glc, occur*)

9-Octadecenoic acid, 9CI O-47

[2027-47-6]
[26764-26-1]

$H_3C(CH_2)_7CH{=}CH(CH_2)_7COOH$

$C_{18}H_{34}O_2$ 282.465

Present in lipids of *Physalia physalis* (Portuguese-man-of-war).

(*Z*)-*form*
Oleic acid. Rapinic acid. Pamolyn 100. MYX 6121. FEMA 2815
[112-80-1]
[27104-13-8]
Major constit. of plant oils e.g. olive oil (*ca.* 80%), almond oil (*ca.* 80%) and many others, mainly as glyceride. Constit. of tall oil and present in fruits. Food additive. Used in manuf. of surfactants, soaps, plasticisers. Emulsifying agent in foods and pharmaceuticals. Skin penetrant. Herbicide, insecticide, fungicide. Oil. Insol. H_2O; sol. EtOH, Et_2O. d_4^{20} 0.9.
Mp 12° (labile form) Mp 16° (stable form). Bp_5 203-205°. n_D^{20} 1.4595. Log P 7.75 (uncertain value) (calc). ^{125}I and ^{131}I labelled cpds. are used as radioactive agents (Oleotope). Undergoes BF_3-catalysed dimerisation.
▶ Skin irritant. LD_{50} (rat, orl) 74000 mg/kg. RG2275000

Tetradecyl ester: Tetradecyl 9-octadecenoate. Tetradecyl oleate
[22393-85-7]
$C_{32}H_{62}O_2$ 478.841
Constit. of the fruit of *Terminalia arjuna* and of the soft coral *Sarcophyton trocheliophorum*.
Mp 22.5°.

[142-17-6, 544-60-5, 557-07-3, 688-37-9, 1555-53-9, 2462-84-2, 2717-15-9, 3687-46-5, 10402-16-1]

Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*Physalia physalis constit*)
Dembitsky, V.M. *et al., Phytochemistry*, 1996, **42**, 1075-1080 (*tetradecyl ester*)

10-Octadecenoic acid O-48

Isooleic acid
[3386-63-8]

$H_3C(CH_2)_6CH{=}CH(CH_2)_8COOH$

$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [5684-82-2]
Found in partially hydrogenated fats as a glyceride. Constit. of rapeseed oil, soybean oil, human milk, butter, sunflower oil and Kangaroo fat. Also isol. from Portuguese Man-of-War *Physalia physalis*, roots of *Oplopanax elatus*, *Daphne bholua*, *Buthus martensii* and *Scolopendra subspinipes mutilans.*
Mp 52-52.6°. Bp_3 208-216°.

Amide:
$C_{18}H_{35}NO$ 281.481
Mp 83°.

(*Z*)-*form* [2442-70-8]
Found in partially hydrogenated fats as a glyceride. Constit. of butter, soybean oil and seed oil from *Zanthoxylum alatum*. Isol. from the sponge *Thalysias juniperina*.
Mp 22.2-22.8°.

Huber, F. *et al., J.A.C.S.*, 1951, **73**, 2730-2733 (*synth*)

Swern, D. *et al., J. Am. Oil Chem. Soc.*, 1955, **32**, 539-540 (*cryst struct*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311-323 (*synth*)
Stillway, L.W. *et al., Comp. Biochem. Physiol.*, 1976, **53B**, 535-537 (*occur*)
Parodi, P.W. *et al., J. Dairy Sci.*, 1976, **59**, 1870-1873 (*glc, occur*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1977, **18**, 115-129 (*cmr*)
Saito, Y. *et al., Biochim. Biophys. Acta*, 1978, **529**, 224-229 (*occur*)
Fogerty, A.C. *et al., Nutr. Rep. Int.*, 1983, **28**, 375-380 (*glc, occur*)
Carballeira, N.M. *et al., Lipids*, 1990, **25**, 235-237 (*Z-form, occur*)
Venkatachalam, S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 515, (*isol, ms*)

11-Octadecenoic acid O-49

[143-25-9]

$H_3C(CH_2)_5CH{=}CH(CH_2)_9COOH$

$C_{18}H_{34}O_2$ 282.465

Present in lipids of *Physalia physalis* (Portuguese-man-of-war).

(*E*)-*form*

Vaccenic acid

[693-72-1]

Occurs in small proportions in ruminant fats (e.g., butter) *via* biohydrogenation of dietary polyene acids. Main component of *Streptomyces pyogenes* protoplast lipids.

Mp 43.5-44.1°.

Me ester: [6198-58-9]
$C_{19}H_{36}O_2$ 296.492
Bp_3 172-173°.

(*Z*)-*form*

Asclepic acid

[506-17-2]

A minor component of various natural fats. Isol. from various sponges.

Cryst. (Me_2CO).

Mp 14.5-15.5°.

[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl] ester: 1-O-(11Z-Octadecenoyl)-β-sophorose
[174661-38-2]
$C_{30}H_{54}O_{12}$ 606.749

Isol. from the bacterium *Sarcina ventriculi*. Incorrect struct. in CA.

Me ester: [1937-63-9] $Bp_{0.1}$ 162-164°. n_D^{20} 1.4500.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 987C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 685A (*ir, Asclepic acid*)
Bounds, D.G. *et al., J.C.S.*, 1954, 4219 (*synth*)
Swern, D. *et al., J. Am. Oil Chem. Soc.*, 1955, **32**, 539 (*cryst struct*)
Cohen, M. *et al., Biochemistry*, 1966, **5**, 2385 (*isol*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311 (*synth*)
Noble, R.C. *et al., Br. J. Nutr.*, 1974, **31**, 99
Bus, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1974, **93**, 213 (*cmr*)
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206 (*isol*)
Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*Physalia physalis constit*)
Saito, Y. *et al., Biochim. Biophys. Acta*, 1978, **529**, 224 (*isol*)
Lee, J. *et al., Tetrahedron*, 1996, **52**, 3873-3878 (*sophorosyl ester*)
Duffy, P.E. *et al., Tetrahedron*, 2006, **62**, 4838-4843 (*synth*)

12-Octadecenoic acid O-50

[7378-88-3]

$H_3C(CH_2)_4CH{=}CH(CH_2)_{10}COOH$

$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [13126-38-0]

Present in partially hydrogenated fat as a glyceride. e.g. kangaroo fat and butter, and in rape seed oil.

Cryst. (petrol).

Mp 39.7-40.1° Mp 52-53°.

(*Z*)-*form* [13126-37-9]

Present in butter, mapara (*Hypophthalmus* spp.), red alga (*Porphyridium cruentum*) and porcine parasitic worms *Oesophagostomum dentatum* and *Oesophagostomum quadrispinulatum*.

Mp 26.5-27.5° Mp 26.8-27.6°. $Bp_{1.5}$ 196°.

Et ester:
$C_{20}H_{38}O_2$ 310.519
$Bp_{0.4}$ 184°.

Huber, F. *et al., J.A.C.S.*, 1951, **73**, 2730-2733 (*synth*)
Baker, C.D. *et al., J.C.S.*, 1963, 489-491 (*synth*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311-323 (*synth*)
Schwartz, D.P. *et al., Anal. Biochem.*, 1976, **74**, 320-328 (*detn*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1977, **18**, 115-129 (*cmr*)
Conacher, H.B.S. *et al., J. Assoc. Off. Anal. Chem.*, 1978, **61**, 702 (*glc*)
Fogerty, A.C. *et al., Nutr. Rep. Int.*, 1983, **28**, 375-380 (*glc, occur*)
Inhamuns, A.J. *et al., J. Agric. Food Chem.*, 2001, **49**, 4859-4863 (*Z-form, occur*)

13-Octadecenoic acid O-51

[7378-89-4]

$H_3C(CH_2)_3CH{=}CH(CH_2)_{11}COOH$

$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [693-71-0]

Mp 43.5-44.5°.

(*Z*)-*form* [13126-39-1]

Constit. of various lipid fractions from algae, bacteria, fish and some cooked foods. Also found in various plant spp. Isol. from *Haliclona cinerea*.

Mp 26.5-27°.

Me ester: [13058-55-4]
$C_{19}H_{36}O_2$ 296.492
Constit. of *Aesculus indica*. Liq. $Bp_{0.4}$ 145°.

Et ester: [101766-90-9]
$C_{20}H_{38}O_2$ 310.519
Constit. of *Aesculus indica*. Viscous liq.

[42199-38-2, 56338-67-1]

Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1967, **1**, 209; 264; 1977, **18**, 115 (*synth, cmr*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311 (*synth*)
Singh, B. *et al., J. Nat. Prod.*, 1989, **52**, 180 (*isol, ir, pmr, cmr, esters*)
Subbaraman, A.S. *et al., Indian J. Chem., Sect. B*, 1991, **30**, 865 (*synth, ir*)
Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*Haliclona, isol*)

9-Octadecen-1-ol, 9CI O-52

[593-47-5]

$H_3C(CH_2)_7CH{=}CH(CH_2)_7CH_2OH$

$C_{18}H_{36}O$ 268.482

(*E*)-*form*

Elaidyl alcohol. Elaidic alcohol

[506-42-3]

Mp 36-37° (34°). Bp_{18} 216°.

(*Z*)-*form*

Oleyl alcohol. Oleic alcohol. Francol OA-95

[143-28-2]

Occurs in fish oils. Also obt. from wood of *Eperua falcata*. Used in the food industry.

Pale yellow, oily liq. Insol. H_2O. d_4^{20} 0.85. Bp 360° Bp_{15} 205-210°. n_D^{20} 1.4607. Oligomerises in the presence of BF_3.

▶ Skin and eye irritant. Fl. p. 184/189°, autoignition temp. 363°.

RG4120000

Ac: [693-80-1]
$C_{20}H_{38}O_2$ 310.519
Liq. $Bp_{0.04}$ 131-135°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 146A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 220B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 215C (*ir*)
Noller, C.R. *et al., J.A.C.S.*, 1934, **56**, 1563 (*synth*)
Org. Synth., 1935, **15**, 72 (*synth*)
Nyström, R.F. *et al., J.A.C.S.*, 1947, **69**, 1197
Blake, S. *et al., J.C.S.*, 1963, 430 (*isol*)
Ghodssi, M.A. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1966, **262**, 269 (*oligomers*)
Bestman, H.J. *et al., Chem. Ber.*, 1971, **104**, 65 (*Ac, synth, pmr*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OBA000

Octadecyl hydrogen sulfate O-53

[143-03-3]

$H_3C(CH_2)_{17}OSO_3H$

$C_{18}H_{38}O_4S$ 350.562

Isol. from the tunicate *Sidnyum turbinatum*. Hygroscopic cryst. Mp 54.1-55.5° (sealed tube).

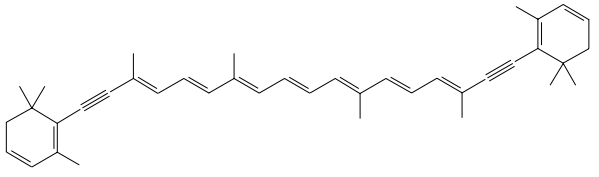
Na salt: [1120-04-3]
Amorph. solid. Mp 211-213°.

▶ WT1170000

Maurer, E.W. *et al., J. Am. Oil Chem. Soc.*, 1960, **37**, 34 (*synth*)
Maurer, E.W. *et al., Biochem. Prep.*, 1966, **11**, 96 (*synth*)
Aiello, A. *et al., J. Nat. Prod.*, 2001, **64**, 219-221 (*isol*)

3,3′,4,4′,7,7′,8,8′-Octadehydro-β,β-carotene O-54

Octadehydro-β-carotene
[116180-16-6]



$C_{40}H_{48}$ 528.819

Constit. of *Euglena viridis* and the sponge *Polymastia granulosa*. Cryst. (Me_2CO/hexane). λ_{max} 327; 445 (sh); 472; 501 (hexane).

Hertzberg, S. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 801-814 (*Polymastia granulosa constit*)
Fiksdahl, A. *et al., Phytochemistry*, 1988, **27**, 1447-1450 (*isol, uv, pmr*)

2,4-Octadien-1-amine O-55

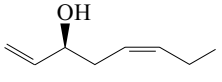
1-Amino-2,4-octadiene
$H_3CCH_2CH_2CH{=}CHCH{=}CHCH_2NH_2$

$C_8H_{15}N$ 125.213

(E,E)-form

N-*(2*R*-Hydroxyheptyl)*: ***Pseudodistamine***
[356522-64-0]
$C_{15}H_{29}NO$ 239.4
Isol. from a *Pseudodistoma* sp. Gum. $[\alpha]_D$ -3 (c, 0.1 in MeOH). λ_{max} 225 (log ϵ 3.72) (MeOH).
Rashid, M.A. *et al., Tetrahedron*, 2001, **57**, 5751-5755 (*Pseudodistamine, isol, pmr, cmr, uv*)

1,5-Octadien-3-ol, 9CI O-56



(S,Z)–form

$C_8H_{14}O$ 126.198

(3S,5Z)-form [56994-74-2]
Constit. of essential oil of *Chondrococcus hornemanni*.
$[\alpha]_D$ -8 (c, 0.5 in CH_2Cl_2).

(3ξ,5E)-form [50306-14-4]
Found in the fungus *Trichothecium roseum*. Insect attractant for *Tyrophagus putrescentiae*.

(3ξ,5Z)-form [50306-18-8]
From *Tyrophagus roseum*. Off-flavour component of cooked prawns and sand-lobsters. Insect attractant.

Woolard, F.X. *et al., Chem. Comm.*, 1975, 486 (*pmr*)
Vanhaelen, M. *et al., J. Chromatogr.*, 1977, **144**, 108
Whitfield, F.B. *et al., Aust. J. Chem.*, 1982, **35**, 373 (*isol*)

2,5-Octadien-1-ol O-57

[83861-75-0]

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2OH$

$C_8H_{14}O$ 126.198

Constit. of various fish and other marine animals.

(2E,5Z)-form [67548-36-1]
Bp_{12} 92-93°.

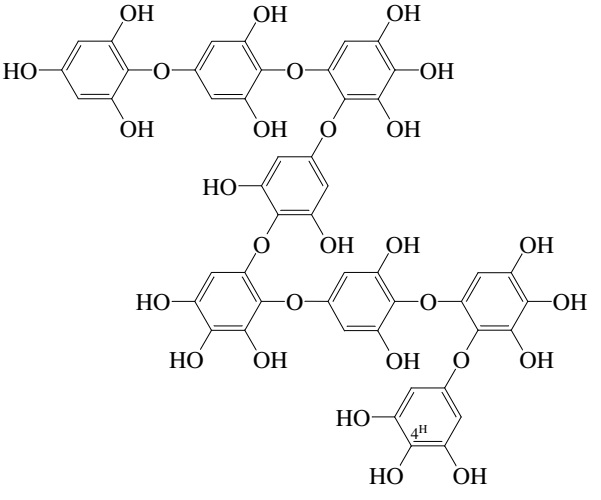
(2Z,5Z)-form [67548-44-1]

[101339-88-2]

Cahiez, C. *et al., Synthesis*, 1978, 528 (*synth, ir, pmr*)
Marner, F.J. *et al., Annalen*, 1982, 579 (*synth*)
Wurzenburger, M. *et al., Lipids*, 1986, **21**, 261
Honda, T. *et al., J.C.S. Perkin 1*, 1999, 23-29 (*synth, ir, pmr, cmr*)

Octafuhalol A O-58

Octafuhalol
[83903-59-7]



$C_{48}H_{34}O_{28}$ 1058.78

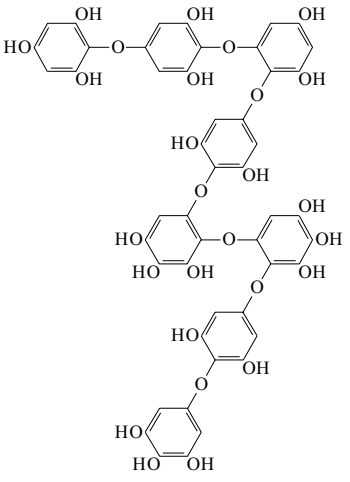
Constit. of brown algae *Sargassum muticum*, *Sargassum spinuligerum*, *Carpophyllum maschalocarpum* and *Carpophyllum angustifolium*.

4^H-Deoxy: ***Deshydroxyoctafuhalol C***
$C_{48}H_{34}O_{27}$ 1042.78
Isol. from *Sargassum spinuligerum*.

Glombitza, K.-W. *et al., Bot. Mar.*, 1982, **25**, 449 (*isol, pmr*)
Glombitza, K.-W. *et al., Phytochemistry*, 1991, **30**, 2741; 1995, **38**, 987-995 (*isol, cmr*)

Octafuhalol B O-59

[164230-58-4]

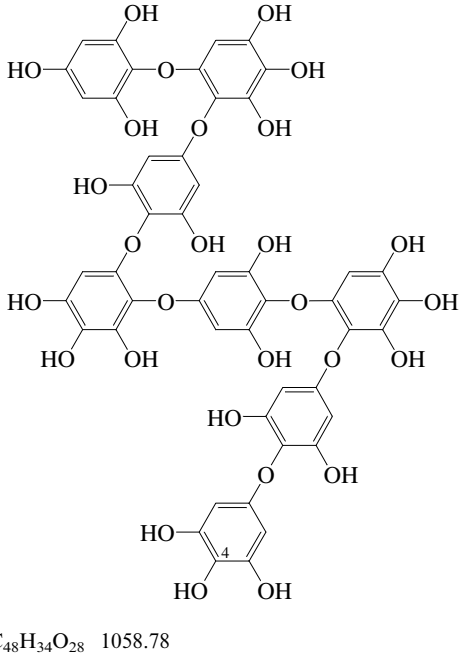


$C_{48}H_{34}O_{27}$ 1042.78

Constit. of the brown alga *Sargassum spinuligerum*.

Glombitza, K.-W. *et al., Phytochemistry*, 1995, **38**, 987-995 (*isol, pmr, cmr, ms*)

Octafuhalol C O-60



$C_{48}H_{34}O_{28}$ 1058.78

Isol. from brown alga *Carpophyllum angustifolium*. Characterised as per-Ac.

4-Deoxy: ***Deshydroxyoctafuhalol C***

$C_{48}H_{34}O_{27}$ 1042.78

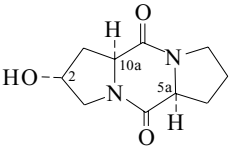
Isol. from *Sargassum spinuligerum* and *Carpophyllum angustifolium*.

Glombitza, K.W. *et al., Phytochemistry*, 1995, **38**, 987-995 (*Deshydroxyoctafuhalol C*)

Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*Octafuhalol C*)

Octahydro-2-hydroxy-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, 9CI O-61

Hydroxyprolylproline anhydride. Cyclo(hydroxyprolylprolyl)



(2*R*,5a*S*,10a*S*)–*form*

$C_{10}H_{14}N_2O_3$ 210.232

(2*R*,5*aR*,10*aR*)-*form*

Mp 174-175°. $[\alpha]_D^{28}$ +90.8 (c, 1 in H_2O).

(2*R*,5*aS*,10*aS*)-*form* [36099-80-6]

Isol. from rabbit skin tissue extract. Prod. by a *Ruegeria* sp. isol. from the sponge *Suberites domuncula*. Plant growth regulator.

Mp 141-142°. $[\alpha]_D^{28}$ -134.7 (c, 1 in H_2O).

(2*S*,5*aR*,10*aS*)-*form* [55903-97-4]

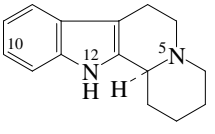
Cryst. (MeOH/Et_2O). Mp 195-198°. $[\alpha]_D$ -10.2 (c, 0.48 in DMF).

Justova, V. *et al., Coll. Czech. Chem. Comm.*, 1975, **40**, 662 (*synth*)
Anteunis, M.J.O. *et al., Bull. Soc. Chim. Belg.*, 1978, **87**, 41 (*pmr, conformn*)
Ienaga, K. *et al., Tet. Lett.*, 1987, **28**, 1285-1286 (*isol, synth, props*)
Mitova, M. *et al., J. Nat. Prod.*, 2004, **67**, 1178-1181 (*isol*)

1,2,3,4,6,7,12,12*b*-Octahydroindolo[2,3-*a*]quinolizine, 9CI O-62

Indoloquinolizidine*. Tetramethylenetetrahydro-β-carboline*

[4802-79-3]



(*S*)-*form*

$C_{15}H_{18}N_2$ 226.321

(*S*)-*form* [10252-12-7]

Main alkaloid from leaves of *Dracontomelon mangiferum* (Anacardiaceae). Also from *Nitraria schoberi*.

Mp 149-151°. $[\alpha]_D$ -86.5 (MeOH). The alkaloid is partly racemic.

λ_{max} 228 (log ϵ 4.43); 284 (log ϵ 3.5); 292 (log ϵ 3.43) (EtOH).

10-Bromo: ***Arborescidine A***

[147395-92-4]

$C_{15}H_{17}BrN_2$ 305.217

Alkaloid from the marine tunicate *Pseudodistoma arborescens.*

Cryst. (MeOH).

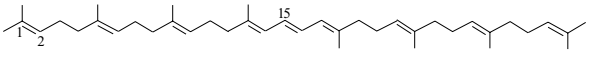
Mp 202°. $[\alpha]_D$ -85 (c, 1 in $CHCl_3$).

Johns, S.R. *et al., Aust. J. Chem.*, 1966, **19**, 1951-1954 (*S-form, isol, uv, ir, pmr, ms, struct*)
Hua, D.H. *et al., J.O.C.*, 1991, **56**, 6998-7007 (*synth*)
Chbani, M. *et al., J. Nat. Prod.*, 1993, **56**, 99-104 (*Arborescidine A*)
Cheng, E. *et al., Tetrahedron*, 1996, **52**, 6725-6732 (*synth*)
Diker, K. *et al., J. Nat. Prod.*, 1997, **60**, 790-793 (*synth, ir, uv, pmr, cmr*)
Burm, B.E.A. *et al., Tetrahedron*, 1998, **54**, 6135-6146 (*Arborescidine A, synth*)
Santos, L.S. *et al., J.O.C.*, 2004, **69**, 1283-1289 (*Arborescidine A, synth*)
Allin, S.M. *et al., Eur. J. Org. Chem.*, 2005, 4179-4186 (*S-form, synth, pmr, cmr*)

7,7′,8,8′,11,11′,12,12′-Octahydrolycopene O-63

7,7′,8,8′,11,11′,12,12′-Octahydro-ψ,ψ-carotene. ***Phytoene***

[540-04-5]



$C_{40}H_{64}$ 544.946

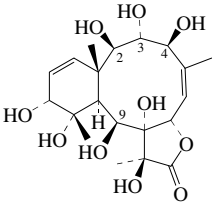
Constit. of *Mycobacterium phlei* and other bacteria. Widespread in plants. Viscous oil with strong uv fluorescence.

1,2-Epoxide: ***Phytoene 1,2-epoxide****. 1,2-Epoxy-1,2,7,7′,8,8′,11,11′,12,12′-decahydro-ψ,ψ-carotene*
[26107-96-0]
$C_{40}H_{64}O$ 560.945
Isol. from ripe tomatoes. λ_{max} 275; 285; 296 (no solvent reported).

(15Z)-Isomer: ***15*-cis-*Pytoene****. 15Z-Phytoene isomer*
[13920-14-4]
Isol. from tomato (*Lycopersicon esculentum* var. 'Tangella'), and *Dunaliella bardawil*. Clear branch point for poly-Z-carotene formation in the tangerine tomato. Pale orange oil. λ_{max} 286; 296 (hexane).

Britton, G. *et al., Phytochemistry*, 1969, **8**, 2257 (*epoxide*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 1817a (*occur*)
Gregonis, D.E. *et al., Biochemistry*, 1974, **13**, 1538 (*biosynth*)
Khan, N. *et al., J.C.S. Perkin 1*, 1975, 1457 (*struct, synth*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97 (*cmr*)
Clough, J.M. *et al., J.C.S. Perkin 1*, 1983, 3011 (*15Z-Phytoene, ir, pmr, cmr*)
Frecknell, E.A. *et al., Phytochemistry*, 1984, **23**, 1707 (*isol, occur*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 44 (*bibl*)
Ebenezer, W.J. *et al., J.C.S. Perkin 1*, 1993, 1869 (*15Z-Phytoene, ir, pmr, cmr*)

2,3,4,8,9,11,12,17-Octahydroxy-5,13-briaradien-18,7-olide O-64



(2β,3α,4β,5Z,7α,8α,9β,11α,12α,17β)-*form*

$C_{20}H_{30}O_{10}$ 430.451

(2β,3α,4β,5*Z*,7α,8α,9β,11α,12α,17β)-*form*

2,3,4,9-Tetra-Ac: ***Violide J***
[252058-36-9]
$C_{28}H_{38}O_{14}$ 598.6
Constit. of a *Briareum* sp. Cryst. (MeOH aq.).
Mp 281-283°. $[\alpha]_D$ +59.8 (c, 0.12 in MeOH). λ_{max} 206 (log ϵ 3.74) (MeOH).

2,3,4,9,12-Penta-Ac: ***Violide O***
[299926-25-3]
$C_{30}H_{40}O_{15}$ 640.637
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ +31 (c, 0.2 in MeOH). λ_{max} 206 (log ϵ 3.79) (MeOH).

3-Butanoyl, 2,4,9-tri-Ac: ***Violide U***
[851723-75-6]
$C_{30}H_{42}O_{14}$ 626.653
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +76 (c, 0.09 in MeOH).

4-Hexanoyl, 2,9-di-Ac: ***Violide L***
[252058-39-2]
$C_{30}H_{44}O_{13}$ 612.67
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ +21 (c, 0.15 in MeOH). λ_{max} 206 (log ϵ 3.85) (MeOH).

4-Octanoyl, 2,9-di-Ac: ***Violide K***
[252058-38-1]
$C_{32}H_{48}O_{13}$ 640.723
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ +29.6 (c, 0.38 in MeOH). λ_{max} 206 (log ϵ 3.91) (MeOH).

4-Octanoyl, 2,3,9-tri-Ac: ***Violide T***
[851723-74-5]
$C_{34}H_{50}O_{14}$ 682.761
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +75 (c, 0.32 in MeOH).

4-Octanoyl, 2,9,17-tri-Ac: ***Violide Z***
[851539-03-2]
$C_{34}H_{50}O_{14}$ 682.761
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +5 (c, 0.19 in MeOH).

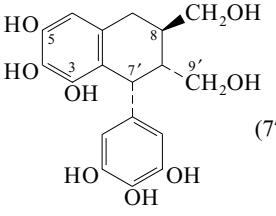
4-Octanoyl, 17-propanoyl, 2,9-di-Ac: ***17-Propanoylviolide K***
[851539-04-3]
$C_{35}H_{52}O_{14}$ 696.787
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +4 (c, 0.11 in MeOH).

(2β,3α,4β,5*Z*,7α,8β,9β,11α,12α,17α)-*form*

4-Octanoyl, 2,3,9-tri-Ac: ***Violide V***
[851723-76-7]
$C_{34}H_{50}O_{14}$ 682.761
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +5 (c, 0.19 in MeOH).

Iwagawa, T. *et al., Heterocycles*, 1999, **51**, 2619-2625; 2000, **53**, 1789-1792 (*isol, pmr, cmr, cryst struct*)
Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 607-617 (*Violides T,U,V,Z, 4-octanoyl esters*)

3,3′,4,4′,5,5′,9,9′-Octahydroxy-2,7′-cyclolignan O-65



(7′*R*,8*R*,8′*R*)−*form*

$C_{18}H_{20}O_8$ 364.351
Lignan numbering shown.

(7′*S*,8*R*,8′*R*)-*form*

3,3′,5,5′-Tetra-Me ether, 9-O-α-D-*galactopyranoside, 9′*-O-β-D-*glucopyranoside:*
$C_{34}H_{48}O_{18}$ 744.742
Constit. of the aerial parts of *Acanthus ilicifolius*. Amorph. powder. $[\alpha]_D^{25}$ +40 (c, 0.6 in MeOH).

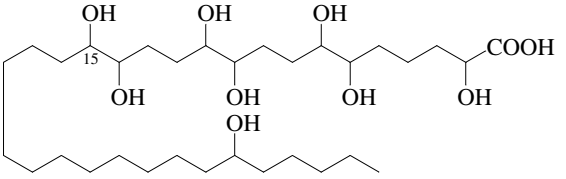
3,3′,5,5′-Tetra-Me ether, 9′-O-*[4-hydroxy-3,5-dimethoxybenzoyl-(→2)-β-D-glucopyranoside]:* ***Acanfolioside***
$C_{37}H_{46}O_{17}$ 762.76
Constit. of *Acanthus ilicifolius*. Amorph. powder. $[\alpha]_D^{22}$ +28.3 (c, 2.7 in MeOH).

3,3′,5,5′-Tetra-Me ether, 9′-O-*[α-D-galactopyranosyl-(1→6)-β-D-glucopyranoside]:*
$C_{34}H_{48}O_{18}$ 744.742
Constit. of the aerial parts of *Acanthus ilicifolius*. Amorph. powder. $[\alpha]_D^{25}$ +36.5 (c, 0.8 in MeOH).

[3737-93-7]

Kanchanapoom, T. *et al., Phytochemistry*, 2001, **56**, 369-372; **57**, 1245-1248 (*Acanfolioside, Fernandoside*)
Wu, J. *et al., Z. Naturforsch., B*, 2004, **59**, 341-344 (*Acanthus ilicifolius glycosides*)

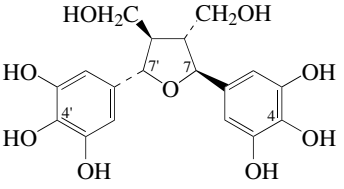
2,6,7,10,11,14,15,27-Octahydroxydotriacontanoic acid O-66



$C_{32}H_{64}O_{10}$ 608.852

Amide, 15-O-*sulfate:* ***Turbinamide***
[366788-20-7]
$C_{32}H_{65}NO_{12}S$ 687.931
Isol. from the tunicate *Sidnyum turbinatum*. Selective cytotoxic agent. Solid (as Na salt). $[\alpha]_D^{25}$ +7.1 (c, 0.003 in MeOH) (Na salt).
Aiello, A. *et al., Org. Lett.*, 2001, **3**, 2941-2944 (*isol, pmr, cmr*)

3,3′,4,4′,5,5′,9,9′-Octahydroxy-7,7′-epoxylignan O-67



(7*S*,7′*S*,8*R*,8′*R*)-*form*

$C_{18}H_{20}O_9$ 380.351

(7*S*,7′*S*,8*R*,8′*R*)-*form*
3,3′,5,5′-Tetra-Me ether: ***Huazhongilexin***
[161657-71-2]
$C_{22}H_{28}O_9$ 436.458
Constit. of *Ilex centrochinensis*.

(7*R,7′*R**,8*R**,8′*R**)-*form***
3,3′,5,5′-Tetra-Me ether, 4-O-*β*-D-*glucopyranoside:*
$C_{28}H_{38}O_{14}$ 598.6
Constit. of the aerial parts of *Phagnalon rupestre*. Amorph. powder. $[\alpha]_D$ -13 (c, 0.1 in MeOH). λ_{max} 212; 273 (MeOH).

(7*R,7′*R**,8*S**,8′*S**)-*form***
3,3′,5,5′-Tetra-Me ether: 4,4′,9,9′-Tetrahydroxy-3,3′,5,5′-tetramethoxy-7,7′-epoxylignan. ***Icariol A$_2$***
[135820-79-0]
$C_{22}H_{28}O_9$ 436.458
Constit. of *Epimedium sagittatum*. Amorph. powder. $[\alpha]_D^{23}$ -22 (c, 0.59 in MeOH). May be identical with Huazhongilexin.

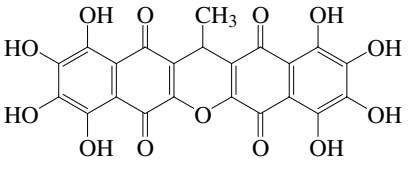
(7*R*,7′*S*,8*S*,8′*R*)-*form*
3,3′,5,5′-Tetra-Me ether, 9- or 9′-O-*β*-D-*glucopyranoside:*
$C_{28}H_{38}O_{14}$ 598.6
Constit. of *Acanthus ilicifolius*. Amorph. powder. $[\alpha]_D^{22}$ -25.5 (c, 1 in MeOH).

(7ξ,7′ξ,8ξ,8′ξ)-*form*
3,3′,5,5′-Tetra-Me ether, 9-O-*β*-D-*xylopyranoside:*
$C_{27}H_{36}O_{13}$ 568.574
Isol. from non-centrifuged cane sugar (*Saccharum officinarum*). Oil.

Matsushita, H. *et al., Phytochemistry*, 1991, **30**, 2025 (*Icariol A2*)
Lin, L.-D. *et al., Huaxue Xuebao*, 1995, **53**, 98; *CA*, **122**, 183194 (*Huazhongilexin*)
Kanchanapoom, T. *et al., Phytochemistry*, 2001, **56**, 369-372 (*Acanthus ilicifolius glucoside*)
Gongora, L. *et al., Phytochemistry*, 2002, **59**, 857-860 (*Phagnalon rupestre glucoside*)
Takara, K. *et al., Biosci., Biotechnol., Biochem.*, 2003, **67**, 376-379 (*cane sugar xyloside*)

1,2,3,4,8,9,10,11-Octahydroxy-13-methyl-12*H*-dibenzo[*b,i*]xanthene-5,7,12,14(13*H*)-tetrone, 8CI O-68

[32669-41-3]

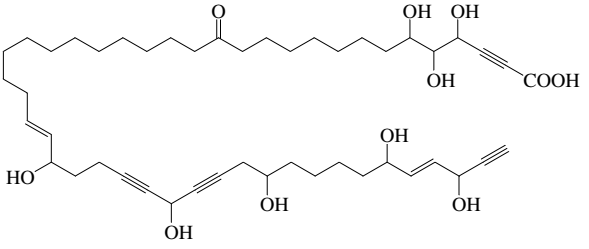


$C_{22}H_{12}O_{13}$ 484.329
Isol. from sea urchins *Spatangus raschi* and *Strongylocentrotus drobachiensis*. Dark red needles (MeOH aq.).
Mp 253-256°. λ_{max} 268 (log ε 4.5); 318 (log ε 4); 468 (log ε 4.12); 491 (log ε 4.1); 523 (log ε 3.95) (EtOH).

Mathieson, J.W. *et al., J.C.S.(C)*, 1971, 153-160 (*isol, ir, pmr, uv*)
Kol'tsova, E.A. *et al., Khim. Prir. Soedin.*, 1978, 438-441; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 371-374 (*isol, pmr*)

4,5,6,28,33,37,42,45-Octahydroxy-14-oxo-26,43-heptatetracontadiene-2,31,34,46-tetraynoic acid O-69

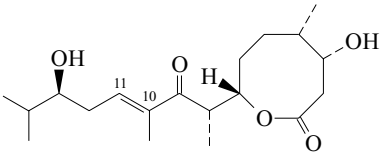
Haliclonyne
[264265-85-2]



$C_{47}H_{72}O_{11}$ 813.079
Isol. from the sponge *Haliclona* sp. Oil.
Chill, L. *et al., J. Nat. Prod.*, 2000, **63**, 523-526

Octalactin B O-70

[133473-07-1]



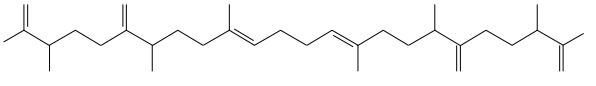
$C_{19}H_{32}O_5$ 340.459
Prod. by a marine *Streptomyces* sp. Cytotoxic agent. Oil. $[\alpha]_D$ -12.3 (c, 5.6 in $CHCl_3$). λ_{max} 236 (ε 10000) (no solvent reported) (Derep).

10β,11β-Epoxide: ***Octalactin A***
[133473-06-0]
$C_{19}H_{32}O_6$ 356.458
Prod. by a marine *Streptomyces* sp. Cryst. ($CHCl_3$/EtOAc). Mp 155-157°. $[\alpha]_D$ -14 (c, 1.8 in $CHCl_3$).

Tapiolas, D.M. *et al., J.A.C.S.*, 1991, **113**, 4682 (*isol, struct*)
Buszek, K.R. *et al., J.A.C.S.*, 1994, **116**, 5511 (*synth*)
McWilliams, J.C. *et al., J.A.C.S.*, 1994, **116**, 8378 (*synth*)
Kodama, M. *et al., Chem. Lett.*, 1997, 117-118 (*Octalactin A, synth*)
Buszek, K.R. *et al., Tet. Lett.*, 2002, **43**, 181-184 (*synth*)
O'Sullivan, P.T. *et al., J.A.C.S.*, 2004, **126**, 2194-2207 (*synth*)
Shiina, I. *et al., Chem. Eur. J.*, 2005, **11**, 6601-6608 (*Octalactin A, synth*)

2,3,7,10,15,18,22,23-Octamethyl-6,19-dimethylene-1,10,14,23-tetracosatetraene O-71

Tetramethylsqualene
[121927-67-1]



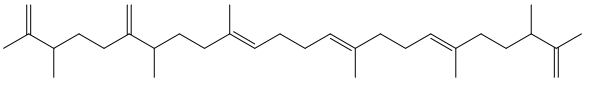
$C_{34}H_{58}$ 466.832
Constit. of *Botryococcus braunii* var. *showa*. Oil. $[\alpha]_D^{25}$ +6 (c, 0.21 in $CHCl_3$).

10,11-Epoxide: 14,15-Epoxy-2,3,7,10,15,18,22,23-octamethyl-6,19-dimethylene-1,10,23-tetracosatriene

[188554-73-6]
$C_{34}H_{58}O$ 482.832
Prod. by *Botryococcus braunii*.
Huang, Z. *et al., Phytochemistry*, 1989, **28**, 1467 (*isol, pmr, ms*)
Delahais, V. *et al., Phytochemistry*, 1997, **44**, 671-678 (*epoxide, pmr, cmr, ms*)
Sato, Y. *et al., Tet. Lett.*, 2003, **44**, 7035-7037 (*biosynth*)

2,3,6,10,15,18,22,23-Octamethyl-19-methylene-1,6,10,14,23-tetracosapentaene O-72

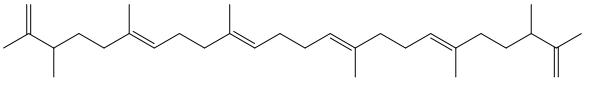
3,7,22-Trimethylsqualene
[827019-99-8]



$C_{33}H_{56}$ 452.805
Constit. of *Botryococcus braunii*.
Achitouv, E. *et al., Phytochemistry*, 2004, **65**, 3159-3165 (*isol, pmr, cmr*)

2,3,6,10,15,19,22,23-Octamethyl-1,6,10,14,18,23-tetracosahexaene O-73

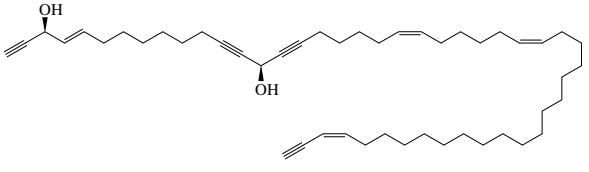
3,22-Dimethylsqualene
[825610-42-2]



$C_{32}H_{54}$ 438.779
Constit. of *Botryococcus braunii*.
Achitouv, E. *et al., Phytochemistry*, 2004, **65**, 3159-3165 (*isol, pmr, cmr*)

4,21,27,45-Octatetracontatetraene-1,12,15,47-tetrayne-3,14-diol O-74

Dihomopetrocortyne A

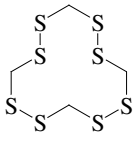


$C_{48}H_{74}O_2$ 683.111

(3S,4E,14S,21Z,27Z,45Z)-form
Isol. from the sponge *Petrosia* sp. Cytotoxic. Yellow oil. $[\alpha]_D^{23}$ +10 (c, 1 in MeOH). λ_{max} 223 (log ϵ 3.9) (MeOH).
Lim, Y.J. *et al., J. Nat. Prod.*, 2001, **64**, 1565-1567

1,2,4,5,7,8,10,11-Octathiacyclododecane O-75

[58966-88-4]



$C_4H_8S_8$ 312.635
Constit. of the red alga *Chondria californica*. Needles (CS_2/$CHCl_3$).
Mp 177-178°. Struct. not fully confirmed.
Wratten, S.J. *et al., J.O.C.*, 1976, **41**, 2465-2467 (*isol, pmr, ms*)

16,23-Octatriacontadien-3-one O-76

[81538-84-3]
[132139-53-8]
$H_3C(CH_2)_{13}CH{=}CH(CH_2)_5CH{=}CH(CH_2)_{12}COCH_2CH_3$
$C_{38}H_{72}O$ 544.986
Constit. of the alga *Emiliania huxleyii*. Also found in various marine sediments.
Volkman, J.K. *et al., Phytochemistry*, 1980, **19**, 2619-2622 (*isol*)

1,15,22-Octatriacontatriene O-77

$H_3C(CH_2)_{14}CH{=}CH(CH_2)_5CH{=}CH(CH_2)_{12}CH{=}CH_2$
$C_{38}H_{72}$ 528.987

(15E,22E)-form [211238-45-8]
Isol. from the haptophyte *Emiliania huxleyi*.
Rieley, G. *et al., Lipids*, 1998, **33**, 617-625 (*isol*)

9,16,23-Octatriacontatrien-3-one O-78

[102037-92-3]
[132139-54-9]
$H_3C(CH_2)_{13}CH{=}CH(CH_2)_5CH{=}CH(CH_2)_5CH{=}CH(CH_2)_5COCH_2CH_3$
$C_{38}H_{70}O$ 542.97
Constit. of the alga *Emiliania huxleyi*. Also found in various marine sediments.
Volkman, J.K. *et al., Phytochemistry*, 1980, **19**, 2619-2622 (*isol*)

1,3,5-Octatriene O-79

$H_3CCH_2CH{=}CHCH{=}CHCH{=}CH_2$
C_8H_{12} 108.183

(3E,5E)-form
Sarohornene B
[33580-04-0]
Constit. of male-attractant pheromone from *Sargassum horneri*.
Bp_{60} 67°.

(3E,5Z)-form
Fucoserratene
[40087-61-4]
Female sex attractant from the ova of *Fucus serratus* and *Fucus vesiculosus*. Sol. MeOH, hexane; poorly sol. H_2O. Bp_{40} 56°. λ_{max} 252 (hexane) (Berdy). λ_{max} 254 (ϵ 28180) (cyclohexane) (Berdy).

(3Z,5E)-form
Sarohornene C
[33580-05-1]
Constit. of male-attractant pheromone from *Sargassum horneri*.

(3Z,5Z)-form [40087-62-5]
No phys. props. reported.
Alder, K. *et al., Annalen*, 1957, **608**, 195 (*synth*)
Jaenicke, L. *et al., Chem. Ber.*, 1975, **108**, 225 (*synth*)
Mueller, D.G. *et al., Naturwissenschaften*, 1978, **65**, 389 (*isol*)
Kajiwara, T. *et al., Naturwissenschaften*, 1980, **67**, 612 (*Sarohornenes*)
Jaenicke, L. *et al., Angew. Chem., Int. Ed.*, 1982, **21**, 643 (*rev*)
Baldwin, J.E. *et al., J.A.C.S.*, 1987, **109**, 8051 (*synth, pmr, props*)
Kishi, N. *et al., Tetrahedron*, 1992, **48**, 4087 (*synth*)
Hombeck, M. *et al., Tetrahedron*, 1998, **54**, 11033-11042 (*biosynth*)
Bender, J.D. *et al., J.O.C.*, 2000, **65**, 5396-5402 (*synth, pmr, cmr*)

2,4,6-Octatriene, 9CI O-80

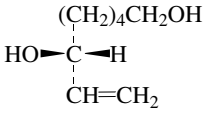
[74842-48-1]
$H_3CCH{=}CHCH{=}CHCH{=}CHCH_3$
C_8H_{12} 108.183
Bp_{100} 84-88° Bp_{44} 66°. Bp refers to isomeric mixt. Pure isomers have been characterised spectroscopically.

(2E,4Z,6Z)-form
Sarohornene
[2417-80-3]
Isol. from brown seaweed *Sargassum horneri*. Gamete attractant present in female receptacles.

[764-75-0, 14947-20-7, 15192-80-0]

Cardenas, C.G. *et al., J.O.C.*, 1970, **35**, 264 (*synth*)
Hasiak, B. *et al., Bull. Soc. Chim. Fr.*, 1974, 2917 (*synth*)
Musco, A. *et al., J. Organomet. Chem.*, 1975, **88**, C41 (*synth*)
Rennekamp, M.E. *et al., Org. Mass Spectrom.*, 1975, **10**, 1075 (*synth, isom*)
Kajiwara, T. *et al., Naturwissenschaften*, 1980, **67**, 612 (*isol*)
Baldwin, J.E. *et al., J.O.C.*, 1988, **53**, 1129 (*synth, pmr, isom*)

7-Octene-1,6-diol O-81



(*R*)-*form*

$C_8H_{16}O_2$ 144.213

(R)-form

6-O-[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]: ***Ebracteatoside D***
[394693-15-3]
$C_{19}H_{34}O_{11}$ 438.471
Constit. of *Acanthus ebracteatus*. Amorph. powder. $[\alpha]_D^{22}$ -57.7 (c, 0.35 in MeOH).

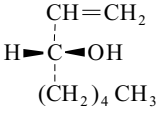
6-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]: ***Ebracteatoside C***
[394693-14-2]
$C_{20}H_{36}O_{12}$ 468.497
Constit. of *Acanthus ebracteatus*. Amorph. powder. $[\alpha]_D^{22}$ -19.8 (c, 2.6 in MeOH).

6-O-[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→6)]-β-D-glucopyranoside]: ***Ilicifolioside B***
[599205-63-7]
$C_{25}H_{44}O_{16}$ 600.613
Constit. of the aerial parts of *Acanthus ilicifolius*. Amorph. powder. $[\alpha]_D^{25}$ -51 (c, 0.6 in MeOH).

Kanchanapoom, T. *et al., Phytochemistry*, 2001, **58**, 811-817 (*Ebracteatosides*)
Wu, J. *et al., Phytochemistry*, 2003, **63**, 491-495 (*Ilicifolioside B*)

1-Octen-3-ol, 9CI O-82

Amyl vinyl carbinol. Matsutake alcohol. Matsutakeol. FEMA 2805
[3391-86-4]



(*R*)–*form*

$C_8H_{16}O$ 128.214
▶ LD_{50} (rat, orl) 340 mg/kg. RH3300000

(R)-form

Isol. from a number of essential oils, e.g. lavender, leek, mint and mushrooms. Food odorant responsible for typical mushroom odour. Flavouring ingredient. Mp 175°. $[\alpha]_D^{20}$ -18.4 (neat) (c, 7.3 in EtOH).

O-*[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→6)]-β-D-glucopyranoside]:* ***Ebracteatoside B***
$C_{25}H_{44}O_{15}$ 584.614
Constit. of *Acanthus ebracteatus*. Amorph. powder. $[\alpha]_D^{22}$ -45 (c, 2.1 in MeOH).

[2442-10-6, 3687-48-7, 24587-53-9, 50999-79-6, 208350-34-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 143C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 215C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 210C (*ir*)
Kanchanapoom, T. *et al., Phytochemistry*, 2001, **58**, 811-817 (*Ebracteatoside B*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ODW000

5-Octen-1-ol, 9CI O-83

$H_3CCH_2CH{=}CH(CH_2)_3CH_2OH$
$C_8H_{16}O$ 128.214

(E)-form [64275-74-7]
Bp_{14} 91.5°.

Ac: [71978-07-9]
$C_{10}H_{18}O_2$ 170.251
Oil.

(Z)-form

FEMA 3722
[64275-73-6]
Constit. of apples, banana, passionfruit and *Michelia champaca*. Liq. with green, fatty odour. d_4^{20} 0.85. Bp_{12} 96-98°. n_D^{20} 1.4472.

Sulfate: [309941-89-7]
$C_8H_{16}O_4S$ 208.278
Isol. from the ascidian *Halocynthia papillosa*. Amorph. solid. Stated as *E*-isomer in parts of text.

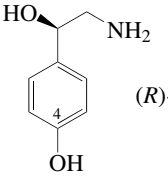
Ac: [71978-00-2]
Constit. of bananas and *Michelia champaca*.
Oil.

Propanoyl: 5-Octenyl propanoate. FEMA 3890
[196109-18-9]
$C_{11}H_{20}O_2$ 184.278
Food flavouring. Liq. with melon, green, fatty odour. $Bp_{0.5}$ 70°.

Ficini, J. *et al., Bull. Soc. Chim. Fr.*, 1956, 119 (*synth*)
Waelchli, P.C. *et al., Helv. Chim. Acta*, 1978, **61**, 885 (*synth, tetrahydropyranyl ethers*)
Brown, D.C. *et al., J.O.C.*, 1979, **44**, 3457 (*E-form, synth*)
Yajima, I. *et al., Agric. Biol. Chem.*, 1984, **48**, 849 (*Z-form, isol, synth, ir, pmr, ms*)
Kaiser, R. *et al., J. Essent. Oil Res.*, 1991, **3**, 129 (*Z-form, isol*)
Aiello, A. *et al., J. Nat. Prod.*, 2000, **63**, 1590-1592 (*isol, sulfate*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1359 (*use*)

Octopamine, INN O-84

*α-(Aminomethyl)-4-hydroxybenzenemethanol, 9CI. α-(Aminomethyl)-*p*-hydroxybenzyl alcohol, 8CI. 2-Amino-1-(4-hydroxyphenyl)ethanol.* p-*(β-Amino-α-hydroxyethyl)phenol. Norden. Norphen. Noroxedrine. Norsympathol. Norsynephrine. WIN 5512. Many other names*
[104-14-3]



(*R*)-*form*

$C_8H_{11}NO_2$ 153.18
▶ LD_{50} (rat, orl) 1240 mg/kg. LD_{50} (mus, ipr) 600 mg/kg. DN7350000

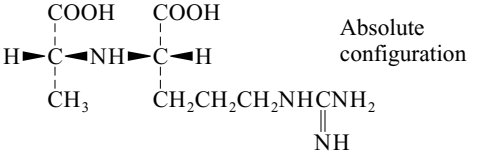
(R)-form [876-04-0]
Alkaloid from leaves of tabasco pepper (*Capsicum frutescens*), leaves or fruit of *Citrus* spp., and leaves of nutgrass (*Cyperus rotundus*) and *Cyperus papyrus* (Solanaceae, Rutaceae, Cyperaceae). Occurs in many animal tissues; found in high concs. in the posterior salivary gland of *Octopus vulgaris*. Invertebrate neurotransmitter. In vertebrates, prob. a cotransmitter with noradrenaline. Adrenergic. Cryst. (H_2O).
Mp 160° approx. $[\alpha]_D^{25}$ -37.4 (c, 1 in H_2O). $[\alpha]_D$ -56 (c, 1 in 1*M* HCl).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1290D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 613B (*nmr*)
Bretschneider, H. *et al., Monatsh. Chem.*, 1949, **80**, 530 (*resoln*)
Corrigan, J.R. *et al., J.A.C.S.*, 1953, **75**, 6258 (*synth*)
Ascher, M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1953, **84**, 1021 (*synth*)
Kappe, T. *et al., J. Med. Chem.*, 1964, **7**, 569 (*resoln*)

Hardwick, B.C. *et al., Plant Physiol.*, 1969, **44**, 1745 (*ir, uv*)
Wheaton, T.A. *et al., Lloydia*, 1970, **33**, 244-254 (*occur*)
Brandau, K. *et al., Naunyn-Schmiedeberg's Arch. Pharmacol.*, 1972, **273**, 123-133 (*biosynth*)
Hengstmann, J.H. *et al., Naunyn-Schmiedeberg's Arch. Pharmacol.*, 1974, **283**, 93 (*metab*)
Paxton, K. *et al., Acta Cryst. B*, 1977, **33**, 2143 (*cryst struct*)
Axelrod, J. *et al., Nature (London)*, 1977, **265**, 501 (*rev*)
Smith, T.A. *et al., Phytochemistry*, 1977, **16**, 9 (*occur*)
Redouane, K. *et al., Agressologie*, 1984, **25**, 3 (*rev*)
Midgley, J.M. *et al., J.C.S. Perkin 2*, 1989, 963-964 (*cryst struct, abs config, bibl*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1250
Lundell, K. *et al., Tetrahedron: Asymmetry*, 2004, **15**, 3723-3729 (*R-form, S-form*)

Octopine O-85

N^2-*(1-Carboxyethyl)arginine, 9CI. Arginine-α-propionic acid. Pectenin*†
[34522-32-2]



$C_9H_{18}N_4O_4$ 246.266
Isol. from aq. extracts of tentacle muscles of *Loligo pealii* and *Octopus vulgaris*, the adductor muscles of the scallop *Pecten magellanicus* and the muscles of the octopod *Eledone moschata*. Needles (H_2O or EtOH aq.).
Mp 281-282° (261-264°). $[\alpha]_D^{17}$ +20.94 (H_2O). Stereoisomers have been synthesised.

Cu salt: Mp 223-227° dec.

Ni salt: Mp 290°.

Picrate: Mp 226-230° dec.

Izumiya, N. *et al., J.A.C.S.*, 1957, **79**, 652 (*synth*)
Biellmann, J.F. *et al., Bioorg. Chem.*, 1977, **6**, 89 (*synth, abs config*)
Goto, K. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 261 (*synth, abs config*)

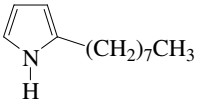
Octopine dehydrogenase O-86

E.C. 1.5.1.11. N^2-*(D-1-Carboxyethyl)-L-arginine:NAD⊕ oxidoreductase (L-arginine-forming). D-Octopine synthase*
[37256-27-2]
Oxidoreductase enzyme. Isol. from the King scallop *Pecten maximus* and from *Nicotiana tabacum* crown gall tumour. Catalyses the reversible reaction of Octopine, O-85 with NAD⊕ and H_2O to give pyruvate and NADH.

Nguyen-Van-Thoai, *et al., Biochim. Biophys. Acta*, 1969, **191**, 46-57 (*Pecten maximus*)
Monneuse-Doublet, M.O. *et al., Eur. J. Biochem.*, 1980, **108**, 261-269 (*Pecten maximus*)
Schrimsher, J.L. *et al., J. Biol. Chem.*, 1982, **257**, 8953-8956 (*Nicotiana tabacum crown gall tumour*)

2-Octylpyrrole, 9CI O-87

[158697-97-3]



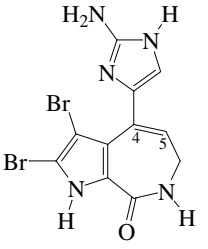
$C_{12}H_{21}N$ 179.305
No phys. props. reported.

N-*Sulfo: 2-Octylpyrrole sulfamate*
[587875-51-2]
$C_{12}H_{21}NO_3S$ 259.369
Alkaloid from the marine annelid *Cirriformia tentaculata*. Glass (as Na salt). CAS no. refers to Na salt.

Garrido, D.O.A. *et al., J.O.C.*, 1984, **49**, 2619-2622 (*synth*)
Barsby, T. *et al., J. Nat. Prod.*, 2003, **66**, 1110-1112 (*sulfamate*)

Odiline O-88

Stevensine
[99102-22-4]



$C_{11}H_9Br_2N_5O$ 387.033
Metab. from the New Caledonian sponge *Pseudaxinyssa cantharella* and from *Ptilocaulis walpersi* and *Teichaxinella morchella*. Also isol. (as Stevensine) from an unidentified Micronesian sponge. Amorph. $[\alpha]_D$ +28 (c, 0.84 in MeOH).

4ξ,5-Dihydro: ***Hymenine***†
[105748-62-7]
$C_{11}H_{11}Br_2N_5O$ 389.049
Isol. from the Okinawan marine sponge *Hymeniacidon* sp. Potent α-adrenoceptor blocking agent. Amorph. solid. $[\alpha]_D^{25}$ -15 (c, 0.5 in MeOH). λ_{max} 274 (ε 9200) (MeOH) (Derep).

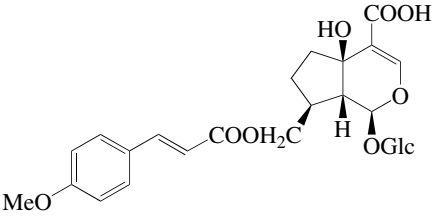
2-Debromo: ***2-Debromoodiline***. *2-Debromostevensine*
$C_{11}H_{10}BrN_5O$ 308.137
Isol. from the sponge *Stylissa carteri*. Amorph. orange solid.
λ_{max} 232 (log ε 3.84); 263 (log ε 3.62); 288 (log ε 3.37) (MeOH).

2-Debromo, 4ξ,5-dihydro: ***2-Debromohymenine***
$C_{11}H_{12}BrN_5O$ 310.153
Isol. from the sponge *Stylissa carteri*. Amorph. brown solid.
λ_{max} 220 (log ε 3.86); 269 (log ε 3.64) (MeOH).

Albizati, K.F. *et al., J.O.C.*, 1985, **50**, 4163-4164 (*isol, uv, ir, pmr, cmr*)
de Nanteuil, G. *et al., Tetrahedron*, 1985, **41**, 6019-6033 (*isol, cd, uv, ir, pmr, cmr, ms*)
Kobayashi, J. *et al., Experientia*, 1986, **42**, 1064-1065 (*Hymenine*)
Xu, Y.-Z. *et al., J.O.C.*, 1997, **62**, 456-464 (*Hymenine, Stevensine, synth*)
Eder, C. *et al., J. Nat. Prod.*, 1999, **62**, 184-187 (*2-Debromoodiline, 2-Debromohymenine*)
Andrade, P. *et al., Tet. Lett.*, 1999, **40**, 4775-4778 (*biosynth*)

Officinosidic acid O-89

[176226-57-6]

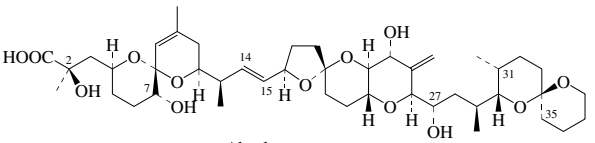


$C_{26}H_{32}O_{13}$ 552.531
Constit. of *Avicennia officinalis*.
$[\alpha]_D^{25}$ -53.1 (c, 0.5 in $CHCl_3$) (penta-Ac).

Sharma, M. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 459-462 (*isol, pmr, cmr*)

Okadaic acid O-90

9,10-Deepithio-9,10-didehydroacanthifolicin. PL toxin II
[78111-17-8]



Absolute Configuration

$C_{44}H_{68}O_{13}$ 805.013
Found in the marine sponges *Halichondria okadai*, *Halichondria melanodocia*, *Pandaros acanthifolium*, *Phakellia* sp., mussel *Mytilus edulis* and other marine organisms. A prod. of symbiotic/endophytic dinoflagellates *Prorocentrum lima* and *Dinophysis fortii*. Diarrhetic shellfish toxin. Mammalian toxin. Shows cytotoxic props. against human epidermoid carcinoma. Cryst. (C_6H_6/$CHCl_3$). Sol. MeOH, hexane; poorly sol. H_2O, hexane. Mp 164-166°. $[\alpha]_D^{20}$ +53.3 (c, 0.182 in $CHCl_3$).

▶ LD_{50} (mus, ipr) 0.192 mg/kg. AA8227800

Me ester: [78111-14-5]
Cryst. (hexane/C_6H_6). Mp 127-133°. $[\alpha]_D^{25}$ +28 (c, 0.38 in $CHCl_3$).

p-*Bromophenacyl ester:* Mp 134-135°.

3-Hydroxy-2-methylenepropyl ester:
$C_{48}H_{74}O_{14}$ 875.104
Isol. from *Prorocentrum lima* strain PLV2. Amorph. powder. $[\alpha]_D^{25}$ -15 (c, 0.02 in $CHCl_3$). CAS No. not found to 2006.

*5-Hydroxy-2-methylene-3*E*-pentenyl ester:* [851596-25-3]
$C_{50}H_{76}O_{14}$ 901.142
Isol. from an artificial culture of *Prorocentrum lima*. Amorph. powder. $[\alpha]_D^{25}$ +26.6 (c, 0.04 in $CHCl_3$). λ_{max} 205 (log ϵ 4.19) (EtOH).

4-Formyl-2-methylene-4-pentenyl ester: ***DTX6***
[379699-87-3]
$C_{51}H_{76}O_{14}$ 913.153
Isol. from a *Prorocentrum lima* strain PLV2. Amorph. powder. $[\alpha]_D^{25}$ +3.3 (c, 0.1 in $CHCl_3$). λ_{max} 242; 270 (EtOH).

6-Hydroxy-2-methylene-4-hexenyl ester: [109137-88-4]
$C_{51}H_{78}O_{14}$ 915.169
Isol. from the benthic dinoflagellate *Prorocentrum lima*.

*6-Hydroxy-2-methyl-2*E*,4*E*-hexadienyl ester:* [145781-81-3]
$C_{51}H_{78}O_{14}$ 915.169
Isol. from *Prorocentrum concavum*.

5ξ,7-Dihydroxy-2,4-bis(methylene)heptyl ester: [851606-66-1]
$C_{53}H_{82}O_{15}$ 959.222
Isol. from an artificial culture of *Prorocentrum lima*. Amorph. powder. $[\alpha]_D^{25}$ +10 (c, 0.1 in $CHCl_3$).

5ξ-Hydroperoxy-7-hydroxy-2,4-bis(methylene)heptyl ester:
[851606-67-2]
$C_{53}H_{82}O_{16}$ 975.221
Isol. from an artificial culture of *Prorocentrum lima*. Amorph. solid. $[\alpha]_D^{25}$ +10 (c, 0.06 in $CHCl_3$).

*7-Hydroxy-2-methyl-2*E*,4*E*-heptadienyl ester:* [145814-30-8]
$C_{52}H_{80}O_{14}$ 929.196
Isol. from the benthic dinoflagellates *Prorocentrum concavum* and *Prorocentrum lima*.

*7-Hydroxy-2,4-dimethyl-2*E*,4*E*-heptadienyl ester:* [157376-74-4]
$C_{53}H_{82}O_{14}$ 943.222
Isol. from the dinoflagellate *Prorocentrum lima*. Enzyme inhibitor. Amorph. powder. $[\alpha]_D$ +21.4 (c, 0.5 in $CHCl_3$). λ_{max} 264 (ϵ 14822) (EtOH) (Berdy).

▶ Toxic, tumour promotor.

*7-Hydroxy-4-methyl-2-methylene-4*E*-heptenyl ester:* [145814-31-9]
$C_{53}H_{82}O_{14}$ 943.222
Isol. from *Prorocentrum lima*. Enzyme inhibitor. Amorph. powder. $[\alpha]_D$ +17.3 (c, 0.1 in $CHCl_3$). λ_{max} 263 (EtOH) (Berdy).

▶ Toxic, tumour promotor.

8-Hydroxy-2,7-bis(methylene)-4Z-octenyl ester: [851596-26-4]
$C_{54}H_{82}O_{14}$ 955.233
Isol. from an artificial culture of *Prorocentrum belizeanum*. Amorph. powder. $[\alpha]_D^{25}$ +8.4 (c, 0.24 in $CHCl_3$).

Glycine amide: ***Glycookadaic acid***
[123764-98-7]
$C_{46}H_{71}NO_{14}$ 862.065
Isol. from *Halichondria melanodocia* and *Halichondria okadai*.

27-Ac: ***27-O-Acetylokadaic acid***
[581784-57-8]
$C_{46}H_{70}O_{14}$ 847.051
Isol. from the marine sponge *Merriamum oxeato*.

Tetra-Ac: [78111-15-6]
$[\alpha]_D^{20}$ +153 (c, 1.4 in $CHCl_3$).

7-Deoxy: ***7-Deoxyokadaic acid***
[136993-62-9]
$C_{44}H_{68}O_{12}$ 789.014
Isol. from *Prorocentrum lima*. Antifungal and cytotoxic agent. Cryst.

Decarboxy, 2-ketone: ***Norokadanone***
[131204-29-0]
$C_{43}H_{66}O_{11}$ 758.988
Isol. from *Prorocentrum lima* strain PLV2. Amorph. powder. $[\alpha]_D^{25}$ +9.8 (c, 0.06 in $CHCl_3$). λ_{max} 242; 270 (EtOH).

*35*R*-Methyl:* ***Dinophysistoxin 1***. *DTX1*
[81720-10-7]
$C_{45}H_{70}O_{13}$ 819.04
Metab. of *Dinophysis fortii*. Found in scallops and mussels. Component toxin in diarrhetic shellfish poisoning. Solid. Sol. MeOH, C_6H_6; poorly sol. hexane.
Mp 134°. $[\alpha]_D^{20}$ +28.

*35*R*-Methyl, 27-Ac:* ***27-O-Acetyldinophysistoxin 1***
[581784-59-0]
$C_{47}H_{72}O_{14}$ 861.077
Isol. from the marine sponge *Merriamum oxeato*.

*35*R*-Methyl, 14,15-dihydro:* ***14,15-Dihydrodinophysistoxin 1***
[165054-89-7]
$C_{45}H_{72}O_{13}$ 821.056
Isol. from a sponge of the *Phakellia* sp. Amorph. solid. $[\alpha]_D^{25}$ +19 (c, 0.4 in $CHCl_3$).

*35*S*-Methyl, 7-*O*-acyl:* ***Dinophysistoxin 3***. *DTX3*
[97559-94-9]
Metab. of *Dinophysis acuminata*. Found in scallops and mussels. Component toxin of diarrhetic shellfish poisoning. Solid. Contains 13% C_{14}, 29% C_{16}, 12% C_{18}, 23% C_{20} and 23% C_{22} fatty acids.

▶ LD_{50} (mus, ipr) 800 mg/kg.

*35*S*-Methyl, 7-*O*-hexadecanoyl:* [97564-96-0]
$C_{61}H_{100}O_{14}$ 1057.453
Rel. nontoxic artifact formed from Dinophysistoxin 3 on standing. Prod. by *Prorocentrum lima* and *Patinopecten yessonensis*. Solid.
Mp 78°. $[\alpha]_D^{20}$ +5.9 (c, 0.041 in $CHCl_3$).

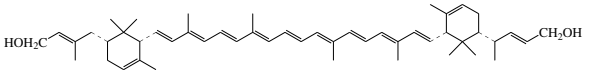
*31-Demethyl, 35*R*-methyl:* ***Dinophysistoxin 2***. *DTX2*
[139933-46-3]
$C_{44}H_{68}O_{13}$ 805.013
Metab. of *Dinophysis* spp. and *Mytilus edulis*. Diarrhetic shellfish poison. Amorph. solid.
Mp 128-130°. $[\alpha]_D$ +15.49 (c, 0.213 in $CHCl_3$).

Tachibana, K. *et al., J.A.C.S.*, 1981, **103**, 2469 (*isol, cryst struct, spectra*)
Japan. Pat., 1982, 82 11 986; *CA*, **96**, 217820
Murakami, W. *et al., Nippon Suisan Gakkaishi*, 1982, **48**, 69; *CA*, **96**, 139; 380 (*isol*)
Muraka, W. *et al., Nippon Suisan Gakkaishi*, 1982, **48**, 549; *CA*, **97**, 52852 (*deriv*)
Yasumoto, T. *et al., Tetrahedron*, 1985, **41**, 1019 (*deriv*)
Yasumoto, T. *et al., Biol. Bull. (Woods Hole, Mass.)*, 1987, **172**, 128-131 (*6-hydroxy-2-methylene-4-hexenyl ester*)
Ichikawa, Y. *et al., Tetrahedron*, 1987, **43**, 4737; 4742; 4749; 4759 (*synth*)
Nagai, H. *et al., J. Appl. Phycol.*, 1990, **2**, 305-308 (*7-Deoxyokadaic acid*)
Norte, M. *et al., Tetrahedron*, 1991, **47**, 7437; 1994, **50**, 9175 (*pmr, cmr, esters*)
Hu, T. *et al., Chem. Comm.*, 1992, 39 (*Dinophysistoxin 2*)
Hu, T. *et al., J. Nat. Prod.*, 1992, **55**, 1631 (*esters*)
Norte, M. *et al., Tet. Lett.*, 1994, **35**, 1441 (*Dinophysistoxin 1*)

Sakai, R. *et al., J. Nat. Prod.*, 1995, **58**, 773 (*Dihydrodinophysistoxin 1*)
Matsumori, N. *et al., Tetrahedron*, 1995, **51**, 12229 (*nmr, conformn*)
Forsyth, C.J. *et al., J.A.C.S.*, 1997, **119**, 8381-8382 (*synth*)
Urbanek, R.A. *et al., J.A.C.S.*, 1998, **120**, 2523-2533; 2534-2542 (*synth*)
Ley, S.V. *et al., J.C.S. Perkin 1*, 1998, 3907-3911 (*synth*)
Perry, N.B. *et al., Nat. Prod. Lett.*, 1998, **11**, 305-312 (*Glycookadaic acid*)
Leftley, J.W. *et al., Natural Toxicants in Food*, (ed. Watson, D.H.), CRC Press, 1998, 182-224 (*rev*)
Dounay, A.B. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 2258-2262, (*7-Deoxyokadaic acid, synth*)
Food Sci. Technol., *Seafood and Freshwater Toxins*, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*revs*)
Suárez-Gómez, B. *et al., J. Nat. Prod.*, 2001, **64**, 1363-1364; **68**, 596-599 (*esters*)
Britton, R. *et al., J. Nat. Prod.*, 2003, **66**, 838-843 (*27-Acetylokadaic acid, 27-Acetyldinophysistoxin 1*)
Fernández, J.J. *et al., J. Nat. Prod.*, 2003, **66**, 1294-1296 (*Me ester, Norokadanone, hydroxymethylenepropyl ester*)

Okadaxanthin O-91

2,2′-Bis(4-hydroxy-2-methyl-2-butenyl)-ϵ,ϵ-carotene

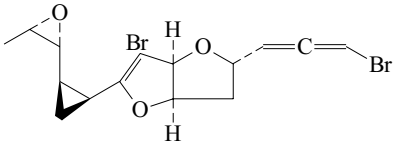


$C_{50}H_{72}O_2$ 705.118
Constit. of *Halichondria okadai* and a *Pseudomonas* sp. Red powder. λ_{max} 414; 437; 467 (hexane). λ_{max} 414; 438; 468 (MeOH).

Miki, W. *et al., Experientia*, 1994, **50**, 684-686 (*isol, pmr*)

Okamurallene O-92

[80539-33-9]

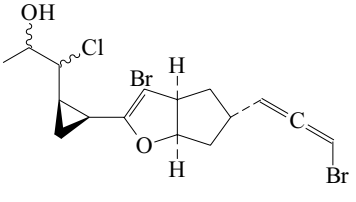


$C_{15}H_{16}Br_2O_3$ 404.098
Constit. of *Laurencia okamurai*. Oil. $[\alpha]_D^{26}$ +160 (c, 1.74 in $CHCl_3$).

Suzuki, M. *et al., Tet. Lett.*, 1981, **22**, 3853 (*isol*)
Suzuki, M. *et al., Phytochemistry*, 1989, **28**, 2145 (*cmr, struct*)
Suzuki, M. *et al., Chem. Lett.*, 1991, 33 (*abs config, cryst struct*)

Okamurallene chlorohydrin O-93

[123297-19-8]

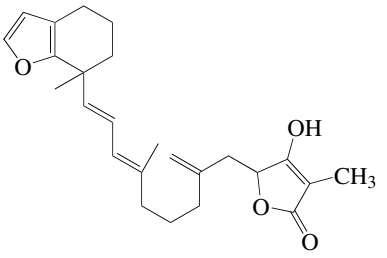


$C_{15}H_{17}Br_2ClO_3$ 440.558
Metab. of *Laurencia intricata*. Cryst. (hexane).
Mp 71-72°. $[\alpha]_D^{18}$ +205 (c, 0.325 in CCl_4).

Suzuki, M. *et al., Phytochemistry*, 1989, **28**, 2145 (*isol, pmr, cmr*)

Okinonellin A O-94

[107656-78-0]

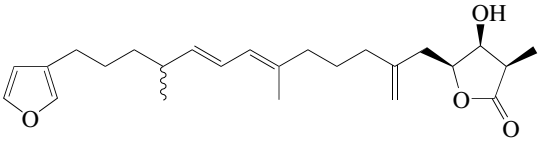


$C_{25}H_{32}O_4$ 396.525
Isol. from the marine sponge *Spongionella* sp. Labile oil. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{20}$ +42.5 (c, 0.08 in EtOH). λ_{max} 243 (ϵ 26000) (EtOH).

Kato, Y. *et al., Experientia*, 1986, **42**, 1299-1300 (*isol, uv, ir, pmr, cmr*)

Okinonellin B O-95

[107585-45-5]

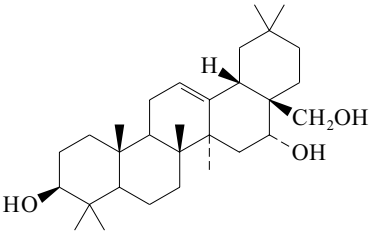


Relative Configuration

$C_{25}H_{36}O_4$ 400.557
Isol. from the marine sponge *Spongionella* sp. Oil. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{20}$ +17.9 (c, 0.15 in EtOH). λ_{max} 240 (ϵ 24000) (EtOH).

Kato, Y. *et al., Experientia*, 1986, **42**, 1299-1300 (*isol, uv, ir, pmr, cmr*)

12-Oleanene-3,16,28-triol O-96



(3β,16α)–*form*

$C_{30}H_{50}O_3$ 458.723

(3β,16α)-*form*
Primulagenin A. *Armillarisgenin C. Schiwalligenin B_1*
[465-95-2]
Constit. of *Primula officinalis, Aegiceras corniculatum, Jacquinia* spp. and other plants.
Cryst. ($CHCl_3$/MeOH).
Mp 249.5-250°. $[\alpha]_D$ +58 (c, 0.7 in $CHCl_3$). Identity of Primulagenin A and Armillarisgenin C not definitely confirmed.

Hensens, O.D. *et al., Tet. Lett.*, 1965, **6**, 4639-4643 (*Aegiceras corniculatum constit*)
Itô, S. *et al., Tet. Lett.*, 1969, 2905-2908 (*pmr*)
Allen, J. *et al., J.C.S. Perkin 1*, 1972, 2994-3001 (*Primulagenin A, synth*)
Baigert, D.R. *et al., Aust. J. Chem.*, 1978, **31**, 1375-1381 (*isol*)

1,3-β-Oligoglucan phosphorylase O-97

E.C. 2.4.1.30. 1,3-β-D-Oligoglucan:phosphate α-D-glucosyltransferase

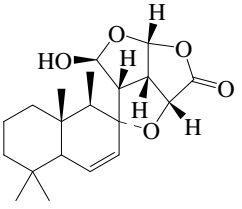
[37257-28-6]

Hexosyltransferase enzyme. Isol. from *Euglena gracilis*. Catalyses the reversible reaction of $[(1,3)\text{-}\beta\text{-D-glucosyl}]_n$ with orthophosphate to give $[(1,3)\text{-}\beta\text{-D-glucosyl}]_{n-1}$ and α-D-glucose 1-phosphate.

Marechal, L.R. *et al., Biochim. Biophys. Acta*, 1967, **146**, 417-430; 431-442
Goldemberg, S.H. *et al., Methods Enzymol.*, 1972, **28**, 953-960

Omriolide A O-98

[871943-97-4]



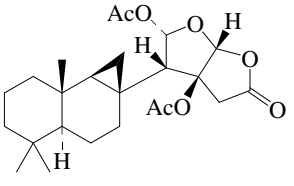
$C_{20}H_{28}O_5$ 348.438

Constit. of *Dictyodendrilla* aff. *retiara*. Oil. $[\alpha]_D$ -18 (c, 0.005 in CH_2Cl_2).

Rudi, A. *et al., Tet. Lett.*, 2005, **46**, 8613-8616 (*Omriolide A*)

Omriolide B O-99

[871943-98-5]



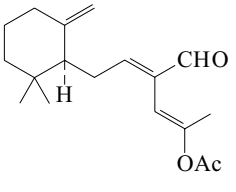
$C_{24}H_{34}O_7$ 434.528

Constit. of *Dictyodendrilla* aff. *retiara*. Oil. $[\alpha]_D$ -10 (c, 0.007 in CH_2Cl_2).

Rudi, A. *et al., Tet. Lett.*, 2005, **46**, 8613-8616 (*Omriolide B*)

Onchidal O-100

[67656-42-2]



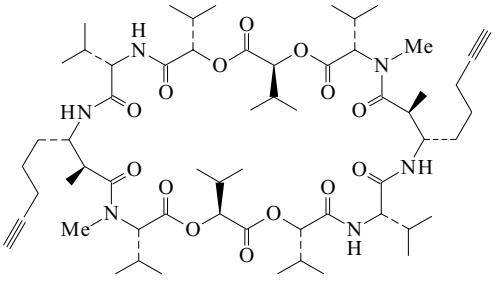
$C_{17}H_{24}O_3$ 276.375

Constit. of *Onchidella binneyi*. Oil. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{22}$ +17.2 (c, 1 in $CHCl_3$). λ_{max} 235; 260 (solvent not reported) (Derep). λ_{max} 235; 260 (MeOH) (Berdy).

Ireland, C. *et al., Bioorg. Chem.*, 1978, **7**, 125-131 (*isol*)

Onchidin O-101

[161779-98-2]



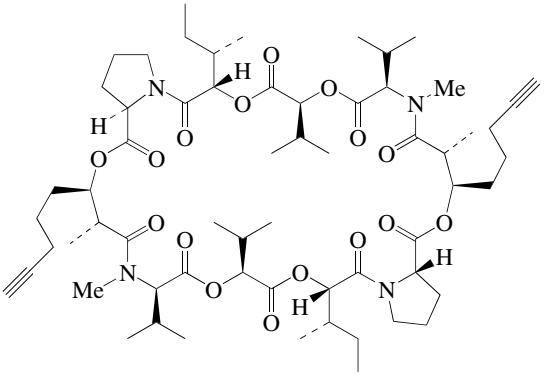
$C_{60}H_{98}N_6O_{14}$ 1127.466

Depsipeptide antibiotic. Stereochemistry assigned above has been shown to be incorrect by synth. (2004). Isol. from a pulmonate mollusc *Onchidium* sp. Cytotoxic agent. Sol. MeOH. $[\alpha]_D^{25}$ -140.9.

Rodriguez, J. *et al., Tet. Lett.*, 1994, **35**, 9239-9242 (*isol, pmr, cmr, ms*)
Peng, Y. *et al., Org. Lett.*, 2004, **6**, 3781-3784 (*synth*)

Onchidin B O-102

[183731-02-4]



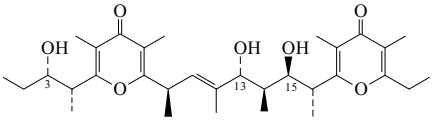
$C_{62}H_{96}N_4O_{16}$ 1153.458

Depsipeptide antibiotic. Isol. from the mollusc *Onchidium* sp. Cytotoxic agent. $[\alpha]_D^{25}$ -220.1 (c, 0.1 in $CHCl_3$).

Fernandez, R. *et al., J.A.C.S.*, 1996, **118**, 11635-11643 (*isol, pmr, cmr*)

Onchitriol I O-103

[140924-47-6]



$C_{32}H_{48}O_7$ 544.727

Stereochem. revised in 1995. Constit. of an *Onchidium* mollusc. $[\alpha]_D$ -20 (c, 0.01 in CH_2Cl_2). λ_{max} 260 (ε 12000) (MeOH) (Derep). λ_{max} 260 (MeOH) (Berdy).

13,15-Di-Ac: ***Onchitriol IA***

[142132-12-5]

$C_{36}H_{52}O_9$ 628.801

Constit. of *Onchidium* sp.

$[\alpha]_D$ -11.5 (c, 0.02 in CH_2Cl_2). λ_{max} 259 (MeOH) (Berdy).

13-Propanoyl, 15-Ac: ***Onchitriol IB***

[142159-63-5]

$C_{37}H_{54}O_9$ 642.828

From *Onchidium* sp.

$[\alpha]_D$ -19.5 (c, 0.01 in CH_2Cl_2). λ_{max} 260 (MeOH) (Berdy).

15-Propanoyl, 13-Ac: ***Onchitriol IC***
[142132-13-6]
$C_{37}H_{54}O_9$ 642.828
From *Onchidium* sp.
$[\alpha]_D$ -18 (c, 0.1 in CH_2Cl_2). λ_{max} 260 (MeOH) (Berdy).

13,15-Dipropanoyl, 3-Ac: ***Onchitriol ID***
[142132-14-7]
$C_{40}H_{58}O_{10}$ 698.892
From *Onchidium* sp.
$[\alpha]_D$ -25.2 (c, 0.01 in CH_2Cl_2). λ_{max} 260 (MeOH) (Berdy).

4,13-Diepimer: ***Onchitriol II***
[140924-48-7]
$C_{32}H_{48}O_7$ 544.727
Constit. of an *Onchidium* mollusc. Cytotoxic agent. $[\alpha]_D$ -33 (c, 0.01 in $CHCl_3$). λ_{max} 260 (ϵ 12000) (MeOH) (Derep). λ_{max} 260 (MeOH) (Berdy).

4,13-Diepimer, 15-Ac: ***Onchitriol IIA***
[140849-45-2]
$C_{34}H_{50}O_8$ 586.764
From *Onchidium* sp.
$[\alpha]_D$ -26 (c, 0.1 in CH_2Cl_2). λ_{max} 260 (MeOH) (Berdy).

4,13-Diepimer, 15-propanoyl: ***Onchitriol IIB***
[142132-15-8]
$C_{35}H_{52}O_8$ 600.791
From *Onchidium* sp.
$[\alpha]_D$ -25.2 (c, 0.01 in CH_2Cl_2). λ_{max} 260 (MeOH) (Berdy).

4,13-Diepimer, tri-Ac: ***Onchitriol IIC***
[142132-16-9]
$C_{38}H_{54}O_{10}$ 670.839
From *Onchidium* sp.
$[\alpha]_D$ -26 (c, 0.01 in CH_2Cl_2). λ_{max} 260 (MeOH) (Berdy).

4,13-Diepimer, 3,15-di-Ac: ***Onchitriol IID***
[85589-35-1]
$C_{36}H_{52}O_9$ 628.801
From *Onchidium* sp.
$[\alpha]_D$ -20 (c, 0.1 in CH_2Cl_2). λ_{max} 260 (MeOH) (Berdy).

3,4,10-Triepimer: ***Peroniatriol I***
[99102-19-9]
$C_{32}H_{48}O_7$ 544.727
Metab. of the mollusc *Peronia peronii*. Cytotoxic agent. Sol. MeOH, $CHCl_3$, CH_2Cl_2; poorly sol. H_2O, hexane. $[\alpha]_D$ -12.4 (c, 1.2 in CH_2Cl_2). λ_{max} 259 (ϵ 13000) (CH_2Cl_2) (Berdy).

3,10,13-Triepimer: ***Peroniatriol II***
[99147-38-3]
$C_{32}H_{48}O_7$ 544.727
Metab. of *Peronia peronii*. Cytotoxic agent. Sol. MeOH, $CHCl_3$, CH_2Cl_2; poorly sol. H_2O, hexane. $[\alpha]_D$ +224.8 (c, 1 in CH_2Cl_2). λ_{max} 259 (ϵ 13000) (CH_2Cl_2) (Berdy).

Biskupiak, J.E. *et al., Tet. Lett.*, 1985, **26**, 4307-4310 (*Peroniatriols*)
Arimoto, H. *et al., Tet. Lett.*, 1990, **31**, 5491; 1995, **36**, 5357-5358 (*Peroniatriols, synth, abs config*)
Rodriguez, J. *et al., J.O.C.*, 1992, **57**, 4624-4632 (*isol, pmr, cmr, ms*)
Rodriguez, J. *et al., Tet. Lett.*, 1992, **33**, 1089-1092 (*abs config*)
Arimoto, H. *et al., Tet. Lett.*, 1993, **34**, 5781-5784 (*Peroniatriols I,II*)

Oncorhyncin II O-104

Peptide contg. 69 amino acid residues, probably phosphorylated at 2 residues; a C-terminal fragment of histone H1. Isol. from an acid extract of skin secretions of the rainbow trout *Oncorhynchus mykiss*. Shows antimicrobial activity.

Fernandes, J.M. *et al., Dev. Comp. Immunol.*, 2004, **28**, 127-138 (*isol, struct*)

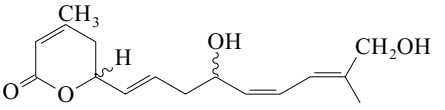
Oncorhyncin III O-105

Peptide comprising residues 1-66 of the non-histone chromosomal protein H6. Isol. from an acid extract of skin secretions of the rainbow trout *Oncorhynchus mykiss*. Shows antimicrobial activity.

Fernandes, J.M. *et al., Biochem. J.*, 2003, **373**, 621-628 (*isol, struct*)

Oncorhyncolide O-106

*6-(4,9-Dihydroxy-8-methyl-1,5,7-nonatrienyl)-5,6-dihydro-4-methyl-2*H*-pyran-2-one, 9CI*
[132916-09-7]

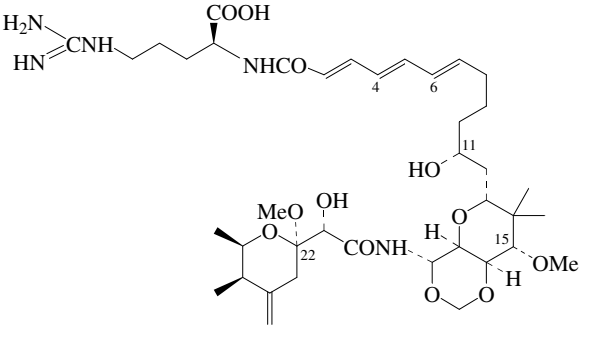


$C_{16}H_{22}O_4$ 278.347
Metab. of a marine bacterium. Unstable oil. $[\alpha]_D$ -36 (c, 3.1 in MeOH).

Needham, J. *et al., Tet. Lett.*, 1991, **32**, 315 (*isol, pmr, cmr*)
Needham, J. *et al., Chem. Comm.*, 1992, 1367 (*biosynth*)

Onnamide A O-107

[115204-07-4]



$C_{39}H_{63}N_5O_{12}$ 793.953
Numbering systems vary. Constit. of the sponge *Theonella* sp. Antitumour and antiviral agent. Pale yellow solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ +99.1 (c, 5.5 in MeOH). Related to Mycalamides. λ_{max} 202 (ϵ 7500); 299 (ϵ 38800) (MeOH) (Derep).

4Z-Isomer: ***4Z-Onnamide A***
$C_{39}H_{63}N_5O_{12}$ 793.953
Isol. from *Theonella* sp. Solid. $[\alpha]_D^{23}$ +81 (c, 0.59 in MeOH). λ_{max} 300 (ϵ 5900) (MeOH) (Berdy).
▶ Exhibits cytotoxicity.

*15-*O*-De-Me:* ***15-De-O-methylonnamide****. 13-*O*-Demethylonnamide*
[145781-30-2]
$C_{38}H_{61}N_5O_{12}$ 779.926
Constit. of *Theonella* sp. Cytotoxic agent. Glassy solid. Sol. MeOH, butanol; poorly sol. H_2O. $[\alpha]_D^{23}$ +70 (c, 0.1 in MeOH). λ_{max} 298 (ϵ 29000) (MeOH).

*22-*O*-De-Me:* ***Pseudoonnamide A***
[145757-40-0]
$C_{38}H_{61}N_5O_{12}$ 779.926
Constit. of the sponge *Theonella* sp. Glassy solid. $[\alpha]_D^{23}$ +64 (c, 0.05 in MeOH). λ_{max} 298 (ϵ 26200) (MeOH).

11-Oxo: ***11-Oxoonnamide A***
$C_{39}H_{61}N_5O_{12}$ 791.937
Isol. from *Theonella* sp. Solid. $[\alpha]_D^{23}$ +90 (c, 0.24 in MeOH). λ_{max} 298 (ϵ 39700) (MeOH) (Berdy).
▶ Exhibits cytotoxicity.

6,7-Dihydro: ***6,7-Dihydroonnamide A***
$C_{39}H_{65}N_5O_{12}$ 795.969
Constit. of the Okinawan marine sponge *Theonella* sp. Sol. MeOH, butanol; poorly sol. H_2O. λ_{max} 260 (ϵ 22000) (MeOH) (Berdy).
▶ Exhibits cytotoxicity. Skin irritant.

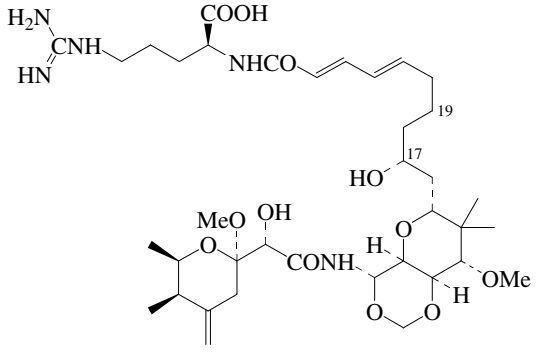
6,7-Dihydro, 11-oxo: ***6,7-Dihydro-11-oxoonnamide A***
$C_{39}H_{63}N_5O_{12}$ 793.953
Isol. from *Theonella* sp. Solid. $[\alpha]_D^{24}$ +39 (c, 0.42 in MeOH). λ_{max} 263 (ϵ 22700) (MeOH) (Berdy).

▶ Exhibits cytotoxicity.

Sakemi, S. *et al., J.A.C.S.*, 1988, **110**, 4851 (*isol, uv, pmr, cmr*)
Hong, C.Y. *et al., J.A.C.S.*, 1991, **113**, 9693 (*synth*)
Matsunaga, S. *et al., Tetrahedron*, 1992, **48**, 8369 (*6,7-Dihydroonnamide A*)
Kobayashi, J. *et al., J. Nat. Prod.*, 1993, **56**, 976 (*6,7-Dihydro-11-oxoonnamide A, 11-Oxoonnamide A, 4Z-Onnamide A*)

Onnamide B O-108

[145757-35-3]



$C_{37}H_{61}N_5O_{12}$ 767.915
Constit. of the sponge *Theonella* sp. Cytotoxic agent. Glassy solid. Sol. MeOH, butanol; poorly sol. H_2O. $[\alpha]_D^{23}$ +61.8 (c, 0.5 in MeOH). λ_{max} 260 (ϵ 16000) (MeOH).

▶ Skin irritant.

17-Ketone: ***17-Oxoonnamide B***
[145757-36-4]
$C_{37}H_{59}N_5O_{12}$ 765.899
Constit. of the sponge *Theonella* sp. Cytotoxic agent. Glassy solid. Sol. MeOH, butanol; poorly sol. H_2O. $[\alpha]_D^{23}$ +59.7 (c, 0.2 in MeOH). λ_{max} 260 (ϵ 20000) (MeOH).

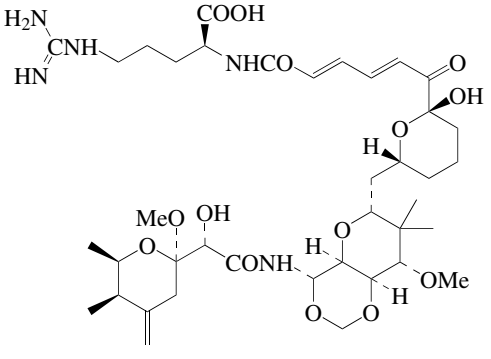
▶ Skin irritant.

*18,19-Didehydro(*E-*):* ***Icadamide A***
[173792-57-9]
$C_{37}H_{59}N_5O_{12}$ 765.899
Constit. of the sponge *Leiosella* sp. Cytotoxic agent, immunostimulant. Oil. Sol. MeOH. $[\alpha]_D$ +81 (c, 0.12 in MeOH). λ_{max} 262 (ϵ 3060) (MeOH).

Matsunaga, S. *et al., Tetrahedron*, 1992, **48**, 8369-8376 (*isol, uv, pmr, cmr*)
U.S. Pat., 1995, 5 476 953; *CA*, **124**, 165232u (*Icadamide A*)

Onnamide C O-109

[145757-37-5]



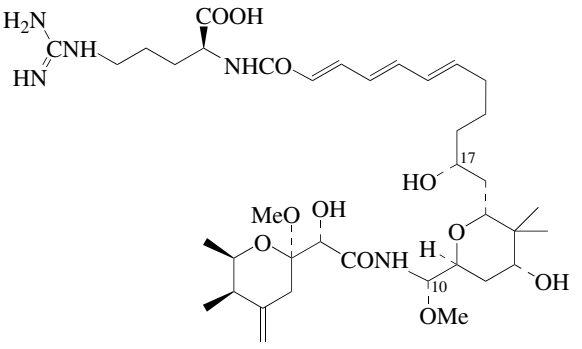
$C_{39}H_{61}N_5O_{14}$ 823.936
Constit. of the sponge *Theonella* sp. Cytotoxic agent. Glassy solid. Sol. MeOH, butanol; poorly sol. H_2O. $[\alpha]_D^{23}$ +45.4 (c, 0.2 in MeOH). λ_{max} 282 (ϵ 16000) (MeOH).

▶ Skin irritant.

Matsunaga, S. *et al., Tetrahedron*, 1992, **48**, 8369-8376 (*isol, uv, pmr, cmr*)

Onnamide D O-110

[145757-38-6]



$C_{38}H_{63}N_5O_{11}$ 765.943
Constit. of the sponge *Theonella* sp. Cytotoxic agent. Glassy solid. Sol. MeOH, butanol; poorly sol. H_2O. $[\alpha]_D^{23}$ +51.4 (c, 0.1 in MeOH). λ_{max} 298 (ϵ 24000) (MeOH).

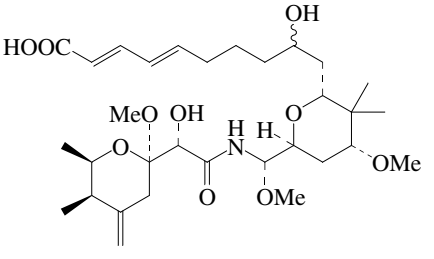
▶ Skin irritant.

10-Demethoxy, 17-ketone: ***Onnamide E***
[145757-39-7]
$C_{37}H_{59}N_5O_{10}$ 733.901
Constit. of the sponge *Theonella* sp. Glassy solid. Sol. MeOH, butanol; poorly sol. H_2O. $[\alpha]_D^{23}$ +64 (c, 0.05 in MeOH). λ_{max} 299 (ϵ 14000) (MeOH).

▶ Skin irritant.

Matsunaga, S. *et al., Tetrahedron*, 1992, **48**, 8369-8376 (*isol, uv, pmr, cmr*)

Onnamide F O-111

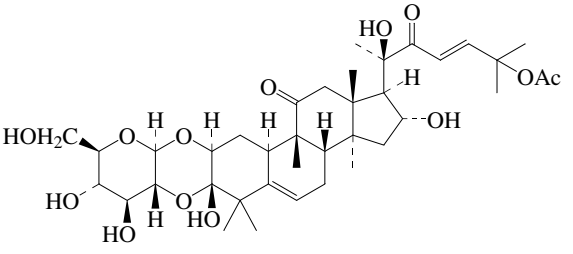


$C_{31}H_{51}NO_{10}$ 597.745
Isol. from the sponge *Trachycladus laevispirulifer*. Nematocidal and antifungal agent. Pale yellow solid. $[\alpha]_D^{22}$ +22 (c, 0.16 in MeOH).

Vuong, D. *et al., J. Nat. Prod.*, 2001, **64**, 640-642,

Opercurin B O-112

[352359-56-9]



$C_{38}H_{56}O_{13}$ 720.853
Constit. of *Luffa operculata*. Amorph. powder. $[\alpha]_D^{20}$ +45.4 (c, 1.42 in Me_2CO). λ_{max} 224 (sh) (log ϵ 4.36); 248 (sh) (log ϵ 3.76) (no solvent reported).

Kawahara, N. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1018-1020 (*isol, pmr, cmr*)

Opheline O-113

[2-[(Aminoiminomethyl)amino]ethyl] methyl phosphate. Guanidinoethyl methyl phosphate

[1119-53-5]

$HN{=}C(N^1H_2)NHCH_2CH_2OP(O)(OH)OMe$

$C_4H_{12}N_3O_4P$ 197.13

Isol. from the worm *Ophelia neglecta*. Cryst. (AcOH aq.).

Mp 271° (253-255° dec.).

N^1*-Phosphono:* **N′*-Phosphonoopheline***. *Phosphorylopheline*

[4294-31-9]

$C_4H_{13}N_3O_7P_2$ 277.11

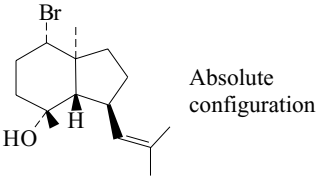
Isol. from the worm *Ophelia neglecta*.

Nguyen-Van-Thoai, *et al., C. R. Hebd. Seances Acad. Sci.*, 1963, **256**, 4525-4528 (*isol, synth*)

Euerby, M.R. *et al., J. Chem. Res., Synop.*, 1988, 394-395 (*synth*)

Oppositol O-114

[50906-52-0]



$C_{15}H_{25}BrO$ 301.266

Constit. of *Laurencia subopposita*.

Mp 54-55°. $[\alpha]_D^{25}$ -232 (c, 0.2 in EtOH).

Hall, S.S. *et al., J.A.C.S.*, 1973, **95**, 7187

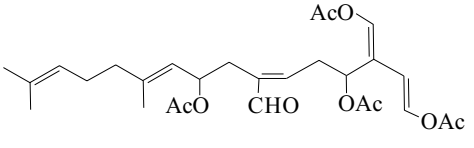
Fukuzawa, A. *et al., Tet. Lett.*, 1987, **28**, 4303 (*synth*)

Sato, Y. *et al., Tetrahedron: Asymmetry*, 1995, **6**, 757 (*synth*)

Kim, D. *et al., Tet. Lett.*, 1997, **38**, 415 (*synth*)

Opuntial O-115

[94480-86-1]



$C_{28}H_{38}O_9$ 518.603

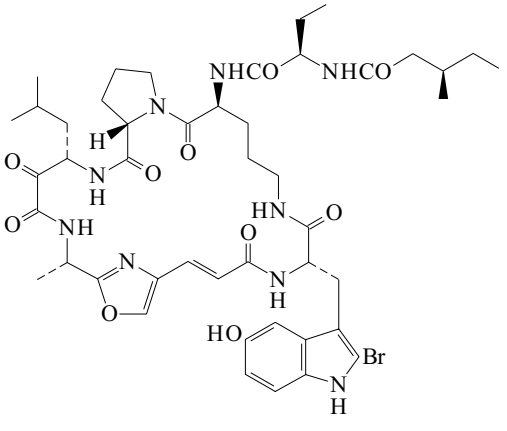
Constit. of *Halimeda opuntia*. Oil. $[\alpha]_D$ -16.6 (c, 2.5 in $CHCl_3$).

Tillekeratne, L.M.V. *et al., Phytochemistry*, 1984, **23**, 1331

Paul, V.J. *et al., Tetrahedron*, 1984, **40**, 3053 (*isol, pmr, cmr*)

Orbiculamide A O-116

[137041-28-2]



$C_{46}H_{62}BrN_9O_{10}$ 980.954

Cyclic peptide antibiotic. Constit. of the marine sponge *Theonella* sp. Cytotoxic agent. Powder. $[\alpha]_D^{23}$ -60 (c, 0.005 in MeOH). λ_{max} 203 (ϵ 14100); 220 (ϵ 10200); 269 (ϵ 6900); 303 (ϵ 1500) (MeOH) (Derep).

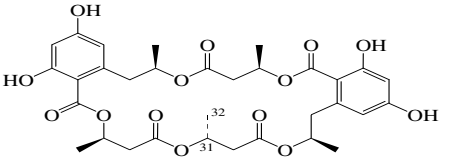
Fusetani, N. *et al., J.A.C.S.*, 1991, **113**, 7811 (*isol, uv, pmr, cmr*)

Orbuticin O-117

Antibiotic BE 26263. Antibiotic BK 223C. Antibiotic 15G256β. BE 26263. BK 223C. 15G256β

[151379-39-4]

[147716-81-2, 184852-27-5]



$C_{32}H_{38}O_{14}$ 646.644

Prod. by *Acremonium butyri*, the marine fungus *Hypoxylon oceanicum*, *Penicillium verruculosum* and *Streptomyces apiospermum*. Antifungal agent. Amorph. solid.

Mp 240° dec. $[\alpha]_D^{25}$ -24.7 (c, 1.25 in MeOH). $[\alpha]_D^{22}$ -21 (c, 0.4 in MeOH). λ_{max} 216 (ϵ 45330); 264 (ϵ 22870); 302 (ϵ 10000) (MeOH).

32-Hydroxy: ***Antibiotic NG 11***. *NG 11. Antibiotic 15G256α1. 15G256α1*

[141731-75-1]

$C_{32}H_{38}O_{15}$ 662.643

Prod. by *Penicillium verruculosum* and the marine fungus *Hypoxylon oceanicum*. Antifungal agent and nerve growth factor potentiator. Powder.

Mp 85-100°. $[\alpha]_D^{26}$ -7.2 (c, 0.25 in EtOH). λ_{max} 217 (ϵ 41900); 264 (ϵ 22400); 302 (ϵ 10000) (MeOH) (Derep). λ_{max} 217 (ϵ 36700); 264 (ϵ 19300); 302 (ϵ 8600) (MeOH) (Berdy).

31-Epimer, 32-hydroxy: Antibiotic BK 223A. Antibiotic NG 012. Antibiotic 15G256α. BK 223A. NG 012. 15G256α

[141731-76-2]

$C_{32}H_{38}O_{15}$ 662.643

Prod. by marine fungus *Hypoxylon oceanicum* and *Penicillium verruculosum*. Antifungal agent and nerve growth factor potentiator. Powder.

Mp 113-120°. $[\alpha]_D^{26}$ -25.2 (c, 0.25 in EtOH). λ_{max} 217 (ϵ 41900); 264 (ϵ 22400); 302 (ϵ 10000) (MeOH) (Derep).

Ito, M. *et al., J. Antibiot.*, 1992, **45**, 1559-1565; 1566-1572 (*NG 012*)

Breinholt, J. *et al., J. Antibiot.*, 1993, **46**, 1101-1108 (*BK 223*)

Japan. Pat., 1993, 93 32 658; *CA*, **118**, 253403 (*BE 26263*)

Roy, K. *et al., J. Antibiot.*, 1996, **49**, 1186-1187 (*Orbuticin*)

Schlingmann, G. *et al., Tetrahedron*, 2002, **58**, 6825-6835 (*15G256 polylactones*)

Orcokinin O-118

[145344-97-4]

H-Asn-Phe-Asp-Glu-Ile-Asp-Arg-Ser-^{9}Gly-Phe-Gly-Phe-^{13}Asn-OH

$C_{67}H_{92}N_{18}O_{23}$ 1517.571

Constit. of the nervous system of *Orconectes limosus*. Myotropic neuropeptide.

9-L-Serine analogue: [161467-63-6]

$C_{68}H_{94}N_{18}O_{24}$ 1547.597

Isol. from the shore crab *Carcinus maenas*.

13-L-Alanine analogue: [161467-64-7]

$C_{66}H_{91}N_{17}O_{22}$ 1474.546

Isol. from *Carcinus maenas*.

13-L-Valine analogue: [161467-65-8]

$C_{68}H_{95}N_{17}O_{22}$ 1502.599

Isol. from *Carcinus maenas*.

Stangier, J. *et al., Peptides (N.Y.)*, 1992, **13**, 859

Bungart, D. *et al., Peptides (N.Y.)*, 1994, **15**, 393; 1995, **16**, 67; 199 (*isol*)

Orcostatin I O-119

Penaeustatin 5

[246221-61-4]

H-Ser-Ala-Gly-Pro-Tyr-Ala-Phe-Gly-Leu-NH_2

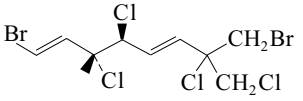
$C_{42}H_{60}N_{10}O_{11}$ 880.996

Allostatin. Isol. from the crayfish *Orconectes limosus* and the tiger prawn *Penaeus monodon*.

Dircksen, H. *et al., Peptides (N.Y.)*, 1999, **20**, 695-712 (*isol*)
Duve, H. *et al., Peptides (N.Y.)*, 2002, **23**, 1039-1051 (*isol*)

Oregonene A O-120

[62416-32-4]



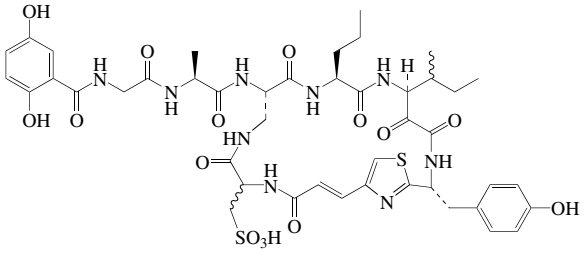
$C_{10}H_{12}Br_2Cl_4$ 433.824

Metab. of *Plocamium oregonum*. Oil.

Crews, P. *et al., J.O.C.*, 1977, **42**, 2634

Oriamide O-121

[200182-07-6]



$C_{44}H_{55}N_9O_{15}S_2$ 1014.102

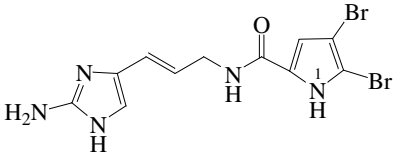
Cyclic peptide antibiotic. Isol. from the sponge *Theonella* sp. Cytotoxic agent. Amorph. powder (as Na salt).

Chill, L. *et al., Tetrahedron*, 1997, **53**, 16147-16152 (*isol, pmr, cmr, ms*)

Oroidine O-122

N-*[3-(2-Amino-1*H*-imidazol-4-yl)-2-propenyl]-4,5-dibromo-1*H*-pyrrole-2-carboxamide, 9CI*

[34649-22-4]



$C_{11}H_{11}Br_2N_5O$ 389.049

Alkaloid from the sponges *Agelas oroides, Agelas sceptrum, Axinella verrucosa*, *Axinella damicornis, Hymeniacidon* sp., *Pseudaxinyssa cantharella, Agelas conifera, Agelas longissima, Agelas mauritiana, Agelas clathrodes, Acanthella carteri, Agelas wiedenmeyeri* and *Acanthella aurantiaca*. Antiserotonergic, adrenergic antagonist, serotonin antagonist, anti-muscarinic, antifouling, antihistamine. Noncryst. Poorly sol. hexane. λ_{max} 296 (ϵ 24500) (MeOH/KOH) (Derep). λ_{max} 278 (ϵ 21000) (MeOH) (Derep).

N-*Ac:* Mp 256-258°.

N^1-*Me:* ***Sventrine***

[392315-92-3]

$C_{12}H_{13}Br_2N_5O$ 403.076

Alkaloid from the sponge *Agelas sventres*. Light yellow powder. λ_{max} 274 (log ϵ 4.27) (MeOH).

2-Debromo: ***Hymenidine***

[107019-95-4]

$C_{11}H_{12}BrN_5O$ 310.153

Isol. from the sponge *Hymeniacidon* sp. and *Agelas clathrodes*. Serotonin receptor antagonist. Antihypertensive, antimuscarinic, smooth muscle contractant. Amorph. solid. Sol. MeOH, butanol. λ_{max} 269 (ϵ 21400) (MeOH) (Derep). λ_{max} 270 (ϵ 23000) (MeOH) (Berdy).

2,3-Didebromo: ***Clathrodine***

[135383-64-1]

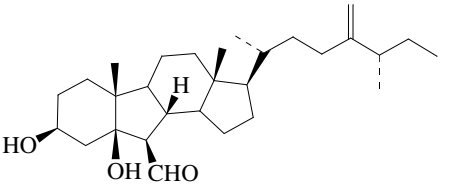
$C_{11}H_{13}N_5O$ 231.257

Isol. from the sponge *Agelas clathrodes*. Cholinergic receptor blocker, antiadrenergic, antimuscarinic neurotoxin. Amorph. solid. λ_{max} 272 (ϵ 24500) (MeOH) (Derep).

Forenza, S. *et al., Chem. Comm.*, 1971, 1129-1130 (*isol, uv, ir, pmr*)
Garcia, E.E. *et al., Chem. Comm.*, 1973, 78-79 (*struct*)
Walker, R.P. *et al., J.A.C.S.*, 1981, **103**, 6772-6773 (*isol*)
Kobayashi, J. *et al., Experientia*, 1986, **42**, 1176-1177 (*Hymenidine*)
Morales, J.J. *et al., J. Nat. Prod.*, 1991, **54**, 629-631 (*Clathrodine*)
Daninos-Zeghal, S. *et al., Tetrahedron*, 1997, **53**, 7605-7614 (*Hymenidine, synth*)
Koenig, G.M. *et al., Planta Med.*, 1998, **64**, 443-447 (*isol, pmr, cmr, ms*)
Lindel, T. *et al., J.O.C.*, 2000, **65**, 2806-2809 (*synth*)
Assmann, M. *et al., J. Nat. Prod.*, 2001, **64**, 1593-1595 (*Sventrine*)
Berré, F. *et al., Tet. Lett.*, 2002, **43**, 4935-4938 (*synth*)
Breckle, G. *et al., Z. Naturforsch., B*, 2003, **58**, 451-456 (*Sventrine, synth*)

Orostanal O-123

[374563-85-6]

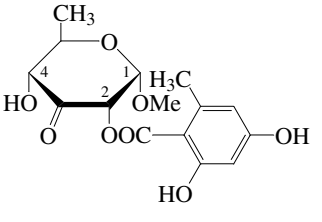


$C_{29}H_{48}O_3$ 444.696

Constit. of *Stelletta hiwasaensis*. Amorph. solid. $[\alpha]_D$ +50.6 (c, 0.3 in $CHCl_3$).

Miyamoto, T. *et al., Tet. Lett.*, 2001, **42**, 6349-6351 (*isol, pmr, cmr*)
Liu, B. *et al., Tet. Lett.*, 2002, **43**, 4187-4189 (*synth*)

Orsellide A O-124



$C_{15}H_{18}O_8$ 326.302

Prod. by a marine-derived *Chaetomium* sp. Gö 100/9. Oil. $[\alpha]_D^{20}$ +58 (c, 0.1 in MeOH). Isol. as a mixt. with Orsellide B, to which data refers. λ_{max} 216 (log ϵ 4.48); 261 (log ϵ 4.17); 299 (log ϵ 3.83) (MeOH).

O^2-*Deacyl,* O^4-*(2,4-dihydroxy-6-methylbenzoyl):* ***Orsellide B***

$C_{15}H_{18}O_8$ 326.302

Prod. by the marine-derived *Chaetomium* sp. Gö 100/9. Isol. as a mixt. with Orsellide A.

4-Deoxy: ***Orsellide C***

$C_{15}H_{18}O_7$ 310.303

Prod. by the marine-derived *Chaetomium* sp. Gö 100/9. Oil. $[\alpha]_D^{20}$ +45 (c, 0.1 in MeOH). λ_{max} 216 (log ϵ 4.39); 265 (log ϵ 4.19); 302 (log ϵ 3.76) (MeOH).

1-Demethoxy, 1,2-didehydro: ***Orsellide D***

$C_{14}H_{14}O_7$ 294.26

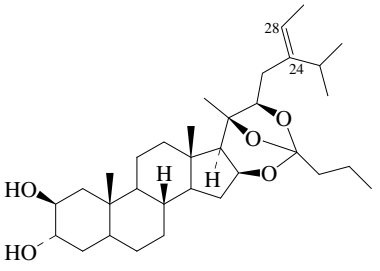
Prod. by the marine-derived *Chaetomium* sp. Gö 100/9.

Amorph. solid.
Mp 81°. $[\alpha]_D^{20}$ +58 (c, 0.1 in MeOH). λ_{max} 215 (log ϵ 4.11); 269 (log ϵ 3.97); 299 (sh) (log ϵ 3.49) (MeOH).

1-Demethoxy, 1,2-didehydro, 4-deoxy: ***Orsellide E***
$C_{14}H_{14}O_6$ 278.261
Prod. by the marine-derived *Chaetomium* sp. Gö 100/9. Oil. $[\alpha]_D^{20}$ +88 (c, 0.1 in MeOH). λ_{max} 215 (log ϵ 4.35); 269 (log ϵ 4.33); 301 (sh) (log ϵ 3.86) (MeOH).

Schlörke, O. *et al., Eur. J. Org. Chem.*, 2006, 1043-1049 (*isol, pmr, cmr*)

Orthoesterol A O-125



$C_{33}H_{54}O_5$ 530.787

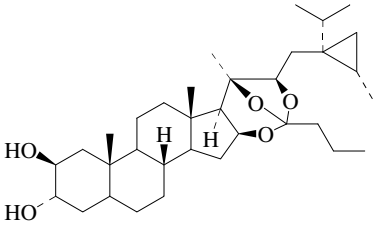
Disulfate: [131010-92-9]
$C_{33}H_{54}O_{11}S_2$ 690.915
Constit. of *Petrosia weinbergi*. Amorph. powder.

*24*R*,28-Dihydro:* ***Orthoesterol C***
$C_{33}H_{56}O_5$ 532.802

24,28-Dihydro, disulfate: [131010-94-1]
$C_{33}H_{56}O_{11}S_2$ 692.931
Constit. of *Petrosia weinbergi*. Shows antiviral props. Amorph. powder.

Koehn, F.E. *et al., J.O.C.*, 1991, **56**, 1322-1325 (*isol, pmr, cmr*)
Giner, J.L. *et al., Steroids*, 1999, **64**, 820-824 (*Orthoesterol C, config*)

Orthoesterol B O-126



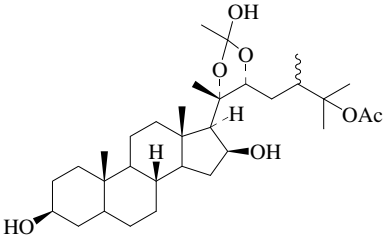
$C_{34}H_{56}O_5$ 544.813

Disulfate: ***Orthoesterol B disulfate***
[131010-93-0]
$C_{34}H_{56}O_{11}S_2$ 704.942
Constit. of *Petrosia weinbergi*. Amorph. powder.

Koehn, F.E. *et al., J.O.C.*, 1991, **56**, 1322-1325 (*isol, pmr, cmr*)
Giner, J.L. *et al., Steroids*, 1999, **64**, 820-824 (*config*)

Orthohippurinsterol A O-127

[346423-92-5]



$C_{32}H_{54}O_7$ 550.774

Constit. of *Isis hippuris*.
$[\alpha]_D^{23}$ +2.67 (c, 0.07 in $CHCl_3$).

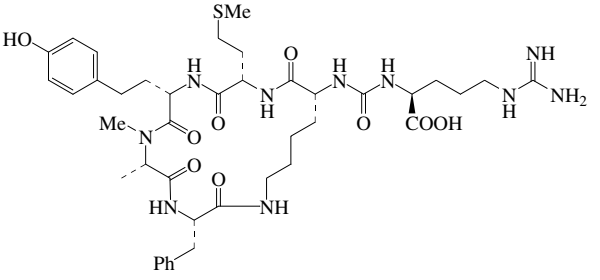
3-Epimer: ***Orthohippurinsterol B***
[346423-93-6]
$C_{32}H_{54}O_7$ 550.774
Constit. of *Isis hippuris*. Powder. $[\alpha]_D^{27}$ +11.7 (c, 0.07 in $CHCl_3$).

3-Ketone: ***Orthohippurinsterone A***
[346423-91-4]
$C_{32}H_{52}O_7$ 548.759
Constit. of *Isis hippuris*. Powder. $[\alpha]_D^{27}$ -58.5 (c, 0.035 in $CHCl_3$).

González, N. *et al., Tetrahedron*, 2001, **57**, 3487-3497 (*isol, pmr, cmr*)

Oscillamide B O-128

[365400-06-2]

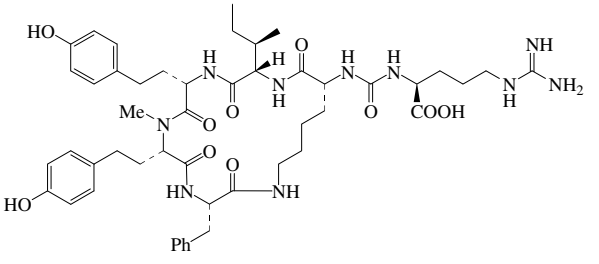


$C_{41}H_{60}N_{10}O_9S$ 869.053
Isol. from the cyanobacteria *Planktothrix agardhii* and *Planktothrix rubescens*. Protein phosphatase inhibitor. Amorph. solid. $[\alpha]_D^{25}$ -83 (c, 0.2 in MeOH). λ_{max} 279 (log ϵ 3.5) (MeOH).

Sano, T. *et al., J. Nat. Prod.*, 2001, **64**, 1052-1055

Oscillamide C O-129

[365400-08-4]

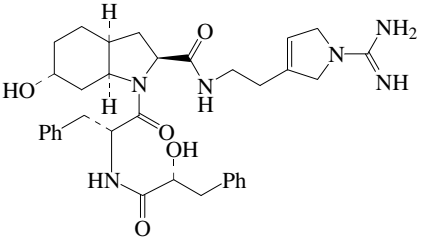


$C_{49}H_{68}N_{10}O_{10}$ 957.137
Isol. from the cyanobacterium *Planktothrix rubescens*. Protein phosphatase inhibitor. Amorph. solid. $[\alpha]_D^{25}$ -111 (c, 0.15 in MeOH). λ_{max} 279 (log ϵ 3.5) (MeOH).

Sano, T. *et al., J. Nat. Prod.*, 2001, **64**, 1052-1055

Oscillarin O-130

[176328-50-0]



Absolute Configuration

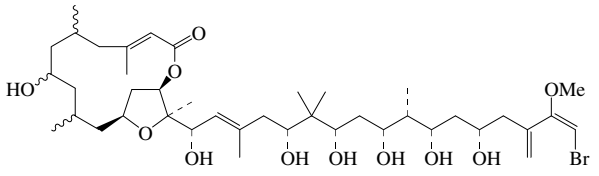
$C_{34}H_{44}N_6O_5$ 616.759

Struct. revised in 2004. Isol. from the cyanobacterium *Oscillatoria agardhii* strain B2 83. Thrombin and trypsin inhibitor, antiinflammatory. Shows cerebroprotective and antiinflammatory props. Sol. MeOH; fairly sol. butanol.

Ger. Pat., 1996, 4 436 772; *CA*, **124**, 315175u (*isol, activity*)
Hanessian, S. *et al., J.A.C.S.*, 2004, **126**, 6064-6065 (*synth, abs config, cryst struct*)

Oscillariolide O-131

[135097-77-7]



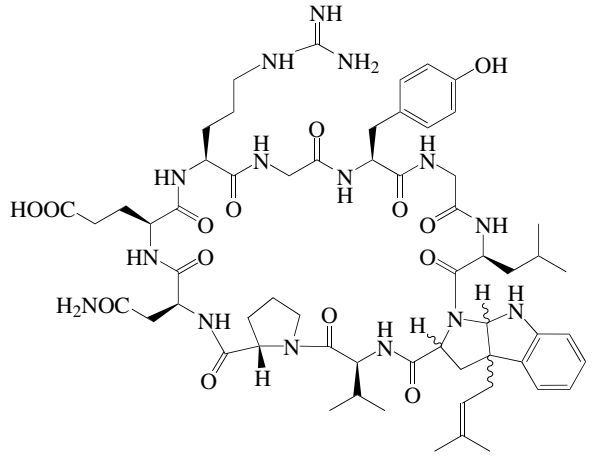
$C_{41}H_{69}BrO_{11}$ 817.893

Macrolide antibiotic. Isol. from a marine blue-green alga *Oscillatoria* sp. Inhibits development of fertilised echinoderm eggs. λ_{max} 225 (ϵ 14000) (MeOH) (Derep).

Murakami, M. *et al., Tet. Lett.*, 1991, **32**, 2391-2394 (*isol, pmr, cmr*)
Williamson, R.T. *et al., J.O.C.*, 2002, **67**, 7927-7936 (*struct*)

Oscillatorin O-132

[182261-00-3]



$C_{60}H_{85}N_{15}O_{14}$ 1240.424

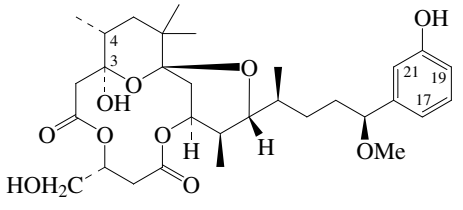
Cyclic peptide antibiotic. Isol. from the cyanobacterium *Oscillatoria agardhii*. Chymotrypsin inhibitor. Amorph. solid. λ_{max} 283 (log ϵ 3.4) (H_2O).

Sano, T. *et al., Tet. Lett.*, 1996, **37**, 6873-6876 (*isol, uv, pmr, cmr*)

Oscillatoxin A O-133

17-Debromo-29-de(1-hydroxyethyl)-29-(hydroxymethyl)aplysiatoxin, 9CI

[66671-95-2]



$C_{31}H_{46}O_{10}$ 578.698

Related to Aplysiatoxin, A-590. Isol. from *Lyngbya majuscula*, *Schizothrix calcicola* and *Oscillatoria negroviridis.*

$[\alpha]_D^{25}$ +67 (c, 0.12 in EtOH). λ_{max} 290 (ϵ 3000) (MeOH/NaOH) (Derep). λ_{max} 283 (ϵ 1950) (MeOH) (Derep).

3-Deoxy, 3,4-didehydro: ***Anhydrooscillatoxin A***

[90359-04-9]

$C_{31}H_{44}O_9$ 560.683

Isol. from *Lyngbya majuscula*.

17-Bromo: ***17-Bromooscillatoxin A***

[66648-16-6]

$C_{31}H_{45}BrO_{10}$ 657.594

Minor component isol. from *Schizothrix calcicola* and *Oscillatoria nitroviridis*. No phys. props. reported. λ_{max} 290 (ϵ 3000) (MeOH/NaOH) (Derep). λ_{max} 283 (ϵ 1950) (MeOH) (Derep).

17,19-Dibromo: ***17,19-Dibromooscillatoxin A***

[66648-17-7]

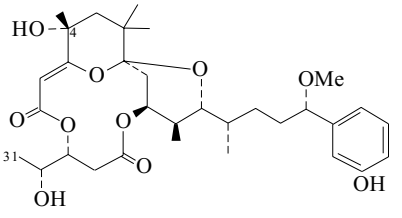
$C_{31}H_{44}Br_2O_{10}$ 736.491

Minor component isol. from *Schizothrix calcicola* and *Oscillatoria nitroviridis*. No phys. props. reported. λ_{max} 283 (ϵ 1950) (MeOH) (Derep).

Mynderse, J.S. *et al., J.O.C.*, 1978, **43**, 2301-2303 (*isol, struct*)
Moore, R.E. *et al., J.O.C.*, 1984, **49**, 2484-2489 (*abs config*)

Oscillatoxin B_1 O-134

[95189-16-5]



$C_{32}H_{46}O_{10}$ 590.709

Constit. of *Lyngbya majuscula*. Solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.

Mp 89° dec. λ_{max} 216 (ϵ 9350); 235 (ϵ 5030); 243 (ϵ 3820); 272 (ϵ 1980); 278 (ϵ 1750) (MeOH) (Derep). λ_{max} 216 (ϵ 9350); 235 (ϵ 3030); 243 (ϵ 3820); 272 (ϵ 2980); 278 (ϵ 1750) (MeOH) (Berdy).

4-Epimer: ***Oscillatoxin B_2***

[95189-17-6]

$C_{32}H_{46}O_{10}$ 590.709

From *Lyngbya majuscula*. Solid. λ_{max} 216 (ϵ 9350); 235 (ϵ 5030); 243 (ϵ 3820); 272 (ϵ 1980); 278 (ϵ 1750) (MeOH) (Derep).

31-De-Me: ***31-Noroscillatoxin B***

[95098-07-0]

$C_{31}H_{44}O_{10}$ 576.683

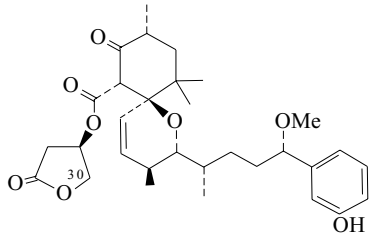
Constit. of *Schizothrix calcicola* and *Oscillatoria nigroviridis*. Gum. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 216 (ϵ 9350); 235 (ϵ 5030); 243 (ϵ 3820); 272 (ϵ 1980); 278 (ϵ 1750) (MeOH) (Derep).

[90359-06-1]

Entzeroth, M. *et al., J.O.C.*, 1985, **50**, 1255

Oscillatoxin D O-135

[95069-53-7]



$C_{31}H_{42}O_8$ 542.668

Constit. of *Schizothrix calcicola* and *Oscillatoria nigroviridis.*

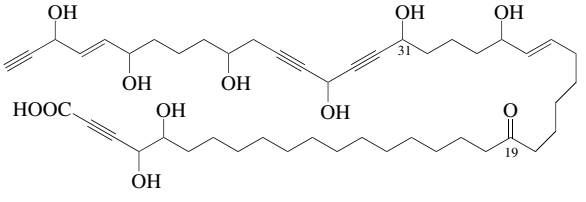
Gum. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 208 (ϵ 24000); 211 (ϵ 8200); 224 (ϵ 5150); 274 (ϵ 2030); 280 (ϵ 1800) (MeOH) (Derep).

30β-Methyl: ***30-Methyloscillatoxin D***
[95069-54-8]
$C_{32}H_{44}O_8$ 556.695
From *Lyngbya majuscula*. Cryst. (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 166°. λ_{max} 208 (ϵ 24000); 211 (ϵ 8200); 224 (ϵ 5150); 274 (ϵ 2030); 280 (ϵ 1800) (MeOH) (Derep).

Entzeroth, M. *et al., J.O.C.*, 1985, **50**, 1255
Toshima, H. *et al., Tet. Lett.*, 1995, **36**, 3373 (*synth*)
Ichihara, A. *et al., Stud. Nat. Prod. Chem.*, 1996, **18**, 269 (*rev, synth*)

Osirisyne A O-136

4,5,27,31,34,38,42,45-Octahydroxy-19-oxo-25,43-heptatetracontadiene-2,32,35,46-tetraynoic acid



$C_{47}H_{72}O_{11}$ 813.079
Constit. of the sponge *Haliclona osiris*. Exhibits moderate cytotoxicity. Toxic to brine shrimp. Solid.
Mp 118-120°. $[\alpha]_D^{25}$ +11.8 (c, 0.1 in MeOH). λ_{max} 209 (log ϵ 3.6) (MeOH).

31-Deoxy: 4,5,27,34,38,42,45-Heptahydroxy-19-oxo-25,43-heptatetracontadiene-2,32,35,46-tetraynoic acid. ***Osirisyne B***
$C_{47}H_{72}O_{10}$ 797.08
Constit. of *Haliclona osiris*. Toxic to brine shrimp. Solid.
Mp 123-124°. $[\alpha]_D^{25}$ +16.1 (c, 0.1 in MeOH). λ_{max} 207 (log ϵ 3.62) (MeOH).

19-Deoxo, 21-oxo: 4,5,27,31,34,38,42,45-Octahydroxy-21-oxo-25,43-heptatetracontadiene-2,32,35,46-tetraynoic acid. ***Osirisyne C***
$C_{47}H_{72}O_{11}$ 813.079
Constit. of *Haliclona osiris*. Toxic to brine shrimp. Na/K-ATPase reverse transcriptase inhibitor. Solid.
Mp 121-122°. $[\alpha]_D^{25}$ +13.4 (c, 0.2 in MeOH). λ_{max} 209 (log ϵ 3.56) (MeOH).

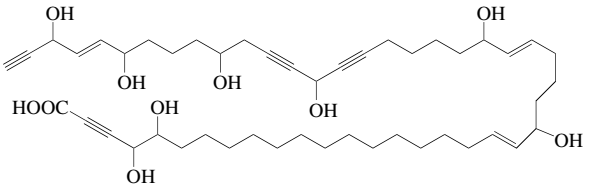
19-Deoxo, 21-oxo, 31-deoxy: 4,5,27,34,38,42,45-Heptahydroxy-21-oxo-25,43-heptatetracontadiene-2,32,35,46-tetraynoic acid. ***Osirisyne D***
$C_{47}H_{72}O_{10}$ 797.08
Constit. of *Haliclona osiris*. Toxic to brine shrimp. Solid.
Mp 138-140°. $[\alpha]_D^{25}$ +10.3 (c, 0.1 in MeOH). λ_{max} 206 (log ϵ 3.72) (MeOH).

6-Hydroxy, 19-deoxo, 21-oxo: 4,5,6,27,31,34,38,42,45-Nonahydroxy-21-oxo-25,43-heptatetracontadiene-2,32,35,46-tetraynoic acid. ***Osirisyne F***
$C_{47}H_{72}O_{12}$ 829.079
Constit. of *Haliclona osiris*. Toxic to brine shrimp. Na/K-ATPase inhibitor. Solid.
Mp 138-140°. $[\alpha]_D^{25}$ +6.8 (c, 0.09 in MeOH). Incorrect struct. shown in ref. λ_{max} 207 (log ϵ 4.01) (MeOH).

Shin, J. *et al., Tetrahedron*, 1998, **54**, 8711-8720 (*isol, uv, ir, pmr, cmr*)

Osirisyne E O-137

4,5,21,27,34,38,42,45-Octahydroxy-19,25,43-heptatetracontatriene-2,32,35,46-tetraynoic acid

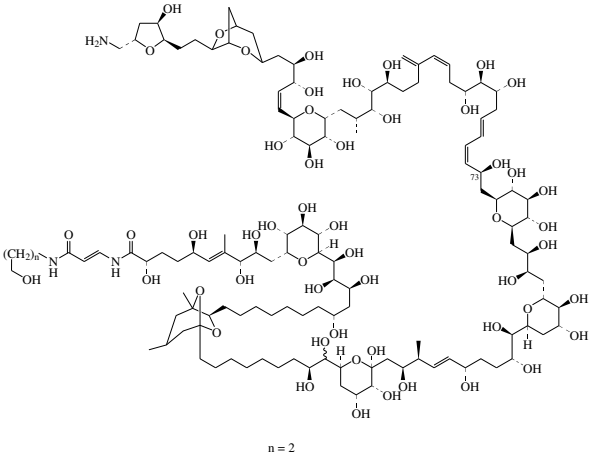


$C_{47}H_{72}O_{10}$ 797.08
Constit. of the sponge *Haliclona osiris*. Toxic to brine shrimp. Na/K-ATPase reverse transcriptase inhibitor. Solid.
Mp 126-128°. $[\alpha]_D^{25}$ +18.5 (c, 0.1 in MeOH). λ_{max} 207 (log ϵ 3.69) (MeOH).

Shin, J. *et al., Tetrahedron*, 1998, **54**, 8711-8720 (*isol, uv, ir, pmr, cmr*)

Ostreocin D O-138

42-Hydroxy-3,26-didemethyl-19,44-dideoxypalytoxin
[163648-25-7]



$C_{127}H_{219}N_3O_{53}$ 2636.115
Related to Palytoxin, P-76. Isol. from the dinoflagellate *Ostreopsis siamensis*. Amorph. powder. $[\alpha]_D^{23}$ +16.6 (c, 0.1 in H_2O). λ_{max} 234 (ϵ 35000); 263 (ϵ 22000) (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 0.75 mg/kg.

Ukena, T. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 2585-2588 (*isol, pmr, cmr*)

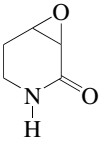
Sepia officinalis Ovotropin O-139

SepOvotropin
[309254-10-2]
Pro-Lys-Asp-Ser-Met-Leu-Leu-Leu-Gln-Val-Pro-Val-Tyr-NH_2
$C_{70}H_{116}N_{16}O_{18}S$ 1501.849
Isol. from vitellogenic ovarian follicles of the cuttlefish *Sepia officinalis*. Regulates oocyte transport.

Zatylny, C. *et al., Biochem. Biophys. Res. Commun.*, 2000, **276**, 1013-1018 (*isol, struct*)

7-Oxa-3-azabicyclo[4.1.0]heptan-2-one, 9CI O-140

3,4-Epoxy-2-piperidone. 3,4-Epoxyvalerolactam. ***Tedanalactam***

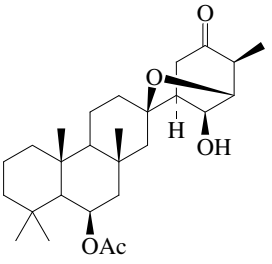


$C_5H_7NO_2$ 113.116

(-)-*form* [159934-17-5]
Isol. from the sponge *Tedania ignis*.
Oil. $[\alpha]_D$ -8.9 (c, 0.3 in MeOH).
Cronan, J.M. *et al., Nat. Prod. Lett.*, 1994, **5**, 85-88; 141-146 (*isol, ir, pmr, cmr*)

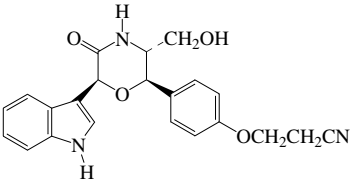
Oxaspirosuberitenone O-141

[720681-62-9]



$C_{27}H_{42}O_5$ 446.626
Constit. of *Suberites caminatus*. Oil. $[\alpha]_D^{25}$ +140 (c, 0.093 in $CHCl_3$).
Díaz-Marrero, A.R. *et al., Tet. Lett.*, 2004, **45**, 4707-4710 (*isol, pmr, cmr*)

Oxazinine 1 O-142



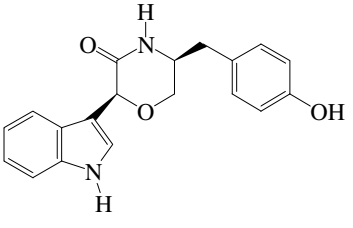
Relative Configuration

$C_{22}H_{21}N_3O_4$ 391.426
Isol. from the digestive glands of *Mytilus galloprovincialis*.
Cytotoxic. $[\alpha]_D^{25}$ +9 (MeOH). λ_{max} 216 (ϵ 46000); 270 (ϵ 5700); 277 (ϵ 5500); 286 (ϵ 3500) (MeOH).

O-*De(cyanoethyl):* ***Oxazinine 2***
$C_{19}H_{18}N_2O_4$ 338.362
Isol. from *Mytilus galloprovincialis*.
$[\alpha]_D^{25}$ +8.7 (MeOH). λ_{max} 216 (ϵ 20400); 275 (ϵ 3200); 377 (ϵ 700) (MeOH).
Ciminiello, P. *et al., Eur. J. Org. Chem.*, 2001, 49-53

Oxazinine 3 O-143

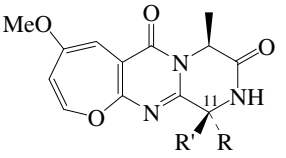
*5-[(4-Hydroxyphenyl)methyl]-2-(1*H*-indol-3-yl)-3-morpholinone, 9CI*
[331836-05-6]



Absolute Configuration

$C_{19}H_{18}N_2O_3$ 322.363
Isol. from the digestive glands of *Mytilus galloprovincialis*.
$[\alpha]_D^{25}$ +12 (MeOH). λ_{max} 220 (ϵ 20600); 270 (ϵ 3100); 375 (ϵ 750) (MeOH).
Ciminiello, P. *et al., Eur. J. Org. Chem.*, 2001, 49-53 (*isol, pmr, cmr*)
Couladouros, E.A. *et al., Tet. Lett.*, 2004, **45**, 7779-7781 (*synth, abs config*)

Oxepinamide A O-144



Relative Configuration

R = $CH(CH_3)CH_2CH_3$, R' = OH

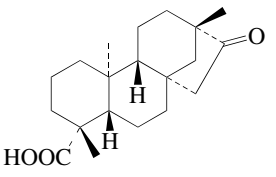
$C_{17}H_{21}N_3O_5$ 347.37
Isol. from an *Acremonium* sp. obt. from the tunicate *Ecteinascidia turbinata*. Antiinflammatory agent. Yellow oil. $[\alpha]_D$ +43 (c, 0.001 in $CHCl_3$). λ_{max} 250 (ϵ 6100); 345 (ϵ 4900) (MeOH).

11-Epimer: ***Oxepinamide B***
$C_{17}H_{21}N_3O_5$ 347.37
Isol. from an *Acremonium* sp. obt. from *Ecteinascidia turbinata*. Yellow oil. $[\alpha]_D$ +52 (c, 0.001 in $CHCl_3$). λ_{max} 252 (ϵ 4900); 347 (ϵ 2600) (MeOH).
Belofsky, G.N. *et al., Chem. Eur. J.*, 2000, **6**, 1355-1360

Oxepinamide C O-145

As Oxepinamide A, O-144 with
R = $CH_2CH(CH_3)_2$, R′ = OMe
$C_{18}H_{23}N_3O_5$ 361.397
Isol. from an *Acremonium* sp. obt. from *Ecteinascidia turbinata*. Yellow oil. $[\alpha]_D$ -35 (c, 0.001 in $CHCl_3$). λ_{max} 250 (ϵ 3000); 345 (ϵ 2100) (MeOH).
Belofsky, G.N. *et al., Eur. J. Org. Chem.*, 2000, **6**, 1355-1360

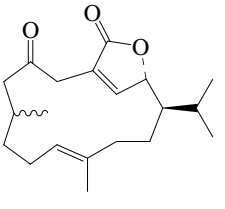
16-Oxo-19-beyeranoic acid O-146



$C_{20}H_{30}O_3$ 318.455

ent-form
Isosteviol
[27975-19-5]
Cryst. Mp 234°. $[\alpha]_D$ -78 (95% EtOH).
19-Aldehyde: 16-Oxo-19-beyeranal. ***Ceriopsin G***
[554412-03-2]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Ceriops decandra*. Oil. $[\alpha]_D^{25}$ -49 (c, 0.25 in $CHCl_3$).
Mosettig, E. *et al., J.A.C.S.*, 1963, **85**, 2305 (*struct*)
Ziegler, F.E. *et al., Tetrahedron*, 1977, **33**, 373 (*synth*)
Snider, B.B. *et al., J.O.C.*, 1998, **63**, 7945-7952 (*synth*)
Anjaneyulu, A.S.R. *et al., Phytochemistry*, 2003, **62**, 1207-1211 (*Ceriopsin G*)

6-Oxo-3,11-cembradien-18,2-olide O-147

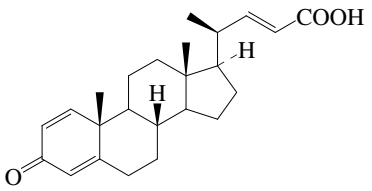


$C_{20}H_{30}O_3$ 318.455

(1*R*,2*R*,8ξ,11*E*)-*form*
Sarcophytonolide C

[862248-73-5]
Constit. of a *Sarcophyton* sp.
Oil. $[\alpha]_D^{20}$ -31 (c, 0.2 in $CHCl_3$). λ_{max} 227 (log ϵ 2.13) (MeOH).
Jia, R. *et al., Helv. Chim. Acta*, 2005, **88**, 1028-1033 (*Sarcophytonolide C*)

3-Oxochola-1,4,22-trien-24-oic acid O-148

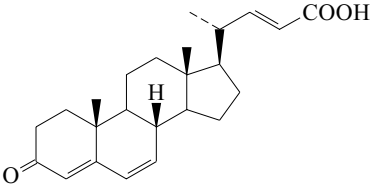


$C_{24}H_{32}O_3$ 368.515

(20S,22E)-form [832723-74-7]
Constit. of an *Eleutherobia* sp.
Glass. $[\alpha]_D^{20}$ -39.6 (c, 0.045 in EtOH).

Me ester: [349104-69-4]
$C_{25}H_{34}O_3$ 382.542
Constit. of *Alcyonium gracillimum* and *Dendronephthya* sp.
$[\alpha]_D^{22}$ +53.6 (c, 0.28 in $CHCl_3$). λ_{max} 215 (ϵ 21000); 243 (ϵ 16000) (MeOH).
Tomono, Y. *et al., J. Nat. Prod.*, 1999, **62**, 1538-1541 (*isol, pmr, cmr*)
Linker, M. *et al., Acta Cryst. E*, 2001, **57**, o574-o575 (*cryst struct*)
Lievens, S.C. *et al., J. Nat. Prod.*, 2004, **67**, 2130-2132 (*Eleutherobia constit.*)

3-Oxochola-4,6,22-trien-24-oic acid O-149



$C_{24}H_{32}O_3$ 368.515

(22E)-form [180603-62-7]
Constit. of *Deltocyathus magnificus.*
$[\alpha]_D^{20}$ -34.1 (c, 0.37 in EtOH).

Me ester: [180603-63-8]
$[\alpha]_D^{20}$ -26.9 (c, 0.13 in EtOH).

22,23-Dihydro: ***3-Oxochola-4,6-dien-24-oic acid***
[88179-71-9]
$C_{24}H_{34}O_3$ 370.531
Constit. of *Deltocyathus magnificus.*

22,23-Dihydro, Me ester: [93800-48-7]
$[\alpha]_D^{20}$ +19.1 (c, 0.11 in EtOH).

6,7-Dihydro: ***3-Oxochola-4,22-dien-24-oic acid***
[82637-22-7]
$C_{24}H_{34}O_3$ 370.531
Constit. of *Deltocyathus magnificus* and *Aldisa sanguinea cooperi.*

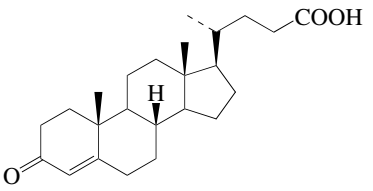
6,7-Dihydro, Me ester: ***Methyl 3-oxochola-4,22-dien-24-oate***
[180603-66-1]
$C_{25}H_{36}O_3$ 384.558
Constit. of a *Dendronephthya* sp.
$[\alpha]_D^{20}$ +55.8 (c, 0.12 in EtOH). λ_{max} 215 (ϵ 21000); 243 (ϵ 16000) (MeOH).

6,7,22,23-Tetrahydro: See 3-Oxochol-4-en-24-oic acid, O-150

Ayer, S.W. *et al., Tet. Lett.*, 1982, **23**, 1039-1042 (*isol, pmr*)
Guirriero, A. *et al., Helv. Chim. Acta*, 1996, **79**, 982-988 (*isol, pmr, cmr*)
Tomono, Y. *et al., J. Nat. Prod.*, 1999, **62**, 1538-1541 (*Methyl 3-oxochola-4,22-dien-24-oate*)

3-Oxochol-4-en-24-oic acid O-150

[1452-29-5]



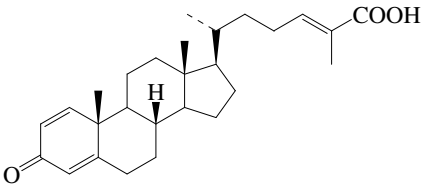
$C_{24}H_{36}O_3$ 372.547
Constit. of *Deltocyathus magnificus* and *Aldisa sanguinea cooperi*.
Ichthyotoxin, antifeedant. Cryst. (EtOH).
Mp 185-187.5°. λ_{max} 240 (MeOH) (Berdy).

Me ester: [1452-33-1]
$C_{25}H_{38}O_3$ 386.573
Cryst. (MeOH or hexane). Mp 125-127°. $[\alpha]_D^{21}$ +61 ($CHCl_3$).
$[\alpha]_D^{20}$ +35.9 (c, 0.05 in EtOH).

Me ester, 2,4-dinitrophenylhydrazone:
Orange-red cryst. (MeOH/$CHCl_3$). Mp 232-233°.

Gallagher, T.F. *et al., J. Biol. Chem.*, 1946, **165**, 365 (*synth*)
Takeda, K. *et al., J. Biochem. (Tokyo)*, 1953, **40**, 477 (*synth*)
Osawa, R. *et al., Bull. Chem. Soc. Jpn.*, 1962, **35**, 381 (*uv, ir, ord*)
Iacona, R.N. *et al., J.O.C.*, 1964, **29**, 3495 (*synth*)
Aries, V. *et al., Biochem. J.*, 1970, **119**, 37P (*synth*)
Ayer, S.W. *et al., Tet. Lett.*, 1982, **23**, 1039 (*isol*)
Nicotra, F. *et al., J.C.S. Perkin 1*, 1983, 787 (*synth*)
Miyamoto, K. *et al., Synth. Commun.*, 1986, **16**, 513 (*synth*)
Demir, A.S. *et al., Org. Prep. Proced. Int.*, 1987, **19**, 197 (*synth*)
Aranda, G. *et al., Tetrahedron*, 1987, **43**, 4147 (*synth, pmr, cmr*)
Guirriero, A. *et al., Helv. Chim. Acta*, 1996, **79**, 982-988 (*isol, pmr, cmr*)

3-Oxocholesta-1,4,24-trien-26-oic acid O-151



$C_{27}H_{38}O_3$ 410.595

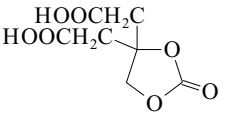
(24E)-form

Me ester: [862286-69-9]
$C_{28}H_{40}O_3$ 424.622
Constit. of *Anthomastus bathyproctus.* Amorph. powder. $[\alpha]_D^{25}$ +8.4 (c, 0.1 in $CHCl_3$). λ_{max} 223 (log ϵ 4.11); 238 (log ϵ 4.02) (MeOH).

24,25ξ-Dihydro: 3-Oxocholesta-1,4-dien-26-oic acid
$C_{27}H_{40}O_3$ 412.611

24,25ξ-Dihydro, Me ester: [862288-89-9]
$C_{28}H_{42}O_3$ 426.638
Constit. of *Anthomastus bathyproctus.* Amorph. powder. $[\alpha]_D^{25}$ -8.8 (c, 0.05 in $CHCl_3$). λ_{max} 244 (log ϵ 3.96) (MeOH).
Mellado, G.G. *et al., J. Nat. Prod.*, 2005, **68**, 1111-1115

2-Oxo-1,3-dioxolane-4,4-diacetic acid O-152



$C_7H_8O_7$ 204.136

Di-Me ester: ***Lyngbyacarbonate***
[164740-29-8]
$C_9H_{12}O_7$ 232.19

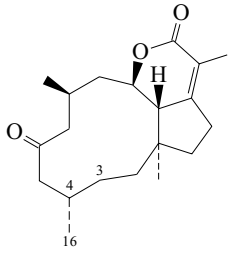
Isol. from the cyanobacterium *Lyngbya majuscula*.
Todd, J.S. *et al., J. Nat. Prod.*, 1995, **58**, 586 (*isol, pmr, ms*)

12-Oxo-5,8,10-dodecatrienoic acid, 9CI O-153

11-Formyl-5,8,10-undecatrienoic acid
OHCCH=CHCH=CHCH$_2$CH=CH(CH$_2$)$_3$COOH
$C_{12}H_{16}O_3$ 208.257

(5*Z*,7*E*,8*E*)-*form* [81892-90-2]
Antimicrobial component of the red alga *Laurencia hybrida*.
Poorly sol. hexane. λ_{max} 274 (ϵ 28500) (MeOH) (Berdy).
Higgs, M.D. *et al., Tetrahedron*, 1981, **24**, 4255 (*isol, pmr, ms*)

6-Oxo-12(18)-dolabellen-19,10-olide O-154



$C_{20}H_{30}O_3$ 318.455

(4α,8β,10β)-*form*
Clavirolide C
[135048-55-4]
Metab. of *Clavularia viridis*.
Cryst.
Mp 124.5-126.5°. $[\alpha]_D^{26.5}$ -38.5 (c, 0.018 in MeOH).

*3,4-Didehydro(*E*-): 6-Oxo-3,12(18)-dolabelladien-19,10-olide.*
Clavirolide B
[135096-90-1]
$C_{20}H_{28}O_3$ 316.439
Isol. from *Clavularia viridis*. Calcium channel blocker. Plates (Me_2CO/petrol).
Mp 143.5-145.5°. $[\alpha]_D^{26.5}$ -392.7 (c, 0.085 in MeOH). λ_{max} 232 (ϵ 9500) (MeOH) (Berdy).

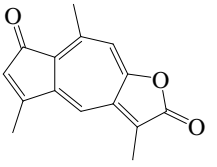
*3,4-Didehydro(*Z*-):* ***Clavulactone***
[113023-71-5]
$C_{20}H_{28}O_3$ 316.439
Isol. from *Clavularia viridis*. Cryst. (Me_2CO/petrol).
Mp 195-197°. $[\alpha]_D^{20}$ -238.5 (c, 0.035 in MeOH). λ_{max} 202 (ϵ 9000); 226 (ϵ 23000) (MeOH) (Derep). λ_{max} 232 (ϵ 13000) (MeOH) (Berdy).

*4,5-Didehydro(*Z*-): 6-Oxo-4,12(18)-dolabelladien-19,10-olide.*
Clavirolide D
[135048-56-5]
$C_{20}H_{28}O_3$ 316.439
Isol. from *Clavularia viridis*. Calcium channel blocker. Syrup.
$[\alpha]_D^{26.5}$ -118.5 (c, 0.08 in MeOH). λ_{max} 234 (ϵ 13900) (MeOH) (Berdy).

4,16-Didehydro: 6-Oxo-4(16),12(18)-dolabelladien-19,10-olide.
Clavirolide E
[135048-57-6]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Clavularia viridis*. Calcium channel blocker. Cryst.
Mp 200-201°. $[\alpha]_D^{20}$ -40 (c, 0.01 in MeOH). λ_{max} 234 (ϵ 12800) (MeOH) (Berdy).
Su, J. *et al., J. Nat. Prod.*, 1991, **54**, 380 (*isol, pmr, cmr*)

2-Oxo-1(10),3,5,7(11),8-guaiapentaen-12,8-olide O-155

[89044-36-0]



$C_{15}H_{12}O_3$ 240.258
Constit. of *Taraxacum wallichii*. Also isol. from the gorgonian *Paramuricea chamaeleon* as artifact derived from Linderazulene, L-174. Yellow cryst. (MeOH).
Mp 107-110°. λ_{max} 272; 285 (sh); 415 (sh); 430 (MeOH).
Alpertunga, B. *et al., Tet. Lett.*, 1983, **24**, 4461-4462 (*isol, cryst struct*)
Li, M.K.W. *et al., Tet. Lett.*, 1984, **25**, 2109-2110 (*isol*)
Ahmad, V.U. *et al., J. Nat. Prod.*, 2000, **63**, 1010-1011 (*isol, pmr, cmr*)

2-Oxohexadecanoic acid, 9CI O-156

2-Oxopalmitic acid
[2570-24-3]
$H_3C(CH_2)_{13}COCOOH$
$C_{16}H_{30}O_3$ 270.411
Constit. of the algae *Porphyra* sp. and *Ulva pertusa*. Needles (petrol).
Mp 69.5°.

Oxime:
$C_{16}H_{31}NO_3$ 285.426
Mp 81-82°.

Me ester: [55836-30-1]
$C_{17}H_{32}O_3$ 284.438
Cryst. (MeOH aq./petrol). Mp 47°.

*Me ester, (*E*)-oxime:* [17589-52-5]
$C_{17}H_{33}NO_3$ 299.453
Needles. Mp 93-94°.

*Me ester, (*Z*)-oxime:* [17589-53-6]
$C_{17}H_{33}NO_3$ 299.453
Leaflets (MeOH). Mp 58.5-59.5°.

Me ester, 2,4-dinitrophenylhydrazone: [18281-57-7]
Yellow needles (MeOH). Mp 130°.

Et ester: [158305-67-0]
$C_{18}H_{34}O_3$ 298.465
Cryst.

Kuwata, T. *et al., J.A.C.S.*, 1938, **60**, 559-560 (*Me ester*)
Reinheckel, H. *et al., Monatsh. Chem.*, 1967, **98**, 1217-1229 (*Me ester*)
Khan, M. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 1043-1046 (*synth*)
Kajiwara, T. *et al., Phytochemistry*, 1991, **30**, 193-195 (*isol*)
Rochat, S. *et al., Helv. Chim. Acta*, 2000, **83**, 1645-1671 (*Et ester, synth, ir, uv, pmr, cmr, ms*)

4-Oxohexadecanoic acid, 9CI O-157

4-Oxopalmitic acid. 4-Ketopalmitic acid
[4144-56-3]
$H_3C(CH_2)_{11}CO(CH_2)_2COOH$
$C_{16}H_{30}O_3$ 270.411
Constit of the marine alga *Gracilaria tenuistiptitata*. Cryst. (petrol).
Mp 91-92°.

Oxime:
$C_{16}H_{31}NO_3$ 285.426
Cryst. (petrol). Mp 54°.

[54527-07-0]

Robinson, G.M. *et al., J.C.S.*, 1925, **127**, 175-180 (*synth*)
Houston, D.F. *et al., J.A.C.S.*, 1947, **69**, 517 (*synth*)
Ahmad, M.U. *et al., J. Am. Oil Chem. Soc.*, 1978, **55**, 491-495 (*synth*)
Granata, A. *et al., Can. J. Chem.*, 1993, **71**, 864-871 (*synth, cmr, ms*)
Xu, S. *et al., Redai Haiyang*, 1993, **12**, 1-9; *CA*, **121**, 77921 (*Gracilaria tenuistipitata constit*)

Bosch, M.P. *et al., Bioorg. Med. Chem.*, 1996, **4**, 467-472 (*Me ester, synth, ir, pmr, cmr*)

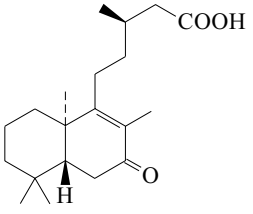
5-Oxohexadecanoic acid, 9CI O-158

5-Oxopalmitic acid. 5-Ketopalmitic acid
[70444-63-2]
$H_3C(CH_2)_{10}CO(CH_2)_3COOH$
$C_{16}H_{30}O_3$ 270.411
Trace constit. of milk fat and the red alga *Gracilaria tenuistipitata*.
Cryst. (MeOH, C_6H_6 or petrol).
Mp 88°.

Me ester: [54527-00-3]
$C_{17}H_{32}O_3$ 284.438
Mp 47.5-48.5°.

Robinson, G.M. *et al., J.C.S.*, 1930, 745-751 (*synth*)
Weihrauch, J.L. *et al., Lipids*, 1974, **9**, 883-890 (*isol*)
Naoshima, Y. *et al., Agric. Biol. Chem.*, 1983, **47**, 1431-1434 (*Me ester, synth, ir, pmr, ms*)
Xu, S. *et al., Redai Haiyang*, 1993, **12**, 1-9; *CA*, **121**, 77921 (*Gracilaria tenuistipitata constit*)
Lhommet, G. *et al., Synth. Commun.*, 1996, **26**, 3897-3901 (*synth, ir, cmr*)

7-Oxo-8-labden-15-oic acid O-159

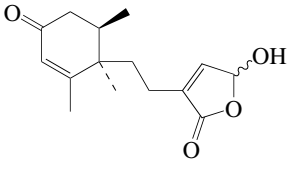


$C_{20}H_{32}O_3$ 320.471

(ent*-13*S*)-*form
2,3-Dihydroxypropyl ester: [138909-53-2]
$C_{23}H_{38}O_5$ 394.55
Constit. of *Austrodoris kerguelensis*. Oil. $[\alpha]_D$ -61 (c, 0.09 in $CHCl_3$).
Davies-Coleman, M.T. *et al., Tetrahedron*, 1991, **47**, 9743 (*isol, pmr, cmr*)

2-Oxomicrocionin 2-lactone O-160

[194020-49-0]

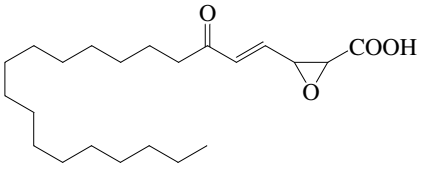


$C_{15}H_{20}O_4$ 264.321
Constit. of *Cadlina luteomarginata*. Oil.

Me ether: [194020-51-4]
$C_{16}H_{22}O_4$ 278.347
Constit. of *Cadlina luteomarginata*. Glass.
Dumdei, E.J. *et al., Can. J. Chem.*, 1997, **75**, 773-789 (*isol, pmr, cmr*)

3-(3-Oxo-1-nonadecenyl)oxiranecarboxylic acid O-161

***Plakortic acid*†**



$C_{22}H_{38}O_4$ 366.54

Not to be confused with Plakortic acid, P-472. Isol. from *Plakortis simplex*. Oil. $[\alpha]_D^{25}$ +36.3 (c, 0.5 in CH_2Cl_2). λ_{max} 204 (log ε 1.89); 221 (log ε 3.14) (MeOH).
Shen, Y.-C. *et al., J. Nat. Prod.*, 2001, **64**, 324-327

4-Oxononanoic acid, 9CI, 8CI O-162

4-Ketopelargonic acid
[6064-52-4]
$H_3C(CH_2)_4COCH_2CH_2COOH$
$C_9H_{16}O_3$ 172.224
Constit of the marine red alga *Gracilaria tenuistipitata*. Cryst. (petrol).
Mp 69-70°.

Phenylhydrazone: Mp 85-87°.

Semicarbazone: Mp 157-159° dec.

Me ester: [33566-57-3]
$C_{10}H_{18}O_3$ 186.25
Oil. Bp_2 96-98° $Bp_{0.2}$ 105-110°.

Et ester: [37174-92-8]
$C_{11}H_{20}O_3$ 200.277
Bp_2 90-92°.

Ernest, I. *et al., Coll. Czech. Chem. Comm.*, 1959, **24**, 3341 (*synth*)
Takeda, A. *et al., J.O.C.*, 1966, **31**, 616 (*synth*)
Steglich, W. *et al., Angew. Chem., Int. Ed.*, 1971, **10**, 655 (*synth*)
Wineburg, J.P. *et al., J. Het. Chem.*, 1975, **12**, 749 (*synth*)
Stetter, H. *et al., Chem. Ber.*, 1976, **109**, 534 (*synth*)
Kawashima, M. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 3255 (*synth*)
Schick, H. *et al., Synthesis*, 1992, 369 (*synth*)
Xu, S. *et al., Redai Haiyang*, 1993, **12**, 1-9; *CA*, **121**, 77921 (*Gracilaria tenuistipitata constit*)
Geraghty, N.W.A. *et al., Synth. Commun.*, 1994, **24**, 1351 (*Me ester*)
Sorokin, V.L. *et al., Synthesis*, 1994, 361 (*Me ester*)

11-Oxo-9,12-octadecadienoic acid O-163

$H_3C(CH_2)_4CH{=}CHCOCH{=}CH(CH_2)_7COOH$
$C_{18}H_{30}O_3$ 294.433

(E,E)*-*form [223754-54-9]
Prod. by *Trichoderma* sp. F5594. Enhances fibrinolytic activity in endothelial cells. Light brown oil. λ_{max} 253 (ε 10100) (MeOH).

(Z,Z)*-*form
11-Oxolinoleic acid
[70247-26-6]
Constit. of the glyceride complex of *Onopordon acanthium*. Metab. of linoleic acid in *Lithothamnion corallioides*.

[158956-80-0]

Ul'chenko, N.T. *et al., Khim. Prir. Soedin.*, 1978, 699-707 (*isol*)
Hamberg, M. *et al., Lipids*, 1992, **27**, 487-493
Muehldorf, A.V. *et al., Tet. Lett.*, 1994, **35**, 6851-6852 (*synth*)
Shinohara, C. *et al., J. Antibiot.*, 1999, **52**, 171-174 (*isol, uv, ir, pmr, cmr, ms*)
Chikanishi, T. *et al., J. Antibiot.*, 1999, **52**, 797-802 (*activity*)

13-Oxo-9,11-octadecadienoic acid O-164

[31385-09-8]

[26474-39-5, 79790-32-2, 119051-89-7]

$H_3C(CH_2)_4COCH{=}CHCH{=}CH(CH_2)_7COOH$
$C_{18}H_{30}O_3$ 294.433

(9E,11E)*-*form [29623-29-8]
Constit. of the processed leaves of *Artemisia argyi. Also from Monnina emarginata*.
Powder. λ_{max} 276 (log ε 4.21) (MeOH).
2,3-Dihydroxypropyl ester:
$C_{21}H_{36}O_5$ 368.512
Isol. from the mushroom *Clitocybe clavipes*. Oil.

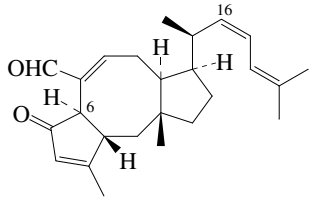
(9Z,11E)*-*form [54739-30-9]
Constit. of the processed leaves of *Artemisia argyi*. Also from the alga *Gracilariopsis lemaneiformis*.
Powder. λ_{max} 278 (log ε 4.15) (MeOH).
Phillips, B.E. *et al., Biochim. Biophys. Acta*, 1970, **210**, 353 (*isol, uv, ir, pmr*)

Jiang, Z.D. *et al., Phytochemistry*, 1991, **30**, 1187 (*isol*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1656 (*isol, uv, ir, pmr, cmr, ms*)
Kawagishi, H. *et al., J. Nat. Prod.*, 2002, **65**, 1712-1714 (*dihydroxypropyl ester*)

5-Oxo-3,7,16,18-ophiobolatetraen-21-al O-165

Ophiobolin G

[90108-63-7]



$C_{25}H_{34}O_2$ 366.542

Sesterterpene antibiotic. Isol. from *Aspergillus ustus* ATCC38849. Phytotoxin. Active against *Bacillus subtilis*. Inhibits etiolated wheat coleoptile growth. Translucent fine needles. Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane.
Mp 131-133°. λ_{max} 235 (ϵ 36300) (EtOH) (Berdy).

6-Epimer: ***6-Epiophiobolin G***
[753457-93-1]
$C_{25}H_{34}O_2$ 366.542
Constit. of the marine derived fungus *Emericella variecolor* GF10. Amorph. powder. $[\alpha]_D^{23}$ +117 (c, 1.05 in MeOH). λ_{max} 228 (ϵ 27000) ($CHCl_3$).

6-Epimer, 16,17-dihydro: ***6-Epiophiobolin N***
[753457-94-2]
$C_{25}H_{36}O_2$ 368.558
Constit. of the marine derived fungus *Emericella variecolor* GF10. Amorph. powder. $[\alpha]_D^{23}$ +88 (c, 0.34 in MeOH).

Cutler, H.G. *et al., J. Agric. Food Chem.*, 1984, **32**, 778 (*isol, uv, ir, pmr, cmr*)
Wei, H. *et al., Tetrahedron*, 2004, **60**, 6015-6019 (*6-Epiophiobolins G and N*)

4-Oxopentanoic acid, 9CI O-166

Levulinic acid, 8CI. 3-Acetylpropionic acid. FEMA 2627
[123-76-2]
$H_3CCOCH_2CH_2COOH$
$C_5H_8O_3$ 116.116
Obt. by the action of dil. acids on carbohydrates, e.g. sucrose, glucose, starch. Isol. from bagasse, the prod. of fermentation of sugar cane. Isol. from lychee (*Litchi chinensis*), Malabar spinach (*Basella rubra*) and prod. by *Phyllophora* spp. Used to make antacids, cathartics and shampoos, nylon, synthetic rubber, plastics and medicines. Flavour ingredient. Reagent for cleavage of oximes and 2,4-dinitrophenylhydrazones. Plates or leaflets with tart, whisky taste. V. sol. H_2O, EtOH, Et_2O; insol. hydrocarbons. Mp 33.5°. Bp 245° Bp_{14} 143-147°. pK_a 4.62.

▶ Skin irritant. LD_{50} (rat, orl) 1850 mg/kg. OI1575000

[591-64-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 531B; 685B; 685C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 823A; 1102B; 1102C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 741D (*ir*)
Sadtler Standard C-13 NMR Spectra, 2217 (*cmr*)
Sah, P.P.T. *et al., J.A.C.S.*, 1930, **52**, 4881 (*synth*)
Org. Synth., Coll. Vol., 1, 1932, 335 (*synth*)
Cowley, M.A. *et al., J.A.C.S.*, 1933, **55**, 3463 (*bibl*)
Mattox, V.R. *et al., J.A.C.S.*, 1948, **70**, 882 (*use*)
Leonard, R.H. *et al., Ind. Eng. Chem.*, 1956, **48**, 1331 (*rev*)
Cooper, A.J.L. *et al., J. Biol. Chem.*, 1975, **250**, 527 (*pmr*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 308
Srzić, D. *et al., Org. Mass Spectrom.*, 1988, **23**, 829 (*ms*)
Sizov, A.Y. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1990, 474; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1990, 412 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EFS600; LFH000

4-Oxo-19-phenyl-5-nonadecenoic acid O-167

$Ph(CH_2)_{13}CH{=}CHCOCH_2CH_2COOH$
$C_{25}H_{38}O_3$ 386.573

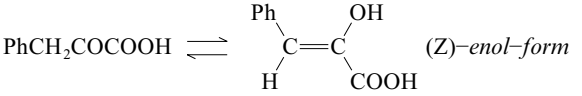
(E)-form
Constit. of *Xylocarpus moluccensis*.
Mp 74-76°.

Me ester:
$C_{26}H_{40}O_3$ 400.6
Constit. of *Xylocarpus moluccensis*. Oil.

Bercich, M.G. *et al., Aust. J. Chem.*, 1998, **51**, 795-797 (*isol, pmr, cmr, ms*)

2-Oxo-3-phenylpropanoic acid O-168

α-Oxobenzenepropanoic acid, 9CI. Phenylpyruvic acid. 2-Hydroxy-3-phenyl-2-propenoic acid, 9CI. α-Hydroxycinnamic acid. FEMA 3892
[156-06-9]



$C_9H_8O_3$ 164.16

Exists as (*Z*)-enol-form in solid state; enol predominates in organic solvents; equilibrium in aq. soln. Occurs in plants, prod. by *Pseudomonas* and other microorganisms. Substrate for microbial production of phenylalanine. Plates ($CHCl_3$). Spar. sol. hot H_2O.
Mp 157° dec. Oxidises in air. Reduces boiling Fehling's soln.

Na salt: [114-76-1]
Cryst. + $1H_2O$. Insol. EtOH. Stable in air. H_2O of cryst. remains at 100°.

Me ester: Methyl phenylpyruvate
[6362-58-9]
$C_{10}H_{10}O_3$ 178.187
Needles. Mp 75°.

Et ester: Ethyl phenylpyruvate
[6613-41-8]
$C_{11}H_{12}O_3$ 192.214
Needles. Insol. H_2O. Mp 45°. Bp_{15} 154.5°. Oxidises in air. Enolic Et esters (*E*- and *Z*-) are also known.

Amide: [6362-62-5]
$C_9H_9NO_2$ 163.176
Sol. hot EtOH; insol. H_2O, Et_2O, C_6H_6. Mp 190°.

Anilide: [6362-61-4]
$C_{15}H_{13}NO_2$ 239.273
Mp 127-129°.

Nitrile: Phenacetyl cyanide
[33472-02-5]
C_9H_7NO 145.16
Bp_3 100-120°.

Oxo-*form* [156-06-9]

Oxime: α-(Hydroxyimino)benzenepropanoic acid, 9CI
[3682-17-5]
$C_9H_9NO_3$ 179.175
Isol. from the sponge *Psammaplysilla purpurea*. Used as a 3% soln. in EtOH for gravimetric detn. of Cu; pptn. of heavy metals. Needles (EtOH aq. or H_2O).
Mp 159° dec.

Semicarbazone: Mp 180° dec.

4-Nitrophenylhydrazone:
Cryst. (EtOH aq.). Mp 187-188° dec.

2-Quinolylhydrazone: See α-(2-Quinolinylhydrazono)benzenepropanoic acid in *The Combined Chemical Dictionary.*

Et ester, oxime:
$C_{11}H_{13}NO_3$ 207.229
Prisms or needles (petrol). Mp 57-58°.

Et ester, phenylhydrazone: Mp 89°.

Et ester, semicarbazone:
Plates (EtOH aq.). Mp 167°.

Amide, oxime: [13942-61-5]
$C_9H_{10}N_2O_2$ 178.19
Needles (H_2O). Mp 147°.

(*Z-enol*)-*form*

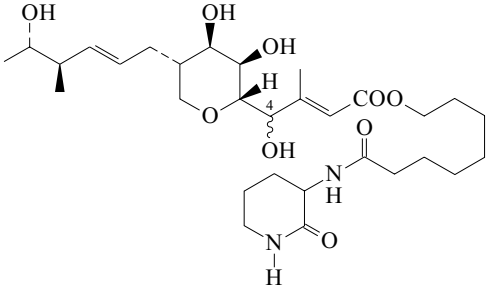
O-*β*-D-*Glucopyranoside:* [180161-92-6]
$C_{15}H_{18}O_8$ 326.302
Constit. of *Aspalathus linearis.*

[52178-60-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 273A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 998B (*nmr*)
Org. Synth., Coll. Vol., 2, 1943, 519 (*synth*)
Weygand, F. *et al., Annalen*, 1962, **658**, 128 (*synth*)
Katyal, M. *et al., Curr. Sci.*, 1962, **31**, 373 (*oxime, detn, Cu*)
Katyal, M. *et al., J. Indian Chem. Soc.*, 1963, **40**, 491 (*pptn*)
Kretovich, V.L. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1964, **158**, 471 (*occur*)
Igarashi, M. *et al., J.O.C.*, 1967, **32**, 3399 (*synth*)
Anatol, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1971, **272**, 1159 (*synth*)
Kulkarni, B.D. *et al., Indian J. Chem.*, 1975, **13**, 1097 (*synth*)
Haider, Q. *et al., J. Indian Chem. Soc.*, 1975, **552**, 881 (*oxime, detn, Cu*)
Sciacovelli, O. *et al., Z. Naturforsch., C*, 1976, **31**, 5 (*ms, cmr, pmr*)
Ramage, R. *et al., J.C.S. Perkin 1*, 1984, 1531 (*synth, ir*)
Fujita, Y. *et al., Chem. Pharm. Bull.*, 1985, **33**, 242 (*anal*)
Hanai, K. *et al., J. Phys. Chem.*, 1989, **93**, 6013 (*ir, Raman*)
Hanai, K. *et al., J. Mol. Struct.*, 1991, **245**, 21 (*ir, pmr, uv*)
Kuwae, A. *et al., Spectrochim. Acta A*, 1993, **49**, 125 (*cmr*)
Yagi, H. *et al., Tetrahedron*, 1993, **49**, 3749-3754 (*oxime, isol*)
Marais, C. *et al., J.C.S. Perkin 1*, 1996, **2915**, (*isol, biosynth, synth*)
Pat. Coop. Treaty (WIPO), 1996, 96 10 927; *CA*, **125**, 56856n (*use*)
Marais, C. *et al., Tet. Lett.*, 1996, **37**, 5763 (*glucoside*)
Okabe, N. *et al., Acta Cryst. C*, 1997, **53**, 1449-1450 (*cryst struct*)
Lu, Y. *et al., Phytochemistry*, 2000, **55**, 67-75 (*glucoside*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1394 (*use*)

8-[(2-Oxo-3-piperidinyl)amino]-8-oxooctyl 5,9-anhydro-2,3,8-trideoxy-8-(5-hydroxy-4-methyl-2-hexenyl)-3-methyl-DL-*glycero*-LD-*allo*-non-2-enoate, 9CI O-169

[147024-92-8]



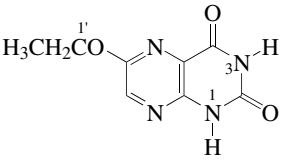
$C_{30}H_{50}N_2O_9$ 582.733
Constit. of the marine bacterium *Alteromonas rava*. Antimicrobial agent. Oil. $[\alpha]_D$ -1.8 (c, 0.003 in MeOH). Related to Pseudomonic acid A. λ_{max} 220 (ϵ 14000) (MeOH) (Berdy).

4-Deoxy: BP 2. NSC 646282
[147024-96-2]
$C_{30}H_{50}N_2O_8$ 566.734
Constit. of *Alteromonas* sp. Antimicrobial agent. Oil. $[\alpha]_D$ -3.1 (c, 0.005 in MeOH). λ_{max} 220 (ϵ 14000) (MeOH) (Berdy).

Stierle, D.B. *et al., Experientia*, 1992, **48**, 1165 (*isol, pmr, cmr*)
Shiozawa, H. *et al., Annu. Rep. Sankyo Res. Lab.*, 1999, **51**, 45-72 (*rev*)

6-(1-Oxopropyl)-2,4(1*H*,3*H*)-pteridinedione, 9CI O-170

6-Propionyllumazine
[126857-77-0]



$C_9H_8N_4O_3$ 220.187
Isol. from the marine polychaete *Odontosyllis undecimdonta*.
Mp 278-280° dec.

*3-Me: 3-Methyl-6-(1-oxopropyl)-2,4(1*H,3H*)-pteridinedione, 9CI.* ***3-Methyl-6-propionyllumazine***
[71014-16-9]
$C_{10}H_{10}N_4O_3$ 234.214
Isol. from *Odontosyllis undecimdonta*. Cryst. ($CHCl_3$/hexane).
Mp 234° (227-228°).

*1,3-Di-Me: 1,3-Dimethyl-6-(1-oxopropyl)-2,4(1*H,3H*)-pteridinedione, 9CI.* ***1,3-Dimethyl-6-propionyllumazine***
[71014-17-0]
$C_{11}H_{12}N_4O_3$ 248.241
Isol. from *Odontosyllis undecimdonta*. Cryst. (C_6H_6/petrol).
Mp 146-147° (141-142°).

3-Me, 3′-hydroxy: ***6-(β-Hydroxypropionyl)-3-methyllumazine***
[135048-63-4]
$C_{10}H_{10}N_4O_4$ 250.213
From *Odontosyllis undecimdonta*.
Mp 200° dec.

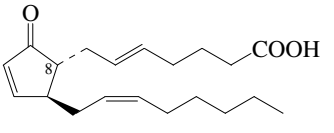
3-Me, 3′-methoxy: ***6-(β-Methoxypropionyl)-3-methyllumazine***
[135048-61-2]
$C_{11}H_{12}N_4O_4$ 264.24
From *Odontosyllis undecimdonta*.
Mp 193-196° dec.

1,3-Di-Me, 3′-hydroxy: ***6-(β-Hydroxypropionyl)-1,3-dimethyllumazine***
[163132-70-5]
$C_{11}H_{12}N_4O_4$ 264.24
From *Odontosyllis undecimdonta*.
Mp 168-169° dec.

1,3-Di-Me, 3′-methoxy: ***6-(β-Methoxypropionyl)-1,3-dimethyllumazine***
[135048-62-3]
$C_{12}H_{14}N_4O_4$ 278.267
From *Odontosyllis undecimdonta*.
Mp 129-130°.

Baur, R. *et al., Annalen*, 1984, 1798 (*synth, deriv*)
Pfleiderer, W. *et al., Tetrahedron*, 1988, **44**, 3373 (*synth, deriv*)
Inoue, S. *et al., Chem. Lett.*, 1990, 367 (*isol*)
Kakoi, H. *et al., Heterocycles*, 1995, **41**, 789-797 (*isol, uv, pmr, cmr, struct*)

9-Oxo-5,10,14-prostatrienoic acid, 9CI O-171



(5*E*,8α,12β,14*Z*)-*form*

$C_{20}H_{30}O_3$ 318.455

(5*E*,8α,12β,14*Z*)-*form*

Me ester.
[289896-07-7]
$C_{21}H_{32}O_3$ 332.482
Isol. from *Plexaura nina*. Yellowish oil. $[\alpha]_D^{20}$ +103 ($CHCl_3$). C-5 config. revised in 2003.

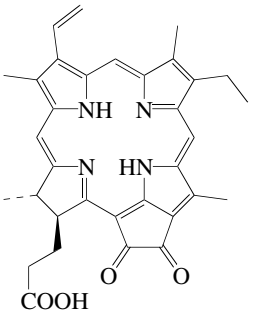
(5*Z*,8α,12α,14*Z*)-*form*
Preclavulone A
[117248-65-4]
Isol. from corals *Clavularia viridis, Pseudoplexaura porosa* and other coral spp.
Me ester: [98964-95-5]
Isol. from *Clavularia viridis.*
$[\alpha]_D^{20}$ -131.8 (c, 1.14 in THF).

(5*Z*,8β,12α,14*Z*)-*form*
Me ester: Isol. from *Clavularia viridis.*
Viscous oil. $[\alpha]_D$ -49.8 (c, 0.08 in THF). λ_{max} 216 (ϵ 9900) (MeOH).

Corey, E.J. *et al., Tet. Lett.*, 1985, **26**, 4171; 1987, **28**, 4247; 1988, **29**, 995 (*isol, synth, biosynth, pmr, cmr, ms*)
Corey, E.J. *et al., J.A.C.S.*, 1987, **109**, 289 (*biosynth*)
Watanabe, K. *et al., Chem. Pharm. Bull.*, 2003, **51**, 909-913 (*isol, pmr, cmr*)
Ito, H. *et al., Tet. Lett.*, 2004, **45**, 1941-1944 (*Me ester, synth*)
Zanoni, G. *et al., J.O.C.*, 2006, **71**, 8459-8466 (*Preclavulone A, synth*)

13²-Oxopyrophaeophorbide a O-172

13²-Oxopyropheophorbide a
[148031-29-2]



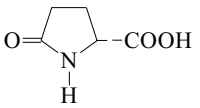
$C_{33}H_{32}N_4O_4$ 548.64
Isol. from the marine bivalve *Ruditapes philipinarum*. Yellow-brown solid. λ_{max} 288; 386; 514; 618; 676 (MeOH).

Me ester: [175275-29-3]
Yellow cryst. (CH_2Cl_2/hexane). Mp 245°.

Watanabe, N. *et al., J. Nat. Prod.*, 1993, **56**, 305 (*isol, uv, pmr*)
Ma, L. *et al., J.O.C.*, 1996, **61**, 2501 (*synth, uv, pmr, cmr*)

5-Oxo-2-pyrrolidinecarboxylic acid O-173

5-Oxoproline, 9CI. ***Pidolic acid, BAN, INN****. α-Aminoglutaric acid lactam. Glutimic acid lactam. Glutimic acid. Glutiminic acid. Pyroglutamic acid. 2-Pyrrolidone-5-carboxylic acid*



(*R*)–*form*

$C_5H_7NO_3$ 129.115
Antihyperlipidaemic agent. Log P -1.27 (calc).

(*R*)-*form*
D-form
[4042-36-8]
Cryst. (H_2O). Mp 182°. $[\alpha]_D$ +10.7 (H_2O).

(*S*)-*form*
L-form
[98-79-3]
Found in substantial amounts in brain tissue and other tissue in bound form, esp. skin. Also present in plant tissues. Isol. from the tunicate *Botryllus schlosseri*. Used in resoln. of amines.
Cryst. (H_2O).
Mp 156-157°. $[\alpha]_D^{20}$ -11.45 (c, 4.44 in H_2O).

(ξ)-*form*
N-*(2,3-Dibromo-4,5-dihydroxybenzyl):*
$C_{12}H_{11}Br_2NO_5$ 409.031
Isol. from the red alga *Rhodomela confervoides*. Cryst. (MeOH aq.).
Mp 172-174°. $[\alpha]_D^{20}$ +24 (c, 5.7 in Me_2CO).

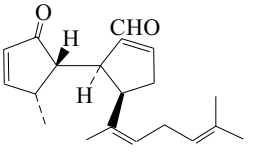
N-*(2,3-Dibromo-4,5-dihydroxybenzyl), Me ester:*
$C_{13}H_{13}Br_2NO_5$ 423.057
Isol. from *Rhodomela confervoides*. Cryst. (MeOH aq.).
Mp 183-185°. $[\alpha]_D^{20}$ +7 (c, 5 in Me_2CO).

N-*[3-Bromo-2-(2,3-dibromo-4,5-dihydroxybenzyl)-4,5-dihydroxybenzyl], Me ester:*
$C_{20}H_{18}Br_3NO_7$ 624.077
Isol. from *Rhodomela confervoides*. Cryst. (MeOH aq.).
Mp 196-198°. $[\alpha]_D^{20}$ -30.9 (c, 9.7 in Me_2CO).

[28874-51-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 791A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1289C; 1290A; 1291A; 1291B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 789C; 789D (*ir*)
Hardegger, E. *et al., Helv. Chim. Acta*, 1955, **38**, 312-320 (*S-form, synth, abs config*)
Gibian, H. *et al., Annalen*, 1961, **640**, 145-156 (*synth, bibl*)
Pattabhi, V. *et al., J.C.S. Perkin 2*, 1974, 1085-1089 (*cryst struct*)
Taira, Z. *et al., Acta Cryst. B*, 1977, **33**, 3823-3827 (*cryst struct*)
Hardy, P.M. *et al., Synthesis*, 1978, 290-291 (*synth*)
Schmidt, U. *et al., Synthesis*, 1978, 752-754 (*synth*)
Abraham, G.N. *et al., Mol. Cell. Biochem.*, 1981, **38**, 181-191 (*rev*)
Rigo, B. *et al., J. Het. Chem.*, 1995, **32**, 1489-1492 (*occur*)
Usov, A.I. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2002, **28**, 147-151 (*Botryllus constit*)
Zhao, J. *et al., J. Nat. Prod.*, 2005, **68**, 691-694 (*Rhodomela dibromobenzyl constits*)

10-Oxo-4,10-seco-2,4,13(15),17-spatatetraen-12-al O-174



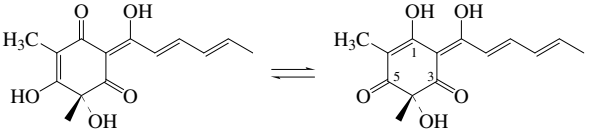
$C_{20}H_{26}O_2$ 298.424

(13(15)*Z*)-*form* [81575-02-2]
Constit. of *Dilophus marginatus.*
Oil. $[\alpha]_D^{20}$ +196 (c, 1 in CCl_4).

12-Carboxylic acid, Me ester: ***Methyl 10-oxo-4,10-seco-2,4,13(15),17-spatatetraen-12-oate***
$C_{21}H_{28}O_3$ 328.45
Metab. of *Dilophus okamurai*. Oil. $[\alpha]_D$ +182 (c, 1.14 in $CHCl_3$).

Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 129 (*isol, struct*)
Kurata, K. *et al., Phytochemistry*, 1990, **29**, 3453 (*isol, pmr, cmr*)

Oxosorbicillinol O-175



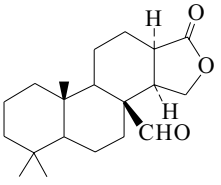
$C_{14}H_{16}O_5$ 264.277
Enolised β-triketone. The isolate from *P. notatum* appears to be the stable 3,5-dioxo tautomer but the evidence is not conclusive. Prod. by *Trichoderma* sp. USF-2690 and a marine-derived *Penicillium chrysogenum*.Also from *Penicillium notatum* GWPA. Antioxidant. Amorph. yellow powder. $[\alpha]_D^{21}$ -65 (c, 0.1 in MeOH). λ_{max} 231 (ϵ 11000); 301 (ϵ 9000); 377 (ϵ 17600) (MeOH).

Abe, N. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 620-622 (*isol, uv, pmr, cmr*)

Maskey, R.P. *et al., J. Nat. Prod.*, 2005, **68**, 865-870 (*isol*)
Bringmann, G. *et al., Tetrahedron*, 2005, **61**, 7252-7265 (*marine isol*)

16-Oxo-17-spongianal O-176

17-Spongianal-16-one. Spongiane lactone 7



$C_{20}H_{30}O_3$ 318.455
Constit. of *Ceratosoma brevicaudatum*. Oil.

Ksebati, M.B. *et al., J.O.C.*, 1987, **52**, 3766
Arnó, M. *et al., Tet. Lett.*, 2001, **42**, 1669-1672 (*synth*)
Arnó, M. *et al., J.O.C.*, 2003, **68**, 1242-1251 (*synth*)

13-Oxotridecanoic acid, 9CI O-177

[65157-88-2]
$OHC(CH_2)_{11}COOH$
$C_{13}H_{24}O_3$ 228.331
Solid. Mp 85°.

Me ester: [1608-77-1]
$C_{14}H_{26}O_3$ 242.358
Present in deep sea bottom sediment. Low-melting solid. d_4^{20} 0.94. Mp 19-20°. Bp_3 152-153° $Bp_{0.01}$ 123-125°. n_D^{20} 1.4469.

Me ester, semicarbazone:
Solid (EtOAc). Mp 116.5-117.5°.

[1119-77-3]

Noller, C.R. *et al., J.A.C.S.*, 1926, **48**, 1074 (*deriv, synth*)
Bestmann, H.J. *et al., Chem. Ber.*, 1979, **112**, 3740 (*synth*)
Leblanc, P. *et al., J. Biol. Chem.*, 1982, **257**, 14586 (*synth*)
Waugh, K.M. *et al., J.O.C.*, 1984, **49**, 873 (*synth, cmr, pmr*)
Subbaraman, A.S. *et al., Indian J. Chem., Sect. B*, 1991, **30**, 865 (*synth, ir*)

11-Oxo-5,9-undecadienoic acid O-178

10-Formyl-5,9-decadienoic acid
$OHCCH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{11}H_{16}O_3$ 196.246

(5Z,9E)-form

Me ester:
$C_{12}H_{18}O_3$ 210.272
Isol. from *Cymathere triplicata*. Cell adhesion inhibitor.

Takamatsu, S. *et al., Planta Med.*, 2004, **70**, 127-131 (*isol, activity*)

6-Oxoundecanoic acid, 9CI O-179

[91214-05-0]
$H_3C(CH_2)_4CO(CH_2)_4COOH$
$C_{11}H_{20}O_3$ 200.277
Present in marine aerosols.

Me ester: [79664-91-8]
$C_{12}H_{22}O_3$ 214.304
Liq. Bp_{19} 133-135°.

Nitrile: 6-Oxoundecanenitrile, 9CI. 1-Cyano-5-decanone
[102503-99-1]
$C_{11}H_{19}NO$ 181.277
Liq. $Bp_{0.05}$ 82-85°.

[72665-99-7]

Torii, S. *et al., J.O.C.*, 1982, **47**, 47; 1986, **51**, 155 (*synth*)
Giese, B. *et al., Tetrahedron*, 1985, **41**, 4025 (*deriv, synth, pmr, ir*)
Kawamura, K. *et al., J. Chromatogr.*, 1988, **438**, 299 (*isol, glc, ms*)

11-Oxoundecanoic acid, 9CI O-180

11-Aldehydoundecanoic acid. 10-Formyldecanoic acid
[53163-99-8]
$OHC(CH_2)_9COOH$
$C_{11}H_{20}O_3$ 200.277
Present in marine sediments.

Trimer:
$C_{33}H_{60}O_9$ 600.832
Solid. Mp 126°.

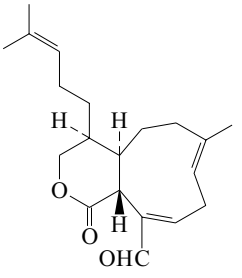
Me ester: [1931-65-3]
$C_{12}H_{22}O_3$ 214.304
Low-melting solid. d_{20}^{20} 0.95. Mp 16°. Bp_5 154° $Bp_{0.02}$ 110-112°. n_D^{20} 1.4432.

Me ester, di-Me acetal: Methyl 11,11-dimethoxyundecanoate
[1931-66-4]
$C_{14}H_{28}O_4$ 260.373
Liq. $Bp_{0.6}$ 151°.

Et ester: [85318-87-2]
$C_{13}H_{24}O_3$ 228.331
Liq. Bp_1 126°.

Tomecko, C.G. *et al., J.A.C.S.*, 1927, **49**, 522 (*Me ester*)
Chang, S.S. *et al., J. Am. Oil Chem. Soc.*, 1978, **55**, 718 (*isol*)
Leblanc, P. *et al., J. Biol. Chem.*, 1982, **257**, 14586 (*synth*)
Mukaiyama, T. *et al., Chem. Lett.*, 1983, 1207 (*Et ester, synth, pmr, ir*)
Waugh, K.M. *et al., J.O.C.*, 1984, **49**, 873 (*synth, pmr, ir, Me ester*)
Brown, H.C. *et al., Tetrahedron*, 1986, **42**, 5515 (*Me ester, synth*)
Danheiser, R.L. *et al., Tet. Lett.*, 1990, **31**, 1527 (*Et ester, synth, cmr, pmr, ir*)

19-Oxo-1(9),6,13-xenicatrien-18,17-olide O-181



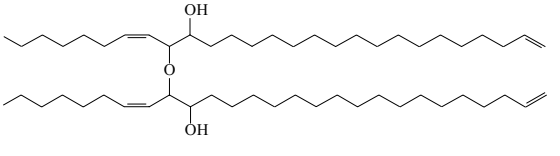
$C_{20}H_{28}O_3$ 316.439

(1(9)E,6E,10S)-form [133585-90-7]
Constit. of *Dictyota divaricata*.
Oil. $[\alpha]_D^{25}$ -189.5 (c, 0.2 in $CHCl_3$). λ_{max} 227 (ϵ 4750) (MeOH) (Berdy).

König, G.M. *et al., Tetrahedron*, 1991, **47**, 1399-1410 (*Dictyota divaricata constit*)

9,9′-Oxybis[7,26-heptacosadien-10-ol] O-182

[2-Hydroxy-1-(1-octenyl)-18-nonadecenyl] ether
[168981-89-3]

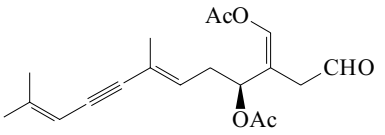


$C_{54}H_{102}O_3$ 799.398

(Z,Z)-form
Constit. of *Botryococcus braunii*.
Oil. A series of 8 long chain mono 10-acyl derivs. has also been isol.

Metzger, P. *et al., Phytochemistry*, 1995, **40**, 543-554 (*isol, pmr, cmr, ms*)

7,7′-Oxybis[6-methyl-5,8-dioxo-1-isoquinoline-methanol] O-183



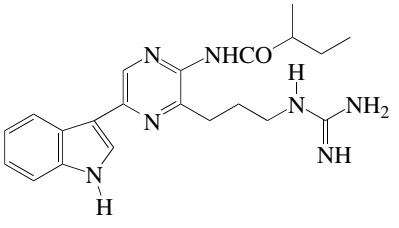
$C_{22}H_{16}N_2O_7$ 420.378
Antibacterial agent. Red cryst. λ_{max} 231 (ϵ 31850); 256 (ϵ 29970); 304 (ϵ 6250); 324 (ϵ 8000); 379 (ϵ 5140); 485 (ϵ 2170) (MeOH).

Diangeloyl: [153585-64-9]
$C_{32}H_{28}N_2O_9$ 584.581
Alkaloid from the sponge *Haliclona* sp.

Parameswaran, P.S. *et al., Oceanogr. Indian Ocean*, 1992, 417; *CA*, **120**, 187482v

Cypridina Oxyluciferin O-184

Cypridina oxyluciferin
[17297-78-8]



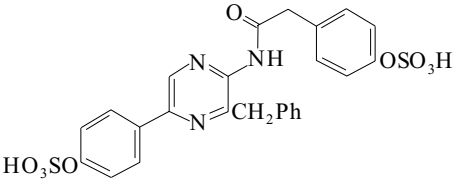
$C_{21}H_{27}N_7O$ 393.491
Isol. from *Cypridina luciferin*. Chemiluminescent agent.

[29066-76-0, 29066-77-1]

Goto, T. *et al., Tet. Lett.*, 1968, 4035-4038 (*struct, uv, fluorescence*)
Sugiura, S. *et al., Yakugaku Zasshi*, 1970, **90**, 711-715 (*synth*)
Suzuki, N. *et al., Heterocycles*, 1983, **20**, 1027-1030 (*fluorescence*)

Watasenia Oxyluciferin O-185

Watasenia oxyluciferin
[54028-46-5]

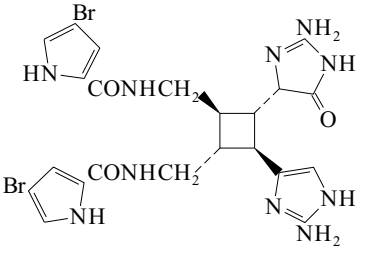


$C_{25}H_{21}N_3O_9S_2$ 571.588
Isol. from the light organs of the squid *Watasenia scintillans*. Possibly involved in bioluminescence.

Goto, T. *et al., Tet. Lett.*, 1974, 2321 (*isol, uv, pmr, struct, synth*)

Oxysceptrin O-186

[117417-62-6]



$C_{22}H_{24}Br_2N_{10}O_3$ 636.305
Alkaloid from the marine sponge *Agelas* cf *nemoechinata*, *Agelas clathrodes*, *Agelas mauritiana* and *Agelas conifera*. Actomyosin ATPase activator. Possesses antiviral and antibacterial props. Antifouling agent. Amorph. solid. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -19.7 (c, 1.02 in MeOH). λ_{max} 203 (ϵ 35100); 221 (ϵ 30700); 267 (ϵ 28100) (MeOH) (Derep). λ_{max} 214 (ϵ 21000); 268 (ϵ 21000) (MeOH) (Derep). λ_{max} 206 (ϵ 35100); 221 (ϵ 30100); 267 (ϵ 23100) (MeOH) (Berdy).

Di-Ac: [117417-63-7]
$[\alpha]_D^{25}$ +4.5 (c, 1.37 in MeOH).

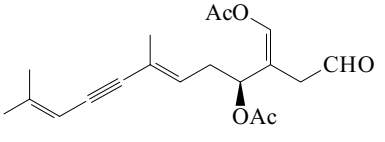
Monodebromo: ***Debromooxysceptrin***
[132911-41-2]
[117472-97-6]
$C_{22}H_{25}BrN_{10}O_3$ 557.409
Alkaloid from *Agelas conifera*, *Agelas clathrodes* and *Agelas mauritiana*. Possesses antiviral and antibacterial props. Sol. MeOH, $CHCl_3$, EtOAc; poorly sol. H_2O. $[\alpha]_D^{25}$ -25 (c, 0.108 in MeOH) (as di-Ac). λ_{max} 203 (ϵ 32400); 220 (ϵ 24600); 265 (ϵ 26600) (MeOH) (Derep).

[117468-53-8]

Kobayashi, J. *et al., Experientia*, 1991, **47**, 301 (*isol, uv, ir, pmr, cmr, ms, struct*)
Keifer, P.A. *et al., J.O.C.*, 1991, **56**, 2965 (*isol, pmr, cmr, struct*)

Oxytoxin 1 O-187

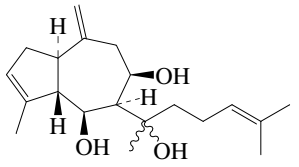
[129932-67-8]



$C_{19}H_{24}O_5$ 332.396
Constit. of *Oxynoe olivacea* and the green alga *Caulerpa taxifolia* on which it feeds. Also from *Ascobulla fragilis* and *Lobiger serradifalci*. Ichthyotoxin. Toxic to brine shrimp. Oil. $[\alpha]_D^{25}$ -70.6 (c, 2 in $CHCl_3$). λ_{max} 270 (ϵ 21600); 283 (ϵ 16500) (MeOH) (Berdy).

Cimino, G. *et al., Experientia*, 1990, **46**, 767-770 (*isol, pmr, cmr*)
Guerriero, A. *et al., Helv. Chim. Acta*, 1992, **75**, 689-695; 1993, **76**, 855-864 (*isol*)
Gavagnin, M. *et al., J. Exp. Mar. Biol. Ecol.*, 1994, **175**, 197-210

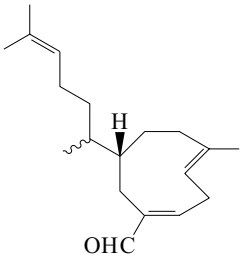
3,10(18),14-Pachdictyatriene-6,8,11-triol P-1



(1α,5β,6β,8β,11ξ)-*form*
8β,11-Dihydroxypachydictyol A
Constit. of *Glossophora kunthii*.
Oil. $[\alpha]_D$ -6 (c, 0.1 in $CHCl_3$).
De Nys, R. *et al., Phytochemistry*, 1993, **32**, 463-465 (*8,11-Dihydroxypachydictyol A*)

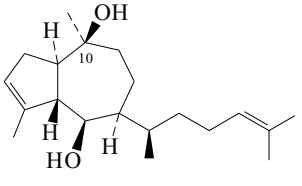
Pachyaldehyde P-2

18-Nor-1(9),6,13-xenicatrien-19-al
[94190-79-1]



$C_{19}H_{30}O$ 274.445
Constit. of *Pachydictyon coriaceum*. Oil. $[\alpha]_D^{23}$ -40 (c, 0.21 in $CHCl_3$). λ_{max} 222 (ϵ 10000) (EtOH) (Derep).
Ishitsuka, M. *et al., Chem. Comm.*, 1984, 906 (*isol, pmr, cmr*)

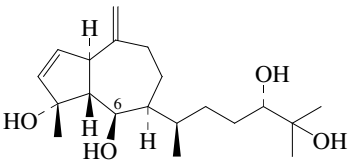
3,14-Pachydictyadiene-6,10-diol P-3



$C_{20}H_{34}O_2$ 306.487

(1α,5β,6β,10β,11*R*)-*form*
Dictyol C
[62820-33-1]
Constit. of *Aplysia depilans*, *Aplysia dactylomela*, *Dictyota dichotoma* and *Dictyota dentata*. Algicide, antimitotic, ichthyotoxin. Cryst. (hexane). Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O.
Mp 68°. $[\alpha]_D$ -16.6 (c, 1 in $CHCl_3$).
10-Ac: ***Acetyldictyol C***
[81575-24-8]
$C_{22}H_{36}O_3$ 348.525
Constit. of *Pachydictyon coriaceum*. Oil. $[\alpha]_D$ -7.2 (c, 0.6 in MeOH).
Danise, B. *et al., Experientia*, 1977, **33**, 413-415 (*isol, pmr, cmr*)
Faulkner, D.J. *et al., Phytochemistry*, 1977, **16**, 991-993 (*isol*)
Amico, V. *et al., Tetrahedron*, 1980, **36**, 1409-1414 (*isol*)
Ishitsuka, M. *et al., Chem. Lett.*, 1982, 1517-1518 (*isol*)
Gonzalez, A.G. *et al., J. Nat. Prod.*, 1987, **50**, 1158-1159 (*isol, Aplysia*)

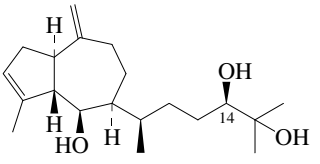
2,10(18)-Pachydictyadiene-4,6,14,15-tetrol P-4



$C_{20}H_{34}O_4$ 338.486

(1α,4α,5β,6β,12*R*,13*S*)-*form*
Cystoseirol
6-Ac: ***Cystoseirol 6-acetate***
[604807-25-2]
$C_{22}H_{36}O_5$ 380.523
Constit. of *Cystoseira myrica*. Oil.
Ayyad, S.E.N. *et al., Z. Naturforsch., C*, 2003, **58**, 33-38 (*isol, pmr, cmr*)

3,10(18)-Pachydictyadiene-6,14,15-triol P-5



(1α,5β,6β,11*R*,14*R*)-*form*

$C_{20}H_{34}O_3$ 322.487

(1α,5β,6β,11*R*,14*R*)-*form*
Dictytriol
[84181-73-7]
Isol. from brown algae *Dictyota dichotoma* and *Dictyota indica*.
Cryst.
Mp 92-93°. $[\alpha]_D^{24}$ +80.7 (c, 0.63 in $CHCl_3$).

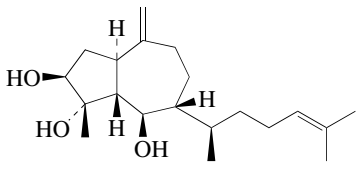
(1α,5β,6β,11*R*,14*S*)-*form*
Isodictytriol
[104113-53-3]
Isol. from *Dictyota dichotoma* and *Dictyota indica*.
Cryst.
Mp 125-126°.
6-Ac: ***Isodictytriol 6-acetate***
[604807-24-1]
$C_{22}H_{36}O_4$ 364.524
Constit. of *Cystoseira myrica*. Oil.

(1α,5β,6β,11*R*,14ξ)-*form*
15-Me ether: [149064-79-9]
$C_{21}H_{36}O_3$ 336.514
Constit. of *Aplysia* sp.
$[\alpha]_D$ +58.1 (c, 1.14 in $CHCl_3$).

(1ξ,5ξ,6ξ,11ξ,14ξ)(1)-*form*
Dictyotriol A†
[95120-01-7]
Constit. of *Dictyota indica*. Not to be confused with 3,10(18),14-Pachydictyatriene-6,9,12-triol, P-25.

(1ξ,5ξ,6ξ,11ξ,14ξ)(2)-*form*
Dictyotriol B
[95120-02-8]
Constit. of *Dictyota indica*.
Enoki, N. *et al., Chem. Lett.*, 1982, 1837-1840 (*Dictytriol, isol, struct, pmr*)
Li, L. *et al., Hydrobiologia*, 1984, **116-7**, 168 (*Dictyotriols*)
Kusumi, T. *et al., Chem. Lett.*, 1986, 1241-1242 (*Isodictytriol*)
Yamaguchi, Y. *et al., Kinki Daigaku Rikogakubu Kenkyu Hokoku*, 1992, **2**, 73-81; *CA*, **119**, 91581e (*15-Me ether*)
Ayyad, S.-E.N. *et al., Z. Naturforsch., C*, 2003, **58**, 33-38 (*Isodictytriol 6-acetate*)

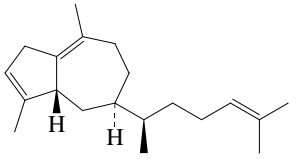
10(18),14-Pachydictyadiene-3,4,6-triol P-6



$C_{20}H_{34}O_3$ 322.487

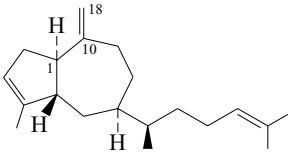
(1α,3β,4α,5β,6β,7β*H*,11*R*)-*form*
Dictyotatriol A
[193975-36-9]
Constit. of *Dictyota dichotoma*.
Amorph. solid. $[\alpha]_D^{25}$ +27.8 (c, 0.09 in $CHCl_3$).
Durán, R. *et al., Tetrahedron*, 1997, **53**, 8675-8688 (*isol, pmr, cmr*)

1(10),3,14-Pachydictyatriene P-7
Dictytriene B
[84164-87-4]



$C_{20}H_{32}$ 272.473
Constit. of *Dictyota dichotoma*. Oil. $[\alpha]_D^{22}$ +54.4 (c, 0.29 in cyclohexane).
Kusumi, T. *et al., Chem. Lett.*, 1986, 1241 (*cryst struct*)

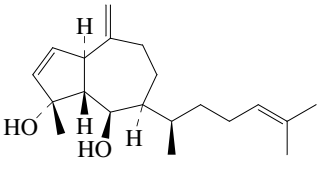
3,10(18),14-Pachydictyatriene P-8



$C_{20}H_{32}$ 272.473

(1α,5β,12*R*)-*form*
Dictyatriene A
[84164-86-3]
Constit. of brown alga *Dictyota dichotoma*.
Oil. $[\alpha]_D^{22}$ +37 (c, 0.28 in $CHCl_3$).
Enoki, N. *et al., Chem. Lett.*, 1982, 1837-1840 (*isol*)
Li, L. *et al., Hydrobiologia*, 1984, **116-117**, 168 (*isol*)

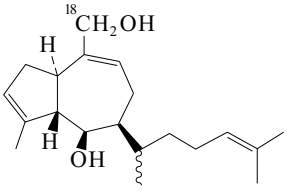
2,10(18),14-Pachydictyatriene-4,6-diol P-9



$C_{20}H_{32}O_2$ 304.472
Revised abs. config. Earlier work by the same authors assigning abs. config. from CD was unreliable.

(1α,4α*OH*,5β,6β,7α*H*,11*R*)-*form*
Dictyotadiol
[63908-63-4]
Constit. of *Dictyota* spp.
Cryst. (Me_2CO/hexane).
Mp 150-151°. $[\alpha]_D$ +1.3 (c, 0.15 in MeOH).
Faulkner, D.J. *et al., Phytochemistry*, 1977, **16**, 991-993 (*isol, pmr, cryst struct*)
Arroyo, J.T. *et al., J.O.C.*, 1991, **56**, 2671-2675 (*abs config*)

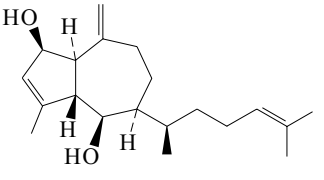
3,9,14-Pachydictyatriene-6,18-diol P-10



$C_{20}H_{32}O_2$ 304.472

(1α,5β,6β,11ξ)-*form*
Dictyol I
Constit. of *Dictyota dichotoma* var. *implexa*.
Oil.
18-Aldehyde: 6-Hydroxy-3,9,14-pachydictyatrien-18-al. ***Isopachydictyolal***
[760996-46-1]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Dictyota dichotoma*.
De Rosa, S. *et al., Phytochemistry*, 1986, **25**, 2179-2181 (*Dyctyol I*)
Siamopoulou, P. *et al., Phytochemistry*, 2004, **65**, 2025-2030 (*Isopachydictyolal*)

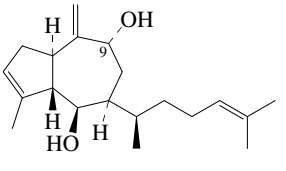
3,10(18),14-Pachydictyatriene-2,6-diol P-11



$C_{20}H_{32}O_2$ 304.472

(1α,2β,5β,6β,11*R*)-*form*
Dictyol D
[62820-34-2]
Constit. of *Aplysia depilans* and *Dictyota dichotoma*.
Oil. $[\alpha]_D$ -80 (c, 2 in $CHCl_3$).
2-Ac: [163089-14-3]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Dictyota dichotoma*.
Danise, B. *et al., Experientia*, 1977, **33**, 413-415 (*isol, pmr, cmr*)
Palermo, J.A. *et al., An. Asoc. Quim. Argent.*, 1994, **82**, 355; *CA*, **122**, 286227p (*2-Ac*)

3,10(18),14-Pachydictyatriene-6,9-diol P-12



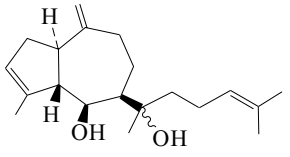
(1α,5β,6β,7α*H*,9α,12*R*)-*form*

$C_{20}H_{32}O_2$ 304.472
Revised abs. configs. Earlier work by the same authors assigning the opposite abs. configs. by CD was unreliable.

(1α,5β,6β,7α*H*,9α,12*R*)-*form*
9-Epidictyol B
Isol. from brown alga *Glossophora kuntii*.
Oil. $[\alpha]_D^{25}$ +45.9 (c, 0.26 in $CHCl_3$).

(1α,5β,6β,7α*H*,9β,12*R*)-*form*
Dictyol B
[61263-83-0]
Constit. of *Dictyota dichotoma* and *Aplysia depilans.*
Cryst. (hexane).
Mp 112-115°. $[\alpha]_D$ +76 ($CHCl_3$).
9-Ac: ***Acetyldictyol B***
$C_{22}H_{34}O_3$ 346.509
Constit. of *Dictyota dichotoma*. Oil. $[\alpha]_D^{25}$ +59 (c, 1.27 in MeOH).
Fattorusso, E. *et al., Chem. Comm.*, 1976, 575-576 (*Dictyols A,B*)
Minale, L. *et al., Tet. Lett.*, 1976, **17**, 2711-2714 (*Aplysia depilans constit*)
Faulkner, D.J. *et al., Phytochemistry*, 1977, **16**, 991 (*Acetyldictyol B*)
Vázquez, J.T. *et al., J.O.C.*, 1991, **56**, 2671-2675 (*abs config*)

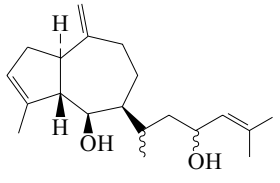
3,10(18),14-Pachydictyatriene-6,11-diol **P-13**



$C_{20}H_{32}O_2$ 304.472

(1α,5β,6β,11ξ)-*form*
Dictyol E
[62858-25-7]
Constit. of *Dilophus ligulatus*, *Aplysia depilans*, *Dilophus guineensis* and *Dictyota dichotoma.*
Oil. $[\alpha]_D$ +26.8 (c, 1 in $CHCl_3$).
Danise, B. *et al., Experientia*, 1977, **33**, 413-415 (*isol, pmr, cmr*)
Sun, H.H. *et al., Phytochemistry*, 1979, **18**, 340-341 (*isol*)
Amico, V. *et al., Tetrahedron*, 1980, **36**, 1409-1414 (*isol*)
Hay, M.E. *et al., Ecology*, 1987, **68**, 1567-1580 (*props*)
Gedara, S.R. *et al., Z. Naturforsch., C*, 2003, **58**, 17-22 (*Dictyota dichotoma constit*)

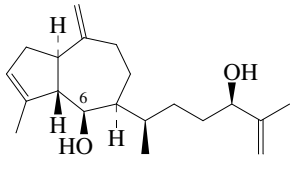
3,10(18),14-Pachydictyatriene-6,13-diol **P-14**



$C_{20}H_{32}O_2$ 304.472

(1α,5β,6β,11ξ,13ξ)-*form*
Dictyol G
[93710-22-6]
13-Ac:
$C_{22}H_{34}O_3$ 346.509
Constit. of *Dictyota binghamiae* and *Dictyota volubilis.* Oil. $[\alpha]_D^{22}$ +50 (c, 0.13 in $CHCl_3$).
Pathirana, C. *et al., Can. J. Chem.*, 1984, **62**, 1666-1671 (*isol, pmr, cmr*)
König, G.M. *et al., Planta Med.*, 1993, **59**, 174-178 (*isol, pmr, cmr*)

3,10(18),15-Pachydictyatriene-6,14-diol **P-15**



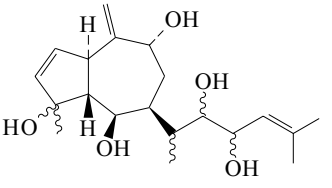
(1α,5β,6β,11*R*,14*R*)-*form*

$C_{20}H_{32}O_2$ 304.472

(1α,5β,6β,11*R*,14*R*)-*form*
Dictyol F
[87980-58-3]
Constit. of the brown alga *Dictyota dichotoma* and the mollusc *Aplysia depilans.* Shows antimicrobial activity. Oil. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D^{25}$ +48.2 (c, 1.5 in $CHCl_3$).
6-Ac: [604807-23-0]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Cystoseira myrica*. Oil.

(1α,5β,6β,11*R*,14*S*)-*form*
Epidictyol F
Constit. of *Dictyota dichotoma* and *Aplysia depilans.* Shows antimicrobial activity. Cryst. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O.
Mp 62-63°. $[\alpha]_D^{25}$ +37.5 (c, 1.1 in $CHCl_3$).
Enoki, N. *et al., Chem. Lett.*, 1983, 1627-1630 (*Dictyol F, Epidictyol F*)
Ayyad, S.E.N. *et al., Z. Naturforsch., C*, 2003, **58**, 33-38 (*6-Ac*)

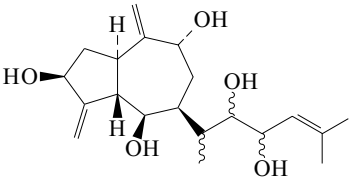
2,10(18),14-Pachydictyatriene-4,6,9,12,13-pentol **P-16**
2,10(18),14-Prenylguaiatriene-4,6,9,12,13-pentol



$C_{20}H_{32}O_5$ 352.47

(1α,4ξ,5β,6β,9α,11ξ,12ξ,13ξ)-*form*
12,13-Di-Ac: [146523-00-4]
$C_{24}H_{36}O_7$ 436.544
Constit. of *Dictyota volubilis.* Oil. $[\alpha]_D^{25}$ -15.3 (c, 0.6 in $CHCl_3$).
Wright, A.D. *et al., Tetrahedron*, 1993, **49**, 571-580 (*isol, pmr, cmr*)

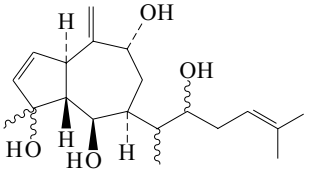
4(17),10(18),14-Pachydictyatriene-3,6,9,12,13-pentol **P-17**
4(17),10(18),14-Prenylguaiatriene-3,6,9,12,13-pentol



$C_{20}H_{32}O_5$ 352.47

(1α,3β,5β,6β,9α,11ξ,12ξ,13ξ)-*form*
12,13-Di-Ac: [146522-99-8]
$C_{24}H_{36}O_7$ 436.544
Constit. of *Dictyota volubilis.* Oil. $[\alpha]_D^{25}$ -8.5 (c, 0.2 in $CHCl_3$).
Wright, A.D. *et al., Tetrahedron*, 1993, **49**, 571-580 (*isol, pmr, cmr*)

2,10(18),14-Pachydictyatriene-4,6,9,12-tetrol **P-18**
2,10(18),14-Prenylguaiatriene-4,6,9,12-tetrol



$C_{20}H_{32}O_4$ 336.47

(1α,4ξ,5β,6β,9α,11ξ,12ξ)-*form*

12-Ac: [149195-81-3]

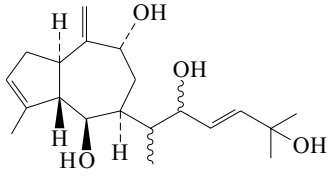
$C_{22}H_{34}O_5$ 378.508

Constit. of *Dictyota volubilis.* Oil. $[\alpha]_D$ -16.6 (c, 0.74 in $CHCl_3$).

König, G.M. *et al., Planta Med.*, 1993, **59**, 174-178 (*isol, pmr, cmr*)

3,10(18),13-Pachydictyatriene-6,9,12,15-tetrol P-19

3,10(18),13-Prenylguaiatriene-6,9,12,15-tetrol



$C_{20}H_{32}O_4$ 336.47

(1α,5β,6β,9α,11ξ,12ξ)-*form*

12-Ac: [149195-80-2]

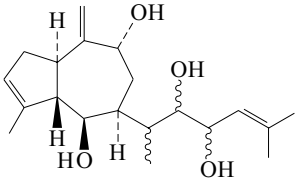
$C_{22}H_{34}O_5$ 378.508

Constit. of *Dictyota volubilis.* Yellow oil. $[\alpha]_D$ +2.1 (c, 0.51 in $CHCl_3$).

König, G.M. *et al., Planta Med.*, 1993, **59**, 174-178 (*isol, pmr, cmr*)

3,10(18),14-Pachydictyatriene-6,9,12,13-tetrol P-20

3,10(18),14-Prenylguaiatriene-6,9,12,13-tetrol



$C_{20}H_{32}O_4$ 336.47

(1α,5β,6β,9α,11ξ,12ξ,13ξ)-*form*

12,13-Di-Ac: [149195-79-9]

$C_{24}H_{36}O_6$ 420.545

Constit. of *Dictyota volubilis.* Yellow oil. $[\alpha]_D$ +4.4 (c, 1.2 in $CHCl_3$).

6,12,13-Tri-Ac: [149195-78-8]

$C_{26}H_{38}O_7$ 462.582

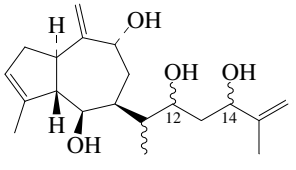
Constit. of *Dictyota volubilis.* Cryst.

Mp 142.4°. $[\alpha]_D$ +21.3 (c, 0.16 in $CHCl_3$).

König, G.M. *et al., Planta Med.*, 1993, **59**, 174-178 (*isol, pmr, cmr*)

3,10(18),15-Pachydictyatriene-6,9,12,14-tetrol P-21

3,10(18),15-Prenylguaiatriene-6,9,12,14-tetrol



$C_{20}H_{32}O_4$ 336.47

(1α,5β,6β,9α,11ξ,12ξ,14ξ)-*form*

12-Ac: [146506-42-5]

$C_{22}H_{34}O_5$ 378.508

Constit. of *Dictyota volubilis.* Oil. $[\alpha]_D^{25}$ +30.5 (c, 0.2 in $CHCl_3$).

14-Epimer, 12-Ac:

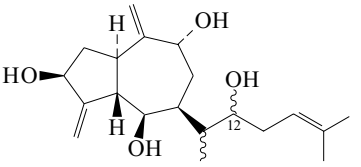
$C_{22}H_{34}O_5$ 378.508

Constit. of *Dictyota volubilis.* Oil. $[\alpha]_D^{25}$ -16.8 (c, 0.22 in $CHCl_3$).

Wright, A.D. *et al., Tetrahedron*, 1993, **49**, 571-580 (*isol, pmr, cmr*)

4(17),10(18),14-Pachydictyatriene-3,6,9,12-tetrol P-22

4(17),10(18),14-Prenylguaiatriene-3,6,9,12-tetrol



$C_{20}H_{32}O_4$ 336.47

(1α,5β,3β,6β,9α,11ξ,12ξ)-*form*

12-Ac: [146506-41-4]

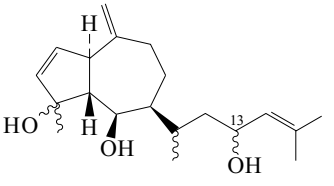
$C_{22}H_{34}O_5$ 378.508

Constit. of *Dictyota volubilis.* Oil. $[\alpha]_D^{25}$ -16.4 (c, 0.25 in $CHCl_3$).

Wright, A.D. *et al., Tetrahedron*, 1993, **49**, 571-580 (*isol, pmr, cmr*)

2,10(18),14-Pachydictyatriene-4,6,13-triol P-23

2,10(18),14-Prenylguaiatriene-4,6,13-triol



$C_{20}H_{32}O_3$ 320.471

(1α,4ξ,5β,6β,11ξ,13ξ)-*form*

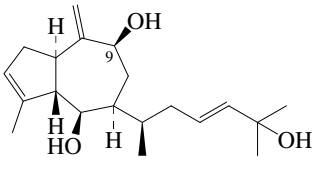
13-Ac: [146506-43-6]

$C_{22}H_{34}O_4$ 362.508

Constit. of *Dictyota volubilis.* Oil. $[\alpha]_D^{25}$ +13 (c, 0.43 in $CHCl_3$).

Wright, A.D. *et al., Tetrahedron*, 1993, **49**, 571-580 (*isol, pmr, cmr*)

3,10(18),13-Pachydictyatriene-6,9,15-triol P-24



$C_{20}H_{32}O_3$ 320.471

(1α,5β,6β,7α*H*,9β,11*R*,13*E*)-*form*

Dictyotriol E

[115890-57-8]

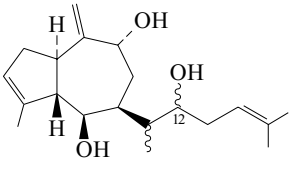
[115890-59-0 (Ac)]

Constit. of *Dictyota* spp.

Oil (as Ac). $[\alpha]_D$ +56.8 (c, 2.29 in $CHCl_3$) (Ac). Revised abs. config. Earlier work by the same authors assigning the opposite abs. config. by CD was unreliable.

Arroyo, P *et al., J.O.C.*, 1991, **56**, 2671-2675 (*abs config*)

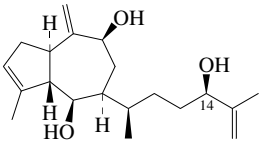
3,10(18),14-Pachydictyatriene-6,9,12-triol P-25



$C_{20}H_{32}O_3$ 320.471

(1α,5β,6β,9α,11ξ,12ξ)-*form*
Dictyotriol A†
[93710-24-8]
Constit. of the brown alga *Glossophora kuntii*.
Amorph. solid. $[\alpha]_D^{25}$ +24.9 (c, 0.47 in $CHCl_3$).
12-Ac: ***Acetyldictyotriol A***
[112523-88-3]
$C_{22}H_{34}O_4$ 362.508
Isol. from *Glossophora kuntii* and *Dictyota volubilis*. Oil. $[\alpha]_D^{25}$ +7.8 (c, 0.017 in $CHCl_3$).
9,12-Di-Ac: ***Diacetyldictyotriol A***
[93710-25-9]
$C_{24}H_{36}O_5$ 404.545
Constit. of *Dictyota binghamiae* and *Glossophora kuntii*. Oil. $[\alpha]_D^{22}$ +12.5 (c, 0.11 in $CHCl_3$).
Pathirana, C. *et al., Can. J. Chem.*, 1984, **62**, 1666-1671 (*9,12-di-Ac*)
Rivera, A.P. *et al., J. Nat. Prod.*, 1987, **50**, 965-967 (*isol*)

3,10(18),15-Pachydictyatriene-6,9,14-triol P-26



(1α,5β,6β,7α*H*,9β,11*R*,14*R*)-*form*

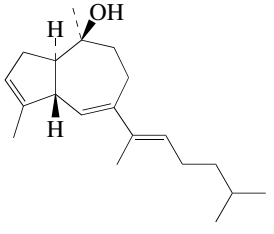
$C_{20}H_{32}O_3$ 320.471
Revised abs. configs. Earlier work by the same authors assigning the opposite abs. configs. by CD was unreliable. Mp 165-167°.

(1α,5β,6β,7α*H*,9β,11*R*,14*R*)-*form*
Dictyotriol C
[115890-56-7]
Constit. of *Dictyota* spp.
Cryst.
Mp 165-167°. $[\alpha]_D$ +77.4 (c, 0.4 in $CHCl_3$).

(1α,5β,6β,7α*H*,11*R*,14*S*)-*form*
Dictyotriol D
[115940-72-2]
Constit. of *Dictyota* spp.
Cryst. ($CHCl_3$/hexane).
Mp 164-166°. $[\alpha]_D$ +72.4 (c, 0.4 in $CHCl_3$).
Vázquez, J.T. *et al., J.O.C.*, 1988, **53**, 4797-4800 (*isol, pmr, cmr*)
Arroyo, P. *et al., J.O.C.*, 1991, **56**, 2671-2675 (*abs config*)

3,6,11-Pachydictyatrien-10-ol P-27

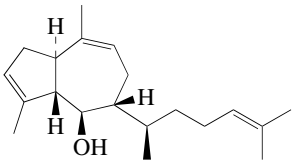
3,6,11-Prenylguaiatrien-10-ol



$C_{20}H_{32}O$ 288.472

(1α,5β,10β,11*E*)-*form*
Nephthol A
[160669-38-5]
Constit. of *Nephthea chabroli*.
Oil. $[\alpha]_D$ +80.7 (c, 0.55 in $CHCl_3$).
10-Hydroperoxide: ***Nephthol B***. *Nephthoxide*
[160669-39-6]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Nephthea chabroli*. Oil. $[\alpha]_D$ +71.5 (c, 0.66 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 32-39 (*isol, pmr, cmr*)

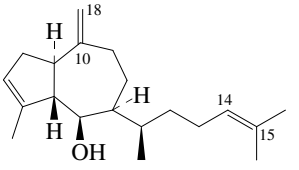
3,9,14-Pachydictyatrien-6-ol P-28



$C_{20}H_{32}O$ 288.472

(1α,5β,6β,7β*H*,12*R*)-*form*
Isopachydictyol A
[61263-84-1]
Constit. of *Dictyota dichotoma*.
Oil. $[\alpha]_D^{25}$ -25.7 (c, 0.28 in $CHCl_3$).
Durán, R. *et al., Tetrahedron*, 1997, **53**, 8675-8688 (*isol, pmr, cmr*)

3,10(18),14-Pachydictyatrien-6-ol P-29

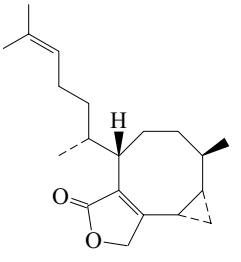


$C_{20}H_{32}O$ 288.472

(1α,5β,6β,11*R*)-*form*
Pachydictyol A
[50299-47-3]
Constit. of *Pachydictyon coriaceum*, *Aplysia depilans*, *Aplysia vaccaria* and a range of *Dictyota* spp. Feeding deterrent, algicide, antimitotic, ichthyotoxic, vasopressin-V1 receptor antagonist, norepinephrine antagonist. Oil. Sol. MeOH, hexane; poorly sol. H_2O. $[\alpha]_D^{20}$ +106 (cyclohexane).
10α,18-Epoxide: ***10,18-Epoxy-3,14-pachydictyadien-6-ol***
[64118-74-7]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Dictyota flabellata*. Vasopressin-V1 receptor antagonist , norepinephrine antagonist. Oil. Poorly sol. hexane. $[\alpha]_D$ +28.6 (c, 3.1 in $CHCl_3$).
*14*R*,15-Epoxide:* ***14,15-Epoxy-3,10(18)-pachydictyadien-6-ol***.
Epoxypachydictyol A
$C_{20}H_{32}O_2$ 304.472
Constit. of *Dictyota dichotoma*.
Hirschfeld, D.R. *et al., J.A.C.S.*, 1973, **95**, 4049-4050 (*Pachydictyol A, isol, cryst struct, abs config*)
Minale, L. *et al., Tet. Lett.*, 1976, **17**, 2711-2714 (*Pachydictyol A*)
Robertson, K.J. *et al., Phytochemistry*, 1977, **16**, 1071-1073 (*10,18-epoxide*)
Greene, A.E. *et al., Tet. Lett.*, 1978, **19**, 851-854 (*Pachydictyol A, synth, abs config*)
De Rosa, S. *et al., Phytochemistry*, 1986, **25**, 2179-2181 (*pmr*)
Banerjee, A.K. *et al., Tetrahedron*, 1993, **49**, 4761-4788 (*synth, rev*)

Pachylactone P-30

1,13-Crenuladien-19,18-olide
[89199-96-2]



$C_{20}H_{30}O_2$ 302.456

Constit. of brown alga *Pachydictyon coriaceum*. Oil. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D^{25}$ -23.3 (c, 0.18 in $CHCl_3$). λ_{max} 209 (ϵ 4310); 231 (ϵ 5790) (MeOH) (Derep). λ_{max} 228 (ϵ 11700) (MeOH) (Berdy).

Ishitsuka, M. *et al., Tet. Lett.*, 1983, **24**, 5117

Pachymatismin P-31

[185702-38-9]

Glycoprotein; MW 46 kDa. Isol. from *Pachymatisma johnstonii*. Shows antitumour activity.

Zidane, M. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1996, **115**, 47-53 (*isol*)

Pachymoside aglycone P-32

N-*(Carboxymethyl)-23-hydroxy*-N-*methyl-14-oxooctacosanamide*
$H_3C(CH_2)_4CH(OH)(CH_2)_8CO(CH_2)_{12}CONMeCH_2COOH$

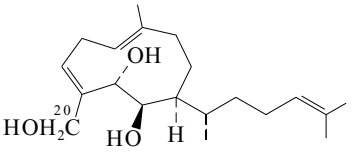
$C_{31}H_{59}NO_5$ 525.811

O-*[6*-O-*Acetyl-β-*D*-glucopyranosyl-(1→4)-β-*D*-glucopyranosyl-(1→4)-[tetra*-O-*acetyl-β-*D*-galactopyranosyl-(1→2)]-6*-O-*acetyl-β-*D*-glucopyranosyl-(1→4)-[tetra*-O-*acetyl-β-*D*-galactopyranosyl-(1→2)]-β-*D*-glucopyranoside]:* ***Pachymoside***
[702700-64-9]
$C_{87}H_{139}NO_{45}$ 1919.035
Isol. from the marine sponge *Pachymatisma johnstonia*.

Warabi, K. *et al., Can. J. Chem.*, 2004, **82**, 102-112 (*isol, pmr, cmr, ms*)

Pachytriol P-33

[110839-03-7]



$C_{20}H_{34}O_3$ 322.487
Constit. of *Dictyota dichotoma*. Oil. $[\alpha]_D$ -46.7 (c, 1.49 in $CHCl_3$).

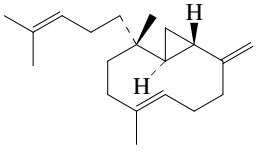
20-Ac: ***Acetoxypachydiol***
$C_{22}H_{36}O_4$ 364.524
Isol. from brown alga *Pachydictyon coriaceum*. Oil. $[\alpha]_D$ -76.4 (c, 0.55 in $CHCl_3$).

[101390-93-6]

Ishitsuka, M. *et al., Tet. Lett.*, 1986, **27**, 2639 (*Acetoxypachydiol*)
González, A.G. *et al., J. Nat. Prod.*, 1987, **50**, 500 (*Pachytriol*)

Pacificin I P-34

[847450-79-7]

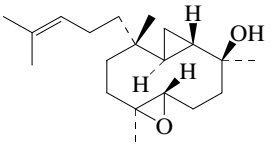


$C_{20}H_{32}$ 272.473
Constit. of *Nephthea pacifica*.
$[\alpha]_D^{25}$ -28 (c, 0.1 in $CHCl_3$).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 74-77 (*isol, pmr, cmr*)

Pacificin A P-35

[847450-71-9]

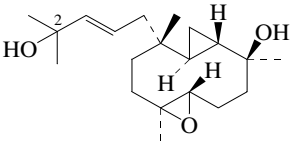


$C_{20}H_{34}O_2$ 306.487
Constit. of *Nephthea pacifica*. Amorph. solid. $[\alpha]_D^{25}$ -62 (c, 0.2 in $CHCl_3$).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 74-77 (*isol, pmr, cmr*)

Pacificin B P-36

[847450-72-0]



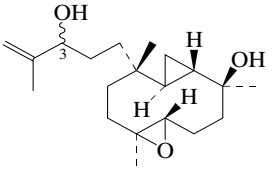
$C_{20}H_{34}O_3$ 322.487
Constit. of *Nephthea pacifica*. Amorph. solid. $[\alpha]_D^{25}$ -53 (c, 0.2 in $CHCl_3$).

2-Hydroperoxide: ***Pacificin C***
[847450-73-1]
$C_{20}H_{34}O_4$ 338.486
Constit. of *Nephthea pacifica*. Amorph. solid. $[\alpha]_D^{25}$ -46 (c, 0.1 in $CHCl_3$).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 74-77 (*isol, pmr, cmr*)

Pacificin D P-37

[847450-74-2]



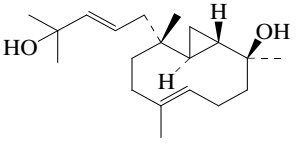
$C_{20}H_{34}O_3$ 322.487
Constit. of *Nephthea pacifica*. Amorph. solid. $[\alpha]_D^{25}$ -43 (c, 0.2 in $CHCl_3$).

3-Hydroperoxide: ***Pacificin E***
[847450-75-3]
$C_{20}H_{34}O_4$ 338.486
Constit. of *Nephthea pacifica*. Amorph. solid. $[\alpha]_D^{25}$ -38 (c, 0.1 in $CHCl_3$).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 74-77 (*isol, pmr, cmr*)

Pacificin F P-38

[847450-76-4]

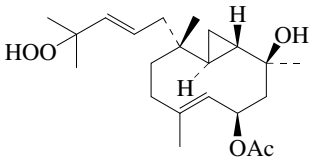


$C_{20}H_{34}O_2$ 306.487
Constit. of *Nephthea pacifica*. Amorph. solid. $[\alpha]_D^{25}$ -51 (c, 0.2 in $CHCl_3$).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 74-77 (*isol, pmr, cmr*)

Pacificin G P-39

[847450-77-5]

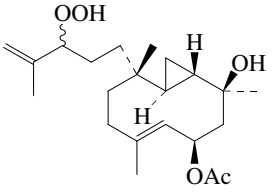


$C_{22}H_{36}O_5$ 380.523
Constit. of *Nephthea pacifica*. Amorph. solid. $[\alpha]_D^{25}$ -26 (c, 0.2 in $CHCl_3$).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 74-77 (*isol, pmr, cmr*)

Pacificin H P-40

[847450-78-6]

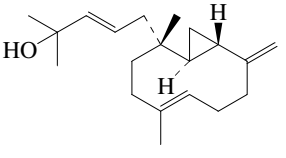


$C_{22}H_{36}O_5$ 380.523
Constit. of *Nephthea pacifica*. Amorph. solid. $[\alpha]_D^{25}$ -18 (c, 0.1 in $CHCl_3$).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 74-77 (*isol, pmr, cmr*)

Pacificin J P-41

[847450-80-0]

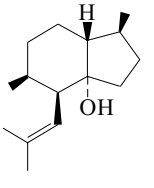


$C_{20}H_{32}O$ 288.472
Constit. of *Nephthea pacifica*.
$[\alpha]_D^{25}$ -22 (c, 0.2 in $CHCl_3$).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2005, **68**, 74-77 (*isol, pmr, cmr*)

Pacifigorgiol P-42

*Octahydro-1,5-dimethyl-4-(2-methyl-1-propenyl)-3*a*H-inden-3*a*-ol, 9CI*



(+)–*form*

$C_{15}H_{26}O$ 222.37

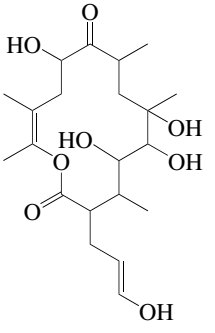
(+)-*form* [84014-68-6]
Constit. of gorgonian coral *Pacifigorgia* cf. *adamsii*. Ichthyotoxin. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ +41 (c, 1.02 in $CHCl_3$).

(-)-*form* [90988-77-5]
Constit. of *Valeriana officinalis* (valerian).
Oil. $[\alpha]_D$ -45.3 (c, 0.724 in $CHCl_3$).

Martin, M. *et al., Pure Appl. Chem.*, 1982, **54**, 1915 (*synth*)
Izac, R.R. *et al., Tet. Lett.*, 1982, **23**, 3743 (*isol, cryst struct*)
Bos, R. *et al., Phytochemistry*, 1986, **25**, 1234 (*isol*)

Paciforgin P-43

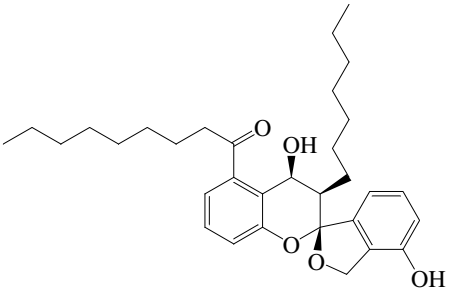
5,6,7,11-Tetrahydroxy-3-(3-hydroxy-2-propenyl)-4,7,9,13,14-pentamethyloxacyclotetradec-13-ene-2,10-dione, 9CI
[136440-72-7]



$C_{21}H_{34}O_8$ 414.495
Macrolide antibiotic. Isol. from the coral *Pacifigorgia* sp. Antifungal agent. Cryst. λ_{max} 227 (MeOH). λ_{max} 229 ($CHCl_3$) (Berdy).

Perez Gutierrez, R.M. *et al., Drugs Exp. Clin. Res.*, 1990, **16**, 505-508 (*isol, struct*)

Paecilospirone† P-44

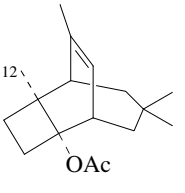


$C_{32}H_{44}O_5$ 508.697
Prod. by a marine-derived fungus, *Paecilomyces* sp.
$[\alpha]_D^{25}$ +202.5 (c, 0.37 in MeOH). λ_{max} 206; 218; 251; 278; 299 (MeOH).

Namikoshi, M. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1452-1457

Paesslerin A P-45

[342373-86-8]



$C_{17}H_{26}O_2$ 262.391
Struct. shown to be incorrect by synth. (2004). Constit. of *Alcyonium paessleri*.

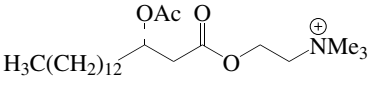
12-Acetoxy: ***Paesslerin B***
[342373-87-9]
$C_{19}H_{28}O_4$ 320.428
Constit. of *Alcyonium paessleri*.
Brasco, M.F.R. *et al., Org. Lett.*, 2001, **3**, 1415-1417 (*isol, pmr, cmr*)
Inanaga, K. *et al., J.A.C.S.*, 2004, **126**, 1352-1353 (*synth*)

PAFYSQRY amide P-46

[638174-64-8]
Pro-Ala-Phe-Tyr-Ser-Gln-Arg-Tyr-NH_2
$C_{49}H_{67}N_{13}O_{12}$ 1030.148
Isol. from the pericardial organs of the crab *Cancer borealis*.
Li, L. *et al., J. Neurochem.*, 2003, **87**, 642-656 (*isol*)

Pahutoxin P-47

*2-[[3-(Acetyloxy)-1-oxohexadecyl]oxy]-*N,N,N*-trimethylethanaminium, 9CI. 3-Acetoxyhexadecanoic acid choline ester*
[122767-82-2]



(*S*)-*form*

$C_{23}H_{46}NO_4^{\oplus}$ 400.621

(S)-form [27742-14-9]
Poison secreted by the blue dogfish (*Ostracion lentiginosus*).
Needles (Me_2CO)(as chloride).
Mp 74-75° (chloride). $[\alpha]_D^{22}$ +3.05 (c, 2.3 in MeOH). CAS no. refers to chloride.
▶ Toxic.

O-*De-Ac,* O-*propanoyl:* ***Homopahutoxin***
[109777-68-6]
$C_{24}H_{48}NO_4^{\oplus}$ 414.648
Isol. from the boxfish *Ostracion immaculatus*. Haemolytic agent.

(ξ)-form [116613-97-9]
Constit. of toxic skin secretions of the trunkfish, *Anoplocapros lenticularis*, *Aracana ornata*, *Lactoria fornasini*, *Ostracion cubicus*, *Rhinesomas reipublicae* and *Strophiurichthys robustus*. CAS no. refers to chloride. Genus name incorr. given as Anoplacapros.

O-*De-Ac:* [116613-93-5]
$C_{21}H_{44}NO_3$ 358.584
Constit. of toxic skin secretions of the trunkfish *Anoplocapros lenticularis*, *Aracana ornata*, *Lactoria fornasini* and *Ostracion cubicus*. CAS no. refers to chloride.

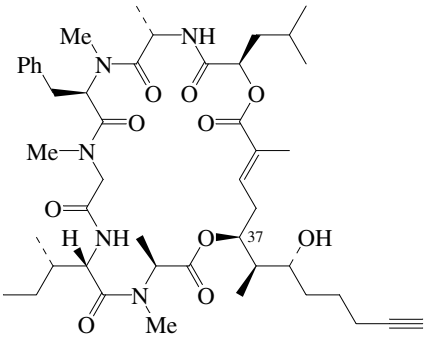
O-*De-Ac,* O-*propanoyl:* [116613-96-8]
$C_{24}H_{48}NO_4$ 414.648
Trace constit. of toxic skin secretions of the trunkfish *Lactoria fornasini* and *Rhinesomas reipublicae*. CAS no. refers to chloride.

O-*De-Ac,* O-*butanoyl:* [116613-95-7]
$C_{25}H_{50}NO_4$ 428.674
Constit. of toxic skin secretions of the trunkfish *Anoplocapros lenticularis* and *Strophiurichthys robustus*. CAS no refers to chloride.

O-*De-Ac,* O-*pentanoyl:* [116613-94-6]
$C_{26}H_{52}NO_4$ 442.701
Constit. of toxic skin secretions of the trunkfish *Anoplocapros lenticularis*, *Rhinesomas reipublicae* and *Strophiurichthys robustus*. CAS no. refers to chloride.

Boylan, D.B. *et al., Science (Washington, D.C.)*, 1967, **155**, 52-56
Fusetani, N. *et al., Toxicon*, 1987, **25**, 459-461 (*Homopahutoxin, isol*)
Goldberg, A.S. *et al., Toxicon*, 1988, **26**, 651-663 (*trunkfish constits*)
Yoshikawa, M. *et al., Agric. Biol. Chem.*, 1989, **53**, 37-40 (*synth, ir, pmr, abs config*)

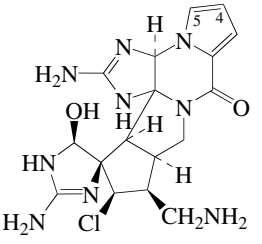
Palauamide P-48



$C_{46}H_{69}N_5O_{10}$ 852.079
Synthesis of the proposed struct. indicates that some stereochemistry needs to be reassigned. Isol. from a Palauan *Lyngbya* sp. Cytotoxic. Oil. $[\alpha]_D^{23}$ -22 (c, 0.4 in MeOH). λ_{max} 202 (log ϵ 4.54); 225 (sh) (MeOH).
Williams, P.G. *et al., J. Nat. Prod.*, 2003, **66**, 1545-1549 (*isol, pmr, cmr*)
Zou, B. *et al., Org. Lett.*, 2005, **7**, 4237-4240 (*synth, stereochem*)

Palauamine P-49

[148717-58-2]



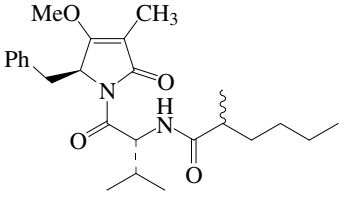
Probable Absolute Configuration

$C_{17}H_{22}ClN_9O_2$ 419.873
Alkaloid from the sponge *Stylotella aurantium* and *Stylotella agminata*. Cytotoxic. Possesses immunosuppressive, antibiotic and antifungal activities. Off-white amorph. powder. $[\alpha]_D^{24}$ -45.2 (c, 3.0 in MeOH). λ_{max} 273 (ϵ 4700) (MeOH) (Derep). λ_{max} 224 (ϵ 7800); 272 (ϵ 7900) (MeOH) (Derep).
▶ LD_{50} (mus, ipr) 13 mg/kg.

4-Bromo: ***4-Bromopalauamine***
$C_{17}H_{21}BrClN_9O_2$ 498.769
Alkaloid from *Stylotella aurantium*. Amorph. tan solid. $[\alpha]_D$ -64.4 (c, 2.6 in MeOH).

4,5-Dibromo: ***4,5-Dibromopalauamine***
$C_{17}H_{20}Br_2ClN_9O_2$ 577.665
Alkaloid from *Stylotella aurantium*. Solid. $[\alpha]_D$ -115.3 (c, 2.7 in MeOH). Dec. on heating.
Kinnel, R.B. *et al., J.O.C.*, 1998, **63**, 3281-3286 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)
Jacquot, D.E.N. *et al., Curr. Org. Chem.*, 2005, **9**, 1551-1566 (*rev, synth*)
Dransfield, P.J. *et al., Tetrahedron*, 2006, **62**, 5223-5247 (*synth*)

Palauimide P-50



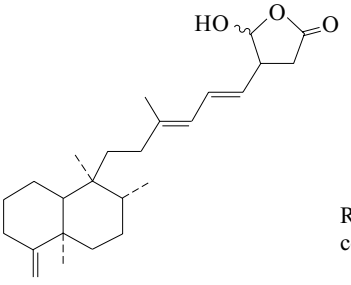
$C_{25}H_{36}N_2O_4$ 428.57

Isol. from a *Lyngbya* sp. Cytotoxic. Amorph. solid. $[\alpha]_D^{25}$ +50 (c, 0.33 in MeOH). CAS no. not found to CA 138. λ_{max} 201 (log ϵ 3.78); 252 (log ϵ 3.44) (MeOH).

Luesch, H. *et al., Tetrahedron*, 2002, **58**, 7959-7966 (*isol, pmr, cmr*)

Palauolide P-51

[82205-22-9]



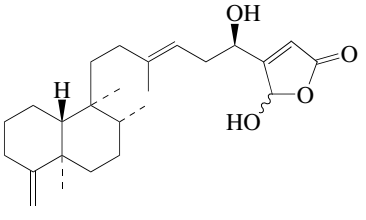
Relative configuration

$C_{25}H_{38}O_3$ 386.573
Constit. of an unidentified Palauan sponge. Antibacterial agent. Yellow oil. Sol. MeOH, EtOAc; poorly sol. hexane, H_2O. $[\alpha]_D$ +1.5 (c, 0.2 in $CHCl_3$). λ_{max} 322 (ϵ 17000) (MeOH) (Derep).

Sullivan, B. *et al., Tet. Lett.*, 1982, **23**, 907 (*isol, struct*)
Piers, E. *et al., Can. J. Chem.*, 1994, **72**, 146 (*synth*)

Palauolol P-52

[178064-14-7]

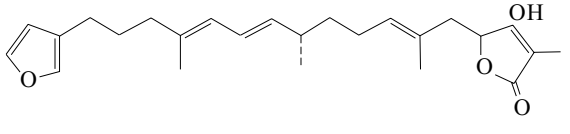


$C_{25}H_{38}O_4$ 402.573
Constit. of a *Fascaplysinopsis* sp. Phospholipase-A2 inhibitor. Antiinflammatory agent. Oil. Sol. MeOH, EtOAc. λ_{max} 206 (ϵ 25000) (MeOH) (Berdy).

Schmidt, E.W. *et al., Tet. Lett.*, 1996, **37**, 3951-3954 (*isol, pmr, cmr*)

Palinurin† P-53

[71947-64-3]



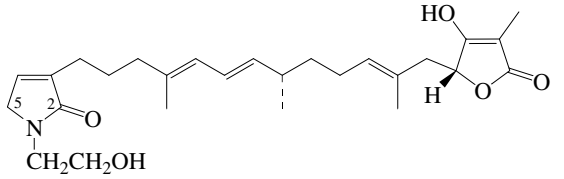
$C_{25}H_{34}O_4$ 398.541
Constit. of *Ircinia echinata* and *Ircinia variabilis*. ACE and Aldose reductase inhibitor. Oil. $[\alpha]_D$ +45.3 ($CHCl_3$). λ_{max} 241 (ϵ 23400) (MeOH) (Derep). λ_{max} 244 (ϵ 46350) (EtOH) (Berdy).

O-*Sulfate:* [192066-73-2]
$C_{25}H_{34}O_7S$ 478.605
Constit. of *Ircinia variabilis*. Amorph. solid. $[\alpha]_D$ +11.3 (c, 2 in $CHCl_3$). λ_{max} 273 (ϵ 17500) (MeOH).

Alfano, G. *et al., Experientia*, 1979, **35**, 1136 (*Palinurin*)
De Rosa, S. *et al., Nat. Prod. Lett.*, 1997, **10**, 7-12 (*sulfate*)

Palinurine A† P-54

[254901-26-3]



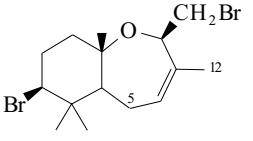
$C_{27}H_{39}NO_5$ 457.609
Microbial metab. of Palinurin, P-53 prod. by *Cunninghamella* sp. NRRL 5695. Yellowish oil. $[\alpha]_D^{25}$ +69.9 (c, 0.25 in $CHCl_3$). λ_{max} 246 (log ϵ 2.87); 268 (log ϵ 2.67) (MeOH).

2-Deoxo, 5-oxo: ***Palinurine B***
[254901-27-4]
$C_{27}H_{39}NO_5$ 457.609
Prod. by *Cunninghamella* sp. NRRL 5695. Yellowish oil. $[\alpha]_D^{25}$ +58.5 (c, 0.38 in $CHCl_3$). λ_{max} 246 (log ϵ 2.87); 268 (log ϵ 2.67) (MeOH).

El Sayed, K.A. *et al., J.O.C.*, 1999, **64**, 9258-9260

Palisadin B P-55

[77249-85-5]



$C_{15}H_{24}Br_2O$ 380.162
Constit. of *Laurencia* cf. *palisada* and *Laurencia karlae*. Cryst. (Me_2CO/petrol).
Mp 94-95°. $[\alpha]_D$ +10 (c, 0.28 in $CHCl_3$). λ_{max} (MeOH) (Berdy).

12-Bromo: ***12-Bromopalisadin B***
$C_{15}H_{23}Br_3O$ 459.058
Constit. of *Laurencia flexilis*. Oil. $[\alpha]_D^{25}$ -16 (c, 0.1 in $CHCl_3$).

12-Hydroxy: ***12-Hydroxypalisadin B***
[77250-03-4]
$C_{15}H_{24}Br_2O_2$ 396.161
Constit. of *Laurencia palisada*. Oil. $[\alpha]_D$ +19.7 (c, 0.4 in $CHCl_3$).

5β-Hydroxy: ***5β-Hydroxypalisadin B***
$C_{15}H_{24}Br_2O_2$ 396.161
Constit. of *Laurencia flexilis*. Oil. $[\alpha]_D^{25}$ -12 (c, 0.1 in $CHCl_3$).

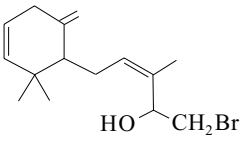
5β-Acetoxy: ***5β-Acetoxypalisadin B***
[77250-04-5]
$C_{17}H_{26}Br_2O_3$ 438.199
Constit. of *Laurencia palisada*. Cryst. (CH_2Cl_2/petrol).
Mp 58-59°. $[\alpha]_D$ -131.7 (c, 0.6 in $CHCl_3$).

$\Delta^{3(12)}$-Isomer, 4α-bromo: ***Palisadin C***
[150998-90-6]
$C_{15}H_{23}Br_3O$ 459.058
Constit. of *Laurencia flexilis*.

Paul, V.J. *et al., Tet. Lett.*, 1980, **21**, 2787-2790 (*isol*)
Tanaka, A. *et al., Agric. Biol. Chem.*, 1986, **50**, 1069 (*synth*)
De Nys, R. *et al., J. Nat. Prod.*, 1993, **56**, 877 (*5β-Hydroxypalisadin B, 12-Bromopalisadin B, Palisadin C*)
Huang, Y. *et al., CA*, 1994, **120**, 270854p (*isol, cryst struct*)
Su, J.-Y. *et al., Phytochemistry*, 1995, **40**, 195 (*isol*)
Couladouros, E.A. *et al., Chem. Eur. J.*, 2004, **10**, 3822-3835 (*synth*)

Palisol P-56

[77249-84-4]



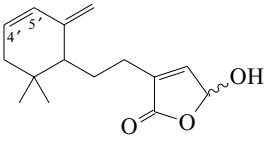
$C_{15}H_{23}BrO$ 299.25
Constit. of *Laurencia palisada*. Oil (as Ac). $[\alpha]_D$ -0.6 (c, 0.51 in $CHCl_3$) (Ac).

E-*Isomer:* ***Isopalisol***
[350483-16-8]
$C_{15}H_{23}BrO$ 299.25
Constit. of *Laurencia luzonensis*. Oil. $[\alpha]_D^{27}$ -31.9 (c, 0.59 in $CHCl_3$).

Paul, V.J. *et al., Tet. Lett.*, 1980, 2787 (*Palisol*)
Kunigoshi, M. *et al., J. Nat. Prod.*, 2001, **64**, 696-700 (*Isopalisol*)

Pallescensin 3 P-57

[56881-46-0]



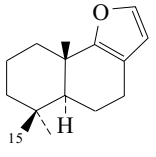
$C_{15}H_{20}O_3$ 248.321
Constit. of *Dysidea pallescens*. Oil. λ_{max} 230 (ϵ 24600) (MeOH) (Derep).

4′,5′-Dihydro: ***3-[2-(2,2-Dimethyl-6-methylenecyclohexyl)ethyl]-5-hydroxy-2(5H)-furanone, 9CI***
[85653-95-8]
$C_{15}H_{22}O_3$ 250.337
Constit. of marine alga *Caulerpa bikinensis*. Viscous oil. $[\alpha]_D$ -5.6 (c, 0.8 in $CHCl_3$). λ_{max} 230 (ϵ 24600) (MeOH) (Derep).

Cimino, G. *et al., Tet. Lett.*, 1975, **16**, 1417-1420
Paul, V.J. *et al., Tet. Lett.*, 1982, **23**, 5017-5020 (*Caulerpa bikinensis constit*)

Pallescensin A P-58

*4,5,5*a*,6,7,8,9,9*a-*Octahydro-6,6,9*a-*trimethylnaphtho[1,2-*b*]furan, 9CI*



(+)–*form*

$C_{15}H_{22}O$ 218.338

(+)-*form* [56881-68-6]
Constit. of *Dysidea pallescens*, *Dysidea amblia* , *Cadlina luteomarginata*, *Hypselodoris californiensis* and *Euryspongia* sp.
Oil. Sol. MeOH, $CHCl_3$; fairly sol. hexane; poorly sol. H_2O.
$[\alpha]_D$ +9.7. λ_{max} 223 (ϵ 9300) (MeOH) (Berdy).

(-)-*form*
ent-*Pallescensin A*
[66101-04-0]
Constit. of *Doriopsilla areolata*.
Oil. $[\alpha]_D^{25}$ -73.8 (c, 0.05 in $CHCl_3$).

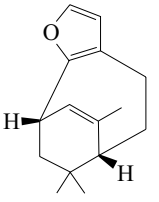
15-Acetoxy: **ent-*15-Acetoxypallescensin A***
[159664-81-0]
$C_{17}H_{24}O_3$ 276.375
Constit. of *Doriopsilla areolata*.
$[\alpha]_D^{25}$ -53.5 (c, 0.74 in $CHCl_3$).

2β,15-Diacetoxy: **ent-*2α,15-Diacetoxypallescensin A***
[159664-82-1]
$C_{19}H_{26}O_5$ 334.411
Constit. of *Doriopsilla areolata*.
$[\alpha]_D^{25}$ -26.8 (c, 0.25 in $CHCl_3$).

Cimino, G. *et al., Tet. Lett.*, 1975, 1425 (*isol, struct*)
Matsumoto, T. *et al., Chem. Lett.*, 1978, 105 (*stereochem, synth*)
Nasipuri, D. *et al., J.C.S. Perkin 1*, 1979, 2776 (*synth*)
Hochlowski, J.E. *et al., J.O.C.*, 1982, **47**, 88
Gariboldi, P. *et al., J.O.C.*, 1982, **47**, 1961 (*synth*)
Smith, A.B. *et al., J.O.C.*, 1984, **49**, 3685 (*synth*)
Shishido, K. *et al., Heterocycles*, 1990, **31**, 597 (*synth*)
Shishido, K. *et al., J. Chem. Res., Synop.*, 1993, 58 (*synth*)
Spinella, A. *et al., Tet. Lett.*, 1994, **35**, 8665-8668 (*ent-Pallescensin A, ent-15-Acetoxypallescensin A, ent-2α,15-Diacetoxypallescensin A*)
Fontana, A. *et al., J.O.C.*, 2003, **68**, 2405-2409 (*biosynth*)
Foot, J.S. *et al., Tet. Lett.*, 2006, **47**, 6817-6820 (*synth*)

Pallescensin B P-59

[56881-69-7]

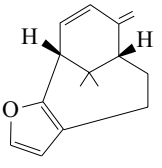


$C_{15}H_{20}O$ 216.322
Constit. of *Dysidea pallescens*. Oil. $[\alpha]_D$ +62.6. Genus name given as Disidea. λ_{max} 230 (ϵ 11800) (MeOH) (Derep).

Cimino, G. *et al., Tet. Lett.*, 1975, 1425
Liu, W.-C. *et al., Chem. Comm.*, 1999, 117-118 (*synth*)

Pallescensin C P-60

[56881-70-0]

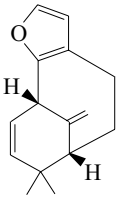


$C_{15}H_{18}O$ 214.307
Constit. of *Dysidea pallescens*. Oil. $[\alpha]_D$ +424. Genus name given as Disidea. λ_{max} 230 (ϵ 11800) (MeOH) (Derep).

Cimino, G. *et al., Tet. Lett.*, 1975, 1425

Pallescensin D P-61

[56881-71-1]



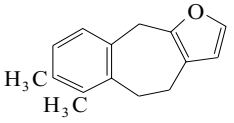
$C_{15}H_{18}O$ 214.307
Constit. of *Dysidea pallescens*. Oil. $[\alpha]_D$ -45.3. Genus name given as Disidea. λ_{max} 230 (ϵ 11800) (MeOH) (Derep).

Cimino, G. *et al., Tet. Lett.*, 1975, 1425

Pallescensin E P-62

*5,10-Dihydro-6,7-dimethyl-4*H*-benzo[5,6]cyclohepta[1,2-*b*]furan, 9CI*

[56881-47-1]



$C_{15}H_{16}O$ 212.291

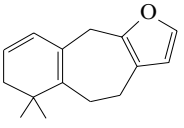
Constit. of *Dysidea pallescens*. Oil. Genus name given as Disidea. λ_{max} 223 (ϵ 9300) (MeOH) (Derep).

Cimino, G. *et al., Tet. Lett.*, 1975, 1421

Baker, R. *et al., J.C.S. Perkin 1*, 1981, 3087 (*struct, synth*)

Pallescensin F P-63

[56881-48-2]



$C_{15}H_{18}O$ 214.307

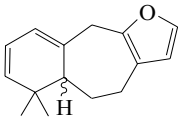
Constit. of *Dysidea pallescens*. Oil. Genus name given as Disidea. λ_{max} 220 (ϵ 10300); 268 (ϵ 7000) (MeOH) (Derep).

Cimino, G. *et al., Tet. Lett.*, 1975, 1421 (*isol*)

Matsumoto, T. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 491 (*synth*)

Pallescensin G P-64

[56881-49-3]



$C_{15}H_{18}O$ 214.307

Constit. of *Dysidea pallescens*. Oil. $[\alpha]_D$ -289. Genus name given as Disidea. λ_{max} 220 (ϵ 10300); 268 (ϵ 7000) (MeOH) (Derep).

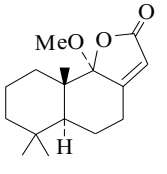
Cimino, G. *et al., Tet. Lett.*, 1975, 1421 (*isol*)

Matsumoto, T. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 491 (*synth*)

Pallescensolide P-65

*5,5*a*,6,7,8,9,9*a*,9*b*-Octahydro-9*b*-methoxy-6,6,9*a*-trimethyl-naphtho[1,2-*b*]furan-2(4*H*)-one, 9CI*

[93474-11-4]



$C_{16}H_{24}O_3$ 264.364

Constit. of *Dysidea amblia*. Ichthyotoxin. Cryst. Sol. $CHCl_3$, hexane; poorly sol. H_2O.

Mp 53-56°. $[\alpha]_D$ -57.4 (c, 0.9 in $CHCl_3$). λ_{max} 205 (ϵ 21800) (pentane) (Berdy).

*3,3*a*-Dihydro: Decahydro-9*b*-methoxy-6,6,9*a*-trimethyl-naphtho[1,2-*b*]furan-2(3*H*)-one, 9CI.* ***Pallescensinolide***

[99132-83-9]

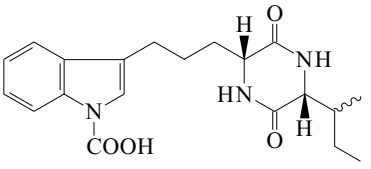
$C_{16}H_{26}O_3$ 266.38

From *Dysidea amblia*.

Walker, R.P. *et al., J.O.C.*, 1984, **49**, 5160-5163 (*isol, uv, pmr, cmr, struct*)

Pallidin† P-66

[174756-39-9]



Relative configuration

$C_{20}H_{25}N_3O_4$ 371.435

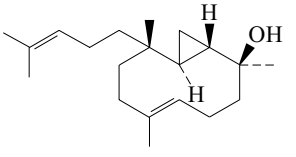
Alkaloid from the marine sponge *Rhaphisia pallida*. Cryst. (MeOH).

Mp 124-125°. $[\alpha]_D^{25}$ -52.4 (c, 0.04 in MeOH).

Su, J. *et al., J. Nat. Prod.*, 1996, **59**, 504 (*isol, uv, ir, pmr, cmr, ms, struct*)

Palmatol P-67

[158846-16-3]



$C_{20}H_{34}O$ 290.488

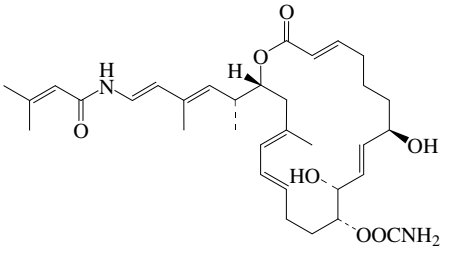
Constit. of *Alcyonium palmatum*. Ichthyotoxic agent. Toxic to brine shrimp. Cryst. (hexane).

Mp 93-94°. $[\alpha]_D^{20}$ -94.7 (c, 2.5 in $CHCl_3$).

Zubía, E. *et al., Tet. Lett.*, 1994, **35**, 7069 (*isol, pmr, cmr*)

Palmerolide A P-68

[863116-48-7]



Absolute Configuration

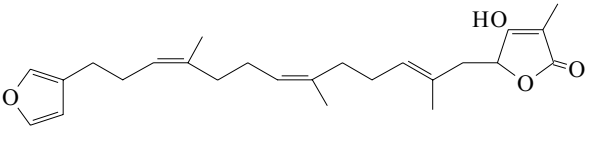
$C_{33}H_{48}N_2O_7$ 584.751

Macrolide antibiotic. Isol. from *Synoicum adareanum*. Cytotoxic. Amorph. solid. $[\alpha]_D^{24}$ -1.6 (c, 0.5 in MeOH). λ_{max} 224 (ϵ 2670); 242 (ϵ 2800); 296 (ϵ 1775) (MeOH).

Diyabalanage, T. *et al., J.A.C.S.*, 2006, **128**, 5630-5631 (*isol, pmr, cmr*)

Palominin P-69

[127486-65-1]



$C_{25}H_{34}O_4$ 398.541

Metab. of sponge *Ircinia* sp. Antioxidant. Unstable oil. λ_{max} 208 (ϵ 21666) (MeOH) (Berdy).

*7*E*-Isomer:*

$C_{25}H_{34}O_4$ 398.541

Constit. of a *Spongia* sp. Pale yellow oil. $[\alpha]_D^{20}$ +17.7 (c, 2.3 in $CHCl_3$).

Garcia, M.O. *et al., Tetrahedron*, 1990, **46**, 1119
Lumsdon, D. *et al., Aust. J. Chem.*, 1992, **45**, 1321 (*isol, pmr, cmr*)

Palystatin P-70

Isol. from *Palythoa liscia*. Cell-growth inhibitors.

Palystatin A [82497-18-5]
Glycopeptide.

Palystatin B [82497-19-6]
Glycopeptide.

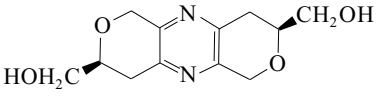
Palystatin C [82497-20-9]
Peptide conjugate.

Palystatin D [82497-21-0]
Peptide conjugate.

Pettit, G.R. *et al., J. Nat. Prod.*, 1982, **45**, 272-276 (*isol*)

Palythazine P-71

*1,3,4,6,8,9-Hexahydrodipyrano[3,4-*b*:3′,4′-*e*]pyrazine-3,8-dimethanol, 9CI*
[72681-96-0]

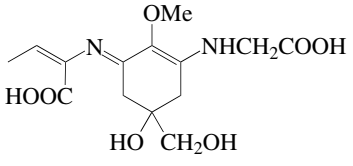


$C_{12}H_{16}N_2O_4$ 252.269
Isol. from the zoanthid *Palythoa tuberculosa*.
Mp 223-225° (169-170°). $[\alpha]_D^{25}$ -199 (MeOH). The abs. config. of (-)-Palythazine is as shown but it is not known whether this is the natural enantiomer.

Uemura, D. *et al., Chem. Lett.*, 1979, 1481 (*isol, uv, cmr, struct, synth*)
Jarglis, P. *et al., Angew. Chem., Int. Ed.*, 1982, **21**, 141 (*struct, synth*)

Palythenic acid P-72

[84621-49-8]
[79876-33-8, 79876-34-9]



(*E*)-*form*

$C_{14}H_{20}N_2O_7$ 328.321

(E)-form [83509-36-8]
[131320-70-2]
Isol. from the ascidian *Halocynthia roretzi* and from *Alexandrium excavatum* and *Noctiluca* sp. Shows radioprotectant props.
Amorph. powder (as Na salt).
Mp 153-156° dec. (Na salt). $[\alpha]_D^{25}$ -50 (c, 0.3 in H_2O).

3′-Hydroxy, 2′,3′-dihydro: 2-[[3-[(Carboxymethyl)amino]-5-hydroxy-5-(hydroxymethyl)-2-methoxy-2-cyclohexen-1-ylidene]amino]-3-hydroxybutanoic acid
$C_{14}H_{22}N_2O_8$ 346.336
Isol. from *Porphyra tenera*.

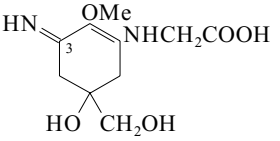
(Z)-form [83456-04-6]
[131320-69-9]
Isol. from *Alexandrium excavatum*, *Halocynthia roretzi* and *Noctiluca* sp.
Amorph. powder (as Na salt). $[\alpha]_D^{25}$ -50 (c, 0.3 in H_2O) (Na salt).
λ_{max} 337 (ε 29200) (H_2O).

[131320-69-9]

Hirata, Y. *et al., Pure Appl. Chem.*, 1979, **51**, 1875 (*isol, uv, cmr, struct, deriv*)
Kobayashi, J. *et al., Tet. Lett.*, 1981, **22**, 3001-3002 (*isol, uv, pmr, cmr*)
Japan. Pat., 1982, 82 62 243; *CA*, **97**, 196864e (*isol*)
Carreto, J.I. *et al., J. Plankton Res.*, 1990, **12**, 909-921 (*isol, uv*)
Bandaranayake, W.M. *et al., Nat. Prod. Rep.*, 1998, **16**, 159-172 (*rev*)

Palythine P-73

N-*[5-Hydroxy-5-(hydroxymethyl)-3-imino-2-methoxy-1-cyclohexen-1-yl]glycine, 9CI. Iminomycosporine-Gly*
[67731-19-5]



$C_{10}H_{16}N_2O_5$ 244.247
Isol. from the red alga *Chondrus yendoi* and the zoanthid *Palythoa tuberculosa*.
Mp 155-156° (142-145°). $[\alpha]_D$ -7.9 (c, 1.5 in H_2O). λ_{max} 320 (MeOH) (Berdy).

Me ester, hydrochloride: Mp 186-189° dec.

3-N-*(2-Hydroxyethyl):* ***Asterina 330***
[84563-31-5]
$C_{12}H_{20}N_2O_6$ 288.3
Constit. of the starfish *Asterina pectinifera*. Syrup. λ_{max} 330 (no solvent reported).

3-N-*(2-Hydroxy-1-methylethyl):* ***Palythinol***
[69281-11-4]
$C_{13}H_{22}N_2O_6$ 302.327
Constit. of *Palythoa tuberculosa*. Yellow cryst.
Mp 154-156° dec. $[\alpha]_D$ -51.9 (c, 1.3 in H_2O). λ_{max} 332 (no solvent reported).

3-N-*(1E-Propenyl):* ***Palythene***
[69281-10-3]
$C_{13}H_{20}N_2O_5$ 284.311
Constit. of *Palythoa tuberculosa*. Yellow cryst. $+1H_2O$.
Mp 145-146°. $[\alpha]_D$ -30.1 (c, 0.8 in H_2O). λ_{max} 359 (no solvent reported).

3-N-*(1Z-Propenyl):* N-*[5-Hydroxy-5-(hydroxymethyl)-2-methoxy-3-(1-propenylimino)-1-cyclohexen-1-yl]glycine, 9CI.* ***Usujirene***
[109361-80-0]
$C_{13}H_{20}N_2O_5$ 284.311
Constit. of *Palmaria palmata*, *Alexandrium excavatum* and a *Dysidea*/*Prochloron* symbiont. Growth factor; uv protectant.
λ_{max} 357 (MeOH) (Berdy).

3-N-*(Carboxymethyl):* ***Mycosporin-2-Gly***
[149092-45-5]
$C_{12}H_{18}N_2O_7$ 302.283
Isol. from *Anthopleura elegantissima*.

3-N-*(1,2-Dicarboxyethyl):* ***Mycosporin-Gly-Asp***
[97148-42-0]
$C_{14}H_{20}N_2O_9$ 360.32
Isol. from a brine shrimp, *Artemia* sp.

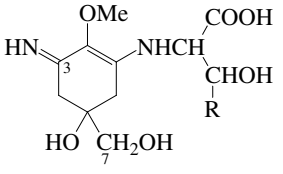
3-N-*(1-Carboxy-2-methylpropyl):* ***Mycosporin-Gly-Val***
[133792-98-0]
$C_{15}H_{24}N_2O_7$ 344.364
Isol. from an Antarctic fish.

Tsujino, I. *et al., Tet. Lett.*, 1978, 1401 (*isol, uv, pmr, cmr, struct*)
Takano, S. *et al., Tet. Lett.*, 1978, 2299; 4909 (*Palythin, Palythinol, isol, uv, ir, pmr, cmr, struct*)
Hirata, Y. *et al., Pure Appl. Chem.*, 1979, **51**, 1875 (*isol*)
Furusaki, A. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 319-323 (*cryst struct*)
Uemura, D. *et al., Chem. Lett.*, 1980, 755 (*Palythene*)
Nakamura, H. *et al., Chem. Lett.*, 1981, 1413-1414 (*Asterina 330*)
Grant, P.T. *et al., Chem. Pharm. Bull.*, 1985, **80**, 755-759 (*Mycosporin-Gly-Asp*)
Chioccara, F. *et al., Gazz. Chim. Ital.*, 1985, **115**, 643 (*isol*)
Sekikawa, I. *et al., Jpn. J. Phycol.*, 1986, **34**, 185 (*Usujirene*)
Dunlap, H. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **93**, 601 (*Asterina 330*)
Carreto, J.I. *et al., J. Plankton Res.*, 1990, **12**, 909 (*Usujirene*)

Karentz, D. *et al., Mar. Biol. (Berlin)*, 1991, **108**, 157-166 (*Mycosporin-Gly-Val*)
Stochaj, W.R. *et al., Mar. Biol. (Berlin)*, 1994, **118**, 149-156 (*Mycosporin-2-Gly*)
Dionisio-See, M.L. *et al., Mar. Biol. (Berlin)*, 1997, **128**, 455-461 (*Usujirin, isol*)
Bandaranayake, W.M. *et al., Nat. Prod. Rep.*, 1998, **16**, 159-172 (*rev*)

Palythine-serine P-74

N-*[5-Hydroxy-5-(hydroxymethyl)-3-imino-2-methoxy-1-cyclohexen-1-yl]serine. Iminomycosporin-Ser*
[195706-18-4]



R = H

$C_{11}H_{18}N_2O_6$ 274.273
Isol. from the coral *Pocillopora eydouxi*. λ_{max} 320 (ϵ 10500) (MeOH).

7-O-*Sulfate: Palythine-serine sulfate*
$C_{11}H_{18}N_2O_9S$ 354.337
Isol. from the coral *Stylophora pistillata*. Sol. H_2O. Not in CA. λ_{max} 320 (MeOH) (Berdy).

3-N-*Me:* **N-*Methylpalythine-serine***. N-*Methyliminomycosporin-Ser*
[195706-20-8]
$C_{12}H_{20}N_2O_6$ 288.3
Isol. from *Pocillopora eydouxi*. λ_{max} 325 (ϵ 16600) (MeOH).
Teai, T.T. *et al., Tet. Lett.*, 1997, **38**, 2525; 5799 (*isol, uv, pmr*)

Palythine-threonine P-75

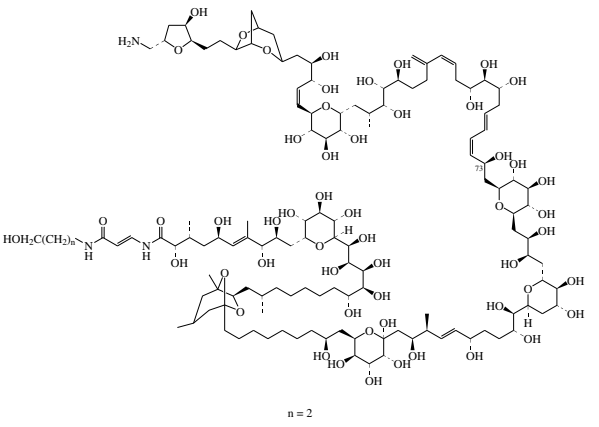
N-*[5-Hydroxy-5-(hydroxymethyl)-3-imino-2-methoxy-1-cyclohexen-1-yl]threonine. Iminomycosporin-Thr*
As Palythine-serine, P-74 with
R = CH_3
$C_{12}H_{20}N_2O_6$ 288.3

7-O-*Sulfate: Palythine-threonine sulfate*
[189812-69-9]
$C_{12}H_{20}N_2O_9S$ 368.364
Isol. from the coral *Stylophora pistillata*. Sol. H_2O. λ_{max} 320 (MeOH) (Berdy).

N^3-*Me:* **N-*Methylpalythine-threonine***. N-*Methyliminomycosporin-Thr. Mycosporin methylamine-Thr*
[166547-39-3]
$C_{13}H_{22}N_2O_6$ 302.327
Isol. from the corals *Pocillopora damicornis*, *Pocillopora eydouxi* and *Stylophora pistillata*. Powder. Delocalised zwitterion.
λ_{max} 313 (ϵ 1900); 320 (ϵ 2800); 330 (ϵ 3300) (MeOH).
Won, J.J.W. *et al., Tet. Lett.*, 1995, **36**, 5255-5256; 1997, **38**, 2525-2526; 5799-5800 (*isol, pmr, cmr*)

Palytoxin P-76

NSC 714361
[77734-91-9]



$C_{129}H_{223}N_3O_{54}$ 2680.168
Prod. by *Palythoa tuberculosa*, *Palythoa toxica* and *Radianthus macrodactylus*; also found in a variety of marine organisms that graze on coral reefs. Toxic. Na/K-ATPase inhibitor, sperm motility inhibitor, cardiotoxic and haemolytic agent, coronary vasoconstrictor. Sol. Py, DMSO, H_2O; fairly sol. MeOH, EtOH; poorly sol. $CHCl_3$, Me_2CO. 2 forms of Palytoxin are known, the one shown and an acetal form, $C_{129}H_{221}N_3O_{53}$. Struct. shown is for Palytoxin from a Tahitian *P.* sp. Palytoxins from *P. toxica* have slightly differing structs. λ_{max} 233; 263 (ϵ 23600) (H_2O) (Berdy).

▶ Highly toxic, LD_{50} 62.5 ng/kg (crab); LD_{50} (mus, ivn) 0.45 mg/kg; LD_{50} (mus, ipr) 0.05 mg/kg.

73-Deoxy: ***Deoxypalytoxin***
[96391-17-2]
$C_{129}H_{223}N_3O_{53}$ 2664.169
Prod. by *Palythoa tuberculosa*. λ_{max} 233; 263 (H_2O).

Homologue (n = 3): ***Homopalytoxin***
[96391-18-3]
$C_{130}H_{225}N_3O_{54}$ 2694.195
Prod. by *Palythoa tuberculosa*. λ_{max} 233; 263 (H_2O).

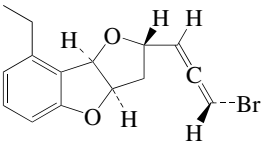
Homologue (n = 4): ***Bishomopalytoxin***
[96411-43-7]
$C_{131}H_{227}N_3O_{54}$ 2708.222
Prod. by *Palythoa tuberculosa*. λ_{max} 233; 263 (H_2O).

[11077-03-5]

Moore, R.E. *et al., J.A.C.S.*, 1981, **103**, 2491-2494; 1982, **104**, 3776-3779 (*struct, abs config*)
Beress, L. *et al., Toxicon*, 1983, **21**, 285 (*isol*)
Uemura, D. *et al., Tetrahedron*, 1985, **41**, 1007-1017 (*isol, struct, rev*)
Armstrong, R.W. *et al., J.A.C.S.*, 1989, **111**, 7525; 7530 (*synth*)
Kishi, Y. *et al., Pure Appl. Chem.*, 1993, **65**, 771-778 (*rev, conformn*)
Gleibs, S. *et al., Toxicon*, 1995, **33**, 1531-1537; 1999, **37**, 1521-1527 (*occur, distribution*)
Nicolaou, K.C. *et al., Classics in Total Synthesis, Targets, Strategies, Methods*, VCH, 1996, 711 (*bibl, synth*)
Food Sci. Technol., *Seafood and Freshwater Toxins*, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*revs*)
Kan, Y. *et al., Tet. Lett.*, 2001, **42**, 3197-3202 (*pmr, cmr*)
Kishi, Y. *et al., Tetrahedron*, 2002, **58**, 6239-6258 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PAF000

Panacene P-77

[66389-39-7]



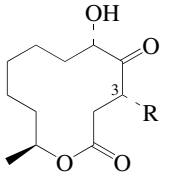
Absolution Configuration

$C_{15}H_{15}BrO_2$ 307.186
Metabolite of the sea hare *Aplysia brasiliana*. Analgesic, tranquilliser. Fish antifeedant. Oil. $[\alpha]_D^{21}$ +382. Log P 3.59 (calc). λ_{max} 224 (ϵ 3470); 279 (ϵ 2510) (EtOH) (Derep).

Kinnel, R.B. *et al., Tet. Lett.*, 1977, 3913-3916 (*isol, struct*)
Feldman, K.S. *et al., J.A.C.S.*, 1982, **104**, 4011 (*synth, config*)
Feldman, K.S. *et al., Tet. Lett.*, 1982, **23**, 3031 (*synth*)
Boukouvalas, J. *et al., Org. Lett.*, 2006, **8**, 3597-3599 (*synth, abs config*)

Pandangolide 1 P-78

4,6-Dihydroxy-12-methyloxacyclododecane-2,5-dione, 9CI



Absolute Configuration

R = OH

$C_{12}H_{20}O_5$ 244.287
Isol. from the fungus *Cladosporium* sp. obt. from a Red Sea sponge. Oil. $[\alpha]_D$ -31 (c, 0.19 in MeOH). λ_{max} 205 (log ϵ 2.9) (MeOH).

3-Benzoyl: ***Sporiolide A***
$C_{19}H_{24}O_6$ 348.395
Isol. from the marine-derived *Cladosporium* sp. Cytotoxic and antifungal agent. Amorph. solid. $[\alpha]_D^{25}$ -14 (c, 0.2 in MeOH). λ_{max} 209 (ϵ 11700); 237 (ϵ 9200) (MeOH).

3-Me ether: ***Sporiolide B***
$C_{13}H_{22}O_5$ 258.314
Isol. from a marine-derived *Cladosporium* sp. Cytotoxic. Amorph. solid. $[\alpha]_D^{25}$ -33 (c, 0.3 in MeOH).

3-Epimer: ***Pandangolide 1a***
$C_{12}H_{20}O_5$ 244.287
Isol. from a marine-derived *Cladosporium* sp. Amorph. solid. $[\alpha]_D^{28}$ -25 (c, 1.6 in MeOH). λ_{max} 205 (log ϵ 2.9) (MeOH).

Smith, C.J. *et al., J. Nat. Prod.*, 2000, **63**, 142-145 (*Pandangolide 1*)
Shigemori, H. *et al., Mar. Drugs*, 2004, **2**, 164-169 (*Sporiolides*)
Gesner, S. *et al., J. Nat. Prod.*, 2005, **68**, 1350-1353 (*Pandangolides, abs config*)
Du, Y. *et al., J.O.C.*, 2006, **71**, 8446-8451 (*Sporiolide A, synth*)

Pandangolide 2 P-79

As Pandangolide 1, P-78 with
R = -SCH_2COOH

$C_{14}H_{22}O_6S$ 318.39
Isol. from a fungus obt. from a marine sponge. Oil. $[\alpha]_D$ -30 (c, 0.07 in MeOH).

Smith, C.J. *et al., J. Nat. Prod.*, 2000, **63**, 142-145

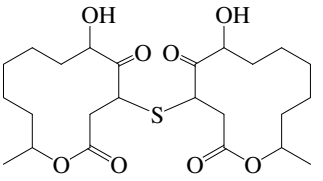
Pandangolide 3 P-80

As Pandangolide 1, P-78 with
R = -$SCH_2CH(OH)COOMe$

$C_{16}H_{26}O_7S$ 362.443
Isol. from a sponge-derived *Cladosporium herbarum*. $[\alpha]_D$ -57.3 (c, 0.72 in MeOH).

Jadulco, R. *et al., J. Nat. Prod.*, 2001, **64**, 527-530

Pandangolide 4 P-81

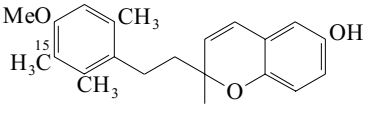


$C_{24}H_{38}O_8S$ 486.625
Isol. from a sponge-derived *Cladosporium herbarum*. $[\alpha]_D$ -55.1 (c, 0.72 in MeOH).

Jadulco, R. *et al., J. Nat. Prod.*, 2001, **64**, 527-530

Panicein A_2 P-82

[157002-42-1]



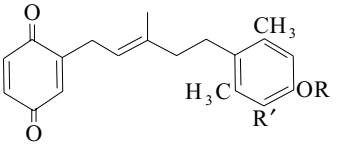
$C_{22}H_{26}O_3$ 338.446
Constit. of *Reniera mucosa*. Oil. λ_{max} 242 (ϵ 5320) ($CHCl_3$) (Berdy).

15-Alcohol: ***Panicein F_2***
[157002-45-4]
$C_{22}H_{26}O_4$ 354.445
Constit. of *Reniera mucosa*. Yellow oil. λ_{max} 243 (ϵ 7990) ($CHCl_3$) (Berdy).

Zubía, E. *et al., Tetrahedron*, 1994, **50**, 8153 (*isol, pmr, cmr*)

Panicein A P-83

2-[5-(4-Methoxy-2,3,6-trimethylphenyl)-3-methyl-2-pentenyl]-2,5-cyclohexadiene-1,4-dione, 9CI
[51847-80-4]



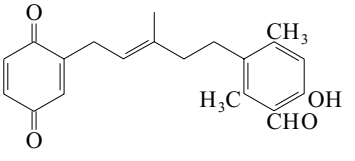
R = R′ = CH_3

$C_{22}H_{26}O_3$ 338.446
Constit. of the marine sponge *Halichondria panicea*.

Cimino, G. *et al., Tetrahedron*, 1973, **29**, 2561 (*isol, spectra, struct*)

Panicein B_1 P-84

3-[5-(3,6-Dioxo-1,4-cyclohexadien-1-yl)-3-methyl-3-pentenyl]-6-hydroxy-2,4-dimethylbenzaldehyde, 9CI
[51918-94-6]

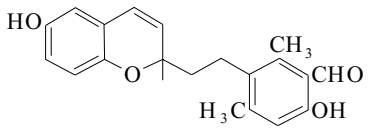


$C_{21}H_{22}O_4$ 338.402
Constit. of the marine sponge *Halichondria panicea*.

Cimino, G. *et al., Tetrahedron*, 1973, **29**, 2561 (*isol, struct*)

Panicein B_2 P-85

6-Hydroxy-3-[2-(6-hydroxy-2-methyl-2H-1-benzopyran-2-yl)ethyl]-2,4-dimethylbenzaldehyde, 9CI
[51847-81-5]

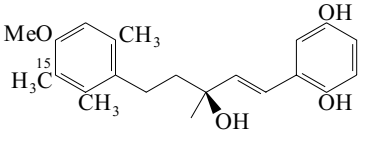


$C_{21}H_{22}O_4$ 338.402
Constit. of the marine sponge *Halichondria panicea*. Sol. MeOH. λ_{max} 273 (ϵ 8100); 340 (ϵ 2800) (MeOH) (Berdy).

Cimino, G. *et al., Tetrahedron*, 1973, **29**, 2565 (*isol, struct*)

Panicein E P-86

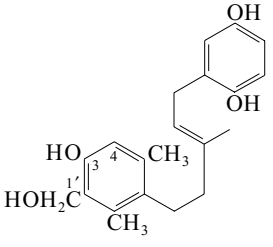
[157002-41-0]



$C_{22}H_{28}O_4$ 356.461
Constit. of *Reniera mucosa*. Yellow oil. $[\alpha]_D$ -8.4 (c, 0.11 in $CHCl_3$). λ_{max} 244 (ϵ 8010) ($CHCl_3$) (Berdy).

15-Oxo, O*-de-Me:* ***Panicein D***
[157002-40-9]
$C_{21}H_{24}O_5$ 356.418
Constit. of *Reniera mucosa*. Orange oil. $[\alpha]_D$ -8 (c, 0.14 in $CHCl_3$). λ_{max} 242 (ϵ 17560); 274 (ϵ 17960) ($CHCl_3$) (Berdy).
Zubía, E. *et al., Tetrahedron*, 1994, **50**, 8153 (*isol, pmr, cmr*)

Panicein G P-87



$C_{21}H_{26}O_4$ 342.434
Constit. of *Reniera mucosa*. Amorph. powder.

3-Me ether: ***Panicein F_1***
$C_{22}H_{28}O_4$ 356.461
Constit. of *Reniera mucosa*. Dihydrofolate reductase inhibitor. Orange oil. λ_{max} 242 (ϵ 7070); 288 (ϵ 7250) ($CHCl_3$) (Berdy).

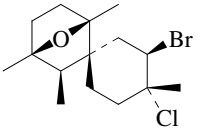
1′-Aldehyde: ***Panicein B_3****. 3-[5-(2,5-Dihydroxyphenyl)-3-methyl-3-pentenyl]-6-hydroxy-2,4-dimethylbenzaldehyde, 9CI*
[51847-82-6]
$C_{21}H_{24}O_4$ 340.418
Constit. of the marine sponge *Halichondria panicea*. λ_{max} 276 (ϵ 12600); 294 (ϵ 5100); 346 (ϵ 3400) (MeOH) (Berdy).

1′-Aldehyde, 4-hydroxy: ***Panicein C***
[51847-83-7]
$C_{21}H_{24}O_5$ 356.418
Constit. of *Halichondria panicea*. λ_{max} 291 (ϵ 15300); 380 (ϵ 2100) (MeOH) (Berdy).

Cimino, G. *et al., Tetrahedron*, 1973, **29**, 2565 (*isol, struct, derivs*)
Zubia, E. *et al., Tetrahedron*, 1994, **50**, 8153 (*Panicein G*)

Pannosane P-88

[348111-21-7]

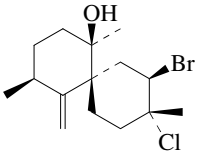


$C_{15}H_{24}BrClO$ 335.711
Constit. of *Laurencia pannosa*. Oil. $[\alpha]_D^{23}$ -6.41 (c, 0.53 in $CHCl_3$).

Suzuki, M. *et al., J. Nat. Prod.*, 2001, **64**, 597-602 (*isol, pmr, cmr*)

Pannosanol P-89

[348111-20-6]

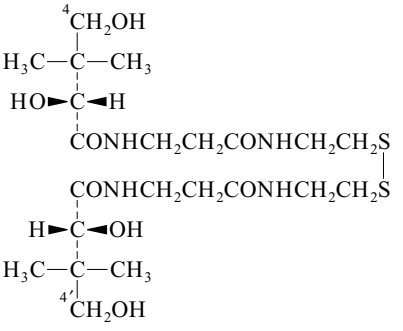


$C_{15}H_{24}BrClO$ 335.711
Constit. of *Laurencia pannosa*. Oil. $[\alpha]_D^{24}$ +4.97 (c, 0.52 in $CHCl_3$).

Suzuki, M. *et al., J. Nat. Prod.*, 2001, **64**, 597-602 (*isol, pmr, cmr*)

Pantethine, JAN P-90

N,N′*-[Dithiobis[2,1-ethanediylimino(3-oxo-3,1-propanediyl)]]-bis[2,4-dihydroxy-3,3-dimethylbutanamide], 9CI.* N,N′*-[Dithiobis(ethyleneiminocarbonylethylene)]bis[2,4-dihydroxy-3,3-dimethylbutyramide], 8CI. Bis(pantothenyl-2-aminoethyl)disulfide*
[303-05-9]



$C_{22}H_{42}N_4O_8S_2$ 554.728

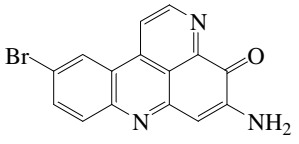
(R,R)-form
D-form. Lipodel. Pantetina. Panthecin. Pantomin. Pantosin
[16816-67-4]
Growth factor for *Lactobacillus bulgaricus* and component of coenzyme A. Occurs in sweet potato, pulses, fermented soybeans (natto), sardines, mackerel, pike, oyster, ear-shell, stone leek, garlic leek and cauliflower. Synth. intermed. for Coenzyme A. Bacterial growth factor. Antihyperlipidaemic agent. Cryst. ($MeOH/Me_2CO$), glass (H_2O). $[\alpha]_D^{22}$ +17.9 (c, 3.2 in H_2O). Hydrol. by acids.
► LD_{50} (mus, ipr) 4800 mg/kg. Exp. reprod. and teratogenic effects. ES4392700

4,4′-Diphosphate: [17451-69-3]
$C_{22}H_{44}N_4O_{14}P_2S_2$ 714.687
Intermed. for synth. of Coenzyme A. Powder (MeOH) (as Ba salt). $[\alpha]_D^{20}$ +12.2 (c, 1 in H_2O).
Brown, G.M. *et al., J.A.C.S.*, 1953, **75**, 1691-1693 (*occur, purifn*)
Viscontini, M. *et al., Helv. Chim. Acta*, 1954, **37**, 375-377 (*synth, tlc, diphosphate*)
Bowman, R.E. *et al., J.C.S.*, 1954, 1171-1176 (*synth, anal, rev, bibl*)

Moffatt, J.G. *et al., J.A.C.S.*, 1961, **83**, 663-675 (*chromatog*)
Ishiguro, K. *et al., J. Exp. Med.*, 1963, **78**, 375-380; *CA*, **59**, 2095h (*occur*)
Shimizu, M. *et al., Chem. Pharm. Bull.*, 1965, **13**, 180-188 (*synth, chromatog, ir, uv*)
Nagase, O. *et al., Chem. Pharm. Bull.*, 1967, **15**, 648-654 (*phosphate, synth*)
Zhdanovich, E.S. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1967, **37**, 337-338 (*synth, ir*)
Hashimoto, M. *et al., Chem. Lett.*, 1972, 595-598 (*synth*)
Wittwer, C.T. *et al., Methods of Enzymzatic Analysis*, 3rd edn., (ed. Bergmeyer, H.U.), Verlag Chemie, 1985, **7**, 244-250 (*anal*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, PAG150

Pantherinine P-91

[152606-66-1]



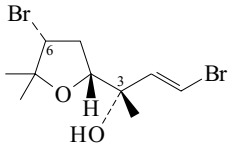
$C_{15}H_8BrN_3O$ 326.152
Alkaloid from the ascidian *Aplidium pantherinum*. Exhibits mild cytotoxicity against P388 murine leukemia cells. Purple powder. λ_{max} 254 (ϵ 16110); 316 (ϵ 3950) (MeOH) (Berdy).

Ac:
Red glass.

Kim, J. *et al., J. Nat. Prod.*, 1993, **56**, 1813-1816 (*isol, uv, ir, pmr, cmr, ms, struct*)
Nakahara, S. *et al., Tet. Lett.*, 1998, **39**, 5531-5522 (*synth*)

Pantofuranoid A P-92

[175889-43-7]



$C_{10}H_{16}Br_2O_2$ 328.043
Constit. of *Pantoneura plocamioides*. Oil. $[\alpha]_D^{25}$ -63 (c, 0.22 in $CHCl_3$).

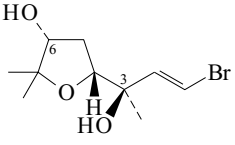
3-Epimer: ***Pantofuranoid B***
[176021-38-8]
$C_{10}H_{16}Br_2O_2$ 328.043
Constit. of *Pantoneura plocamioides*. Oil. $[\alpha]_D^{25}$ -63 (c, 0.22 in $CHCl_3$).

3,6-Diepimer: ***Pantofuranoid C***
[176021-39-9]
$C_{10}H_{16}Br_2O_2$ 328.043
Constit. of *Pantoneura plocamioides*. Oil. $[\alpha]_D^{25}$ -100 (c, 0.2 in $CHCl_3$).

Cueto, M. *et al., Tetrahedron*, 1996, **52**, 5899 (*isol, pmr, cmr*)

Pantofuranoid D P-93

[176021-40-2]



$C_{10}H_{17}BrO_3$ 265.146
Constit. of *Pantoneura plocamioides*. Oil. $[\alpha]_D^{25}$ -29 (c, 0.77 in $CHCl_3$).

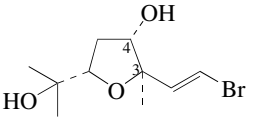
3-Epimer: ***Pantofuranoid E***
[176590-79-7]
$C_{10}H_{17}BrO_3$ 265.146
Constit. of *Pantoneura plocamioides*. Oil. $[\alpha]_D^{25}$ -27 (c, 1 in $CHCl_3$).

3,6-Diepimer: ***Pantofuranoid F***
[176021-41-3]
$C_{10}H_{17}BrO_3$ 265.146
Constit. of *Pantoneura plocamioides*. Oil. $[\alpha]_D^{25}$ -48 (c, 0.33 in $CHCl_3$).

Cueto, M. *et al., Tetrahedron*, 1996, **52**, 5899 (*isol, pmr, cmr*)

Pantoisofuranoid A P-94

[199603-74-2]



$C_{10}H_{17}BrO_3$ 265.147
Constit. of *Pantoneura plocamioides*. Oil. $[\alpha]_D^{25}$ -72 (c, 0.4 in $CHCl_3$).

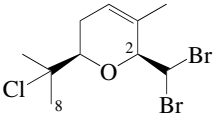
4-Epimer: ***Pantoisofuranoid B***
[199603-75-3]
$C_{10}H_{17}BrO_3$ 265.147
Constit. of *Pantoneura plocamioides*. Oil. $[\alpha]_D^{25}$ -147 (c, 0.2 in $CHCl_3$).

3,4-Diepimer: ***Pantoisofuranoid C***
[199603-76-4]
$C_{10}H_{17}BrO_3$ 265.147
Constit. of *Pantoneura plocamioides*. Oil. $[\alpha]_D^{25}$ -45 (c, 0.6 in $CHCl_3$).

Cueto, M. *et al., J. Nat. Prod.*, 1998, **61**, 17-21 (*isol, pmr, cmr*)

Pantoneurine A P-95

[218603-43-1]



$C_{10}H_{15}Br_2ClO$ 346.489
Constit. of *Pantoneura plocamioides*. Oil.

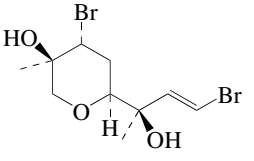
2-Epimer: ***Pantoneurine B***
[218603-49-7]
$C_{10}H_{15}Br_2ClO$ 346.489
Constit. of *Pantoneura plocamioides*. Oil.

2-Epimer, 8-chloro: [218603-39-5]
$C_{10}H_{14}Br_2Cl_2O$ 380.933
Constit. of *Plocamium cartilagineum*. Oil. $[\alpha]_D^{25}$ +14 (c, 0.01 in $CHCl_3$).

Cuerto, M. *et al., J. Nat. Prod.*, 1998, **61**, 1466-1468 (*isol, pmr, cmr*)

Pantopyranoid A P-96

[199603-71-9]

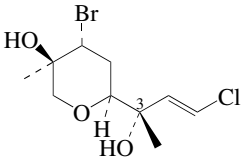


$C_{10}H_{16}Br_2O_3$ 344.043
Constit. of *Pantoneura plocamioides*. Oil. $[\alpha]_D^{25}$ -93 (c, 0.45 in $CHCl_3$).

Cueto, M. *et al., J. Nat. Prod.*, 1998, **61**, 17-21 (*isol, pmr, cmr*)

Pantopyranoid B P-97

[199603-72-0]



$C_{10}H_{16}BrClO_3$ 299.591
Constit. of *Pantoneura plocamioides*. Oil. $[\alpha]_D$ -83 (c, 5 in $CHCl_3$).

3-Epimer: ***Pantopyranoid C***
[199603-73-1]
$C_{10}H_{16}BrClO_3$ 299.591
Constit. of *Pantoneura plocamioides*. Oil. $[\alpha]_D$ -205 (c, 0.2 in $CHCl_3$).

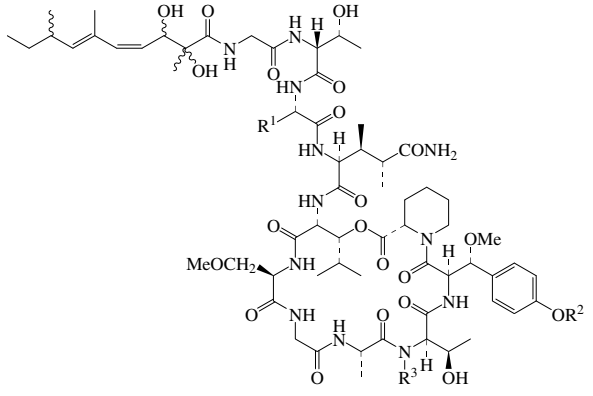
Cueto, M. *et al., J. Nat. Prod.*, 1998, **61**, 17-21 (*isol, pmr, cmr*)

Paolins P-98

Three fractions isol. with MWs 9000-10000, 1400-1700, and 700. Structs. unknown. Isol. from the common clam *Mercenaria mercenaria*. Shows antiviral activity. Sol. H_2O.

Li, C.P. *et al., Ann. N.Y. Acad. Sci.*, 1965, **130**, 374-382 (*isol*)

Papuamides P-99



Papuamide A R^1 = -$CH(CH_3)NH_2$(*S*-), R^2 = H, R^3 = CH_3
Papuamide B R^1 = -$CH(CH_3)NH_2$(*S*-), R^2 = R^3 = H
Papuamide C R^1 = =$CHCH_3$ R^2 = H, R^3 = CH_3
Papuamide D R^1 = =$CHCH_3$ R^2 = R^3 = H

Depsipeptide antibiotics. Cytotoxic agents.

Papuamide A [240427-03-6]
$C_{66}H_{105}N_{13}O_{21}$ 1416.63
Isol. from the sponges *Theonella mirabilis* and *Theonella swinhoei*. Amorph. glass. $[\alpha]_D^{25}$ +12 (c, 3.5 in MeOH). λ_{max} 227 (ϵ 22800); 274 (ϵ 1400) (MeOH).

Papuamide B [240427-04-7]
$C_{65}H_{103}N_{13}O_{21}$ 1402.603
Isol. from *Theonella mirabilis* and *Theonella swinhoei*. Amorph. glass. $[\alpha]_D^{25}$ +12.9 (c, 0.13 in MeOH). λ_{max} 225 (ϵ 24000); 274 (ϵ 1900) (MeOH).

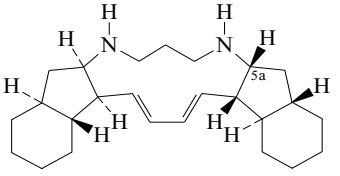
Papuamide C [240427-05-8]
$C_{66}H_{102}N_{12}O_{21}$ 1399.6
Isol. from *Theonella swinhoei*. Glass. $[\alpha]_D^{25}$ +4.4 (c, 1.14 in MeOH). λ_{max} 229 (ϵ 18470); 276 (ϵ 2720) (MeCN aq.).

Papuamide D [240427-06-9]
$C_{65}H_{100}N_{12}O_{21}$ 1385.573
Isol. from *Theonella swinhoei*. Glass. $[\alpha]_D^{25}$ +16.1 (c, 0.68 in MeOH). λ_{max} 226 (ϵ 18490); 274 (ϵ 2270) (MeCN aq.).

Ford, P.W. *et al., J.A.C.S.*, 1999, **121**, 5899-5909 (*isol*)
Makino, K. *et al., Tet. Lett.*, 2005, **46**, 6827-6830 (*config*)

Papuamine P-100

[112455-84-2]



$C_{25}H_{40}N_2$ 368.604
Alkaloid from a marine sponge *Haliclona* sp. Antifungal. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 167.5-169°. $[\alpha]_D$ -150 (c, 1.5 in MeOH). λ_{max} 241 (ϵ 3000) (MeOH) (Derep). λ_{max} 236; 240 (ϵ 3000) (MeOH) (Berdy). λ_{max} 240 (MeOH/HCl) (Berdy).

Hydrochloride (1:2): Mp 230° dec. $[\alpha]_D$ -140 (c, 1.3 in MeOH).

*5*a-*Epimer:* ***Haliclonadiamine***
[117065-24-4]
$C_{25}H_{40}N_2$ 368.604
Alkaloid from a marine sponge *Haliclona* sp. Shows antimicrobial activity. Oil. Sol. MeOH. $[\alpha]_D$ -18.2. λ_{max} 241 (ϵ 3000) (MeOH) (Derep). λ_{max} 241 (ϵ 10700) (MeOH) (Berdy).

*5*a-*Epimer, di-Ac:* Mp 96-98°.

Baker, B.J. *et al., J.A.C.S.*, 1988, **110**, 965 (*isol, uv, ir, pmr, cmr, ms, struct*)
Fahy, E. *et al., Tet. Lett.*, 1988, **29**, 3427 (*Haliclonadiamine*)
Borzilleri, R.M. *et al., J.A.C.S.*, 1995, **117**, 10905 (*synth, abs config*)
Barrett, A.G.M. *et al., J.O.C.*, 1996, **61**, 685 (*synth, enantiomer*)
McDermott, T.S. *et al., J.O.C.*, 1996, **61**, 700 (*synth*)
Taber, D.F. *et al., J.A.C.S.*, 1997, **119**, 22 (*synth, Haliclonadiamine*)
Matzanke, N. *et al., Org. Prep. Proced. Int.*, 1998, **30**, 3-51 (*rev, synth*)
Adlington, R.M. *et al., Tetrahedron*, 2000, **56**, 623-628 (*synth*)

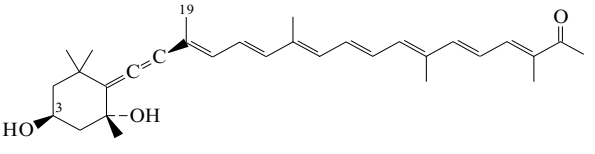
Papyraceabromine A P-101

$C_{22}H_{17}Br_4N_3O_5$ 723.009
Struct. unknown. Metab. from the marine bryozoan *Flustra papyracea (Chartella papyracea)*. Wide-spectrum *in vitro* antibacterial alkaloid. Unstable. Minor alkaloids of structurally different type, Papyraceabromine B (with 5 bromine atoms) and Papyraceabromine C, were also isol.

Pietra, F. *et al., Gazz. Chim. Ital.*, 1985, **115**, 443

Paracentrone P-102

6,7-Didehydro-5,6-dihydro-3,5-dihydroxy-7′-apo-β-caroten-8′-one
[31190-20-2]



$C_{31}H_{42}O_3$ 462.671
Pigment from *Paracentrotus lividus*. Cryst. (EtOAc/MeOH). Mp 147-149°.

19-Hexanoyloxy, 3-Ac: ***19-Hexanoyloxyparacentrone***
[60147-89-9]
$C_{39}H_{54}O_6$ 618.852
Isol. from *Coccolithus huxleyi*. λ_{max} 423; 450 (Me_2CO).

Galasko, G. *et al., J.C.S.(C)*, 1969, 1264 (*isol, struct*)
Hora, J. *et al., J.C.S.(C)*, 1970, 241 (*synth*)
Arpin, N. *et al., Phytochemistry*, 1976, **15**, 529 (*deriv*)
Matsuno, T. *et al., J. Nat. Prod.*, 1985, **48**, 606
Haugan, J.A. *et al., J.C.S. Perkin 1*, 1997, 2731-2737 (*synth*)
Murakami, Y. *et al., Org. Biomol. Chem.*, 2005, **3**, 1372-1374 (*synth*)

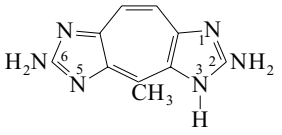
Parasitoxin P-103

Polypeptide, MW 17000-19000 Da, containing no half-cystine. Isol. from the sea anemone *Parasicyonis actinostoloides*. Shows haemolytic activity.

Shiomi, K. *et al., Toxicon*, 1985, **23**, 865-874 (*isol*)

Parazoanthoxanthin A P-103a

*4-Methyl-1*H-*cyclohepta[1,2*-d:*4,5*-d′*]diimidazole-2,6-diamine, 9CI. 2,6-Diamino-4-methyl-1*H-*cyclohepta[1,2*-d:*4,5*-d′*]diimidazole*
[53823-11-3]



$C_{10}H_{10}N_6$ 214.229

Complex tautomerism possible with 1*H* and 3*H* tautomers. The parent compd. is symmetrical by tautomerism between the two imidazole rings but substitution can destroy this symmetry. Fluorescent pigment from *Parazoanthus axinellae adriaticus, Zoanthus sociatus* and *Zoanthus* cfr. *pacificus*. Yellow cryst. (EtOH). Mp 310°.

3-Me: ***Parazoanthoxanthin B***
[53571-91-8]
$C_{11}H_{12}N_6$ 228.256
Isol. from *Parazoanthus axinellae adriaticus* and *Zoanthus* cfr. *pacificus*.

3,N^6*-Di-Me:* ***Parazoanthoxanthin G***
[71827-19-5]
$C_{12}H_{14}N_6$ 242.283
Isol. from *Parazoanthus axinellae adriaticus* and *Zoanthus sociatus*.

N^6,N^6*-Di-Me:* ***Parazoanthoxanthin D***
[53941-25-6]
$C_{12}H_{14}N_6$ 242.283
Constit. of *Parazoanthus axinellae adriaticus, Zoanthus sociatus, Zoanthus* cfr. *pacificus, Palythoa mammilosa* and *Palythoa tuberculosa*. Yellow needles (H_2O). Mp 303-304° dec. λ_{max} 255 (ϵ 13200); 300 (ϵ 39800); 394 (ϵ 15100) (MeOH/HCl) (Derep). λ_{max} 296 (sh) (ϵ 28800); 306 (ϵ 36300); 415 (ϵ 17800) (MeOH) (Derep).

N,N′*-Di-Me:* ***Parazoanthoxanthin C***
$C_{12}H_{14}N_6$ 242.283
Isol. from *Parazoanthus axinellae*. Exact struct. not determined. λ_{max} 302; 412 (MeOH). λ_{max} 297; 392 (MeOH/acid).

1,N^6,N^6*-Tri-Me:* ***Palyzoanthoxanthin A***
[55084-57-6]
$C_{13}H_{16}N_6$ 256.31
Pigment from *Palythoa mammilosa*, *Palythoa tuberculosa* and *Zoanthus pacificus*. Cryst. (MeOH). Mp 310°.

3,N^6,N^6*-Tri-Me:* ***Zoanthoxanthin***. *Parazoanthoxanthin E*
[40451-47-6]
$C_{13}H_{16}N_6$ 256.31
Isol. from *Parazoanthus axinellae*. Yellow needles (MeOH). Mp 275-276°. Highly fluorescent. λ_{max} 259 (ϵ 7410); 293 (ϵ 17800); 392 (ϵ 8710) (1*M* HCl) (Derep). λ_{max} 293 (ϵ 33100); 427 (ϵ 22400) (MeOH) (Derep).

▶ GU3100500

N^2,N^2,N^6*-Tri-Me:* ***Epizoanthoxanthin A***
[55084-60-1]
$C_{13}H_{16}N_6$ 256.31
Pigment from *Parazoanthus axinellae* and *Zoanthus pacificus*. Orange-yellow needles (H_2O). Mp 191-192°.

1,3,N^6,N^6*-Tetra-Me:* ***Parazoanthoxanthin F***
[55084-58-7]
$C_{14}H_{18}N_6$ 270.336
Isol. from *Parazoanthus axinellae adriaticus* and *Palythoa mammilosa*. Cryst. (EtOH). Mp 310° (darkens above 220°). Conts. =NH at C(2).

1,N^2,N^2,N^6*-Tetra-Me:* ***Epizoanthoxanthin B***
[55827-10-6]
$C_{14}H_{18}N_6$ 270.336
Pigment from *Parazoanthus axinellae* and *Palythoa mammilosa*. Amorph. yellow powder.

3,N^2,N^6,N^6*-Tetra-Me:* ***Parazoanthoxanthin E***
[55084-59-8]
$C_{14}H_{18}N_6$ 270.336
Isol. from *Parazoanthus axinellae*. Yellow cryst. (EtOH). Mp >310° (darkens >220°). CAS gives incorrect struct.

N^2,N^2,N^6,N^6*-Tetra-Me:* ***Palyzoanthoxanthin B***
[55084-61-2]
$C_{14}H_{18}N_6$ 270.336
Pigment from *Palythoa tuberculosa*. Cryst. (EtOH). Mp 310° (darkens >220°).

3,N^2,N^2,N^6,N^6*-Penta-Me:* ***Palyzoanthoxanthin C***
[71827-20-8]
$C_{15}H_{20}N_6$ 284.363
Pigment from *Palythoa mammilosa*. Cryst. (EtOH). Mp 180-181°.

Cariello, L. *et al., Experientia*, 1974, **30**, 849 (*Zoanthoxanthin, cryst struct, Parazoanthoxanthins A-D*)
Cariello, L. *et al., Tetrahedron*, 1974, **30**, 3281-3287; 3611-3614; 4191-4196 (*Parazoanthoxanthins E-F, Palyzoanthoxanthins, Epizoanthoxanthins*)
Braun, M. *et al., J.A.C.S.*, 1976, **98**, 3049 (*Parazoanthoxanthin A*)
Cariello, L. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1979, **63**, 77 (*occur*)
Jiménez, C. *et al., J. Nat. Prod.*, 1993, **56**, 9-14 (*Zoanthoxanthin, cmr*)

Parbolysin P-104

Basic protein consisting of a few very similar isotoxins. Isol. from mucus of the Antarctic heteronemertine *Parborlasia corrugatus*. Cytolytic.

Berne, S. *et al., Toxicon*, 2003, **41**, 483-491 (*isol*)

Pardaxin P-105

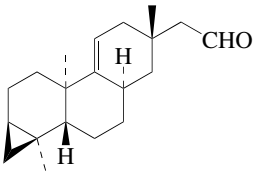
H-Gly-Phe-Phe-Ala-Leu-Ile-Pro-Lys-Ile-Ile-Ser-Ser-Pro-Leu-Phe-Lys-Thr-Leu-Leu-Ser-Ala-Val-Gly-Ser-Ala-Leu-Ser-Ser-Ser-Gly-Glu-Gln-Glu-OH

A group of surfactant polypeptides containing 33 amino acid residues. Struct. of Pardaxin P1 shown. Isol. from the toxic secretion of the Red Sea Moses sole *Pardachirus marmoratus* and the western Pacific Peacock sole *Pardachirus pavoninus*. Shark-repellant. Icthyotoxic agent.

[67995-63-5, 104833-59-2, 104916-49-6, 105184-54-1, 105269-81-6, 105269-82-7, 115537-80-9]

Lazarovici, P. *et al., J. Biol. Chem.*, 1986, **261**, 16704-16713 (*isol*)
Thompson, S.A. *et al., Science (Washington, D.C.)*, 1986, **233**, 341-343 (*isol*)
Thompson, S.A. *et al., Pept. Chem.*, 1987, 127 (*Pardaxin M1*)
Shei, Y. *et al., FEBS Lett.*, 1988, **242**, 161-166 (*synth*)
Adermann, K. *et al., FEBS Lett.*, 1998, **435**, 173-177 (*isol*)
Lazarovici, P. *et al., J. Toxicol., Toxin Rev.*, 2002, **21**, 391-421 (*rev*)

9(11)-Pargueren-16-al P-106

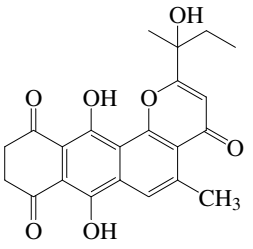


$C_{20}H_{30}O$ 286.456

ent-form [202870-61-9]
Constit. of *Laurencia saitoi*. Oil. $[\alpha]_D^{26}$ -13 (c, 1.54 in $CHCl_3$).
Kurata, K. *et al., Phytochemistry*, 1998, **47**, 363-369 (*isol, pmr, cmr*)

Parimycin P-107

*9,10-Dihydro-7,12-dihydroxy-2-(1-hydroxy-1-methylpropyl)-5-methyl-4*H*-anthra[1,2-*b*]pyran-4,8,11-trione*



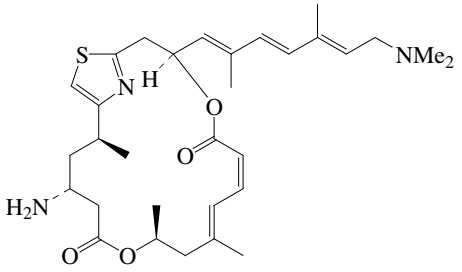
$C_{22}H_{20}O_7$ 396.396

Related to Antibiotic SS 43405E, A-558. Prod. by the marine *Streptomyces* sp. B8652. Cytotoxic and antibacterial agent. Pale orange solid. $[\alpha]_D^{20}$ +60 (c, 0.03 in MeOH). λ_{max} 260 (log ϵ 4.28); 423 (log ϵ 3.88); 447 (log ϵ 3.9) (MeOH).

Maskey, R.P. *et al., J. Antibiot.*, 2002, **55**, 1031-1035 (*isol, uv, pmr, cmr*)

Pateamine A P-108

[139220-18-1]



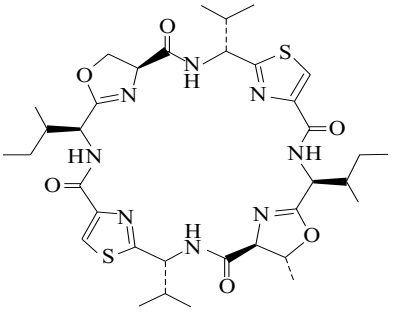
$C_{31}H_{45}N_3O_4S$ 555.78

Rare dilactone functionality. Isol. from the New Zealand marine sponge *Mycale* sp. Potent cytotoxin and immunosuppressant. $[\alpha]_D$ -253 (MeOH). λ_{max} 274 (ϵ 47000); 285 (ϵ 42000) (MeOH) (Berdy).

Northcote, P.T. *et al., Tet. Lett.*, 1991, **32**, 6411-6414 (*isol, uv, cd, ir, pmr, cmr, ms, struct*)
Stirling, D.J. *et al., Ph.D. Thesis*, 1996, (*activity*)
Remuiñán, M.J. *et al., Tet. Lett.*, 2000, **41**, 7367-7371 (*synth*)
Pattenden, G. *et al., Can. J. Chem.*, 2004, **82**, 353-365 (*synth*)
Romo, D. *et al., J.A.C.S.*, 2004, **126**, 10582-10588 (*synth*)

Patellamide A P-109

[81120-73-2]



$C_{35}H_{50}N_8O_6S_2$ 742.962

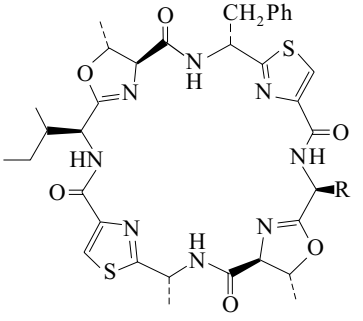
Struct. revised in 1985. Cyclopeptide from the marine tunicate *Lissoclinum patella*. Shows selective metal binding props. Cytotoxic, shows antineoplastic props. MDR inhibitor. Cryst. (C_6H_6). Sol. MeOH, EtOAc; poorly sol. hexane, H_2O.

Mp 228-229°. $[\alpha]_D^{24}$ +140.7 (c, 0.27 in $CHCl_3$) (+113.9). λ_{max} 232 (ϵ 21000) (MeOH) (Derep).

Ireland, C.M. *et al., J.O.C.*, 1982, **47**, 1807-1811 (*isol, ir, pmr, cmr*)
Biskupiak, J.E. *et al., J.O.C.*, 1983, **48**, 2302-2304 (*abs config*)
Hamada, Y. *et al., Tet. Lett.*, 1985, **26**, 6501-6504 (*synth*)
In, Y. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1686-1690 (*conformn, cryst struct*)
In, Y. *et al., Acta Cryst. C*, 1994, **50**, 432-434 (*cryst struct*)
Morris, L.A. *et al., Tetrahedron*, 2001, **57**, 3185-3197 (*activity*)
Salomon, C.E. *et al., J. Nat. Prod.*, 2002, **65**, 689-692 (*isol*)
Schmidt, E.W. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2005, **102**, 7315-7320 (*biosynth*)

Patellamide B P-110

[81098-23-9]



R = $CH_2CH(CH_3)_2$

$C_{38}H_{48}N_8O_6S_2$ 776.979

Cyclopeptide from the marine tunicate *Lissoclinum patella*. Cytotoxic, shows antineoplastic props. MDR inhibitor. Sol. MeOH, $CHCl_3$; poorly sol. hexane, H_2O. $[\alpha]_D$ +29.4 (c, 0.34 in CH_2Cl_2). λ_{max} 248 (ϵ 8000) (MeOH) (Derep).

Ireland, C.M. *et al., J.O.C.*, 1982, **47**, 1807-1811 (*isol, ir, pmr, cmr*)
Biskupiak, J.E. *et al., J.O.C.*, 1983, **48**, 2302-2304 (*abs config*)
Hamada, Y. *et al., Tet. Lett.*, 1985, **26**, 5155-5158; 5159-5162 (*synth, struct*)
Schmidt, U. *et al., Tet. Lett.*, 1986, **27**, 163-166; 179 (*synth, struct*)
Salomon, C.E. *et al., J. Nat. Prod.*, 2002, **65**, 689-692 (*isol*)

Patellamide C P-111

[81120-74-3]

As Patellamide B, P-110 with

R = –$CH(CH_3)_2$

$C_{37}H_{46}N_8O_6S_2$ 762.952

Cyclopeptide from the marine tunicate *Lissoclinum patella*. Shows selective metal binding props. Antineoplastic agent. MDR inhibitor. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D$ +19 (c, 0.21 in CH_2Cl_2). λ_{max} 248 (ϵ 8000) (MeOH) (Derep).

Ireland, C.M. *et al., J.O.C.*, 1982, **47**, 1807-1811; 1983, **48**, 2302-2304 (*isol, ir, pmr, cmr, abs config*)
Hamada, Y. *et al., Tet. Lett.*, 1985, **26**, 5155-5158; 5159-5162 (*synth, struct*)
Morris, L.A. *et al., Tetrahedron*, 2001, **57**, 3185-3197 (*activity*)
Salomon, C.E. *et al., J. Nat. Prod.*, 2002, **65**, 689-692 (*isol*)
Schmidt, E.W. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2005, **102**, 7315-7320 (*biosynth*)

Patellamide D P-112

[120853-15-8]

As Patellamide B, P-110 with

R = –$CH(CH_3)CH_2CH_3$

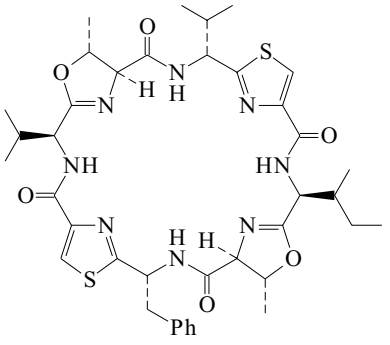
$C_{38}H_{48}N_8O_6S_2$ 776.979

Cyclopeptide from the ascidian *Lissoclinum patella*. Cytotoxic. Mp 144-145°. $[\alpha]_D$ +32 (c, 0.37 in $CHCl_3$).

Degnan, B.M. *et al., J. Med. Chem.*, 1989, **32**, 1349-1354 (*isol, pmr, cmr, struct*)
Schmitz, F.J. *et al., J.O.C.*, 1989, **54**, 3463-3472 (*isol, ir, pmr, cmr, cryst struct*)

Patellamide E P-113

[140430-46-2]



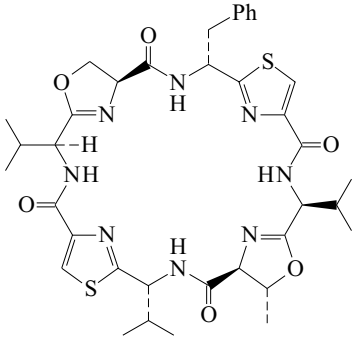
$C_{39}H_{50}N_8O_6S_2$ 791.006

Cyclic peptide antibiotic. Isol. from the ascidian *Lissoclinum patella*. Weakly cytotoxic. Amorph. $[\alpha]_D^{25}$ +48.6 (c, 0.58 in $CHCl_3$). λ_{max} 235 (ϵ 12300) (MeOH) (Berdy).

McDonald, L.A. *et al., J. Nat. Prod.*, 1992, **55**, 376-379 (*isol, cmr, struct*)

Patellamide F P-114

[164803-18-3]



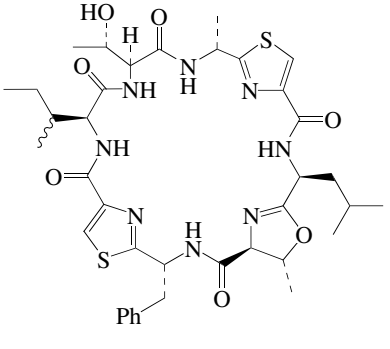
$C_{37}H_{46}N_8O_6S_2$ 762.952

Cyclopeptide from the marine tunicate *Lissoclinum patella*. Cytotoxic. Amorph. solid. Sol. MeOH. $[\alpha]_D$ +40 (c, 0.1 in MeOH). λ_{max} 235 (ϵ 13700) (MeOH) (Berdy).

Rashid, M.A. *et al., J. Nat. Prod.*, 1995, **58**, 594-597 (*isol, ir, pmr, cmr, struct*)

Patellamide G P-115

[218916-91-7]



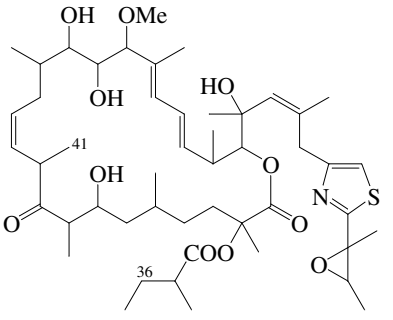
$C_{38}H_{50}N_8O_7S_2$ 794.994

Cyclic peptide. Isol. from the ascidian *Lissoclinum patella*. Amorph. solid. $[\alpha]_D$ +40.6 (c, 0.35 in MeOH).

Fu, X. *et al., J. Nat. Prod.*, 1998, **61**, 1547-1551 (*isol, ir, pmr, cmr, ms*)

Patellazole A P-116

[117527-05-6]



$C_{49}H_{77}NO_{11}S$ 888.213

Macrolide antibiotic. Isol. from the didemnid tunicate *Lissoclinum patella*. Cytotoxic. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 241 (ϵ 26000) (MeOH) (Derep).

36-Hydroxy: ***Patellazole B****. Patellide*

[117527-06-7]

$C_{49}H_{77}NO_{12}S$ 904.213

Isol. from *Lissoclinum patella*. Cytotoxic. λ_{max} 241 (ϵ 26000) (MeOH).

36,41-Dihydroxy: ***Patellazole C***

[117527-07-8]

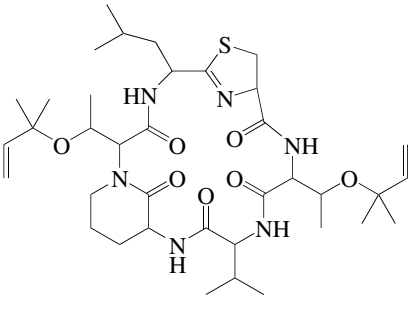
$C_{49}H_{77}NO_{13}S$ 920.212

Isol. from *Lissoclinum patella*. Cytotoxic. $[\alpha]_D$ -100 (c, 1.06 in CH_2Cl_2). λ_{max} 241 (ϵ 26000) (MeOH).

Zabriskie, T.M. *et al., J.A.C.S.*, 1988, **110**, 7919-7920; 7920-7922 (*isol*)

Patellin 1 P-117

[181758-78-1]



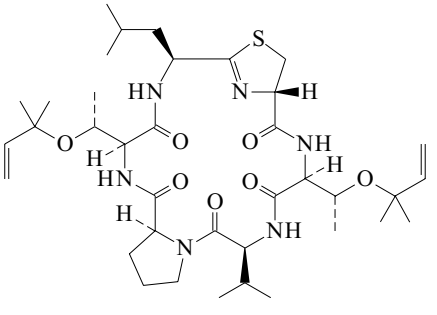
$C_{37}H_{60}N_6O_7S$ 732.983

Cyclic hexapeptide. Isol. from the ascidian *Lissoclinum patella*. Glass. λ_{max} 220 (ϵ 3800) (MeOH).

Carroll, A.R. *et al., Aust. J. Chem.*, 1996, **49**, 659-667 (*isol, uv, ir, pmr, cmr, ms*)

Patellin 2 P-118

[129216-76-8]



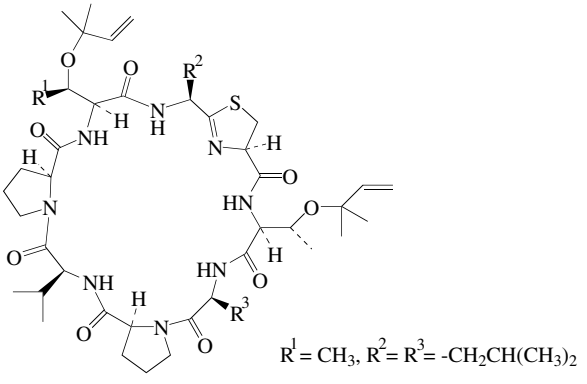
$C_{37}H_{60}N_6O_7S$ 732.983

Modified cyclic peptide. Constit. of *Lissoclinum patella*. Cryst. Mp 128-130°. $[\alpha]_D^{25}$ -110 (c, 1.48 in MeOH). λ_{max} 210 (ϵ 3400); 248 (MeOH) (Berdy).

Zabriskie, T.M. *et al., J.A.C.S.*, 1990, **112**, 8080-8084 (*isol*)

Patellin 3 P-119

[181758-79-2]



$C_{48}H_{78}N_8O_9S$ 943.258

Cyclic octapeptide. Isol. from the ascidian *Lissoclinum patella*. Oil. $[\alpha]_D$ -63 (c, 0.09 in $CHCl_3$). λ_{max} 242 (ϵ 10100) (EtOH).

Carroll, A.R. *et al., Aust. J. Chem.*, 1996, **49**, 659-667 (*isol, uv, ir, ms, struct*)

Patellin 4 P-120

[181758-80-5]

As Patellin 3, P-119 with

R^1=CH_3, R^2=-$CH(CH_3)_2$, R^3=-$CH_2CH(CH_3)_2$

$C_{47}H_{76}N_8O_9S$ 929.232

Cyclic octapeptide, stereochem. not assigned. Isol. from the ascidian *Lissoclinum patella*.

Carroll, A.R. *et al., Aust. J. Chem.*, 1996, **49**, 659-667 (*isol*)

Patellin 5 P-121

[181758-81-6]

As Patellin 3, P-119 with

R^1=H, R^2=-CH_2Ph, R^3=-$CH(CH_3)_2$

$C_{49}H_{72}N_8O_9S$ 949.222

Cyclic octapeptide. Isol. from the ascidian *Lissoclinum patella*. Oil. $[\alpha]_D$ -36 (c, 0.05 in $CHCl_3$). λ_{max} 245 (ϵ 12500) (EtOH).

Carroll, A.R. *et al., Aust. J. Chem.*, 1996, **49**, 659-667 (*isol, ur, ir, pmr, cmr, ms*)

Patellin 6 P-122

[181758-82-7]

As Patellin 3, P-119 with

R^1=CH_3, R^2=-$CH(CH_3)_2$, R^3=-CH_2Ph

$C_{50}H_{74}N_8O_9S$ 963.249

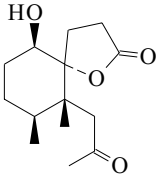
Cyclic octapeptide. Isol. from the ascidian *Lissoclinum patella*. Oil. $[\alpha]_D$ -50 (c, 0.04 in $CHCl_3$). λ_{max} 248 (ϵ 12400) (EtOH).

Carroll, A.R. *et al., Aust. J. Chem.*, 1996, **49**, 659-667 (*isol, uv, ir, pmr, cmr, ms*)

Pathylactone A P-123

1-Hydroxy-13-nor-11-oxo-6,7-seco-7,10-nardosinanolide

[140165-43-1]



$C_{14}H_{22}O_4$ 254.325

A seconardosinane terpenoid. Constit. of *Paralemnalia thyrsoides*. Needles.

Mp 44.5-47°. $[\alpha]_D$ -7.8 (c, 0.041 in MeOH).

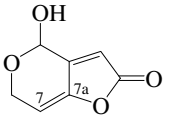
Su, J.-Y. *et al., J. Nat. Prod.*, 1993, **56**, 288 (*isol, pmr, cmr*)

Coelho, F. *et al., Tetrahedron*, 2002, **58**, 1647-1656 (*synth*)

Patulin P-124

*4-Hydroxy-4*H*-furo[3,2-c]pyran-2(6*H*)-one, 9CI, 8CI. Clavacin. Clavatin. Claviformin. Expansin. Flavicin. Gigantic acid†. Mycoin C_3. Penicidin. Terinin. YS 1649. Antibiotic YS 1649. Sch 351633. Antibiotic Sch 351633*

[149-29-1]



$C_7H_6O_4$ 154.122

Antibiotic produced by several fungi, e.g. *Aspergillus clavatus*, *Aspergillus terreus*, a marine *Aspergillus varians*, *Penicillium patulum*, *Penicillium griseofulvum* and *Byssochlamys nivea*. Seed germination inhibitor. Shows antibacterial props. Inhibitor of hepatitis C virus protease. Mycotoxin, found as a contaminant of foods. Prisms or plates (Et_2O or $CHCl_3$).

Mp 111°. $[\alpha]_D^{21}$ -6.2 ($CHCl_3$). Log P -2.4 (uncertain value) (calc). Occurs as a racemate or partial racemate. λ_{max} 292 (ϵ 13400) (0.1*M* NaOH) (Derep). λ_{max} 276 (ϵ 14800) (H_2O or MeOH) (Derep).

▶ Exp. neoplastic agent and teratogen. LD_{50} (rat, orl) 27.8 mg/kg. Exp. kidney and gastrointestinal effects. LV2625000

Phenylhydrazone: Mp 149-150°.

Ac: [6192-26-3]

Prisms (EtOH aq.). Mp 118-120°.

*7,7*a-*Epoxide:* ***3,4-Epoxypatulin***

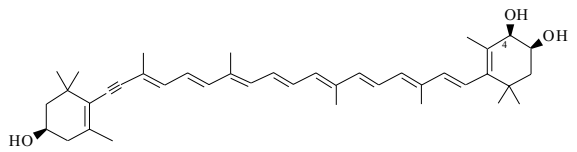
$C_7H_6O_5$ 170.121

Isol. from samples of Patulin as minor contaminant. Tentative struct.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1151C (*nmr*)
Birkinshaw, J.H. *et al., Lancet*, 1943, **245**, 625 (*isol, struct*)
Bergel, F. *et al., J.C.S.*, 1944, 415-421 (*isol, struct*)
Woodward, R.B. *et al., J.A.C.S.*, 1950, **72**, 1428 (*synth*)
Lalau-Kéraly, F. *et al., C. R. Hebd. Seances Acad. Sci.*, 1965, **261**, 4028-4030 (*ir*)
Ciegler, A. *et al., Microb. Toxins*, (eds. Ciegler, A. *et al*), Academic Press, 1971, **V1**, 409 (*rev*)
Scott, P.M. *et al., Mycotoxins*, (ed. Purchase, I.F.H.), Elsevier, 1974, 383 (*rev*)
Wilson, D.M. *et al., Adv. Chem. Ser.*, 1976, **149**, 90-109 (*rev*)
Hubbard, C.R. *et al., Acta Cryst. B*, 1977, **33**, 928-931 (*cryst struct*)
Sekiguchi, J. *et al., Tet. Lett.*, 1979, 41-42 (*biosynth*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2219-2284 (*uv, ir, pmr, ms*)
Iijima, H. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3534-3537 (*biosynth*)
IARC Monog., 1986, **40**, 83-98; *Suppl.* 7, 69 (*rev, tox*)
Gill, G.B. *et al., Tet. Lett.*, 1988, **29**, 2875-2878 (*synth*)
Sejas, J.A. *et al., Heterocycles*, 1989, **29**, 181-184 (*synth*)
Tarter, E.J. *et al., J. Chromatogr.*, 1991, **538**, 441-446 (*glc*)
Bennett, M. *et al., J.C.S. Perkin 1*, 1991, 929-937 (*synth*)
Tada, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 2167-2169 (*synth*)
Yoo, S.-J. *et al., J. Microb. Biotechnol.*, 1995, **5**, 31-35 (*YS 1649*)
Boukouvalas, J. *et al., Tet. Lett.*, 1995, **36**, 7175-7176 (*synth, bibl*)
Chu, M. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 1949-1952 (*Sch 351633, activity, isol*)
Ghisalberti, E.L. *et al., Aust. J. Chem.*, 2000, **53**, 995-997 (*3,4-Epoxypatulin*)
Dai, J.R. *et al., J. Nat. Prod.*, 2001, **64**, 125-126 (*activity*)
Smetanina, O.F. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 243-244 (*marine isol*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 511
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials 10th edn., J. Wiley*, 2000, CMV000

Pectenol A P-125

7′,8′-Didehydro-β,β-carotene-3,3′,4-triol
[81704-35-0]



$C_{40}H_{54}O_3$ 582.865
Isol. from bivalve molluscs.

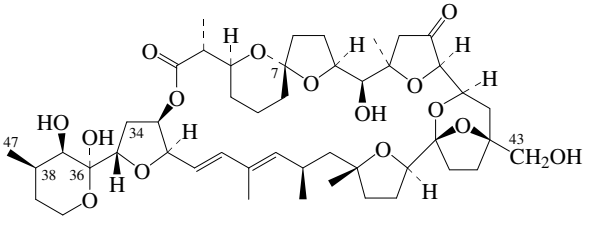
4-Epimer: ***Pectenol B***
[93920-58-2]
Constit. of *Mytilus coruscus*.

4-Ketone: 7′,8′-Didehydro-3,3′-dihydroxy-β,β-caroten-4-one. ***Pectenolone***
[16913-24-9]
$C_{40}H_{52}O_3$ 580.849
Constit. of the giant scallop (*Pecten maximus*) and the tunicates *Halocynthia papillosa* and *Halocynthia roretzi*. Reddish needles (petrol).
Mp 162-163°.

Campbell, S.A. *et al., Chem. Comm.*, 1967, 941 (*Pectenolone*)
Matsuno, T. *et al., Nippon Suisan Gakkaishi*, 1981, **47**, 143; 501; 1984, **50**, 1251 (*Pectenol*)
Hiraoka, K. *et al., Nippon Suisan Gakkaishi*, 1982, **48**, 215; *CA*, **97**, 56060g (*abs config, Pectenolone*)
Matsuno, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 4315 (*isol*)
Davies, A.J. *et al., J.C.S. Perkin 1*, 1984, 2147 (*isol, pmr*)
Maoka, T. *et al., CA*, 1988, **109**, 226980a (*Pectenol B*)

Pectenotoxin 1 P-126

PTX1
[97564-90-4]



Absolute configuration

$C_{47}H_{70}O_{15}$ 875.061
Polyether antibiotic. Found in scallops. Metab. of *Dinophysis acuminata*. Ichthyotoxin. Component toxin of shellfish poisoning. Cytotoxic agent. Cryst. (MeCN aq.). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 208-209°. $[\alpha]_D^{20}$ +17.1 (c, 0.41 in MeOH). Pectenotoxin 8 and Pectenotoxin 9 have been isol. and identified as artifacts. λ_{max} 235 (ϵ 12400) (MeOH) (Berdy).

43-Aldehyde: ***Pectenotoxin 3***. *PTX3*
[97560-25-3]
$C_{47}H_{68}O_{15}$ 873.045
Metab. of *Dinophysis acuminata* and *Dinophysis fortii*. Shellfish toxin. Ichthyotoxin. Amorph. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 159-160°. $[\alpha]_D^{20}$ +2.22 (c, 0.135 in MeOH). λ_{max} 235 (ϵ 11000) (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 0.35 mg/kg.

43-Carboxylic acid: ***Pectenotoxin 6***. *PTX6*
[124843-18-1]
$C_{47}H_{68}O_{16}$ 889.045
Constit. of *Dinophysis* sp. Shellfish toxin. Phycotoxin. $[\alpha]_D^{20}$ +8.8 (c, 0.11 in MeOH). $[\alpha]_D^{20}$ +37.1 (c, 1.5 in $CHCl_3$). λ_{max} 237 (ϵ 37000) (MeOH) (Berdy).

Dihydro (?): ***Pectenotoxin 5***. *PTX5*
[97560-27-5]
$C_{47}H_{72}O_{15}$ 877.077
Metab. of *Dinophysis acuminata* and *Dinophysis fortii*. Shellfish toxin. Ichthyotoxin. Amorph. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 235 (MeOH) (Berdy).

43-Deoxy: ***Pectenotoxin 2***. *PTX2*
[97564-91-5]
$C_{47}H_{70}O_{14}$ 859.062
From *Dinophysis acuminata* and *Dinophysis fortii*. Shellfish toxin. Ichthyotoxin, hepatotoxin and nephrotoxin. Shows cytotoxic activity against KB cells. Amorph. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ +16.2 (c, 0.105 in MeOH). λ_{max} 235 (ϵ 16000) (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 0.2 mg/kg.

43-Deoxy, parent hydroxyacid: ***Pectenotoxin 2 secoacid***. *PTX2-SA*
[212502-87-9]
$C_{47}H_{72}O_{15}$ 877.077
From *Dinophysis acuta* and *Perna canaliculus* (New Zealand green mussel). Ring-opened parent hydroxyacid of the lactone.

*43-Deoxy, 34*S*-hydroxy:* ***Pectenotoxin 11***. *PTX11*
[635678-86-3]
$C_{47}H_{70}O_{15}$ 875.061
Isol. from *Dinophysis acuta*. Shellfish toxin.

*43-Deoxy, 34*S*-hydroxy, parent hydroxyacid:* ***Pectenotoxin 11 secoacid***. *PTX11-SA*
[848656-06-4]
$C_{47}H_{72}O_{16}$ 893.076
Isol. from *Dinophysis* sp.

7-Epimer: ***Pectenotoxin 4***. *PTX4*
[97560-26-4]
$C_{47}H_{70}O_{15}$ 875.061
From *Dinophysis acuminata*. Shellfish toxin. Ichthyotoxin. Solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ +2.07 (c, 0.193 in MeOH).

7-Epimer, 43-carboxylic acid: ***Pectenotoxin 7***. *PTX7*
$C_{47}H_{68}O_{16}$ 889.045
From *Dinophysis* sp. Phycotoxin. λ_{max} 237 (ϵ 37000) (MeOH) (Berdy).

7-Epimer, 43-deoxy, parent hydroxyacid: ***7-Epipectenotoxin 2 secoacid***. *7*-epi-*PTX2-SA*
[212502-88-0]
$C_{47}H_{72}O_{15}$ 877.077
From *Dinophysis acuta* and *Perna canaliculus* (New Zealand green mussel).

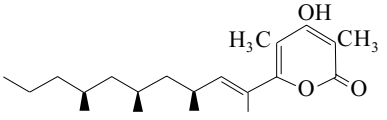
7-Epimer, 43-deoxy, 38,47-didehydro: ***Pectenotoxin 12***. *PTX12*
[809272-79-5 (36*S*-), 809272-80-8 (36*R*-)]
$C_{47}H_{68}O_{14}$ 857.046
Isol. from *Dinophysis acuminata* and *Dinophysis norvegica*. Shellfish toxin. Isol. as a mixt. of 36-epimers.

*7-Epimer, 43-deoxy, 34*S*-hydroxy, parent hydroxyacid:* ***7-Epipectenotoxin 11 secoacid***. *7*-epi-*PTX11-SA*
[862892-28-2]
$C_{47}H_{72}O_{16}$ 893.076
Isol. from *Dinophysis* sp.

Yasumoto, T. *et al., Tetrahedron*, 1985, **41**, 1019-1025 (*isol, cryst struct, spectra*)
Murata, M. *et al., Agric. Biol. Chem.*, 1986, **50**, 2693-2695 (*deriv*)
Lee, J.S. *et al., Bioact. Mol.*, 1989, **10**, 327 (*Pectenotoxin 6*)
Jung, J.H. *et al., J. Nat. Prod.*, 1995, **58**, 1722 (*Pectenotoxin 2, pmr, cmr, activity*)
Sasaki, K. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1783-1785 (*pmr, abs config*)
Daiguji, M. *et al., Chem. Lett.*, 1998, 653-654 (*isol, secoacids, activity*)
Jacobs, M.F. *et al., Curr. Org. Chem.*, 1998, **2**, 395-436 (*rev*)
Suzuki, T. *et al., J. Chromatogr., A*, 1998, **815**, 155-160
Sasaki, K. *et al., J.O.C.*, 1998, **63**, 2475-2480 (*isol, struct*)
Food Sci. Technol., Seafood and Freshwater Toxins, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*revs*)
Suzuki, T. *et al., Toxicon*, 2001, **39**, 507-514 (*Pectenotoxin 2, isol*)
Miles, C.O. *et al., Chem. Res. Toxicol.*, 2004, **17**, 1423-1433 (*Pectenotoxin 12*)
Suzuki, T. *et al., Chem. Res. Toxicol.*, 2006, **19**, 310-318 (*Pectenotoxin 11*)

Pectinatone P-127

*4-Hydroxy-3,5-dimethyl-6-(1,3,5,7-tetramethyl-1-decenyl)-2*H*-pyran-2-one, 9CI*
[87168-18-1]



$C_{21}H_{34}O_3$ 334.498

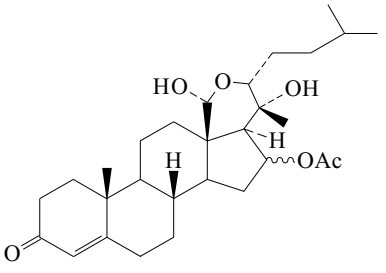
Struct. revised in 1990. Prod. by *Siphonaria pectinata* and *Siphonaria grisea*. Active against gram-positive bacteria. Cryst. (CH_2Cl_2). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 127-129°. $[\alpha]_D$ +62 (c, 0.184 in $CHCl_3$). λ_{max} 301 (ϵ 5060) (MeOH) (Derep).

Me ether: $[\alpha]_D$ +69.6 (c, 1.13 in CH_2Cl_2). λ_{max} 313 (no solvent reported).

(Z)-Isomer: ***Isopectinatone***
$C_{21}H_{34}O_3$ 334.498
Metab. of *Streptomyces pectinata*. Oil. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{25}$ +35 (c, 0.1 in $CHCl_3$). λ_{max} 238 (ϵ 2879); 294 (ϵ 6596) ($CHCl_3$).

Biskupiak, J.E. *et al., Tet. Lett.*, 1983, **24**, 3055-3058 (*isol, struct*)
Garson, M.J. *et al., J.C.S. Perkin 1*, 1990, 805-807 (*cryst struct, abs config*)
Norte, M. *et al., Tetrahedron*, 1990, **46**, 1669-1678 (*cryst struct, abs config*)
Paul, M.C. *et al., Tetrahedron*, 1997, **53**, 2303-2308 (*Isopectinatone*)
Zhu, Y. *et al., Tet. Lett.*, 1998, **39**, 7823-7826 (*synth*)

Pectinoacetal A P-128

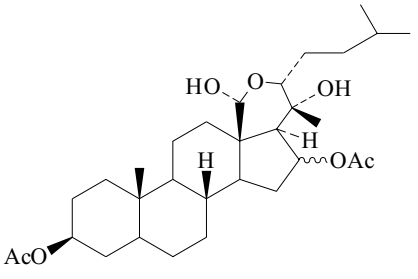


$C_{29}H_{44}O_6$ 488.663
Constit. of *Ctenocella pectinata*.

18-Epimer: ***Pectinoacetal B***
$C_{29}H_{44}O_6$ 488.663
Constit. of *Ctenocella pectinata*.

Roussis, V. *et al., Experientia*, 1993, **49**, 265 (*isol, pmr, cmr*)

Pectinoacetal C P-129



$C_{31}H_{50}O_7$ 534.732
Constit. of *Ctenocella pectinata*.

Roussis, V. *et al., Experientia*, 1993, **49**, 265 (*isol, pmr, cmr*)

Tritonia Pedal ganglion peptides P-130

TPep
H-Pro-Tyr-Asp-Gln-Ile-Thr-Gly-Leu-His-Gly-Leu-Ser-Gly-Phe-Ala-OH
Struct. of TPep-PLS shown. Isol. from the marine mollusc *Tritonia diomedea*. Neuropeptides.

TPep-PLS [173866-35-8]
$C_{72}H_{106}N_{18}O_{22}$ 1575.737

TPep-PAR [173866-36-9]
$C_{72}H_{107}N_{21}O_{21}$ 1602.765

TPep-NLS [173866-37-0]
$C_{71}H_{105}N_{19}O_{23}$ 1592.724

Lloyd, P.E. *et al., Peptides (N.Y.)*, 1996, **17**, 17-23 (*isol*)

Aplysia Pedal peptide P-131

[119975-71-2]
H-Pro-Leu-Asp-Ser-Val-Tyr-Gly-Thr-His-Gly-Met-Ser-Gly-Phe-Ala-OH
$C_{68}H_{99}N_{17}O_{22}S$ 1538.697
Present in v. high concentrations in the central nervous system and 2 peripheral tissues of *Aplysia californica*.

[119758-47-3]

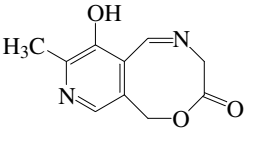
Lloyd, P.F. *et al., J. Neurosci.*, 1989, **9**, 312-317 (*isol*)
Pearson, W.L. *et al., J. Neurobiol.*, 1990, **21**, 883-892 (*isol*)

Peditoxin P-132

[158210-95-8]
Protein toxin (Pedin) non-covalently attached to an active prosthetic group (Pedoxin, P-133); pedin is a cytochrome b-like haem protein and contains 82 amino acid residues. Isol. from the sea urchin *Toxopneustes pileolus*. Toxin. λ_{max} 265; 335; 435; 535; 566 (pH 2 buffer) (Berdy). λ_{max} 280; 415; 525; 558 (pH 7 buffer) (Berdy).
▶ LD_{50} (mus, ipr) 70 mg/kg.
Kuwabara, K. *et al., J. Biol. Chem.*, 1994, **269**, 26734-26738 (*isol*)

Pedoxin P-133

*3,6-Dihydro-10-hydroxy-9-methyl-4*H*-pyrido[4,3-*f*][1,4]oxazocin-4-one, 9CI*
[158365-17-4]



$C_{10}H_{10}N_2O_3$ 206.201
Isol. from the sea urchin *Toxopneustes pileolus*. Prosthetic group of the protein toxin, Peditoxin. Sedative, anaesthetic. Yellow cryst. λ_{max} 256; 330 (pH 2 buffer) (Berdy). λ_{max} 334 (pH 7 buffer) (Berdy).
▶ LD_{50} (mus, scu) 250 mg/kg.
Kuwabara, S. *et al., J. Biol. Chem.*, 1994, **269**, 26734-26738

Pelamitoxin a P-134

*Neurotoxin 5 (*Enhydrina schistosa *reduced), 9CI. Hydrophitoxin b*
[39297-58-0]
Consists of a 60 amino acid sequence. Constit. of the venom of *Enhydrina schistosa*, sea snake *Hydrophis cyanocinctus* and *Pelamis platurus*.

[54990-78-2, 55963-83-2]

Frykland, L. *et al., Biochemistry*, 1972, **11**, 4633 (*isol*)
Liu, C.S. *et al., Toxicon*, 1974, **12**, 543; 1975, **13**, 31; 1976, **14**, 459 (*isol, struct*)

Pellynol I P-135

?-Methyl-27-hentriacontene-2,4,30-triyne-1,6,29-triol

$HC{\equiv}CCH(OH)CH{=}CH(CH_2)_mCH(CH_3)(CH_2)_nCH(OH)C{\equiv}CC{\equiv}CCH_2OH$

$C_{32}H_{52}O_3$ 484.761

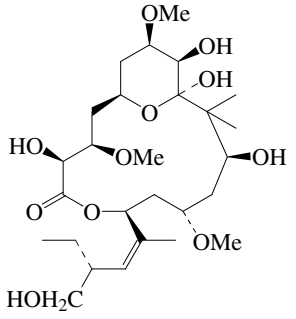
m + n = 19.

(-)-(E)-form

Constit. of the sponge *Pellina* sp. Cytotoxic agent. Amorph. powder. $[\alpha]_D$ -13.5 (c, 0.1 in $CHCl_3$).

Rashid, M.A. *et al., Nat. Prod. Lett.*, 2000, **14**, 387-392

Peloruside A P-136



Absolute Configuration

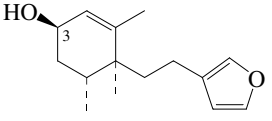
$C_{27}H_{48}O_{11}$ 548.67

Isol. from the marine sponge *Mycale hentscheli*. Cytotoxic agent. Antimitotic agent with Taxol -like microtubule stabilising activity. Oil. $[\alpha]_D^{20}$ +16 (c, 0.3 in CH_2Cl_2).

West, L.M. *et al., J.O.C.*, 2000, **65**, 445-449 (*isol, pmr, cmr*)
Hood, K.A. *et al., Cancer Res.*, 2002, **62**, 3356-3360 (*activity*)
Liao, X. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 1648-1652 (*synth, abs config*)
Jin, M. *et al., Org. Lett.*, 2005, **7**, 1303-1305 (*synth*)
Jiménez-Barbero, J. *et al., J.A.C.S.*, 2006, **128**, 8757-8765 (*pmr, conformn*)

Pelseneeriol 1 P-137

[871261-80-2]



$C_{15}H_{22}O_2$ 234.338

Constit. of *Doriopsilla pelseneeri*. Oil. $[\alpha]_D$ +9.4 (c, 0.04 in $CHCl_3$).

3-Epimer: ***Pelseneeriol 2***
[871261-81-3]
$C_{15}H_{22}O_2$ 234.338
Constit. of *Doriopsilla pelseneeri*. Oil. $[\alpha]_D$ -89.9 (c, 0.03 in $CHCl_3$).

Gaspar, H. *et al., Tetrahedron*, 2005, **61**, 11032-11037 (*Pelseneeriols*)

Pelvetian, 8CI P-138

Pelvecyan. *Pelvecian*

[39421-88-0]

Branched sulfated polysaccharide based on a linear glucurono-mannan chain. Isol. from the brown alga *Pelvetia wrightii*. $[\alpha]_D^{20}$ -57 (H_2O).

Ovodov, Y.S. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 408 (*isol*)
Khomenko, V.A. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 375; 378 (*struct*)
Pavlenko, A.F. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 155 (*struct*)
Ovodov, Y.S. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 317 (*struct, rev*)
Pavlenko, A.F. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1976, **12**, 515 (*struct*)

Penaeidin P-139

A family of peptides, Penaeidins 1 (50 residues), 2 (50 residues), 3 (62 residues) and 4 (47 residues); several isoforms have been isol. Isol. from the haemolymph of shrimps *Litopenaeus vannamei* and *Penaeus setiferus*. Antibacterial and antifungal agent.

[199877-63-9, 199877-64-0, 199877-65-1, 199877-66-2, 220381-72-6, 220381-86-2, 220382-52-5]

Destoumieux, D. *et al., J. Biol. Chem.*, 1997, **272**, 28398-28406 (*isol*)
Destoumieux, D. *et al., Cell Mol. Life Sci.*, 2000, **57**, 1260-1271 (*rev*)
Cuthbertson, B.J. *et al., Immunogenetics*, 2002, **54**, 442-445 (*isol*)
Yang, Y. *et al., J. Biol. Chem.*, 2003, **278**, 36859-36867 (*Penaeidin 3, soln struct*)
Cuthbertson, B.J. *et al., Biochem. J.*, 2004, **381**, 79-86 (*Penaeidin 4, synth*)

Penaeustatins P-140

Ala-Asn-Glu-Asp-Glu-Asp-Ala-Ala-Ser-Leu-Phe-Ala-Phe-Gly-Leu-NH_2

Peptides of the allatostatin superfamily; struct. of Penaeustatin 1 shown. Isol. from the CNS of the tiger prawn *Penaeus monodon*. Neuropeptides. See also Orcostatin I, O-119.

Penaeustatin 1 [474794-36-0]
$C_{69}H_{101}N_{17}O_{25}$ 1568.656

Penaeustatin 2 [474794-37-1]
$C_{86}H_{134}N_{26}O_{28}$ 1980.162

Penaeustatin 3 [158789-30-1]
$C_{45}H_{68}N_{12}O_{11}$ 953.106

Penaeustatin 4 [474794-39-3]
$C_{42}H_{60}N_{10}O_{11}$ 880.996

Penaeustatin 7 [474794-40-6]
$C_{40}H_{55}N_{11}O_{10}$ 849.942

Penaeustatin 8 [474794-42-8]
$C_{41}H_{59}N_{11}O_{11}$ 881.984

Penaeustatin 9 [474794-44-0]
$C_{39}H_{56}N_{10}O_{10}$ 824.932

Penaeustatin 10 [474794-46-2]
$C_{41}H_{59}N_9O_{11}$ 853.971

Penaeustatin 11 [474794-47-3]
$C_{44}H_{62}N_{12}O_{12}$ 951.047

Penaeustatin 12 [474794-48-4]
$C_{36}H_{50}N_8O_{11}$ 770.838

Penaeustatin 14 [474794-50-8]
$C_{42}H_{61}N_{11}O_{12}$ 912.01

Penaeustatin 15 [474794-51-9]
$C_{41}H_{60}N_{10}O_{12}$ 884.985

Penaeustatin 16 [474794-52-0]
$C_{38}H_{55}N_9O_{11}$ 813.906

Penaeustatin 17 [474794-53-1]
$C_{30}H_{42}N_6O_7$ 598.698

Penaeustatin 18 [474794-54-2]
$C_{41}H_{56}N_{12}O_{11}$ 892.967

Penaeustatin 19 [474794-56-4]
$C_{38}H_{51}N_{11}O_9$ 805.889

Penaeustatin 20 [474794-58-6]
$C_{41}H_{57}N_9O_{11}$ 851.955

Penaeustatin 21 [474794-59-7]
$C_{40}H_{55}N_9O_{11}$ 837.928

Penaeustatin 22 [474794-60-0]
$C_{42}H_{59}N_9O_{11}$ 865.982

Penaeustatin 23 [474794-61-1]
$C_{38}H_{52}N_8O_{10}$ 780.876

Penaeustatin 24 [474794-62-2]
$C_{39}H_{54}N_8O_{11}$ 810.903

Penaeustatin 25 [474794-63-3]
$C_{40}H_{55}N_9O_{11}$ 837.928

Penaeustatin 26 [474794-64-4]
$C_{85}H_{125}N_{23}O_{32}$ 1981.057

Penaeustatin 27 [474794-65-5]
$C_{81}H_{119}N_{21}O_{30}$ 1866.954

Penaeustatin 28 [474794-66-6]
$C_{62}H_{91}N_{17}O_{22}$ 1426.502

Penaeustatin 29 [474794-67-7]
$C_{37}H_{51}N_9O_{12}$ 813.863

Penaeustatin 30 [196201-72-6]
$C_{30}H_{40}N_6O_8$ 612.681

Penaeustatin 31 [474794-68-8]
$C_{40}H_{55}N_{11}O_{10}$ 849.942

Penaeustatin 32 [474794-70-2]
$C_{43}H_{64}N_{12}O_{13}$ 957.051

Penaeustatin 33 [474794-71-3]
$C_{40}H_{57}N_9O_{11}$ 839.944

Penaeustatin 34 [474794-72-4]
$C_{43}H_{60}N_{10}O_{12}S$ 941.073

Penaeustatin 36 [474794-73-5]
$C_{136}H_{213}N_{39}O_{45}$ 3114.413

Penaeustatin 37 [474794-74-6]
$C_{136}H_{215}N_{39}O_{44}$ 3100.429

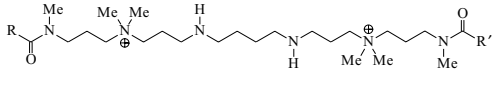
Penaeustatin 38 [474794-76-8]
$C_{39}H_{57}N_9O_{10}$ 811.934

Penaeustatin 39 [474794-78-0]
$C_{40}H_{59}N_9O_{10}$ 825.96

Duve, H. *et al., Peptides (N.Y.)*, 2002, **23**, 1039-1051 (*isol*)

Penaramides P-141

Penaresamides



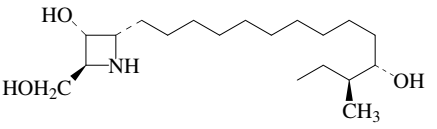
R, R′ = $(CH_2)_9CH_3$; $(CH_2)_7CH(CH_3)_2$; $(CH_2)_6CH(CH_3)CH_2CH_3$; $(CH_2)_2CH(CH_3)(CH_2)_5CH_3$; $CH_2CH(CH_3)(CH_2)_6CH_3$

Inseparable mixt. The simplest component Penaramide A has been synthesised. Isol. from the marine sponge *Penares* aff. *incrustans*. Inhibits binding of ω-Conotoxin GVIA to N-type Ca channels. Yellowish oil. $[\alpha]_D^{20}$ -11 (c, 0.39 in $CHCl_3$/MeOH 1:1).

Ushio-Sata, N. *et al., Tet. Lett.*, 1996, **37**, 225 (*isol, ir, pmr, cmr, synth, struct*)

Penaresidin A P-142

3-Hydroxy-4-(hydroxymethyl)-α-(1-methylpropyl)-2-azetidineundecanol, 9CI
[135574-62-8]



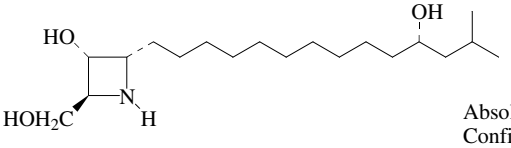
Absolute Configuration

$C_{19}H_{39}NO_3$ 329.522
Alkaloid from the marine sponge *Penares* sp. Potent ATPase activator. Isol. as an insep. mixt. with Penaresidin B, P-143.

Kobayashi, J. *et al., J.C.S. Perkin 1*, 1991, 1135-1137 (*isol, struct*)
Kobayashi, J. *et al., Tet. Lett.*, 1996, **37**, 6775-6776 (*abs config*)
Takikawa, H. *et al., J.C.S. Perkin 1*, 1997, 97-111 (*synth*)
Knapp, S. *et al., Tet. Lett.*, 1997, **38**, 3813-3816 (*synth*)
Lin, G.-Q. *et al., Heterocycles*, 1998, **47**, 337-348 (*synth*)
Liu, D.G. *et al., Tet. Lett.*, 1999, **40**, 337-340 (*synth, bibl*)

Penaresidin B P-143

3-Hydroxy-4-(hydroxymethyl)-α-(2-methylpropyl)-2-azetidineundecanol, 9CI
[135574-63-9]

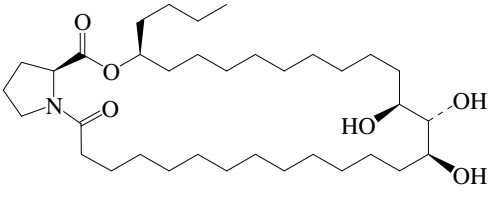


Absolute Configuration

$C_{19}H_{39}NO_3$ 329.522
Alkaloid from the marine sponge *Penares* sp. Potent ATPase activator. Isol. as an inseparable mixt. with Penaresidin A, P-142.

Kobayashi, J. *et al., J.C.S. Perkin 1*, 1991, 1135-1137 (*isol, struct*)
Kobayashi, J. *et al., Tet. Lett.*, 1996, **37**, 6775-6776 (*abs config*)
Takikawa, H. *et al., J.C.S. Perkin 1*, 1997, 97-111 (*synth*)
Yoda, H. *et al., Tet. Lett.*, 1997, **38**, 3283-3284 (*synth*)
Liu, D.-G. *et al., Tet. Lett.*, 1999, **40**, 337-340 (*synth*)
Yoda, H. *et al., Tet. Lett.*, 2003, **44**, 977-979 (*synth*)

Penarolide A_1 P-144

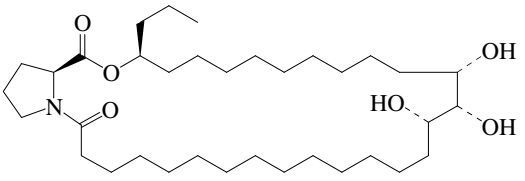


$C_{35}H_{65}NO_6$ 595.902

Tri-O-*sulfate:* ***Penarolide sulfate A_1***
[329019-71-8]
$C_{35}H_{65}NO_{15}S_3$ 836.094
Isol. from the marine sponge *Penares* sp. α-Glucosidase inhibitor. Amorph. solid (as tri-Na salt). $[\alpha]_D^{29}$ -25.7 (c, 0.5 in MeOH) (tri-Na salt). λ_{max} 204 (ϵ 9100) (MeOH) (tri-Na salt).

Nakao, Y. *et al., Tetrahedron*, 2000, **56**, 8977-8987

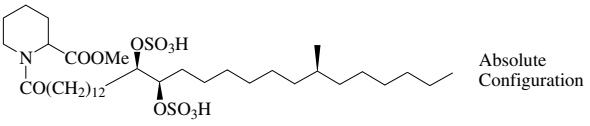
Penarolide A_2 P-145



$C_{35}H_{65}NO_6$ 595.902

Tri-O-*sulfate:* ***Penarolide sulfate A_2***
[329019-70-7]
$C_{35}H_{65}NO_{15}S_3$ 836.094
Isol. from the marine sponge *Penares* sp. α-Glucosidase inhibitor. Amorph. solid (as tri-Na salt). $[\alpha]_D^{29}$ -25.2 (c, 0.3 in MeOH) (tri-Na salt). λ_{max} 205 (ϵ 9000) (MeOH) (tri-Na salt).
Nakao, Y. *et al., Tetrahedron*, 2000, **56**, 8977-8987

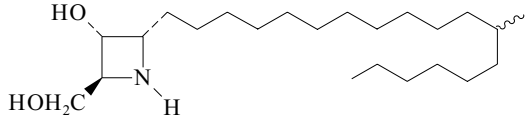
Penasulfate A P-146



$C_{36}H_{69}NO_{11}S_2$ 756.073
Isol. as a 4:1 mixt. of 2*R*- and 2*S*-stereoisomers. Alkaloid from the sponge *Penares* sp. α-Glucosidase inhibitor. Amorph. solid (as di-Na salt). $[\alpha]_D^{29}$ +10 (c, 0.03 in MeOH) (di-Na salt). λ_{max} 203 (ϵ 9700) (MeOH) (di-Na salt).
Nakao, Y. *et al., J. Nat. Prod.*, 2004, **67**, 1346-1350

Penazetidine A P-147

3-Hydroxy-4-(12-methyloctadecyl)-2-azetidinemethanol, 9CI
[160098-77-1]

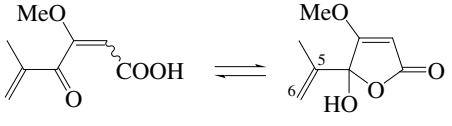


$C_{23}H_{47}NO_2$ 369.63
Isol. from the Indo-Pacific marine sponge *Penares sollasi*. Protein kinase C inhibitor. $[\alpha]_D$ -16.9 (c, 0.04 in MeOH).

Alvi, K.A. *et al., Bioorg. Med. Chem. Lett.*, 1994, **4**, 2447 (*isol, pmr, cmr, activity*)
Yajima, A. *et al., Annalen*, 1996, 1083 (*synth*)
Liu, D.-G. *et al., Tet. Lett.*, 1999, **40**, 337-340 (*synth*)
Li, Z.M. *et al., Chin. Chem. Lett.*, 2004, **15**, 138-140 (*synth*)

Penicillic acid P-148

*3-Methoxy-5-methyl-4-oxo-2,5-hexadienoic acid, 9CI. 5-Hydroxy-5-isopropenyl-4-methoxy-2(5*H*)-furanone*
[90-65-3]



$C_8H_{10}O_4$ 170.165
Toxic metab. of various *Penicillium* and *Aspergillus* spp. Rhombic or hexagonal plates + $1H_2O$ (H_2O). Spar. sol. H_2O; sol. EtOH; Et_2O; insol. petrol.
Mp 64-65° (hydrate) Mp 87° (anhyd.). pK_a 5.9. λ_{max} 218 (ϵ 16000) (pH 7 phosphate buffer) (Derep). λ_{max} 218 (sh) (ϵ 16000) (0.1*N* NaOH) (Derep). λ_{max} 228 (ϵ 11100) (MeOH) (Derep). λ_{max} 226 (ϵ 12750) (H_2O) (Berdy). λ_{max} 221 (ϵ 12500); 295 (ϵ 9800) (NaOH) (Berdy). λ_{max} 224 (ϵ 10500) (EtOH) (Berdy).
▶ LD_{50} (mus, orl) 600 mg/kg. Exp. neoplastic agent. Exp. reprod. and teratogenic effects. Hepatotoxic. LD_{50} (mus, ivn) 250 mg/kg , LD_{50} (mus, scu) 110 mg/kg. MM2625000

Me ester:
$C_9H_{12}O_4$ 184.191
Prisms. Mp 35°.

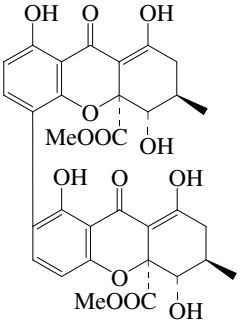
*5,6-Dihydro: 3-Methoxy-5-methyl-4-oxo-2-hexenoic acid. 5-Hydroxy-5-isopropyl-4-methoxy-2(5*H*)-furanone.* ***5,6-Dihydropenicillic acid***
$C_8H_{12}O_4$ 172.18
Prod. by *Aspergillus melleus*. Needles.
Mp 83-85°.

*6-Hydroxy, 5,6-dihydro: 5-Hydroxy-5-(2-hydroxy-1-methylethyl)-4-methoxy-2(5*H*)-furanone.* ***5,6-Dihydro-6-hydroxypenicillic acid***
$C_8H_{12}O_5$ 188.18
Prod. by *Penicillium* sp. F-4273. Nerve growth factor activator. λ_{max} 224 (ϵ 8300) (MeOH).

6-Methoxy, 5,6-dihydro: ***5,6-Dihydro-6-methoxypenicillic acid***
$C_9H_{14}O_5$ 202.207
Prod. by *Aspergillus cervinus*. Oil. $[\alpha]_D^{20}$ +19.8 (c, 0.19 in $CHCl_3$). λ_{max} 249 (log ϵ 4.46) (MeOH).

Raphael, R.A. *et al., J.C.S.*, 1948, 1508 (*synth*)
Kovac, S. *et al., Tetrahedron*, 1969, **25**, 3617 (*ir, uv*)
Suzuki, S. *et al., Agric. Biol. Chem.*, 1971, **35**, 287 (*ms*)
Kobayashi, H. *et al., Chem. Pharm. Bull.*, 1971, **19**, 839 (*pmr*)
Wilson, D.M. *et al., Adv. Chem. Ser.*, No. 170, 1976, 90 (*rev*)
IARC Monog., 1976, **10**, 211; *Suppl.* 7, 69 (*rev, tox*)
Yeh, C. *et al., Tet. Lett.*, 1978, 3987 (*synth*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2220 (*uv, ir, pmr, ms, cd*)
Japan. Pat., 1991, 91 184 968; *CA*, **116**, 82223a (*deriv*)
Kimura, Y. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 1375 (*5,6-Dihydropenicillic acid*)
Abrell, L.M. *et al., Tet. Lett.*, 1996, **37**, 2331-2334 (*marine Aspergillus metab*)
He, J. *et al., J. Nat. Prod.*, 2004, **67**, 1985-1991 (*5,6-Dihydro-6-methoxypenicillic acid*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 520
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PAP750

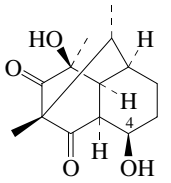
Penicillixanthone A P-149



$C_{32}H_{30}O_{14}$ 638.581
Prod. by the marine fungus *Penicillium thomii*.
Mp 235-237°. $[\alpha]_D^{25}$ -2.2 (c, 0.25 in Me_2CO).

Jiang, T. *et al., Yaoxue Xuebao*, 2002, **37**, 271-274 (*isol, pmr, cmr*)

Penicillone B P-150



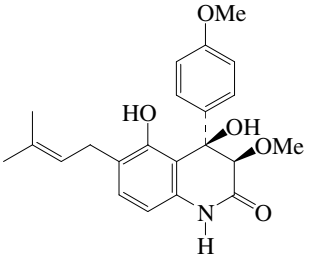
Relative Configuration

$C_{14}H_{20}O_4$ 252.31
Isol. from a marine-derived *Penicillium terrestre*. Needles (Me_2CO).
Mp 193° dec. $[\alpha]_D^{20}$ -13.7 (c, 0.2 in MeOH).

4-Ketone: ***Penicillone A***
$C_{14}H_{18}O_4$ 250.294
Isol. from *Penicillium terrestre*. Plates (Me_2CO).
Mp 200-201°. $[\alpha]_D^{20}$ +169.7 (c, 0.2 in MeOH).

Liu, W.-H. *et al., Tet. Lett.*, 2005, **46**, 4993-4996 (*isol, cd, pmr, cmr*)

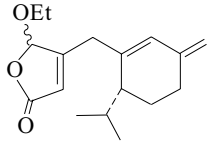
Peniprequinolone P-151



$C_{22}H_{25}NO_5$ 383.443
Prod. by *Penicillium* cf. *simplicissimum* and a marine-derived *Penicillium janczewski*. Pale yellowish solid.
Mp 191-194°. $[\alpha]_D^{20}$ -0.3 (c, 0.6 in $CHCl_3$). λ_{max} 206 (ε 74000); 222 (ε 65000); 302 (ε 19000) (EtOH).

Kusano, M. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 2559-2568 (*isol, cd, pmr, cmr, ms*)
Hu, J. *et al., J. Nat. Prod.*, 2005, **68**, 1397-1399 (*isol*)

Penlanbutenolide P-152



$C_{17}H_{24}O_3$ 276.375
Isol. from *Dysidea fragilis*. Oil. $[\alpha]_D$ +22.8 (c, 0.07 in $CHCl_3$). Artifact of ethanolic extraction. The nat. prods. are prob. the hydroxybutenolides. λ_{max} 238 (ε 11000) (MeOH).

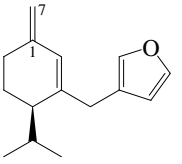
4-Epimer: ***4-Epipenlanbutenolide***
$C_{17}H_{24}O_3$ 276.375
Artifact isol. from *Dysidea fragilis*. Liq. $[\alpha]_D^{20}$ -5 (c, 0.2 in $CHCl_3$). More polar isomer. λ_{max} 238 (ε 11000) (MeOH).

[95653-88-6, 95653-89-7]

Guella, G. *et al., Helv. Chim. Acta*, 1985, **68**, 39-48

Penlanfuran P-153

3-[[3-Methylene-6-(1-methylethyl)-1-cyclohexen-1-yl]methyl] furan, 9CI



$C_{15}H_{20}O$ 216.322

(R)-form [87896-23-9]
Constit. of sponge *Dysidea fragilis*.
Oil. $[\alpha]_D^{20}$ -68 (c, 2.4 in $CHCl_3$).

1,7α-Dihydro, 7-acetoxy: ***Acetoxydihydropenlanfuran***
[95653-85-3]
$C_{17}H_{24}O_3$ 276.375
Isol. from *Dysidea fragilis*. Liq. λ_{max} 221 (ε 2500) (MeOH).

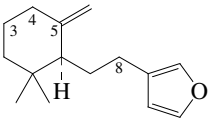
*1,7-Dihydro, 1*R*,7-dihydroxy: 3-(3-Furanylmethyl)-*p*-menth-2-ene-1,7-diol*
[95653-84-2]
$C_{15}H_{22}O_3$ 250.337
Isol. from *Dysidea fragilis*. Liq. (as Ac). $[\alpha]_D^{20}$ -54.1 (c, 0.44 in $CHCl_3$) (Ac). Isol. as a mixt. with its 1*S*-epimer, separated as their Ac derivs.

*1,7-Dihydro, 1*S*,7-dihydroxy:*
[95653-84-2]
$C_{15}H_{22}O_3$ 250.337
Isol. from *Dysidea fragilis*. Liq. (as Ac). $[\alpha]_D$ -39.2 (c, 0.67 in $CHCl_3$) (Ac).

Guella, G. *et al., Tet. Lett.*, 1983, **24**, 3897 (*isol*)
Guella, G. *et al., Helv. Chim. Acta*, 1985, **68**, 39-48 (*Acetoxydihydropenlanfuran, furanylmethylmenthenediols*)
Mancini, I. *et al., Helv. Chim. Acta*, 1990, **73**, 652 (*abs config*)
Takano, D. *et al., J. Het. Chem.*, 1997, **34**, 1111-1114 (*synth, pmr, cmr*)

Penlanpallescensin P-154

3-[2-(2,2-Dimethyl-6-methylenecyclohexyl)ethyl]furan, 9CI. Dihydropallescensin 2



(*S*)-*form*

$C_{15}H_{22}O$ 218.338

(S)-form [83631-17-8]
Constit. of *Dysidea fragilis*.
Oil. $[\alpha]_D^{20}$ +6 (c, 0.3 in $CHCl_3$).

Δ^4-Isomer: ***Pallescensin 1***
[56881-44-8]
$C_{15}H_{22}O$ 218.338
Constit. of *Dysidea pallescens*. Oil. $[\alpha]_D$ -89.5 ($CHCl_3$). λ_{max} 223 (ε 9300) (MeOH) (Derep).

3,4-Didehydro: ***Pallescensin 2***
[56881-45-9]
$C_{15}H_{20}O$ 216.322
Constit. of *Dysidea pallescens*. Oil. $[\alpha]_D$ +39.5. λ_{max} 230 (ε 11800) (MeOH) (Derep).

8-Oxo: ***Pallescensone***
[112137-03-8]
$C_{15}H_{20}O_2$ 232.322
Constit. of the sponge *Dictyodendrilla cavernosa*. Cryst.
Mp 42.5-43°. $[\alpha]_D$ +36 (c, 1 in $CHCl_3$). λ_{max} 252 (ε 5100) ($CHCl_3$) (Derep).

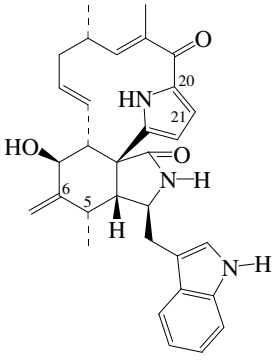
(ξ)-*form*

Isol. from mollusc *Cadlina luteomarginata*.

Cimino, G. *et al., Tet. Lett.*, 1975, 1417 (*isol, struct*)
Tius, M.A. *et al., J.O.C.*, 1982, **47**, 3166 (*synth*)
Thompson, J.E. *et al., Tetrahedron*, 1982, **38**, 1865-1873 (*isol*)
Matsumoto, T. *et al., Bull. Chem. Soc. Jpn.*, 1983, **46**, 491 (*synth*)
Guella, G. *et al., Helv. Chim. Acta*, 1985, **68**, 39 (*isol*)
Cambie, R.C. *et al., J. Nat. Prod.*, 1987, **50**, 948 (*Pallescensone*)
Kurth, M.J. *et al., Tet. Lett.*, 1987, **28**, 1031 (*synth*)
Vidori, G. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 3009 (*synth*)

Penochalasin C P-155

[173792-72-8]



$C_{32}H_{35}N_3O_3$ 509.647

Prod. by a marine *Penicillium* sp. Mycotoxin. Powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 173-178°. $[\alpha]_D$ -6.2 (c, 0.1 in $CHCl_3$). λ_{max} 208 (log ϵ 4.5); 222 (log ϵ 4.59); 284 (log ϵ 3.92); 293 (log ϵ 3.96); 315 (log ϵ 3.87) (EtOH).

$\Delta^{5,6}$-Isomer: ***Penochalasin B***

[173792-71-7]

$C_{32}H_{35}N_3O_3$ 509.647

Prod. by a marine *Penicillium* sp. Mycotoxin. Powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 177-179°. $[\alpha]_D$ -6.2 (c, 0.2 in $CHCl_3$). λ_{max} 206 (log ϵ 4.1); 222 (log ϵ 4.1); 284 (log ϵ 4.08); 293 (log ϵ 4.5); 312 (log ϵ 4.45) (EtOH).

7-Deoxy, 6,12-dihydro, 6β,7β-epoxide: ***Penochalasin A***

[173792-70-6]

$C_{32}H_{35}N_3O_3$ 509.647

Prod. by a marine *Penicillium* sp. Mycotoxin. Needles (Me_2CO). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 222-224°. $[\alpha]_D$ -10 (c, 0.2 in $CHCl_3$). λ_{max} 206 (log ϵ 4.58); 222 (log ϵ 4.66); 285 (log ϵ 4.4); 292 (log ϵ 4.09); 313 (log ϵ 4.13) (EtOH).

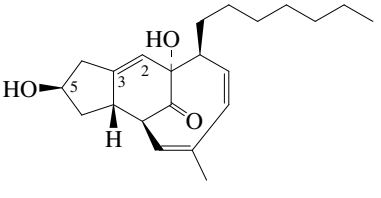
7-Deoxy, 6,12,20β,21-tetrahydro, 6β,7β-epoxide: ***Penochalasin D***

$C_{32}H_{37}N_3O_3$ 511.663

Prod. by a marine *Penicillium* sp. Cytotoxic. Oil. $[\alpha]_D$ +10.8 (c, 0.2 in $CHCl_3$). λ_{max} 221 (log ϵ 4.33); 242 (sh) (log ϵ 3.72); 280 (log ϵ 3.58); 292 (log ϵ 3.48) (EtOH).

Numata, A. *et al., J.C.S. Perkin 1*, 1996, 239-245 (*Penochalasins A-C*)
Iwamoto, C. *et al., Tetrahedron*, 2001, **57**, 2997-3004 (*Penochalasin D*)

Penostatin I P-156



(+)-*form*

$C_{22}H_{32}O_3$ 344.493

Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 230; 278 (ϵ 4786) (MeOH) (Berdy).

(+)-form [204198-97-0]

Prod. by a *Penicillium* sp. isol. from the alga *Enteromorpha intestinalis*. Cytotoxic agent. Oil. $[\alpha]_D$ +13.3 (c, 0.3 in $CHCl_3$). λ_{max} 230 (sh) (log ϵ 4.01) (EtOH).

2,3-Dihydro, 3α-hydroxy: ***Penostatin J***

$C_{22}H_{34}O_4$ 362.508

Prod. by a *Penicillium* sp. isol. from a marine alga.

(-)-*form*

5-Epimer: ***Penostatin F***

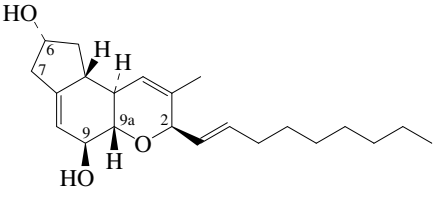
[183659-20-3]

$C_{22}H_{32}O_3$ 344.493

Prod. by a *Penicillium* sp. isol. from *Enteromorpha intestinalis*. Cytotoxic agent. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -12.5 (c, 0.2 in $CHCl_3$). λ_{max} 232 (sh) (log ϵ 3.93) (EtOH). λ_{max} 232; 281 (ϵ 646) (MeOH) (Berdy).

Iwamoto, C. *et al., J.C.S. Perkin 1*, 1998, 449-456 (*isol, uv, cd, pmr, cmr, ms*)
Iwamoto, C. *et al., Tennen Yuki Kagobutsu Toronkai Koen Yoshishu*, 1999, **41**, 601-606; *CA*, **132**, 262418 (*Penostatin J*)

Penostatin D P-157



(-)-*form*

$C_{22}H_{34}O_3$ 346.509

(-)-form [173560-29-7]

Isol. from a *Penicillium* sp. found in a marine alga *Enteromorpha* sp. Cytotoxic agent. Powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 106-110°. $[\alpha]_D$ -26.7 (c, 0.1 in $CHCl_3$).

9-Ketone: ***Penostatin B***

[173655-56-6]

$C_{22}H_{32}O_3$ 344.493

Isol. from a *Penicillium* sp. Cytotoxic agent. Powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 63-66°. $[\alpha]_D$ -103 (c, 0.5 in $CHCl_3$). λ_{max} 230 (log ϵ 4.1) (no solvent reported). λ_{max} 230 (ϵ 12590) (MeOH) (Berdy).

(+)-*form*

6-Deoxy, 6,7-didehydro, 9-ketone: ***Penostatin C***

[173485-71-7]

$C_{22}H_{30}O_2$ 326.478

Isol. from a *Penicillium* sp. Cytotoxic agent. Powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 63-65°. $[\alpha]_D$ +120 (c, 1 in $CHCl_3$). λ_{max} 283 (log ϵ 4.3) (no solvent reported). λ_{max} 283 (ϵ 19952) (MeOH) (Berdy).

9aβ-Hydroxy, 6-deoxy, 6,7-didehydro, 9-ketone: ***Penostatin L***

$C_{22}H_{30}O_3$ 342.477

Isol. from a *Penicillium* sp. separated from a marine alga.

6-Epimer, 9-ketone: ***Penostatin A***

[173485-70-6]

$C_{22}H_{32}O_3$ 344.493

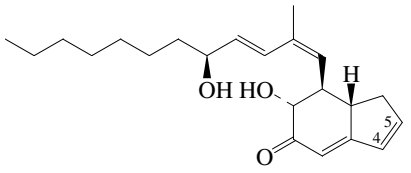
Isol. from a *Penicillium* sp. Cytotoxic agent. Needles. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 73-75°. $[\alpha]_D$ +133 (c, 0.2 in $CHCl_3$). λ_{max} 232 (log ϵ 4.22) (MeOH).

Takahashi, C. *et al., Tet. Lett.*, 1996, **37**, 655 (*isol, uv, ir, pmr, cmr*)
Iwamoto, C. *et al., Tennen Yuki Kagobutsu Toronkai Koen Yoshishu*, 1999, **41**, 601-606; *CA*, **132**, 262418 (*Penostatin L*)
Iwamoto, C. *et al., Tetrahedron*, 1999, **55**, 14353-14368 (*abs config*)
Snider, B.B. *et al., J.O.C.*, 2000, **65**, 8490-8498 (*synth*)

Penostatin E P-158

[256463-57-7]



Absolute Configuration

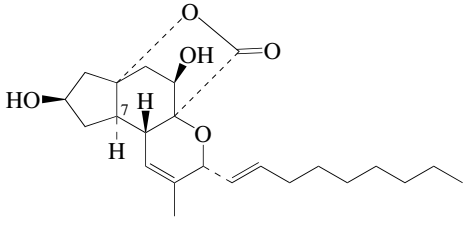
$C_{22}H_{32}O_3$ 344.493
Prod. by a *Penicillium* sp. isol. from the microalga *Enteromorpha* sp. Cytotoxic agent. Oil. $[\alpha]_D$ +48.5 (c, 0.16 in $CHCl_3$). λ_{max} 235 (log ϵ 4.4); 281 (log ϵ 4.23) (EtOH).

4,5-Dihydro, 5β-hydroxy: ***Penostatin O***
$C_{22}H_{34}O_4$ 362.508
Isol. from a *Penicillium* sp. separated from a marine alga.

Iwamoto, C. *et al., Tennen Yuki Kagobutsu Toronkai Koen Yoshishu*, 1999, **41**, 601-606; *CA*, **132**, 262418 (*Penostatin O*)
Iwamoto, C. *et al., Tetrahedron*, 1999, **55**, 14353-14368 (*Penostatin E, abs config*)

Penostatin G P-159

[183659-21-4]

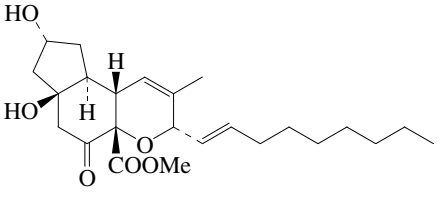


$C_{23}H_{34}O_5$ 390.519
Prod. by a *Penicillium* sp. isol. from the alga *Enteromorpha intestinalis*. Cytotoxic agent. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -35.1 (c, 0.3 in $CHCl_3$).

7-Epimer: ***Penostatin H***
[204198-96-9]
$C_{23}H_{34}O_5$ 390.519
Prod. by a *Penicillium* sp. isol. from *Enteromorpha intestinalis*. Cytotoxic agent. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -11.4 (c, 0.2 in $CHCl_3$).

Iwamoto, C. *et al., J.C.S. Perkin 1*, 1998, 449-456 (*isol, cd, pmr, cmr, ms*)

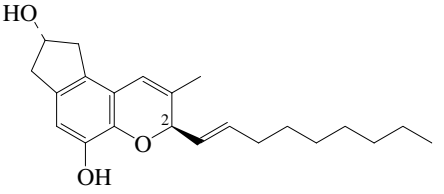
Penostatin K P-160



$C_{24}H_{36}O_6$ 420.545
Isol. from a *Penicillium* sp. separated from a marine alga.

Iwamoto, C. *et al., Tennen Yuki Kagobutsu Toronkai Koen Yoshishu*, 1999, **41**, 601-606; *CA*, **132**, 262418

Penostatin M P-161

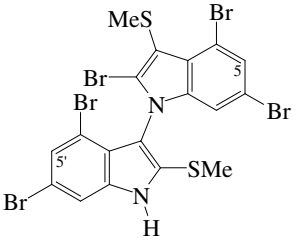


$C_{22}H_{30}O_3$ 342.477
Isol. from a *Penicillium* sp. separated from a marine alga.

2-Epimer: ***Penostatin N***
$C_{22}H_{30}O_3$ 342.477
Isol. from a *Penicillium* sp. separated from a marine alga.

Iwamoto, C. *et al., Tennen Yuki Kagobutsu Toronkai Koen Yoshishu*, 1999, **41**, 601-606; *CA*, **132**, 262418

2,4,4′,6,6′-Pentabromo-2′,3-bis(methylthio)-1,3′-bi-1*H*-indole P-162



$C_{18}H_{11}Br_5N_2S_2$ 718.95
Alkaloid from *Laurencia brongniartii*. Plates (hexane/EtOAc). Mp 243-245°. λ_{max} 231 (ϵ 83300); 302 (ϵ 28300) (MeOH).

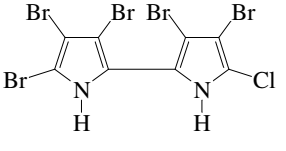
*5-Bromo: 2,4,4′,5,6,6′-Hexabromo-2′,3-bis(methylthio)-1,3′-bi-1*H*-indole*
$C_{18}H_{10}Br_6N_2S_2$ 797.846
Alkaloid from *Laurencia brongniartii*. λ_{max} 233 (ϵ 51800); 303 (ϵ 16200) (MeOH).

*5′-Bromo: 2,4,4′,5′,6,6′-Hexabromo-2′,3-bis(methylthio)-1,3′-bi-1*H*-indole*
$C_{18}H_{10}Br_6N_2S_2$ 797.846
Alkaloid from *Laurencia brongniartii*. λ_{max} 233 (ϵ 89400); 300 (ϵ 26700) (MeOH).

*5,5′-Dibromo: 2,4,4′,5,5′,6,6′-Heptabromo-2′,3-bis(methylthio)-1,3′-bi-1*H*-indole*
$C_{18}H_9Br_7N_2S_2$ 876.743
Alkaloid from *Laurencia brongniartii*. λ_{max} 236 (ϵ 43700); 298 (ϵ 10200) (MeOH).

Kubota, N.K. *et al., Heterocycles*, 2005, **65**, 2675-2682 (*isol, pmr, cmr, ms, cryst struct*)

3,3′,4,4′,5-Pentabromo-5′-chloro-2,2′-bi-1*H*-pyrrole P-163



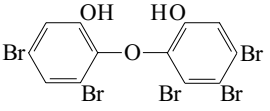
$C_8H_2Br_5ClN_2$ 561.09

*N,N′-Di-Me: 3,3′,4,4′,5-Pentabromo-5′-chloro-1,1′-dimethyl-2,2′-bi-1*H*-pyrrole. DBP-Br_5Cl*
[400767-00-2]
$C_{10}H_6Br_5ClN_2$ 589.144
Marine natural product of unknown biogenic origin. Present in marine or freshwater fish, shrimps, seabirds and seal blubber.

Tittlemier, S.A. *et al., Environ. Pollut.*, 2002, **116**, 85-93 (*N,N′-di-Me, occur, detn*)
Tittlemier, S.A. *et al., J. Agric. Food Chem.*, 2004, **52**, 2010-2015 (*N,N′-di-Me, occur*)

2,2′,3,4,4′-Pentabromo-6,6′-dihydroxydiphenyl ether P-164

3,4,5-Tribromo-2-(2,4-dibromo-6-hydroxyphenoxy)phenol
[170473-64-0]

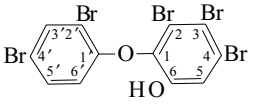


$C_{12}H_5Br_5O_3$ 596.69
Metab. of the sponge *Dysidea* sp. Amorph. powder.

Fu, X. *et al., J. Nat. Prod.*, 1995, **58**, 1384 (*isol, ir, pmr, props*)

2,2′,3,4,4′-Pentabromo-6-hydroxydiphenyl ether P-165

3,4,5-Tribromo-2-(2,4-dibromophenoxy)phenol, 9CI
[35162-01-7]



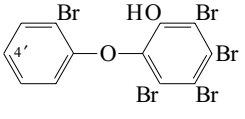
$C_{12}H_5Br_5O_2$ 580.69
Constit. of *Dysidea herbacea* and *Chromodoris funerea*. Cryst. (hexane).
Mp 195-196° (185-186°).

Me ether: [38926-88-4]
$C_{13}H_7Br_5O_2$ 594.717
Mp 155°.

Sharma, G.M. *et al., Tet. Lett.*, 1972, 1715 (*isol, struct*)
Carté, B. *et al., J.O.C.*, 1986, **51**, 3528
Fu, X. *et al., J. Nat. Prod.*, 1995, **58**, 1384 (*isol*)
Marsh, G. *et al., Eur. J. Org. Chem.*, 2003, 2566-2576 (*synth, pmr, ms, Me ether*)

2,2′,3,4,5-Pentabromo-6-hydroxydiphenyl ether P-166

2,3,4,5-Tetrabromo-6-(2-bromophenoxy)phenol, 9CI
[129602-13-7]



$C_{12}H_5Br_5O_2$ 580.69
Constit. of a marine sponge *Dysidea* sp. Cryst. (EtOAc/hexane).
Mp 143-145°. λ_{max} 295 (ϵ 4500) (MeOH) (Berdy). λ_{max} 310 (MeOH/NaOH) (Berdy).

4′-Bromo: 2,3,4,5-Tetrabromo-6-(2,4-dibromophenoxy)phenol, 9CI. 2,2′,3,4,4′,5-Hexabromo-6-hydroxydiphenyl ether
[111863-67-3]
$C_{12}H_4Br_6O_2$ 659.586
Constit. of *Dysidea fragilis*. Cryst. (hexane).
Mp 151-153°.

3-Debromo: 2,3,5-Tribromo-6-(2-bromophenoxy)phenol. 2′,3,4,6-Tetrabromo-2-hydroxydiphenyl ether
[198275-05-7]
$C_{12}H_6Br_4O_2$ 501.794
Constit. of *Dysidea herbacea*. λ_{max} 220 (MeOH) (Berdy).

4-Debromo: 3,4,6-Tribromo-2-(2-bromophenoxy)phenol. 2,2′,3,5-Tetrabromo-6-hydroxydiphenyl ether
[198275-06-8]
$C_{12}H_6Br_4O_2$ 501.794
Constit. of *Dysidea herbacea*. λ_{max} 222 (MeOH) (Berdy).

4-Debromo, Me ether: 2,2′,3,5-Tetrabromo-6-methoxydiphenyl ether
[198275-07-9]
$C_{13}H_8Br_4O_2$ 515.821
Constit. of *Dysidea herbacea*. Viscous oil. λ_{max} 226 (MeOH).

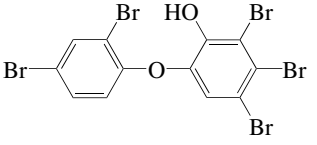
4-Debromo, 4′-bromo: 3,4,6-Tribromo-2-(2,4-dibromophenoxy)-phenol. 2,2′,3,4′,5-Pentabromo-6-hydroxydiphenyl ether
$C_{12}H_5Br_5O_2$ 580.69
Constit. of *Dysidea herbacea*.

5-Debromo: 3,4,5-Tribromo-2-(2-bromophenoxy)phenol. 2,2′,3,4-Tetrabromo-6-hydroxydiphenyl ether
[198275-04-6]
$C_{12}H_6Br_4O_2$ 501.794
Constit. of *Dysidea herbacea*. Viscous oil. λ_{max} 209 (MeOH).

Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1987, **23**, 603-605; *Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 508-509 (*4′-bromo*)
Salver, J. *et al., J. Nat. Prod.*, 1990, **53**, 757-760 (*isol, synth*)
Handayani, D. *et al., J. Nat. Prod.*, 1997, **60**, 1313-1316 (*debromo derivs*)
Agrawal, M.S. *et al., Mar. Drugs*, 2005, **3**, 9-14 (*4-debromo-4′-bromo*)

2′,3,4,4′,5-Pentabromo-2-hydroxydiphenyl ether P-167

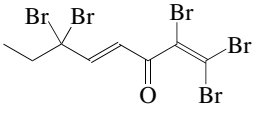
2,3,4-Tribromo-6-(2,4-dibromophenoxy)phenol
[80246-24-8]



$C_{12}H_5Br_5O_2$ 580.69
Metab. of the sponges *Dysidea* spp.
Mp 138-140°.

Carte, B. *et al., Tetrahedron*, 1981, **37**, 2335-2339 (*isol*)
Fu, X. *et al., J. Nat. Prod.*, 1995, **58**, 1384-1391 (*isol*)

1,1,2,6,6-Pentabromo-1,4-octadien-3-one P-168



$C_8H_7Br_5O$ 518.663

(E)-form [69267-73-8]
Constit. of the red alga *Ptilonia australasica*.

Kazlauskas, R. *et al., Tet. Lett.*, 1978, 3165-3168 (*isol, struct*)
Naylor, S. *et al., J. Nat. Prod.*, 1985, **48**, 72-75 (*cmr*)

1,1,2,4,4-Pentabromo-1-octen-3-one P-169

[69267-72-7]
$H_3C(CH_2)_3CBr_2COCBr{=}CBr_2$
$C_8H_9Br_5O$ 520.678
Constit. of the red alga *Ptilonia australasica*.

Kazlauskas, R. *et al., Tet. Lett.*, 1978, 3165 (*isol*)

Pentabromo-2-propanone, 9CI P-170

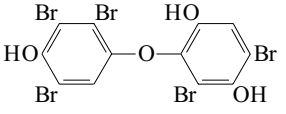
Pentabromoacetone
[79-49-2]
$Br_3CCOCHBr_2$
C_3HBr_5O 452.56
Constit. of the red alga *Asparagopsis taxiformis*. Needles (H_2O or EtOH), prisms (Et_2O).
Mp 79-80°. Steam-volatile. Subl.

Enol dibromoacetate: Pentabromo-2-propenyl dibromoacetate
[130034-39-8]
$C_5HBr_7O_2$ 652.39
Constit. of *Asparagopsis taxiformis*. Aldose reductase inhibitor. Oil.

Enol tribromoacetate: Pentabromo-2-propenyl tribromoacetate
[130034-38-7]
$C_5Br_8O_2$ 731.286
Constit. of *Asparagopsis taxiformis*. Aldose reductase inhibitor. Mp 120-121°.
Jackson, C.L. *et al., J.A.C.S.*, 1915, **37**, 2532 (*synth*)
Rappe, C. *et al., Acta Chem. Scand.*, 1964, **18**, 1998 (*synth*)
McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367 (*isol*)
Sugano, M. *et al., Tet. Lett.*, 1990, **31**, 7015 (*isol, derivs*)

2,2′,3,4′,5-Pentabromo-3′,4,6′-trihydroxydiphenyl ether P-171

3,5-Dibromo-2-(2,3,5-tribromo-4-hydroxyphenoxy)-1,4-benzenediol
[74092-58-3]



$C_{12}H_5Br_5O_4$ 612.689
Constit. of an acorn worm.

5′-Bromo: 3,5,6-Tribromo-2-(2,3,5-tribromo-4-hydroxyphenoxy)-1,4-benzenediol. 2,2′,3′,4,5,5′-Hexabromo-3,4′,6-trihydroxydiphenyl ether
$C_{12}H_4Br_6O_4$ 691.585
Isol. from acorn worm *Ptychodera flava*.
Higa, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **65**, 525 (*isol*)
Kanakubo, A. *et al., Bioorg. Med. Chem.*, 2005, **13**, 2741-2747 (*5′-bromo*)

1,16-Pentacosadiene P-172

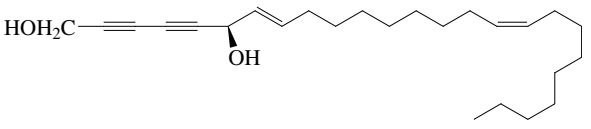
[99461-72-0]
$H_3C(CH_2)_7CH{=}CH(CH_2)_{13}CH{=}CH_2$
$C_{25}H_{48}$ 348.654

(*E*)-*form* [104899-44-7]
Isol. from the green alga *Botryococcus braunii*.

(*Z*)-*form* [104899-39-0]
Isol. from *Botryococcus braunii*.
Metzger, P. *et al., Phytochemistry*, 1986, **25**, 1869; 1993, **33**, 1125 (*isol, pmr, cmr*)

7,16-Pentacosadiene-2,4-diyne-1,6-diol P-173

Strongylodiol H



$C_{25}H_{40}O_2$ 372.59

(6*R*,7*E*,16*Z*)-*form*
Isol. from the sponge *Strongylophora* sp.
Oil. $[\alpha]_D^{22}$ -43.8 (c, 0.35 in $CHCl_3$). Obt. as a partial racemate (94% op). λ_{max} 208 (log ϵ 3.79) (MeOH).
Watanabe, K. *et al., J. Nat. Prod.*, 2005, **68**, 1001-1005 (*isol, pmr, cmr*)

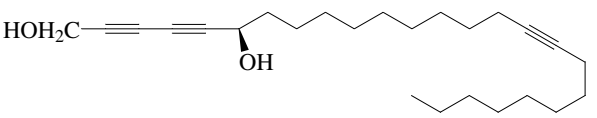
5,9-Pentacosadienoic acid P-174

[59708-82-6]
$H_3C(CH_2)_{14}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{25}H_{46}O_2$ 378.637

(*Z*,*Z*)-*form* [124029-64-7]
Constit. of various sponges incl. *Dysidea fragilis* and *Hymeniacidon sanguinea*.
Christie, W.W. *et al., Lipids*, 1992, **27**, 640-644 (*isol*)
Duque, C. *et al., Lipids*, 1993, **28**, 767-769 (*isol*)
Christie, W.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1994, **109**, 245-252 (*isol*)

2,4,16-Pentacosatriyne-1,6-diol P-175

Strongylodiol B



(*R*)-*form*

$C_{25}H_{40}O_2$ 372.59

(*R*)-*form*
Isol. from the sponge *Strongylophora* sp. Cytotoxic agent. $[\alpha]_D^{22}$ -7.1 (c, 0.42 in $CHCl_3$).

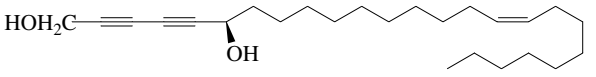
(*S*)-*form*
Isol. from *Strongylophora* sp. Cytotoxic agent. $[\alpha]_D^{22}$ +7.7 (c, 0.01 in $CHCl_3$).
Watanabe, K. *et al., Tet. Lett.*, 2000, **41**, 9271-9276 (*isol*)
Reber, S. *et al., Tetrahedron*, 2003, **59**, 6813-6817 (*synth*)
Kirkham, J.E.D. *et al., Tetrahedron*, 2005, **61**, 7219-7232 (*synth*)

1-Pentacosene P-176

[16980-85-1]
$H_3C(CH_2)_{22}CH{=}CH_2$
$C_{25}H_{50}$ 350.67
Isol. from the alga *Botryococcus braunii* and various plant spp. Fp 48.7. Bp_{30} 271.2°.
Dreisbach, R.R. *et al., Adv. Chem. Ser.*, 1959, **22**, 390 (*props*)
MacLeod, G. *et al., Phytochemistry*, 1990, **29**, 1197 (*isol*)
Metzger, P. *et al., Phytochemistry*, 1993, **33**, 1125 (*isol*)

16-Pentacosene-2,4-diyne-1,6-diol P-177

Strongylodiol A



(6*R*,16*Z*)-*form*

$C_{25}H_{42}O_2$ 374.606

(6*R*,16*Z*)-*form*
Isol. from the sponge *Strongylophora* sp. Cytotoxic agent. $[\alpha]_D^{22}$ -7.2 (c, 1.1 in $CHCl_3$). λ_{max} 231 (log ϵ 2.68); 243 (log ϵ 2.63); 257 (log ϵ 2.41) (EtOH).

(6*S*,16*Z*)-*form*
Isol. from *Strongylophora* sp. Cytotoxic agent. $[\alpha]_D^{22}$ +7.5 (c, 0.07 in $CHCl_3$).
Watanabe, K. *et al., Tet. Lett.*, 2000, **41**, 9271-9276 (*isol*)
Yadav, J.S. *et al., Tet. Lett.*, 2002, **43**, 1739-1741 (*synth*)
Reber, S. *et al., Tetrahedron*, 2003, **59**, 6813-6817 (*synth*)
Kirkham, J.E.D. *et al., Tetrahedron*, 2005, **61**, 7219-7232 (*synth*)

5-Pentacosenoic acid P-178

$H_3C(CH_2)_{18}CH{=}CH(CH_2)_3COOH$
$C_{25}H_{48}O_2$ 380.653

(*Z*)-*form* [173866-83-6]
Constit. of the sponge *Pseudaxinella* cf. *lunaecharta*.
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol, ms*)

16-Pentacosenoic acid P-179

$H_3C(CH_2)_7CH{=}CH(CH_2)_{14}COOH$
$C_{25}H_{48}O_2$ 380.653

(*Z*)-*form* [140163-39-9]
Constit. of the sponge *Mycale laevis*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1992, **55**, 333

17-Pentacosenoic acid P-180

$H_3C(CH_2)_6CH{=}CH(CH_2)_{15}COOH$
$C_{25}H_{48}O_2$ 380.653

(*Z*)-*form* [134394-72-2]
Constit. of the lichens *Cladonia* sp. and *Parmelia* sp. and from the sponge *Geodia gibberosa*.
Carballeira, N.M. *et al., Lipids*, 1991, **26**, 324
Dembitskii, V.M. *et al., Phytochemistry*, 1991, **30**, 4015; 1992, **31**, 841 (*isol*)

18-Pentacosenoic acid P-181

$H_3C(CH_2)_5CH{=}CH(CH_2)_{16}COOH$
$C_{25}H_{48}O_2$ 380.653

(*Z*)-*form* [138282-15-2]
Constit. of the sponges *Euspongilla lacustris* and *Mycale laevis*.
Dembitskii, V.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **100**, 185 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1992, **55**, 333

19-Pentacosenoic acid P-182

$H_3C(CH_2)_4CH{=}CH(CH_2)_{17}COOH$
$C_{25}H_{48}O_2$ 380.653

(*Z*)-*form* [140163-40-2]
Constit. of the sponge *Amphimedon compressa*.
Me ester: [443965-82-0]
$C_{26}H_{50}O_2$ 394.68
Constit. of the seeds of *Papaver somniferum* (opium poppy). Solid. Mp 45-47°.
Aldehyde: ***19-Pentacosenal***
[140163-48-0]
$C_{25}H_{48}O$ 364.654
Constit. of *Amphimedon compressa*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1992, **55**, 333
Agarwal, S.K. *et al., Indian J. Chem., Sect. B*, 2002, **41**, 1061-1063 (*Me ester*)

Pentadecane P-183

[629-62-9]
$H_3C(CH_2)_{13}CH_3$
$C_{15}H_{32}$ 212.418
Found in numerous plants and waxes. Prod. by blue-green algae *Oscillatoria splendida*, *Oscillatoria amoena*, *Oscillatoria geminata* and *Aphanizomenon* sp. Oil of *Rumex japonicus* and *Vallisneria denseserrulate*, fungus *Trametes lilacino-gilva*, *Agaricus bisporus*. Defensive secretions of bombadier beetles and ponerine ant *Rhytidoponera metallica*.
Mp 10°. Bp 270° Bp_{10} 136°.
▶ LD_{50} (mus, ivn) 3494 mg/kg. RZ1800000
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 3D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 4B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 4D (*ir*)
Vogel, A.I. *et al., J.C.S.*, 1946, 133-139 (*synth*)
Bergmann, G. *et al., Angew. Chem., Int. Ed.*, 1972, **11**, 1032-1033 (*cmr*)
Tsuchiya, Y. *et al., CA*, 1981, **95**, 200575 (*occur*)
Brophy, J.J. *et al., Insect Biochem.*, 1981, **11**, 307-310 (*occur*)
Yamaguchi, K. *et al., J. Agric. Food Chem.*, 1981, **29**, 366-370 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, PAY750

Pentadecanoic acid P-184

[1002-84-2]
$H_3C(CH_2)_{13}COOH$
$C_{15}H_{30}O_2$ 242.401
Isol. from some plants, e.g. bark of *Zanthoxylum carolinianum*. Occurs in lichens. Present in lipids of *Physalia physalis* (Portuguese-man-of-war). Cryst. (Me_2CO aq.).
Mp 53°. Bp_{100} 257° $Bp_{0.05}$ 138-139°.
▶ LD_{50} (mus, ivn) 54 mg/kg. RZ1925000
Me ester: [7132-64-1]
$C_{16}H_{32}O_2$ 256.428
Cryst. (EtOH aq.). Mp 18.5°.
Et ester: [41114-00-5]
$C_{17}H_{34}O_2$ 270.454
Cryst. (EtOH aq.). Mp 14°.
Amide: [3843-51-4]
$C_{15}H_{31}NO$ 241.416
Cryst. (EtOH aq.). Mp 103-104°.
Nitrile: Pentadecanenitrile. 1-Cyanotetradecane
[18300-91-9]
$C_{15}H_{29}N$ 223.401
Oil or solid. Mp 20-24°. Bp_{23} 181-185°. n_D^{25} 1.4413.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 484D; 609A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 756A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 577A; 629C (*ir*)
Majima, R. *et al., Ber.*, 1913, **46**, 4089 (*nitrile*)
Wynberg, H. *et al., J.A.C.S.*, 1956, **78**, 1958 (*synth*)
Corey, E.J. *et al., J.A.C.S.*, 1968, **90**, 5615 (*synth*)
Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*Physalia physalis constit*)
Boivin, J. *et al., Tetrahedron*, 1995, **51**, 2573 (*nitrile*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PAZ000

2-Pentadecanone, 9CI P-185

FEMA 3724
[2345-28-0]
$H_3C(CH_2)_{12}COCH_3$
$C_{15}H_{30}O$ 226.401
Isol. from hop (*Humulus lupulus*), coconut (*Cocos nucifera*) and other oils and fruits. Constit. of male mandibular gland secretions of the Hymenoptera *Philanthus basilaris* and *Philanthus bicinctus*. Prod. by a marine bacterium and the marine sponge *Spheciospongia vagunda*. Flavouring ingredient.
Mp 39°. Bp 294° $Bp_{0.7}$ 104-106°.
Oxime:
$C_{15}H_{31}NO$ 241.416
Mp 63-65°.
Semicarbazone: Mp 124-125°.
Krafft, F. *et al., Ber.*, 1879, **12**, 1668
Baumgarten, P. *et al., Ber.*, 1943, **76**, 213
Weichet, J. *et al., Chem. Listy*, 1957, **51**, 127-132 (*synth*)
Rieche, A. *et al., Z. Chem.*, 1964, **4**, 177-180 (*synth*)
Czech. Pat., 1969, 131 766; *CA*, **72**, 132025
McDaniel, C.A. *et al., J. Chem. Ecol.*, 1987, **13**, 227-235 (*Philanthus constit*)
Xiao, D. *et al., Fenxi Huaxue*, 2004, **32**, 1621-1623; *CA*, **143**, 23210 (*Spheciospongia vagabunda constit*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*marine bacterium constit*)

1,3,6,9,12-Pentadecapentaen-14-yne P-186

$H_2C{=}CHCH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHC{\equiv}CH$
$C_{15}H_{18}$ 198.307

(3*E*,6*Z*,9*Z*,12*E*)-*form* [148084-31-5]
Constit. of the red alga *Laurencia majuscula*.
Oil.
Wright, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 394

3,6,9,12-Pentadecatetraen-1-yne P-187

Laurencenyne
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHC{\equiv}CH$
$C_{15}H_{20}$ 200.323

(*all-Z*)-*form* [81371-19-9]
Metab. of *Laurencia okamurai*.
Liq.

(3*E*,6*Z*,9*Z*,12*Z*)-*form*
trans-*Laurencenyne*
[81066-46-8]
Isol. from *Laurencia okamurai*. Possible precursor of a wide range of C_{15}-halogenated cyclic ethers found in marine red algae. Liq.

(3*E*,6*Z*,9*Z*,12*E*)-*form* [148152-79-8]
Isol. from *Laurencia majuscula*.
Oil.
Kigoshi, H. *et al., Tetrahedron*, 1986, **47**, 3781 (*struct, synth, bibl*)
Wright, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 394 (*isol, pmr, cmr*)

3,6,9-Pentadecatrien-1-yne P-188

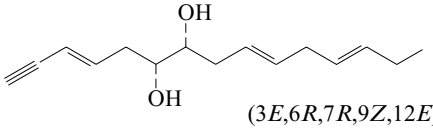
$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CHCH_2CH{=}CHC{\equiv}CH$
$C_{15}H_{22}$ 202.339

(all-*Z*)-*form*
Neolaurencenyne
[81344-95-8]
Isol. from *Laurencia okamurai*.

(3*E*,6*Z*,9*Z*)-*form*
trans-*Neolaurencenyne*
Constit. of *Laurencia okamurai*. Possible precursor of a wide range of C_{15}-halogenated cyclic ethers found in marine red algae.
Liq.
Kigoshi, H. *et al., Tetrahedron*, 1986, **42**, 3781 (*struct, synth, bibl*)

3,9,12-Pentadecatrien-1-yne-6,7-diol P-189

Laurediol



(3*E*,6*R*,7*R*,9*Z*,12*E*)–*form*

$C_{15}H_{22}O_2$ 234.338

(3*E*,6*R*,7*R*,9*Z*,12*E*)-*form* [37866-22-1]
Constit. of *Laurencia nipponica* (Yamada oil).
Unstable cryst.
Mp 26-28°. $[\alpha]_D$ +27.2.

(3*Z*,6*S*,7*S*,9*Z*,12*E*)-*form* [37866-25-4]
Constit. of *Laurencia nipponica*.
Unstable oil. $[\alpha]_D$ -19.6.
Kurosawa, E. *et al., Tet. Lett.*, 1972, 2121 (*synth*)
Fukuzawa, A. *et al., Phytochemistry*, 1993, **32**, 1435 (*isol, pmr*)
Martin, T. *et al., Tet. Lett.*, 2000, **41**, 2503-2505 (*synth*)

3-Pentadecene-5,7-diyn-2-one P-190

$H_3C(CH_2)_6C{\equiv}CC{\equiv}CCH{=}CHCOCH_3$
$C_{15}H_{20}O$ 216.322

(*E*)-*form*
Montiporyne A
Isol. from the stony coral *Montipora* sp. Cytotoxic agent. Yellow gum. λ_{max} 209 (log ϵ 4.4); 218 (log ϵ 4.4); 227 (log ϵ 4.4); 294 (log ϵ 4.2); 309 (log ϵ 3.2) (EtOH).
14,15-Didehydro: 3,14-Pentadecadiene-5,7-diyn-2-one. ***Montiporyne L***
$C_{15}H_{18}O$ 214.307
Isol. from *Montipora* sp. Cytotoxic. Light yellow oil.

(*Z*)-*form*
Montiporyne B
Isol. from the stony coral *Montipora* sp.
Yellow gum.
14,15-Didehydro: ***Montiporyne M***
Isol. from *Montipora* sp. Cytotoxic. Light yellow oil.
Bae, B.H. *et al., J. Nat. Prod.*, 2000, **63**, 1511-1514; 2001, **64**, 1059-1063 (*isol*)
Speed, T.J. *et al., Tet. Lett.*, 2002, **43**, 367-369 (*synth*)
Fiandanese, V. *et al., Tetrahedron*, 2006, **62**, 5126-5132 (*synth*)

4-Pentadecenoic acid P-191

[66086-78-0]
[26444-04-2]
$H_3C(CH_2)_9CH{=}CHCH_2CH_2COOH$
$C_{15}H_{28}O_2$ 240.385

(*Z*)-*form* [64252-91-1]
[29255-62-7]
Isol. from various sponge spp. and the seed oil of *Hydnocarpus anthelmintica*. $Bp_{0.04}$ 131-135°.
Ger. Pat., 1979, 2 758 882; *CA*, **92**, 6394c (*synth*)
Christie, W.W. *et al., Lipids*, 1989, **24**, 116-120 (*isol*)
Keinan, E. *et al., Tet. Lett.*, 1992, **33**, 6411-6414 (*ester, synth*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1994, **57**, 1152-1159 (*isol*)

5-Pentadecenoic acid P-192

$H_3C(CH_2)_8CH{=}CH(CH_2)_3COOH$
$C_{15}H_{28}O_2$ 240.385

(*E*)-*form* [69861-66-1]
Constit. of *Brassica campestris*.

(*Z*)-*form* [69861-65-0]
Constit. of *Brassica campestris*. Also isol. from various marine sponges.
Sebedio, J.L. *et al., J. Am. Oil Chem. Soc.*, 1979, **56**, 15-21 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*isol*)

6-Pentadecenoic acid P-193

[89747-95-5]
[26444-04-2, 26764-41-0, 29255-62-7]
$H_3C(CH_2)_7CH{=}CH(CH_2)_4COOH$
$C_{15}H_{28}O_2$ 240.385

(*Z*)-*form* [45210-00-2]
Constit. of various marine sponges. Also from the seed oil of *Microula sikkimensis*.
Scholz, D. *et al., Annalen*, 1984, 264-272 (*synth, ir, pmr*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*isol*)

8-Pentadecen-2-one P-194

$H_3C(CH_2)_5CH{=}CH(CH_2)_5COCH_3$
$C_{15}H_{28}O$ 224.386

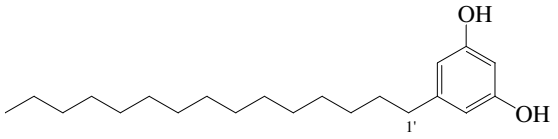
(*Z*)-*form* [76963-26-3]
Constit. of the root oil of *Echinacea* spp. Prod. by a marine bacterium. Component of the defence secretion of the termite *Acorhinotermes subfusciceps*.
Oil.
Prestwich, G.D. *et al., J.O.C.*, 1981, **46**, 2383-2385 (*synth, pmr, cmr*)
Prestwich, G.D. *et al., J. Chem. Ecol.*, 1982, **8**, 147-161 (*isol*)
Heinzer, F. *et al., Pharm. Acta Helv.*, 1988, **63**, 132-136 (*isol*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol, synth, pmr, cmr, ms*)

Pentadecylbenzene, 9CI P-195

1-Phenylpentadecane
[2131-18-2]
$Ph(CH_2)_{14}CH_3$
$C_{21}H_{36}$ 288.515
Rather poorly documented. Constit. of the mussel (*Mytilus galloprovincialis*).
U.K. Pat., 1961, 884 700; *CA*, **57**, 4591b (*synth*)
Mironov, O.G. *et al., CA*, 1991, **114**, 161123 (*isol*)

5-Pentadecyl-1,3-benzenediol, 9CI P-196

5-Pentadecylresorcinol. ***Adipostatin A***
[3158-56-3]



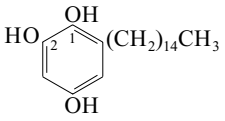
$C_{21}H_{36}O_2$ 320.514
Constit. of several Proteaceae spp. Prod. by *Streptomyces cyaneus*. Isol. from cereals and other plants. Inhibitor of glycerol 3-phosphate dehydrogenase, shows cytotoxic and antifungal props. Cryst. (petrol or C_6H_6).
Mp 95.5-96° (91-92°). λ_{max} 221 (sh) (ϵ 7000); 272 (ϵ 1590); 278 (ϵ 1570) (MeOH) (Derep).

4′,5′Z-Didehydro: 5-(4-Pentadecenyl)-1,3-benzenediol
[138168-56-6]
$C_{21}H_{34}O_2$ 318.498
Constit. of the sponge *Haliclona* sp.

6′,7′-Didehydro: 5-(6-Pentadecenyl)-1,3-benzenediol
[138168-57-7]
$C_{21}H_{34}O_2$ 318.498
Constit. of *Haliclona* sp.

Barrow, R.A. *et al., Aust. J. Chem.*, 1991, **44**, 1393 (*4′,5′-didehydro, 6′,7′-didehydro*)

6-Pentadecyl-1,2,4-benzenetriol P-197



$C_{21}H_{36}O_3$ 336.514

1-Ac: ***Ardisiphenol A***
$C_{23}H_{38}O_4$ 378.551
Constit. of the fruit of *Ardisia colorata*. Cytotoxic. Oil. Darkens in air. λ_{max} 224 (log ϵ 3.85); 279 (log ϵ 3.44) (MeOH).

1,2-Di-Me ether: 3,4-Dimethoxy-5-pentadecylphenol
[144089-13-4]
$C_{23}H_{40}O_3$ 364.567
Constit. of *Iris* spp.

2,4-Di-Me ether: 2,4-Dimethoxy-6-pentadecylphenol. ***Hierridin B***
$C_{23}H_{40}O_3$ 364.567
Prod. by the marine cyanobacterium *Phormidium ectocarpi*. Antiplasmodial agent. λ_{max} 222; 254; 263; 274 (MeOH) (Berdy).

8′,9′-Didehydro(Z-), 1-Ac: ***Ardisiphenol B***
$C_{23}H_{36}O_4$ 376.535
Constit. of the fruit of *Ardisia colorata*. Cytotoxic. Oil. Darkens in air. λ_{max} 224 (log ϵ 3.85); 279 (log ϵ 3.39) (MeOH).

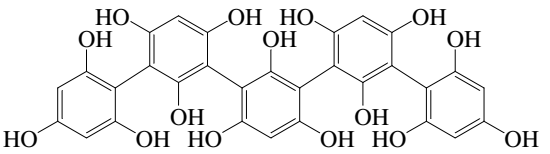
10′,11′-Didehydro(Z-), 2,4-di-Me ether: 2,4-Dimethoxy-6-(10-pentadecenyl)phenol. ***Belamcandol A***. *Belamcandaphenol*
[137786-93-7]
$C_{23}H_{38}O_3$ 362.551
Constit. of *Belamcanda chinensis*. Oil.

2′-Acetoxy, 2-Me ether, O^4*-Ac: 2-[2-(Acetyloxy)pentadecyl]-6-methoxy-1,4-benzenediol 4-acetate, 9CI*. ***Ardisianol***
[66398-67-2]
$C_{26}H_{42}O_6$ 450.614
Constit. of *Ardisia quinquegona*. Needles (hexane).
Mp 82-84°.

Kusami, T. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 943 (*Ardisianol*)
Fukujama, Y. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1877; 1993, **41**, 561 (*Belamcandol A*)
Marner, F.J. *et al., Helv. Chim. Acta*, 1992, **75**, 1557 (*1,2-di-Me ether*)
Seki, K. *et al., Phytochemistry*, 1995, **38**, 703 (*isol*)
Papendorf, O. *et al., Phytochemistry*, 1998, **49**, 2383-2386 (*Hierridin B*)
Sumino, M. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1484-1487 (*Ardisiphenols*)

Pentafucol A P-198

[123237-91-2]

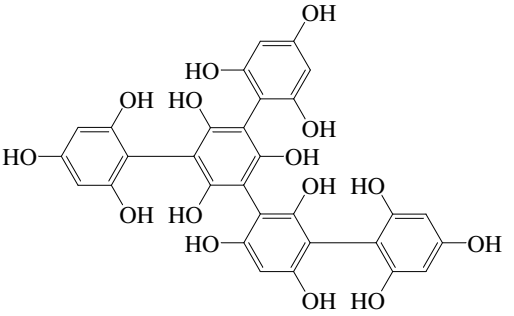


$C_{30}H_{22}O_{15}$ 622.495
Isol. from the brown algae *Scytothamnus australis* and *Analipus japonicus*. Isol. as pentadeca-Ac to which CAS no. refers.

Glombitza, K.W. *et al., Planta Med.*, 1989, **55**, 171-175 (*isol, pmr*)
Glombitza, K.W. *et al., Bot. Mar.*, 2003, **46**, 315-320 (*isol*)

Pentafucol B P-199

[642487-13-6]

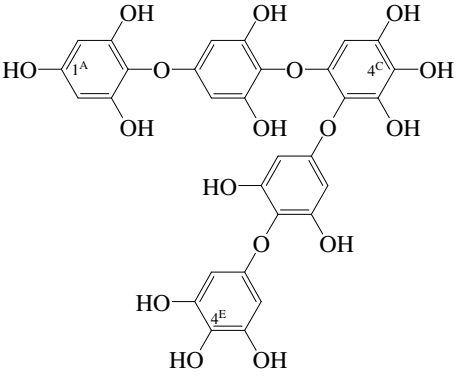


$C_{30}H_{22}O_{15}$ 622.495
Isol. from the brown alga *Scytothamnus australis*. Isol. as pentadeca-Ac to which CAS no. refers.

Glombitza, K.-W. *et al., Bot. Mar.*, 2003, **46**, 315-320 (*isol, pmr, cmr*)

Pentafuhalol A P-200

5-[2,6-Dihydroxy-4-(2,4,6-trihydroxyphenoxy)phenoxy]-4-[3,5-dihydroxy-4-(3,4,5-trihydroxyphenoxy)phenoxy]-1,2,3-benzenetriol, 9CI
[76265-29-7]



$C_{30}H_{22}O_{17}$ 654.494
Isol. from *Sargassum muticum*, *Sargassum spinuligerum* and *Carpophyllum maschalocarpum*.

4^C*-Deoxy:* ***Deshydroxypentafuhalol***. *Dehydroxypentafuhalol*
[137809-90-6]
$C_{30}H_{22}O_{16}$ 638.494
Constit. of *Carpophyllum maschalocarpum*.

4^E*-O-(3,4,5-Trihydroxyphenyl):* ***Phlorethopentafuhalol A***
[138529-06-3]
$C_{36}H_{26}O_{20}$ 778.589

Constit. of *Carpophyllum maschalocarpum*. Isol. as pentadeca-Ac.

1^A-O-*(2,4,6-Trihydroxyphenyl), 4^E*-O-*(3,4,5-trihydroxyphenyl):* ***Diphlorethopentafuhalol A***
[138529-07-4]
$C_{42}H_{30}O_{23}$ 902.685
Constit. of *Carpophyllum maschalocarpum*. Isol. as heptadeca-Ac.

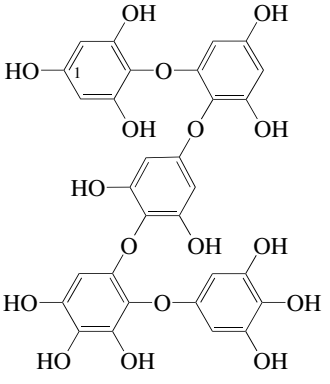
2^C-Hydroxy: ***Hydroxypentafuhalol B***
$C_{30}H_{22}O_{18}$ 670.493
Isol. from *Sargassum spinuligerum*. Care needed with nomenclature. Hydroxypentafuhalol B is a hydroxy deriv. of Pentafuhalol A, but Hydroxypentafuhalol A is not.

[61470-22-2]

Glombitza, K.W. *et al., Bot. Mar.*, 1982, **25**, 449; *CA*, **98**, 14341x
Glombitza, K.W. *et al., Phytochemistry*, 1991, **30**, 2741; 1995, **38**, 975-985; 987-995 (*isol, pmr, Hydroxypentafuhalol B*)
Li, S.-M. *et al., Phytochemistry*, 1991, **30**, 3417-3421 (*Phlorethopentafuhalol, Diphlorethopentafuhalol*)
Keusgen, M. *et al., Phytochemistry*, 1995, **38**, 975 (*isol, pmr*)

Pentafuhalol B P-201

[164176-24-3]

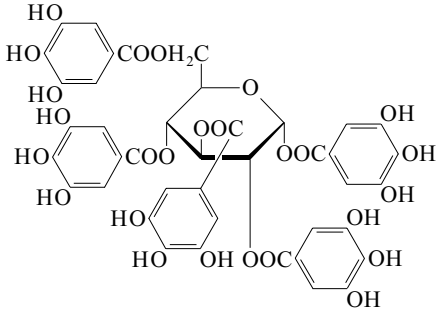


$C_{30}H_{22}O_{17}$ 654.494
Constit. of the brown alga *Sargassum spinuligerum*.

1-O-*(2,4,6-Trihydroxyphenyl):* ***Phlorethopentafuhalol B***
[138551-15-2]
$C_{36}H_{26}O_{20}$ 778.589
Constit. of *Carpophyllum maschalocarpum*. Isol. as pentadeca-Ac.

Li, S.M. *et al., Phytochemistry*, 1991, **30**, 3417-3421 (*Phlorethopentafuhalol B*)
Keusgen, M. *et al., Phytochemistry*, 1995, **38**, 975 (*isol, pmr, cmr, ms*)

1,2,3,4,6-Pentagalloylglucose P-202



α–D–Pyranose–*form*

$C_{41}H_{32}O_{26}$ 940.688
Possesses antiviral props. Log P 2.4 (calc).

β-D-Pyranose-*form* [14937-32-7]
Isol. from several *Acer* spp., *Quercus* spp., *Rhus* spp. and *Rubus* spp.
Off-white amorph. powder. $[\alpha]_D^{20}$ +20.5 (c, 1.0 in Me_2CO).

Bis(3,4,5-trihydroxybenzoyl) (1): 2,3-Di-O-*digalloyl-1,4,6-tri*-O-*galloyl-β-D-glucopyranose*
[85199-91-3]
$C_{55}H_{40}O_{34}$ 1244.901
Constit. of twig galls from *Rhus semialata* and of green alga (*Spirogyra* sp.).
$[\alpha]_D^{20}$ +24.4 (c, 1.35 in Me_2CO). Contains digalloyl residues at C-2 and C-3.

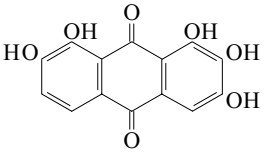
Bis(3,4,5-trihydroxybenzoyl) (2): 2,4-Di-O-*digalloyl-1,3,6-tri*-O-*galloyl-β-D-glucopyranose*
[85249-29-2]
$C_{55}H_{40}O_{34}$ 1244.901
Gallotannin from *Rhus semialata* and from green alga *Spirogyra* sp. Light brown amorph. powder. $[\alpha]_D^{20}$ +12 (c, 1.27 in Me_2CO). Contains digalloyl residues at C-2 and C-4.

Bis(3,4,5-trihydroxybenzoyl) (4): 3,4-Di-O-*digalloyl-1,2,6-tri*-O-*galloyl-β-D-glucopyranose*
[85249-28-1]
$C_{55}H_{40}O_{34}$ 1244.901
Gallotannin from *Rhus semialata* and from green alga *Spirogyra* sp. Light brown amorph. powder. $[\alpha]_D^{20}$ +36.4 (c, 1.62 in Me_2CO). Contains digalloyl residues at C-3 and C-4.

[52238-31-0, 86747-19-5, 99877-82-4, 99877-84-6, 99877-86-8, 99877-87-9]

Nishizawa, M. *et al., Phytochemistry*, 1985, **24**, 2411-2413 (*Spirogyra constits*)

1,2,3,7,8-Pentahydroxyanthraquinone P-203



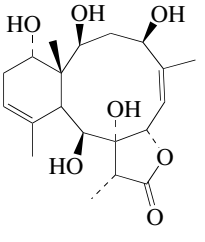
$C_{14}H_8O_7$ 288.213
Anthraquinone. Defence chemical prod. by *Tubastrea micrantha*.

2,3-Di-Me ether: 1,7,8-Trihydroxy-2,3-dimethoxyanthraquinone
$C_{16}H_{12}O_7$ 316.267
Constit. of *Cassia obtusifolia*.

2,3-Methylene, 1,8-di-Me ether: 7-Hydroxy-1,8-dimethoxy-2,3-methylenedioxyanthraquinone
[108615-35-6]
$C_{17}H_{12}O_7$ 328.278
Prod. by *Tubastrea micrantha*. Defence chemical. Mp 206°.

Sanduja, R. *et al., J. Chem. Res., Synop.*, 1986, 450-451 (*isol, struct*)
Guo, H. *et al., Phytochemistry*, 1998, **49**, 1623-1625 (*isol*)

2,4,8,9,14-Pentahydroxy-5,11-briaradien-18,7-olide P-204



$C_{20}H_{30}O_7$ 382.453

(2β,4β,5*Z*,7α,8α,9β,14α)-*form*
2,4,14-Tri-Ac: ***4-Acetoxy-9-deacetylstylatulide lactone***
[182482-67-3]
$C_{26}H_{36}O_{10}$ 508.564
Constit. of a *Briareum* sp. Cryst. Mp 216-217°. $[\alpha]_D^{26}$ +44 (c, 0.12 in $CHCl_3$).

2,4,9,14-Tetra-Ac: ***Milolide M***
[438552-16-0]
$C_{28}H_{38}O_{11}$ 550.602
Constit. of *Briareum stechei*. $[\alpha]_D^{23}$ +31.1 (c, 0.47 in CH_2Cl_2).

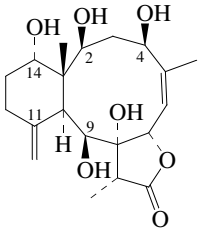
4-Butanoyl, 2,9,14-tri-Ac: ***Milolide N***
[438552-19-3]
$C_{30}H_{42}O_{11}$ 578.655
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ +61.7 (c, 0.6 in CH_2Cl_2).

4-(3-Acetoxybutanoyl), 2,9,14-tri-Ac: ***Erythrolide M***
[410096-43-4]
$C_{32}H_{44}O_{13}$ 636.692
Constit. of *Erythropodium caribaeorum*. Gum. $[\alpha]_D^{25}$ +55 (c, 0.4 in $CHCl_3$).

11β,12β-Epoxide, 2,4,9,14-tetra-Ac: ***Milolide A***
[352335-80-9]
$C_{28}H_{38}O_{12}$ 566.601
Constit. of *Briareum stechei*. $[\alpha]_D^{23}$ +47.7 (c, 0.65 in CH_2Cl_2).

Sheu, J.-H. *et al., J. Nat. Prod.*, 1996, **59**, 935 (*Acetoxydeactylstylatulide lactone*)
Kwak, J.H. *et al., J. Nat. Prod.*, 2001, **64**, 754-760; 2002, **65**, 704-708 (*Milolides*)
Banjoo, D. *et al., J. Nat. Prod.*, 2002, **65**, 314-318 (*Erythrolide M*)

2,4,8,9,14-Pentahydroxy-5,11(20)-briaradien-18,7-olide P-205



$C_{20}H_{30}O_7$ 382.453

2,9,14-Tri-Ac: ***4-Deacetyljunceellolide D***
[221056-37-7]
$C_{26}H_{36}O_{10}$ 508.564
Constit. of *Junceella fragilis*. Powder. $[\alpha]_D^{22}$ -54.1 (c, 0.3 in CH_2Cl_2).

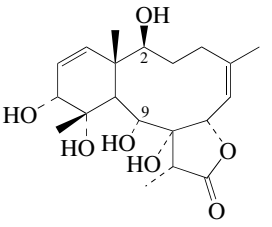
2,4,9,14-Tetra-Ac: ***Junceellolide D***
[121798-81-0]
$C_{28}H_{38}O_{11}$ 550.602
Constit. of *Junceella fragilis*. Antiinflammatory agent. Inhibits phospholipase A and phospholipase A_2. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 208-209°. $[\alpha]_D$ -7.7 (c, 2.5 in $CHCl_3$).

11α,20-Epoxide,2,9,14-tri-Ac: ***11,20-Epoxy-4-deacetyljunceellolide D***
[221056-47-9]
$C_{26}H_{36}O_{11}$ 524.564
Constit. of *Junceella fragilis*. Powder. $[\alpha]_D^{22}$ -12.6 (c, 0.15 in CH_2Cl_2).

11α,20-Epoxide, 2,4,9,14-tetra-Ac: ***11,20-Epoxyjunceelloloide D***
[221056-42-4]
$C_{28}H_{38}O_{12}$ 566.601
Constit. of *Junceella fragilis*. Powder. $[\alpha]_D^{22}$ +5.3 (c, 0.4 in CH_2Cl_2).

Shin, J. *et al., Tetrahedron*, 1989, **45**, 1633-1638 (*Junceellolide D*)
García, M. *et al., J. Nat. Prod.*, 1999, **62**, 257-260 (*tri-Ac, epoxides*)

2,8,9,11,12-Pentahydroxy-5,13-briaradien-18,7-olide P-206



$C_{20}H_{30}O_7$ 382.453

2,9-Di-Ac: ***Minabein 7***
[104993-13-7]
$C_{24}H_{34}O_9$ 466.527
Constit. of *Minabea* sp. Cryst. ($CHCl_3$).
Mp 278-280°.

2,9,12-Tri-Ac: ***Minabein 6***
[104993-12-6]
$C_{26}H_{36}O_{10}$ 508.564
Constit. of *Minabea* sp. Powder.
Mp 259-262°. $[\alpha]_D$ -204 (c, 1.2 in $CHCl_3$).

12-Ketone, 2,9-di-Ac: ***Renillafoulin A***. *Minabein 8*
[104715-93-7]
$C_{24}H_{32}O_9$ 464.511
Isol. from *Minabea* sp. and *Renilla reniformis*. Antifouling agent. Cryst. (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 203 (ϵ 15300); 220 (ϵ 9500) (MeOH) (Berdy).

12-Ketone, 2-propanoyl, 9-Ac: ***Renillafoulin B***
[104715-94-8]
$C_{25}H_{34}O_9$ 478.538
Isol. from *Renilla reniformis*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 204 (ϵ 12600); 219 (ϵ 9400) (MeOH) (Berdy).

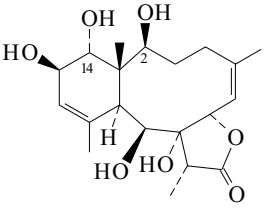
12-Ketone, 9-propanoyl, 2-Ac: [120893-76-7]
$C_{25}H_{34}O_9$ 478.538
Isol. from a coelenterate.

12-Ketone, 2-butanoyl, 9-Ac: ***Renillafoulin C***
[104715-95-9]
$C_{26}H_{36}O_9$ 492.565
Isol. from *Renilla reniformis*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 202 (ϵ 13000); 220 (ϵ 7300) (MeOH) (Berdy).

12-Ketone, 9-butanoyl, 2-Ac: [120909-04-8]
$C_{26}H_{36}O_9$ 492.565
Isol. from a coelenterate.

Ksebati, M.B. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 835-851 (*isol, pmr, cmr*)
Kiefer, P.A. *et al., J.O.C.*, 1986, **51**, 4450 (*isol, cryst struct, uv, cmr*)
U.S. Pat., 1988, 4 788 302; *CA*, **111**, 2684k

2,8,9,13,14-Pentahydroxy-5,11-briaradien-18-7-olide P-207



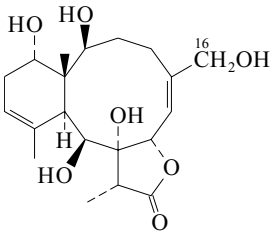
$C_{20}H_{30}O_7$ 382.453

2-Hexanoyl, 13,14-di-Ac: ***Cavernulin***
[90052-73-6]
$C_{30}H_{44}O_{10}$ 564.672
Isol. from the sea pen *Cavernulina grandiflora*. Cryst. (Me_2CO/hexane).
Mp 251-253°. $[\alpha]_D$ -19.6 (c, 0.52 in $CHCl_3$).

2-Hexanoyl, 14-propanoyl, 13-Ac: **O-*Deacetylpropionylcavernulin***
[90052-70-3]
$C_{31}H_{46}O_{10}$ 578.698
Isol. from *Cavernulina grandiflora*. Cryst. (Me_2CO/hexane).
Mp 262-264°. $[\alpha]_D$ -24 (c, 0.5 in $CHCl_3$).

13,14-Dibutanoyl, 2-propanoyl: ***Cavernulinin***
[90052-74-7]
$C_{31}H_{46}O_{10}$ 578.698
Isol. from *Cavernulina grandiflora*. Cryst. (Me_2CO/hexane).
Mp 275-277°. $[\alpha]_D$ -24.3 (c, 0.3 in $CHCl_3$).
Clastres, A. *et al., J. Nat. Prod.*, 1984, **47**, 162 (*isol, pmr, cmr*)

2,8,9,14,16-Pentahydroxy-5,11-briaradien-18,7-olide P-208



$C_{20}H_{30}O_7$ 382.453

(2β,5*E*,7α,8α,9β,14α)-*form*

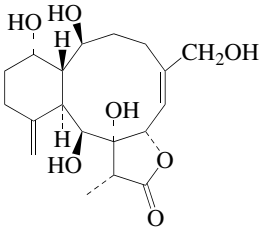
2,9,14-Tri-Ac: ***Stylatula lactone B***. Stylatula *Lactone B*
[74269-52-6]
$C_{26}H_{36}O_{10}$ 508.564
Isol. from *Stylatula* spp. Oil. $[\alpha]_D^{20}$ -13 (c, 1 in $CHCl_3$).

2,14,16-Tri-Ac: ***Milolide K***
[438552-14-8]
$C_{26}H_{36}O_{10}$ 508.564
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ -20.7 (c, 0.59 in CH_2Cl_2).

16-Carboxylic acid, 2,9,14-tri-Ac, Me ester: ***Stylatula lactone C***. Stylatula *Lactone C*
[74269-40-2]
$C_{27}H_{36}O_{11}$ 536.575
Isol. from *Stylatula* spp. Oil. $[\alpha]_D^{20}$ -31 (c, 1 in $CHCl_3$).

11β,12β-Epoxide, 2,14,16-tri-Ac: ***16-Acetoxymilolide B***
[352273-96-2]
$C_{26}H_{36}O_{11}$ 524.564
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ -0.8 (c, 0.38 in CH_2Cl_2).
Wratten, S.J. *et al., Tetrahedron*, 1979, **35**, 1907 (*Stylatula lactones*)
Kwak, J.H. *et al., J. Nat. Prod.*, 2001, **64**, 754-760 (*16-Acetoxymilolide B*)
Kwak, J.H. *et al., J. Nat. Prod.*, 2002, **65**, 704-708 (*Milolide K*)

2,8,9,14,16-Pentahydroxy-5,11(20)-briaradien-18,7-olide P-209

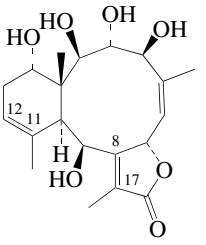


$C_{20}H_{30}O_7$ 382.453

(2β,5*E*,7α,8α,9β,14α,17α)-*form*

2,9,14,16-Tetra-Ac: ***Junceellonoid B***
[804557-38-8]
$C_{28}H_{38}O_{11}$ 550.602
Constit. of *Junceella fragilis*. Cryst.
Mp 135-136° dec. $[\alpha]_D^{20}$ -29 (c, 0.13 in $CHCl_3$).
Zhang, W. *et al., Helv. Chim. Acta*, 2004, **87**, 2341-2345 (*Junceellonoid B*)

2,3,4,9,14-Pentahydroxy-5,8(17),11-briaratrien-18,7-olide P-210



$C_{20}H_{28}O_7$ 380.437

(2β,3α,4β,5Z,7α,9β,14α)-*form*

8,17-Epoxide: 8,17-Epoxy-2,3,4,9,14-pentahydroxy-5,11-briaradien-18,7-olide

8α,17α-Epoxide, 2,4,9,14-tetra-Ac: ***Briarlide P***
[845641-26-1]
$C_{28}H_{36}O_{12}$ 564.585
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +49 (c, 0.39 in MeOH).

8α,17α-Epoxide, penta-Ac: ***Excavatolide O***
[247158-34-5]
$C_{30}H_{38}O_{13}$ 606.622
Constit. of *Briareum excavatum*. Cryst. (EtOH aq.).
Mp 193-195°. $[\alpha]_D$ -102 (c, 0.05 in $CHCl_3$).

8α,17α-Epoxide, 4-octanoyl, 2,9,14-tri-Ac: ***Briarlide O***
[845641-25-0]
$C_{34}H_{48}O_{12}$ 648.746
Constit. of a *Briareum* sp. Amorph. solid. $[\alpha]_D$ -106 (c, 0.12 in MeOH).

8α,17α-Epoxide, 4-octanoyl, 3,9,14-tri-Ac: ***Briarlide Q***
[845641-27-2]
$C_{34}H_{48}O_{12}$ 648.746
Constit. of a *Briareum* sp. Amorph. solid. $[\alpha]_D$ -50 (c, 0.08 in MeOH).

11,12-Epoxide: 11,12-Epoxy-2,3,4,9,14-pentahydroxy-5,8(17)-briaradien-18,7-olide

11β,12β-Epoxide, 4-octanoyl, 2,9,14-tri-Ac: ***Briviolide F***
[868526-13-0]
$C_{34}H_{48}O_{12}$ 648.746
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +104 (c, 0.1 in MeOH). λ_{max} 213 (ϵ 10700) (MeOH).

8,17:11,12-Diepoxide: 8,17:11,12-Diepoxy-2,3,4,9,14-pentahydroxy-5-briaren-18,7-olide

8α,17α:11β,12β-Diepoxide, penta-Ac: ***Excavatolide R***
[247158-43-6]
$C_{30}H_{38}O_{14}$ 622.622
Constit. of *Briareum excavatum*. Cryst.
Mp 183-186°. $[\alpha]_D$ +34 (c, 0.05 in $CHCl_3$).

(2β,3β,4α,5*Z*,7α,9β,14α)-*form*

8α,17α-Epoxide, penta-Ac: ***Briaranolide A***
[866087-85-6]
$C_{30}H_{38}O_{13}$ 606.622
Constit. of a *Briareum* sp. Powder.
Mp 230-233°. $[\alpha]_D^{27}$ +41.2 (c, 1 in $CHCl_3$).

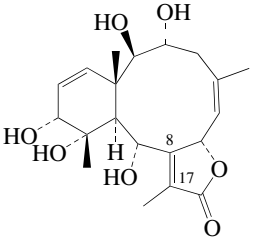
8α,17α-Epoxide, 4-butanoyl, 2,9,14-tri-Ac: ***Briaranolide D***
[866087-88-9]
$C_{30}H_{40}O_{12}$ 592.639
Constit. of a *Briareum* sp. Amorph. solid. $[\alpha]_D^{23}$ +53 (c, 1 in $CHCl_3$).

8α,17α-Epoxide, 4-butanoyl, 2,3,9,14-tetra-Ac: ***Briaranolide B***
[866087-86-7]
$C_{32}H_{42}O_{13}$ 634.676
Constit. of a *Briareum* sp. Cryst.
Mp 224-228°. $[\alpha]_D^{24}$ +50.4 (c, 0.4 in $CHCl_3$).

8α,17α-Epoxide, 3,4-dibutanoyl, 2,9,14-tri-Ac: ***Briaranolide C***
[866087-87-8]
$C_{34}H_{46}O_{13}$ 662.73
Constit. of a *Briareum* sp. Cryst.
Mp 149-152°. $[\alpha]_D^{25}$ +44.3 (c, 1.1 in $CHCl_3$).

Neve, J.E. *et al., Aust. J. Chem.*, 1999, **52**, 359-366 (*Excavatolides O,R*)
Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 2083-2093 (*Briviolide F*)
Iwagawa, T. *et al., J. Nat. Prod.*, 2005, **68**, 31-35 (*Briarlides O,P,Q*)
Hoshino, A. *et al., J. Nat. Prod.*, 2005, **68**, 1328-1335 (*Briaranolides A-D*)

2,3,9,11,12-Pentahydroxy-5,8(17),13-briaratrien-18,7-olide P-211



$C_{20}H_{28}O_7$ 380.437

(2β,3α,5*Z*,7α,9α,11α,12α)-*form*

8α,17α-Epoxide: 8,17-Epoxy-2,3,9,11,12-pentahydroxy-5,13-briaradien-18,7-olide

8α,17α-Epoxide, 3,9-di-Ac: ***Briarlide H***
[610311-51-8]
$C_{24}H_{32}O_{10}$ 480.511
Constit. of a *Briareum* sp. Amorph. $[\alpha]_D$ -106.4 (c, 0.14 in MeOH).

8α,17α-Epoxide, 2,3,9-tri-Ac: ***Violide G***
[243972-86-3]
$C_{26}H_{34}O_{11}$ 522.548
Constit. of a *Briareum* sp. Cryst. (C_6H_6/hexane).
Mp 131-133°. $[\alpha]_D$ -10 (c, 0.58 in MeOH). λ_{max} 205 (ϵ 6800) (MeOH).

8α,17α-Epoxide, 2,3,9,12-tetra-Ac: ***Tubiporein***. *Briarlide G*
[126784-38-1]
[610311-50-7]
$C_{28}H_{36}O_{12}$ 564.585
Constit. of soft coral *Tubipora* sp. and of a *Briareum* sp.
Cytotoxic. Needles (MeOH). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 71-71.5°. $[\alpha]_D^{27.5}$ -36.6 (c, 1.0 in $CHCl_3$). $[\alpha]_D$ -73 (c, 0.2 in MeOH).

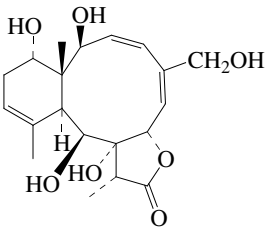
(2β,3α,5*Z*,7α,9β,11α,12α)-*form*

2,3,9-Tri-Ac: ***Briviolide D***
[868526-11-8]
$C_{26}H_{34}O_{10}$ 506.549
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +9.4 (c, 0.12 in MeOH). λ_{max} 213 (ϵ 10400) (MeOH).

2,3,9,12-Tetra-Ac: ***12-O-Acetylbriviolide D***
[868281-72-5]
$C_{28}H_{36}O_{11}$ 548.586
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ -21 (c, 0.06 in MeOH). λ_{max} 215 (ϵ 8900) (MeOH).

Natori, T. *et al., Tet. Lett.*, 1990, **31**, 689-690 (*Tubiporein*)
Iwagawa, T. *et al., Heterocycles*, 1999, **51**, 1653-1659 (*Violide G*)
Iwagawa, T. *et al., J. Nat. Prod.*, 2003, **66**, 1412-1415 (*Briarlides*)
Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 2083-2093 (*Briviolide D, 12-Acetylbriviolide D*)

2,8,9,14,16-Pentahydroxy-3,5,11-briaratrien-18,7-olide P-212



$C_{20}H_{28}O_7$ 380.437

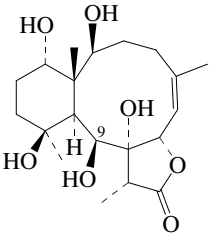
(2β,3*Z*,5*E*,7α,8α,9β,14α)-*form*

2,9,14-Tri-Ac: ***Pachyclavulide B***
[877669-13-1]
$C_{26}H_{34}O_{10}$ 506.549
Constit. of *Pachyclavularia violacea*. Amorph. solid. $[\alpha]_D^{25}$ -2.9 (c, 0.27 in $CHCl_3$).

2,9,14,16-Tetra-Ac: ***Pachyclavulide C***
[877669-15-3]
$C_{28}H_{36}O_{11}$ 548.586
Constit. of *Pachyclavularia violacea*. Amorph. solid. $[\alpha]_D^{25}$ -19.8 (c, 0.81 in $CHCl_3$).

Iwasaki, J. *et al., J. Nat. Prod.*, 2006, **69**, 2-6

2,8,9,11,14-Pentahydroxy-5-briaren-18,7-olide P-213



$C_{20}H_{32}O_7$ 384.469

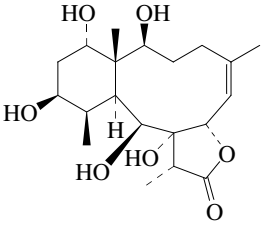
(2β,7α,8α,9β,11β,14α)-*form*

9-Ac: ***Junceellolide G***
[303963-53-3]
$C_{22}H_{34}O_8$ 426.506
Constit. of *Junceella fragilis.* Powder.
Mp 128-130°. $[\alpha]_D^{26}$ -71 (c, 0.2 in $CHCl_3$).

2,9-Di-Ac: ***Junceellolide I***
[848415-37-2]
$C_{24}H_{36}O_9$ 468.543
Constit. of *Junceella fragilis.* Powder.
Mp 210-212°. $[\alpha]_D^{25}$ -77 (c, 0.7 in $CHCl_3$).

Sung, P.-J. *et al., J. Nat. Prod.*, 2000, **63**, 1483-1487 (*Junceellolide G*)
Sung, P.-J. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1504-1506 (*Junceellolide I*)

2,8,9,12,14-Pentahydroxy-5-briaren-18,7-olide P-214

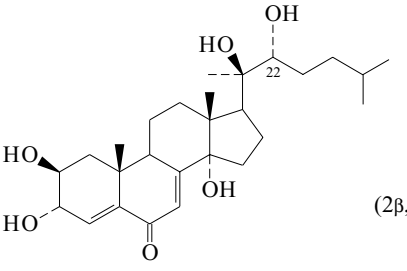


$C_{20}H_{32}O_7$ 384.469

(2β,5*Z*,7α,8α,9β,11β,12β,14α,17α)-*form*

2,9,14-Tri-Ac: ***Pachyclavulide A***
[877669-12-0]
$C_{26}H_{38}O_{10}$ 510.58
Constit. of *Pachyclavularia violacea*. Amorph. solid. $[\alpha]_D^{25}$ -4.7 (c, 0.58 in $CHCl_3$).
Iwasaki, J. *et al., J. Nat. Prod.*, 2006, **69**, 2-6 (*Pachyclavulide A, cryst struct*)

2,3,14,20,22-Pentahydroxycholesta-4,7-dien-6-one P-215



(2β,3α,20*R*,22*R*)–*form*

$C_{27}H_{42}O_6$ 462.625

(2β,3α,20*R*,22*R*)-*form*
14-Hydroxypinnasterol
[104406-80-6]
Constit. of *Laurencia pinnata*.
Cryst. (MeOH aq.).
Mp 210-212°. $[\alpha]_D^{22}$ +39 (c, 0.35 in MeOH). λ_{max} 256 (log ε 3.88) (EtOH).

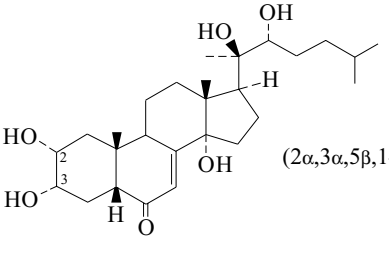
2-Ac: ***14-Hydroxyacetylpinnasterol***
[104387-07-7]
$C_{29}H_{44}O_7$ 504.662
From *Laurencia pinnata*. Cryst. ($CHCl_3/Et_2O$).
Mp 174-176°. $[\alpha]_D$ +91 (c, 0.55 in MeOH). λ_{max} 257 (log ε 3.99) (EtOH).

3-Ac: ***3*-O-*Acetyl-14-hydroxypinnasterol***
[104387-08-8]
$C_{29}H_{44}O_7$ 504.662
From *Laurencia pinnata*. Oil. $[\alpha]_D^{20}$ +92 (c, 0.5 in $CHCl_3$). λ_{max} 255 (log ε 4) (EtOH).

(2β,3α,14α,20*R*,22*S*)-*form*

2-Ac: ***22-Epi-14-hydroxyacetylpinnasterol***
[104418-60-2]
$C_{29}H_{44}O_7$ 504.662
From *Laurencia pinnata*. Cryst. (Me_2CO/hexane).
Mp 144-145°. $[\alpha]_D^{20}$ +65 (c, 0.23 in MeOH). λ_{max} 253 (log ε 3.93) (EtOH).
Fukuzawa, A. *et al., Phytochemistry*, 1986, **25**, 1305-1307 (*isol, pmr*)

2,3,14,20,22-Pentahydroxycholest-7-en-6-one P-216



(2α,3α,5β,14α,20*R*,22*R*)–*form*

$C_{27}H_{44}O_6$ 464.641

(2α,3α,5β,14α,20*R*,22*R*)-*form*
Ponasterone B
[19338-77-3]
From *Podocarpus nakaii*. Shows strong insect-moulting activity.
Noncryst.

2,3,22-Tri-Ac:
Cryst. Mp 128-130°.

(2β,3β,5β,14α,20*R*,22*R*)-*form*
Ponasterone A
[13408-56-5]
Isol. from leaves of *Podocarpus nakaii*. Also found in various ferns such as *Woodwardia orientalis*. Insect moulting hormone. Cryst. (EtOH).
Mp 259-260° dec. $[\alpha]_D^{15}$ +90 (MeOH). λ_{max} 244 (ε 12400); 326 (ε 130) (MeOH) (Berdy).

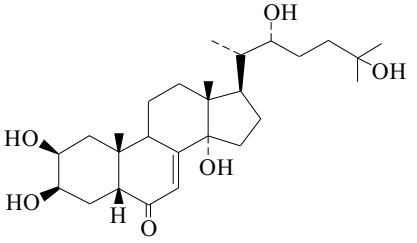
3-O-β-D-Xylopyranoside: ***Limnantheoside B***
$C_{32}H_{52}O_{10}$ 596.757
Constit. of *Limnanthes douglasii*. Gum. λ_{max} 242 (log ε 4) (no solvent reported).

3-O-β-D-Glucopyranoside: ***Ponasteroside A***. *Warabisterone*
[20117-33-3]
$C_{33}H_{54}O_{11}$ 626.783
Isol. from *Pteridium aquilinum* (bracken fern). Insect moulting hormone. Cryst.
Mp 278-279.5°. $[\alpha]_D$ +28.5 (Py).

22-O-(Hydroxyacetyl): ***22-O-Hydroxyacetylponasterone A***
[264189-83-5]
$C_{29}H_{46}O_8$ 522.678
Isol. from the sponge *Iotrochota birotulata*. Solid. λ_{max} 242 (ε 4200) (MeOH).

Hüppi, G. *et al., Tet. Lett.*, 1968, 1113 (*synth*)
Nakanishi, K. *et al., Bull. Soc. Chim. Fr.*, 1969, 3475
Hikino, H. *et al., Phytochemistry*, 1970, **9**, 367 (*biosynth*)
Koreeda, M. *et al., J.A.C.S.*, 1971, **93**, 4085 (*abs config*)
Takemoto, T. *et al., Chem. Pharm. Bull.*, 1973, **21**, 2336 (*isol*)
Hikino, H. *et al., Chem. Pharm. Bull.*, 1975, **23**, 125 (*cmr*)
Murakami, T. *et al., Prog. Chem. Org. Nat. Prod.*, 1988, **54**, 1 (*occur*)
Sarker, S.D. *et al., Phytochemistry*, 1997, **44**, 513 (*Limnatheoside B*)
Vokáč, K. *et al., Phytochemistry*, 1998, **49**, 2109-2114 (*Ponasterone A, pmr, cmr*)
Costantino, V. *et al., Steroids*, 2000, **65**, 138-142 (*22-Hydroxyacetylponasterone A*)

2,3,14,22,25-Pentahydroxycholest-7-en-6-one P-217



$C_{27}H_{44}O_6$ 464.641

(2β,3β,5β,22*R*)-*form*
α-Ecdysone. *Ecdysone*
[3604-87-3]
Isol. from various plants, e.g. ferns, and from silkworm pupae and present in the 'organ Y' of crustaceans. Moulting hormone of insects and crustaceans. Cryst. (THF/petrol).
Mp 242°. $[\alpha]_D^{26}$ +64.7 (c, 1 in EtOH).
▶ FZ8170000

22-Sulfate: α-Ecdysone 22-sulfate
$C_{27}H_{44}O_9S$ 544.705
Constit. of *Silene brahuica*. Cryst. (MeOH)(as Na salt).
Mp 224-226° (Na salt). $[\alpha]_D^{20}$ +63.3 (c, 0.91 in MeOH) (Na salt).

Karlson, P. *et al., Chem. Ber.*, 1965, **98**, 2394 (*struct*)
Huber, R. *et al., Chem. Ber.*, 1965, **98**, 2403 (*cryst struct*)
Kerb, U. *et al., Helv. Chim. Acta*, 1966, **49**, 1601 (*synth*)
Siddall, J.B. *et al., J.A.C.S.*, 1966, **88**, 862 (*synth*)
Mori, H. *et al., Chem. Pharm. Bull.*, 1968, **16**, 563 (*synth*)
Chang, Y.K. *et al., Chem. Comm.*, 1970, 1217 (*isol, struct*)
Koreeda, M. *et al., J.A.C.S.*, 1971, **93**, 4084 (*config*)
Nakanishi, K. *et al., Pure Appl. Chem.*, 1971, **25**, 167 (*rev*)
Hikino, H. *et al., Chem. Pharm. Bull.*, 1975, **23**, 125 (*cmr*)

Lee, E. *et al., J.A.C.S.*, 1976, **98**, 1634 (*synth*)
Krepinsky, J. *et al., Org. Magn. Reson.*, 1977, **10**, 25 (*cmr*)
Tsoupras, G. *et al., Tetrahedron*, 1983, **39**, 1789 (*conjugates*)
Saatov, Z. *et al., Khim. Prir. Soedin.*, 1984, **20**, 467; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 441 (*isol*)
Koolman, J. *et al., Ecdysone*, Thieme, 1989, 74; *CA*, **112**, 217330y (*rev*)
Coll, J. *et al., Tetrahedron*, 1994, **50**, 7247 (*isol, cmr*)
Devarenne, T.P. *et al., Phytochemistry*, 1995, **40**, 1125 (*biosynth*)
Blais, C. *et al., Biochem. J.*, 1996, **320**, 413 (*biosynth*)

3,14,20,22,25-Pentahydroxycholest-7-en-6-one, 9CI P-218

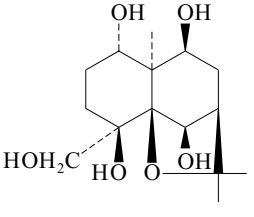
$C_{27}H_{44}O_6$ 464.641

(3α,5β,22*R*)-*form*
2-Deoxy-3-epicrustecdysone
[22785-88-2]
Isol. from *Tinospora capillipes*.
Needles (EtOAc/EtOH).
Mp 234-237° (230-231°).

(3β,5α,22*R*)-*form* [102976-85-2] Obt. as a mixt. with 5β-form.
3,22-Di-Ac: [102942-11-0]
$C_{31}H_{48}O_8$ 548.715
Needles (EtOAc). Mp 214-215°.

(3β,5β,20*R*,22*R*)-*form*
2-Deoxycrustecdysone. *2-Deoxy-20-hydroxyecdysone*
[17942-08-4]
Constit. of the pupae of *Antheraea pernyi*, of the eggs of *Schistocerca gregaria*, the langoustine crayfish *Jasus lalandii* and isol. from the plants *Murdannia triquetra, Blechnum minus* and various *Silene* spp.
Mp 250-252°. Present only in very minute traces in crustaceans, greater amounts in insects and readily obtainable from plants.
3-O-*β*-D-*Glucopyranoside:* [136849-87-1]
$C_{33}H_{54}O_{11}$ 626.783
Constit. of *Tinospora capillipes*.
25-Ac: ***2-Deoxyecdysterone 25-acetate***
[478809-55-1]
$C_{29}H_{46}O_7$ 506.678
Constit. of *Silene wallichiana*. Cryst. (MeOH aq.).
Mp 192-196°.
3-Benzoyl: [345958-46-5]
$C_{34}H_{48}O_7$ 568.749
Constit. of *Silene wallichiana*. Cryst. (EtOH aq.).
Mp 210-212°. $[\alpha]_D^{23}$ +72.3 (c, 0.5 in MeOH).
Galbraith, M.N. *et al., Chem. Comm.*, 1966, 339; 1968, 83; 1970, 1217 (*isol*)
Galbraith, M.N. *et al., Aust. J. Chem.*, 1969, **22**, 1059 (*synth, pmr, ms*)
Rashkes, Y.V. *et al., Khim. Prir. Soedin.*, 1980, **16**, 518; *Chem. Nat. Compd. (Engl. Transl.)*, 1980, **16**, 372 (*ms*)
Isaac, R.E. *et al., Chem. Comm.*, 1981, 418 (*isol*)
Isaac, R.E. *et al., J. Chromatogr.*, 1982, **246**, 317 (*hplc*)
Kametani, T. *et al., J.O.C.*, 1986, **51**, 2932 (*synth, pmr*)
Saatov, Z. *et al., Khim. Prir. Soedin.*, 1986, **22**, 323; 1987, **23**, 852; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 297; 1987, **23**, 708 (*isol*)
Song, C. *et al., Chin. Chem. Lett.*, 1991, **2**, 13; *CA*, **115**, 203297t (*isol, pmr*)
Suksamrarn, A. *et al., Tetrahedron*, 1996, **52**, 12623; 1997, **53**, 3145 (*synth*)
Mamadalieva, N.Z. *et al., Khim. Prir. Soedin.*, 2000, **36**, 405-407; *Chem. Nat. Compd. (Engl. Transl.)*, 2000, **36**, 513-515 (*3-benzoyl*)
Mamadalieva, N.Z. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2002, **38**, 179-181 (*25-Ac*)

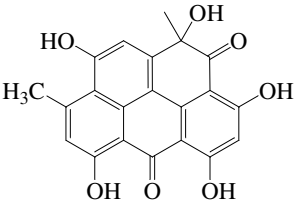
1,4,6,9,15-Pentahydroxydihydro-β-agarofuran P-219



$C_{15}H_{26}O_6$ 302.367

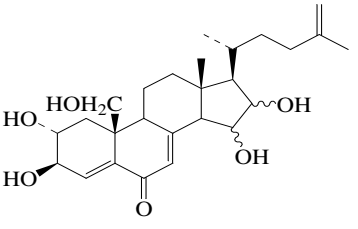
(1α,6β,9β)-*form*
1-Benzoyl, 6,9,15-tri-Ac: [107602-73-3]
$C_{28}H_{36}O_{10}$ 532.586
Constit. of *Orthosphenia mexicana*. Cryst.
Mp 188-190°. Called 6,9,15-Trihydroxy in the ref.
González, A.G. *et al., Phytochemistry*, 1988, **27**, 473

1,3,5,7,10-Pentahydroxy-1,9-dimethyl-2*H*-benzo[*cd*]pyrene-2,6(1*H*)-dione P-220
1-Hydroxy-1-norresistomycin



$C_{21}H_{14}O_7$ 378.337
Prod. by the marine-derived *Streptomyces chibaensis* AUBN$_1$/7 and *Streptomyces* sp. B8005. Cytotoxic. Orange solid. λ_{max} 204; 288; 464; 516 (MeOH).
Gorajana, A. *et al., J. Antibiot.*, 2005, **58**, 526-529 (*isol, pmr, cmr*)
Kock, I. *et al., J. Antibiot.*, 2005, **58**, 530-534 (*isol, cd, pmr, cmr*)

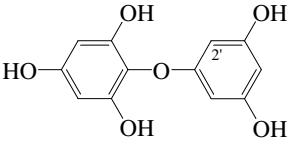
2,3,15,16,19-Pentahydroxy-26,27-dinorergosta-4,7,24-trien-6-one P-221



$C_{26}H_{38}O_6$ 446.583

(2α,3β,15ξ,16ξ)-*form* [193285-27-7]
Isol. from soft coral *Nephthea bayeri*.
Li, R. *et al., CA*, 1996, **127**, 147220

2,3′,4,5′,6-Pentahydroxydiphenyl ether P-222
2-(3,5-Dihydroxyphenoxy)-1,3,5-benzenetriol, 9CI. ***Diphlorethol***
[61237-21-6]



$C_{12}H_{10}O_6$ 250.207
Constit. of brown algae including *Analipus japonicus*, *Laminaria ochroleuca*, *Sargassum thunbergii*, *Ecklonia bicyclis*, *Himanthalia elongata*, *Bifurcaria bifurcata*, *Cystoseira tamariscifolia*, *Cystophora congesta* and *Sargassum muticum*. Antioxidant. λ_{max} 236 (ϵ 15000); 266 (ϵ 2500) (MeCN) (Berdy).
Penta-Ac: [56318-97-9]
Cryst. (MeOH). Mp 121-123° (113-114°).
Monochloro: ***Chlorodiphlorethol***
[63267-57-2]
$C_{12}H_9ClO_6$ 284.652
Constit. of *Laminaria ochroleuca*. Posn. of Cl atom not determined. CAS no. refers to penta-Ac.

4′-Chloro: ***4′-Chlorodiphlorethol***
[256448-74-5]
$C_{12}H_9ClO_6$ 284.652
Constit. of *Cystophora retroflexa*. Isol. as penta-Ac, to which CAS no. refers.

2′-Bromo: ***2′-Bromodiphlorethol***
[248600-48-8]
$C_{12}H_9BrO_6$ 329.104
Isol. from *Cystophora congesta* and *Cystophora retroflexa*. Called 2[D′]-bromo in the lit., by analogy with compds. having a greater number of rings. Isol. as penta-Ac, to which CAS no. refers.

3-Bromo: ***3-Bromodiphlorethol***
[256448-72-3]
$C_{12}H_9BrO_6$ 329.104
Constit. of *Cystophora retroflexa*. Isol. as penta-Ac, to which CAS no. refers.

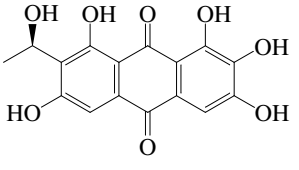
4′-Bromo: ***4′-Bromodiphlorethol***
[256448-73-4]
$C_{12}H_9BrO_6$ 329.104
Constit. of *Cystophora retroflexa*. Isol. as penta-Ac, to which CAS no. refers.

2′-Iodo: ***2′-Iododiphlorethol***
[248600-44-4]
$C_{12}H_9IO_6$ 376.104
Minor constit. of brown alga *Carpophyllum angustifolium* and *Cystophora congesta*. Isol. as penta-Ac.

Glombitza, K.-W. *et al., Phytochemistry*, 1975, **14**, 1115-1116; 1976, **15**, 1082-1083; 1978, **17**, 579-580; 1999, **50**, 869-881 (*isol, brown algae*)
Craigie, J.S. *et al., Can. J. Chem.*, 1977, **55**, 1575 (*pmr, cmr*)
Glombitza, K.W. *et al., Phytochemistry*, 1977, **16**, 796-798 (*Chlorodiphlorethol*)
Koch, M. *et al., Phytochemistry*, 1984, **23**, 2633-2637 (*2′-Bromodiphlorethol*)
Glombitza, K.W. *et al., Planta Med.*, 1985, **51**, 42; 116; 1989, **55**, 171 (*isol*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*2′-Iododiphlorethol*)
Sailler, B. *et al., Nat. Toxins*, 1999, **7**, 57-62 (*Cystophora retroflexa constits*)

1,2,3,6,8-Pentahydroxy-7-(1-hydroxyethyl)anthraquinone P-223

1,2,3,6,8-Pentahydroxy-7-(1-hydroxyethyl)-9,10-anthracenedione



$C_{16}H_{12}O_8$ 332.266

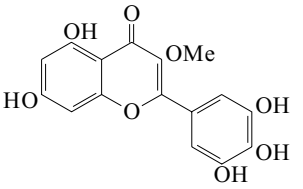
(R)-form

1′-Me ether: 1,2,3,6,8-Pentahydroxy-7-(1-methoxyethyl)anthraquinone
$C_{17}H_{14}O_8$ 346.293
Prod. by a *Microsphaeropsis* sp. from *Aplysia aerophoba*. Inhibitor of protein kinases. Orange-yellow powder. $[\alpha]_D$ -380.2 (c, 0.1 in EtOH). λ_{max} 225; 295; 330; 450 (MeOH).

Brauers, G. *et al., J. Nat. Prod.*, 2000, **63**, 739-745 (*isol, uv, cd, pmr, cmr, abs config*)

3′,4′,5,5′,7-Pentahydroxy-3-methoxyflavone P-224

*5,7-Dihydroxy-3-methoxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Annulatin****. Myricetin 3-methyl ether*
[1486-67-5]



$C_{16}H_{12}O_8$ 332.266
Isol. from *Aegialitis annulata*, *Oenothera speciosa*, *Cereus* spp., *Cleistocereus* sp., (preferred genus name *Cleistocactus*), *Mammillaria elongata* and *Solanum* spp.

*3′-*O*-β-D-Glucopyranoside:* [31105-82-5]
$C_{22}H_{22}O_{13}$ 494.408
Isol. from *Oenothera speciosa*. Yellow cubes (EtOH) (synthetic). Mp 300°.

*7-*O*-α-L-Rhamnopyranoside:* [93373-17-2]
$C_{22}H_{22}O_{12}$ 478.409
Isol. from *Dacrycarpus dacrydioides.*

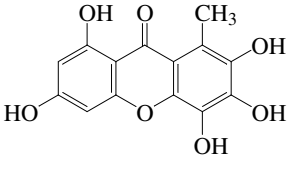
*3′-*O*-β-D-Xylopyranoside:* [76010-06-5]
$C_{21}H_{20}O_{12}$ 464.382
Isol. from *Ledum palustre* and *Dacrycarpus dacrydioides.*

*7-*O*-L-Rhamnopyranoside, 3′-*O*-β-D-xylopyranoside:* [93373-15-0]
$C_{27}H_{30}O_{16}$ 610.524
Isol. from *Dacrycarpus dacrydioides.*

Grouiller, A. *et al., Bull. Soc. Chim. Fr.*, 1967, 1938 (*pmr*)
Howard, G. *et al., Phytochemistry*, 1970, **9**, 2413; 1972, **11**, 289 (*isol*)
Chhabra, S.C. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 384 (*synth*)
Burret, F. *et al., J. Nat. Prod.*, 1982, **45**, 687 (*isol*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Markham, K.R. *et al., Phytochemistry*, 1984, **23**, 1931 (*glycosides*)
Seidel, V. *et al., Phytochemistry*, 2000, **55**, 439-446 (*isol, pmr, cmr*)

2,3,4,6,8-Pentahydroxy-1-methylxanthone P-225

*2,3,4,6,8-Pentahydroxy-1-methyl-9*H*-xanthen-9-one, 9CI.* ***Anomalin B***

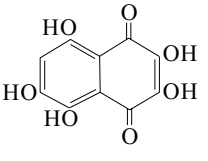


$C_{14}H_{10}O_7$ 290.229
Prod. by an algicolous marine fungus *Wardomyces anomalus.* Yellow-brown powder. λ_{max} 258 (log ϵ 4.7); 327 (log ϵ 4.48); 370 (sh) (MeOH).

Abdel-Lateff, A. *et al., J. Nat. Prod.*, 2003, **66**, 706-708 (*isol, pmr, cmr*)

2,3,5,6,8-Pentahydroxy-1,4-naphthoquinone P-226

2,3,5,6,8-Pentahydroxy-1,4-naphthalenedione, 9CI. ***Spinochrome D***
[1143-11-9]



$C_{10}H_6O_7$ 238.153
Tautomeric with the 2,5,6,7,8-pentahydroxy isomer. Pigment from the sea urchins *Spatangus purpureus, Pseudocentrotus depressus*

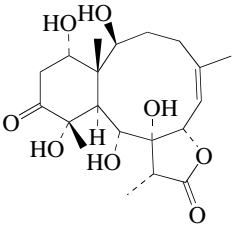
and *Strongylocentrotus droebachiensis*. Red cryst. Sublimes at 285-290° without melting. λ_{max} 266 (ϵ 12600); 333 (ϵ 2760); 463 (ϵ 2580); 530 (ϵ 1820) (MeOH) (Berdy).

Penta-Ac:
$C_{20}H_{16}O_{12}$ 448.339
Yellow cryst. (MeOH). Mp 179-180°.

2,3,6-Tri-Me ether: 5,8-Dihydroxy-2,3,6-trimethoxy-1,4-naphthoquinone. ***Tricrozarin B***
[3560-71-2]
$C_{13}H_{12}O_7$ 280.234
Constit. of *Tritonia crocosmaeflora*. Potent antitumour agent. Sol. MeOH, C_6H_6; poorly sol. H_2O. Potentially tautomeric with the 5,8-dihydroxy-2,6,7-trimethoxy struct. λ_{max} 232; 318; 492 (MeOH) (Berdy). λ_{max} 232; 317; 497 (MeOH/HCl) (Berdy). λ_{max} 232; 322; 532 (MeOH/NaOH) (Berdy).

Kuroda, C. *et al., Proc. Imp. Acad. (Tokyo)*, 1944, **20**, 23 (*isol*)
Singh, I. *et al., J.A.C.S.*, 1965, **87**, 4023-4024 (*synth*)
Anderson, H.A. *et al., J.C.S.*, 1965, 2141-2144 (*synth*)
Mathieson, J.W. *et al., J.C.S.(C)*, 1971, 153-160 (*isol*)
Kol'tsova, E.A. *et al., Khim. Prir. Soedin.*, 1978, 438-441; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 371-374 (*isol*)
Masuda, K. *et al., J. Nat. Prod.*, 1987, **50**, 958-960 (*2,3,6-tri-Me ether, isol, activity*)

2,8,9,11,14-Pentahydroxy-12-oxo-5-briaren-18,7-olide P-227



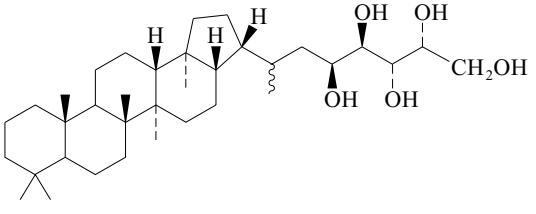
$C_{20}H_{30}O_8$ 398.452

(2β,5*Z*,7α,8α,9α,11α,14α)-*form*
2,9,14-Tri-Ac: ***Minabein 9***
[104993-14-8]
$C_{26}H_{36}O_{11}$ 524.564
Constit. of *Minabea* sp. Powder.
Mp 190-193°.

Ksebati, M.B. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 835-851 (*isol, pmr, cmr*)

29-(1,2,3,4,5-Pentahydroxypentyl)hopane P-228

31,32,33,34,35-Bacteriohopanepentol

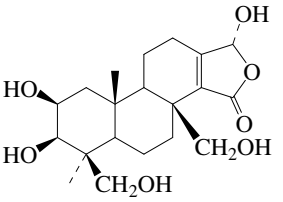


$C_{35}H_{62}O_5$ 562.872

(22ξ,31*S*,32*R*,33*S*,34*R*)-*form* [175669-46-2]
Constit. of *Nostoc* PCC 6720. Component of cell wall lipids.

Zhao, N. *et al., Tetrahedron*, 1996, **52**, 2777 (*isol, pmr, cmr*)

2,3,16,17,19-Pentahydroxy-13-spongien-15-one P-229



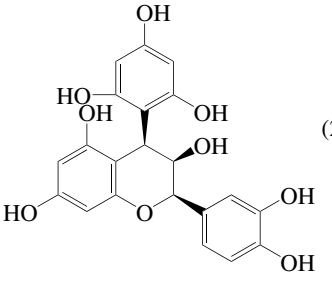
$C_{20}H_{30}O_7$ 382.453

(2β,3β,16α)-*form*
Zimoclactone C
[384828-99-3]
Constit. of *Spongia zimocca* ssp. *irregularia*.
Cryst. (EtOH aq.).
Mp 243-244°. $[\alpha]_D^{25}$ -56.47 (c, 0.028 in EtOH).

Zeng, L.-M. *et al., Huaxue Xuebao*, 2001, **59**, 1675-1679 (*isol, pmr, cmr, cryst struct*)

3,3′,4′,5,7-Pentahydroxy-4-(2,4,6-trihydroxyphenyl)flavan P-230

2-(3,4-Dihydroxyphenyl)-3,4-dihydro-4-(2,4,6-trihydroxyphenyl)-2H-1-benzopyran-3,5,7-triol, 9CI. 4-(2,4,6-Trihydroxyphenyl)-3,3′,4′,5,7-flavanpentol



(2*R*,3*R*,4*R*)-*form*

$C_{21}H_{18}O_9$ 414.368

(2*R*,3*R*,4*R*)-*form*
Epicatechin(4α→2)phloroglucinol
[104320-35-6]
Isol. from *Pseudotsuga menziesii*.
Off-white solid. $[\alpha]_D$ +64 (c, 0.08 in MeOH).

3-O-α-L-Rhamnopyranoside: [154849-41-9]
$C_{27}H_{28}O_{13}$ 560.51
Constit. of *Bruguiera gymnorrhiza*. Incorr. struct. given in CA.

(2*R*,3*R*,4*S*)-*form*
Prodelphinidin B6. *Epicatechin(4β→2)phloroglucinol*
[61541-02-4]
Constit. of *Nelia meyeri* and *Pseudotsuga menziesii*.
$[\alpha]_D$ +122 (H_2O).

3′-Deoxy: 3,4′,5,7-Tetrahydroxy-4-(2,4,6-trihydroxyphenyl)flavan. Epiafzelechin(4β→2)phloroglucinol
[173293-94-2]
$C_{21}H_{18}O_8$ 398.368
Constit. of *Lotus corniculatus* (Leguminosae). Light brown powder. $[\alpha]_D$ +113 (c, 0.1 in MeOH).

(2*R*,3*S*,4*R*)-*form* [78284-51-2]
Amorph. solid.

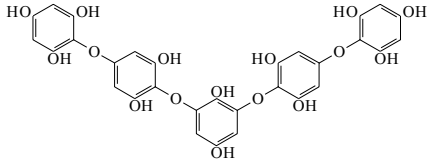
(2*R*,3*S*,4*S*)-*form*
Catechin(4α→2)phloroglucinol
[61541-06-8]
Isol. from *Pseudotsuga menziesii*.
Amorph. solid. $[\alpha]_D$ -188 (c, 0.17 im MeOH).

[79199-52-3, 79199-53-4]

Fletcher, A.C. *et al., J.C.S. Perkin 1*, 1977, 1628 (*synth, cmr*)
Botha, J.J. *et al., J.C.S. Perkin 1*, 1981, 1213 (*synth, cd*)
Foo, L.Y. *et al., Chem. Comm.*, 1983, 672; 1035 (*synth*)
Kolodziej, H. *et al., Tet. Lett.*, 1983, **24**, 1825 (*isol, synth*)
Foo, L.Y. *et al., Phytochemistry*, 1984, **23**, 2915; 1989, **28**, 3185; 1996, **41**, 617 (*isol, pmr, cmr*)
Porter, L.J. *et al., J. Chem. Res., Synop.*, 1986, 86 (*pmr, conformn*)
Newman, R.H. *et al., Magn. Reson. Chem.*, 1987, **25**, 118 (*cmr*)
Achmaldi, S. *et al., Phytochemistry*, 1994, **35**, 217 (*3-rhamnoside*)
Roussow, W. *et al., Tetrahedron*, 1994, **50**, 12477 (*pmr, abs config*)

Pentaisofuhalol P-231

2,2′-[(2,5-Dihydroxy-1,3-phenylene)bis[oxy(3,5-dihydroxy-4,1-phenylene)oxy]]bis[1,3,5-benzenetriol], 9CI
[94513-77-6]



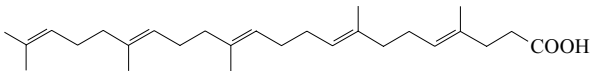
$C_{30}H_{22}O_{16}$ 638.494
Isol. from *Chorda filum* (as per-Ac).

[94513-78-7]

Grosse-Damhues, J. *et al., Phytochemistry*, 1984, **23**, 2639 (*isol, cmr*)

4,8,13,17,21-Pentamethyl-4,8,12,16,20-docosapentaenoic acid P-232

Turbinaric acid

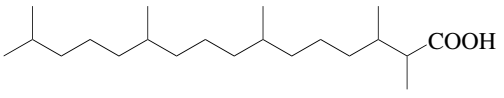


$C_{27}H_{44}O_2$ 400.643
Constit. of *Turbinaria ornata*.

van Tamelen, E.E. *et al., Tet. Lett.*, 1962, 121 (*synth*)
Asari, F. *et al., J. Nat. Prod.*, 1989, **52**, 1167 (*isol, pmr, cmr*)

2,3,7,11,15-Pentamethylhexadecanoic acid P-233

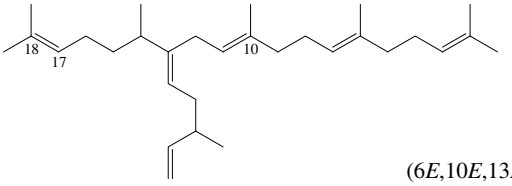
[122706-68-7]



$C_{21}H_{42}O_2$ 326.562
Isol. from the oil of the redfish (*Sebastes* sp.).

Ratnayake, W.M.N. *et al., Lipids*, 1989, **24**, 630 (*isol*)

2,6,10,14,18-Pentamethyl-13-(3-methyl-4-pentenylidene)-2,6,10,17-nonadecatetraene P-234



(6*E*,10*E*,13*E*)-*form*

$C_{30}H_{50}$ 410.725

(6*E*,10*E*,13*E*)-*form* [367939-68-2]
Constit. of *Rhizosolenia setigera*.

17,18-Dihydro: ***2,6,10,14,18-Pentamethyl-13-(3-methyl-4-pentenylidene)-2,6,10-nonadecatriene***
[367939-70-6]
$C_{30}H_{52}$ 412.741
Constit. of *Rhizosolenia setigera*.

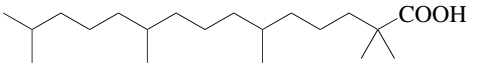
(6*E*,10*Z*,13*E*)-*form* [367939-69-3]
Constit. of *Rhizosolenia setigera*.

17,18-Dihydro: [367939-71-7]
$C_{30}H_{52}$ 412.741
Constit. of *Rhizosolenia setigera*.

Belt, S.T. *et al., Tet. Lett.*, 2001, **42**, 5583-5585 (*isol, pmr, cmr*)
Massé, G. *et al., Phytochemistry*, 2004, **65**, 1101-1106

2,2,6,10,14-Pentamethylpentadecanoic acid P-235

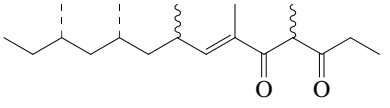
[122706-67-6]



$C_{20}H_{40}O_2$ 312.535
Isol. from the oil of the redfish (*Sebastes* sp.).

Ratnayake, W.M.N. *et al., Lipids*, 1989, **24**, 630 (*isol*)

4,6,8,10,12-Pentamethyl-6-tetradecene-3,5-dione P-236

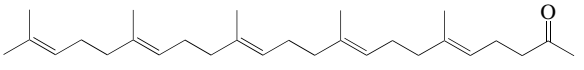


$C_{19}H_{34}O_2$ 294.476
Constit. of *Siphonaria lessoni*. Ref. not seen, not in CAS. Data obtained from review.

Rovirosa, J. *et al., Bol. Soc. Chil. Quim.*, 1991, **36**, 233-238 (*isol*)

6,10,14,18,22-Pentamethyl-5,9,13,17,21-tricosapentaen-2-one P-237

Geranylfarnesylacetone
[86541-61-9]



$C_{28}H_{46}O$ 398.671
Constit. of *Sarcotragus spinulosus*. Oil.

Ponomarenko, L.P. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1998, **47**, 2017-2019 (*isol, pmr, ms*)

Pentanal, 9CI P-238

n-*Valeraldehyde, 8CI. Valeric aldehyde. FEMA 3098*
[110-62-3]
$H_3CCH_2CH_2CH_2CHO$
$C_5H_{10}O$ 86.133
Found in olive oil and several essential oils. Also present in coriander leaf, rice, Bourbon vanilla, scallops, apple and banana, sweet cherry, blackcurrant and other sources. Used to make flavouring compounds and resins. Liq. d_4^{20} 0.81.
Fp -92. Bp 102.5-103°. n_D^{20} 1.3947.

▶ Highly flammable, fl. p. 12°, autoignition temp. 222°. Eye, skin and respiratory tract irritant. LD_{50} (rat, orl) 3200 mg/kg. LD_{50} (rbt, skn) 4857 mg/kg. YV3600000

Oxime: [628-79-5]
$C_5H_{11}NO$ 101.148
Cryst. Mp 52°.

2,4-Dinitrophenylhydrazone: [2057-84-3]
Yellow cryst. Mp 106-107°.

Di-Me acetal: 1,1-Dimethoxypentane
[26450-58-8]
$C_7H_{16}O_2$ 132.202
Liq. Bp 120-129°.

Di-Et acetal: 1,1-Diethoxypentane
[3658-79-5]
$C_9H_{20}O_2$ 160.256
Volatile component of strawberries and other fruits. Liq. d_4^{22} 0.83. Bp 162.5-163.5° Bp_{12} 59°. n_D^{23} 1.4029.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 729C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 467B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 553B (*ir*)
Blaise, E.E. *et al., C. R. Hebd. Seances Acad. Sci.*, 1904, **138**, 698 (*synth*)
Bruylants, P. *et al., CA*, 1932, **26**, 3232 (*synth*)
Org. Synth., 1971, **51**, 31 (*synth*)
Zeidler, U. *et al., CA*, 1974, **81**, 91007 (*synth*)
Roberts, J.D. *et al., J.O.C.*, 1974, **39**, 1017 (*cmr*)
Savoia, D. *et al., J.O.C.*, 1978, **43**, 2907; 1980, **45**, 3227 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 919 (*rev, tox*)
Maccoll, A. *et al., Org. Mass Spectrom.*, 1986, **21**, 251 (*ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VAG000
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1312

1,5-Pentanediamine, 9CI P-239

Pentamethylenediamine. 1,5-Diaminopentane. Cadaverine
[462-94-2]
$H_2NCH_2(CH_2)_3CH_2NH_2$
$C_5H_{14}N_2$ 102.179
Found in nature as bacterial decarboxylation prod. of Lysine, e.g. in putrefaction. Anal sac secretion of the red fox *Vulpes vulpes*. Monomer for polyamides. Syrupy fuming liq. d^{20} 0.84. Bp 178-180°. n_D^{20} 1.4582. pK_{a1} 10.92; pK_{a2} 10.05 (25°, 0.5*M* KNO_3).
▶ Skin irritant. SA0200000

Hydrochloride (1:2): [1476-39-7]
Needles (H_2O). Mp 226° Mp 260-262°.

N-*Benzoyl:* [29833-52-1]
$C_{12}H_{18}N_2O$ 206.287
Oil. $Bp_{0.5}$ 202°.

N,N′-*Dibenzoyl:* [31991-79-4]
$C_{19}H_{22}N_2O_2$ 310.395
Cryst. (C_6H_6). Mp 135°.

N,N′-*Bis(4-nitrobenzoyl):* [81852-10-0]
Cryst. (Me_2CO aq.). Mp 185-185.5°.

N-*Me:* [32752-52-6]
$C_6H_{16}N_2$ 116.206
Liq. Bp 177-178° Bp_{12} 55°.

N,N′-*Di-Me:* [56992-95-1]
$C_7H_{18}N_2$ 130.233
Liq. Bp 190° Bp_{10} 74°.

N,N,N-*Tri-Me: 5-Amino*-N,N,N-*trimethylpentanaminium, 9CI. **Ascophylline***
[83524-44-1]
[4175-13-7, 30835-02-0]
$C_8H_{21}N_2^{\oplus}$ 145.267
Constit. of the alga *Ascophyllum nodosum* and isol. from the beetle *Platyphora opima*.

N,N,N′,N′-*Tetra-Me:* [44994-28-7]
$C_9H_{22}N_2$ 158.286
Liq. Bp 192-194° Bp_{15} 85-95°.

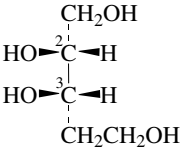
N-*Hexa-Me:* See Pentamethonium(2+) in *The Combined Chemical Dictionary.*

N-tert-*Butyloxycarbonyl:* [51644-96-3]
$C_{10}H_{22}N_2O_2$ 202.296
Oil.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 292B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 466A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 376B (*ir*)
Putochin, N. *et al., Ber.*, 1926, **59**, 625 (*synth*)
Korshak, V.V. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1955, 756; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1955, 673 (*polyamides*)
Ger. Pat., 1971, 2 043 141; *CA*, **75**, 6884 (*N-Me*)
Sarneski, J.E. *et al., Anal. Chem.*, 1975, **47**, 2116 (*cmr*)
Mayerl, F. *et al., Helv. Chim. Acta*, 1976, **59**, 127 (*ms*)
Albone, E.S. *et al., J. Chem. Ecol.*, 1976, **2**, 167
Richter, R. *et al., J.O.C.*, 1978, **43**, 4150 (*synth*)
Abd-alla, M.F. *et al., Phytochemistry*, 1980, **19**, 2629 (*Ascophylline*)
Battersby, A.R. *et al., J.C.S. Perkin 1*, 1982, 449 (*biosynth*)
Blunden, G. *et al., Magn. Reson. Chem.*, 1986, **24**, 965-971 (*Ascophylline*)
Thalladi, V.R. *et al., Angew. Chem., Int. Ed.*, 2000, **39**, 918-922 (*cryst struct*)
Gardner, R. *et al., J. Med. Chem.*, 2004, **47**, 4933-4940 (*N-Boc*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PBK500

1,2,3,5-Pentanetetrol P-240

2-Deoxypentitol, 9CI



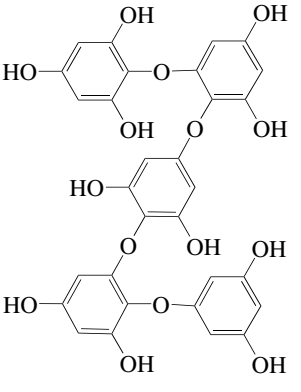
$C_5H_{12}O_4$ 136.147
The pentitol numbering starts at the other end of the chain.

(2*R*,3*S*)-*form*
2-Deoxy-D-ribitol
Constit. of the fruit of *Foeniculum vulgare* (fennel).
Syrup. $[\alpha]_D^{22}$ -20 (c, 0.3 in H_2O). $[\alpha]_D$ -17 (c, 0.3 in MeOH).

Tetrakis(4-hydroxybenzoyl): ***Kelletinin II***
[87698-01-9]
$C_{33}H_{28}O_{12}$ 616.577
Metab. of the marine mollusc, *Kelletia kelletii*. Antibacterial, cytotoxic. Sol. MeOH, bases, Et_2O; poorly sol. H_2O. λ_{max} 258 (ϵ 63100) (EtOH/HCl) (Derep). λ_{max} 301 (ϵ 100000) (EtOH/NaOH) (Derep). λ_{max} 258 (ϵ 50100) (EtOH) (Derep). λ_{max} 259 (ϵ 24700) (EtOH) (Berdy). λ_{max} 257 (ϵ 33900) (HCl) (Berdy). λ_{max} 302 (ϵ 45600) (NaOH) (Berdy).
Tymiak, A.A. *et al., J.A.C.S.*, 1983, **105**, 7396-7401 (*Kelletinin II*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1999, **47**, 988-992 (*isol, pmr, cmr*)

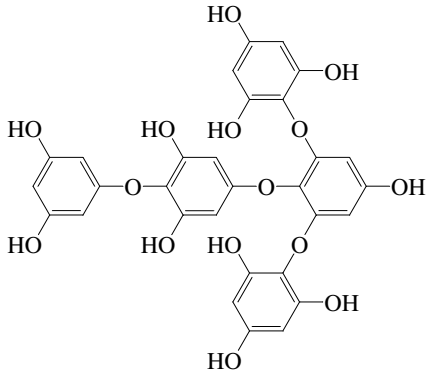
Pentaphlorethol A P-241

[164176-23-2]



$C_{30}H_{22}O_{15}$ 622.495
Constit. of the brown alga *Sargassum spinuligerum*.
Keusgen, M. *et al., Phytochemistry*, 1995, **38**, 975 (*isol, pmr, ms*)

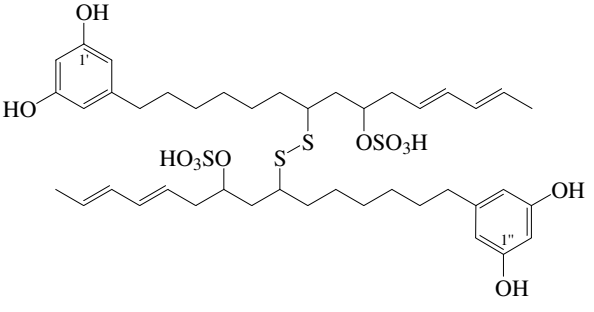
Pentaphlorethol B P-242



$C_{30}H_{22}O_{15}$ 622.495
Isol. from *Cystophora retroflexa*.

Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol, pmr, cmr, ms*)

Pentaporin A P-243



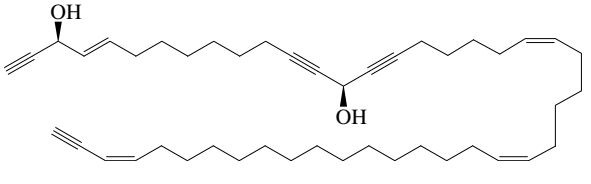
$C_{42}H_{62}O_{12}S_4$ 887.209
Isol. from the marine bryozoan *Pentapora fascialis*. Shows anthelmintic activity. $[\alpha]_D^{25}$ -13.1 (c, 0.006 in MeOH) (as di-Na salt). λ_{max} 202 (log ϵ 7.95); 223 (log ϵ 7.77); 274 (log ϵ 6.59) (MeOH) (di-Na salt).

1′-Sulfate: ***Pentaporin B***
$C_{42}H_{62}O_{15}S_5$ 967.273
Isol. from *Pentapora fascialis*.
$[\alpha]_D^{25}$ -13 (c, 0.006 in MeOH) (as tri-Na salt). λ_{max} 202 (log ϵ 8.19); 224 (log ϵ 7.95); 271 (log ϵ 6.83) (MeOH) (tri-Na salt).

1′,1′′-Disulfate: ***Pentaporin C***
$C_{42}H_{62}O_{18}S_6$ 1047.337
Isol. from *Pentapora fascialis*.
$[\alpha]_D^{25}$ -11 (c, 0.002 in MeOH) (as tetra-Na salt). λ_{max} 202 (log ϵ 6.97); 222 (log ϵ 6.75); 272 (log ϵ 6.01) (MeOH) (tetra-Na salt).

Eisenbarth, S. *et al., Tetrahedron*, 2002, **58**, 8461-8464 (*isol, cd, uv, pmr, cmr, ms*)

4,21,27,42-Pentatetracontatetraene-1,12,15,44-tetrayne-3,14-diol P-244

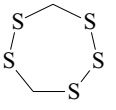


$C_{45}H_{68}O_2$ 641.031

(3*S*,4*E*,14*S*,21*Z*,27*Z*,42*Z*)-*form*
Norpetrocortyne A
[246240-53-9]
Constit. of a sponge *Petrosia* sp. Cytotoxic agent. Yellow oil. $[\alpha]_D^{23}$ +10 (c, 1 in MeOH). λ_{max} 223 (log ϵ 3.9) (MeOH).
Lim, Y.J. *et al., J. Nat. Prod.*, 1999, **62**, 1215-1217; 2001, **64**, 46-53 (*isol,pmr,cmr*)

1,2,3,5,6-Pentathiepane, 9CI, 8CI P-245

1,2,3,5,6-Pentathiacycloheptane. ***Lenthionine***
[292-46-6]



$C_2H_4S_5$ 188.384
Constit. of the edible mushroom Shiitake *Lentinus edodes*, responsible for its characteristic odour. Also found in the alga *Chondria californica* and in *Parkia speciosa*. Active against gram-positive and -negative bacteria and *Candida albicans*. Cryst. (CH_2Cl_2). Prac. insol. H_2O, polar org. solvs.; sol. oils. Mp 60-61°.

Morita, K. *et al., Chem. Pharm. Bull.*, 1967, **15**, 988 (*synth, isol, ms*)
Wada, S. *et al., J. Food Sci.*, 1967, **32**, 559 (*isol, synth*)
Wratten, S.J. *et al., J.O.C.*, 1976, **41**, 2465 (*isol*)
Iwami, K. *et al., CA*, 1978, **89**, 161546 (*rev, bibl*)
Nixon, L.N. *et al., J. Agric. Food Chem.*, 1979, **27**, 355 (*isol*)
Gmelin, R. *et al., Phytochemistry*, 1981, **20**, 2521 (*isol, props*)
Still, I.W.J. *et al., Tet. Lett.*, 1981, 1939 (*synth*)
Holzmann, G. *et al., Org. Mass Spectrom.*, 1982, **17**, 165 (*ms*)
Bannister, R.M. *et al., J.C.S. Perkin 1*, 1990, 509 (*synth*)
Ritzau, M. *et al., Annalen*, 1993, 871 (*isol*)

20,31-Pentatriacontadiene-2,4,22,34-tetrayne-1,6,33-triol P-246

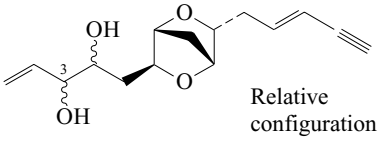
$HC{\equiv}CCH(OH)CH{=}CH(CH_2)_7C{\equiv}CCH{=}CH(CH_2)_{13}CH(OH)C{\equiv}CC{\equiv}CCH_2OH$

$C_{35}H_{52}O_3$ 520.794

(-)-(20*Z*,31*E*)-*form*
Pellynol D
[186248-12-4]
Isol. from the sponge *Pellina triangulata*. Exhibits cytotoxic activity to human cell lines. $[\alpha]_D$ -9.8 (c, 0.6 in $CHCl_3$).
Fu, X. *et al., Tetrahedron*, 1997, **53**, 799 (*isol, ir, pmr, cmr*)
Rashid, M.A. *et al., Nat. Prod. Lett.*, 2000, **14**, 387-392 (*isol, activity*)

1-[6-(2-Penten-4-ynyl)-2,5-dioxabicyclo[2.2.1]hept-3-yl]-4-pentene-2,3-diol P-247

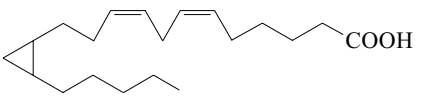
6,9:7,10-Diepoxy-1,12-pentadecadien-14-yne-3,4-diol
[148084-33-7]



$C_{15}H_{20}O_4$ 264.321
Isol. from the red alga *Laurencia majuscula*. Oil. $[\alpha]_D^{22}$ +47 (c, 0.1 in $CHCl_3$).

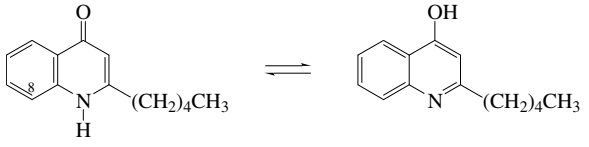
3-Deoxy, 3-chloro: ***3-Chloro-1-[6-(2-penten-4-ynyl)-2,5-dioxabicyclo[2.2.1]hept-3-yl]-4-penten-2-ol***
[148084-32-6]
$C_{15}H_{19}ClO_3$ 282.766
Isol. from *Laurencia majuscula*. Oil. $[\alpha]_D^{22}$ +53.4 (c, 0.29 in $CHCl_3$).
Wright, A.D. *et al., J. Nat. Prod.*, 1993, **56**, 394 (*isol, pmr, struct*)

12-(2-Pentylcyclopropyl)-6,9-dodecadienoic acid P-248
13,14-Methylene-6,9-nonadecadienoic acid
[73414-50-3]



$C_{20}H_{34}O_2$ 306.487
Constit. of the mollusc *Bursatella leachii*.
Fenical, W. *et al., Pure Appl. Chem.*, 1979, **51**, 1865 (*isol*)

2-Pentyl-4(1*H*)-quinolinone P-249
2-Pentyl-4-quinolinol. 4-Hydroxy-2-pentylquinoline
[62869-70-9]



$C_{14}H_{17}NO$ 215.294
Alkaloid from a yellow marine pseudomonad. Active against *Staphylococcus aureus* and *Vibrio* sp. Cryst. Sol. MeOH, $CHCl_3$. Mp 141-142° (135°). λ_{max} 235; 315; 326 (MeOH) (Berdy).

NH-form
8-Methoxy, N-*Me:* ***8-Methoxy-1-methyl-2-pentyl-4(1H)-quinolinone***
$C_{16}H_{21}NO_2$ 259.347
Alkaloid from trunk bark of *Esenbeckia almawillia* (Rutaceae). Oil.

OH-form
Me ether: ***4-Methoxy-2-pentylquinoline***
[22048-99-3]
$C_{15}H_{19}NO$ 229.321
Alkaloid from *Galipea officinalis* and *Galipea longiflora*. Oil. $Bp_{0.14}$ 135°.
1′,2′-Didehydro, Me ether: ***4-Methoxy-2-(1-pentenyl)quinoline***
[124902-97-2]
$C_{15}H_{17}NO$ 227.305
Alkaloid from stem bark of *Galipea bracteata* (Rutaceae). Amorph.
Buu-Hoï, Ng.Ph. *et al., J.O.C.*, 1953, **18**, 1209 (*synth*)
Werner, W. *et al., Tetrahedron*, 1969, **25**, 255-261 (*synth*)
Wratten, S.J. *et al., Antimicrob. Agents Chemother.*, 1977, **11**, 411 (*isol, struct*)
Thomsen, I. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 309 (*synth, pmr*)
Fournet, A. *et al., Can. J. Chem.*, 1989, **67**, 2116-2118 (*4-Methoxy-2-pentylquinoline, 4-Methoxy-2-(1-pentenyl)quinoline*)
Guilhon, G.M.S.P. *et al., Phytochemistry*, 1994, **37**, 1193 (*8-Methoxy-1-methyl-2-pentyl-4(1H)-quinolinone*)

***Homarus americanus* Peptide F_1** P-250
Lobster peptide F_1
[113611-68-0]
H-Thr-Asn-Arg-Asn-Phe-Leu-Arg-Phe-NH_2
$C_{48}H_{75}N_{17}O_{11}$ 1066.228
Neurohormone isol. from the nervous system of the lobster *Homarus americanus* and from the crab *Cancer borealis*. Immunoreactive agent.
Trimmer, B.A. *et al., J. Comp. Neurol.*, 1987, **266**, 16-26 (*isol, Homarus constit*)
Wiemann, J.M. *et al., J. Exp. Biol.*, 1993, **181**, 1-26 (*isol, Cancer constit*)

***Homarus americanus* Peptide G_1** P-251
Peptide. Chain contains =61 residues. The complete amino-acid sequence was not reported. Isol. from the secretory gland of the American lobster *Homarus americanus*. Increases the cyclic GMP content of every lobster tissue studied.
Pavloff, M.S. *et al., J. Neurochem.*, 1990, **55**, 788 (*isol*)

Peptide Mo 1659 P-252
Mo 1659
H-Phe-His-Gly-Gly-Ser-Trp-Tyr-Arg-Phe-Pro-Trp-Gly-Tyr-amide
Isol. from the venom of the snail *Conus monile*. Targets potassium channels.
Sudarslal, S. *et al., Biochem. Biophys. Res. Commun.*, 2004, **317**, 682-688 (*isol, struct, props*)

Peptide RHM 1 P-253
RHM 1. Antibiotic RHM 1
Ac-Gln-Ile-MeLeu-Ile-MeVal-MeIle-MeIle-MeIle-OH
$C_{53}H_{97}N_9O_{11}$ 1036.403
Prod. by an *Acremonium* sp. isol. from a *Teichaxinella* sp. Cryst. $[\alpha]_D^{25}$ -125 (c, 0.08 in MeOH). λ_{max} 205 (log ϵ 4.33) (MeOH).
Boot, C.M. *et al., J. Nat. Prod.*, 2006, **69**, 83-92 (*isol, pmr, cmr*)

Peptide RHM 2 P-254
RHM 2. Antibiotic RHM 2
Ac-Gln-Val-MeLeu-MeVal-Ile-MeIle-MeIle-MeIle-OH
$C_{52}H_{95}N_9O_{11}$ 1022.376
Prod. by an *Acremonium* sp. isol. from a *Teichaxinella* sp. Cryst. $[\alpha]_D^{25}$ -137.5 (c, 0.08 in MeOH). λ_{max} 207 (log ϵ 4.47) (MeOH).
Boot, C.M. *et al., J. Nat. Prod.*, 2006, **69**, 83-92 (*isol, pmr, cmr*)

***Antheopsis maculata* Peptide toxins** P-255
Isol. from the sea anemone *Antheopsis maculata*. Toxic to crabs.

Am I
$C_{117}H_{184}N_{34}O_{38}S_4$ 2803.21

Am II
Peptide containing 46 amino acid residues.

Am III
Peptide containing 47 amino acid residues.
Honma, T. *et al., Toxicon*, 2005, **45**, 33-41 (*isol*)

***Penaeus monodon* Peptide tyrosine-phenylalanine** P-256
Pem-PYF
Arg-Ala-Arg-Pro-Arg-Phe-NH_2
Struct. of Pem-PYF 1 shown. Isol. from the eyestalk of the giant tiger prawn *Penaeus monodon*.

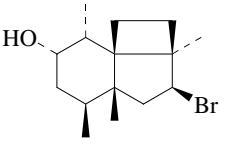
Pem-PYF 1 [499132-01-3]
$C_{35}H_{60}N_{16}O_6$ 800.963

Pem-PYF 2 [499132-02-4]
$C_{51}H_{79}N_{17}O_{13}$ 1138.291

Pem-PYF 3 [499132-03-5]
$C_{49}H_{76}N_{16}O_{10}$ 1049.241

Pem-PYF 4 [499132-04-6]
$C_{53}H_{85}N_{19}O_{11}$ 1164.375
Sithigorngul, P. *et al., Peptides (N.Y.)*, 2002, **23**, 1895-1906 (*isol*)

Perforatol P-257
[539824-92-5]



Relative Configuration

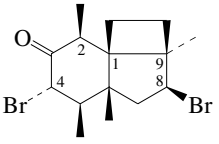
$C_{15}H_{25}BrO$ 301.266

Isol. from *Aplysia punctata*. Semi-solid. $[\alpha]_D$ +14.8 (c, 0.002 in $CHCl_3$).

Findlay, J.A. *et al., Can. J. Chem.*, 2002, **80**, 1697-1707 (*isol, pmr, cmr, ms*)

Perforatone P-258

[57566-98-0]



$C_{15}H_{22}Br_2O$ 378.146

Stereochem. revised in 2002. Constit. of *Laurencia perforata* and *Laurencia obtusa*. Cryst.
Mp 106-108°. $[\alpha]_D$ +186 (c, 1.58 in $CHCl_3$).

4-Debromo: [474511-68-7]
$C_{15}H_{23}BrO$ 299.25
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ +42.3 (c, 0.17 in $CHCl_3$).
λ_{max} 202 (log ϵ 3); 207 (log ϵ 3.01) (hexane).

2-Epimer:
$C_{15}H_{22}Br_2O$ 378.146
Constit. of *Laurencia tenera*. Cryst.
Mp 112-113°. $[\alpha]_D$ -25 (c, 0.002 in $CHCl_3$).

2-Epimer, 4-debromo: [474511-70-1]
$C_{15}H_{23}BrO$ 299.25
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ -11.6 (c, 0.31 in $CHCl_3$).
λ_{max} 203 (log ϵ 2.91); 207 (log ϵ 2.91) (hexane).

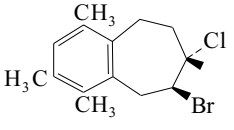
2-Epimer, 4-debromo, 4β-methoxy: [474511-66-5]
$C_{16}H_{25}BrO_2$ 329.276
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ -5.7 (c, 0.07 in $CHCl_3$).

2,4-Diepimer: [132342-61-1]
$C_{15}H_{22}Br_2O$ 378.146
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ -94 (c, 0.35 in $CHCl_3$).
λ_{max} 202 (log ϵ 3.05); 207 (log ϵ 3.06) (hexane).

González, A.G. *et al., Tet. Lett.*, 1975, **16**, 2499-2502 (*isol, pmr*)
Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1695-1703 (*Laurencia tenera constits, cryst struct*)
Iliopoulou, D. *et al., Tetrahedron*, 2002, **58**, 6749-6755 (*Laurencia obtusa constits, pmr, cmr, struct*)

Perforene P-259

[59557-94-7]

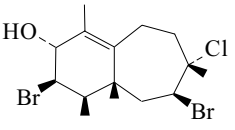


$C_{15}H_{20}BrCl$ 315.68
Constit. of *Laurencia perforata*. Oil. $[\alpha]_D$ -3.

González, A.G. *et al., Tet. Lett.*, 1976, 205

Perforenol P-260

[70073-12-0]



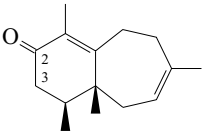
Absolute configuration

$C_{15}H_{23}Br_2ClO$ 414.607
Constit. of *Laurencia perforata* and *Laurencia obtusa*. Cryst.
Mp 105-107°. $[\alpha]_D$ -107. λ_{max} 204 (log ϵ 3.79) (hexane).

González, A.G. *et al., Tet. Lett.*, 1978, 3931 (*isol, pmr, cmr, cryst struct*)
Iliopoulou, D. *et al., Tetrahedron*, 2002, **58**, 6749-6755 (*isol, pmr, cmr*)

Perforenone P-261

[66113-28-8]



$C_{15}H_{22}O$ 218.338
Constit. of *Laurencia perforata*. Oil. $[\alpha]_D$ -120.

2α-Alcohol: ***Guadalupol***
[66113-20-0]
$C_{15}H_{24}O$ 220.354
Constit. of *Laurencia snyderae*. Oil.

2β-Alcohol: ***Epiguadalupol***
[66113-19-7]
$C_{15}H_{24}O$ 220.354
Constit. of *Laurencia snyderae*. Oil.

3α-Hydroxy: ***Perforenone A***
[57566-99-1]
$C_{15}H_{22}O_2$ 234.338
Constit. of *Laurencia perforata*.
Mp 120-121°. $[\alpha]_D$ -116.

3β-Hydroxy: ***Perforenone C***
[66141-71-7]
$C_{15}H_{22}O_2$ 234.338
Constit. of *Laurencia perforata*. Cryst.
Mp 67-68°. $[\alpha]_D$ -29.

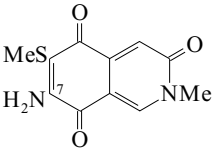
3β-Methoxy: ***3β-Methoxyperforenone***
[474511-71-2]
$C_{16}H_{24}O_2$ 248.364
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ -2.7 (c, 0.33 in $CHCl_3$).
λ_{max} 246 (log ϵ 3.91) (hexane).

3α-Chloro: ***Perforenone B***
[57567-00-7]
$C_{15}H_{21}ClO$ 252.783
Constit. of *Laurencia perforata*. Cryst.
Mp 190°. $[\alpha]_D$ -117.

Gonzalez, A.G. *et al., Tet. Lett.*, 1975, 2499; 1977, 3375; 1978, 481 (*isol, struct, synth*)
Howard, B.M. *et al., Phytochemistry*, 1979, **18**, 1224-1225 (*Guadalupol, Epiguadalupol*)
Majetich, G. *et al., Heterocycles*, 1987, **25**, 271 (*synth*)
Iliopoulou, D. *et al., Tetrahedron*, 2002, **58**, 6749-6755 (*Perforenone, 3β-Methoxyperforenone*)

Perfragilin A P-262

*7-Amino-2-methyl-6-(methylthio)-3,5,8(2*H*)-isoquinolinetrione, 9CI*
[129722-94-7]



$C_{11}H_{10}N_2O_3S$ 250.278
Alkaloid from the bryozoan *Membranipora perfragilis*. Cytotoxic agent. Red needles.
Mp 219-220°. λ_{max} 212 (ϵ 12616); 248 (ϵ 7000); 330 (ϵ 15140); 362 (ϵ 8785); 440 (ϵ 2224) (EtOH) (Berdy).

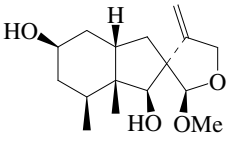
Deamino: ***2-Methyl-6-(methylthio)-3,5,8(2H)-isoquinolinetrione***
$C_{11}H_9NO_3S$ 235.263
Isol. from bryozoan *Biflustra perfragilis*. Yellow powder.
λ_{max} 367 (ϵ 10594) (no solvent reported).

7-Deamino, 7-(methylthio): 2-Methyl-6,7-bis(methylthio)-3,5,8(2H)-isoquinolinetrione, 9CI. ***Perfragilin B***
[146764-79-6]
$C_{12}H_{11}NO_3S_2$ 281.356
Alkaloid from *Membranipora perfragilis* and *Biflustra perfragilis*. Cytotoxic (considerably more potent than Perfragilin A). Red needles or orange plates.
Mp 163° Mp 170-172°. Also obt. as a metastable green powder. λ_{max} 214 (ϵ 14941); 235 (ϵ 10504); 332 (ϵ 8227); 382 (ϵ 5946); 465 (ϵ 1848) (EtOH) (Berdy).

Rizvi, S.K. *et al., Acta Cryst. C*, 1993, **49**, 151 (*cryst struct*)
Blackman, A.J. *et al., Aust. J. Chem.*, 1993, **46**, 213-220 (*7-deamino, 7-deamino-7-methylthio, isol, cryst struct*)
Choi, Y.-H. *et al., J. Nat. Prod.*, 1993, **56**, 1431-1433 (*isol, uv, ir, pmr, cmr, ms, struct*)
Ferreira, V.F. *et al., Tetrahedron*, 2003, **59**, 1349-1357 (*synth*)

Peribysin E P-263

[859509-60-7]



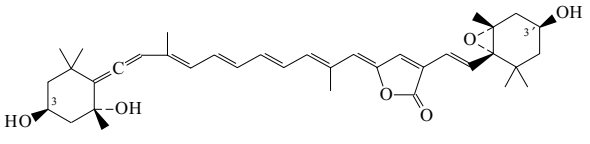
Absolute Configuration

$C_{16}H_{26}O_4$ 282.379
Prod. by a marine-derived *Periconia byssoides* OUPS-N133. Pale yellow oil. $[\alpha]_D$ -262.2 (c, 0.11 in EtOH). λ_{max} 208 (log ϵ 3.79); 261 (log ϵ 2.97); 311 (log ϵ 2.64) (EtOH).

Yamada, T. *et al., J. Antibiot.*, 2005, **58**, 185-191 (*isol, pmr, cmr*)

Peridininol P-264

[54369-14-1]

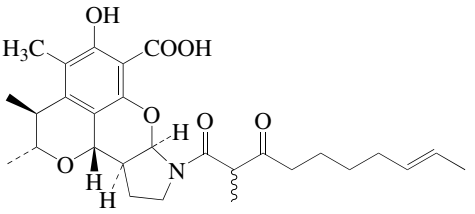


$C_{37}H_{48}O_6$ 588.783
Constit. of the Dinophyceae.

3-Ac: ***Peridinin***. *Sulcatoxanthin*
[33281-81-1]
$C_{39}H_{50}O_7$ 630.82
Constit. of the Dinophyceae. Also isol. from the sea squirt *Botrylloides violaceus* and coelenterate *Anemonia sulcata*. Pigment responsible for 'red tide' algal blooms. Purple cryst. (Et_2O/hexane).
Mp 128-132°. λ_{max} 472 (EtOH). λ_{max} 458; 485 (hexane).

Johansen, J.E. *et al., Phytochemistry*, 1974, **13**, 2261; 1980, **19**, 441 (*isol, abs config*)
Kjosen, H. *et al., Acta Chem. Scand., Ser. B*, 1976, **30**, 157 (*struct*)
Swift, I.E. *et al., Phytochemistry*, 1982, **21**, 2859 (*biosynth*)
Skjenstad, T. *et al., Biochem. Syst. Ecol.*, 1984, **12**, 149 (*isol, pmr, cmr*)
Matsuno, T. *et al., Nippon Suisan Gakkaishi*, 1984, **50**, 1267 (*Peridinin, isol, sea squirt*)
Ito, M. *et al., J.C.S. Perkin 1*, 1990, 197 (*synth*)
Krane, J. *et al., Magn. Reson. Chem.*, 1992, **30**, 1169 (*pmr, cmr*)
Yamano, Y. *et al., J.C.S. Perkin 1*, 1993, 1599 (*synth*)
Furuichi, N. *et al., J.O.C.*, 2004, **69**, 7949-7959 (*synth*)
Vaz, B. *et al., Org. Lett.*, 2005, **7**, 545-548 (*synth*)
Olpp, T. *et al., Angew. Chem., Int. Ed.*, 2006, **45**, 4023-4027 (*synth*)

Perinadine A P-265



$C_{28}H_{37}NO_7$ 499.603
Prod. by a marine-derived *Penicillium citrinum* strain N055. Amorph. solid. $[\alpha]_D^{22}$ -33 (c, 1 in $CHCl_3$). λ_{max} 215 (ϵ 16000); 252 (ϵ 3600); 315 (ϵ 1700) (MeOH).

Sasaki, M. *et al., Org. Lett.*, 2005, **7**, 4261-4264 (*isol, pmr, cmr*)

Perinerin P-266

Peptide containing 51 amino acid residues. Isol. from the clamworm *Perinereis aibuhitensis*. Shows antimicrobial activity.

Pan, W. *et al., J. Biochem. (Tokyo)*, 2004, **135**, 297-304 (*isol*)

Perlucin P-267

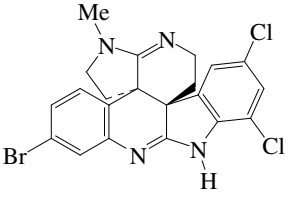
[330492-46-1]

Protein containing 155 amino acid residues including a glycosylated asparagine. Isol. from shell of abalone (*Haliotis laevigata*).

Weiss, I.M. *et al., Biochem. Biophys. Res. Commun.*, 2000, **267**, 17-21 (*isol*)
Mann, K. *et al., Eur. J. Biochem.*, 2000, **267**, 5257-5264 (*struct*)

Perophoramidine P-268

[474779-75-4]

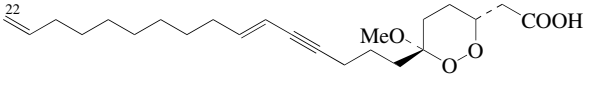


$C_{21}H_{17}BrCl_2N_4$ 476.202
Alkaloid from the Philippine ascidian *Perophora namei*. Cytotoxic. Amorph. off-white solid. λ_{max} 220 (ϵ 13300); 240 (sh) (ϵ 10300); 298 (sh) (ϵ 5800); 308 (ϵ 6800); 338 (ϵ 4600) (MeOH).

Verbitski, S.M. *et al., J.O.C.*, 2002, **67**, 7124-7126 (*isol, uv, cd, pmr, cmr, ms*)
Fuchs, J.R. *et al., J.A.C.S.*, 2004, **126**, 5068-5069 (*synth*)

Peroxyacarnoic acid A P-269

6-(6,15-Hexadecadien-4-ynyl)-6-methoxy-1,2-dioxane-3-acetic acid. 3,6-Epidioxy-6-methoxy-12,21-docosadien-10-ynoic acid
[203793-30-0]



$C_{23}H_{36}O_5$ 392.534
Isol. from the marine sponge *Acarnus* cf. *bergquistae*. Oil (as Me ester). $[\alpha]_D$ -26 (c, 0.2 in $CHCl_3$)(Me ester). CAS no. refers to Me ester. λ_{max} 204; 288 (EtOH) (Me ester).

21,22-Dihydro: ***Peroxyacarnoic acid D***
$C_{23}H_{38}O_5$ 394.55
Isol. from *Acarnus bicladotylata*. Powder (as Me ester). $[\alpha]_D$ -10.1 (c, 0.2 in $CHCl_3$) (Me ester).

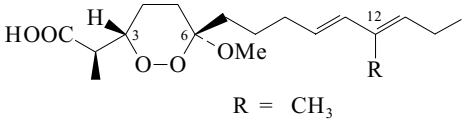
21,22-Dihydro, 21-oxo: ***Peroxyacarnoic acid C***
$C_{23}H_{36}O_6$ 408.534
Isol. from *Acarnus bicladotylata*. Pale yellow powder (as Me ester). $[\alpha]_D$ -12.1 (c, 0.09 in $CHCl_3$) (Me ester). λ_{max} 206 (ϵ 46000); 230 (ϵ 32000) (EtOH) (Me ester).

21,22-Didehydro: 6-(6-Hexadecene-4,15-diynyl)-6-methoxy-1,2-dioxane-3-acetic acid. 3,6-Epidioxy-6-methoxy-12-docosene-10,21-diynoic acid. ***Peroxyacarnoic acid B***
[203793-33-3]
$C_{23}H_{34}O_5$ 390.519
Isol. from the marine sponge *Acarnus* cf. *bergquistae*. Oil (as Me ester). $[\alpha]_D$ -26 (c, 0.2 in $CHCl_3$)(Me ester). CAS no. refers to Me ester. λ_{max} 204; 228 (EtOH) (Me ester).

Yosief, T. *et al., J. Nat. Prod.*, 1998, **61**, 491-493 (*isol, pmr, cmr, ms*)
Fontana, A. *et al., J. Nat. Prod.*, 2001, **64**, 131-133 (*isol, pmr, cmr, ms, abs config*)
Xu, C. *et al., Org. Lett.*, 2005, **7**, 2509-2511 (*synth*)

Peroxyplakoric acid A_1 P-270

[155866-97-0]



$C_{18}H_{30}O_5$ 326.432
Isol. from the sponge *Plakortis* sp. Antifungal agent. Amorph. solid (as Me ester). $[\alpha]_D$ -164 ($CHCl_3$) (as Me ester). λ_{max} 235 (ϵ 22000) (MeOH) (Berdy).

12Z-Isomer: ***Peroxyplakoric acid A_2***
[155900-14-4]
Isol. from a *Plakortis* sp.
$[\alpha]_D$ -163 ($CHCl_3$) (as Me ester). λ_{max} 237 (ϵ 20000) (MeOH) (Berdy).

3-Epimer: ***Peroxyplakoric acid B_1***
[155900-15-5]
$C_{18}H_{30}O_5$ 326.432
Isol. from a *Plakortis* sp.
$[\alpha]_D$ -197 ($CHCl_3$) (as Me ester). λ_{max} 235 (ϵ 22000) (MeOH) (Berdy).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1324 (*isol, pmr, struct*)

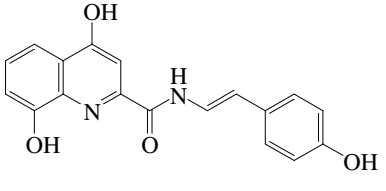
Peroxyplakoric acid A_3 P-271

[155866-98-1]
As Peroxyplakoric acid A_1, P-270 with
R = H
$C_{17}H_{28}O_5$ 312.405
Isol. from the sponge *Plakortis* sp. Antifungal agent. $[\alpha]_D$ -167 ($CHCl_3$) (as Me ester). λ_{max} 230 (ϵ 21000) (MeOH) (Berdy).

3-Epimer: ***Peroxyplakoric acid B_3***
[155900-16-6]
$C_{17}H_{28}O_5$ 312.405
Isol. from a *Plakortis* sp.
$[\alpha]_D$ -191 ($CHCl_3$) (as Me ester). λ_{max} 230 (ϵ 21000) (MeOH) (Berdy).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1324 (*isol, pmr, struct*)

Perspicamide A P-272



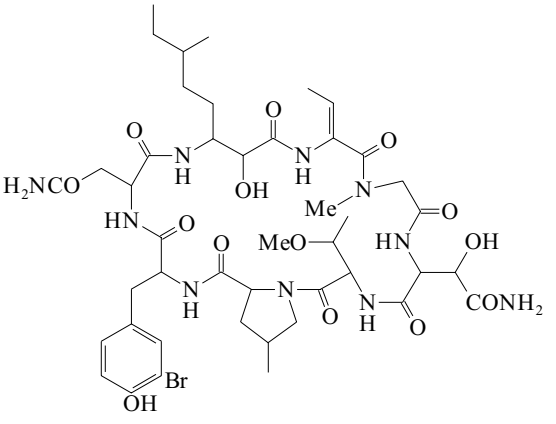
$C_{18}H_{14}N_2O_4$ 322.32
Isol. from *Botrylloides perspicum*. Pale yellow solid. λ_{max} 230 (ϵ 15830); 246 (ϵ 16000); 314 (ϵ 6620); 349 (ϵ 7460) (MeOH).

Z-Isomer: ***Perspicamide B***
$C_{18}H_{14}N_2O_4$ 322.32
Isol. from *Botrylloides perspicum*. Pale yellow solid. λ_{max} 221 (ϵ 17725); 246 (ϵ 16645); 315 (ϵ 6800); 347 (ϵ 7680) (MeOH).

McKay, M.J. *et al., J. Nat. Prod.*, 2005, **68**, 1776-1778 (*isol, pmr, cmr, ms*)

Perthamide B P-273

[158204-53-6]

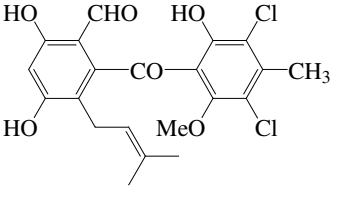


$C_{44}H_{65}BrN_{10}O_{14}$ 1037.96
Cyclic peptide antibiotic. Isol. from the sponge *Theonella* sp. Amorph. solid.
Mp 228-231°. $[\alpha]_D^{23}$ +19.8 (c, 0.2 in Py). λ_{max} 202 (ϵ 54000); 225 (sh) (ϵ 23000); 281 (ϵ 1600); 290 (ϵ 1300) (MeOH).

Gulavita, N.K. *et al., Tet. Lett.*, 1994, **35**, 6815-6 (*isol, uv, ir, pmr, cmr*)

Pestalone P-274

2-(3,5-Dichloro-2-hydroxy-6-methoxy-4-methylbenzoyl)-4,6-dihydroxy-3-(3-methyl-2-butenyl)benzaldehyde. 3,5-Dichloro-2′-formyl-2,3′,5′-trihydroxy-6-methoxy-4-methyl-6′-prenylbenzophenone



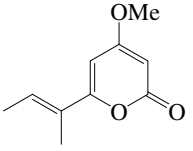
$C_{21}H_{20}Cl_2O_6$ 439.291
Prod. by a marine *Pestalotia* sp. isol. from the alga *Rosenvingea* sp., in response to bacterial challenge. Antibacterial agent active against MRSA. Cytotoxic. Yellow cryst.
Mp 153-155°. λ_{max} 238 (log ϵ 4.24); 281 (log ϵ 4.29); 340 (log ϵ 3.75) (CH_2Cl_2).

O-*De-Me:* ***De-O-methylpestalone***. *SB87-Cl*
[163768-83-0]
$C_{20}H_{18}Cl_2O_6$ 425.264
Prod. by *Chrysosporium* sp. Inhibitor of testosterone 5α-reductase.

Japan. Pat., 1995, 95 61 950; *CA*, **123**, 8034t (*De-O-methylpestalone*)
Cueto, M. *et al., J. Nat. Prod.*, 2001, **64**, 1444-1446 (*isol, uv, ir, pmr, cmr*)
Iijima, D. *et al., Tet. Lett.*, 2004, **45**, 5469-5471 (*synth*)

Pestalopyrone P-275

*4-Methoxy-6-(1-methyl-1-propenyl)-2*H*-pyran-2-one, 9CI. Demethylnectriapyrone*
[134956-10-8]



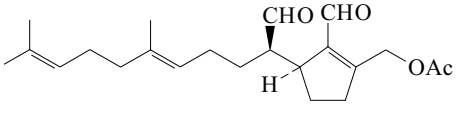
$C_{10}H_{12}O_3$ 180.203
Metab. of *Pestalotiopsis oenotherae* and prod. by an unidentified fungus from a marine sponge. Cryst. (MeOH/hexane).
Mp 101°. λ_{max} 223 (ϵ 37000); 309 (ϵ 10000) (MeOH) (Derep).

3′-Hydroxy: ***Hydroxypestalopyrone***
[171297-98-6]
$C_{10}H_{12}O_4$ 196.202
Prod. by *Pestalotiopsis microspora*. Antifungal agent. Powder.

Venkatasubbaiah, P. *et al., Phytochemistry*, 1991, **30**, 1471 (*isol, pmr, cmr*)
Abrell, L.M. *et al., Tet. Lett.*, 1994, **35**, 9159 (*isol*)
Lee, J.C. *et al., Chem. Biol.*, 1995, **2**, 721-727 (*Hydroxypestalopyrone*)

Petiodial P-276

[88192-90-9]



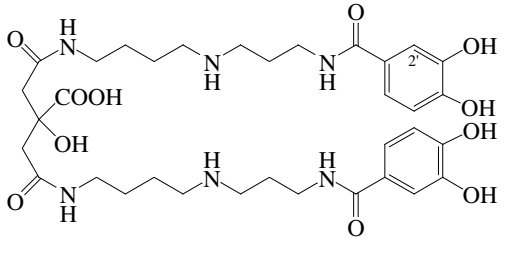
$C_{22}H_{32}O_4$ 360.492
Constit. of *Udotea petiolata*. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -25.7 (c, 0.5 in $CHCl_3$). λ_{max} 248 (ϵ 6500) (MeOH) (Berdy).

[93922-83-9, 115403-94-6, 122741-37-1, 122741-38-2]

Fattorusso, E. *et al., Experientia*, 1983, **39**, 1275 (*isol*)
Trost, B.M. *et al., J.A.C.S.*, 1988, **110**, 5233 (*synth*)
Isoe, S. *et al., Tet. Lett.*, 1988, **29**, 4591 (*synth, abs config*)

Petrobactin P-277

[545434-89-7]



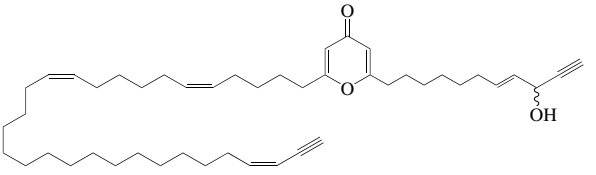
$C_{34}H_{50}N_6O_{11}$ 718.803
Struct. revised in 2003; formerly assigned as bis(2,3-dihydroxybenzoyl). Prod. by *Marinobacter hydrocarbonoclasticus*. Photoreactive siderophore.

2′-Sulfo: ***Petrobactin sulfonate***
$C_{34}H_{50}N_6O_{14}S$ 798.867
Prod. by *Marinobacter hydrocarbonoclasticus*. Amorph. solid. $[\alpha]_D^{20}$ -2.5 (c, 0.013 in DMSO). λ_{max} 229 (log ϵ 3.95); 253 (log ϵ 3.83); 291 (log ϵ 3.74) (DMSO).

Barbeau, K. *et al., J.A.C.S.*, 2002, **124**, 378-379 (*isol, pmr, cmr, ms*)
Bergeron, R.J. *et al., Tetrahedron*, 2003, **59**, 2007-2014 (*synth, struct*)
Hickford, S.J.H. *et al., J. Nat. Prod.*, 2004, **67**, 1897-1899 (*Petrobactin sulfonate*)
Gardner, R.A. *et al., J.O.C.*, 2004, **69**, 3530-3537 (*synth, pmr, cmr*)

Petrocortyne C P-278

*2-(9-Hydroxy-7-undecen-10-ynyl)-6-(5,11,27-tricosatrien-29-ynyl)-4*H*-pyran-4-one*

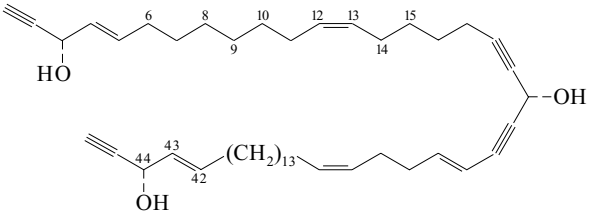


$C_{46}H_{70}O_3$ 671.057
Isol. from the sponge *Petrosia* sp. Cytotoxic agent. Yellow oil. $[\alpha]_D^{25}$ +6.2 (c, 0.2 in MeOH). λ_{max} 223 (log ϵ 4.31); 252 (log ϵ 4.04) (MeOH). λ_{max} 222 (log ϵ 4.1); 255 (log ϵ 3.8) (MeOH).

Seo, Y. *et al., Tetrahedron*, 1998, **54**, 447-462 (*isol, uv, ir, pmr, cmr, ms*)
Lim, Y.J. *et al., J. Nat. Prod.*, 2001, **64**, 46-53 (*isol, uv, pmr, cmr, ms*)
Young, J.L. *et al., J. Nat. Prod.*, 2001, **64**, 46-53 (*isol, props, activity*)

Petroformyne 1 P-279

4,12,23,27,42-Hexatetracontapentaene-1,18,21,45-tetrayne-3,20,44-triol, 9CI
[124739-43-1]



$C_{46}H_{68}O_3$ 669.041
Constit. of *Petrosia ficiformis*. Cytotoxic, inhibits sea urchin egg development. Sol. Me_2CO, hexane; poorly sol. H_2O. $[\alpha]_D^{25}$ +12.5 (c, 10 in $CHCl_3$). λ_{max} 232 (ϵ 15600) (MeOH) (Derep).

3- or 44-Ketone: ***Petroformyne 10***
$C_{46}H_{66}O_3$ 667.026
Constit. of *Petrosia ficiformis*. Pale yellow oil. $[\alpha]_D^{21}$ -3.5 (c, 1 in $CHCl_3$). Struct. not fully known. λ_{max} 230 (ϵ 31000) (MeOH) (Berdy).

3,44-Diketone: 20-Hydroxy-4,12,23,27,42-hexatetracontapentaene-1,18,21,45-tetrayne-3,44-dione. ***3,44-Dioxopetroformyne 1***
$C_{46}H_{64}O_3$ 665.01
Constit. of *Petrosia ficiformis*. Pale yellow oil. $[\alpha]_D^{21}$ -2.5 (c, 0.9 in $CHCl_3$). λ_{max} 232 (ϵ 38000) (MeOH) (Berdy).

23,24-Dihydro, 44-deoxy, Δ^{43}-isomer: ***23,24-Dihydropetroformyne 4***
$C_{46}H_{70}O_2$ 655.058
Isol. from *Petrosia ficiformis*. Oil. $[\alpha]_D^{21}$ +5 (c, 0.05 in $CHCl_3$). λ_{max} 228 (ϵ 27000) (MeOH). λ_{max} 228 (ϵ 27000) (MeOH) (Berdy).

42,43-Dihydro, 44-deoxy: ***Petroformyne 3***
[124739-45-3]
$C_{46}H_{70}O_2$ 655.058
Constit. of *Petrosia ficiformis*. Cytotoxic agent. Sol. Me_2CO, hexane; poorly sol. H_2O. $[\alpha]_D$ +10 ($CHCl_3$). λ_{max} 232 (ϵ 15600) (MeOH) (Derep).

42,43-Dihydro, 44-deoxy, 20-ketone: 3-Hydroxy-4,12,23,27-hexatetracontatetraene-1,18,21,45-tetrayn-20-one. ***20-Oxopetroformyne 3***
$C_{46}H_{68}O_2$ 653.042
Constit. of *Petrosia ficiformis*. Pale yellow oil. $[\alpha]_D^{21}$ -1 (c, 0.3 in $CHCl_3$). λ_{max} 230 (ϵ 19000) (MeOH) (Berdy).

42,43-Dihydro, 44-deoxy, 23-isomer: ***Isopetroformyne 3***
$C_{46}H_{70}O_2$ 655.058
Constit. of *Petrosia ficiformis*. Pale yellow oil. $[\alpha]_D^{21}$ +20 (c, 0.06 in $CHCl_3$). λ_{max} 231 (ϵ 40000) (MeOH) (Berdy).

42,43-Dihydro, 44-deoxy, 20-ketone, 23Z-isomer: ***20-Oxoisopetroformyne 3***
$C_{46}H_{68}O_2$ 653.042
Isol. from *Petrosia ficiformis*. Oil. $[\alpha]_D^{21}$ +2.7 (c, 0.1 in $CHCl_3$). λ_{max} 228 (ϵ 21000) (MeOH). λ_{max} 228 (ϵ 19000) (MeOH) (Berdy).

44-Deoxy, Δ^{43}-isomer: ***Petroformyne 4***
[124764-12-1]
$C_{46}H_{68}O_2$ 653.042
Constit. of *Petrosia ficiformis*. Cytotoxic agent. Sol. Me_2CO, hexane; poorly sol. H_2O. $[\alpha]_D$ +6 ($CHCl_3$). λ_{max} 232 (ϵ 15600) (MeOH) (Derep).

44-Deoxy, Δ^{43}-isomer, 23Z-isomer: ***Isopetroformyne 4***
$C_{46}H_{68}O_2$ 653.042
Constit. of *Petrosia ficiformis*. Pale yellow oil. $[\alpha]_D^{21}$ +25 (c, 0.1 in $CHCl_3$). λ_{max} 228 (ϵ 41000) (MeOH) (Berdy).

44-Deoxy, Δ^{43}-isomer, 23Z-isomer, 20-ketone: ***20-Oxoisopetroformyne 4***
$C_{46}H_{66}O_2$ 651.026
Isol. from *Petrosia ficiformis*. Oil. $[\alpha]_D$ +0.25 ($CHCl_3$). λ_{max} 228 (ϵ 19000) (MeOH). λ_{max} 228 (ϵ 21000) (MeOH) (Berdy).

4,5,42,43-Tetrahydro, 44-deoxy, 23Z-isomer: 12,23,27-Hexatetracontatriene-1,18,21,45-tetrayne-3,20-diol. ***4,5-Dihydroisopetroformyne 3***
$C_{46}H_{72}O_2$ 657.074
Constit. of *Petrosia ficiformis*. Oil. $[\alpha]_D^{21}$ +1.8 (c, 0.2 in $CHCl_3$). λ_{max} 230 (ϵ 32000) (MeOH) (Berdy).

8,9,14,15-Tetradehydro(Z,Z-), 12,13-dihydro, 3,44-diketone: 20-Hydroxy-4,8,14,23,27,42-hexatetracontahexaene-1,18,21,45-tetrayne-3,44-dione. ***3,44-Dioxopetroformyne 2***
$C_{46}H_{62}O_3$ 662.994
Constit. of *Petrosia ficiformis*. Oil. $[\alpha]_D^{21}$ +2.3 (c, 0.6 in $CHCl_3$). λ_{max} 232 (ϵ 42000) (MeOH) (Berdy).

8,9,14,15-Tetradehydro(Z,Z-), 12,13-dihydro: ***Petroformyne 2***
[124739-44-2]
$C_{46}H_{66}O_3$ 667.026
Constit. of *Petrosia ficiformis*. Cytotoxic agent, inhibits sea-urchin egg development. Sol. Me_2CO, hexane; poorly sol. H_2O. $[\alpha]_D^{25}$ +15 ($CHCl_3$). λ_{max} 232 (ϵ 15600) (MeOH) (Derep).

8,9,14,15-Tetradehydro(Z,Z-), 12,13-dihydro, 3-ketone: 20,44-Dihydroxy-4,8,14,23,27,42-hexatetracontahexaene-1,18,21,45-tetrayn-3-one. ***Petroformyne 8***
[161238-91-1]
$C_{46}H_{64}O_3$ 665.01
Constit. of *Petrosia ficiformis*. Oil. $[\alpha]_D^{21}$ +3.6 (c, 0.7 in $CHCl_3$). λ_{max} 231 (ϵ 30000) (MeOH) (Berdy).

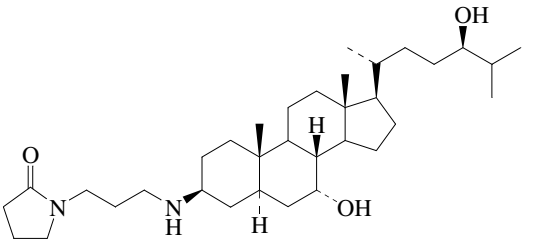
23,24,42,43-Tetrahydro, 44-deoxy, 20-ketone: 3-Hydroxy-4,12,27-hexatetracontatriene-1,18,21,45-tetrayn-20-one. ***23,24-Dihydro-20-oxopetroformyne 3***
$C_{46}H_{70}O_2$ 655.058
Constit. of *Petrosia ficiformis*. Oil. $[\alpha]_D^{21}$ +6.8 (c, 0.3 in $CHCl_3$). λ_{max} 231 (ϵ 15700) (MeOH) (Berdy).

6S-Hydroxy: 4,12,23,27,42-Hexatetracontapentaene-1,18,21,45-tetrayne-3,6,20,44-tetrol. ***Petroformyne 5***
[128646-05-9]
$C_{46}H_{68}O_4$ 685.041
Constit. of *Petrosia ficiformis*.

Cimino, G. *et al., Tet. Lett.*, 1989, **30**, 3563
Cimino, G. *et al., J. Nat. Prod.*, 1990, **53**, 345 (*Petroformyne 5*)
Guo, Y. *et al., Tetrahedron*, 1994, **50**, 13261 (*abs config*)
Guo, Y. *et al., J. Nat. Prod.*, 1995, **58**, 713; 1998, **61**, 333-337 (*isol, pmr, cmr, derivs*)

Petromyzonamine P-280

[871332-07-9]



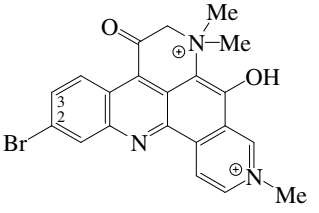
$C_{34}H_{60}N_2O_3$ 544.86

7,24-Disulfate: ***Petromyzonamine disulfate***
[871543-67-8]
$C_{34}H_{60}N_2O_9S_2$ 704.988
Pheromone of the sea lamprey (*Petromyzon marinus*).

Sorensen, P.W. *et al., Nat. Chem. Biol.*, 2005, **1**, 324-328

Petrosamine P-281

[113403-19-3]



$C_{21}H_{18}BrN_3O_2^{\oplus}$ 424.296

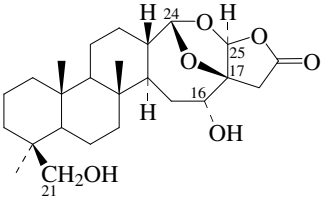
Minor struct. revision in 2005. Originally descr. as the 5-oxo monocation tautomer. Props. given refer to the chloride, which should presumably be reassigned as dichloride (or chloride-hydrochloride). Alkaloidal pigment from the marine sponge *Petrosia* sp. Dark green cryst. (CH_2Cl_2/MeOH) (as dichloride). Mp 330° (chloride). λ_{max} 284 (ϵ 32000); 345 (ϵ 10900); 574 (ϵ 4700) (H_2O). λ_{max} 289 (ϵ 42600); 346 (ϵ 12400); 414 (sh) (ϵ 6900); 595 (ϵ 5300) (MeOH).

Debromo, 3-bromo: ***Petrosamine B***
$C_{21}H_{18}BrN_3O_2^{\oplus}$ 424.296
Alkaloid from the Australian sponge *Oceanapia* sp. Weak inhibitor of aspartyl semialdehyde dehydrogenase. Blue solid (as bis(trifluoroacetate)). λ_{max} 205 (ϵ 34610); 288 (ϵ 30460); 378 (ϵ 15845); 609 (ϵ 4385) (MeOH) (bis(trifluoroacetate)).

Molinski, T.F. *et al., J.O.C.*, 1988, **53**, 1340-1341 (*isol, uv, ir, pmr, cmr, cryst struct*)
Carroll, A.R. *et al., J. Nat. Prod.*, 2005, **68**, 804-806 (*tautom, Petrosamine B*)

Petrosaspongiolide G P-282

[194198-89-5]



$C_{25}H_{38}O_6$ 434.572
Isol. from the New Caledonian marine sponge *Petrosaspongia nigra*. Cytotoxic agent. $[\alpha]_D$ -25.2 (c, 0.002 in MeOH). Indexed as its 21-Ac in CA.

16-Ac: ***Petrosaspongiolide D***
[194148-83-9]
$C_{27}H_{40}O_7$ 476.609
Isol. from *Petrosaspongia nigra*.
$[\alpha]_D$ -27 (c, 0.003 in $CHCl_3$).

16,21-Di-Ac: ***Petrosaspongiolide C***
[194148-82-8]
$C_{29}H_{42}O_8$ 518.646
Isol. from *Petrosaspongia nigra*.
$[\alpha]_D$ -12.5 (c, 0.003 in $CHCl_3$).

21-Aldehyde, 16-Ac: ***Petrosaspongiolide E***
[194148-84-0]
$C_{27}H_{38}O_7$ 474.593
Isol. from *Petrosaspongia nigra*.
$[\alpha]_D$ -19.4 (c, 0.003 in $CHCl_3$).

21-Carboxylic acid: ***Petrosaspongiolide H***
[194148-91-9]
$C_{25}H_{36}O_7$ 448.555
Isol. from *Petrosaspongia nigra*.
$[\alpha]_D$ +4.3 (c, 0.003 in MeOH).

21-Carboxylic acid, 16-Ac: ***Petrosaspongiolide F***
[194148-87-3]
$C_{27}H_{38}O_8$ 490.592
Isol. from *Petrosaspongia nigra*.
$[\alpha]_D$ -17.8 (c, 0.002 in MeOH).

21-Deoxy, 16-Ac: ***Petrosaspongiolide A***. *Ircinolide A*
[152110-09-3]
$C_{27}H_{40}O_6$ 460.609
Isol. from *Petrosaspongia nigra*, a *Dactylospongia* sp. and an *Ircinia* sp. Antitumour agent. Cryst.
Mp 248-251°. $[\alpha]_D$ -15 (c, 0.02 in $CHCl_3$).

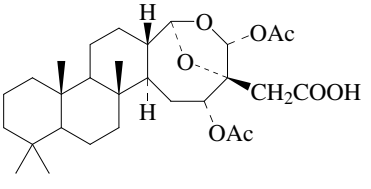
17,24,25-Triepimer, 16,21-di-Ac: ***Petrosaspongiolide I***
[194148-93-1]
$C_{29}H_{42}O_8$ 518.646
Isol. from *Petrosaspongia nigra*.
$[\alpha]_D$ -28 (c, 0.001 in $CHCl_3$).

17,24,25-Triepimer, 21-deoxy, 16-Ac: ***Petrosaspongiolide B***. *Ircinolide B*
[152186-77-1]
$C_{27}H_{40}O_6$ 460.609
Isol. from *Petrosaspongia nigra* and an *Ircinia* sp. Antitumour agent. Cryst.
Mp 238-240°. $[\alpha]_D$ -71 (c, 0.03 in $CHCl_3$).

Japan. Pat., 1993, 213 988; *CA*, **120**, 45936x (*Ircinolides*)
Lal, A.R. *et al., Tet. Lett.*, 1994, **35**, 2603-2606 (*isol, pmr, cmr*)
Cambie, R.C. *et al., Acta Cryst. C*, 1996, **52**, 709-711 (*cryst struct*)
Paloma, L.G. *et al., Tetrahedron*, 1997, **53**, 10451-10458 (*isol, pmr, cmr*)

Petrosaspongiolide J P-283

[194148-95-3]

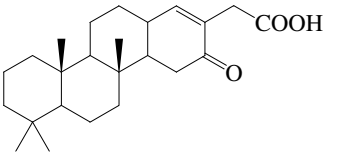


$C_{29}H_{44}O_8$ 520.662
Isol. from the marine sponge *Petrosaspongia nigra*. Cytotoxic.
Amorph. solid. $[\alpha]_D$ -14.5 (c, 0.003 in $CHCl_3$).

Paloma, L.G. *et al., Tetrahedron*, 1997, **53**, 10451-10458 (*isol, pmr, cmr*)

Petrosaspongiolide K P-284

[194148-97-5]

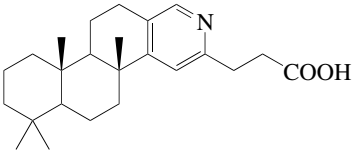


$C_{24}H_{36}O_3$ 372.547
Isol. from the marine sponge *Petrosaspongia nigra*. Cytotoxic.
$[\alpha]_D$ -15.4 (c, 0.004 in $CHCl_3$).

Paloma, L.G. *et al., Tetrahedron*, 1997, **53**, 10451-10458 (*isol, pmr, cmr*)

Petrosaspongiolide L P-285

[194148-99-7]

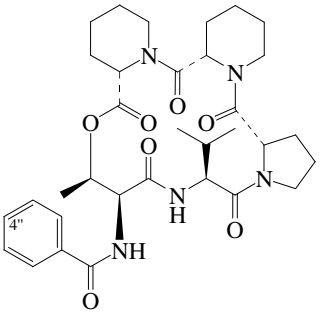


$C_{24}H_{35}NO_2$ 369.546
Alkaloid from the sponge *Petrosaspongia nigra*. Cytotoxic agent.
$[\alpha]_D$ -33.3 (c, 0.001 in MeOH). λ_{max} 210 (ϵ 5545); 266 (ϵ 2375) (no solvent reported).

N-*(Carboxymethyl)*: ***Spongidine C***
$C_{26}H_{38}NO_4^{\oplus}$ 428.591
Alkaloid from a *Spongia* sp. Inhibits human phospholipase A_2.
$[\alpha]_D$ -10 (c, 0.01 in MeOH). Counterion not specified. CAS no. not found 14CI.

Paloma, L.G. *et al., Tetrahedron*, 1997, **53**, 10451-10458 (*isol, uv, pmr, cmr*)
De Marino, S. *et al., J. Nat. Prod.*, 2000, **63**, 323-326 (*Spongidine C*)

Petrosifungin A P-286



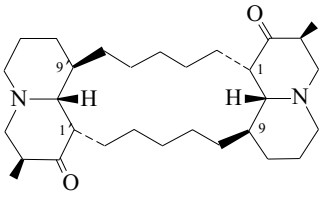
$C_{33}H_{45}N_5O_7$ 623.748
Prod. by a *Penicillium brevicompactum* isol. from the sponge *Petrosia ficiformis*. Amorph. solid.
Mp 162-164°. $[\alpha]_D^{25}$ -56.2 (c, 0.5 in MeOH).

4″-Hydroxy: ***Petrosifungin B***
$C_{33}H_{45}N_5O_8$ 639.747
Prod. by *Penicillium brevicompactum* from *Petrosia ficiformis*. Amorph. solid.
Mp 210-212°. $[\alpha]_D^{25}$ -37.9 (c, 0.5 in MeOH).

Bringmann, G. *et al., J. Nat. Prod.*, 2004, **67**, 311-315 (*isol, cd, pmr, cmr, ms*)

Petrosine P-287

[84679-41-4]



$C_{30}H_{50}N_2O_2$ 470.737

Alkaloid from the Papua-New Guinean marine sponge *Petrosia seriata* and from an Okinawan sponge *Xestospongia* sp. Ichthyotoxin.

Mp 215-216°. Petrosine C and Petrosine D are synthetic diastereoisomers of Petrosin A and B.

1,9-Diepimer: ***Petrosine B***

[95189-04-1]

$C_{30}H_{50}N_2O_2$ 470.737

From *Petrosia seriata*. Ichthyotoxin. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -12 (c, 0.79 in CH_2Cl_2).

1,3,9,10-Tetraepimer: ***Petrosine A***

[95189-03-0]

$C_{30}H_{50}N_2O_2$ 470.737

From *Petrosia seriata* and the *Xestospongia* sp. Ichthyotoxin. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Struct. revised in 1988. Originally described as the 1,1′,9,9′-tetraepimer. Opt. inactive (*meso* compd.). The low opt. rotn. originally reported refers to a sample contaminated with traces of Petrosine B.

3,3′,9,10-Tetraepimer: ***Xestosine A***

[290820-78-9]

$C_{30}H_{50}N_2O_2$ 470.737

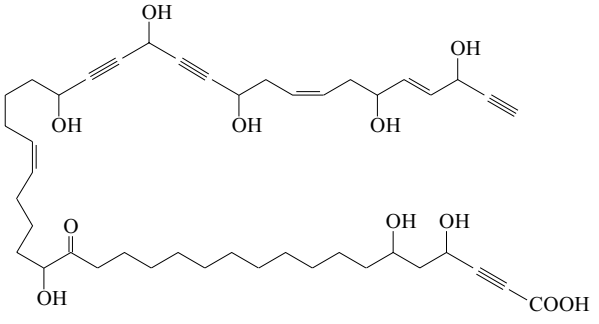
Alkaloid from *Xestospongia exigua*. Prisms (CH_2Cl_2/hexane). Mp 175-177°.

Braekman, J.C. *et al., Tet. Lett.*, 1982, **23**, 4277-4280 (*isol*)
Braekman, J.C. *et al., Bull. Soc. Chim. Belg.*, 1984, **93**, 941-944; 1988, **97**, 519-524 (*isol, pmr, cmr, cryst struct*)
Kobayashi, M. *et al., Tet. Lett.*, 1989, **30**, 4149-4152 (*isol, pmr, cmr, struct, Petrosine, Petrosine A*)
Heathcock, C.H. *et al., J.O.C.*, 1998, **63**, 5001-5012; 5013-5030 (*synth*)
Matzanke, N. *et al., Org. Prep. Proced. Int.*, 1998, **30**, 3-51 (*rev, synth*)
Iwagawa, T. *et al., J. Nat. Prod.*, 2000, **63**, 1310-1311 (*Xestosine A*)

Petrosolic acid P-288

4,6,19,28,31,34,39,42-Octahydroxy-18-oxo-23,36,40-tetratetracontatriene-2,29,32,43-tetraynoic acid, 9CI

[153127-40-3]



$C_{44}H_{64}O_{11}$ 768.983

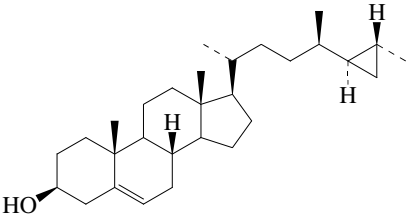
Isol. from the sponge *Petrosia* sp. Inhibitor of HIV reverse transcriptase. Amorph. powder. $[\alpha]_D^{22}$ +7 (c, 2.9 in MeOH).

Isaacs, S. *et al., Tetrahedron*, 1993, **49**, 10435 (*isol*)

Petrosterol P-289

24-(2-Methylcyclopropyl)-26,27-dinorcholest-5-en-3-ol, 9CI. 26,27-Cyclo-24,26-dimethylcholest-5-en-3-ol. 26,27-Cyclo-26-methylergost-5-en-3-ol. 26,27-Cycloaplysterol

[67314-15-2]



$C_{29}H_{48}O$ 412.698

Constit. of *Petrosia ficiformis* and *Peltodoris atromaculata*. Cryst. Mp 123-125°.

Ac:

Cryst. Mp 112-114°. $[\alpha]_D$ -41.5 ($CHCl_3$).

5α,6-Dihydro: ***5α-Petrostan-3β-ol***

[106566-89-6]

$C_{29}H_{50}O$ 414.713

Constit. of *Petrosia hebes*. Cryst. Mp 122-123°.

5β,6-Dihydro: ***5β-Petrostan-3β-ol***

[106518-69-8]

$C_{29}H_{50}O$ 414.713

Constit. of *Petrosia ficiformis*, prob. as endobacterial metab.

3-Epimer, 5β,6-dihydro: ***5β-Petrostan-3α-ol***

[106566-88-5]

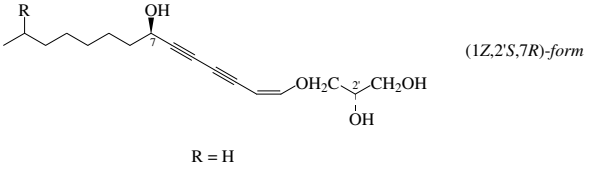
$C_{29}H_{50}O$ 414.713

Minor sterol from *Petrosia ficiformis*, prob. as endobacterial metab.

Sica, D. *et al., Tet. Lett.*, 1978, 837-838 (*isol*)
Mattia, C.A. *et al., Tet. Lett.*, 1978, 3953-3954 (*cryst struct*)
Ravi, B.N. *et al., Tet. Lett.*, 1978, 4379-4380 (*struct*)
Fujimoto, Y. *et al., Tet. Lett.*, 1985, **26**, 3239-3242 (*synth*)
Seidel, S.B. *et al., Steroids*, 1986, **47**, 49-62 (*5β-Petrostanols*)
Cho, J.-H. *et al., J.C.S. Perkin 1*, 1987, 1307-1318 (*5α-Petrostanol*)
Honda, T. *et al., J.C.S. Perkin 1*, 1996, 2291-2296 (*synth*)

Petrosyne I P-290

3-[(7-Hydroxy-1-tetradecene-3,5-diynyl)oxy]-1,2-propanediol, 9CI



(1*Z*,2′*S*,7*R*)-*form*

R = H

$C_{17}H_{26}O_4$ 294.39

Isol. from the sponge *Petrosia* sp. Oil (as tri-Ac). $[\alpha]_D$ -9.8 (c, 0.16 in MeOH) (tri-Ac). Isol. as a mixt. of Ia and Ib.

(1*Z*,2′*S*,7*R*)-*form*

Petrosyne Ia

[150999-01-2]

Oil. $[\alpha]_D$ +5.9 (c, 0.5 in MeOH) (synthetic).

(1*Z*,2′*S*,7*S*)-*form*

Petrosyne Ib

[150999-02-3]

Oil. $[\alpha]_D$ +7.2 (c, 0.21 in MeOH) (synthetic).

Iguchi, K. *et al., J.O.C.*, 1993, **58**, 5690-5698 (*isol, synth, pmr, cmr, ms*)

Petrosyne II P-291

3-[(7-Hydroxy-13-methyl-1-tetradecene-3,5-diynyl)oxy]-1,2-propanediol, 9CI. 1-O-(7-Hydroxy-13-methyl-1-tetradecene-3,5-diynyl)glycerol

[129602-14-8]

As Petrosyne I, P-290 with

R = CH_3

$C_{18}H_{28}O_4$ 308.417

Isol. from a New Zealand sponge, *Petrosia hebes*. Oil (as tri-Ac). $[\alpha]_D$ -9.1 (c, 0.09 in MeOH) (tri-Ac). Isol. as a mixt. of IIa and IIb. λ_{max} 223 (ϵ 14200); 262 (ϵ 6100); 276 (ϵ 8150); 292 (ϵ 6800) (MeOH) (Berdy).

(1*Z*,2′*S*,7*R*)-*form*

Petrosyne IIa

[151063-14-8]

(1*Z*,2′*S*,7*S*)-*form*

Petrosyne IIb

[151063-15-9]

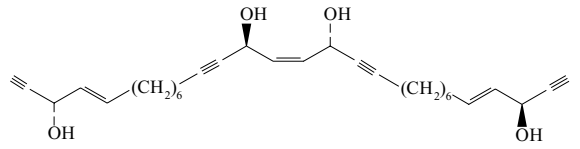
Perry, N.B. *et al., J. Nat. Prod.*, 1990, **53**, 732 (*isol, struct, pmr, cmr, ms, ir, uv*)

Iguchi, K. *et al., J.O.C.*, 1993, **58**, 5690-5698 (*isol, synth, pmr, cmr, ms*)

Petrosynol P-292

4,15,26-Triacontatriene-1,12,18,29-tetrayne-3,14,17,28-tetrol

[111554-19-9]



Absolute configuration

$C_{30}H_{40}O_4$ 464.644

Isol. from marine sponge *Petrosia* sp. and from *Adocia* sp. Exhibits antifungal props. HIV reverse transcriptase (HIV-rt) inhibitor. Oil. $[\alpha]_D^{22}$ +111 (c, 1.3 in $CHCl_3$).

3-Ac: ***Adociacetylene C***

[176182-12-0]

$C_{32}H_{42}O_5$ 506.681

Constit. of the sponge *Adocia* sp. Endothelial cell-neutrophil leukocyte adhesion inhibitor. Oil. $[\alpha]_D^{20}$ +90 (c, 0.5 in $CHCl_3$).

3-Ketone: 14,17,28-Trihydroxy-4,15,26-triacontatriene-1,12,18,29-tetrayn-3-one. ***Adociacetylene A***

[176227-11-5]

$C_{30}H_{38}O_4$ 462.628

Constit. of the sponge *Adocia* sp. Oil. $[\alpha]_D^{22}$ +110 (c, 0.3 in $CHCl_3$).

3,28-Diketone: ***14,17-Dihydroxy-4,15,16-triacontatriene-1,12,18,29-tetrayne-3,28-dione***

$C_{30}H_{36}O_4$ 460.612

Isol. from a sponge of the Niphatidae.

$[\alpha]_D$ +93 ($CHCl_3$).

Tetraketone: 4,15,26-Triacontatriene-1,12,18,29-tetrayne-3,14,17,28-tetrone, 9CI. ***Petrosynone***

[111397-55-8]

$C_{30}H_{32}O_4$ 456.58

From *Petrosia* sp. Active against *Bacillus subtilis*. Yellow oil. λ_{max} 261 (ϵ 6700) (MeOH) (Derep).

15,16-Dihydro, 14,17-diketone: 3,28-Dihydroxy-4,26-triacontadiene-1,12,18,29-tetrayne-14,17-dione. ***Adociacetylene D***

[155624-59-2]

$C_{30}H_{38}O_4$ 462.628

Constit. of the sponges *Adocia* sp. and *Petrosia* sp. Endothelial cell-neutrophil leukocyte adhesion inhibitor. Pale yellow oil. $[\alpha]_D^{22}$ +18.1 (c, 1 in $CHCl_3$). $[\alpha]_D^{22}$ +6 (c, 0.1 in $CHCl_3$). λ_{max} 221 (ϵ 22400); 225 (ϵ 21500) (MeOH) (Berdy).

15,16-Dihydro, tetraketone: ***4,26-Triacontadiene-1,12,18,29-tetrayne-3,14,17,28-tetrone***

$C_{30}H_{34}O_4$ 458.596

Isol. from a sponge of the family Niphatidae.

*15*E*-Isomer, tetraketone:*

$C_{30}H_{32}O_4$ 456.58

Isol. from a sponge of the family Niphatidae.

[86533-12-2]

Fusetani, N. *et al., Tet. Lett.*, 1987, **28**, 4313 (*isol, config*)

Isaacs, S. *et al., Tetrahedron*, 1993, **49**, 10435-10438 (*Petrosynol, activity*)

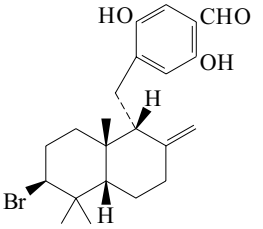
Ochi, M. *et al., Chem. Lett.*, 1994, 89 (*isol, uv, pmr, cmr, ms, deriv*)

Guyot, M. *et al., Pure Appl. Chem.*, 1994, **66**, 2223-2226 (*isol, derivs*)

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 720 (*isol, uv, ir, pmr, cmr, derivs*)

Peyssonol A P-293

[156848-67-8]



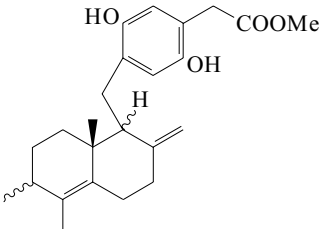
$C_{22}H_{29}BrO_3$ 421.373

Constit. of a *Peyssonnelia* sp. HIV reverse transcriptase (HIV-rt) inhibitor. Oil. $[\alpha]_D^{25}$ +2 (c, 0.1 in $CHCl_3$).

Talpir, R. *et al., Tetrahedron*, 1994, **50**, 4179 (*isol, pmr, cmr, activity*)

Peyssonol B P-294

[156848-68-9]



$C_{24}H_{32}O_4$ 384.514

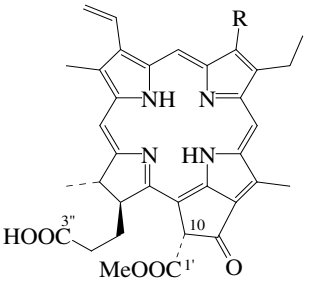
Constit. of a *Peyssonnelia* sp. Oil. $[\alpha]_D^{25}$ -57 (c, 0.1 in $CHCl_3$).

Talpir, R. *et al., Tetrahedron*, 1994, **50**, 4179 (*isol, pmr, cmr*)

Phaeophorbide a P-295

Pheophorbide a_5. Pheophorbide a

[15664-29-6]



R = CH_3

$C_{35}H_{36}N_4O_5$ 592.693

Chlorophyll degradation prod. Formed by enzymic hydrol. of Phaeophytin a, P-297 by chlorophyllase, or by mild acid or alkaline hydrol. Isol. from *Clerodendrum calamitosum*, *Undaria pinnatifida* , *Sargassum tortile*, *Trididemnum solidum*, *Psychotria acuminata* and other spp. Cytotoxic. Apoptosis inducer. MDR pump inhibitor in *Staphylococcus aureus.* Shows photosensitising effect; antipsoriatic agent. Synergistic with Berberine. Blue-black cryst. ($CHCl_3$). $[\alpha]_{Hg}^{20}$ -342 (Me_2CO). λ_{max} 408 (ϵ 84500); 666 (ϵ 38000) (MeOH) (Berdy).

3′′-Me ester: ***Methyl phaeophorbide a***
[5594-30-9]
$C_{36}H_{38}N_4O_5$ 606.72
Isol. from *Cupressus funebris* and *Tapura fischeri*. Deep blue-black microcryst. (CH_2Cl_2/MeOH).
Mp 228°.

3′′-Et ester: ***Ethyl phaeophorbide a***
[55100-98-6]
$C_{37}H_{40}N_4O_5$ 620.747
Constit. of *Tapura fischeri*. Amorph. $[\alpha]_D$ +7.8 (c, 1.6 in $CHCl_3$).

10-Hydroxy: ***10-Hydroxyphaeophorbide a***
[83688-53-3]
$C_{35}H_{36}N_4O_6$ 608.693
Isol. from *Clerodendrum calamitosum*, *Neptunia oleracea*, cells of *Chlorella* sp. and from the tunicate *Trididemnum solidum*. Cytotoxic agent. Dark green amorph. solid.

10-Hydroxy, 3′′-Me ester: ***Methyl 10-hydroxyphaeophorbide a***
[79733-03-2]
$C_{36}H_{38}N_4O_6$ 622.719
Isol. from *Clerodendrum cyrtophyllum* and the green alga *Dunaliella primolecta*. Dark green amorph. solid.

10-Hydroxy, 3′′-Et ester: ***Ethyl 10-hydroxyphaeophorbide a***
$C_{37}H_{40}N_4O_6$ 636.746
Isol. from the sponge *Dysidea* sp. Dark brown solid. $[\alpha]_D^{25}$ -6.5 (c, 0.2 in $CHCl_2$).

1′-Parent acid, 3′′-Et ester: [220969-03-9]
$C_{36}H_{38}N_4O_5$ 606.72
Constit. of *Tapura fischeri*. Amorph.

10-Epimer: ***10-Epiphaeophorbide a***. *Phaeophorbide a′*. *Pheophorbide a′*
[78964-31-5]
$C_{35}H_{36}N_4O_5$ 592.693
Constit. of the aerial parts of *Saussurea medusa*. Black-green powder. λ_{max} 318 (log ϵ 3.97); 421 (log ϵ 5.1); 533 (log ϵ 3.5); 566 (log ϵ 3.32); 605 (log ϵ 3.52); 657 (log ϵ 4.52) (MeOH).

10-Epimer, 3′′-Me ester: ***Methyl 10-epiphaeophorbide a***
[64070-09-3]
$C_{36}H_{38}N_4O_5$ 606.72
Constit. of the aerial parts of *Saussurea medusa*. Black-green powder. λ_{max} 276 (log ϵ 4.05); 329 (log ϵ 4.27); 414 (log ϵ 4.93); 508 (log ϵ 3.9); 539 (log ϵ 3.89); 610 (log ϵ 3.83); 669 (log ϵ 4.59) (MeOH).

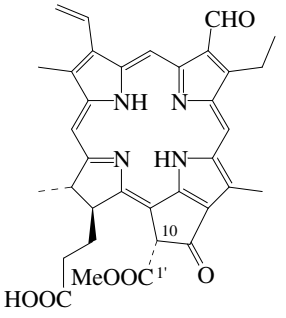
10-Epimer, 3′′-Et ester: ***Ethyl 10-epiphaeophorbide a***
$C_{37}H_{40}N_4O_5$ 620.747
Isol. from the sponge *Dysidea* sp.

10-Epimer, 10-hydroxy, 3′′-Me ester: ***Methyl 10-epi-10-hydroxyphaeophorbide a***
[53358-14-8]
$C_{36}H_{38}N_4O_6$ 622.719
Isol. from *Dunaliella primolecta*.

Strell, M. *et al., Angew. Chem.*, 1960, **72**, 169 (*synth*)
Kenner, G.W. *et al., J.C.S. Perkin 1*, 1973, 2517
Smith, K.M. *et al., Tetrahedron*, 1975, **31**, 367 (*cmr*)
Smith, K.M. *et al., Tet. Lett.*, 1981, **22**, 4873 (*pmr*)
Endo, H. *et al., Agric. Biol. Chem.*, 1982, **46**, 2183 (*10-Hydroxyphaeophorbide a*)
Smith, K.M. *et al., J.A.C.S.*, 1985, **107**, 4946 (*synth*)
Rinehart, K.L. *et al., J. Nat. Prod.*, 1988, **51**, 1 (*10-Hydroxyphaeophorbide a*)
Okazaki, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 3303 (*synth, cmr*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 3348 (*Me ester, isol*)
Ohta, S. *et al., J. Appl. Phycol.*, 1998, **10**, 349-355 (*Dunaliella primolecta constits*)
Schwikkard, S.L. *et al., Phytochemistry*, 1998, **49**, 2391-2394 (*Tapura fischeri constits*)
Matsunaga, T. *et al., CA*, 1999, 49637e (*activity*)
Stermitz, F.R. *et al., J. Nat. Prod.*, 2000, **63**, 1146-1149 (*activity*)
Cheng, H.-H. *et al., J. Nat. Prod.*, 2001, **64**, 915-919 (*isol, pmr, cmr, activity*)
Duan, H. *et al., Phytochemistry*, 2002, **59**, 85-90 (*10-epimers*)
Jin, P.F. *et al., Chin. Chem. Lett.*, 2005, **16**, 209-211 (*Dysidea constits*)

Phaeophorbide b P-296

Pheophorbide b
[20239-99-0]



$C_{35}H_{34}N_4O_6$ 606.677
Hydrol. (acid, alkaline or chlorophyllase) prod. of Phaeophytin b. Constit. of various plant spp. incl. *Brassica* spp. and *Neptunia* sp. Grey-black cryst. (CH_2Cl_2/petrol). Sol. $CHCl_3$.
Mp 220-223°. λ_{max} 439 (ϵ 154000); 530 (ϵ 12300); 553 (ϵ 9320); 602 (ϵ 9270); 653 (ϵ 39800) (Me_2CO).

Me ester: Methyl phaeophorbide b
[5522-71-4]
$C_{36}H_{36}N_4O_6$ 620.704
Obt. by methanolysis of Phaeophytin b. Grey plates (CH_2Cl_2/MeOH).
Mp 269°. $[\alpha]_{Hg}^{20}$ -128 (c, 1.56 in Me_2CO).

Et ester: ***Ethyl phaeophorbide b***
[26287-50-3]
$C_{37}H_{38}N_4O_6$ 634.73
Constit. of *Tapura fischeri*. Amorph. $[\alpha]_D$ +366.7 (c, 0.3 in $CHCl_3$).

10-Hydroxy, Me ester: ***Methyl 10-hydroxyphaeophorbide b***
[79684-25-6]
$C_{36}H_{36}N_4O_7$ 636.703
Isol. from *Dunaliella primolecta*.

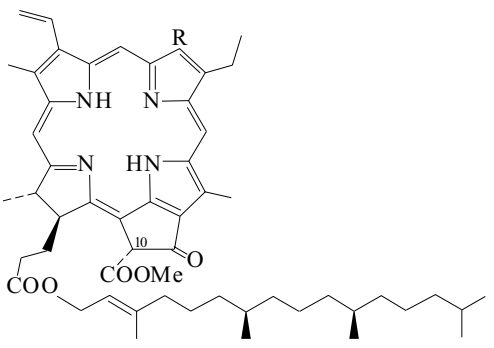
10-Methoxy, Me ester: ***Petasiphyll A***
$C_{37}H_{38}N_4O_7$ 650.73
Constit. of the leaves of *Petasites formosanus.* Deep green powder. λ_{max} 212; 240; 270; 325; 360; 407; 428; 521; 557; 600; 655 (MeOH).

[92935-95-0]

Fischer, H. *et al., Die Chemie des Pyrrols*, Akademische Verlag, Leipzig, Vol. II, (ii), 1940, 245-249 (*rev*)
Kenner, G.W. *et al., J.C.S. Perkin 1*, 1973, 2517-2523 (*synth*)
Smith, K.M. *et al., Porphyrins and Metalloporphyrins*, (ed. Smith, K.M.), Elsevier Elsevier, Amsterdam, 1975, 776 (*synth*)
Smith, K.M. *et al., Tetrahedron*, 1975, **31**, 367-375 (*cmr*)
Wasielewski, M.R. *et al., J.O.C.*, 1980, **45**, 1969-1974 (*synth, uv, pmr*)
Nakamura, Y. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 1028-1030 (*isol*)
Ohta, S. *et al., J. Appl. Phycol.*, 1998, **10**, 349-355 (*Methyl 10-hydroxyphaeophorbide b*)
Schwikkard, S.L. *et al., Phytochemistry*, 1998, **49**, 2391-2394 (*Et ester*)
Lin, C.-H. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1151-1152 (*Petasiphyll A*)

Phaeophytin a P-297

Pheophytin a_5. Pheophytin a
[603-17-8]



R = CH_3

$C_{55}H_{74}N_4O_5$ 871.213
Constit. of numerous plant spp. Mg free deriv. of Chlorophyll a, C-416 obt. by acid treatment. Deep-greenish-black cryst. (petrol). Mp 109-110°. $[\alpha]_D^{20}$ -126. λ_{max} 414 (log ϵ 1.03); 507 (log ϵ 0.11); 538 (log ϵ 0.1); 612 (log ϵ 0.08); 670 (log ϵ 0.46) (EtOH). λ_{max} 413 (ϵ 10); 507; 538; 612; 670 (MeOH) (Berdy).

*10*R-*Hydroxy: 10-Hydroxypheophytin a*
[79733-01-0]
$C_{55}H_{74}N_4O_6$ 887.213
Isol. from the leaves of *Cupressus funebris*, the liverwort *Plagiochila ovalifolia* and the excreta of the silkworm *Bombyx mori*. Cytotoxic agent. Amorph. solid.

*10*S-*Hydroxy: 10*S-*Hydroxypheophytin a*
[20240-17-9]
$C_{55}H_{74}N_4O_6$ 887.213
Isol. from the tunicate *Tridemnum solidum*, from *Plagiochila ovalifolia* and leaves of *Cupressus funebris*. Amorph. solid.

*10*R-*(Methyldioxy):* ***Phaeophytin a hydroperoxide***
[177602-11-8]
$C_{56}H_{76}N_4O_7$ 917.239
Isol. from *Plagiochila ovalifolia*. Contains an Me–O–O– substituent at C-10. The name Phaeophytin a hydroperoxide is not strictly correct. λ_{max} 409 (ϵ 48); 505; 547; 684 (MeOH) (Berdy).

Parent acid: [220969-02-8]
$C_{54}H_{72}N_4O_5$ 857.187
Constit. of *Tapura fischeri*. Amorph.

Fischer, H. *et al., Die Chemie des Pyrrols*, Akademische Verlag, Leipzig, Vol. II, (ii), 1940, 55
Hendrickson, H.R. *et al., J.O.C.*, 1959, **24**, 710
Jackson, A.H. *et al., Chem. Biochem. Plant Pigm.*, (Goodwin, T.W., Ed.), Academic Press, 1976, 1
Nakatani, Y. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2261-2269 (*10-Hydroxypheophytin a*)
Lotjonen, S. *et al., Org. Magn. Reson.*, 1983, **21**, 757 (*cmr*)
Lotjonen, S. *et al., Synthesis*, 1983, 708 (*synth*)
Smith, K.M. *et al., Org. Magn. Reson.*, 1984, **22**, 779 (*pmr*)
Fujiwara, M. *et al., J. Phys. Chem.*, 1986, **90**, 5646 (*ir, Raman*)
Grotemeyer, J. *et al., Angew. Chem., Int. Ed.*, 1988, **27**, 447 (*ms*)
Rinehart, K.L. *et al., J. Nat. Prod.*, 1988, **51**, 1-21 (*10-Hydroxypheophytin a*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 3348 (*10-Hydroxypheophytin a*)
Matsuo, A. *et al., Phytochemistry*, 1996, **42**, 427-430 (*isol, uv, ir, pmr, cmr*)
Schwikkard, S.L. *et al., Phytochemistry*, 1998, **49**, 2391-2394 (*1′-free acid*)

Phakellistatin 1 P-298

[147395-10-6]

Pro–Ile–Pro–Ile
|
Tyr–Pro–Phe

$C_{45}H_{61}N_7O_8$ 828.019
Cyclic peptide antibiotic. Constit. of the sponges *Phakellia costata* and *Stylotella aurantium*. Cytotoxic. Amorph. solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 247-249°. $[\alpha]_D^{25}$ -50.5 (c, 0.33 in $CHCl_3$). λ_{max} (solvent not reported) (Derep). λ_{max} 228 (ϵ 3060); 278 (ϵ 1630) (MeOH) (Derep). λ_{max} 228 (ϵ 3063); 278 (ϵ 1031) (MeOH) (Berdy).

Pettit, G.R. *et al., J. Nat. Prod.*, 1993, **56**, 260 (*isol, pmr, cmr, cryst struct*)

Phakellistatin 2 P-299

[155661-19-1]

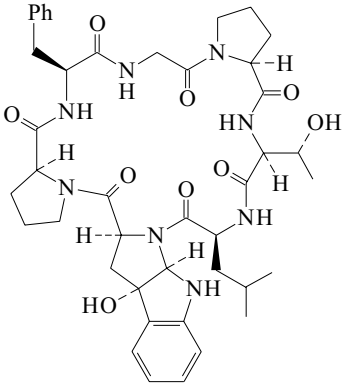
Ile–Ile–Pro–Tyr
|
Pro–Phe–Pro

$C_{45}H_{61}N_7O_8$ 828.019
Cyclic peptide antibiotic. Isol. as a chromatographically separable mixt. of two conformers which appear to have distinct biol. props. Isol. from the sponges *Phakellia carteri* and *Stylotella aurantium*. Cytotoxic agent. Amorph. solid.
Mp 199-201°. $[\alpha]_D^{23}$ -148 (c, 0.34 in MeOH). Biol. activity is mainly due to the less polar conformer, the conc. of which depends on solvent and time. λ_{max} 228 (ϵ 3060); 278 (ϵ 1630) (MeOH) (Derep). λ_{max} 224 (ϵ 8317); 275 (ϵ 708) (MeOH) (Berdy).

Pettit, G.R. *et al., Bioorg. Med. Chem. Lett.*, 1993, **3**, 2869 (*isol, uv, pmr, cmr, activity*)
Pettit, G.R. *et al., J. Nat. Prod.*, 1999, **62**, 409-414 (*synth, pmr, cmr*)
Tabudravu, J.N. *et al., J.O.C.*, 2002, **67**, 8593-8601 (*isol, conformn*)

Phakellistatin 3, 9CI P-300

[153603-87-3]



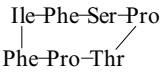
$C_{42}H_{54}N_8O_9$ 814.937
Isol. from the Western Indian ocean sponge *Phakellia carteri*. Shows significant cytotoxicity against murine P388 lymphocytic leukaemia. Amorph. powder. Sol. MeOH, $CHCl_3$.
Mp 178-180°. $[\alpha]_D^{24}$ -147 (c, 0.22 in MeOH). New type of cycloheptapeptide containing an amino acid unit apparently derived from a photooxidn. prod. of Tryptophan. λ_{max} 211 (ϵ 25700); 238 (ϵ 8130); 295 (ϵ 2340) (no solvent reported) (Derep). λ_{max} 214 (ϵ 14800); 234 (ϵ 11000); 291 (ϵ 3310) (MeOH) (Derep).

cis-*Isomer:* ***Isophakellistatin 3***
[153667-40-4]
$C_{42}H_{54}N_8O_9$ 814.937
From *Phakellia carteri*. Cryst. (Me_2CO). Sol. MeOH, $CHCl_3$.
Mp 218-220°. $[\alpha]_D^{23}$ -138 (c, 0.21 in MeOH). Isomeric at the photo-Trp indole ring juncture. Does not show cytotoxicity against P388 cell line. λ_{max} 211 (ϵ 25700); 238 (ϵ 8130); 295 (ϵ 2340) (no solvent reported) (Derep). λ_{max} 214 (ϵ 14800); 234 (ϵ 11000); 291 (ϵ 3310) (MeOH) (Derep). λ_{max} 211 (ϵ 25700); 238 (ϵ 8130); 295 (ϵ 2344) (MeOH) (Berdy).

Pettit, G.R. *et al., J.O.C.*, 1994, **59**, 1593 (*isol, uv, ir, cryst struct*)
Greeman, K.L. *et al., Org. Lett.*, 2004, **6**, 1713-1716 (*synth*)

Phakellistatin 4 P-301

[162763-61-3]



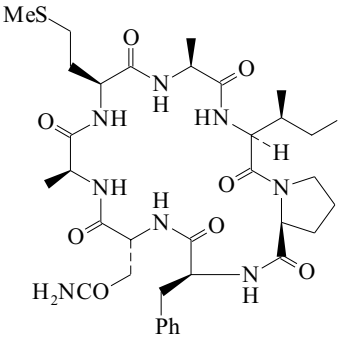
$C_{41}H_{55}N_7O_9$ 789.927

Cyclic heptapeptide antibiotic. Isol. from the sponge *Phakellia costata*. Cytotoxic agent. Amorph. powder. $[\alpha]_D$ -97 (c, 2 in MeOH). λ_{max} 225; 259 (MeOH) (ref. gives uv ranges).

Pettit, G.R. *et al., Heterocycles*, 1995, **40**, 501-506 (*isol, pmr, cmr, struct*)

Phakellistatin 5 P-302

[159850-99-4]



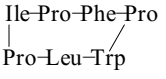
$C_{35}H_{52}N_8O_8S$ 744.911

Cyclic peptide antibiotic. Isol. from the sponge *Phakellia costata*. Cytotoxic agent. Powder.
Mp 216-218° (synthetic). $[\alpha]_D$ -102 (c, 2 in MeOH).

Pettit, G.R. *et al., Bioorg. Med. Chem. Lett.*, 1994, **4**, 2091-2096 (*isol, pmr, cmr, ms*)
Pettit, G.R. *et al., J. Nat. Prod.*, 2000, **63**, 22-28 (*synth, cmr*)

Phakellistatin 6 P-303

[160072-82-2]



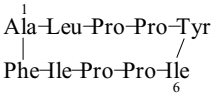
$C_{47}H_{62}N_8O_7$ 851.056

Cyclic peptide antibiotic. Isol. from the sponge *Phakellia costata*. Cytotoxic agent. Powder. $[\alpha]_D$ -129 (c, 0.4 in MeOH). λ_{max} 213; 273 (sh); 280; 289 (prob. MeOH) (Derep).

Pettit, G.R. *et al., Bioorg. Med. Chem. Lett.*, 1994, **4**, 2677 (*isol, uv, pmr, cmr*)

Phakellistatin 7 P-304

[166334-51-6]



$C_{59}H_{84}N_{10}O_{11}$ 1109.373

Cyclic peptide antibiotic. Isol. from the marine sponge *Phakellia costata*. Cytotoxic agent. Amorph. powder.
Mp 192-195°. $[\alpha]_D$ -106 (c, 0.2 in MeOH).

1-L-Valine analogue: ***Phakellistatin 8***
[166334-52-7]
$C_{61}H_{88}N_{10}O_{11}$ 1137.427
Isol. from *Phakellia costata*. Cytotoxic agent. Cryst. (MeOH aq.).
Mp 188-191°. $[\alpha]_D$ -112 (c, 0.2 in MeOH).

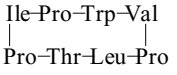
1,6-Di-L-valyl analogue: ***Phakellistatin 9***
[166334-53-8]
$C_{60}H_{86}N_{10}O_{11}$ 1123.4
Isol. from *Phakellia costata*. Cytotoxic agent. Amorph. powder.
Mp 184-188°. $[\alpha]_D$ -113 (c, 0.7 in MeOH).

1-L-Threonine analogue: ***Phakellistatin 12***
[528604-44-6]
$C_{60}H_{86}N_{10}O_{12}$ 1139.399
Isol. from a *Phakellia* sp. Cytotoxic. Amorph. solid. $[\alpha]_D^{25}$ -132 (c, 0.1 in MeOH). λ_{max} 222 (log ϵ 4.31); 254 (log ϵ 3.58); 269 (log ϵ 3.52) (MeOH).

Pettit, G.R. *et al., Bioorg. Med. Chem. Lett.*, 1995, **5**, 1339-1344 (*isol, pmr, cmr, ms, Phakellistatins 8,9*)
Herald, D.L. *et al., J.A.C.S.*, 1997, **119**, 6962-6973 (*cryst struct, Phakellistatin 8*)
Pettit, G.R. *et al., Bioorg. Med. Chem. Lett.*, 2003, **13**, 685-688 (*Phakellistatin 12*)
Napolitano, A. *et al., Tetrahedron*, 2005, **61**, 6808-6815 (*synth*)

Phakellistatin 10 P-305

[167710-82-9]



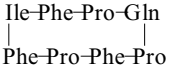
$C_{47}H_{69}N_9O_9$ 904.117

Cyclic peptide antibiotic. Isol. from the sponge *Phakellia* sp. Cytotoxic agent. Amorph. powder.
Mp 217-219°. $[\alpha]_D^{25}$ -128 (c, 0.2 in MeOH).

Pettit, G.R. *et al., J. Nat. Prod.*, 1995, **58**, 961-965 (*isol, pmr, cmr*)

Phakellistatin 11 P-306

[167710-83-0]

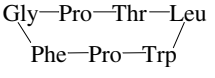


$C_{53}H_{67}N_9O_9$ 974.167

Cyclic peptide antibiotic. Isol. from the sponge *Phakellia* sp. Cytotoxic agent. Amorph. solid.
Mp 194-196°. $[\alpha]_D^{25}$ -163 (c, 0.08 in MeOH).

Pettit, G.R. *et al., J. Nat. Prod.*, 1995, **58**, 961-965 (*isol, pmr, cmr*)
Pettit, G.R. *et al., J. Nat. Prod.*, 2001, **64**, 883-891 (*synth, pmr*)

Phakellistatin 13 P-307

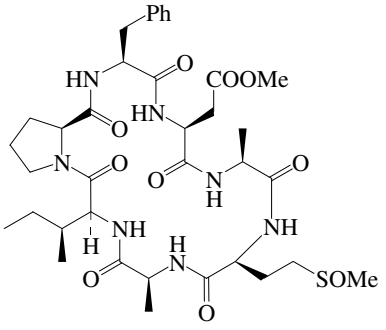


$C_{42}H_{54}N_8O_8$ 798.937

Cyclic peptide antibiotic. Isol. from the sponge *Phakellia fusca*. Cytotoxic. Glassy amorph. solid.
Mp 198-200°. $[\alpha]_D^{25}$ -136 (c, 0.09 in MeOH). λ_{max} 214 (log ϵ 4.34); 240 (log ϵ 3.5); 283 (log ϵ 3.47) (MeOH).

Li, W.-L. *et al., J. Nat. Prod.*, 2003, **66**, 146-148 (*isol, pmr, cmr*)
Greenman, K.L. *et al., Org. Lett.*, 2004, **6**, 1713-1716 (*synth*)

Phakellistatin 14 P-308

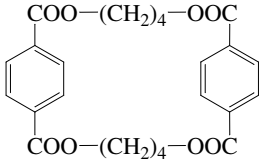


$C_{36}H_{53}N_7O_{10}S$ 775.922
Isol. from the sponge *Phakellia* sp. Cytotoxic. Amorph. powder. Mp 189-191°. $[\alpha]_D^{25}$ -64.9 (c, 0.28 in MeOH). λ_{max} 220 (log ϵ 3.45); 268 (sh) (log ϵ 2.73) (MeOH).

Pettit, G.R. *et al., J. Nat. Prod.*, 2005, **68**, 60-63 (*isol, pmr, cmr, ms*)

Pharacin P-309

3,8,15,20-Tetraoxatricyclo[20.2.2.2^{10,13}]octacosa-10,12,22,24,25,27-hexaene-2,9,14,21-tetrone. Cyclobis(1,4-butylene terephthalate). 2,7,16,21-Tetraoxa[8.8]paracyclophane-1,8,15,22-tetrone
[63440-93-7]



$C_{24}H_{24}O_8$ 440.449
Prod. by *Cytophaga marinoflava* sp. AM13.1 and *Vibrio parahaemolyticus* Bio249.
Mp 199°. Possible artifact - however isol. has been repeated avoiding contact with plastics.

Mueller, F.J. *et al., Makromol. Chem.*, 1983, **184**, 2487-2495 (*synth*)
Shaaban, M. *et al., J. Nat. Prod.*, 2002, **65**, 1660-1663 (*isol*)
Veluri, R. *et al., J. Nat. Prod.*, 2003, **66**, 1520-1523 (*isol*)

Phascoline P-310

*3-[(Aminoiminomethyl)amino]-*N*-(2-hydroxyheptyl)propanamide, 9CI.* N-*(3-Guanidinopropionyl)-2-hydroxyheptylamine*
$H_3C(CH_2)_4CH(OH)CH_2NHCOCH_2CH_2NHC(NH_2)$═NH
$C_{11}H_{24}N_4O_2$ 244.336

(-)-*form* [50767-84-5]
Constit. of the sipunculid worm *Phascolion strombi*.
Oil; yellow needles (as picrate).
Mp 73° (picrate). $[\alpha]_D^{25}$ -8.7 (H_2O).
Guillou, Y. *et al., J. Biol. Chem.*, 1973, **248**, 5668 (*isol*)

Phascolosomine P-311

*3-[(Aminoiminomethyl)amino]-*N*-(2-methoxyheptyl)-2-methylpropanamide, 9CI.* N-*(3-Guanidinoisobutyryl)-2-methoxyheptylamine*
[50767-86-7]
$H_3C(CH_2)_4CH(OMe)CH_2NHCOCH(CH_3)CH_2NH$
$C(NH_2)$═NH
$C_{13}H_{28}N_4O_2$ 272.39

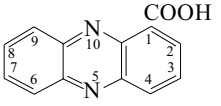
(-)-*form*
[50767-87-8 (picrate)]
Constit. of the marine sipunculan worm *Phascolion strombi*.
Oil; yellow needles (as picrate).
Mp 152° (picrate). $[\alpha]_D^{25}$ -37 (H_2O).
Guillou, Y. *et al., J. Biol. Chem.*, 1973, **248**, 5668 (*isol*)

Phasvatocin P-312

[144334-53-2]
Cys-Tyr-Phe-Asn-Asn-Cys-Pro-Val-Gly-NH_2
$C_{44}H_{60}N_{12}O_{12}S_2$ 1013.163
Peptide of the oxytocin/vasopressin family; struct. of reduced form shown. Isol. from the pituitary of the spotted dogfish *Scyliorhinus caniculus*. Neurohypophysial hormone.
Chauvet, J. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1994, **91**, 11266-11270 (*isol, struct*)

1-Phenazinecarboxylic acid, 9CI P-313

Tubermycin B. *X-Pigment*
[2538-68-3]



$C_{13}H_8N_2O_2$ 224.218
Prod. by *Pseudomonas* spp., *Streptomyces cinnamonensis, Streptomyces misakiensis*, *Bacillus* sp. B-6 and *Actinomadura dassonvillei*. Weakly active against gram-positive bacteria and *Candida albicans*. Inhibits acyl-CoA synthetase. Greenish-yellow needles (EtOH). Mp 241-242° (237-239°). λ_{max} 251 (ϵ 97000); 364 (sh) (ϵ 10000); 370 (ϵ 19000) (CH_2Cl_2/pH 2) (Derep). λ_{max} 250 (ϵ 84900); 364 (ϵ 13400) (MeOH/pH 11) (Derep). λ_{max} 248 (ϵ 65000); 354 (sh) (ϵ); 364 (ϵ 13400) (MeOH) (Derep).
▶ LD_{50} (mus, ipr) 400 mg/kg. SG1576000

5-Oxide: [27210-90-8]
$C_{13}H_8N_2O_3$ 240.218
Photographic bleaching agent. Mp 223°.

10-Oxide:
$C_{13}H_8N_2O_3$ 240.218
Yellow needles (AcOH). Mp 233-234°.

Me ester: Methyl 1-phenazinecarboxylate
[3225-19-2]
$C_{14}H_{10}N_2O_2$ 238.245
Isol. from *Streptomyces luteoreticuli*. Active against mycobacteria. Mp 123-124°.

Amide: 1-Phenazinecarboxamide. ***Oxychlororaphine.*** *Xanthoraphine*
[550-89-0]
$C_{13}H_9N_3O$ 223.234
Prod. by *Pseudomonas chlororaphis* and *Pseudomonas aeruginosa*. Active against phytopathogenic fungi and *Candida albicans*. Yellow needles. Mp 245-246° (237°).
▶ SG1575530

Nitrile: 1-Cyanophenazine
$C_{13}H_7N_3$ 205.218
Needles. Mp 171-172°.

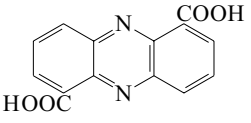
5,10-Dihydro, carboxymethyl ester: Carboxymethyl 5,10-dihydro-1-phenazinecarboxylate. ***Endophenazine D***
$C_{15}H_{12}N_2O_4$ 284.271
Prod. by various strains of the endosymbiotic *Streptomyces anulatus*. Active against gram-positive bacteria. Amorph. solid. λ_{max} 293 (log ϵ 3.82); 351 (log ϵ 3.63) (MeOH).

Kögl, F. *et al., Annalen*, 1930, **480**, 280 (*deriv*)
Vivian, D.L. *et al., J.O.C.*, 1955, **20**, 797 (*synth*)
Isono, K. *et al., J. Antibiot., Ser. A*, 1958, **11**, 264 (*struct*)
Chaim, S. *et al., Spectrochim. Acta*, 1963, **19**, 1625 (*ir*)
Levitch, M.E. *et al., Arch. Biochem. Biophys.*, 1964, **106**, 194 (*biosynth*)
Mokrushin, V.S. *et al., CA*, 1970, **72**, 31750 (*synth*)
Hollstein, U. *et al., J.O.C.*, 1972, **37**, 3510 (*synth*)
Breitmaier, E. *et al., J.O.C.*, 1976, **41**, 2104 (*cmr*)
Kiprianova, E.A. *et al., CA*, 1978, **88**, 11570 (*use*)
Tax, J. *et al., Coll. Czech. Chem. Comm.*, 1983, **48**, 527 (*isol*)

Brisbane, P.G. *et al., Antimicrob. Agents Chemother.*, 1987, **31**, 1967 (*isol, struct*)
Rewcastle, G.W. *et al., Synth. Commun.*, 1987, **17**, 1171 (*synth*)
Jones, G.P. *et al., Acta Cryst. C*, 1988, **44**, 2220 (*cryst struct*)
Ji, X. *et al., Acta Cryst. C*, 1992, **48**, 109 (*cryst struct*)
Jayatilake, G.S. *et al., J. Nat. Prod.*, 1996, **59**, 293-296 (*isol, pmr, cmr*)
Kim, K.-J. *et al., Yakhak Hoeji*, 1998, **42**, 552-557; *CA*, **130**, 14939z (*isol, activity*)
Kim, K.-J. *et al., J. Biochem. Mol. Biol.*, 2000, **33**, 332-336 (*occur, activity*)
Gebhardt, K. *et al., J. Antibiot.*, 2002, **55**, 794-800; 801-806 (*Endophenazine D*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 898
Hazards in the Chemical Laboratory, 3rd edn., (ed. Bretherick, L.), Royal Society of Chemistry, 1981, 437

1,6-Phenazinedicarboxylic acid P-314

[23462-25-1]



$C_{14}H_8N_2O_4$ 268.228

Phenazine antibiotic. Fermentation prod. of *Pseudomonas* and *Streptomyces* spp. Inhibits xanthine oxidase. Shows antibiotic props. by interacting with RNA. Intermed. in the biosynth. of Lomofungin and other phenazines. Green cryst. Sol. EtOH, $CHCl_3$. Mp 325° dec. λ_{max} 250; 370 (MeOH) (Berdy).

Mono-Me ester: ***Phencomycin***
$C_{15}H_{10}N_2O_4$ 282.255
Prod. by a *Streptomyces* sp. Shows antibacterial and anti-tumour props. Yellow cryst. or yellow-green needles ($CHCl_3$/MeOH). Sol. MeCN, $CHCl_3$, MeOH, CH_2Cl_2, EtOAc, DMSO; fairly sol. MeOH; poorly sol. acids, hexane. Mp 263°. λ_{max} 256 (log ϵ 4.87); 368 (log ϵ 4.2) (MeOH). λ_{max} 250; 371 (MeOH/HCl) (Berdy). λ_{max} 258; 366 (MeOH/NaOH) (Berdy).

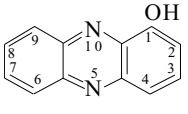
Di-Me ester: [23531-24-0]
$C_{16}H_{12}N_2O_4$ 296.282
Mp 228-230°.

5,10-Dihydro, di-Me ester: 5,10-Dihydrophencomycin methyl ester
$C_{16}H_{14}N_2O_4$ 298.298
Prod. by a marine *Streptomyces* sp. Orange needles ($CHCl_3$/MeOH). Mp 231°. λ_{max} 216 (log ϵ 4.51); 245 (log ϵ 4.48); 450 (log ϵ 4.04) (MeOH).

Gerber, N.N. *et al., J. Het. Chem.*, 1969, **6**, 297 (*isol, synth, uv*)
Breitmaier, E. *et al., J.O.C.*, 1976, **41**, 2104 (*synth, uv, cmr*)
Kimura, Y. *et al., Tet. Lett.*, 1977, 4515 (*biosynth*)
Messenger, A.J. *et al., Biochem. Soc. Trans.*, 1978, **6**, 1326 (*biosynth*)
Buckland, P.R. *et al., J. Chem. Res., Synop.*, 1981, 362 (*biosynth*)
Roemer, A. *et al., Org. Magn. Reson.*, 1982, **19**, 118 (*nmr*)
Chatterjee, S. *et al., J. Antibiot.*, 1995, **48**, 1353 (*Phencomycin*)
Pusecker, K. *et al., J. Antibiot.*, 1997, **50**, 479 (*Phencomycin, Dihydrophencomycin*)
Maul, C. *et al., J. Antibiot.*, 1999, **52**, 1124-1134 (*activity*)

1-Phenazinol, 9CI P-315

1-Hydroxyphenazine. Hemipyocyanine
[528-71-2]



$C_{12}H_8N_2O$ 196.208
Prod. by *Pseudomonas aeruginosa*, *Pseudomonas pyocyanea*, *Pseudomonas aurantiaca* and *Streptomyces thioluteus*. Active against gram-positive bacteria and fungi. Shows some antiviral activity. Algicide. Fluffy yellow needles (EtOH aq.). Sol. MeOH, bases, Et_2O, Py, phenol; fairly sol. EtOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 157-159°. pK_{a1} 1.61; pK_{a2} 8.33 (15°). λ_{max} 264; 368 (MeOH) (Berdy). λ_{max} 264; 352; 360; 384; 425 (hexane) (Berdy). λ_{max} 263; 358 (EtOH) (Berdy). λ_{max} 298 (MeOH/NaOH) (Berdy).

▶ LD_{50} (mus, ipr) 500 mg/kg. SG1647000

5-Oxide: [6479-82-9]
$C_{12}H_8N_2O_2$ 212.207
Yellow. Mp 190-191°.

10-Oxide: ***1-Hydroxyphenazine 10-oxide***
[14994-67-3]
$C_{12}H_8N_2O_2$ 212.207
Prod. by microorganisms, e.g. *Microbispora aerata*. Active against gram-positive bacteria. Orange cryst. Sol. $CHCl_3$; poorly sol. hexane.
Mp 165-167°. λ_{max} 279; 326; 334; 368; 380; 387; 468 (ϵ 2120) (EtOH) (Berdy).

5,10-Dioxide: [18274-55-0]
$C_{12}H_8N_2O_3$ 228.207
Red. Mp 185-186°.

Ac: [6033-10-9]
$C_{14}H_{10}N_2O_2$ 238.245
Mp 120°.

Benzoyl: [6055-50-1]
$C_{19}H_{12}N_2O_2$ 300.316
Mp 173°.

Me ether: ***1-Methoxyphenazine***
[2876-17-7]
$C_{13}H_{10}N_2O$ 210.235
From *Streptomyces luteoreticuli*. Active against mycobacteria. Cryst. (Py).
Mp 167-169°. λ_{max} 261 (ϵ 60250); 395 (ϵ 8310); 407 (ϵ 3020) (MeOH) (Berdy).

Me ether, 5-Me: 1-Methoxy-5-methylphenazinium(1+)
[65162-13-2]
$C_{14}H_{13}N_2O^{\oplus}$ 225.27
Synthetic electron carrier for redox mediated enzymatic reactions. Red cryst. (EtOAc/EtOH) (methanesulfonate). Mp 171-172° (as methanesulfonate salt). CAS no. refers to the methanesulfonate salt.

Et ether: 1-Ethoxyphenazine
[23169-51-9]
$C_{14}H_{12}N_2O$ 224.262
Mp 126-127°.

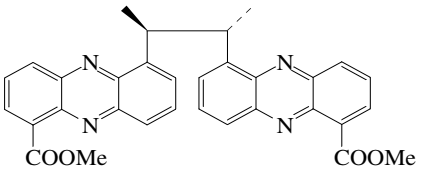
(Methoxycarbonylmethyl) ether: (Methoxycarbonylmethoxy)phenazine. Antibiotic K_3-Ye. K_3-Ye
[159068-58-3]
$C_{15}H_{12}N_2O_3$ 268.271
Isol. from the culture of a genetically engineered *Streptomyces* sp. Inhibitor of nucleoside transport.

Hays, E.E. *et al., J. Biol. Chem.*, 1945, **159**, 725 (*isol*)
Badger, G.M. *et al., J.C.S.*, 1951, 3204
Org. Synth., Coll. Vol., 3, 1955, 753-756 (*1-methoxy-5-Me*)
Gerber, N.N. *et al., Biochemistry*, 1966, **5**, 3824 (*oxides*)
Gerber, N.N. *et al., J.O.C.*, 1967, **32**, 4055 (*isol, props*)
Wake, S. *et al., Tet. Lett.*, 1970, 2415 (*synth*)
Kiprianova, E.A. *et al., Mikrobiol. Zh. (Kiev)*, 1971, **33**, 12; *CA*, **84**, 130344 (*isol, props*)
Breitmaier, E. *et al., J.O.C.*, 1976, **41**, 2104 (*cmr*)
Hisada, R. *et al., J. Biochem. (Tokyo)*, 1977, **82**, 1469-1473 (*1-methoxy-5-Me, synth, pmr, props*)
Issidorides, C.H. *et al., Tetrahedron*, 1979, **34**, 217 (*synth*)
Chen, W.P. *et al., Yaoxue Xuebao*, 1994, **29**, 585 (*K_3-Ye*)

Phenazostatin B P-316

Dimethyl 6,6′-(1,2-dimethyl-1,2-ethanediyl)bis[1-phenazinecarboxylate], 9CI

[73649-05-5]



Relative Configuration

$C_{32}H_{26}N_4O_4$ 530.582

Prod. by *Streptomyces* sp. 833 and *Streptomyces* sp. ME679m4. Neuronal cell protecting agent and free radical scavenger. Phosphodiesterase inhibitor. Yellow cryst. Racemic. λ_{max} 253 (ϵ 89000); 366 (ϵ 19000) (MeOH).

Epimer: ***Phenazostatin D***

[639512-19-9]

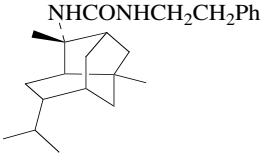
$C_{32}H_{26}N_4O_4$ 530.582

Prod. by the marine *Pseudonocardia* sp. B6273. Yellow solid. *meso*-form. λ_{max} 256 (log ϵ 3.95); 350 (sh) (log ϵ 3.16); 366 (log ϵ 3.34); 385 (sh) (log ϵ 2.92) ($CHCl_3$).

Japan. Pat., 1980, 80 03733; *CA*, **92**, 213541p (*isol*)
Kim, W.-G. *et al., J. Antibiot.*, 1997, **50**, 715-721 (*isol, uv, ir, pmr*)
Maskey, R.P. *et al., Z. Naturforsch., B*, 2003, **58**, 692-694 (*Phenazostatin D*)

N-Phenethyl-*N′*-2-trachyopsanylurea P-317

[189818-49-3]



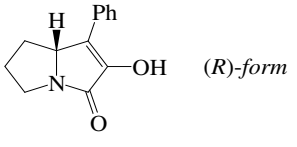
$C_{24}H_{36}N_2O$ 368.561

Constit. of *Axinyssa aplysinoides*. Oil. $[\alpha]_D$ -28.6 (c, 0.14 in MeoH). λ_{max} 211; 342 (br) (MeOH).

Patil, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 507-510 (*isol, pmr, cmr*)

Phenopyrrozin P-318

*5,6,7,7*a-*Tetrahydro-2-hydroxy-1-phenyl-3*H-*pyrrolizin-3-one. Antibiotic FO 2047. FO 2047*



(*R*)-*form*

$C_{13}H_{13}NO_2$ 215.251

(R)-form [172923-76-1]

Prod. by *Penicillium* sp. FO-2047 and the marine-derived *Chromocleista* sp. strain R721. Radical scavenger. Antioxidant. Powder. Sol. MeOH, $CHCl_3$, EtOAc; poorly sol. H_2O. Mp 147-152°. $[\alpha]_D$ -10.2 (c, 0.6 in MeOH). λ_{max} 206 (ϵ 7960); 215 (ϵ 7850); 225 (sh) (ϵ 5810); 240 (ϵ 3870); 295 (ϵ 3810); 340 (sh) (ϵ 650) (EtOH).

(S)-form

*4′-Hydroxy: 5,6,7,7*a-*Tetrahydro-2-hydroxy-1-(4-hydroxyphenyl)-3*H-*pyrrolizin-3-one.* **p-*Hydroxyphenopyrrozin***

[887602-12-2]

$C_{13}H_{13}NO_3$ 231.251

Prod. by the marine-derived *Chromocleista* sp. strain R721. Amorph. solid. $[\alpha]_D^{25}$ +34 (c, 0.34 in MeOH). λ_{max} 198 (log ϵ 4.5); 222 (log ϵ 1.3); 307 (log ϵ 1.8) (MeOH).

Shiomi, K. *et al., J. Antibiot.*, 1995, **48**, 1413-1418 (*isol, uv, pmr, cmr*)
Japan. Pat., 1996, 96 127 583; *CA*, **125**, 112919n
Park, Y.C. *et al., J. Nat. Prod.*, 2006, **69**, 580-584 (*isol, Chromocleista*)

Phenylacetic acid P-319

Benzeneacetic acid, 9CI. Phenylethanoic acid. α-Toluic acid. FEMA 2878

[103-82-2]

$PhCH_2COOH$

$C_8H_8O_2$ 136.15

Found in essential oils, e.g. neroli, rose oil, free and as esters and in many fruits. Also prod. by microorganisms, e.g. by *Fusarium oxysporum*, *Glomerella cingulata* and a marine derived *Streptomyces* sp. Volatile component of tail gland secretion from red deer *Cervus elaphus*. Used as 1*M* soln. in $CHCl_3$ for selective extraction separation of Cu and U ($CHCl_3$). Important industrial intermediate. Perfumery and flavouring ingredient. Incorporation in fermentation of penicillin results in production of Benzylpenicillin. Phytotoxin, germination inhibitor. Plates (petrol) with sweet taste at low conc. and rose-like odour.

Mp 77-78.5°. Bp 265.5° $Bp_{0.01}$ 65-70°. pK_a 4.31 (H_2O).

▶ Fl. p. 102°. LD_{50} (rat, orl) 2250 mg/kg. Exp. teratogenic effects. AJ2430000

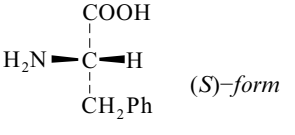
[114-70-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 137A; 278C; 278D; 337A; 381A; 423A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 981A; 1209B; 1209C; 1331A; 1376A; 1411B; 1479A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1315A; 1343B; 1343C (*ir*)
Sadtler Standard C-13 NMR Spectra, 4213 (*cmr*)
Org. Synth., Coll. Vol., 1, 1932, 436 (*synth*)
Johns, S.R. *et al., Aust. J. Chem.*, 1969, **22**, 1315 (*isol*)
El-Bayoumi, M.A. *et al., J.A.C.S.*, 1971, **93**, 6396 (*uv*)
Scott, K.N. *et al., J. Magn. Reson.*, 1972, **6**, 55 (*pmr*)
Harrison, A.G. *et al., J.O.C.*, 1984, **49**, 4993 (*ms*)
Hodgson, D.J. *et al., Acta Cryst. C*, 1991, **47**, 1986 (*cryst struct*)
Hirota, A. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 492-494 (*isol*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1415
Okano, T. *et al., Bull. Chem. Soc. Jpn.*, 1994, **67**, 2339 (*synth*)
Maskey, R.P. *et al., Z. Naturforsch., B*, 2002, **57**, 823-829 (*marine, isol*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2747
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 997; 998
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BQJ350; EOH000; MHA500; PDX750; PEA750; PDY850,

Phenylalanine, 9CI, USAN P-320

α-Aminobenzenepropanoic acid. 2-Amino-3-phenylpropanoic acid. β-Phenylalanine. α-Aminohydrocinnamic acid. FN 1636. Antibiotic FN 1636. Phe

[3617-44-5]



(*S*)−*form*

$C_9H_{11}NO_2$ 165.191

Log P -1.56 (uncertain value) (calc).

(S)-form

L-form. L-Phenylalanine, JAN. FEMA 3585

[63-91-2]

Widely distributed in proteins. Dietary supplement, nutrient. Needles (H_2O). Spar. sol. H_2O (2.97 g/100 g at 25°).

Mp 283-284° (rapid heat). $[\alpha]_D^{20}$ -34.3 (c, 1 in H_2O) (98% op). pK_{a1} 1.83; pK_{a2} 9.13 (NH_2). Isoelectric point 5.48. Bitter taste.

▶ LD_{50} (rat, ipr) 5287 mg/kg. AY7535000

N-*Ac, Me ester:* [3618-96-0]

Isol. from an undescribed Jaspidae sponge collected from the Benga lagoon, Fiji islands.

Viscous oil ($CHCl_3$); needles (petrol); prisms (Et_2O).
Mp 91-92°. $[\alpha]_D$ +101.5 (c, 1 in $CHCl_3$). $[\alpha]_D^{25}$ +19.5 (c, 2 in MeOH).

[60058-39-1, 65864-22-4, 146815-23-8]

Adamczeski, M. *et al., J.A.C.S.*, 1989, **111**, 647-654 (*N-Ac Me ester, isol*)

Phenylalanylglycylalanylserylthreoninylargininyl-glycylalanine P-321

Phe-Gly-Ala-Ser-Thr-Arg-Gly-AlaIsol. from *Theragra chalcogramma* (pollock). ACE inhibitor.

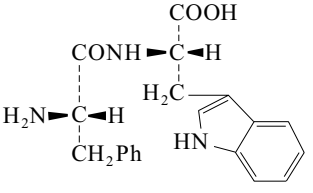
Je, J.-Y. *et al., J. Agric. Food Chem.*, 2004, **52**, 7842-7845 (*isol, struct*)

Phenylalanylthreonylarginylphenylalaninamide, 9CI P-322

FTRF-amide
[135014-49-2]
H-Phe-Thr-Arg-Phe-NH_2Isol. from *Nereis diversicolor*.

Boratte, B. *et al., Eur. J. Biochem.*, 1991, **198**, 627 (*isol, synth, ms*)

N-Phenylalanyltryptophan, 9CI P-323



$C_{20}H_{21}N_3O_3$ 351.404

L-L-*form* [24587-41-5]
Isol. from the annelid *Perinereis vancaurica*.
Cryst. (MeOH/EtOH). $[\alpha]_D^{25}$ +6 (c, 1 in MeOH).
▶ LD_{50} (rat, ivn) 300 mg/kg. YN7405800

[108787-56-0]

Kimmel, H.S. *et al., Anal. Biochem.*, 1969, **32**, 1 (*ir*)
U.K. Pat., 1975, 1 415 506; *CA*, **84**, 126765f (*synth*)
Guarnaccia, R. *et al., Biopolymers*, 1976, **15**, 1103 (*synth, uv*)
Pavo, I. *et al., Acta Chim. Hung.*, 1986, **122**, 261 (*synth*)
Takahashi, T. *et al., Pept. Chem.*, 1993, **31**, 169 (*isol*)

Phenylalanyltyrosylglutamylglycylaspartylvalylprolyltyrosine P-324

FYEGDVPY
[157724-15-7]
H-Phe-Tyr-Glu-Gly-Asp-Val-Pro-Tyr-OH
$C_{48}H_{60}N_8O_{15}$ 989.047
Isol. from the annelid *Perinereis vancaurica*.

Takahashi, T. *et al., Pept. Chem.*, 1993, **31**, 169-174 (*isol, struct*)
Takahashi, T. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1995, **110**, 297-304 (*isol, struct*)

4-Phenyl-3-buten-2-one, 9CI P-325

Benzylideneacetone. Methyl styryl ketone. Benzalacetone. FEMA 2881
[122-57-6]
PhCH=CHCOCH$_3$
$C_{10}H_{10}O$ 146.188
Constit. of *Amomum globosum*, *Comptonia peregrina* and *Scutellaria baicalensis*. Present in hydrolysed soy protein. Flavouring ingredient.
▶ Fl. p. 66°. Mild skin irritant. LD_{50} (rat, orl) 2031 mg/kg. EN0330000

(*E*)-*form* [1896-62-4]
Isol. from the marine sponge *Plakortis halichondrioides*.
Lustrous plates.
Mp 42°. Bp 260-262° Bp_9 126-128°.
▶ EN0330050

Oxime: [1721-83-1]
[21613-44-5, 21613-45-6]
$C_{10}H_{11}NO$ 161.203
Needles. Mp 116°.

Phenylhydrazone:
Yellow needles. Mp 156-157°.

Semicarbazone: [1722-63-0]
Mp 187°.

Ethylene dithioacetal: 2-Methyl-2-(2-phenylethenyl)-1,3-dithiolane
[107389-59-3]
$C_{12}H_{14}S_2$ 222.375
Solid. Mp 52-53°. $Bp_{0.16}$ 109-112°.

(*Z*)-*form* [937-53-1]
Liq. Mp -21.5°. $Bp_{0.2}$ 67-68°.

Semicarbazone: [1722-65-2]
Mp 177.5°.

[2887-98-1, 5468-31-5, 13387-22-9, 22921-89-7, 61210-87-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 7C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 799C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1227D (*ir*)
Grignard, V. *et al., Ann. Chim. (Paris)*, 1928, **9**, 5-54 (*synth*)
Schinz, H. *et al., CA*, 1955, **49**, 6874 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 1011-1081 (*rev, tox*)
Baas, P. *et al., Tetrahedron*, 1977, **33**, 1509-1511 (*conformn, pmr*)
Ravi, B.N. *et al., J.O.C.*, 1979, **44**, 3109-3113 (*isol, ir, pmr*)
Fischer, H. *et al., Chem. Ber.*, 1990, **123**, 399-404 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 661
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2188-2189
Org. Synth., Coll. Vol., 9, 1998, 649-652
Tietze, L.F. *et al., Angew. Chem., Int. Ed.*, 1999, **5**, 297-304 (*synth, ir, uv, pmr, ms*)
Zhong, P. *et al., Synth. Commun.*, 2000, **30**, 3245-3253 (*synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SMS500,

10-Phenyldecanoic acid P-326

Benzenedecanoic acid, 9CI. 10-Phenylcapric acid
[18017-73-7]
Ph$(CH_2)_9$COOH
$C_{16}H_{24}O_2$ 248.364
Constit. of *Trichilia claussenii* and *Vibrio alginolyticus* associated with the alga *Cladophora coelothrix*. Waxy solid.
Mp 42-43°. Bp_{18} 228-230° $Bp_{0.4}$ 196-198°.

Et ester: [58380-63-5]
$C_{18}H_{28}O_2$ 276.418
Bp_{20} 220-224°.

Chloride: [38877-44-0]
$C_{16}H_{23}ClO$ 266.81
Bp_{12} 185-190°.

[21056-10-0, 92410-98-5, 123953-51-5]

Papa, D. *et al., J.A.C.S.*, 1947, **69**, 3018-3022 (*synth*)
Huisgen, R. *et al., Annalen*, 1954, **586**, 52-69 (*synth*)
Eberhardt, H. *et al., Annalen*, 1972, **760**, 157-170 (*synth*)
Pupo, M.T. *et al., Phytochemistry*, 1996, **42**, 795-798 (*isol*)
Carballeira, N.M. *et al., Lipids*, 1997, **32**, 1271-1275 (*occur*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 256-259 (*occur*)

10-Phenyl-3,5,7,9-decatetraen-2-one P-327

PhCH=CHCH=CHCH=CHCH=CHCOCH$_3$
$C_{16}H_{16}O$ 224.302

(*all-E*)-*form*
Navenone B
[62695-68-5]
Trail-breaking hormone of mollusc *Navanax inermis*.
Cryst. (CH_2Cl_2).
Mp 125-140° dec. λ_{max} 389 (ε 18000) (MeOH) (Berdy).

(3*Z*,5*Z*,7*E*,9*E*)-*form* [73952-90-6]
Constit. of the pheromone of *Navanax inermis*.

Sleeper, H.L. *et al., J.A.C.S.*, 1977, **99**, 2367-2368 (*isol*)
Fenical, W. *et al., Pure Appl. Chem.*, 1979, **51**, 1865 (*struct*)
Sleeper, H.L. *et al., J. Chem. Ecol.*, 1980, **6**, 57 (*isol*)
Duhamel, L. *et al., Tet. Lett.*, 1989, **30**, 7377 (*synth*)
Soullez, D. *et al., Nat. Prod. Lett.*, 1994, **4**, 203 (*synth*)

12-Phenyldodecanoic acid P-328

Benzenedodecanoic acid, 9CI
[14507-27-8]
$Ph(CH_2)_{11}COOH$
$C_{18}H_{28}O_2$ 276.418
Constit. of *Trichilia claussenii*, *Vibrio alginolyticus* associated with the alga *Cladophora coelothrix* and halophilic *Bacillus* spp.
Mp 57-58°.

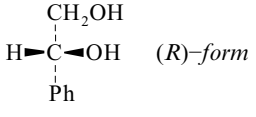
Me ester: [38795-65-2]
$C_{19}H_{30}O_2$ 290.445
Oil. Bp_9 193-196°.

[38795-65-2, 107259-53-0, 107259-54-1, 107259-55-2, 117104-15-1, 125009-69-0, 125009-70-3, 127308-23-0]

Huisgen, R. *et al., Annalen*, 1954, **586**, 52-69 (*synth*)
Goodman, M.M. *et al., J. Med. Chem.*, 1984, **27**, 390-397 (*synth, pmr, ms*)
Pupo, M.T. *et al., Phytochemistry*, 1996, **42**, 795-798 (*occur*)
Carballeira, N.M. *et al., Lipids*, 1997, **32**, 1271-1275 (*occur*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 256-259 (*occur*)

1-Phenyl-1,2-ethanediol, 9CI, 8CI P-329

α,β-Dihydroxyethylbenzene. Styrene glycol. Phenylethylene glycol
[93-56-1]



(*R*)–*form*

$C_8H_{10}O_2$ 138.166
▶ KI2500000

(*S*)-*form* [25779-13-9]
Mp 65-66°. $[\alpha]_D^{24}$ +40.7 (H_2O).

Dibenzoyl: [123725-11-1]
$C_{22}H_{18}O_4$ 346.382
Isol. from the starfish *Pteraster militaris.*

[10522-02-8, 25496-78-0, 115482-82-1, 115482-83-2, 138877-10-8, 147441-61-0, 147441-62-1]

Yayli, N. *et al., Turk. J. Chem.*, 1993, **17**, 208-214 (*Pteraster militaris constit*)

2-Phenylethylamine P-330

Benzeneethanamine, 9CI. Phenethylamine, 8CI. β-Aminoethylbenzene. FEMA 3220. β-Phenethylamine
[64-04-0]
$PhCH_2CH_2NH_2$
$C_8H_{11}N$ 121.182
Very widely distributed alkaloid, esp. in *Acacia* spp. and *Crataegus* spp. Also present in animal tissues, some algae, fungi and cacti (Leguminosae, Rosaceae, Cactaceae). Metab. of *Prosopis alba*. Prod. by *Streptomyces* 699-A3. Shows DNA binding activity. Monoamine oxidase inhibitor. Liq. with a fish odour. d_4^{24} 0.96. Bp 197-198° Bp_7 70-71°. n_D^{25} 1.5290. Absorbs CO_2 from air.
▶ Fl. p. 84°. Skin irritant and possible sensitiser. SG8750000

N-*(3-Methylbutanoyl): 3-Methyl*-N-*(2-phenylethyl)butanamide. 3-Methyl*-N-*phenethylbutyramide.* N-*Phenethylisovaleramide*
$C_{13}H_{19}NO$ 205.299
Prod. by a North sea bacterium *Cytophaga marinoflava* sp. AM13.1. Also prod. by a limnic bacterial strain GW90a.
Amorph.
Mp 64°.

N-*(9-Hydroxyhexadecanoyl):* **N-*(2-Phenylethyl)-9-hydroxyhexadecacarboxamide***
[172303-93-4]
$C_{24}H_{41}NO_2$ 375.593
Isol. from *Telesto riisei*. Mildly cytotoxic to murine leukaemia cells (P-388) in culture. Cryst.
Mp 78°. $[\alpha]_D^{25}$ -2.68 (c, 0.41 in $CHCl_3$). Erroneous struct. diag. in paper.

N-*(9-Oxohexadecanoyl):* **N-*(2-Phenylethyl)-9-oxohexadecacarboxamide***
[172303-92-3]
$C_{24}H_{39}NO_2$ 373.578
Isol. from the coelenterate *Telesto riisei*. Mildly cytotoxic to murine leukaemia cells (P-388) in culture. Cryst.
Mp 85°. Erroneous struct. diag. in paper.

[1077-11-8, 6068-85-5, 62510-53-6, 75337-06-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1269D; 1270A; 1275D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 570C; 571A; 583C; 584A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1164C; 1166D (*ir*)
Sadtler Standard C-13 NMR Spectra, 68 (*cmr*)
Org. Synth., Coll. Vol., 3, 1955, 720-722 (*synth*)
Mosnaim, A. *et al., Clin. Chim. Acta*, 1973, **46**, 407-413 (*ir, ms*)
Smith, T.A. *et al., Phytochemistry*, 1977, **16**, 9-18 (*rev, occur*)
Iwase, H. *et al., Chem. Pharm. Bull.*, 1979, **27**, 1009-1014 (*glc, ms*)
Doetsch, P.W. *et al., J. Chromatogr.*, 1980, **189**, 79-85 (*occur*)
Purchase, C.F. *et al., J.O.C.*, 1991, **56**, 457-459 (*synth, ir, pmr*)
Liyanage, G.K. *et al., J. Nat. Prod.*, 1996, **59**, 148-151 (*9-oxohexadecanoyl, 9-hydroxyhexadecanoyl*)
Luis-Astudillo, S. *et al., Planta Med.*, 1999, **65**, 161-162 (*activity*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*Cytophaga marinoflava amide*)

N-(2-Phenylethyl)carbamic acid P-331

$PhCH_2CH_2NHCOOH$
$C_9H_{11}NO_2$ 165.191

Et ester: Ethyl N-*(2-phenylethyl)carbamate*
$C_{11}H_{15}NO_2$ 193.245
Isol. from a culture medium of the marine bacterium *Cytophaga* sp. Inhibitor of biofilm formation and marine fouling.
Isol. and props. not fully descr.

Butyl ester: Butyl N-*(2-phenylethyl)carbamate. TMC 49A. Antibiotic TMC 49A*
[205594-32-7]
$C_{13}H_{19}NO_2$ 221.299
Prod. by *Streptomyces* sp. AS1345. Transcriptional up-regulator of low density lipoprotein receptor. Oil. Sol. MeOH, EtOAc, DMSO, $CHCl_3$; poorly sol. H_2O, Me_2CO.
Mp 6-7°. Bp 120-122°. λ_{max} 260 (ϵ 270) (MeOH).

Shriner, R.L. *et al., J.A.C.S.*, 1952, **74**, 549-550 (*butyl ester, synth*)
Yamada, A. *et al., Bull. Chem. Soc. Jpn.*, 1997, **70**, 3061-3069 (*Et ester, isol*)
Koguchi, Y. *et al., J. Antibiot.*, 1998, **51**, 107-111 (*butyl ester, isol, pmr, cmr, ms*)

16-Phenylhexadecanoic acid P-332

Benzenehexadecanoic acid, 9CI
[19629-78-8]
$Ph(CH_2)_{15}COOH$
$C_{22}H_{36}O_2$ 332.525
Constit. of *Vibrio alginolyticus* associated with the alga *Cladophora coelothrix*. Cryst. (MeOH).
Mp 76-77°.

Huisgen, R. *et al., Chem. Ber.*, 1960, **93**, 2693-2704 (*synth*)
Protiva, J. *et al., Coll. Czech. Chem. Comm.*, 1986, **51**, 872-878 (*synth, pmr, ms*)
Carballeira, N.M. *et al., Lipids*, 1997, **32**, 1271-1275 (*occur*)

Phenylmethanethiol P-333

Benzenemethanethiol, 9CI. α-Toluenethiol, 8CI. Benzyl mercaptan. Thiobenzyl alcohol. Benzyl thiol. (Mercaptomethyl)benzene. (Thiomethyl)benzene. FEMA 2147
[100-53-8]
$PhCH_2SH$
C_7H_8S 124.206
Isol. from the marine sponge *Crella spinulata*. Flavouring agent.

Liq. with a repulsive, garlic-like odour. d^{20} 1.06. Bp 194-195°. n_D^{20} 1.5748. pK_{a1} 9.43 (25°).

▶ Fl. p. 70°. Eye irritant. LD_{50} (rat, orl) 493 mg/kg. XT8650000

S-*Me:* See Benzyl methyl sulfide, B-64

S-*Et: [(Ethylthio)methyl]benzene. Benzyl ethyl sulfide*
[6263-62-3]
$C_9H_{12}S$ 152.26
Bp 214-216°.

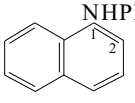
S-*Et,* S,S-*dioxide: Benzyl ethyl sulfone*
[772-47-4]
$C_9H_{12}O_2S$ 184.259
Cryst. Mp 83°.

[3492-64-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1173C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 415C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1089C (*ir*)
Sadtler Standard C-13 NMR Spectra, 1022 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 1822 (*uv*)
Tatematsu, A. *et al., Tet. Lett.*, 1966, 4609 (*ms*)
Bittel, J.E. *et al., J.O.C.*, 1978, **43**, 1687 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 62
Choi, J. *et al., Synthesis*, 1995, 373 (*synth, ir, pmr, ms*)
Bandaranayake, W.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1996, **113**, 499 (*isol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 272
Aitken, R.A. *et al., Synthesis*, 1997, 787-791 (*benzyl ethyl sulfone*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TGO750

N-Phenyl-1-naphthylamine P-334

1-Anilinonaphthalene. Antioxidant PAN. Neozone A. Nocrac PA. Nonox A. Nonox AN. Vulkanox PAN
[90-30-2]



$C_{16}H_{13}N$ 219.285
Constit. of *Eichhornia crassipes* and *Narcissus tazetta*. Prod. by the marine *Streptomyces* sp. B8335. Rubber vulcanisation accelerator. Antioxidant. Indicator used in the anal. of organometallic reagents. Fluorescent probe for detn. of detergent critical micelle concentrations. Electrochem. homopolym. gives a semiconducting polymer film. Prisms or needles (EtOH), leaflets (petrol).
Mp 62°. Bp_{528} 335° Bp_8 226°. Isol. not well documented. Possible contaminant.

▶ Exp. carcinogen. LD_{50} (rat, orl) 1625 mg/kg. QM4500000

Hydrochloride: [43072-28-2]
Light pink leaflets. Mp 164-167°.

N-*Ac:* N-*1-Naphthalenyl*-N-*phenylacetamide, 9CI*
[59130-78-8]
$C_{18}H_{15}NO$ 261.323
Cryst. (EtOH). Sol. EtOH, $CHCl_3$, C_6H_6; spar. sol. Et_2O. Mp 115° Mp 124-125°.

N-*Benzoyl:* N-*1-Naphthalenyl*-N-*phenylbenzamide, 9CI*
[108438-83-1]
$C_{23}H_{17}NO$ 323.393
Cryst. (EtOH). Sol. EtOH, Et_2O, C_6H_6. Mp 152°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 1059A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1251B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1159C (*ir*)
Sadtler Standard C-13 NMR Spectra, 4628 (*cmr*)
Streiff, J. *et al., Annalen*, 1881, **209**, 151 (*synth, N-Ac, N-benzoyl*)
Knoevenagel, E. *et al., J. Prakt. Chem.*, 1914, **89**, 1 (*synth*)
Hodgson, H.H. *et al., J. Soc. Chem. Ind., London*, 1939, **58**, 154 (*synth*)
Nakamura, K. *et al., Synthesis*, 1974, 882 (*synth*)
Riepe, W. *et al., Org. Mass Spectrom.*, 1978, **13**, 57 (*ms*)
Cheung, H.T.A. *et al., J. Labelled Compd. Radiopharm.*, 1980, **17**, 21 (*N-Ac*)
Bergbreiter, D.E. *et al., J.O.C.*, 1981, **46**, 219 (*use*)
Brito, R.M.M. *et al., Anal. Biochem.*, 1986, **152**, 250 (*use*)
Peters, A.T. *et al., Dyes Pigm.*, 1987, **8**, 99 (*synth*)
Guay, J. *et al., Macromolecules*, 1990, **23**, 3598 (*polym*)
Olah, G.A. *et al., J.O.C.*, 1993, **58**, 6900 (*synth*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PFT250

3-Phenyl-2-propen-1-ol, 9CI P-335

Cinnamyl alcohol, 8CI. Cinnamic alcohol. 3-Phenylallyl alcohol. Styrone. Styryl alcohol. FEMA 2294
[104-54-1]
$PhCH{=}CHCH_2OH$
$C_9H_{10}O$ 134.177

▶ Fl. p. >106°. Skin irritant. LD_{50} (rat, orl) 2000 mg/kg. GE2200000

(*E*)-*form* [4407-36-7]
Manuf. by reduction of 3-Phenyl-2-propenal. Constit. of storax and Peruvian balsam, mainly as ester of Cinnamic acid. Used in perfumery industry.
Needles with attractive mild odour. Sol. H_2O. d_4^{20} 1.04.
Mp 33°. Bp 258° Bp_{14} 142-145°.

(3-Phenylpropanoyl): Cinnamyl dihydrocinnamate
[140671-25-6]
$C_{18}H_{18}O_2$ 266.339
Constit. of *Caulerpa racemosa*. Oil.

(1-Phenyl-2-propenyl) ether:
$C_{18}H_{18}O$ 250.34
Constit. of *Caulerpa racemosa*. Oil. $[\alpha]_D^{32}$ +1.67 (c, 0.06 in $CHCl_3$).

(3-Phenyl-1-propenyl) ether: [140671-24-5]
$C_{18}H_{18}O$ 250.34
Constit. of *Caulerpa racemosa*. Oil.

*(3-Phenyl-2*E*-propenyl) ether: Cinnamyl ether. Dicinnamyl ether*
[56759-09-2]
$C_{18}H_{18}O$ 250.34
Constit. of *Caulerpa racemosa*. Cryst. (MeOH) (synthetic).
Mp 43.5-44.8° (synthetic).

[103-54-8, 5320-75-2, 77134-01-1]

Wittig, G. *et al., Annalen*, 1955, **594**, 1 (*cinnamyl ether*)
Staab, H.A. *et al., Chem. Ber.*, 1960, **93**, 2902 (*cinnamyl ether*)
Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 1992, **55**, 496-499 (*Caulerpa racemosa constits*)

14-Phenyltetradecanoic acid P-336

Benzenetetradecanoic acid. 14-Phenylmyristic acid
[24065-50-7]
$Ph(CH_2)_{13}COOH$
$C_{20}H_{32}O_2$ 304.472
Constit. of *Trichilia claussenii*, *Vibrio alginolyticus* associated with the alga *Cladophora coelothrix* and halophilic *Bacillus* spp. Cryst. (cyclohexane).
Mp 69.5-70°. $Bp_{0.007}$ 180-190°.

Et ester: [88336-97-4]
$C_{22}H_{36}O_2$ 332.525
Oil.

Huisgen, R. *et al., Annalen*, 1954, **586**, 52-69 (*synth*)
Ishizawa, A. *et al., CA*, 1969, **71**, 101376y (*synth*)
Goodman, M.M. *et al., J. Med. Chem.*, 1984, **27**, 390-397 (*Et ester, pmr, ms*)
Pupo, M.T. *et al., Phytochemistry*, 1996, **42**, 795-798 (*occur*)
Carballeira, N.M. *et al., Lipids*, 1997, **32**, 1271-1275 (*occur*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 256-259 (*occur*)

13-Phenyltridecanoic acid, 8CI P-337

Benzenetridecanoic acid, 9CI. 13-Phenyltridecoic acid
[20913-07-9]
$Ph(CH_2)_{12}COOH$
$C_{19}H_{30}O_2$ 290.445
Constit. of *Trichilia claussenii*, *Typhonium flagelliforme* and halophilic *Bacillus* spp. Cryst. (petrol).
Mp 55.1-55.6° (52-52.5°). Bp_{10} 236-237°.

[123953-55-9]

Huisgen, R. *et al., Annalen*, 1954, **586**, 52-69 (*synth*)
Dmitriev, S.A. *et al., CA*, 1962, **56**, 7207g (*synth*)
Ishizawa, A. *et al., CA*, 1969, **70**, 11178k; **71**, 101376y (*synth*)
Pupo, M.T. *et al., Phytochemistry*, 1996, **42**, 795-798 (*occur*)
Schmid, P.C. *et al., Phytochemistry*, 1997, **45**, 1173-1175 (*isol*)
Chen, S.-X. *et al., Planta Med.*, 1997, **63**, 580 (*isol, pmr, cmr*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 256-259 (*occur*)

Sepia officinalis Pheromone peptide P-338

[301316-34-7]

Ile-Leu-Met-Glu

$C_{22}H_{40}N_4O_7S$ 504.647

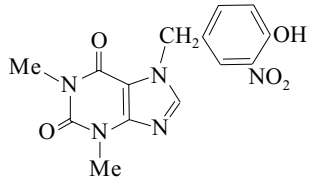
Isol. from the egg mass of *Sepia officinalis*. Exhibits both paracrine and pheromonal activity. All-L-config.

Zatylny, C. *et al., Biochem. Biophys. Res. Commun.*, 2000, **275**, 217-222 (*isol*)

Phidolopin P-339

*3,7-Dihydro-7-[(4-hydroxy-3-nitrophenyl)methyl]-1,3-dimethyl-1*H*-purine-2,6-dione, 9CI*

[92014-27-2]



$C_{14}H_{13}N_5O_5$ 331.287

Found in the marine bryozoan *Phidolopora pacifica*. Shows antifungal and antialgal props. Cryst. (MeOH). Sol. MeOH, EtOAc; poorly sol. H_2O.

Mp 226-227°. λ_{max} 275 (ϵ 16800); 353 (ϵ 3300) (MeCN) (Derep).

N^1,N^3-*Di-de-Me:* ***Desmethylphidolopin***

[103545-34-2]

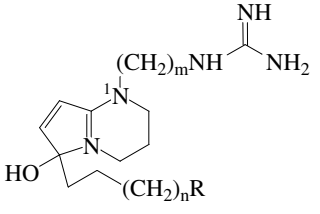
$C_{12}H_9N_5O_5$ 303.234

From the marine bryozoans *Phidolopora pacifica* and *Diaperoecia californica*. Antifungal agent. Yellow amorph. powder.

Ayer, S.W. *et al., J.O.C.*, 1984, **49**, 3869-3870 (*isol, uv, ir, pmr, ms, cryst struct*)
Hirota, K. *et al., Tet. Lett.*, 1985, **26**, 2355 (*synth*)
Tischler, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **84**, 43 (*deriv*)
Avasthi, K. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 437 (*synth, pmr, cmr, ms*)

Phloeodictyne A P-340

Phloeodictine A



Naming system and numbering revised in 2004. Under the revised numbering scheme, the number before the comma indicates *m*, the number after the comma indicates *n*, and the suffix *a* or *i* indicates the end-group *R* (*a* = allyl, -$CH_2CH{=}CH_2$, *i* = isopropyl, -$CH(CH_3)_2$). The +ve charge is delocalised over the two ring nitrogens. Isol. from the New Caledonian deep water sponge *Phloeodictyon* sp. and shallow-water sponge *Oceanapia fistulosa* (*Phloeodictyon fistulosa*). Shows *in vitro* antibacterial activity and mod. cytotoxicity against KB cells. Shows antiplasmodial props.

Phloeodictyne 4,5a

Phloeodictine A4

[155070-26-1]

$C_{22}H_{41}N_5O$ 391.599

λ_{max} 224 (ϵ 6700); 274 (ϵ 2200) (MeOH) (Berdy).

Phloeodictyne 4,5i

$C_{22}H_{43}N_5O$ 393.615

Phloeodictyne 4,6a

$C_{23}H_{43}N_5O$ 405.626

Phloeodictyne 4,6i

$C_{23}H_{45}N_5O$ 407.641

Phloeodictyne 4,7a

Phloeodictine A2

[155070-28-3]

$C_{24}H_{45}N_5O$ 419.652

Amorph. solid (as dichloride). Mixt. with Phloeodictine A1.

λ_{max} 224 (ϵ 6700); 274 (ϵ 2200) (MeOH) (Berdy).

Phloeodictyne 4,7i

$C_{24}H_{47}N_5O$ 421.668

Phloeodictyne 4,8a

$C_{25}H_{47}N_5O$ 433.679

Phloeodictyne 4,8i

Phloeodictine A7

[155070-24-9]

$C_{25}H_{49}N_5O$ 435.695

λ_{max} 224 (ϵ 6700); 274 (ϵ 2200) (MeOH) (Berdy).

Phloeodictyne 4,9a

Phloeodictine A (obsol.)†

[142260-80-8]

$C_{26}H_{49}N_5O$ 447.706

Amorph. solid (as dichloride). λ_{max} 224 (ϵ 6700); 274 (ϵ 2200) (MeOH) (Derep).

Phloeodictyne 4,10a

$C_{27}H_{51}N_5O$ 461.733

Phloeodictyne 4,10i

$C_{27}H_{53}N_5O$ 463.749

Phloeodictyne 4,11a

$C_{28}H_{53}N_5O$ 475.76

Phloeodictyne 5,4a

Phloeodictine A5

[155070-27-2]

$C_{22}H_{41}N_5O$ 391.599

λ_{max} 224 (ϵ 6700); 274 (ϵ 2200) (MeOH) (Berdy).

Phloeodictyne 5,4i

$C_{22}H_{43}N_5O$ 393.615

Phloeodictyne 5,5a

Phloeodictine A3

[155112-61-1]

$C_{23}H_{43}N_5O$ 405.626

Amorph. solid (as dichloride). Initially isol. as a *ca.* 2.6:0.7:0.3 insep. mixt. with Phloeodictines A4 and A5. λ_{max} 224 (ϵ 6700); 274 (ϵ 2200) (MeOH) (Berdy).

Phloeodictyne 5,5i

$C_{23}H_{45}N_5O$ 407.641

Phloeodictyne 5,6i

$C_{24}H_{47}N_5O$ 421.668

Phloeodictyne 5,7a
Phloeodictine A1
[155070-29-4]
$C_{25}H_{47}N_5O$ 433.679
Amorph. solid (as dichloride). Isol. as a *ca.* 2.6:1 insep. mixt. with Phloeodictine A2. λ_{max} 224 (ϵ 6700); 274 (ϵ 2200) (MeOH) (Berdy).

Phloeodictyne 5,7i
$C_{25}H_{49}N_5O$ 435.695

Phloeodictyne 5,8a [690654-91-2]
$C_{26}H_{49}N_5O$ 447.706

Phloeodictyne 5,8i
Phloeodictine A6
[155070-25-0]
$C_{26}H_{51}N_5O$ 449.722
Amorph. solid (as dichloride). Initially isol. as a *ca.* 1:1.4 insep. mixt. with Phloeodictine A7. λ_{max} 224 (ϵ 6700); 274 (ϵ 2200) (MeOH) (Berdy).

Phloeodictyne 5,9a
$C_{27}H_{51}N_5O$ 461.733

Phloeodictyne 5,9i
$C_{27}H_{53}N_5O$ 463.749

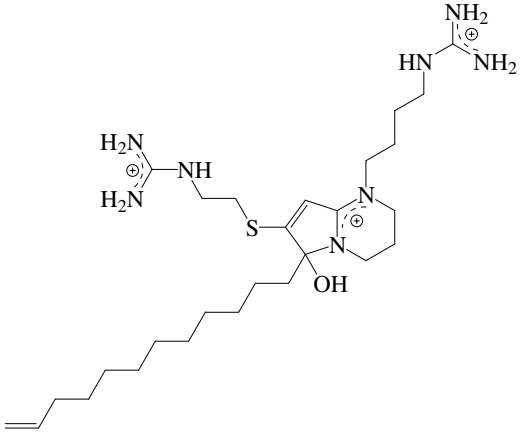
Phloeodictyne 5,10a
$C_{28}H_{53}N_5O$ 475.76

Phloeodictyne 5,10i
$C_{28}H_{55}N_5O$ 477.775

Kourany-Lefoll, E. *et al., Tetrahedron*, 1994, **50**, 3415-3426 (*isol*)
Neubert, B.J. *et al., Org. Lett.*, 2003, **5**, 765-768 (*synth*)
Mancini, I. *et al., Org. Biomol. Chem.*, 2004, **2**, 783-787 (*isol, ms*)

Phloeodictyne B P-341

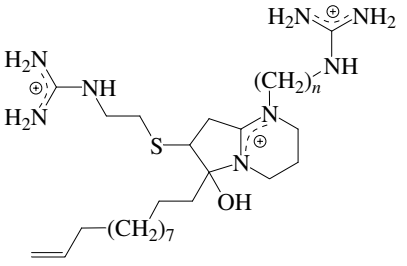
[142260-81-9]



$C_{27}H_{53}N_8OS^{3\oplus}$ 537.835
Isol. from a New Caledonian sponge *Phloeodictyon* sp. Amorph. solid (as trichloride). CAS no. refers to trichloride. λ_{max} 202 (ϵ 5500); 279 (ϵ 7100) (MeOH) (Derep).

Kourany-Lefoll, E. *et al., J.O.C.*, 1992, **57**, 3832 (*isol, uv, pmr, cmr, cd, struct*)

Phloeodictyne C P-342



Phloeodictyne C1, $n = 5$
C2, $n = 4$

Exhibits *in vitro* antibacterial activity and is moderately cytotoxic against KB cells.

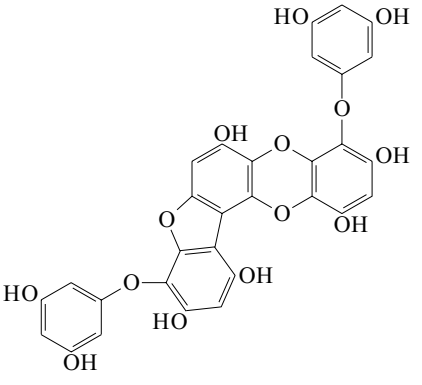
Phloeodictyne C1 [155070-23-8]
$C_{28}H_{57}N_8OS$ 553.877
Alkaloid from the New Caledonian sponge *Phloeodictyon* sp. Amorph. solid (as trichloride) (mixt. with C2). Isol. as a *ca.* 1:1 insep. mixt. of homologues. λ_{max} 219 (ϵ 9100) (MeOH) (Berdy).

Phloeodictyne C2 [155070-22-7]
$C_{27}H_{55}N_8OS$ 539.85
From *Phloeodictyon* sp. Amorph. solid (as trichloride) (mixt. with C1). λ_{max} 219 (ϵ 9100) (MeOH) (Berdy).

Kourany-Lefoll, E. *et al., Tetrahedron*, 1994, **50**, 3415 (*isol, uv, ir, pmr, cmr, struct*)

Phlorofucofuroeckol A P-343

*4,9-Bis(3,5-dihydroxyphenoxy)benzo[*b*]benzofuro[3,2-*f*][1,4]benzodioxin-1,3,6,10,12-pentol, 9CI*
[128129-56-6]

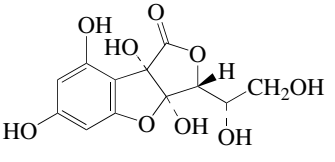


$C_{30}H_{18}O_{14}$ 602.464
Isol. from the brown alga *Ecklonia kurome*. Potent anti-plasmin inhibitor. Amorph. solid. λ_{max} 244 (ϵ 58000); 292 (ϵ 6800); 317 (ϵ 3100) (MeOH) (Berdy).

Fukuyama, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 133 (*isol, pmr, cmr*)

Phloroscorbinol P-344

[197630-93-6]



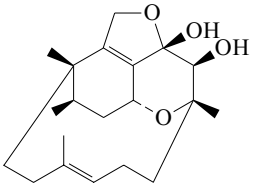
$C_{12}H_{12}O_9$ 300.221

Isol. from the brown alga *Sargassum spinuligerum*. Amorph. (as hexa-Ac).

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 341-345 (*isol, ir, pmr, cmr, ms*)

Phomactin A P-345

Antibiotic Sch 49028. Sch 49028
[130595-24-3]
[149008-34-4]



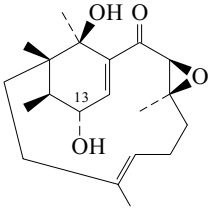
$C_{20}H_{30}O_4$ 334.455

Nmr studies suggest that Phomactin A and Sch 49028 are identical. Metab. of a marine *Phoma* sp. (SANK11486; P10364). Platelet activating factor antagonist. Oil. Sol. MeOH, Et_2O, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ +175 (c, 0.75 in $CHCl_3$) (Phomactin A). $[\alpha]_D$ +245.6 (c, 0.3 in $CHCl_3$) (Sch 49028).

Sugano, M. *et al., J.A.C.S.*, 1991, **113**, 5463-5464 (*Phomactin A, isol, pmr, cmr, cryst struct*)
Chu, M. *et al., J. Antibiot.*, 1993, **46**, 554-563 (*Sch 49028*)
Goldring, W.P.D. *et al., Chem. Comm.*, 2002, 1736-1737 (*synth*)
Mohr, P.J. *et al., J.A.C.S.*, 2003, **125**, 1712-1713 (*synth*)
Diaper, C.M. *et al., Org. Biomol. Chem.*, 2003, 3949-3956 (*synth*)

Phomactin B P-346

[130566-37-9]



$C_{20}H_{30}O_4$ 334.455
Metab. of a marine *Phoma* sp. Platelet activating factor inhibitor. Cryst. Sol. MeOH, Et_2O, C_6H_6; poorly sol. H_2O.
Mp 180-182°. $[\alpha]_D$ +146 (c, 0.75 in $CHCl_3$). λ_{max} 238 (ϵ 3350) (EtOH) (Derep). λ_{max} 240 (ϵ 2500) (EtOH) (Berdy).

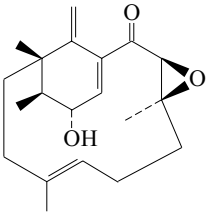
13-Epimer: ***Phomactin B1***
[141361-13-9]
$C_{20}H_{30}O_4$ 334.455
Metab. of a marine *Phoma* sp. Platelet activating factor inhibitor. Cryst.
Mp 203-205°. $[\alpha]_D$ +167.3 (c, 1 in $CHCl_3$). λ_{max} 238 (ϵ 3350) (EtOH) (Derep). λ_{max} 235 (ϵ 3600) (MeOH) (Berdy).

[130566-46-0]

Eur. Pat., 1990, 371 762; *CA*, **113**, 229691a (*isol*)
Sugano, M. *et al., J.O.C.*, 1994, **59**, 564 (*isol, pmr, cmr, cryst struct, abs config*)

Phomactin B2 P-347

[141361-14-0]

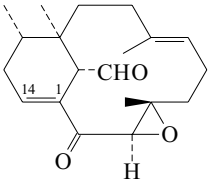


$C_{20}H_{28}O_3$ 316.439
Metab. of a *Phoma* sp. Platelet activating factor inhibitor. Oil. $[\alpha]_D$ +173 (c, 5 in $CHCl_3$). λ_{max} 221 (ϵ 8700); 262 (ϵ 3600) (EtOH) (Derep). λ_{max} 221 (ϵ 8700); 262 (ϵ 3600) (MeOH) (Berdy).

Sugano, M. *et al., J.O.C.*, 1994, **59**, 564 (*isol, pmr, cmr*)

Phomactin C P-348

Antibiotic Sch 47918. Sch 47918
[143903-06-4]



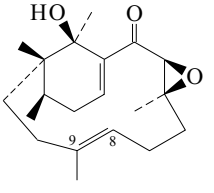
$C_{20}H_{28}O_3$ 316.439
Prod. by a marine *Phoma* sp. Platelet activating factor antagonist. Cryst.
Mp 204-205°. $[\alpha]_D^{22}$ +222.4 (c, 0.3 in $CHCl_3$). λ_{max} 244 (ϵ 6350) (MeOH) (Derep).

1,14-Dihydro: ***Phomactin D***
[154512-14-8]
$C_{20}H_{30}O_3$ 318.455
Metab. of a marine *Phoma* sp. Cryst.
Mp 97-98°. $[\alpha]_D$ +114.3 (c, 1 in $CHCl_3$).

Chu, M. *et al., J.O.C.*, 1992, **57**, 5817 (*isol, pmr, cmr, cryst struct*)
Chu, M. *et al., J. Antibiot.*, 1993, **46**, 554 (*isol, props*)
Sugano, M. *et al., J.O.C.*, 1994, **59**, 564 (*isol, pmr, cmr*)
Miyaoka, H. *et al., Tet. Lett.*, 1996, **37**, 7107-7110 (*synth*)

Phomactin E P-349

16-Hydroxy-5,9,12,13,16-pentamethyl-4-oxatricyclo[10.3.1.0^{3,5}]-hexadeca-1(15),8-dien-2-one, 9CI
[163597-60-2]



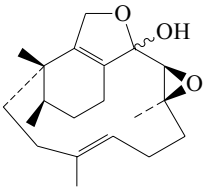
$C_{20}H_{30}O_3$ 318.455
Prod. by a marine *Phoma* sp. Platelet activating factor antagonist. Sol. MeOH, $CHCl_3$, C_6H_6, DMSO, Et_2O, Me_2CO, EtOH; poorly sol. H_2O.
Mp 148-149°. $[\alpha]_D^{25}$ +178.4 ($CHCl_3$).

8β,9β-Epoxide: ***Phomactin F***
[163597-59-9]
$C_{20}H_{30}O_4$ 334.455
Prod. by a marine *Phoma* sp. Platelet activating factor antagonist. Sol. MeOH, $CHCl_3$, Et_2O, C_6H_6, Me_2CO, EtOH; poorly sol. H_2O.

Mp 199-202°. $[\alpha]_D^{25}$ +120.9 ($CHCl_3$).
Sugano, M. *et al., J. Antibiot.*, 1995, **48**, 1188 (*isol, uv, pmr, cmr*)

Phomactin G **P-350**

[163597-61-3]

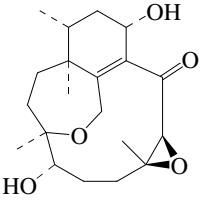


$C_{20}H_{30}O_3$ 318.455
Prod. by a marine *Phoma* sp. Platelet activating factor antagonist. Mp 131-132°. $[\alpha]_D^{25}$ +96.9 ($CHCl_3$).

Sugano, M. *et al., J. Antibiot.*, 1995, **48**, 1188 (*isol, pmr, cmr*)
Goldring, W.P.D. *et al., Org. Biomol. Chem.*, 2004, **2**, 466-473 (*synth*)

Phomactin H **P-351**

[785785-54-8]

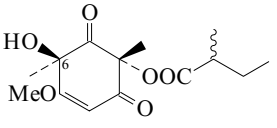


$C_{20}H_{30}O_5$ 350.454
Prod. by a marine-derived fungus. Cryst. $[\alpha]_D^{20}$ +204 (c, 0.18 in MeOH). λ_{max} 250 (log ϵ 3.84) (MeOH).

Koyama, K. *et al., Tet. Lett.*, 2004, **45**, 6947-6948 (*isol, pmr, cmr, cryst struct*)

Phomaligol A **P-352**

[152204-32-5]



$C_{14}H_{20}O_6$ 284.308
Isol. from the asexual stage of *Phoma lingam* (*Leptosphaeria maculens*). Also isol. from a marine-derived *Alternaria* sp. Oil. $[\alpha]_D^{24}$ -79 (c, 1.13 in $CHCl_3$).

6-Epimer: ***Phomaligol A$_1$***
[152053-11-7]
$C_{14}H_{20}O_6$ 284.308
Isol. from *Phoma lingam*. Oil. $[\alpha]_D^{24}$ -32 (c, 0.54 in $CHCl_3$).

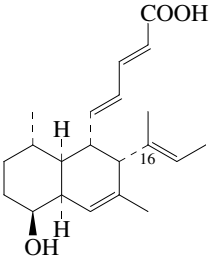
6-Deoxy: ***Phomaligadione A***
[152053-12-8]
$C_{14}H_{20}O_5$ 268.309
Isol. from *Phoma lingam*. Pale yellow oil. Mixt. of C-6 epimers. Obt. as a mixt. with Phomaligadione B.

6-Deoxy, $\Delta^{5,6}$-Isomer: ***Phomaligadione B***
[152053-13-9]
$C_{14}H_{20}O_5$ 268.309
Isol. from *Phoma lingam*.

Pedras, M.S.C. *et al., Tetrahedron*, 1993, **49**, 8317-8322 (*isol, pmr, cmr*)
Li, X. *et al., Arch. Pharmacal Res.*, 2003, **26**, 532-534 (*isol*)

Phomopsidin **P-353**

Antibiotic TUF 95F47. TUF 95F47
[199173-60-9]



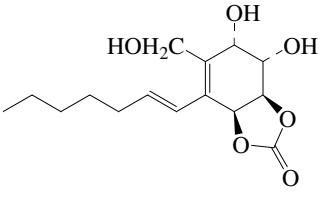
Absolute Configuration

$C_{21}H_{30}O_3$ 330.466
Prod. by a *Phomopsis* sp. strain TUF 95F47 isol. from a coral reef. Antifungal and antibiotic agent. $[\alpha]_D^{27}$ +31 (c, 0.1 in MeOH). λ_{max} 260 (ϵ 23000) (MeOH).

(16Z)-Isomer: ***Antibiotic MK 8383***. *MK 8383*
[165689-16-7]
$C_{21}H_{30}O_3$ 330.466
Prod. by a *Phoma* sp. Antifungal agent. λ_{max} 260 (MeOH) (Berdy).

Japan. Pat., 1995, 95 126 211; *CA*, **123**, 105272b (*MK 8383*)
Namikoshi, M. *et al., J. Antibiot.*, 1997, **50**, 890-892 (*isol, uv, pmr, cmr*)
Japan. Pat., 1999, 99 29 520; *CA*, **130**, 181564h (*TUF 95F47*)
Namikoshi, M. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1452-1457 (*isol, uv, pmr, cmr*)
Kobayashi, H. *et al., Tetrahedron*, 2003, **59**, 455-459 (*abs config, biosynth*)
Suzuki, T. *et al., Org. Lett.*, 2004, **6**, 553-556 (*synth, abs config*)

Phomoxin **P-354**



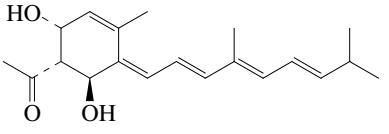
Relative Configuration

$C_{15}H_{22}O_6$ 298.335
Related to Eupenoxide, E-894. Isol. from a marine-derived *Phoma* sp. (strain CNC-651). Amorph. powder. $[\alpha]_D$ -24.4 (c, 0.04 in MeOH). λ_{max} 207 (log ϵ 3.6) (MeOH).

Liu, Z. *et al., Phytochemistry*, 2003, **64**, 571-574 (*isol, pmr, cmr, ms*)

Phorbasin A **P-355**

[313503-37-6]

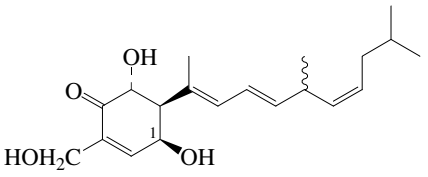


$C_{20}H_{28}O_3$ 316.439
Constit. of a *Phorbas* sponge. Yellow solid. $[\alpha]_D^{22}$ +2 (c, 0.38 in MeOH). λ_{max} 232 (ϵ 11000); 312 (ϵ 25500); 326 (ϵ 20300) (MeOH).

Vuong, D. *et al., J. Nat. Prod.*, 2000, **63**, 1684-1685 (*isol, pmr, cmr*)

Phorbasin B P-356

[346585-46-4]

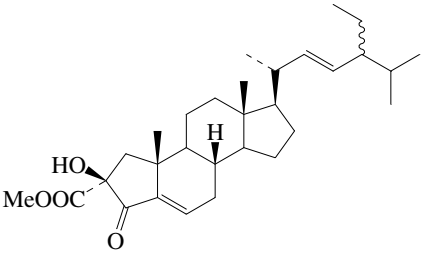


$C_{20}H_{30}O_4$ 334.455
Constit. of a *Phorbas* sponge. Yellow oil. $[\alpha]_D$ -60.2 (c, 0.064 in MeOH). λ_{max} 234 (log ϵ 9.33); 279 (log ϵ 7.74) (no solvent reported).

1-Ac: ***Phorbasin C***
[346585-47-5]
$C_{22}H_{32}O_5$ 376.492
Constit. of a *Phorbas* sponge. Yellow oil.
McNally, M. *et al., J. Nat. Prod.*, 2001, **64**, 645-647 (*isol, pmr, cmr*)

Phorbasterone C P-357

[682808-89-5]
[682808-91-9]

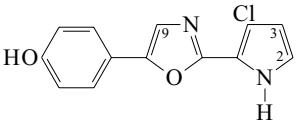


$C_{30}H_{46}O_4$ 470.691
Constit. of *Phorbas amaranthus.* Solid. Mixture of 24-epimers. λ_{max} 250 (ϵ 9100) (MeCN).

22,23-Dihydro: ***Phorbasterone D***
[682808-90-8]
[682808-92-0]
$C_{30}H_{48}O_4$ 472.707
Constit. of *Phorbas amaranthus.* Solid. Mixt. of 24-epimers. λ_{max} 250 (ϵ 9000) (MeCN).
Masuno, M.N. *et al., J. Nat. Prod.*, 2004, **67**, 731-733 (*isol, pmr, cmr*)

Phorbazole D P-358

[156280-94-3]



$C_{13}H_9ClN_2O_2$ 260.679
Isol. from the marine sponge *Phorbas* aff. *clathrata.* Immunomodulator. Amorph. powder.
Mp 210°.

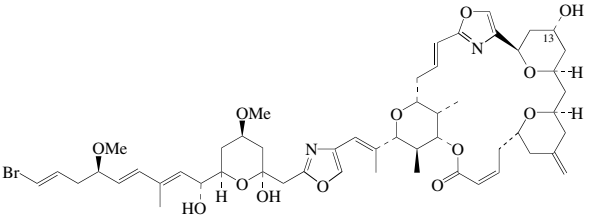
3-Chloro: ***Phorbazole C***
[156280-93-2]
$C_{13}H_8Cl_2N_2O_2$ 295.124
From *Phorbas* aff. *clathrata.* Immunomodulator. Amorph. powder.
Mp 240°.

2,3-Dichloro: ***Phorbazole B***
[156280-92-1]
$C_{13}H_7Cl_3N_2O_2$ 329.569
From *Phorbas* aff. *clathrata*. Immunomodulator. Amorph. off-white powder.
Mp 270°.

3,9-Dichloro: ***Phorbazole A***
[156280-91-0]
$C_{13}H_7Cl_3N_2O_2$ 329.569
From *Phorbas* aff. *clathrata*. Immunomodulator. Powder.
Mp 240°.
Rudi, A. *et al., Tet. Lett.*, 1994, **35**, 2589 (*isol, ir, pmr, cmr, struct*)

Phorboxazole A P-359

[165883-76-1]

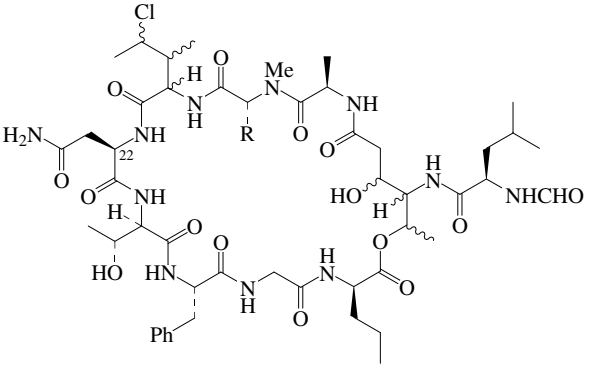


$C_{53}H_{71}BrN_2O_{13}$ 1024.054
Isol. from the sponge *Phorbas* sp. Antifungal and cytostatic agent. Pale yellow solid. $[\alpha]_D$ +44.8 (c,1 in MeOH). λ_{max} 235 (log ϵ 4.9) (MeOH).

13-Epimer: ***Phorboxazole B***
[165689-31-6]
$C_{53}H_{71}BrN_2O_{13}$ 1024.054
Isol. from *Phorbas* sp. Antifungal and cytostatic agent. Pale yellow solid. $[\alpha]_D$ +44.4 (c, 1 in MeOH). λ_{max} 235 (log ϵ 4.8) (MeOH).

Searle, P.A. *et al., J.A.C.S.*, 1995, **117**, 8126 (*isol, uv, ir, pmr, cmr, ms*)
Searle, P.A. *et al., J.A.C.S.*, 1996, **118**, 9422 (*abs config*)
Molinski, T.F. *et al., Tet. Lett.*, 1996, **37**, 7879 (*abs config*)
Evans, D.A. *et al., J.A.C.S.*, 2000, **122**, 10033-10046 (*synth*)
Smith, A.B. *et al., J.A.C.S.*, 2001, **123**, 10942-10953 (*synth, bibl*)
Williams, D.R. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 1258-1262 (*synth*)
Haustedt, L.O. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 2711-2716 (*rev, synth*)
Pattenden, G. *et al., Org. Biomol. Chem.*, 2003, **1**, 4173-4208 (*synth*)
Smith, A.B. *et al., Org. Lett.*, 2005, **7**, 4399-4402 (*synth*)
Li, D.-R. *et al., Chem. Eur. J.*, 2006, **12**, 1185-1204 (*synth*)

Phoriospongin A P-360



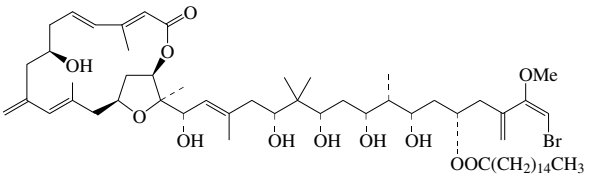
R = $CH_2CH_2CH_3$

$C_{52}H_{82}ClN_{11}O_{15}$ 1136.737

Depsipeptide antibiotic. Related to Cyclolithistide A, C-1027. Isol. from the sponges *Callyspongia bilamellata* and *Phoriospongia* spp. Nematocidal agent. Amorph. solid. $[\alpha]_D^{20}$ +18 (c, 0.08 in MeOH). λ_{max} 204 (ϵ 13750); 229 (ϵ 4100); 273 (ϵ 1300) (MeOH).

Homologue (R = $CH_2CH(CH_3)_2$), 22-epimer: ***Phoriospongin B***
$C_{53}H_{84}ClN_{11}O_{15}$ 1150.764
Isol. from *Callyspongia bilamellata* and *Phoriospongia* spp. Nematocidal agent. Amorph. solid. $[\alpha]_D^{20}$ -6.2 (c, 0.13 in MeOH). λ_{max} 207 (ϵ 16350); 229 (ϵ 3750); 273 (ϵ 1000) (MeOH).
Capon, R.J. *et al., J. Nat. Prod.*, 2002, **65**, 358-363 (*isol, pmr, cmr*)

Phormidolide P-361

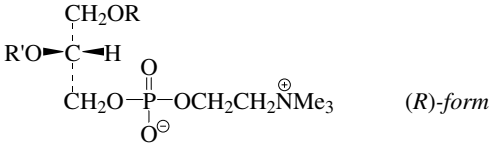


Absolute Configuration

$C_{59}H_{97}BrO_{12}$ 1078.312
Macrolide antibiotic. Related to Oscillariolide, O-131. Isol. from the marine cyanobacterium *Phormidium* sp. Cytotoxic. Oil. $[\alpha]_D^{25}$ +48 (c, 0.25 in $CHCl_3$). λ_{max} 240 (log ϵ 4.2); 270 (log ϵ 4.02) (no solvent reported).
Williamson, R.T. *et al., J.O.C.*, 2002, **67**, 7927-7936; 2003, **68**, 2060 (*isol, pmr, cmr*)

Phosphatidylcholine P-362

1,2-Diacylglycero-3-phosphocholine. Lecithin. Vitellin. Kelecin. Granulestin. Lecithol. Diacyllecithin. Diacylphosphatidylcholine. E322. PC
[8002-43-5]



(*R*)-*form*

R, R' = acyl groups

The naturally occurring (*R*)-form is equivalent to 1,2-diacyl-*sn*-glycero-3-phosphocholine (*sn*-3-phosphatidylcholine). First identified in egg yolk, ox brain and soybean oil. Present in microorganisms and throughout the animal and vegetable kingdoms; structural component of intracellular membranes and the plasma membrane. Major phospholipid in lung surfactant, component of bile. Emollient, emulsifying and solubilising agent. Used in food processing. Involved in permeability, oxidative phosphorylation, phagocytosis and chemical and electrical excitation. Forms bilayers in aq. dispersions which are used to model biol. membranes and to prepare liposomes for drug delivery systems and cosmetics. The degree of unsaturation and chain length result in distinct physical and biol. props. Mammalian phosphatidylcholine usually has a saturated acyl group at *sn*-1 and and an unsaturated group at *sn*-2. The term lecithin is also used to describe a mixture of phosphatidyl esters isolated from vegetable oils and consisting mainly of phosphatidyl-choline, -serine, -ethanolamine and -inositols with some triglycerides, fatty acids and carbohydrates. There is extensive proliferation of CAS numbers for phosphatidylcholines owing to specification of stereochemistry at different levels of precision in the literature.

Glycerol 2-(8,11,14-eicosatrienoate) 1-hexadecanoate 3-phosphocholine
1-O-*Hexadecyl-2*-O-*dihomogammalinolenoylglycero-3-phosphocholine*
[131907-73-8]
$C_{44}H_{84}NO_7P$ 770.124
Isol. from the Japanese oyster *Crassostrea gigas*. PAF precursor.

Glycerol 2-(5,8,11,14,17-eicosapentaenoate) 1-hexadecanoate 3-phosphocholine
2-O-*(5,8,11,14,17-Eicosapentaenoyl)-1*-O-*hexadecylglycero-3-phosphocholine*
[132196-28-2]
Isol. from the Japanese oyster *Crassostrea gigas*. PAF precursor.

Glycerol 2-(4,7,10,13,16,19-docosahexaenoate) 1-hexadecanoate 3-phosphocholine
2-O-*(4,7,10,13,16,19-Docosahexaenoyl)-1*-O-*hexadecylglycero-3-phosphocholine*
[97717-93-6]
Isol. from the Japanese oyster *Crassostrea gigas*. PAF precursor.

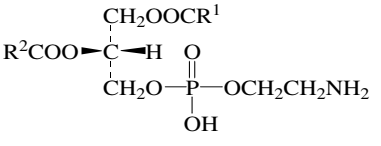
Glycerol 1,2-di(5*Z*,8*Z*,11*Z*,14*Z*-docosatetraenoate) 3-phosphocholine
1,2-Di-5,8,11,14-dicosatetraenoyl-sn-*glycero-3-phosphocholine*
$C_{52}H_{88}NO_8P$ 886.243
Isol. from sponges.

[70094-88-1]

Baer, E. *et al., Biochemistry*, 1962, **1**, 518-521 (*synth*)
Vilallonga, F. *et al., Biochim. Biophys. Acta*, 1968, **163**, 290-300 (*props*)
Saunders, D.R. *et al., Biochim. Biophys. Acta*, 1969, **176**, 828-835 (*props*)
Stoffel, W. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1969, **350**, 1385-1393; 1972, **353**, 1962-1969 (*props, cmr*)
Klein, R.A. *et al., J. Lipid Res.*, 1971, **12**, 123-131; 628-634; 1972, **13**, 672-679 (*ms*)
Demel, R.A. *et al., Biochim. Biophys. Acta*, 1972, **266**, 26-40 (*synth*)
Birdsall, N.J.M. *et al., J.C.S. Perkin 2*, 1972, 1441-1445 (*conformn, pmr, cmr*)
Pons, M. *et al., Biochim. Biophys. Acta*, 1983, **730**, 306-312 (*cmr*)
Dasgupta, A. *et al., Chem. Phys. Lipids*, 1987, **43**, 101-111 (*occur, sponges*)
Burgos, C.E. *et al., J.O.C.*, 1987, **52**, 4973-4977 (***synth***)
Jeong, B.Y. *et al., Lipids*, 1990, **25**, 624-632 (*Crassostrea gigas constits*)
Han, X. *et al., J.A.C.S.*, 1991, **113**, 7104-7109 (*pmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **15**, 192-210 (*rev, props, use, isol, activity*)
Cubre, F. *et al., Biochim. Biophys. Acta*, 1992, **1124**, 297-299 (*biochem*)
Martin, S.F. *et al., J.O.C.*, 1994, **59**, 4805-4820 (***synth***)
Ishihara, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1096-1098 (***synth***)
Lie Ken Jie, M.S.F. *et al., Nat. Prod. Rep.*, 1998, **15**, 607-629 (*rev, occur, synth, anal*)
IUPAC-IUBMB Nomenclature of Lipids, (*nomenclature*)

Phosphatidylethanolamine P-363

1,2-Diacylglycero-3-phosphoethanolamine. Cephalin (obsol.). Kephalin (obsol.). PE



The naturally occurring *R*-form is equivalent to 1,2-diacyl-*sn*-glycero-3-phosphoethanolamine. The nature of R^1 and R^2, including degree of unsaturation and chain length, result in distinct biol. and phys. props. Mammalian phosphatidylethanolamine normally has a saturated acyl group at *sn*-1 and an unsaturated group at *sn*-2. A prominent constit. of the membranes of eukaryotic and prokaryotic cells. Isol. from egg yolk, soya bean lecithin, brain tissue and other biol. sources. Biosynthetic precursor of phosphatidylcholines in eukaryotes. Various members show renin-inhibitory props. Racemates and other stereoisomers are mostly known but phys. props. are not given here.

Glycerol 1,2-bis(5*Z*,9*Z*,19*Z*-octacosatrienoate)
1,2-Di-5,9,19-octacosatrienoyl-sn-*glycero-3-phosphoethanolamine*
$C_{61}H_{110}NO_8P$ 1016.516
Present in sponges.

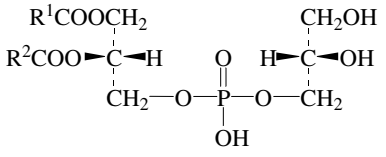
Glycerol 1,2-bis(5*Z*,9*Z*,23*Z*-triacontatrienoate)
1,2-Di-5,9,23-triacontatrienoyl-sn-*glycero-3-phosphoethanolamine*
$C_{65}H_{118}NO_8P$ 1072.623
Present in sponges.

[78535-48-5]

Ansell, G.B. *et al., Phospholipids: Chemistry, Metabolism and Function*, Elsevier, 1964, 85-113 (*bibl, isol*)
Ansell, G.B. *et al., Phospholipids*, (eds. Hawthorne, J.N. *et al*), Elsevier, 1982, 1-49 (*rev*)
Dasgupta, A. *et al., Chem. Phys. Lipids*, 1987, **43**, 101-111 (*sponge phospholipids*)
Paltauf, F. *et al., Prog. Lipid Res.*, 1994, **33**, 239-328 (*synth, rev*)
Kent, C. *et al., Annu. Rev. Biochem.*, 1995, **64**, 315-343 (*biosynth, rev*)
Dowhan, W. *et al., Annu. Rev. Biochem.*, 1997, **66**, 199-232 (*rev, biochem*)
Biochim. Biophys. Acta, 1997, **1348**, 1-256 (*biochem, biosynth, rev*)
McKeone, B.J. *et al., J. Lipid Res.*, 1997, **38**, 429-436 (*hplc, bibl*)

Phosphatidylglycerol P-364

1,2-Diacylglycero-3-phosphoglycerol. PG



Naturally occurring phosphatidylglycerols have the (2*R*,2′*S*)-config. illus. (1,2-diacyl-*sn*-glycero-3-phospho-1′-*sn*-glycerol). Phosphatidylglycerol prepared by phospholipase-catalysed transphosphatidylation of phosphatidylcholine and glycerol is a mixt. of diastereomers at C-2′. Component of adult lung surfactant.

Glycerol 1,2-ditetradecanoate 3-phosphoglycerol
Dimyristoylphosphatidylglycerol. DMPG
[61361-72-6]
[67232-80-8]
$C_{34}H_{67}O_{10}P$ 666.871
Cryst. (CCl_4/EtOH/H_2O)(as Na salt).

Glycerol 1,2-dihexadecanoate 3-phosphoglycerol
1-[[[(2,3-Dihydroxypropoxy)hydroxyphosphinyl]oxy]methyl]-1,2-ethanediyl hexadecanoate. Dipalmitoylphosphatidylglycerol
[4537-77-3]
[58530-79-3, 67232-81-9, 74300-16-6, 74313-95-4, 121236-80-4]
$C_{38}H_{75}O_{10}P$ 722.978
No phys. props. reported.

Glycerol 1,2-di(3,7,11,15-tetramethylhexadecanoate) 3-phosphoglycerol
Present in sponges. Stereochem. not determined.

Glycerol 1,2-dioctadecanoate 3-phosphoglycerol
1-[[[(2,3-Dihydroxypropoxy)hydroxyphosphinyl]oxy]methyl]-1,2-ethanediyl octadecanoate. Distearoylphosphatidylglycerol
[4537-78-4]
[67232-82-0, 120576-51-4]
$C_{42}H_{83}O_{10}P$ 779.085
Cryst. (Me_2CO). Mp 66.5-67°. $[\alpha]_D^{22}$ +2 (c, 10 in $CHCl_3$).
Ba salt: Mp 166°. $[\alpha]_D^{25}$ +9.2 (c, 1 in Py).

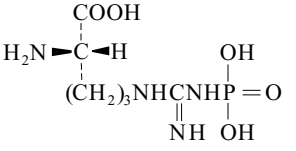
Glycerol 1-(9*Z*-octadecenoate) 2-hexadecanoate 3-phosphoglycerol
Olein 2-palmito-1-(2,3-dihydroxypropyl)hydrogen phosphate
[81490-05-3]
[13879-80-6]
$C_{40}H_{77}O_{10}P$ 749.016
Mp 176-179° (as Na salt). $[\alpha]_D^{20}$ +1.02 (c, 10 in $CHCl_3$) (Na salt).

Glycerol 1,2-di-9*Z*-octadecenoate 3-phosphoglycerol [62700-69-0]
[66322-31-4, 109009-74-7]
$C_{42}H_{79}O_{10}P$ 775.054

Baer, E. *et al., J. Biol. Chem.*, 1958, **232**, 895-901 (*synth*)
Baer, E. *et al., Prog. Chem. Fats Other Lipids*, 1963, **6**, 31-86 (*rev*)
Saunders, R.M. *et al., J.A.C.S.*, 1966, **88**, 3844-3847 (*dioctadecanoyl*)
Joutti, A. *et al., Chem. Phys. Lipids*, 1976, **17**, 262-266 (*dihexadecanoyl, dioctadecanoyl, struct*)
Lammers, J.G. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1977, **96**, 216-218; 1979, **98**, 243-250 (*dihexadecanoyl, dioctadecanoyl, synth, cmr*)
Wohlgemuth, R. *et al., Biochemistry*, 1980, **19**, 3315-3321 (*dihexadecanoyl, H-2 nmr, P-31 nmr*)
Stepanov, A.E. *et al., Zh. Org. Khim.*, 1984, **20**, 985-988; *J. Org. Chem. USSR (Engl. Transl.)*, 1984, **20**, 896-899 (*dihexadecanoyl*)
Pascher, I. *et al., Biochim. Biophys. Acta*, 1987, **896**, 77-88 (*ditetradecanoyl Na salt, cryst struct*)
Demirev, P.A. *et al., Biomed. Environ. Mass Spectrom.*, 1987, **14**, 241-246 (*dioctadecanoyl, ms*)
Dasgupta, A. *et al., Chem. Phys. Lipids*, 1987, **43**, 101-111 (*occur, sponges*)
Jensen, N.J. *et al., Lipids*, 1987, **22**, 480-489 (*dihexadecanoyl, ms*)
Calderon, J. *et al., Chem. Phys. Lipids*, 1988, **46**, 121-125 (*dioctadecanoyl*)
Woolley, P. *et al., Chem. Phys. Lipids*, 1988, **47**, 55-62 (*ditetradecanoyl, synth*)
Hayashi, H. *et al., Biochim. Biophys. Acta*, 1990, **1042**, 126-131 (*occur*)

Phosphoarginine P-365

N^5-*[Imino(phosphonoamino)methyl]ornithine, 9CI.* N^5-*(Phosphonoamidino)ornithine, 8CI.* N-*Phosphonoarginine*



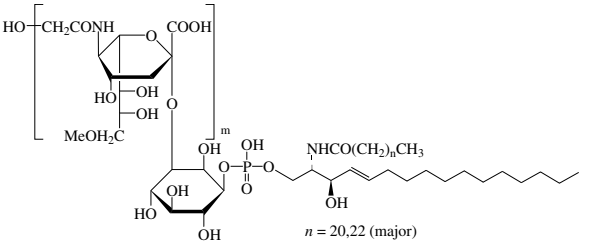
$C_6H_{15}N_4O_5P$ 254.182
Mp 175-180°.

(*S*)-*form*
L-form
[1189-11-3]
Constit. of crayfish muscle. Occurs in human brain. Energy store in invertebrates.
Cryst. + $2H_2O$ (Me_2CO aq.).
Mp 175-180°. Stored as Ba salt; rapidly dec. at -10° in free state.
P,P-*Dibenzyl ester,* C-*Me ester. Dibenzyl [[[(4-amino-4-methoxycarbonyl)butyl]amino](imino)methyl]phosphoramidate*
$C_{21}H_{29}N_4O_5P$ 448.458
Solid. Mp 91-93°.

(±)-*form*
Cryst. (Me_2CO aq.). Mp 175-180°.

Si-Oh, L. *et al., J.A.C.S.*, 1955, **77**, 1866 (*ester*)
Cramer, F. *et al., Chem. Ber.*, 1962, **95**, 1670 (*synth*)
Marcus, F. *et al., Biochem. J.*, 1964, **92**, 429 (*isol, synth*)
Poat, P.C. *et al., Biochim. Biophys. Acta*, 1980, **613**, 410 (*synth*)

Comanthus japonica Phosphoceramides P-366



CJP 1, m = 0
CJP 2, m = 1
CJP 3, m = 2
CJP 4, m = 3

Sphingolipid complex. Major components shown. Isol. from the starfish *Comanthus japonica*. Neuritogenic agent.

CJP 1 [239090-47-2]
$[C_{44\text{-}46}H_{86\text{-}90}NO_{11}P]$ 836.137
Amorph. powder. Mp 173-176°. $[\alpha]_D^{24}$ +3.6 (c, 0.71 in $CHCl_3$/MeOH).

CJP 2
$[C_{56\text{-}58}H_{105\text{-}109}N_2O_{20}P]$ 1157.421
Amorph. powder. Mp 203-208°.

CJP 3

$[C_{68\text{-}70}H_{124\text{-}128}N_3O_{29}P]$ 1478.704
Amorph. powder. Mp 203-208°.

CJP 4

$[C_{80\text{-}82}H_{143\text{-}147}N_4O_{38}P]$ 1799.988
Neuritogenic agent. Amorph. powder. Mp 205-210°.

Arao, K. *et al., Chem. Pharm. Bull.*, 1999, **47**, 687-689; 2001, **49**, 695-698; 2004, **52**, 1140-1142 (*isol, pmr, ms, struct*)

Aiptasia pallida Phospholipase A2 P-367

A phospholipase A_2 existing in 2 isozymic forms with MW 45000 and 43000. Component of the venom of the sea anemone *Aiptasia pallida*. Shows haemolytic activity.

Grotendorst, G.R. *et al., Toxicon*, 1999, **37**, 1779-1796; 2000, **38**, 931-943

O-Phosphoserine sulfhydrylase P-368

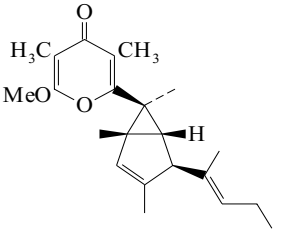
E.C. 2.5.1.65. O-*Phospho*-L-*serine:hydrogen-sulfide 2-amino-2-carboxyethyltransferase*

Enzyme. Isol. from *Aeropyrum pernix*. Catalyses the reaction of *O*-phospho-L-serine with hydrogen sulfide to give L-cysteine and phosphate. Also acts on O^3-acetyl-L-serine.

Mino, K. *et al., Acta Cryst. D*, 2003, **59**, 338-340 (*cryst struct*)
Mino, K. *et al., J. Bacteriol.*, 2003, **185**, 2277-2284 (*isol*)

Photodeoxytridachione P-369

*2-Methoxy-3,5-dimethyl-6-[1,3,6-trimethyl-4-(1-methyl-1-butenyl)bicyclo[3.1.0]hex-2-en-6-yl]-4*H-*pyran-4-one, 9CI*
[71726-12-0]

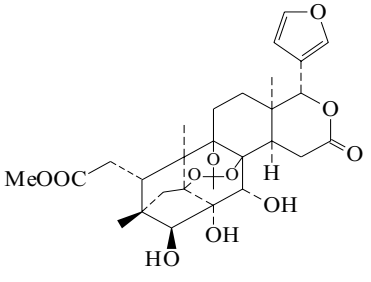


$C_{22}H_{30}O_3$ 342.477
Isol. from *Elysia timida* and *Placobranchus ocellatus*. Ichthyotoxin. $[\alpha]_D^{25}$ +14.4 (c, 0.6 in $CHCl_3$). Similar to Crispatene, C-917. λ_{max} 255 (ϵ 13700) (MeOH) (Berdy).

Ireland, C. *et al., Science (Washington, D.C.)*, 1979, **205**, 922-923 (*isol*)
Gavagnin, M. *et al., J. Nat. Prod.*, 1994, **57**, 298 (*isol, pmr, cmr*)

Phragmalin P-370

[35183-64-3]



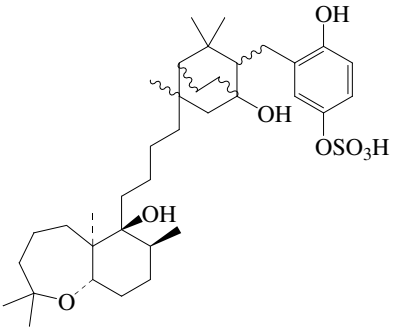
$C_{29}H_{36}O_{11}$ 560.597
Constit. of *Entandrophragma caudatum*. Cryst. (Et_2O aq.). Mp 150-155° dec. $[\alpha]_D$ -77 (c, 1.3 in MeOH).

Tri-Ac: ***Xyloccensin E***
[37665-92-2]
$C_{35}H_{42}O_{14}$ 686.708
Constit. of *Xylocarpus moluccensis*. Cryst. (MeOH). Mp 212-215°.

Arndt, R.R. *et al., Tetrahedron*, 1972, **28**, 2333-2340 (*Phragmalin, cryst struct*)
Connolly, J.D. *et al., J.C.S. Perkin 1*, 1976, 1993-1996 (*Xyloccensin E*)

Phuklona sulfate P-371

[444987-63-7]

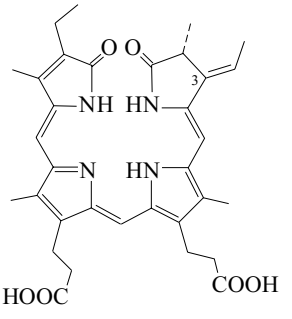


$C_{36}H_{58}O_8S$ 650.915
Constit. of a *Haliclona* sp. Glass. $[\alpha]_D$ -17.4 (c, 0.91 in MeOH). λ_{max} 208 (log ϵ 4.22); 209 (log ϵ 4.04); 280 (log ϵ 3.25) (MeOH).

Bokesch, H.R. *et al., Tet. Lett.*, 2002, **43**, 3079-3081 (*isol, pmr, cmr*)

Phycocyanobilin P-372

[20298-86-6]



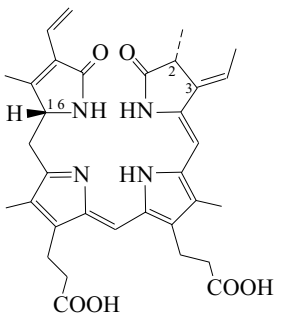
$C_{33}H_{38}N_4O_6$ 586.686
Both 3*E* and 3*Z* isomers have been observed. Chromophore of the photosynthetic (protein) pigment Phycocyanin present in blue-green algae, e.g. *Phormidium luridum*, *Synechococcus lividus* and *Plectonema boryanum*. Covalently linked to protein by thioether linkage to C-3^1. (cleaved by hot MeOH). Also present in red algae. Blue-green solid. $[\alpha]_D$ +660 ($CHCl_3$).

Di-Me ester: [43155-04-0]
$C_{35}H_{42}N_4O_6$ 614.74
Dark-green cryst. ($CHCl_3$/MeOH). Mp 205-206°.

Cole, W.J. *et al., J.A.C.S.*, 1967, **89**, 3643 (*struct, pmr*)
Rüdiger, W. *et al., Nature (London)*, 1967, **215**, 1477
Gossauer, A. *et al., J.O.C.*, 1978, **43**, 283 (*synth*)
Gossauer, A. *et al., The Porphyrins*, (Dolphin, D., Ed.), Academic Press, N.Y., Vol. VI, 1979, 585
Beale, S.I. *et al., Plant Physiol.*, 1984, **76**, 7 (*E/Z isomers*)
Holroyd, J.A. *et al., Biochem. Soc. Trans.*, 1985, **13**, 209 (*biosynth*)
Cheng, L. *et al., Chin. Chem. Lett.*, 1991, **2**, 589 (*uv*)
Micura, R. *et al., Enantiomer*, 1996, **1**, 109-113 (*resoln, abs config*)
Kakiuchi, T. *et al., Chem. Lett.*, 1998, 1001-1002 (*synth*)

Phycoerythrobilin P-373

Phycobiliviolin
[18097-67-1]



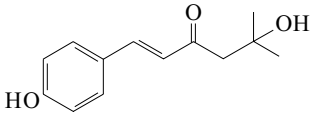
$C_{33}H_{38}N_4O_6$ 586.686
Chromophore of C- and R-Phycoerythrins, photosynthetic red pigments (biliprotein) from blue-green algae as well as most red algae. Mauve solid. $[\alpha]_{Hg}^{25}$ -8300. pK_a 6.4. Covalently bound to the protein *in vivo* by thioether linkage to C-3[1], cleaved by hot MeOH.

Di-Me ester:
Pink cryst. (Me_2CO aq.). Mp 183-184°.

O'Carra, P. *et al., Biochemistry*, 1964, **3**, 1343
Chapman, D.J. *et al., J.A.C.S.*, 1967, **89**, 5976 (*struct, pmr*)
Gossauer, A. *et al., Chem. Ber.*, 1979, **12**, 2243
Gossauer, A. *et al., The Porphyrins*, (Dolphin, D., Ed.), Academic Press, N.Y., 1979, 585 (*struct, synth*)
Cheng, L. *et al., Chin. Chem. Lett.*, 1991, **2**, 589 (*uv*)

Phycopsisenone P-374

5-Hydroxy-1-(4-hydroxyphenyl)-5-methyl-1-hexen-3-one, 9CI
[162857-70-7]

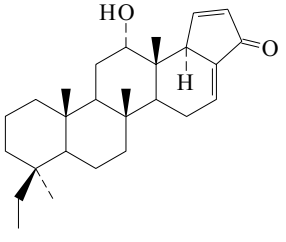


$C_{13}H_{16}O_3$ 220.268
Isol. from the sponge *Phycopsis* sp. Cryst.
Mp 135°. λ_{max} 225 (ϵ 7949) (MeOH) (Berdy).

Venkateswarlu, Y. *et al., J. Nat. Prod.*, 1995, **58**, 269 (*isol, uv, ir, pmr, cmr*)
Kad, G.L. *et al., J. Nat. Prod.*, 1998, **61**, 297-298 (*synth*)

Phyllofenone B P-375

[134985-06-1]

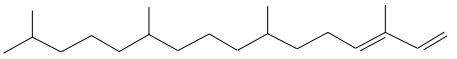


$C_{27}H_{40}O_2$ 396.612
Constit. of *Phyllospongia foliascens*. Cryst. (EtOH).
Mp 241-243°. $[\alpha]_D^{20}$ +133 (c, 0.0047 in $CHCl_3$). λ_{max} 248 (ϵ 21879) (MeOH) (Berdy).

Zeng, L. *et al., J. Nat. Prod.*, 1991, **54**, 421 (*isol, pmr, cmr*)

1,3-Phytadiene P-376

3,7,11,15-Tetramethyl-1,3-hexadecadiene



$C_{20}H_{38}$ 278.52

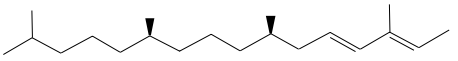
(E)-form [67669-03-8]
Constit. of zooplankton.
Oil.

(Z)-form [67710-88-7]
Constit. of zooplankton.
Oil.

Blumer, M. *et al., Science (Washington, D.C.)*, 1965, **147**, 1148 (*isol, struct*)
Hites, R.A. *et al., J.O.C.*, 1974, **39**, 2634 (*synth*)

2,4-Phytadiene P-377

3,7,11,15-Tetramethyl-2,4-hexadecadiene

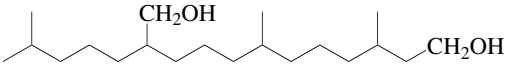


$C_{20}H_{38}$ 278.52

(2E,4E,7R,11R)-form [58864-82-7]
Constit. of zooplankton.
Oil.

Blumer, M. *et al., Science (Washington, D.C.)*, 1965, **147**, 1148 (*isol, struct*)
Scott, J.W. *et al., Helv. Chim. Acta*, 1976, **59**, 290 (*synth*)

1,18-Phytanediol P-378



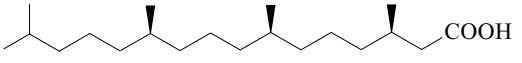
$C_{20}H_{42}O_2$ 314.551

Disulfate: [189883-33-8]
$C_{20}H_{42}O_8S_2$ 474.679
Constit. of *Ascidia mentula* and *Sidnyum turbinatum*. Antiproliferative agent. Amorph. solid. $[\alpha]_D^{25}$ +7 (c, 0.004 in MeOH).

Aiello, A. *et al., Tetrahedron*, 1997, **53**, 5877-5882 (*disulfate, isol, pmr, cmr*)
Aiello, A. *et al., J. Nat. Prod.*, 2001, **64**, 219-221 (*disulfate*)

1-Phytanoic acid P-379

3,7,11,15-Tetramethylhexadecanoic acid. ***Phytanic acid***



(3*R*,7*R*,11*R*)–*form*

$C_{20}H_{40}O_2$ 312.535

(3R,7R,11R)-form [18654-64-3]
Isol. from the liver of patients with Refsum's disease and constit. of oil shale and butter. Also occurs in lipids of *Halobacterium cutirubrum*.
Oil. Sol. MeOH, Et_2O. $Bp_{7.5}$ 221°. $[\alpha]_{500}^{20}$ -3.8 (c, 4 in MeOH/$CHCl_3$). λ_{max} 215 (ϵ 28400); 231 (ϵ 28300); 420 (ϵ 7660) (MeOH) (Berdy).

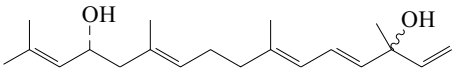
(3S,7R,11R)-form [14721-66-5]
Constit. of oil shale.
Oil.

(3ξ,7ξ,11ξ)-form
Found in fish oils.
*2-Phytenyl ester(*E-*):* ***2-Phytenyl phytanoate***
$C_{40}H_{78}O_2$ 591.055

Constit. of *Megaceros flagellaris.*
$[\alpha]_D$ 0.

Kates, M. *et al., Biochemistry*, 1967, **6**, 3329-3338 (*struct*)
Cox, R.E. *et al., Chem. Comm.*, 1970, 1639 (*isol, struct*)
Lough, A.K. *et al., Prog. Chem. Fats Other Lipids*, Part 1, 1973, **14**, (*rev*)
Ratanayake, W.M.N. *et al., Lipids*, 1989, **24**, 630-637 (*occur, fish oil*)
Sita, L.R. *et al., J.O.C.*, 1993, **58**, 5285 (*synth*)
Buchanan, M.S. *et al., Phytochemistry*, 1996, **41**, 1373 (*2-phytenyl ester*)

1,4,6,10,14-Phytapentaene-3,13-diol P-380

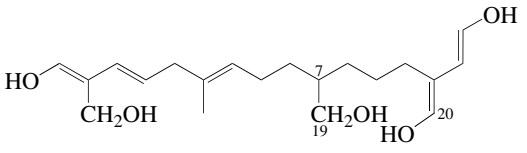


$C_{20}H_{32}O_2$ 304.472

(3ξ,*4E*,*6E*,10*E*,13*R*)-*form* [149415-82-7]
Constit. of *Myrmekioderma styx*.
Oil. $[\alpha]_D$ +4.6 (c, 0.002 in hexane).
Albrizio, S. *et al., Z. Naturforsch., B*, 1993, **48**, 488 (*isol, pmr, cmr*)

1,3(20),10,13,15-Phytapentaene-1,16,17,19,20-pentol P-381

16,19-Dihydroxy-10,13-phytadiene-1,16,20-trial

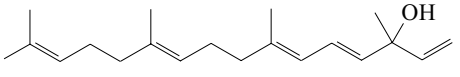


$C_{20}H_{32}O_5$ 352.47
Enol. The synonym refers to the trioxo form.

(1*E*,3*E*,7ξ,10*E*,13*E*,15*Z*)-*form*
1,16,17,20-Tetra-Ac: 1,16,17,20-Tetraacetoxy-1,3(20),10,13,15-phytapentaen-19-ol
[99694-98-1]
$C_{28}H_{40}O_9$ 520.619
Constit. of the alga *Tydemania expeditionis.* Oil. $[\alpha]_D$ -0.8 (c, 1.5 in $CHCl_3$). λ_{max} 243 (ε 11000) (MeOH).
Paul, V.J. *et al., Phytochemistry*, 1985, **24**, 2239-2243 (*isol*)

1,4,6,10,14-Phytapentaen-3-ol P-382

3,7,11,15-Tetramethyl-1,4,6,10,14-hexadecapentaen-3-ol

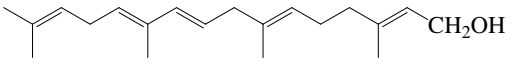


$C_{20}H_{32}O$ 288.472

(4*E*,6*E*,10*E*)-*form* [144101-95-1]
Constit. of *Myrmekioderma styx*.
$[\alpha]_D^{25}$ +13.1 (c, 0.001 in hexane).
Albrizio, S. *et al., J. Nat. Prod.*, 1992, **55**, 1287 (*isol, pmr, cmr*)

2,6,9,11,14-Phytapentaen-1-ol P-383

3,7,11,15-Tetramethyl-2,6,9,11,14-hexadecapentaen-1-ol

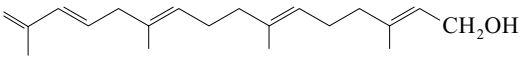


$C_{20}H_{32}O$ 288.472

(2*E*,6*E*,9*E*,11*E*)-*form* [353750-04-6]
Constit. of *Bifurcaria bifurcata*.
Oil.
Culioli, G. *et al., Phytochemistry*, 2001, **57**, 529-535 (*isol, pmr, cmr*)

2,6,10,13,15-Phytapentaen-1-ol P-384

3,7,11,15-Tetramethyl-2,6,10,13,15-hexadecapentaen-1-ol, 9CI

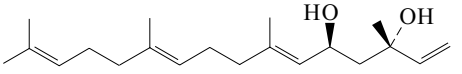


$C_{20}H_{32}O$ 288.472

(2*E*,6*E*,10*E*,13*E*)-*form* [116988-16-0]
Constit. of *Bifurcaria bifurcata*.
Oil.
Semmak, L. *et al., Phytochemistry*, 1988, **27**, 2347

1,6,10,14-Phytatetraene-3,5-diol P-385

3,7,11,15-Tetramethyl-1,6,10,14-hexadecatetraene-3,5-diol, 9CI

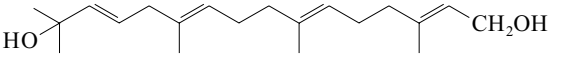


$C_{20}H_{34}O_2$ 306.487

(3*S*,5*S*,6*E*,10*E*)-*form*
5-Hydroxygeranyllinalol
[84093-63-0]
Constit. of *Geigeria burkei* and *Myrmekioderma styx*.
Gum. $[\alpha]_D$ +17.65 (c, 0.005 in hexane).
9-Acetoxy: ***9-Acetoxy-5-hydroxygeranyllinalol***
$C_{22}H_{36}O_4$ 364.524
Constit. of *Geigeria burkei*. Gum.
9-Acetoxy, 5-Ac: ***5,9-Diacetoxygeranyllinalol***
[84093-65-2]
$C_{24}H_{38}O_5$ 406.561
Constit. of *Geigeria burkei*. Gum.
13-Acetoxy: ***13-Acetoxy-5-hydroxygeranyllinalol***
[84093-66-3]
$C_{22}H_{36}O_4$ 364.524
Constit. of *Geigeria burkei*. Gum.
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1679
Albrizio, S. *et al., Z. Naturforsch., B*, 1993, **48**, 488 (*struct*)

2,6,10,13-Phytatetraene-1,15-diol P-386

3,7,11,15-Tetramethyl-2,6,10,13-hexadecatetraene-1,15-diol

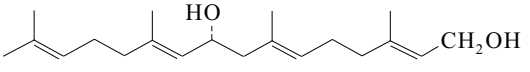


$C_{20}H_{34}O_2$ 306.487

(2*E*,6*E*,10*E*,13*E*)-*form*
Bifurcanol
[153050-23-8]
Constit. of *Bifurcaria bifurcata*. Toxic to sea urchins. Oil. λ_{max} 245 (ε 12200); 285 (ε 8500) ($CHCl_3$) (Berdy).
Valls, R. *et al., Phytochemistry*, 1993, **34**, 1585 (*isol, pmr, cmr*)

2,6,10,14-Phytatetraene-1,9-diol P-387

3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraene-1,9-diol

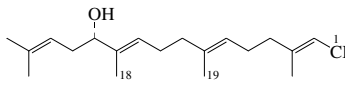


$C_{20}H_{34}O_2$ 306.487

(2*E*,6*E*,9*R*,10*E*)-*form*
Crinitol
[60346-04-5]
Constit. of *Cystoseira crinita* and *Sargassum tortile*. Shows antibacterial activity. Oil. $[\alpha]_D$ -3.
Fattorusso, E. *et al., Tet. Lett.*, 1976, 937
Kubo, I. *et al., Chem. Lett.*, 1985, 249 (*abs config*)
Kubo, I. *et al., J. Nat. Prod.*, 1992, **55**, 780 (*cmr, biochem*)

2,6,10,14-Phytatetraene-1,12-diol P-388

3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraene-1,12-diol



(2*E*,6*E*,10*E*,12*S*)-*form*

$C_{20}H_{34}O_2$ 306.487

(2*E*,6*E*,10*E*,12*S*)-*form*

12-Hydroxygeranylgeraniol. ***Bifurcadiol***
Constit. of *Bifurcaria bifurcata* and *Carpesium divaricatum* (Compositae). Cytotoxic agent. Oil. $[\alpha]_D$ -12.47 (c, 0.93 in $CHCl_3$).

1-Carboxylic acid: ***12-Hydroxy-2,6,10,14-phytatetraen-1-oic acid***. *12-Hydroxygeranylgeranic acid*
[117007-28-0]
$C_{20}H_{32}O_3$ 320.471
Isol. from *Bifurcaria bifurcata*. Oil. $[\alpha]_D$ +4.19 (c, 8.1 in CH_2Cl_2).

1-Carboxylic acid, Me ester: [116988-18-2]
$C_{21}H_{34}O_3$ 334.498
Constit. of *Bifurcaria bifurcata*. Oil. $[\alpha]_D^{25}$ -7.7 (c, 5.5 in CH_2Cl_2).

1-Aldehyde: ***12-Hydroxy-2,6,10,14-phytatetraen-1-al***
[353750-05-7]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Bifurcaria bifurcata*. Oil. λ_{max} 245 (log ϵ 4.18) (EtOH).

(2*E*,6*Z*,10*Z*,12ξ)-*form*

18-Hydroxy: 2,6,10,14-Phytatetraene-1,12,18-triol. ***12,18-Dihydroxygeranylgeraniol***
$C_{20}H_{34}O_3$ 322.487
Isol. from *Zinnia tenuifolia*. Gum. $[\alpha]_D^{24}$ +35.9 (c, 0.3 in $CHCl_3$).

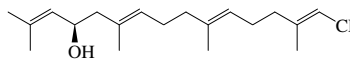
(2*Z*,6*E*,10*E*,12*S*)-*form*

1-Aldehyde: [353750-06-8]
Constit. of *Bifurcaria bifurcata*.
Oil. $[\alpha]_D^{25}$ -3 (c, 1 in CH_2Cl_2).

Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 1613; 1623
Valls, R. *et al., Phytochemistry*, 1986, **25**, 751
Semmak, L. *et al., Phytochemistry*, 1988, **27**, 2347
Zee, O.P. *et al., Arch. Pharmacal Res.*, 1999, **22**, 225 (*Bifurcadiol, isol, activity*)
Di Guardia, S. *et al., Tet. Lett.*, 1999, 8359-8360 (*synth*)
Culioli, G. *et al., Phytochemistry*, 2001, **57**, 529-535 (*Bifurcaria bifurcata constits*)

2,6,10,14-Phytatetraene-1,13-diol P-389

3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraene-1,13-diol. 13-Hydroxygeranylgeraniol



(2*E*,6*E*,10*E*,13*R*)-*form*

$C_{20}H_{34}O_2$ 306.487

(2*E*,6*E*,10*E*,13*R*)-*form*
Eleganediol
[75225-31-9]
Constit. of *Bifurcaria bifurcata*.

13-Ketone: ***1-Hydroxy-2,6,10,14-phytatetraen-13-one***. ***Eleagnolone***
[67880-32-4]
Constit. of *Cystoseira elegans*, *Cystoseira balearica* and *Bifurcaria bifurcata*. Relaxant. Antihypertensive and anticontractive agent. Acetylcholine-histamine antagonist. Oil. λ_{max} 248 (ϵ 12000) ($CHCl_3$) (Derep). λ_{max} 239 (ϵ 12000); 331 (ϵ 760) (EtOH) (Berdy).
▶ LD_{50} (mus, ipr) 100 - 200 mg/kg. MM0340000

13-Ketone, 2,3-epoxide: 2,3-Epoxy-1-hydroxy-6,10,14-phytatrien-13-one. ***Epoxyeleganolone***
[75225-32-0]
$C_{20}H_{32}O_3$ 320.471
Constit. of *Bifurcaria bifurcata* and *Cystoseira elegans*. Antihypertensive and anticontractive agent. λ_{max} 248 (ϵ 12000) ($CHCl_3$) (Derep).

13-Ketone, 1-aldehyde: 13-Oxo-2,6,10,14-phytatetraen-1-al. ***Eleganonal***
[111950-82-4]
$C_{20}H_{30}O_2$ 302.456
Isol. from *Cystoseira balearica*. Antihypertensive and anticontractive agent. Acetylcholine-histamine antagonist. Inotropic activity blocker.

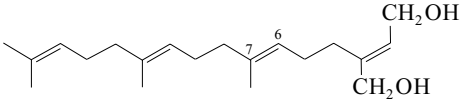
2,3-Dihydro, 13-ketone: 16-Hydroxy-2,6,10,14-tetramethyl-2,6,10-hexadecatrien-4-one. ***1-Hydroxy-6,10,14-phytatrien-13-one***
[80368-36-1]
$C_{20}H_{34}O_2$ 306.487
Constit. of *Koanophyllon conglobatum*. Gum. $[\alpha]_D$ -1.6 (c, 0.5 in $CHCl_3$).

(2*Z*,6*E*,10*E*,13ξ)-*form*

13-Ketone, 1-aldehyde: ***Isoeleganonal***
[111997-20-7]
$C_{20}H_{30}O_2$ 302.456
From *Cystoseira balearica*. Oil.

Francisco, C. *et al., Phytochemistry*, 1978, **17**, 1003
Biard, J.F. *et al., Tet. Lett.*, 1980, 1849-1852 (*Eleganediol*)
Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 1903 (*2,3-dihydro-13-ketone*)
Amico, V. *et al., Phytochemistry*, 1987, **26**, 2637 (*Eleganonal, Isoeleganonal*)
Valls, R. *et al., Phytochemistry*, 1995, **39**, 145-149 (*Eleganediol*)
Li, J. *et al., J. Nat. Prod.*, 1998, **61**, 92-95 (*synth*)
Ortalo-Magné, A. *et al., Phytochemistry*, 2005, **66**, 2316-2323 (*Eleganediol, abs config*)

2,6,10,14-Phytatetraene-1,20-diol P-390



$C_{20}H_{34}O_2$ 306.487

(2*E*,6*E*,10*E*)-*form*
20-Hydroxygeranylnerol
Constit. of *Kingianthus paradoxus*.
Gum.

Di-Ac: [79421-71-9]
$C_{24}H_{38}O_4$ 390.562
Metab. of *Chlorodesmis fastigiata* and *Caulerpa brownii*. Gum.

1-Aldehyde, 20-Ac: [849475-57-6]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Caulerpa brownii*.

1,20-Dialdehyde: ***2,6,10,14-Phytatetraene-1,20-dial***
[79421-72-0]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Caulerpa brownii*. Oil.

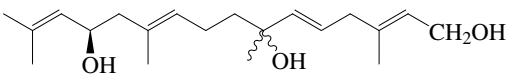
1,20-Dicarboxylic acid: 2,6,10,14-Phytatetraene-1,20-dioic acid. ***Schizostatin***
[163564-55-4]
$C_{20}H_{30}O_4$ 334.455
Constit. of *Schizophyllum commune*. Squalene synthase inhibitor. Cryst. Sol. MeOH, $CHCl_3$, EtOAc, bases, EtOH; poorly sol. hexane, H_2O.
Mp 119-122°. λ_{max} 215 (EtOH). λ_{max} 214 (EtOH) (Berdy).

6ξ,7ξ-Epoxide: 6,7-Epoxy-2,10,14-phytatriene-1,20-diol. ***Zoapatol B***
[135447-92-6]
$C_{20}H_{34}O_3$ 322.487
Isol. from *Montanoa tomentosa*. Gum.

Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 1146 (*isol*)
Wright, A.D. *et al., J. Nat. Prod.*, 1990, **52**, 845-861 (*di-Ac*)
Quijano, L. *et al., Phytochemistry*, 1991, **30**, 1947 (*epoxide*)
Tanimoto, T. *et al., J. Antibiot.*, 1996, **49**, 617; 624 (*Schizostatin, isol, synth, uv, ir, pmr, cmr, ms, activity*)
Handley, J.T. *et al., Aust. J. Chem.*, 2005, **58**, 39-46 (*Caulerpa brownii constits*)

2,5,10,14-Phytatetraene-1,7,13-triol P-391

3,7,11,15-Tetramethyl-2,5,10,14-hexadecatetraene-1,7,13-triol

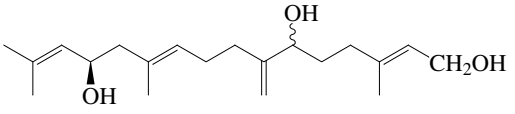


$C_{20}H_{34}O_3$ 322.487

(2*E*,5*E*,7ξ,10*E*,13*R*)-*form* [869482-01-9]
Constit. of *Bifurcaria bifurcata*.
Oil. $[\alpha]_D^{25}$ -7 (c, 0.2 in $CHCl_3$).
Ortalo-Magné, A. *et al., Phytochemistry*, 2005, **66**, 2316-2323 (*Bifurcaria bifurcata constit*)

2,7(19),10,14-Phytatetraene-1,6,13-triol P-392

3,11,15-Trimethyl-7-methylene-2,10,14-hexadecatriene-1,6,13-triol



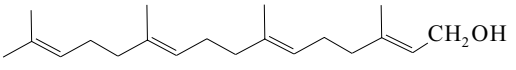
$C_{20}H_{34}O_3$ 322.487

(2*E*,6ξ,10*E*,13*R*)-*form* [869482-00-8]
Constit. of *Bifurcaria bifurcata*.
Oil. $[\alpha]_D^{25}$ -3 (c, 0.15 in $CHCl_3$).

14,15-Dihydro, 13-ketone: ***1,6-Dihydroxy-2,7(19),10-phytatrien-13-one****. 11,16-Dihydroxy-2,6,14-trimethyl-10-methylene-6,14-hexadecadien-4-one*
[869481-99-2]
$C_{20}H_{34}O_3$ 322.487
Constit. of *Bifurcaria bifurcata*. Oil. $[\alpha]_D^{25}$ +12 (c, 0.25 in $CHCl_3$).
Ortalo-Magné, A. *et al., Phytochemistry*, 2005, **66**, 2316-2323 (*Bifurcaria bifurcata constits*)

2,6,10,14-Phytatetraen-1-ol P-393

3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraen-1-ol



$C_{20}H_{34}O$ 290.488

(2*E*,6*E*,10*E*)-*form*
Geranylgeraniol
[24034-73-9]
Widespread in plants, e.g. found in linseed oil. Constit. of thoracic gland secretions of male *Xylocopa* spp.
Oil. $Bp_{0.35}$ 145°. n_D^{30} 1.4932.

O-*[2,3-Di-*O*-acetyl-α-L-rhamnopyranosyl-(1→3)-4,6-di-*O*-acetyl-β-D-glucopyranoside]:* ***Vernanolide***
[353759-45-2]
$C_{40}H_{62}O_{14}$ 766.921
Constit. of *Cupania vernalis*. Powder.

O-*(2,3-Dihydroxypropyl)(*R-*):* ***1-O-Geranylgeranylglycerol***
[64604-13-3]
$C_{23}H_{40}O_3$ 364.567
Constit. of *Dilophus fasciola*. Viscous liq. $[\alpha]_D$ -2.1 (c, 1.5 in $CHCl_3$).

Aldehyde: 2,6,10,14-Phytatetraen-1-al. 3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraen-1-al. ***Geranylgeranial***
[13920-12-2]
$C_{20}H_{32}O$ 288.472
Constit. of *Mikania sessilifolia*. Oil. $Bp_{0.5}$ 150°.

Aldehyde, semicarbazone: Mp 118°.

Aldehyde, 14ξ,15ξ-epoxide: 13-(3,3-Dimethyloxiranyl)-3,7,11-trimethyl-2,6,10-tridecatrienal, 9CI. ***14,15-Epoxy-2,6,10-phytatrien-1-al****. Geranylgeranal epoxide*
[108613-62-3]
$C_{20}H_{32}O_2$ 304.472
Isol. from *Cystophora moniliformis*. Oil. $[\alpha]_D$ -17 (c, 0.98 in $CHCl_3$).

*Aldehyde, 4*S*-hydroxy: 4-Hydroxy-2,6,10,14-phytatetraen-1-al*
[80442-67-7]
$C_{20}H_{32}O_2$ 304.472
Constit. of *Mikania sessilifolia*. Gum.

1-Carboxylic acid: 3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraen-1-oic acid. Geranylgeranic acid
[35750-48-2]
$C_{20}H_{32}O_2$ 304.472

*1-Carboxylic acid, 3-acetoxy-2-hydroxypropyl ester(*S-*):* ***Verrucosin 4***
[188405-17-6]
$C_{25}H_{40}O_5$ 420.588
Constit. of *Doris verrucosa*. Protein kinase C activator. Tumour promoter. Oil. $[\alpha]_D$ -9.7 (c, 0.35 in $CHCl_3$). λ_{max} 223 (ϵ 8930) (MeOH).

(2*Z*,6*E*,10*E*)-*form*

Aldehyde: ***Geranylneral***
[57784-38-0]
$C_{20}H_{32}O$ 288.472
Constit. of *Mikania sessilifolia*. Oil. λ_{max} 232 (hexane).

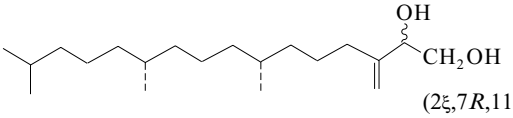
Aldehyde, 14ξ,15ξ-epoxide: [115075-54-2]
Isol. from *Cystophora moniliformis*.
Oil. $[\alpha]_D$ -22 (c, 0.4 in $CHCl_3$).

[32480-11-8, 132513-59-8]

Nagasampagi, B.A. *et al., Tet. Lett.*, 1967, 189 (*pmr*)
Buggy, M.J. *et al., Phytochemistry*, 1974, **13**, 125 (*biosynth*)
Khan, N. *et al., J.C.S. Perkin 1*, 1975, 1457 (*aldehyde*)
Amico, V. *et al., Experientia*, 1977, **33**, 989 (*deriv*)
Altman, L.J. *et al., J.A.C.S.*, 1978, **100**, 6174 (*aldehyde*)
Coates, R.M. *et al., J.O.C.*, 1978, **43**, 4915 (*cmr*)
Ahlqvist, L. *et al., Prog. Chem. Fats Other Lipids*, 1978, **16**, 231 (*rev*)
Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 1899 (*aldehyde*)
Van Altena, I.A. *et al., Aust. J. Chem.*, 1988, **41**, 49 (*aldehyde epoxides*)
Anderson, J.F. *et al., J. Chem. Ecol.*, 1988, **14**, 1153
Mu, Y. *et al., Tet. Lett.*, 1995, **36**, 5669 (*synth*)
Gavagnin, M. *et al., Tetrahedron*, 1997, **53**, 1491-1504 (*Verrucosin 4*)
Huang, Q. *et al., Tet. Lett.*, 1998, **39**, 2033-2036 (*biosynth*)
Cavalcanti, S.B.T. *et al., J. Braz. Chem. Soc.*, 2001, **12**, 413-416 (*Vernanolide*)
Nualkaew, N. *et al., Tet. Lett.*, 2005, **46**, 8727-8731 (*synth*)

3(20)-Phytene-1,2-diol P-394

7,11,15-Trimethyl-3-methylene-1,2-hexadecanediol, 9CI



(2ξ,7*R*,11*R*)–*form*

$C_{20}H_{40}O_2$ 312.535

(2ξ,7*R*,11*R*)-*form* [625454-33-3]
Constit of seeds of *Artemisia annua*.
Oil. Mixture of epimers at C-2.

2-Hydroperoxide: ***2-Hydroperoxy-3(20)-phyten-1-ol***
[100605-94-5]
[100605-81-0]
$C_{20}H_{40}O_3$ 328.534
Constit. of *Artemisia annua*. Oil. Struct. revised 2002, formerly thought to be the 1,2-diol.

(2ξ,7ξ,11ξ)(1)-*form*
Constit. of *Senecio gallicus*.
Oil. $[\alpha]_D$ -1.2 (c, 0.5 in $CHCl_3$).

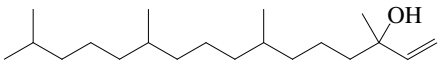
Di-Ac:

$C_{24}H_{44}O_4$ 396.609
Constit. of *Senecio gallicus*. Oil.

(2ξ,7ξ,11ξ)(2)-*form*
Constit. of *Eunicea succinea*.
Oil. $[\alpha]_D^{25}$ +1 (c, 3.9 in $CHCl_3$).
Urones, J.G. *et al., Phytochemistry*, 1987, **26**, 1113
Brown, G.D. *et al., Phytochemistry*, 1994, **36**, 1553 (*isol, pmr, cmr*)
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 1134-1138 (*Eunicea succinea constit*)
Wong, H.-F. *et al., J. Chem. Res., Synop.*, 2002, 30-33 (*2-hydroperoxide, synth, struct*)
Brown, G.D. *et al., Phytochemistry*, 2003, **64**, 303-323 (*Artemisia annua constit*)

1-Phyten-3-ol P-395

3,7,11,15-Tetramethyl-1-hexadecen-3-ol
[505-32-8]



$C_{20}H_{40}O$ 296.535
Constit. of *Laurencia pinnatifida*. Intermed. in the synth. of vitamins A and E. Oil. d_4^{20} 0.85. $Bp_{0.06}$ 125-128°. n_D^{20} 1.4571.

Semicarbazone: Mp 85.1°.

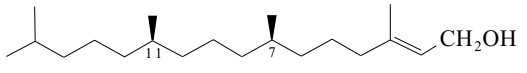
Ac:
$C_{22}H_{42}O_2$ 338.573
$Bp_{0.2}$ 140-142°. n_D^{25} 1.4488.

[60046-87-9, 80736-12-5]

Sato, K. *et al., J.O.C.*, 1963, **28**, 45 (*synth, ir*)
Akutagawa, S. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 1158 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **22**, 731; 753 (*uses*)
Mandai, T. *et al., Tet. Lett.*, 1981, **22**, 763 (*synth*)
Sarandeses, L.A. *et al., Chem. Comm.*, 1991, 818 (*synth*)
Ahmad, V.U. *et al., Phytochemistry*, 1991, **30**, 4172 (*isol, pmr, cmr*)

2-Phyten-1-ol P-396

3,7,11,15-Tetramethyl-2-hexadecen-1-ol. ***Phytol***
[7541-49-3]



(2*E*,7*R*,11*R*)–*form*

$C_{20}H_{40}O$ 296.535
Used in preparation of vitamins E and K. Anticancer agent (colon and gastric cancer).

(2*E*,7*R*,11*R*)-*form* [150-86-7]
Constit. of nettles, *Leucas volkensii*, alga *Gracillaria* sp., *Perilla* spp., *Solidago virga-aurea* and other plants. Anticancer agent (colon and gastric cancer). Oil. $Bp_{0.02}$ 132°. $[\alpha]_D^{18}$ +0.2. λ_{max} 240 (MeOH) (Berdy).
▶ Skin irritant. LD_{50} (rat, orl) >5000 mg/kg. TJ3490000

Heptanoyl: Phytyl heptanoate
[145613-68-9]
$C_{27}H_{52}O_2$ 408.707
Constit. of *Bidens pilosa* and *Rosa roxburghii*. Oil. Bp 159°. $[\alpha]_D^{28}$ -0.89 (EtOH).

Hexadecanoyl: Palmitoylphytol. Codioester
[53950-58-6]
$C_{36}H_{70}O_2$ 534.948
Constit. of *Pentatropis spiralis* and *Codium iyengarii*. Gum. $[\alpha]_D$ -14.28 (c, 0.018 in $CHCl_3$). Abs. config. not clear.

*5,8,11,14,17-Eicosapentaenoyl(*all-Z*): Phytyl 5,8,11,14,17-eicosapentaenoate*
[94035-77-5]
$C_{40}H_{68}O_2$ 580.976
Isol. from *Navicula delognei*. Antibacterial agent. Oil. Sol. $CHCl_3$, hexane; poorly sol. H_2O.

1-Aldehyde: 2-Phyten-1-al. 3,7,11,15-Tetramethyl-2-hexadecenal. ***Phytal***
[13754-69-3]
$C_{20}H_{38}O$ 294.52
Constit. of *Tetragonia tetragonoides* (New Zealand spinach). Oil.

(2*Z*,7*R*,11*R*)-*form* [5492-30-8]
Constit. of *Gracilaria andersoniana*.
Oil.

(2*E*,7ξ,11ξ)-*form*

*1-Carboxylic acid, 2-phytenyl ester(*E-*): 2-Phytenyl 2-phytenoate*
$C_{40}H_{76}O_2$ 589.039
Constit. of *Megaceros flagellaris*. Oil. $[\alpha]_D$ 0.

2,3-Epoxide: ***2,3-Epoxy-1-phytanol***
[107438-44-8]
$C_{20}H_{40}O_2$ 312.535
Constit. of *Bryopsis pennata* and *Valoniopsis pachynema*.

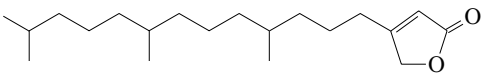
*1-Aldehyde. 2*R**,3*R**-epoxide:* ***2,3-Epoxy-1-phytanal***
[243869-17-2]
$C_{20}H_{38}O_2$ 310.519
Constit. of *Porphyra yezoensis*.

*1-Aldehyde, 2*R**,3*S**-epoxide:*
$C_{20}H_{38}O_2$ 310.519
Constit. of *Porphyra yezoensis*.

Burrell, J.W.K. *et al., J.C.S.(C)*, 1966, 2144 (*Phytal, synth, abs config*)
Shilleter, D.N. *et al., Phytochemistry*, 1970, **9**, 153 (*biosynth*)
Goodman, R.A. *et al., J.A.C.S.*, 1973, **95**, 7553 (*cmr*)
Sims, J.J. *et al., Phytochemistry*, 1976, **15**, 1076 (*isol*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 811 (*rev, tox*)
Schmid, M. *et al., Helv. Chim. Acta*, 1982, **65**, 684 (*synth*)
Aoki, T. *et al., Phytochemistry*, 1982, **21**, 1361 (*isol*)
Findlay, J.A. *et al., J. Nat. Prod.*, 1984, **47**, 815-818 (*Phytyl eicosapentaenoate*)
Gramatica, P. *et al., Tetrahedron*, 1987, **43**, 4481 (*synth*)
Rasool, N. *et al., Phytochemistry*, 1991, **30**, 1331 (*deriv*)
Brown, G.D. *et al., Phytochemistry*, 1994, **36**, 1553 (*pmr, cmr*)
Nabeta, K. *et al., Chem. Comm.*, 1995, 2529 (*biosynth*)
Zulueta, M.C.A. *et al., Phytochemistry*, 1995, **38**, 1449 (*Phytyl heptanoate*)
Buchanan, M.-S. *et al., Phytochemistry*, 1996, **41**, 1373 (*Phytenyl phytenoate*)
Nabeta, K. *et al., J.C.S. Perkin 1*, 1997, 261 (*biosynth*)
Proteau, P.J. *et al., J. Nat. Prod.*, 1998, **61**, 841-843 (*biosynth*)
Arai, Y. *et al., Phytochemistry*, 1998, **48**, 471-474 (*2-Phytenyl 2-phytenoate*)
Proteau, P.J. *et al., Tet. Lett.*, 1998, **39**, 9373-9376 (*biosynth*)
Agatsuma, K. *et al., Fish. Sci.*, 1999, **65**, 494-495; *CA*, **131**, 225864 (*Porphyra yezoensis constits*)
Aliya, R. *et al., Pak. J. Mar. Biol.*, 1999, **5**, 65-76 (*2,3-epoxide*)
Lee, K.-I. *et al., CA*, 2000, **132**, 216670k (*isol, activity*)
Itoh, D. *et al., J. Nat. Prod.*, 2000, **63**, 1090-1093 (*biosynth*)
Huo, S. *et al., Org. Lett.*, 2001, 3253-3256 (*synth*)
Hertewich, U. *et al., Phytochemistry*, 2001, **58**, 1049-1054 (*biosynth*)
Ali, M.S. *et al., Z. Naturforsch., B*, 2001, **56**, 837-841 (*Codioester*)
Thiel, R. *et al., Phytochemistry*, 2002, **59**, 269-274 (*biosynth*)
Itoh, D. *et al., J. Nat. Prod.*2003, **66**, 332-336 (*biosynth*)
Kim, D. *et al., J. Nat. Prod.*, 2004, **67**, 1067-1069 (*biosynth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PIB600

2-Phyten-1,20-olide P-397

*4-(4,8,12-Trimethyltridecyl)-2-(5*H*)-furanone.* ***Luffarin X***
[145398-74-9]

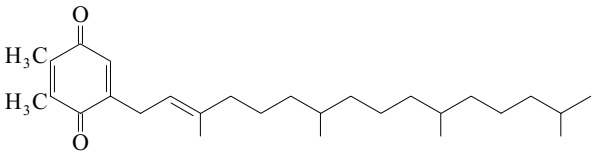


$C_{20}H_{36}O_2$ 308.503
Constit. of *Luffariella geometrica*. Oil. $[\alpha]_D^{20}$ +13.2 (c, 0.7 in $CHCl_3$).

Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1705 (*isol, pmr, cmr*)

Phytylplastoquinone P-398

[1177-24-8]

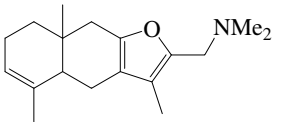


$C_{28}H_{46}O_2$ 414.67
Isol. from two strains of *Euglena gracilis.* Oil. λ_{max} 254; 261 (hexane).

Whistance, G.R. *et al., Phytochemistry*, 1970, **9**, 213

Piccolamine P-399

[139742-31-7]



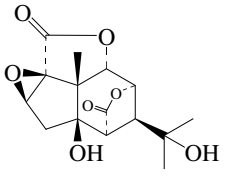
$C_{18}H_{27}NO$ 273.417
Isol. from the Senegalese gorgonian *Leptogorgia piccola.*
$[\alpha]_D$ -22 (c, 0.022 in $CHCl_3$). λ_{max} 204 (ϵ 10500); 208 (ϵ 8600); 228 (ϵ 3250) (MeOH).

N-*Oxide:* ***Piccolamine* N-*oxide***
[139742-32-8]
$C_{18}H_{27}NO_2$ 289.417
Isol. from the gorgonian *Leptogorgia piccola.*
$[\alpha]_D$ -47 (c, 0.012 in $CHCl_3$). λ_{max} 204 (ϵ 11200); 207 (ϵ 3100) (MeOH).

Roussis, V. *et al., New J. Chem.*, 1991, **15**, 959-961 (*isol, pmr, cmr, struct*)

Picrotin P-400

[21416-53-5]

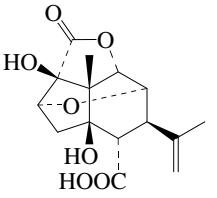


$C_{15}H_{18}O_7$ 310.303
Component of Picrotoxin. See also Picrotoxinin, P-402. Isol. from *Anamirta cocculus, Menispermum cocculus* and others, as component of Picrotoxin. Also isol. from marine sponge *Spirastrella inconstans.* $GABA_A$ receptor antagonist. Convulstant but less active than Picrotoxinin P-402. Cryst. (H_2O). Mp 255°. $[\alpha]_D^{16}$ -70 (EtOH). Log P -3.86 (uncertain value) (calc).
▶ LD_{50} (mus, ipr) 135 mg/kg. TJ8800000

Clark, E.P. *et al., J.A.C.S.*, 1935, **57**, 1111 (*isol*)
Craven, B.M. *et al., Acta Cryst.*, 1962, **15**, 387-396 (*struct*)
Jarboe, C.H. *et al., J. Med. Chem.*, 1968, **11**, 729-731 (*pharmacol*)
Corey, E.J. *et al., Tet. Lett.*, 1980, 1823-1824 (*synth*)
Sarma, N.S. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 189-190 (*isol, Spirastrella*)
Soto-Otero, R. *et al., J. Pharm. Biomed. Anal.*, 1989, **7**, 369-375 (*hplc*)
Miyashita, M. *et al., J.A.C.S.*, 1989, **111**, 3728-3734 (*synth*)

Picrotoxic acid† P-401

*Decahydro-5*a,*7*a-*dihydroxy-7*b-*methyl-4-(1-methylethenyl)-1-oxo-3,7-epoxyindeno[7,1-*bc*]furan-5-carboxylic acid, 9CI*
[111588-72-8]



Absolute Configuration

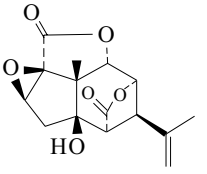
$C_{15}H_{18}O_7$ 310.303
Obt. from Picrotoxinin, P-402 by treatment with dil. acid. Cryst. + $2H_2O$ (H_2). Mp 230-231°. $[\alpha]_D^{17.5}$ +79 (c, 4.23 in EtOH).

Me ester: Methyl picrotoxate
[21412-43-1]
$C_{16}H_{20}O_7$ 324.33
Isol. from the berries of *Anamirta cocculus* and the marine sponge *Spirastrella inconstans.* Cryst. (Me_2CO/hexane).
Mp 174° (natural) Mp 171.5° (synthetic). $[\alpha]_D^{17.5}$ +87 (c, 5 in EtOH).

Harrmann, P. *et al., Annalen*, 1916, **411**, 273-314 (*synth*)
Benstead, J.C. *et al., J.C.S.*, 1952, 2292-2299 (*Me ester, synth*)
Conroy, H. *et al., J.A.C.S.*, 1957, **79**, 5550-5553 (*struct, bibl*)
Hathway, D.E. *et al., J.C.S.*, 1957, 4953-4957 (*Picrotoxic acid*)
Sarma, N.S. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 189-190 (*Me ester, isol, Spirastrella, pmr*)
Pradhan, P. *et al., Indian J. Chem., Sect. B*, 1990, **29**, 676-677 (*Me ester, isol, Anamirta, pmr*)
Krische, M.J. *et al., Tetrahedron*, 1998, **54**, 3693-3704 (*synth*)
Trost, B. *et al., J.A.C.S.*, 1999, **121**, 6131-6141 (*synth*)
Agarwal, S.K. *et al., Phytochemistry*, 1999, **50**, 1365-1368 (*Me ester, isol, Anamirta*)

Picrotoxinin P-402

[17617-45-7]



Absolute configuration

$C_{15}H_{16}O_6$ 292.288
Isol. from *Anamirta cocculus*, *Menispermum cocculus* and others, as component of Picrotoxin. Also isol. from desmosponge*Spirastrella inconstans.* An ichthyotoxin. Potent convulsant drug. Cryst. (H_2O).
Mp 209.5°. $[\alpha]_D$ -5.85 (c, 3.65 in $CHCl_3$).
▶ LD_{50} (mus, ipr) 3 mg/kg. PC5150000

Compd. with Picrotin, P-400 (1:1): ***Picrotoxin***. *Cocculin*†
[124-87-8]
$C_{30}H_{34}O_{13}$ 602.591
Bitter principle from berries of the shrubs *Anamirta cocculus, Menispermum cocculus* and other spp. Powerful nonspecific CNS stimulant; $GABA_A$-receptor antagonist. Anticonvulsant, antiepileptic agent. Used in neurochemical research. Cryst. (EtOH).
Mp 203-204°. $[\alpha]_D^{12}$ -30 (H_2O).
▶ Convulsant toxin, very toxic if swallowed. LD_{Lo} (hmn, orl) 0.4 mg/kg. LD_{50} (rat, ivn) 1.6 mg/kg. TJ9100000

8,9-Dihydro: ***α-Dihydropicrotoxinin***
[17617-46-8]
$C_{15}H_{18}O_6$ 294.304
Constit. of *Dendrobium moniliforme.* Gum. $[\alpha]_D^{24}$ -3.5 (c, 0.51 in Me_2CO).

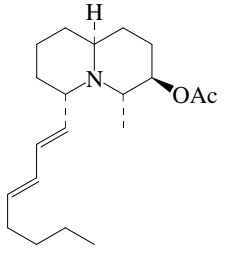
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 701B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1143A (*nmr*)
Clark, E.P. *et al., J.A.C.S.*, 1935, **57**, 1111 (*isol*)

Conroy, H. *et al., J.A.C.S.*, 1957, **79**, 5550-5553 (*struct*)
Porter, L.A. *et al., Chem. Rev.*, 1967, **67**, 441-464 (*rev*)
Jarboe, C.H. *et al., J. Med. Chem.*, 1968, **11**, 729-731 (*pharmacol*)
Coscia, C.J. *et al., Cyclopentanoid Terpene Deriv.*, (Eds. Taylor, W.I. *et al*), Dekker, N.Y., 1969, 147 (*rev*)
Corey, E.J. *et al., J.A.C.S.*, 1979, **101**, 5841-5843 (*synth*)
Mackay, M.F. *et al., Aust. J. Chem.*, 1983, **36**, 2111-2117; 2219-2225 (*cryst struct, conformn, pmr*)
Benzodiazepine/GABA Recept. Chloride Channels: 1986, (Eds. Olsen, R.W. *et al*), A.R. Liss, New York, 1986, (*pharmacol, book*)
Sarma, N.S. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 189-190; 1989, 189-190 (*isol, Spirastrella, pmr, ms*)
Soto-Otero, R. *et al., J. Pharm. Biomed. Anal.*, 1989, **7**, 369-375 (*hplc*)
Miyashita, M. *et al., J.A.C.S.*, 1989, **111**, 3728-3734 (*synth*)
Newland, C.F. *et al., J. Physiol. (London)*, 1992, **447**, 191 (*pharmacol, picrotoxin*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1231
Trost, B.M. *et al., J.A.C.S.*, 1999, **121**, 6183-6192 (*synth*)
Zhao, W. *et al., Planta Med.*, 2003, **69**, 1136-1140 (*α-Dihydropicrotoxinin*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, PIE500; 1992, PIE510

Pictamine P-403

*Octahydro-4-methyl-6-(1,3-octadienyl)-2*H*-quinolizin-3-ol acetate, 9CI*

[136945-62-5]



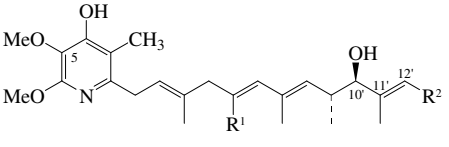
Absolute Configuration

$C_{20}H_{33}NO_2$ 319.486

Alkaloid from the tunicate *Clavelina picta*. Oil. $[\alpha]_D$ -87 (c, 0.1 in EtOAc). λ_{max} 230 (ϵ 19000) (EtOH) (Derep). λ_{max} 231 (MeOH) (Berdy).

Kong, F. *et al., Tet. Lett.*, 1991, **32**, 3667-3668 (*isol, uv, ir, pmr, cmr, ms, struct*)
Toyooka, N. *et al., Tetrahedron*, 1999, **55**, 15209-15224 (*synth, abs config*)

Piericidin P-404



Relative Configuration

Piericidin A_1, $R^1 = H$, $R^2 = CH_3$
A_2, $R^1 = R^2 = CH_3$
A_3, $R^1 = H$, $R^2 = CH(CH_3)_2$
A_4, $R^1 = CH_3$, $R^2 = CH(CH_3)_2$
A_5, $R^1 = H$, $R^2 = CH_2CH_3$
A_6, $R^1 = CH_3$, $R^2 = CH_2CH_3$
Antibiotic IT 143A, $R^1 = CH_3$, R^2 = -C(CH_3)=CHCH_3(*E*-)
IT 143B, $R^1 = H$, R^2 = -C(CH_3)=CHCH_3(*E*-)

Pyridine antibiotic family. Sol. MeOH, hexane; poorly sol. H_2O. λ_{max} 205 (ϵ 40800); 237 (ϵ 41800); 267 (ϵ 6600) (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 0.87 mg/kg.

Piericidin A_5

$C_{26}H_{39}NO_4$ 429.598

This component not yet characterised.

*11′*S*,12′*S*-Epoxide:* ***Piericidin C5***

$C_{26}H_{39}NO_5$ 445.598

Prod. by a marine-derived *Streptomyces* sp. Cell division inhibitor. Pale yellow oil. $[\alpha]_D^{25}$ +7 (c, 0.12 in MeOH). λ_{max} 231 (ϵ 32000); 236 (ϵ 32300); 267 (ϵ 5100) (MeOH).

Piericidin A_6

$C_{27}H_{41}NO_4$ 443.625

Component not yet characterised.

*11′*S*,12′*S*-Epoxide:* ***Piericidin C6***

$C_{27}H_{41}NO_5$ 459.625

Prod. by a marine-derived *Nocardioides* sp. Cell division inhibitor. Pale yellow oil. $[\alpha]_D^{25}$ +34 (c, 0.03 in MeOH). λ_{max} 225 (ϵ 20600); 267 (ϵ 6000) (MeOH).

Kubota, N.K. *et al., Bioorg. Med. Chem.*, 2003, **11**, 4569-4575 (*Piericidins C5, C6*)

Callinectes sapidus Pigment-dispersing hormone P-405

[160871-93-2]

$C_{80}H_{138}N_{22}O_{28}S$ 1888.167

Isol. from the eyestalk of the blue crab *Callinectes sapidus*.

Klein, J.M. *et al., Biochem. Biophys. Res. Commun.*, 1994, **205**, 410-416 (*isol*)

Pandalus borealis Pigment-dispersing hormone P-406

Distal retinal pigment. α-PDH. Pab-α-PDH. DRPH

[58561-85-6]

H-Asn-Ser-Gly-Met-Ile-Asn-Ser-Ile-Leu-Gly-Ile-Pro-Arg-Val-Met-Thr-Glu-Ala-NH_2

$C_{80}H_{140}N_{24}O_{25}S_2$ 1902.264

Isol. from eyestalks of the shrimp *Pandalus borealis*; also found in *Pandalus jordani*. Adapts the shrimp to brighter light conditions by causing the distal retinal pigment cells of the eye to move to a more proximal position.

Fernlund, P. *et al., Biochim. Biophys. Acta*, 1976, **439**, 17-25 (*isol, Pandalus constit*)
Josefsson, L. *et al., Am. Zool.*, 1983, **23**, 507 (*rev*)
Rao, K.R. *et al., Prog. Clin. Biol. Res.*, 1988, **256**, 407 (*rev*)

Pandalus jordani Pigment-dispersing hormone P-407

Paj-PDH

Asn-Ser-Gly-Met-Ile-Asn-Ser-Ile-Leu-Gly-Ile-Pro-Lys-Val-Met-Ala-Asp-Ala-NH_2

Struct. of Paj-PDH-II shown. Isol. from the pink shrimp *Pandalus jordani*. Paj-PDH-I is identical to *Pandalus borealis* Pigment-dispersing hormone, P-406.

Paj-PDH-II

$C_{78}H_{136}N_{22}O_{24}S_2$ 1830.197

Paj-PDH-III

$C_{83}H_{144}N_{22}O_{24}S$ 1866.25

Rao, K.R. *et al., Ann. N.Y. Acad. Sci.*, 1993, **680**, 78-88 (*isol*)

Penaeus aztecus Pigment-dispersing hormone P-408

[176677-91-1]

Asn-Ser-Glu-Leu-Ile-Asn-Ser-Leu-Leu-Gly-Ile-Pro-Lys-Val-Met-Asn-Asp-Ala-NH_2

$C_{83}H_{143}N_{23}O_{27}S$ 1927.247

Isol. from the brown shrimp *Penaeus aztecus* and the white shrimp *Penaeus vannamei*.

Rao, K.R. *et al., Ann. N.Y. Acad. Sci.*, 1993, **680**, 78-88 (*isol*)
Desmoucelles-Carette, C. *et al., Biochem. Biophys. Res. Commun.*, 1996, **221**, 739-743 (*isol*)

Penaeus vannamei Pigment-dispersing hormone P-409

[176677-92-2]

Asn-Ser-Glu-Leu-Ile-Asn-Ser-Leu-Leu-Gly-Leu-Pro-Lys-Val-Met-Asn-Asp-Ala-NH_2

$C_{83}H_{143}N_{23}O_{27}S$ 1927.247

Isol. from the white shrimp *Penaeus vannamei*.

Desmoucelles-Carette, C. *et al., Biochem. Biophys. Res. Commun.*, 1996, **221**, 739-743 (*isol*)

Uca pugilator Pigment-dispersing hormone P-410

Uca-PDH. Cancer magister *Pigment-dispersing hormone. Cam-PDH*

[98798-59-5]

Asn-Ser-Glu-Leu-Ile-Asn-Ser-Ile-Leu-Gly-Leu-Pro-Lys-Val-Met-Asn-Asp-Ala-NH_2

$C_{83}H_{143}N_{23}O_{27}S$ 1927.247

Isol. from the edible crab *Cancer magister*; also present in the Atlantic sand fiddler *Uca pugilator*, the shore crab *Carcinus maenas*, the signal crayfish *Pacifastacus leniusculus* and the blue crab *Callinectes sapidus*.

17-Glutamic acid analogue: Procambarus clarkii *Pigment-dispersing hormone. Prc-β-PDH*

[144078-27-3]

$C_{84}H_{145}N_{23}O_{27}S$ 1941.273

Isol. from eyestalks of the crayfish *Procambarus clarkii*; also present in the crayfish *Orconectes limosus* and *Orconectes immunis*.

Rao, K.R. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1985, **82**, 5319-5322 (*isol, Uca pugilator*)
Kleinholz, L.H. *et al., Biol. Bull. (Woods Hole, Mass.)*, 1986, **170**, 135-143 (*isol, Cancer magister*)
McCallum, M.L. *et al., Pigment Cell Res.*, 1991, **4**, 201-208 (*isol, Procambarus clarkii constit*)
De Klein, D.P.V. *et al., Biochem. Biophys. Res. Commun.*, 1992, **189**, 1505-1514 (*isol, Orconectes immunis*)
Klein, J.M. *et al., Biochem. Biophys. Res. Commun.*, 1992, **189**, 1509-1514; 1994, **205**, 410-416 (*isol, Carcinus maenas, Collinectes sapidus*)
Rao, K.R. *et al., Ann. N.Y. Acad. Sci.*, 1993, **680**, 78-88 (*isol,* Pacifastacus leniusculus, Orconectes immunis)
Lohr, J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1993, **104**, 699-700 (*isol, Cancer maenas*)

Penaeus japonicus Pigment-dispersing hormones P-411

Asn-Ser-Glu-Leu-Ile-Asn-Ser-Leu-Leu-Gly-Ile-Pro-Lys-Val-Met-Thr-Asp-Ala-NH_2

Two octadecapeptides designated Pej-PDH-I and -II; struct. of Pej-PDH-I shown. Isol. from sinus glands of the kuruma prawn *Penaeus japonicus*. Neuropeptides.

Pej-PDH-I

NSELINSLLGIPKVMTDA amide

[235743-39-2]

$C_{83}H_{144}N_{22}O_{27}S$ 1914.248

Pej-PDH-II

NSELINSLLGLPKFMIDA amide

[235743-40-5]

$C_{89}H_{148}N_{22}O_{26}S$ 1974.346

Yang, W.J. *et al., Gen. Comp. Endocrinol.*, 1999, **114**, 415-424 (*isol, struct*)

Piguamerin P-412

[211735-16-9]

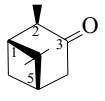
Large peptide containing 48 amino acids. Isol. from the leech *Hirudo nipponia*. Serine protease inhibitor.

Kim, D.R. *et al., Eur. J. Biochem.*, 1998, **254**, 692-697 (*isol, struct*)

3-Pinanone P-413

2,6,6-Trimethylbicyclo[3.1.1]heptan-3-one, 9CI

[15358-88-0]



(1*R*,2*R*,5*S*)–*form*

$C_{10}H_{16}O$ 152.236

Detected by gc-ms in the Black Sea bryozoan *Conopeum seuratum*.

(1*R*,2*R*,5*S*)-*form*

(+)-Isopinocamphone

[473-62-1]

Oil. Bp 213°. $[\alpha]_D^{20}$ +10.5.

Semicarbazone:

Cryst. Mp 219-220°.

(1*R*,2*S*,5*S*)-*form*

(+)-Pinocamphone

[18492-59-6]

Oil. Bp 211-211.5°. $[\alpha]_D^{20}$ +21.3.

Semicarbazone:

Cryst. Mp 227°.

(1*S*,2*R*,5*R*)-*form*

(-)-Pinocamphone

[22339-21-5]

Constit. of the oils of *Hyssopus officinalis* (hyssop) and ground ivy. Also from *Tanacetum fastigiatum, Luvunga scandens* and others.

Oil. Bp 212-214°. $[\alpha]_D^{25}$ -15.2 (c, 0.42 in MeOH).

Semicarbazone:

Cryst. (MeOH aq.). Mp 227.5-228°.

(1*S*,2*S*,5*R*)-*form*

(-)-Isopinocamphone

[14575-93-0]

Constit. of *Mentha aquatica* (water mint).

Oil. Bp 211-211.5°. $[\alpha]_D^{15}$ -7.3.

Semicarbazone:

Cryst. Mp 232°.

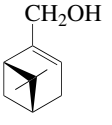
[547-60-4]

Hückel, W. *et al., Annalen*, 1966, **697**, 69 (*synth, config, bibl*)
Banthorpe, D.V. *et al., Chem. Rev.*, 1966, **66**, 643 (*rev*)
Brown, H.C. *et al., J.O.C.*, 1971, **36**, 387 (*synth*)
Hadjieva, P. *et al., Z. Naturforsch., C*, 1987, **42**, 1019-1022 (*occur, Conopeum*)

2-Pinen-10-ol P-414

6,6-Dimethylbicyclo[3.1.1]hept-2-ene-2-methanol, 9CI. Myrtenol. FEMA 3439

[515-00-4]



(+)-*form*

$C_{10}H_{16}O$ 152.236

(+)-*form*

Darwinol

[6712-78-3]

Isol. from oil of myrtle (*Myrtus communis*), *Darwinia grandiflora, Leptospermum lanigerum, Chamaecyparis formosensis* and others.

Oil. Bp_{11} 103-104°. $[\alpha]_D^{22}$ +44.3 (c, 3.21 in $CHCl_3$).

10-Aldehyde: ***Myrtenal***. *FEMA 3395*

[23727-16-4]

[564-94-3]

$C_{10}H_{14}O$ 150.22

Occurs in eucalyptus, orange, lemon, spearmint, pepper, thyme, juniper, calamus, ginger, myrtle, lemon balm, calabash, nutmeg, parsley seed and other plant oils. Unstable oil with cinnamon odour. Bp_{15} 99-100°. $[\alpha]_D^{20}$ +14.75.

(ξ)-*form*

10-Aldehyde:

$C_{10}H_{14}O$ 150.22

Occurs in Black Sea bryozoan *Conopeum seuratum*.

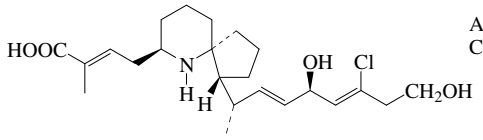
[19250-17-0, 117872-96-5]

Banthorpe, D.V. *et al., Chem. Rev.*, 1966, **66**, 643-656 (*rev*)
Bates, R.B. *et al., J.O.C.*, 1968, **33**, 1730-1732 (*Myrtenal, pmr*)
Borowiecki, L. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1971, **45**, 573-580 (*Myrtenic acid, synth, 10-aldehyde*)

Kergomard, A. *et al., Bull. Soc. Chim. Fr.*, 1974, 2572-2574 (*10-aldehyde, synth*)
Hadjieva, P. *et al., Z. Naturforsch., C*, 1987, **42**, 1019-1022 (*Myrtenal, occur, Conopeum*)

Pinnaic acid P-415

[178115-91-8]



Absolute Configuration

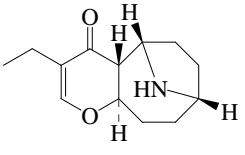
$C_{23}H_{36}ClNO_4$ 425.994
Alkaloid from the Okinawan bivalve *Pinna muricata*. Phospholipase A2 inhibitor. Antiinflammatory agent.

Taurine amide: ***Tauropinnaic acid***
[178115-92-9]
$C_{25}H_{41}ClN_2O_6S$ 533.127
Alkaloid from *Pinna muricata*. Phospholipase A2 inhibitor. Antiinflammatory agent.

Chou, T. *et al., Tet. Lett.*, 1996, **37**, 3871-3874 (*isol, pmr, cmr, struct*)
Carson, M.W. *et al., Angew. Chem., Int. Ed.*, 2001, **40**, 4450-4452; 4453-4456 (*synth, abs config*)
Hayakawa, I. *et al., Heterocycles*, 2003, **59**, 441-444 (*synth*)
Matsumura, Y. *et al., Org. Lett.*, 2004, **6**, 965-968 (*synth*)
Zhang, H.-L. *et al., J.O.C.*, 2005, **70**, 4954-4961 (*synth*)
Andrade, R.B. *et al., Org. Lett.*, 2005, **7**, 5733-5735 (*synth*)

Pinnamine P-416

[298197-30-5]



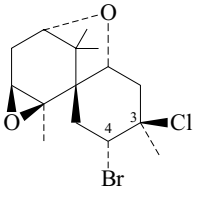
Absolute Configuration

$C_{13}H_{19}NO_2$ 221.299
Alkaloid from the Okinawan bivalve *Pinna muricata*. Toxin. Oil. $[\alpha]_D^{27}$ +71.2 (c, 0.04 in MeOH) (synthetic).

Takada, N. *et al., Tet. Lett.*, 2000, **41**, 6425-6428 (*isol, abs config*)
Kigoshi, H. *et al., Tet. Lett.*, 2001, **42**, 7469-7471 (*synth*)

Pinnatazane P-417

2-Bromo-3-chloro-5,10:7,8-diepoxychamigrane
[119765-94-5]



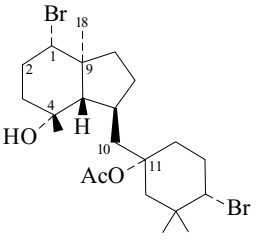
$C_{15}H_{22}BrClO_2$ 349.694
Constit. of *Laurencia pinnatifida*. Cryst. (MeOH).
Mp 190-192°. $[\alpha]_D$ +4.34 (c, 0.23 in $CHCl_3$).

3,4-Diepimer: ***Almadioxide***
$C_{15}H_{22}BrClO_2$ 349.694
Constit. of *Laurencia intricata*. Cryst. (CH_2Cl_2/hexane).
Mp 206°. $[\alpha]_D$ +4 (c, 0.7 in $CHCl_3$).

Atta-ur-Rahman, *et al., Phytochemistry*, 1988, **27**, 3879 (*isol, cryst struct*)
Aknin, M. *et al., Tet. Lett.*, 1989, **30**, 559 (*cryst struct*)

Pinnaterpene A P-418

[81474-79-5]



Absolute configuration

$C_{22}H_{36}Br_2O_3$ 508.333
Constit. of red alga *Laurencia pinnata*. Cryst. (hexane/CH_2Cl_2). Mp 89-93°. $[\alpha]_D$ -23.5 ($CHCl_3$).

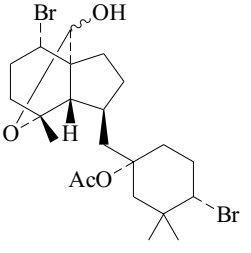
O-*De-Ac:* ***Irieol C***
[67506-19-8]
$C_{20}H_{34}Br_2O_2$ 466.295
Isol. from *Laurencia irieii*. Cryst.
Mp 136-137°. $[\alpha]_D$ -35.2 ($CHCl_3$).

18-Hydroxy: ***Pinnaterpene B***
[81474-78-4]
$C_{22}H_{36}Br_2O_4$ 524.332
Isol. from *Laurencia pinnata*. Cryst. (C_6H_6/hexane). Sol. MeOH. Mp 152-154°. $[\alpha]_D$ -20.6 ($CHCl_3$). λ_{max} 228 (ϵ 8100) (MeOH) (Berdy).

Fukuzawa, A. *et al., Chem. Lett.*, 1982, 1389 (*cryst struct*)

Pinnaterpene C P-419

[81474-77-3]

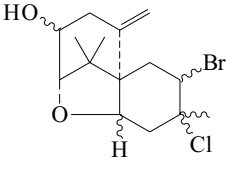


$C_{22}H_{34}Br_2O_4$ 522.316
Isol. from red alga *Laurencia pinnata*. Amorph. solid. $[\alpha]_D$ +29.2 ($CHCl_3$).

Fukuzawa, A. *et al., Chem. Lett.*, 1982, 1389

Pinnatifenol P-420

[140400-47-1]

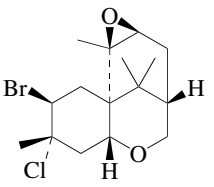


$C_{15}H_{22}BrClO_2$ 349.694
Metab. of *Laurencia pinnatifida*. Gum. $[\alpha]_D$ +14.02 (c, 0.417 in $CHCl_3$).

Ahmad, V.U. *et al., Phytochemistry*, 1991, **30**, 4172-4174 (*isol, pmr, cmr*)

Pinnatificin P-421

[122398-24-7]



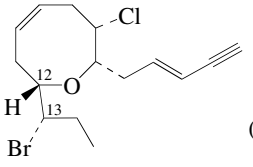
Relative Configuration

$C_{16}H_{24}BrClO_2$ 363.721
Isol. from *Laurencia pinnatifida*.

Ahmad, V.U. *et al., Nat. Prod. Chem. 3*, 1988, 355-358 (*isol*)

Pinnatifidenyne P-422

*8-(1-Bromopropyl)-3-chloro-3,4,7,8-tetrahydro-2-(2-penten-4-ynyl)-2*H*-oxocin, 9CI. 13-Bromo-7-chloro-6,12-epoxy-3,9-pentadecadien-1-yne. Pinnatifidienyne*



(*E*)-*form*

$C_{15}H_{20}BrClO$ 331.679
Abs. configs. revised in 1991.

(*E*)-*form* [83060-13-3]
Metab. of *Laurencia pinnatifida*.
Cryst. (hexane).
Mp 57-58°. $[\alpha]_D^{25}$ +62 (c, 8.9 in $CHCl_3$).

12-Epimer: **trans-*12-Epipinnatifidenyne***. trans-*Dihydrorhodophytin*
[83060-14-4]
$C_{15}H_{20}BrClO$ 331.679
Constit. of *Laurencia pinnatifida*. Solid.
Mp 40-41°. $[\alpha]_D$ +33.19 (c, 0.95 in $CHCl_3$).

13-Epimer: **trans-*13-Epipinnatifidenyne***
$C_{15}H_{20}BrClO$ 331.679
Constit. of *Laurencia obtusa*. Powder. $[\alpha]_D$ +16 (c, 0.1 in $CHCl_3$). λ_{max} 226 (log ϵ 4.07) (hexane).

6,7-Diepimer: **trans-*6,7-Diepipinnatifidenyne***
[860797-04-2]
$C_{15}H_{20}BrClO$ 331.679
Constit. of *Aplysia dactylomela*. Cryst. $[\alpha]_D$ -17.2 (c, 2.2 in $CHCl_3$).

(*Z*)-*form* [82769-15-1]
Metab. of *Laurencia pinnatifida*.
Cryst. (hexane).
Mp 47.5-48.5°. $[\alpha]_D^{25}$ +39 (c, 13.8 in $CHCl_3$).

12-Epimer: **cis-*12-Epipinnatifidenyne***. cis-*Dihydrorhodophytin*
[71778-85-3]
$C_{15}H_{20}BrClO$ 331.679
Constit. of *Aplysia brasiliana* and *Laurencia pinnatifida*. Solid.
Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 37-39°. $[\alpha]_D^{25}$ +74.8. λ_{max} 224 (ϵ 11600) (MeOH) (Berdy).

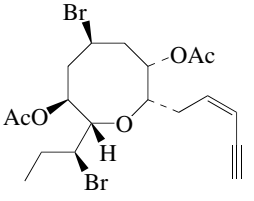
13-Epimer: **cis-*13-Epipinnatifidenyne***
$C_{15}H_{20}BrClO$ 331.679
Constit. of *Laurencia claviformis*. Cryst. (hexane).
Mp 64-65°. $[\alpha]_D^{25}$ +13.4 (c, 1.3 in $CHCl_3$).

Diastereoisomer: **cis-*Isodihydrorhodophytin***
[71806-88-7]
$C_{15}H_{20}BrClO$ 331.679
Minor constit. of *Aplysia brasiliana*. Oil. $[\alpha]_D^{25}$ +71.4 (c, 0.0042 in $CHCl_3$). Abs. config. needs clarifying in the light of recent revisions.

Kinnel, R.B. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1979, **76**, 3576-3579, (*cis-Isodihydrorhodophytin*)
Gonzalez, A.G. *et al., Tetrahedron*, 1982, **38**, 1009-1014 (*isol*)
Norte, M. *et al., Phytochemistry*, 1989, **28**, 647-649 (*12-Epipinnatifidenynes*)
Norte, M. *et al., Tetrahedron*, 1991, **47**, 9411-9418 (*isol, cryst struct, abs config*)
San-Martin, A. *et al., Nat. Prod. Lett.*, 1997, **10**, 303-311 (*cis-13-Epipinnatifidenyne*)
Iliopoulou, D. *et al., Phytochemistry*, 2002, **59**, 111-116 (*trans-13-Epipinnatifidenyne*)
Kim, H. *et al., J.A.C.S.*, 2003, **125**, 10238-10240 (*synth*)
Manzo, E. *et al., Tetrahedron*, 2005, **61**, 7456-7460 (*6,7-Diepipinnatifidenyne*)

Pinnatifidine† P-423

7,11-Diacetoxy-9,13-dibromo-6,12-epoxy-3-pentadecen-1-yne
[123942-27-8]

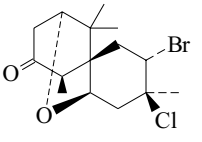


$C_{19}H_{26}Br_2O_5$ 494.219
Isol. from *Laurencia pinnatifida*.

Atta-ur-Rahman, *et al., Pure Appl. Chem.*, 1989, **61**, 453-456

Pinnatifidone P-424

[119400-88-3]

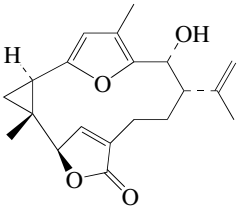


$C_{15}H_{22}BrClO_2$ 349.694
Metab. of *Laurencia pinnatifida*. Semi-cryst. $[\alpha]_D$ +36.03 (c, 0.33 in MeOH).

Bano, S. *et al., Z. Naturforsch., B*, 1988, **43**, 1347 (*isol, pmr, cmr*)

Pinnatin A P-425

[209969-38-0]

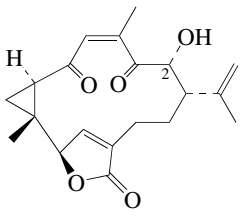


$C_{20}H_{24}O_4$ 328.407
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 189-211° (dec.). $[\alpha]_D^{24}$ +225.4 (c, 0.55 in $CHCl_3$). Related to Gersolide, G-74. λ_{max} 216 (ϵ 12800) (MeOH).

Rodríguez, A.D. *et al., J.O.C.*, 1998, **63**, 4425-4432 (*isol, pmr, cmr, cryst struct*)

Pinnatin C P-426

[209969-40-4]



$C_{20}H_{24}O_5$ 344.407
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 217-237° (dec.). $[\alpha]_D^{24}$ -140 (c, 0.3 in $CHCl_3$). λ_{max} 216 (ϵ 7800) (MeOH). λ_{max} 216 (ϵ 7800) (MeOH) (Berdy).

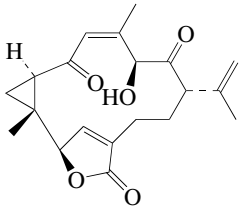
2-Ac: ***Pinnatin B***
[209969-39-1]
$C_{22}H_{26}O_6$ 386.444
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 212-249° (dec.). $[\alpha]_D^{24}$ -80.6 (c, 0.9 in $CHCl_3$). λ_{max} 214 (ϵ 5300) (MeOH). λ_{max} 214 (ϵ 5300) (MeOH) (Berdy).

2-Epimer: ***Pinnatin D***
[209969-42-6]
$C_{20}H_{24}O_5$ 344.407
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 213-220° (dec.). $[\alpha]_D^{24}$ +32.5 (c, 0.4 in $CHCl_3$). λ_{max} 210 (ϵ 12200) (MeOH). λ_{max} 210 (ϵ 12000) (MeOH) (Berdy).

Rodríguez, A.D. *et al., J.O.C.*, 1998, **63**, 4425-4432 (*isol, pmr, cmr, cryst struct*)

Pinnatin E P-427

[209969-43-7]

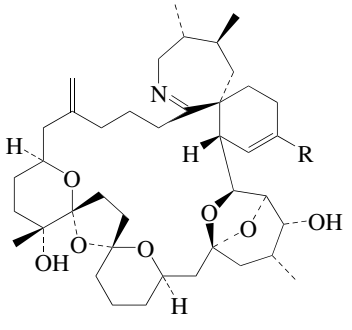


$C_{20}H_{24}O_5$ 344.407
Constit. of *Pseudopterogorgia bipinnata*. Cryst.
Mp 185°. $[\alpha]_D^{24}$ -290 (c, 0.4 in $CHCl_3$). λ_{max} 214 (ϵ 19000) (MeOH). λ_{max} 214 (ϵ 19000) (MeOH) (Berdy).

Rodriguez, A.D. *et al., J.O.C.*, 1998, **63**, 4425-4432 (*isol, pmr, cmr, cryst struct*)

Pinnatoxin A P-428

[160759-36-4]



Absolute Configuration

R = COOH

$C_{41}H_{61}NO_9$ 711.934
Exists as zwitterion. Neutral form shown. Principal toxin from the bivalves *Pinna muricata*, *Pinna attenuata* and *Pinna atropurpurea*. Calcium channel activating agent, smooth muscle contractant showing tetrodotoxin-like effect. λ_{max} 216 (EtOH) (Berdy).
▶ Toxin.

Uemura, D. *et al., J.A.C.S.*, 1995, **117**, 1155-1158 (*isol, pmr, cmr, struct*)
Chou, T. *et al., Tet. Lett.*, 1996, **37**, 4023-4026 (*stereochem*)
McCauley, J.A. *et al., J.A.C.S.*, 1998, **120**, 7647-7648 (*synth*)
Falk, M. *et al., Tetrahedron*, 2001, **57**, 8659-8665 (*abs config*)
Sakamoto, S. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 6505-6510 (*synth*)

Pinnatoxin B P-429

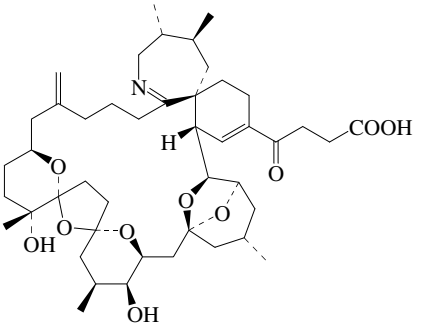
[160903-44-6]
As Pinnatoxin A, P-428 with
R = - $^{34}CH(NH_2)COOH$(*S*-)
$C_{42}H_{64}N_2O_9$ 740.976
Exists as a zwitterion. Minor toxin from *Pinna muricata*.

34-Epimer: ***Pinnatoxin C***
[167228-66-2]
$C_{42}H_{64}N_2O_9$ 740.976
Minor toxin from *Pinna muricata*.

Takada, N. *et al., Tet. Lett.*, 2001, **42**, 3491-3494 (*isol*)
Matsuura, F. *et al., Org. Lett.*, 2006, **8**, 3327-3330 (*synth, abs config*)

Pinnatoxin D P-430

[167228-67-3]



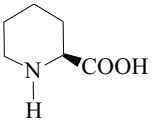
Absolute Configuration

$C_{45}H_{67}NO_{10}$ 782.025
Exists as zwitterion. Neutral form shown. Toxin from the bivalves *Pinna muricata*, *Pinna attenuata* and *Pinna atropurpurea*. Calcium channel activating agent. Solid. $[\alpha]_D$ +42.5 (c, 0.5 in MeOH). λ_{max} 226 (MeOH).
▶ Toxic.

Chou, T. *et al., Tet. Lett.*, 1996, **37**, 4023-4026; 4027-4030 (*isol, uv, pmr, cmr, struct*)
Falk, M. *et al., Tetrahedron*, 2001, **57**, 8659-8665 (*abs config*)

2-Piperidinecarboxylic acid, 9CI P-431

Pipecolic acid. *Hexahydropicolinic acid. Pipecolinic acid. Homoproline*†
[535-75-1]



(*S*)–*form*

$C_6H_{11}NO_2$ 129.158
▶ TK6021000

(S)-form
L-form
[3105-95-1]
Present in beans and other legumes, and in lesser quantities in other plants including barley, hops, teak and mushrooms. Also

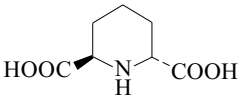
from the red alga *Amphiroa beauvoisii*.
Needles (MeOH/Et_2O). Sol. H_2O.
Mp 259-260°. $[\alpha]_D^{20}$ -30.6 (c, 1 in H_2O).

[41994-45-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 585B; 585C; 585D; 682B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 889A; 889B; 889C; 1085B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 737B (*ir*)
Rodwell, V.W. *et al., Methods Enzymol., Part B*, 1971, **17**, 174 (*rev*)
Fujii, T. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 1341 (*synth*)
Aketa, K. *et al., Chem. Pharm. Bull.*, 1976, **24**, 621 (*synth*)
Bhattacharjee, S.K. *et al., Acta Cryst. B*, 1979, **35**, 396 (*cryst struct*)
Kisfaludy, L. *et al., Synthesis*, 1982, 163 (*synth*)
Shuman, R.T. *et al., J.O.C.*, 1990, **55**, 738 (*synth*)
Ng-Youn-Chen, M.C. *et al., J.O.C.*, 1994, **59**, 2075 (*resoln*)
Berrien, J.-F. *et al., J.O.C.*, 1994, **59**, 3769 (*synth*)
Agami, C. *et al., Synth. Commun.*, 2000, **30**, 2565-2572 (*S-form, synth, pmr*)

2,6-Piperidinedicarboxylic acid P-432

Hexahydrodipicolinic acid. Dipipecolinic acid
[499-82-1]



(2*RS*,6*RS*)–*form*

$C_7H_{11}NO_4$ 173.168
Isol. from *Porphyra tenera*.

(2*RS*,6*RS*)-*form*
(±)-trans-*form*
Powder. Mp 276-279°.

Di-Me ester:
$C_9H_{15}NO_4$ 201.222
Mp 93°.

N-*Me: Scopolinic acid. Teneraic acid*
$C_8H_{13}NO_4$ 187.195
Plates + $1H_2O$. Sol. hot H_2O; spar. sol. Et_2O. Mp 225° dec. (hydrate) Mp 230° (anhyd.).

N-*Me, di-Me ester: Dimethyl scopolinate*
$C_{10}H_{17}NO_4$ 215.249
$Bp_{0.14}$ 71-76°. n_D^{25} 1.4659.

Diamide:
$C_7H_{13}N_3O_2$ 171.199
Cryst. Mp 265-269°.

(2*RS*,6*SR*)-*form*
cis-*form*
[59234-40-1]
Powder. Mp 290-295°.

Di-Me ester: [59234-46-7]
$C_9H_{15}NO_4$ 201.222
Cryst. (hexane or MeOH). Mp 91.5-92.5° Mp 210-212°. No explanation for large discrepancy in Mp's.

Diamide: Mp 226-238°.

N-*Me: Isoscopolinic acid*
Mp 263° (dec. from 253°).

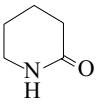
N-*Me, di-Me ester: Dimethyl isoscopolinate*
$Bp_{0.2}$ 85°. n_D^{25} 1.4665.

[6039-37-8, 21495-53-4, 59234-46-7]

Singer, A. *et al., J.A.C.S.*, 1935, **57**, 1137 (*synth*)
Barnes, R.A. *et al., J.A.C.S.*, 1953, **75**, 975 (*synth, config*)
Hermann, K. *et al., Helv. Chim. Acta*, 1976, **59**, 626 (*synth*)
Kawanchi, H. *et al., Nippon Suisan Gakkaishi*, 1978, **44**, 1371 (*isol, synth*)
Wasserman, H.H. *et al., Tet. Lett.*, 1989, **30**, 6077 (*synth*)
Chrystal, E.J.T. *et al., Tetrahedron*, 1995, **51**, 10241 (*synth, acid, diamides*)
Chênevert, R. *et al., J.O.C.*, 1996, **61**, 3332 (*Di-Me ester, synth, ir, pmr, cmr*)

2-Piperidinone, 9CI P-433

δ-Valerolactam. α-Piperidone. 2-Oxopiperidine. 5-Aminopentanoic acid lactam
[675-20-7]



C_5H_9NO 99.132
Isol. from the ascidian *Atriolum robustum* and the sponge *Tedania ignis*. Hygroscopic cryst. Sol. H_2O, Et_2O, EtOH.
Mp 39-40°. Bp 256° $Bp_{0.4}$ 64-65°.

▶ TO0110000

Hydrochloride: [5174-67-4]
Cryst. (EtOH/Et_2O). Mp 182-183°.

N-*Benzoyl:* [4252-56-6]
$C_{12}H_{13}NO_2$ 203.24
Cryst. ($CHCl_3$/petrol). Mp 112° (104-106°).

N-*(4-Methylbenzenesulfonyl):* [23438-61-1]
$C_{12}H_{15}NO_3S$ 253.321
Solid (toluene). Mp 148°.

N-*Me:* [931-20-4]
$C_6H_{11}NO$ 113.159
Hygroscopic liq. Misc. H_2O. Bp_{14} 104°.

N-*Me; hydrochloride:* [87243-73-0]
Cryst. (EtOH/Et_2O). Mp 104°.

N-*Et:* [4789-07-5]
$C_7H_{13}NO$ 127.186
Bp_{12} 109°.

N-*Et; hydrochloride:*
Hygroscopic needles (EtOH/Et_2O). Mp 108°.

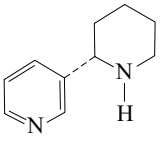
N-*Benzyl:* [4783-65-7]
$C_{12}H_{15}NO$ 189.257
Liq. Bp_4 156°.

N-*Hydroxy:*
$C_5H_9NO_2$ 115.132
Mp 44-45°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 791D; 792A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1292C; 1293A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 790A (*ir*)
Fischer, E. *et al., Ber.*, 1909, **42**, 4878 (*synth*)
Fischer, E. *et al., Annalen*, 1913, **398**, 96 (*synth, N-Me*)
Donaruma, L.G. *et al., J.O.C.*, 1956, **21**, 965 (*synth*)
Smeykal, K. *et al., J. Prakt. Chem.*, 1965, **30**, 126 (*synth*)
Sheehan, J.C. *et al., J.O.C.*, 1974, **39**, 2264 (*synth*)
Williamson, K.L. *et al., J.A.C.S.*, 1976, **98**, 5082 (*synth*)
Kribovian, S.E. *et al., Spectrochim. Acta A*, 1976, **32**, 1447 (*ir*)
Rae, I.D. *et al., Aust. J. Chem.*, 1979, **32**, 567 (*cmr*)
Schmitz, F.J. *et al., J.O.C.*, 1983, **48**, 3941-3945 (*isol*)
Neset, S.M. *et al., Acta Chem. Scand.*, 1993, **47**, 1141 (*N-hydroxy*)
Kehraus, S. *et al., J. Med. Chem.*, 2004, **47**, 2243-2255 (*isol*)
de Filippis, A. *et al., Synthesis*, 2004, 2930-2933 (*N-benzoyl, N-4-methylbenzenesulfonyl, N-benzyl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PIU000

3-(2-Piperidinyl)pyridine, 9CI P-434

2-(3-Pyridinyl)piperidine. ***Anabasine, JMAF.*** *Nicotimine. Neonicotine*
[40774-73-0]



(*S*)–*form*

$C_{10}H_{14}N_2$ 162.234
The name neonicotine refers primarily to the racemate.

(*R*)-*form* [34366-21-7]
Isol. from *Malacocarpus crithmifolius*.
Oil. Bp_{15} 145-150°. $[\alpha]_D^{20}$ +10.1 (neat). n_D^{20} 1.5412. Clearly of low opt. purity.

(*S*)-*form* [494-52-0]
Alkaloid from *Anabasis aphylla, Nicotiana tabacum*, many other *Nicotiana* spp. (Chenopodiaceae, Solanaceae) and many other spp. in several families. Also in marine ribbon worms and a component of ant venoms. Insecticide. Now superseded. Sol. H_2O.
Mp 25-30°. Bp 276° Bp_2 104-105°. $[\alpha]_D^{24}$ -79.2 (c, 0.5 in MeOH) (synthetic). $[\alpha]_D^{24}$ -41.5 (c, 1.0 in C_6H_6). pK_{a1} 11; pK_{a2} 3.21 (30°).
▶ Exp. reprod. effects and teratogen. LD_{50} (gpg, scu) 22 mg/kg. BV4375000

Dipicrate:
Mp 205°.

N-*Ac:* [3350-86-5]
$C_{12}H_{16}N_2O$ 204.271
Used as 0.5*M* aq. soln. for extraction-photometric detn. of Ti. Cryst. Sol. EtOH; sl. sol. H_2O.

N-*Me:* **N-*Methylanabasine***
[24380-92-5]
$C_{11}H_{16}N_2$ 176.261
Occurs in traces in crude nicotine and in *Anabasis aphylla*. Oil. Bp_{12} 127-128°. $[\alpha]_D^{15}$ -85.1.

N-*Me, picrate:*
Cryst. (EtOH). Mp 287-288° dec.

Tetrahydro: ***Tetrahydroanabasine***
[64191-30-6]
$C_{10}H_{18}N_2$ 166.266
Alkaloid from *Adenocarpus complicatus* subsp. *aureus* (Leguminosae). No details. Struct. not fully descr.

(±)-*form* [13078-04-1]
Alkaloid from *Duboisia myoporoides, Nicotiana glauca* and other spp. (Solanaceae). Bp_{775} 280-282° Bp 106-108°.

Dipicrate:
Mp 213-214°.

N-*Me:* [2055-12-1]
$Bp_{0.4}$ 62°.

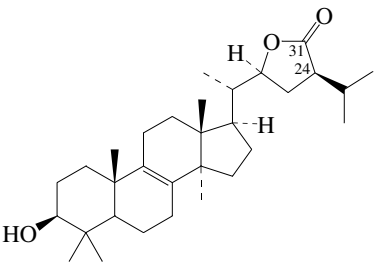
N-*Me, dipicrate:*
Yellow needles (EtOH). Mp 237-239°.

[15251-47-5]

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 295A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1537D (*ir*)
Orechoff, A. *et al., Ber.*, 1931, **64**, 266-274; 1932, **65**, 232-234 (*isol*)
Späth, E. *et al., Ber.*, 1937, **70**, 70-72 (*resoln*)
Otroshchenko, O.S. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1954, **24**, 1847-1849; *Zh. Obshch. Khim.*, 1954, **24**, 1884-1886 (*N-Ac, synth*)
Linnell, R.H. *et al., J.A.C.S.*, 1954, 1391-1393 (*uv*)
Lukeš, R. *et al., Coll. Czech. Chem. Comm.*, 1962, **27**, 751-756 (*config*)
Talipov, S.T. *et al., Zh. Anal. Khim.*, 1963, **18**, 178-181; *J. Anal. Chem. USSR (Engl. Transl.)*, 1963, **18**, 161-164 (*N-Ac, use*)
Duffield, A.M. *et al., J.A.C.S.*, 1965, **87**, 2926-2932 (*ms*)
Zharekeev, V.Kh. *et al., Khim. Prir. Soedin.*, 1971, **7**, 538-539; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 524 (*R-form, isol*)
Aslanov, Kh.A. *et al., Khim. Prir. Soedin.*, 1972, **8**, 324-328; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 319-321 (*isol, manuf*)
Testa, B. *et al., Mol. Pharmacol.*, 1973, **9**, 10-16 (*cd*)
Fitch, W.L. *et al., J.O.C.*, 1974, **39**, 2974-2979 (*S-form, isol*)
Leete, E. *et al., Chem. Comm.*, 1975, 9-10 (*biosynth*)
Nehme, M. *et al., An. Quim.*, 1977, **73**, 307-308; *CA*, **87**, 114689h (*Tetrahydroanabasine*)
Alberici, G.F. *et al., Tet. Lett.*, 1983, **24**, 1937-1940 (*synth*)
Strunz, G.M. *et al., Alkaloids (N.Y.)*, 1985, **26**, 89-183 (*rev*)
Pfrengle, W. *et al., J.O.C.*, 1989, **54**, 4261-4263 (*S-form, synth*)
Pesticide Manual, 9th edn., 1991, No. 380 (*anabasine*)
Hattori, K. *et al., Tetrahedron*, 1993, **49**, 1749-1760 (*S-form, synth*)
Deo, N.M. *et al., Tet. Lett.*, 1996, **37**, 1137-1140 (*synth*)
Yang, C.-M. *et al., Can. J. Chem.*, 1997, **75**, 616-620 (*synth, ir, pmr, cmr, ms*)
Felpin, F.-X. *et al., J.O.C.*, 2001, **66**, 6305-6312 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 0th edn., J. Wiley*, 2000, AON875

Pisolactone P-435

[87164-33-8]



$C_{31}H_{50}O_3$ 470.734
Constit. of fungus *Pisolithus tinctorius*. Prisms (MeOH). Mp 279-280°. $[\alpha]_D^{28}$ +60 (c, 1 in $CHCl_3$).

3-Ketone: ***3-Oxopisolactone***
[119539-75-2]
$C_{31}H_{48}O_3$ 468.718
Metab. of *Pisolithus tinctorius*. Cryst. (MeOH). Mp 248-250°. $[\alpha]_D$ +79 (c, 1.4 in $CHCl_3$).

*31*S-*Alcohol:*
$C_{31}H_{52}O_3$ 472.75
Constit. of *Pisolithus tinctorius*.

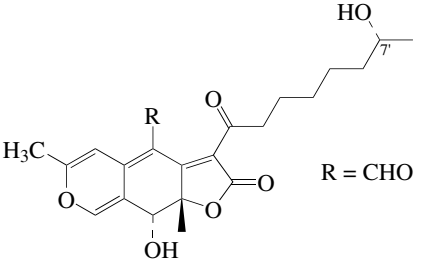
*24-Epimer, 31*R-*alcohol:*
$C_{31}H_{52}O_3$ 472.75
Constit. of *Pisolithus tinctorius*.

22,24-Diepimer: ***22,24-Diepipisolactone***
[362526-07-6]
$C_{31}H_{50}O_3$ 470.734
Isol. from the red alga *Hypnea cerricornis*. Needles (MeOH). Mp 278-280°. $[\alpha]_D^{26}$ +60 ($CHCl_3$).

Lobo, A.M. *et al., Tet. Lett.*, 1983, **24**, 2205-2208 (*isol, cryst struct*)
Lobo, A.M. *et al., Phytochemistry*, 1988, **27**, 3569-3574 (*3-Oxopisolactone*)
Fujimoto, H. *et al., Chem. Pharm. Bull.*, 1994, **42**, 694-697 (*31-alcohols*)
Baumert, A. *et al., Phytochemistry*, 1997, **45**, 499-504 (*isol, pmr, cmr*)
Xu, X.-H. *et al., Chin. J. Chem.*, 2001, **19**, 702-704 (*22,24-Diepipisolactone*)

Pitholide A P-436

[200936-84-1]



$C_{22}H_{26}O_7$ 402.443
Related to Monascorubrin. Prod. by the fungus *Pithomyces* sp. isol. from a marine tunicate (*Oxycorynia fascicularis*). Red oil. $[\alpha]_D$ -84 (c, 0.6 in MeOH).

7′-Deoxy: ***Pitholide B***
[200931-52-8]
$C_{22}H_{26}O_6$ 386.444
Prod. by *Pithomyces* sp. from *Oxycorynia fascicularis*. Red oil. $[\alpha]_D$ -158 (c, 0.8 in MeOH).

Wang, G.-Y.-S. *et al., Tet. Lett.*, 1997, **38**, 8449-8452 (*isol, pmr, cmr*)

Pitholide C P-437

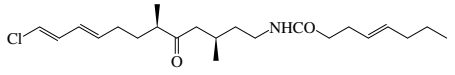
[200936-85-2]
As Pitholide A, P-436 with
R = H
$C_{21}H_{26}O_6$ 374.433

Related to Ankaflavin. Prod. by the fungus *Pithomyces* sp. isol. from a marine tunicate (*Oxycorynia fascularis*). Red oil.

7′-Deoxy: ***Pitholide D***
[200936-86-3]
$C_{21}H_{26}O_5$ 358.433
Prod. by *Pithomyces* sp. from *Oxycorynia fascicularis.* Red oil. $[\alpha]_D$ -248 (c, 0.5 in MeOH).
Wang, G. Y. S. *et al., Tet. Lett.*, 1997, **38**, 8449-8452 (*isol, pmr, cmr*)

Pitiamide A P-438

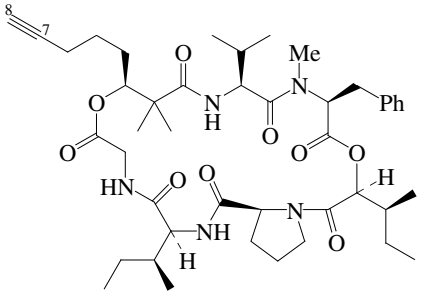
[198416-38-5]



Absolute Configuration

$C_{22}H_{36}ClNO_2$ 381.985
Isol. from a mixt. of *Lyngbya majuscula* and *Microcoleus* sp. growing on coral.
$[\alpha]_D$ -10.3 (c, 3 in $CHCl_3$). λ_{max} 223 (MeOH).
Nagle, D.G. *et al., Tet. Lett.*, 1997, **38**, 6969-6972 (*isol, uv, ir, pmr, cmr*)
Ribe, S. *et al., J.A.C.S.*, 2000, **122**, 4608-4617 (*synth, cd, ir, pmr, abs config*)

Pitipeptolide A P-439

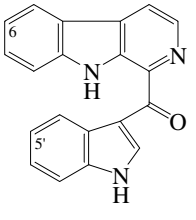


$C_{44}H_{65}N_5O_9$ 808.026
Isol. from *Lyngbya majuscula*. Shows moderate antimycobacterial activity and stimulates elastase activity. Amorph. solid. $[\alpha]_D^{25}$ -109 (c, 1 in MeOH). λ_{max} 202 (log ϵ 4.48) (MeOH).

7,8-Dihydro: ***Pitipeptolide B***
$C_{44}H_{67}N_5O_9$ 810.041
Isol. from *Lyngbya majuscula.* Amorph. solid. $[\alpha]_D^{25}$ -109 (c, 1 in MeOH). λ_{max} 202 (log ϵ 4.48) (MeOH).
Luesch, H. *et al., J. Nat. Prod.*, 2001, **64**, 304-307

Pityriacitrin P-440

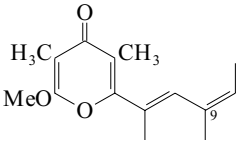
*1-(1*H*-Indole-3-carbonyl)-9*H*-pyrido[3,4-*b*]indole. 1-(1*H*-Indole-3-carbonyl)-β-carboline*
[244295-64-5]



$C_{20}H_{13}N_3O$ 311.342
Prod. by the yeast *Malassezia furfur* and the marine bacterium *Paracoccus* sp. Uv protectant.
Mp 227-230°. λ_{max} 193 (log ϵ 4.24); 216 (log ϵ 4.47); 262 (sh) (log ϵ 3.91); 281 (sh) (log ϵ 3.95); 289 (log ϵ 3.99); 310 (log ϵ 3.86); 389 (log ϵ 3.88) (MeCN).

*5′,6-Dihydroxy: 1-(5-Hydroxy-1*H*-indole-3-carbonyl)-9*H*-pyrido[3,4-*b*]indol-6-ol.* ***Hyrtiosulawesine***
[452067-33-3]
$C_{20}H_{13}N_3O_3$ 343.341
Isol. from the sponge *Hyrtios erectus.* λ_{max} 217 (ϵ 145000); 260 (sh); 305 (ϵ 53000); 325 (sh); 403 (ϵ 22700) (MeOH).
Japan. Pat., 1999, 99 269 175; *CA*, **131**, 242087z (*isol, activity*)
Mayser, P. *et al., Arch. Dermatol. Res.*, 2002, **294**, 131-134 (*isol, ir, pmr, cmr, ms*)
Salmoun, M. *et al., J. Nat. Prod.*, 2002, **65**, 1173-1176 (*Hyrtiosulawesine*)

Placidene B P-441

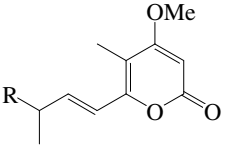


$C_{15}H_{20}O_3$ 248.321
Constit. of *Placida dendritica*. Ichthyotoxic. λ_{max} 260 (ϵ 11200) (base in MeOH) (Derep). λ_{max} 262 (ϵ 9400) (acidic MeOH) (Derep). λ_{max} 260 (ϵ 11200) (MeOH) (Berdy).

*9*E*-Isomer:* ***Isoplacidene B***
[142878-36-2]
$C_{15}H_{20}O_3$ 248.321
Constit. of *Placida dendritica*. Ichthyotoxic. λ_{max} 251 (ϵ 14000) (MeOH) (Berdy).
Vardaro, R.R. *et al., Tet. Lett.*, 1992, **33**, 2875-2878 (*isol, pmr, cmr*)
Liang, G. *et al., Org. Lett.*, 2005, **7**, 819-821 (*synth*)

Placidene C P-442

*4-Methoxy-5-methyl-6-(3-methyl-1-pentenyl)-2*H*-pyran-2-one*



R = CH_2CH_3

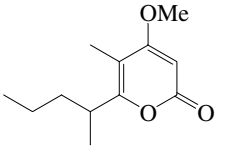
$C_{13}H_{18}O_3$ 222.283
Isol. from *Placida dendritica*. Amorph. solid. $[\alpha]_D$ +22.8 (c, 0.01 in MeOH). λ_{max} 226 (ϵ 21200); 319 (ϵ 6400) (MeOH).
Cutignano, A. *et al., J. Nat. Prod.*, 2003, **66**, 1399-1401 (*isol, pmr, cmr*)

Placidene D P-443

*4-Methoxy-5-methyl-6-(3-methyl-1-hexenyl)-2*H*-pyran-2-one*
As Placidene C, P-442 with
R = $CH_2CH_2CH_3$
$C_{14}H_{20}O_3$ 236.31
Isol. from *Placida dendritica*. Amorph. solid. $[\alpha]_D$ +30 (c, 0.01 in MeOH). λ_{max} 226 (ϵ 15900); 319 (ϵ 4500) (MeOH).
Cutignano, A. *et al., J. Nat. Prod.*, 2003, **66**, 1399-1401 (*isol, pmr, cmr*)

Placidene E P-444

*4-Methoxy-5-methyl-6-(1-methylbutyl)-2*H*-pyran-2-one*



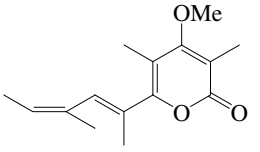
$C_{12}H_{18}O_3$ 210.272

Isol. from *Placida dendritica*. Amorph. solid. $[\alpha]_D$ -56.3 (c, 0.02 in MeOH). λ_{max} 286 (ϵ 4200) (MeOH).

Cutignano, A. *et al., J. Nat. Prod.*, 2003, **66**, 1399-1401 (*isol, pmr, cmr*)

Placidene F **P-445**

*6-(1,3-Dimethyl-1,3-pentadienyl)-4-methoxy-3,5-dimethyl-2*H*-pyran-2-one*



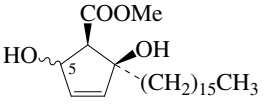
$C_{15}H_{20}O_3$ 248.321

Isol. from *Placida dendritica*. Amorph. solid. λ_{max} 203 (ϵ 9200); 230 (ϵ 5000); 312 (ϵ 5600) (MeOH).

Cutignano, A. *et al., J. Nat. Prod.*, 2003, **66**, 1399-1401 (*isol, pmr, cmr*)

Plakevulin A **P-446**

Methyl 2-hexadecyl-2,5-dihydroxy-3-cyclopentene-1-carboxylate



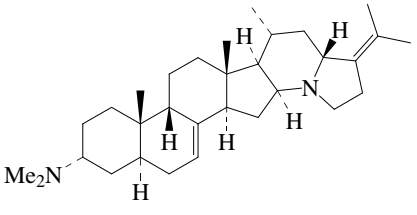
$C_{23}H_{42}O_4$ 382.582

Struct. revised in 2004. Isol. as a mixt. of C-5 epimers. Related to Untenone A, U-49. Isol. from a sponge *Plakortis* sp. Inhibitor of DNA polymerases. $[\alpha]_D^{22}$ -25 (c, 0.1 in $CHCl_3$).

Saito, M. *et al., Tet. Lett.*, 2004, **45**, 8069-8071 (*synth, pmr, cmr, struct*)

Plakinamine I† **P-447**

[640734-86-7]

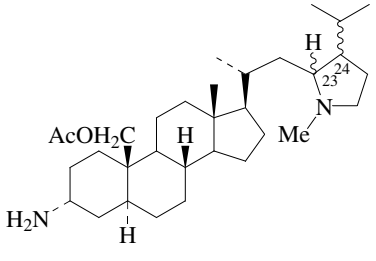


$C_{31}H_{50}N_2$ 450.749

Alkaloid from the sponge *Corticium niger*. Cytotoxic. Oil (as dihydrochloride). $[\alpha]_D$ +45.2 (c, 0.32 in MeOH) (dihydrochloride). λ_{max} 202 (ϵ 49800); 247 (ϵ 1500) (MeOH) (dihydrochloride).

Ridley, C.P. *et al., J. Nat. Prod.*, 2003, **66**, 1536-1539 (*isol, pmr, cmr*)

Plakinamine I† **P-448**



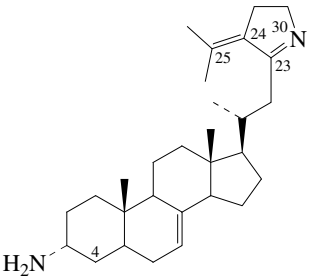
$C_{32}H_{56}N_2O_2$ 500.807

Alkaloid from the sponge *Corticium* sp. Gum. $[\alpha]_D^{25}$ -18.3 (c, 0.03 in MeOH). Rel. config. of C-23/C-24 is *trans*-.

Zampella, A. *et al., Eur. J. Org. Chem.*, 2005, 4359-4363 (*isol, pmr, cmr*)

Plakinamine A **P-449**

[93474-13-6]



$C_{29}H_{46}N_2$ 422.696

Alkaloid from a sponge *Plakina* sp. Active against *Staphylococcus aureus* and *Candida albicans*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 120-130° dec. $[\alpha]_D$ +16 (c, 1.02 in $CHCl_3$). First report of a steroidal alkaloid from a marine organism. Acetylation causes rearrangement and ring opening of the pyrroline system. λ_{max} 246 (ϵ 7100) (MeOH) (Derep).

24,25-Dihydro: ***24,25-Dihydroplakinamine A***
[224576-02-7]
$C_{29}H_{48}N_2$ 424.712
Alkaloid from a *Corticium* sp. Cytotoxic agent. $[\alpha]_D$ +7.4 (c, 0.01 in $CHCl_3$/MeOH). C-24 config. not determined.

23ξ,24ξ,25,30-Tetrahydro: ***Tetrahydroplakinamine A***
[454476-89-2]
$C_{29}H_{50}N_2$ 426.727
Alkaloid from a *Corticium* sp. Gum. $[\alpha]_D^{22}$ +23.2 (c, 0.19 in MeOH).

23ξ,24ξ,25,30-Tetrahydro, N^{30}*-Me:* [224576-05-0]
$C_{30}H_{52}N_2$ 440.754
Alkaloid from a *Corticium* sp. Cytotoxic agent. $[\alpha]_D$ +23 (c, 0.02 in $CHCl_3$/MeOH).

4β-Acetoxy, 23ξ,30-dihydro, N^3*-Me:* ***Plakinamine K***
[64734-88-9]
$C_{32}H_{52}N_2O_2$ 496.775
Alkaloid from the sponge *Corticium niger*. Cytotoxic. Oil. $[\alpha]_D$ +38.4 (c, 0.25 in MeOH). λ_{max} 203 (ϵ 59200); 246 (ϵ 1200) (MeOH).

4β-Acetoxy, 23ξ,24ξ,25,30-tetrahydro, N^3*-Me:* ***Dihydroplakinamine K***
[640734-89-0]
$C_{32}H_{54}N_2O_2$ 498.791
Alkaloid from the sponge *Corticium niger*. Cytotoxic. Oil (as dihydrochloride). $[\alpha]_D$ +5.7 (c, 0.05 in MeOH) (dihydrochloride). λ_{max} 203 (ϵ 54800); 247 (ϵ 1350) (MeOH) (dihydrochloride).

3-Epimer, 4-oxo, N^3,N^3*-di-Me:* ***Plakinamine F***
[383859-60-7]
$C_{31}H_{48}N_2O$ 464.733
Alkaloid from an undescribed sponge of the genus *Corticium*. Gum. $[\alpha]_D^{25}$ +8.4 (c, 0.1 in MeOH). λ_{max} 245 (log ϵ 3.97) (MeOH).

3-Epimer, 4β-hydroxy, N^3*-Ac:* ***Lokysterolamine B***
[159934-15-3]
$C_{31}H_{48}N_2O_2$ 480.732
Alkaloid from the sponge *Corticium* sp. Immunosuppressive agent. Semicryst. solid. $[\alpha]_D^{26}$ -3.1 (c, 1.6 in $CHCl_3$). λ_{max} 247 (ϵ 8750) (MeOH) (Berdy).

3-Epimer, 4β-hydroxy, N^3,N^3*-di-Me:* ***Lokysterolamine A***
[159934-14-2]
$C_{31}H_{50}N_2O$ 466.749
Alkaloid from an undescribed sponge of the genus *Corticium*. Immunosuppressant. Oil. $[\alpha]_D^{25}$ +17.7 (c, 0.1 in MeOH). λ_{max} 247 (log ϵ 3.91) (MeOH).

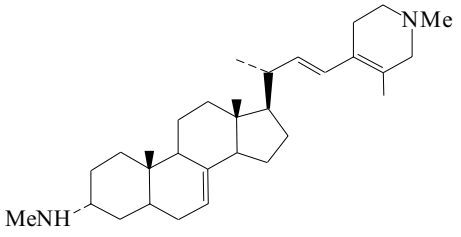
3-Epimer, 4β-hydroxy, N^3,N^3*-di-Me,* N^{30}*-oxide:* ***Plakinamine E***. *Lokysterolamine A* N^{30}*-oxide*
[383859-59-4]
$C_{31}H_{50}N_2O_2$ 482.748

Alkaloid from an undescribed sponge of the genus *Corticium*. Gum. $[\alpha]_D^{25}$ +9.3 (c, 0.2 in MeOH). λ_{max} 249 (log ϵ 3.85); 279 (sh) (log ϵ 3.56) (MeOH).

Rosser, R.M. *et al., J.O.C.*, 1984, **49**, 5157-5160 (*isol, ir, uv, pmr, cmr, struct*)
Jurek, J. *et al., J. Nat. Prod.*, 1994, **57**, 1004-1007 (*Lokysterolamines*)
De Marino, S. *et al., Eur. J. Org. Chem.*, 1999, 697-701 (*derivs*)
Lee, H.-S. *et al., J. Nat. Prod.*, 2001, **64**, 1474-1476 (*Plakinamine E, Plakinamine F*)
Borbone, N. *et al., J. Nat. Prod.*, 2002, **65**, 1206-1209 (*Tetrahydroplakinamine A*)
Ridley, C.P. *et al., J. Nat. Prod.*, 2003, **66**, 1536-1539 (*Plakinamine K, Dihydroplakinamine K*)

Plakinamine B P-450

[93474-14-7]



$C_{31}H_{50}N_2$ 450.749
Alkaloid from a marine sponge *Plakina* sp. Active against *Staphylococcus aureus* and *Candida albicans*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 180-200° dec. (as hydrochloride). $[\alpha]_D$ +29 (c, 1.19 in MeOH). λ_{max} 241 (ϵ 2700) (MeOH) (Derep).

4α-Hydroxy, N^3*-de-Me:* ***4α-Hydroxy-*** $\mathbf{N^3}$***-demethylplakinamine B***
$C_{30}H_{48}N_2O$ 452.722
Alkaloid from the sponge *Corticium* sp. Gum. $[\alpha]_D^{22}$ +6.7 (c, 0.09 in MeOH). λ_{max} 241 (log ϵ 3.8) (MeOH).

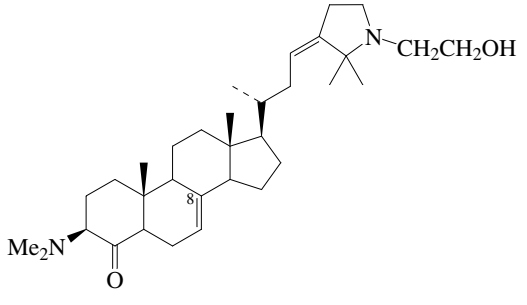
3-Epimer, 4-oxo, N^3*-Me:* $\mathbf{N^3}$***-Methyl-4-oxo-3-epiplakinamine B***
$C_{32}H_{50}N_2O$ 478.76
Alkaloid from the sponge *Corticium* sp. Cytotoxic agent. $[\alpha]_D$ +35.4 (c, 0.01 in $CHCl_3$/MeOH).

3-Epimer, 4-oxo, N^{27}*-de-Me,* N^3*-Me:* ***Plakinamine H***
$C_{31}H_{48}N_2O$ 464.733
Alkaloid from a *Corticium* sp. Gum. $[\alpha]_D^{22}$ +29 (c, 0.1 in MeOH). λ_{max} 250 (log ϵ 3.77) (MeOH).

Rosser, R.M. *et al., J.O.C.*, 1984, **49**, 5157-5160 (*isol, ir, uv, pmr, cmr, struct*)
De Marino, S. *et al., Eur. J. Org. Chem.*, 1999, 697-701 (*deriv, pmr, cmr*)
Borbone, N. *et al., J. Nat. Prod.*, 2002, **65**, 1206-1209 (*4-Hydroxy-*N^3*-demethylplakinamine B, Plakinamine H*)

Plakinamine C P-451

[224575-95-5]



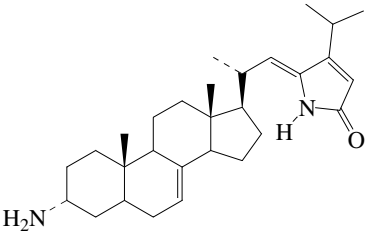
$C_{33}H_{54}N_2O_2$ 510.802
Alkaloid from the sponge *Corticium* sp. Cytotoxic agent. $[\alpha]_D$ +29.4 (c, 0.02 in $CHCl_3$/MeOH).

Δ^8*-Isomer:* ***Plakinamine D***
[224575-99-9]
$C_{33}H_{54}N_2O_2$ 510.802
Alkaloid from *Corticium* sp. Cytotoxic agent. $[\alpha]_D$ +25.2 (c, 0.01 in $CHCl_3$/MeOH).

De Marino, S. *et al., Eur. J. Org. Chem.*, 1999, 697-701 (*isol, pmr, cmr*)

Plakinamine G P-452

[454476-87-0]

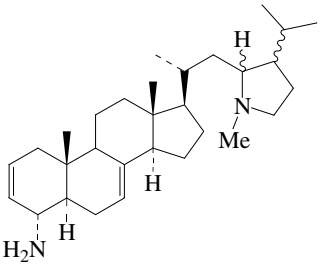


$C_{29}H_{44}N_2O$ 436.679
Alkaloid from the sponge *Corticium* sp. Gum. $[\alpha]_D^{22}$ -24.4 (c, 0.09 in MeOH). λ_{max} 276 (log ϵ 4.11) (MeOH).

Borbone, N. *et al., J. Nat. Prod.*, 2002, **65**, 1206-1209 (*isol, pmr, cmr*)

Plakinamine J P-453

[640734-87-8]

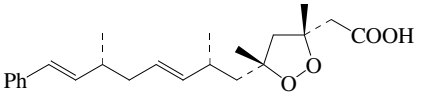


$C_{30}H_{50}N_2$ 438.738
Alkaloid from the sponge *Corticium niger*. Cytotoxic. Oil (as dihydrochloride). $[\alpha]_D$ +25 (c, 0.1 in MeOH) (dihydrochloride). λ_{max} 203 (ϵ 56800); 249 (ϵ 2030) (MeOH) (dihydrochloride).

Ridley, C.P. *et al., J. Nat. Prod.*, 2003, **66**, 1536-1539 (*isol, pmr, cmr*)

Plakinic acid A P-454

[87803-05-2]



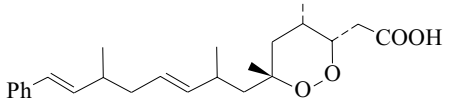
Probable Absolute Configuration

$C_{23}H_{32}O_4$ 372.503
Isol. from a Caribbean sponge, family Plakinidae. Antifungal agent. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{21}$ -57.8 (as Me ester). λ_{max} 246 (ϵ 20000); 282 (sh); 291 (sh) (95% EtOH) (Derep).

Phillipson, D.W. *et al., J.A.C.S.*, 1983, **105**, 7735-7736 (*isol, ir, uv, pmr, ms*)
Bloodworth, A.J. *et al., Tet. Lett.*, 1996, **37**, 1885-1888 (*synth*)
Dai, P. *et al., J.O.C.*, 2006, **71**, 2283-2292 (*synth, abs config*)

Plakinic acid B P-455

[87803-07-4]



$C_{24}H_{34}O_4$ 386.53

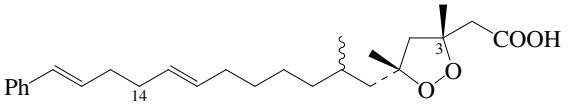
Isol. from a Caribbean sponge, family Plakinidae. Antifungal. Sol. MeOH, C_6H_6; poorly sol. H_2O. λ_{max} 246 (ϵ 20000); 282 (sh); 291 (sh) (95% EtOH) (Derep).

Me ester: $[\alpha]_D^{21}$ -186.

Phillipson, D. *et al., J.A.C.S.*, 1983, **105**, 7735 (*isol, ir, uv, ms, pmr*)

Plakinic acid C P-456

[136707-69-2]



$C_{26}H_{38}O_4$ 414.584
Constit. of a *Plakortis* sponge.
$[\alpha]_D^{27}$ +31.71 (c, 0.098 in $CHCl_3$) (as Me ester). λ_{max} 204; 249 (MeOH) (Berdy).

*14,15-Didehydro(*E-*), 12,13-dihydro:* [473256-23-4]
$C_{26}H_{38}O_4$ 414.584
Isol. from *Plakinastrella onkodes*. Oil.

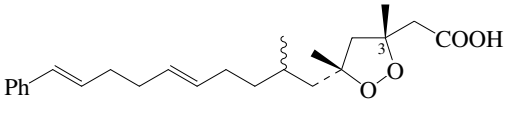
3-Epimer: ***Epiplakinic acid C***
[136780-75-1]
$C_{26}H_{38}O_4$ 414.584
Constit. of a *Plakortis* sponge.
$[\alpha]_D^{26}$ -22.66 (c, 0.11 in $CHCl_3$) (as Me ester). λ_{max} 205; 249 (MeOH) (Berdy).

*3-Epimer, 14,15-didehydro(*E-*), 12,13-dihydro:* [473256-22-3]
$C_{26}H_{38}O_4$ 414.584
Isol. from *Plakinastrella onkodes*. Oil.

Davidson, B.S. *et al., J.O.C.*, 1991, **56**, 6722 (*isol, pmr, cmr*)
Bloodworth, A.J. *et al., Tet. Lett.*, 1996, **37**, 1885 (*synth*)
Chen, Y. *et al., J. Nat. Prod.*, 2002, **65**, 1509-1512 (*Plakinastrella derivs*)

Plakinic acid D P-457

[136780-74-0]

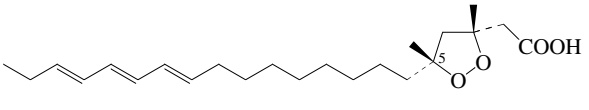


$C_{24}H_{34}O_4$ 386.53
Constit. of a *Plakortis* sponge.
$[\alpha]_D^{27}$ +40.53 (c, 0.12 in $CHCl_3$) (as Me ester). λ_{max} 204; 250 (MeOH) (Berdy).

3-Epimer: ***Epiplakinic acid D***
[136707-70-5]
$C_{24}H_{34}O_4$ 386.53
Constit. of a *Plakortis* sponge.
$[\alpha]_D^{26}$ -16.73 (c, 0.13 in $CHCl_3$) (as Me ester). λ_{max} 204; 250 (MeOH) (Berdy).

Davidson, B.S. *et al., J.O.C.*, 1991, **56**, 6722 (*isol, pmr, cmr*)
Bloodworth, A.J. *et al., Tet. Lett.*, 1996, **37**, 1885 (*synth*)

Plakinic acid F P-458



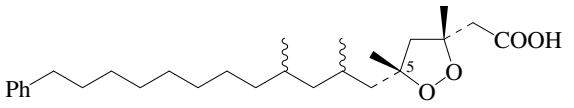
$C_{23}H_{38}O_4$ 378.551
Isol. from the sponge *Plakinastrella* sp. Antifungal agent. Oil.

5-Epimer: ***Epiplakinic acid F***
$C_{23}H_{38}O_4$ 378.551
Isol. from *Plakinastrella* sp. Antifungal agent.

Chen, Y. *et al., J. Nat. Prod.*, 2001, **64**, 262-264

Plakinic acid G P-459

5-(2,4-Dimethyl-12-phenyldodecyl)-3,5-dimethyl-1,2-dioxolane-3-acetic acid. Epiplakinic acid H



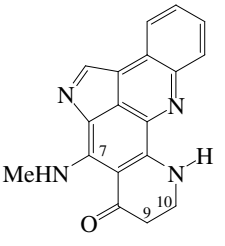
$C_{27}H_{44}O_4$ 432.642
Isol. from the sponge *Plakortis nigra*. Oil. $[\alpha]_D$ +33 (c, 0.07 in MeOH). λ_{max} 254 (ϵ 269); 259 (ϵ 270); 268 (ϵ 212) (MeOH).

5-Epimer: ***Epiplakinic acid G***
Isol. from the sponge *Plakortis nigra*.
Oil. $[\alpha]_D$ -17.2 (c, 0.3 in MeOH). λ_{max} 255 (ϵ 253); 260 (ϵ 276); 269 (ϵ 218) (MeOH).

Sandler, J.S. *et al., J. Nat. Prod.*, 2002, **65**, 1258-1261 (*isol, pmr, cmr*)

Plakinidine A P-460

*10,11-Dihydro-7-(methylamino)benzo[*b*]pyrrolo[4,3,2-*de*][1,10]-phenanthrolin-8(9*H*)-one, 9CI*
[124512-44-3]



$C_{18}H_{14}N_4O$ 302.335
First reported natural pyrrolo[2,3,4-*kl*]acridines. Alkaloid from the sponge *Plakortis* sp. Exhibits *in vitro* activity against the parasite *Hippostrongylus brasiliensis* and shows weak activity against reverse transcriptase. Flat purple plates ($CHCl_3$). Fairly sol. AcOH; poorly sol. MeOH, hexane.
Mp 248-250°. λ_{max} 226 (ϵ 15800); 247 (ϵ 20400); 279 (ϵ 11600); 336 (ϵ 22700); 378 (ϵ 6200); 537 (ϵ 3600) (MeOH) (Derep).

N^7-*Me:* ***Plakinidine B***
[124512-45-4]
$C_{19}H_{16}N_4O$ 316.362
Alkaloid from the sponge *Plakortis* sp. Exhibits *in vitro* activity against the parasite *Nocardia brasiliensis*. Reverse transcriptase inhibitor. Purple oil. Fairly sol. AcOH; poorly sol. MeOH, hexane. λ_{max} 226 (ϵ 13800); 248 (ϵ 17500); 283 (ϵ 9100); 347 (ϵ 19700); 383 (ϵ 4700); 544 (ϵ 4000) (MeOH) (Derep).

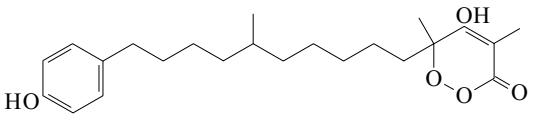
9,10-Didehydro: ***Plakinidine C***
[129744-15-6]
$C_{18}H_{12}N_4O$ 300.319
Alkaloid from the sponge *Plakortis* sp. Cytotoxic, anthelmintic. Reverse transcriptase inhibitor. λ_{max} 244 (ϵ 42800); 254 (ϵ 39100); 323 (ϵ 25200); 370 (ϵ 10900); 508 (ϵ 13800); 541 (ϵ 11400) (MeOH) (Derep).

N^7-*De-Me:* ***Plakinidine D***
[197234-19-8]
$C_{17}H_{12}N_4O$ 288.308
Alkaloid from *Didemnum rubeum* and an unidentified *Didemnum* sp. Dark red solid. λ_{max} 250 (ϵ 4770); 282 (ϵ 3500); 328 (ϵ 2980); 388 (ϵ 1940); 436 (ϵ 820); 514 (ϵ 926) ($CHCl_3$/MeOH).

Inman, W.D. *et al., J.A.C.S.*, 1990, **112**, 1 (*isol, pmr, cmr, ms, struct*)
West, R.R. *et al., Tet. Lett.*, 1990, **31**, 3271 (*isol, uv, ir, pmr, cmr, struct*)
Smith, C.J. *et al., J. Nat. Prod.*, 1997, **60**, 1048-1050 (*Plakinidine D*)
Ford, P.W. *et al., J. Nat. Prod.*, 1997, **60**, 1051-1053 (*Plakinidine D*)

Plakinidone P-461

[137319-23-4]

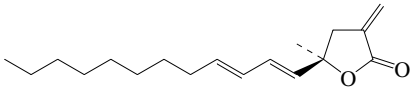


$C_{23}H_{34}O_5$ 390.519
Metab. of *Plakortis angulospiculatus*. Oil. $[\alpha]_D$ +7.9 (c, 0.61 in MeOH). λ_{max} 224 (ϵ 6740); 279 (ϵ 1710) (MeOH) (Derep).

Kushlan, D.M. *et al., J. Nat. Prod.*, 1991, **54**, 1451 (*isol, pmr, cmr*)

Plakolide A P-462

*5-(1,3-Dodecadienyl)dihydro-5-methyl-3-methylene-2(3*H*)-furanone*



Absolute Configuration

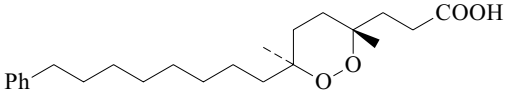
$C_{18}H_{28}O_2$ 276.418
Abs. config. revised in 2006.

(R)-form
Isol. from the sponge *Plakortis* sp. Inhibitor of inducible nitric oxide (iNOS) activity. Gum. $[\alpha]_D^{24}$ -41 (c, 1 in MeOH). λ_{max} 208 (log ϵ 4.36); 230 (log ϵ 4.47) (MeOH).

Gunasekera, S.P. *et al., J. Nat. Prod.*, 2004, **67**, 110-111 (*isol, cd, pmr, cmr*)
Matsuo, K. *et al., Heterocycles*, 2006, **68**, 1401-1407 (*synth, abs config*)

Plakoric acid P-463

3,6-Dimethyl-6-(8-phenyloctyl)-1,2-dioxane-3-propanoic acid, 9CI
[162559-03-7]

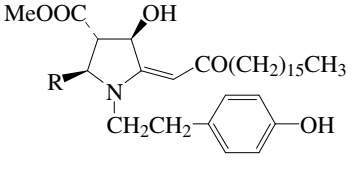


$C_{23}H_{36}O_4$ 376.535
Isol. from the sponge *Plakortis* sp. Brown waxy solid. $[\alpha]_D$ -18.7 (c, 1 in CH_2Cl_2).

Varoglu, M. *et al., J. Nat. Prod.*, 1995, **58**, 27 (*isol, pmr, cmr*)

Plakoridine A P-464

[155944-28-8]



Relative Configuration

R = -$CH_2CH_2CH_3$

$C_{35}H_{57}NO_5$ 571.839
Alkaloid from the Okinawan marine sponge *Plakortis* sp. Weakly cytotoxic against murine lymphoma L1210 cells *in vitro*. Oil. $[\alpha]_D^{19}$ -0.4 (c, 0.5 in $CHCl_3$). λ_{max} 317 (ϵ 22000) (MeOH) (Derep).

Takeuchi, S. *et al., J.O.C.*, 1994, **59**, 3712-3713 (*isol, uv, ir, pmr, cmr, ms, struct*)
Ma, D. *et al., Tet. Lett.*, 2000, **41**, 1947-1950 (*synth*)

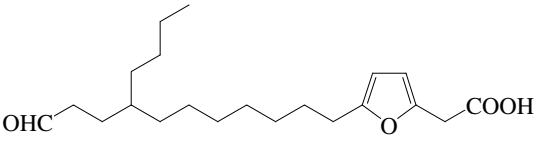
Plakoridine B P-465

[164415-61-6]
As Plakoridine A, P-464 with
R = -$(CH_2)_{14}CH_3$
$C_{47}H_{81}NO_5$ 740.161
Alkaloid from an Okinawan sponge *Plakortis* sp. Oil. λ_{max} 224 (ϵ 12200); 318 (ϵ 16000) (MeOH).

Takeuchi, S. *et al., Tetrahedron*, 1995, **51**, 5979-5986 (*isol, pmr, cmr*)

Plakorsin C P-466

5-(8-Butyl-11-oxoundecyl)-2-furanacetic acid

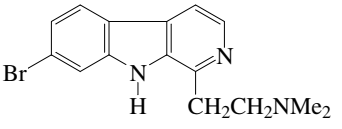


$C_{21}H_{34}O_4$ 350.497
Isol. from *Plakortis simplex*. Oil (as Me ester). $[\alpha]_D^{25}$ +25.8 (c, 0.5 in CH_2Cl_2) (Me ester). λ_{max} 219 (log ϵ 2.93); 282 (log ϵ 3.14) (MeOH) (Me ester).

Shen, Y.-C. *et al., J. Nat. Prod.*, 2001, **64**, 324-327

Plakortamine A P-467

*7-Bromo-*N,N*-dimethyl-9*H*-pyrido[3,4-*b*]indole-1-ethanamine. 7-Bromo-1-[2-(dimethylamino)ethyl]-β-carboline*
[467419-71-2]

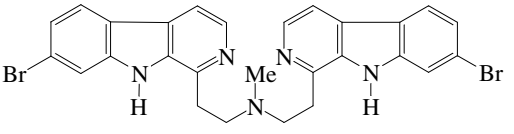


$C_{15}H_{16}BrN_3$ 318.216
Alkaloid from the sponge *Plakortis nigra*. Cytotoxic. Pale yellow oil. λ_{max} 243 (ϵ 20000); 295 (ϵ 11700) (MeOH).

Sandler, J.S. *et al., J. Nat. Prod.*, 2002, **65**, 1258-1261 (*isol, pmr, cmr*)

Plakortamine C P-468

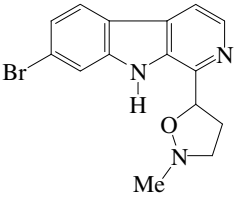
[467419-73-4]



$C_{27}H_{23}Br_2N_5$ 577.32
Alkaloid from the sponge *Plakortis nigra*. Cytotoxic. Pale yellow gum. λ_{max} 243 (ϵ 57400); 296 (ϵ 29000) (MeOH).

Sandler, J.S. *et al., J. Nat. Prod.*, 2002, **65**, 1258-1261 (*isol, pmr, cmr*)

Plakortamine D P-469

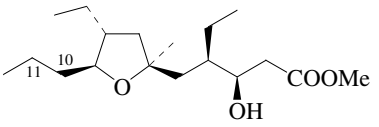


$C_{15}H_{14}BrN_3O$ 332.199

(ξ)-form [467419-74-5]
Alkaloid from the sponge *Plakortis nigra*. Cytotoxic agent. Pale yellow oil. $[\alpha]_D$ -2.1 (c, 0.6 in MeOH). λ_{max} 243 (ϵ 26600); 296 (ϵ 14700) (MeOH).

Sandler, J.S. *et al., J. Nat. Prod.*, 2002, **65**, 1258-1261 (*isol, pmr, cmr*)

Plakortether B P-470



Absolute Configuration

$C_{18}H_{34}O_4$ 314.464
Isol. from *Plakortis simplex*. Oil. $[\alpha]_D$ -13 (c, 0.12 in $CHCl_3$).

*10,11-Didehydro(*E-*):* ***Plakortether A***
$C_{18}H_{32}O_4$ 312.448
Isol. from *Plakortis simplex*. Oil. $[\alpha]_D^{25}$ +2 (c, 0.18 in $CHCl_3$).

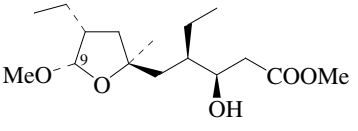
*10*R*-Chloro:* ***Plakortether C***
$C_{18}H_{33}ClO_4$ 348.909
Isol. from *Plakortis simplex*. Oil. $[\alpha]_D^{25}$ -3 (c, 0.14 in $CHCl_3$).

*10*S*-Hydroxy:* ***Plakortether E***
$C_{18}H_{34}O_5$ 330.464
Isol. from *Plakortis simplex*. Oil. $[\alpha]_D^{25}$ +40 (c, 0.02 in $CHCl_3$).

10-Oxo: ***Plakortether D***
$C_{18}H_{32}O_5$ 328.448
Isol. from *Plakortis simplex*. Oil. $[\alpha]_D^{25}$ +7 (c, 0.09 in $CHCl_3$).

Campagnuolo, C. *et al., Eur. J. Org. Chem.*, 2002, 61-69 (*isol, pmr, cmr, abs config*)

Plakortether F P-471



Absolute Configuration

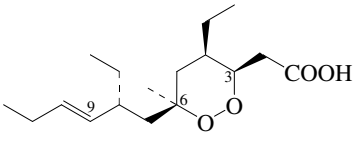
$C_{16}H_{30}O_5$ 302.41
Isol. from *Plakortis simplex*. Oil. $[\alpha]_D^{25}$ +40 (c, 0.02 in $CHCl_3$).

9-Epimer: ***Plakortether G***
$C_{16}H_{30}O_5$ 302.41
Isol. from *Plakortis simplex*. Oil. $[\alpha]_D^{25}$ -14 (c, 0.02 in $CHCl_3$).

Campagnuolo, C. *et al., Eur. J. Org. Chem.*, 2002, 61-69 (*isol, pmr, cmr, abs config*)

Plakortic acid† P-472

[87803-10-9]



Absolute Configuration

$C_{17}H_{30}O_4$ 298.422
Isol. from the sponge *Plakortis zyggompha*. Shows antibacterial and antifungal props.

Me ester: ***Plakortin***
[66940-35-0]
$C_{18}H_{32}O_4$ 312.448
Isol. from *Plakortis halichondrioides*. Biol. inactive. Sol. MeOH, C_6H_6. $[\alpha]_D^{20}$ +189 (c, 2.9 in $CHCl_3$).

9,10-Dihydro, Me ester: ***Dihydroplakortin***
$C_{18}H_{34}O_4$ 314.464
Isol. from *Plakortis simplex*. Oil. $[\alpha]_D^{25}$ +49 (c, 0.002 in $CHCl_3$).

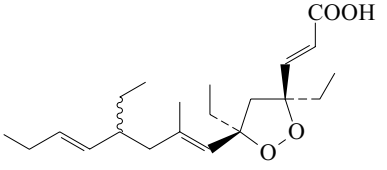
3-Epimer, Me ester: ***3-Epiplakortin***
[874161-22-5]
[74164-09-3]
Isol. from *Plakortis halichondrioides* and *Plakortis simplex*. Poorly sol. hexane. $[\alpha]_D$ +22.1 (c, 2.5 in CCl_4).

3-Epimer, 9,10-dihydro, Me ester: ***9,10-Dihydro-3-epiplakortin***
[74096-80-3]
$C_{18}H_{34}O_4$ 314.464
Constit. of *Plakortis halichondrioides*. Poorly sol. hexane. $[\alpha]_D$ +11.9 (c, 2.2 in CCl_4). Abs. config. not confirmed.

Higgs, M.D. *et al., J.O.C.*, 1978, **43**, 3454-3457 (*Plakortin*)
Faulkner, D.J. *et al., Colloq. Int. C.N.R.S.*, 1979, **291**, 401-406; *CA*, **95**, 21538h (*6-Et analogue Me ester*)
Stierle, D.B. *et al., J.O.C.*, 1980, **45**, 3396-3401 (*3-Epiplakortin, 9,10-Dihydro-3-epiplakortin*)
Phillipson, D.W. *et al., J.A.C.S.*, 1983, **105**, 7735-7736 (*isol, struct*)
Cafieri, F. *et al., Tetrahedron*, 1999, **55**, 7045-7056 (*Dihydroplakortin, abs config*)
Campagnuolo, C. *et al., Eur. J. Org. Chem.*, 2005, 5077-5083, (*3-Epiplakortin*)

Plakortide E P-473

[173075-27-9]

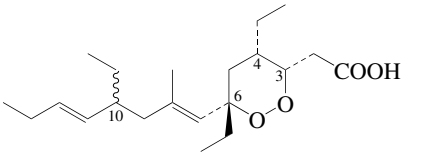


$C_{21}H_{34}O_4$ 350.497
MF given in ref. is incorrect. Isol. from the sponge *Plakortis halichondrioides*. Oil. $[\alpha]_D^{25}$ +63.9 (c, 2 in $CHCl_3$). λ_{max} 219; 244 ($CHCl_3$).

Patil, A.D. *et al., Tetrahedron*, 1996, **52**, 377 (*isol, uv, ir, pmr, cmr*)

Plakortide H P-474

4,6-Diethyl-6-(4-ethyl-2-methyl-1,5-octadienyl)-1,2-dioxane-3-acetic acid. 3,6-Epidioxy-4,6,10-triethyl-8-methyl-7,11-tetradecadienoic acid
[173075-48-4 (Me ester)]



Probable Absolute Configuration

$C_{21}H_{36}O_4$ 352.513
Information on abs. configs. not certain. Isol. from *Plakortis halichondrioides* and *Plakortis simplex*. Oil (as Me ester). $[\alpha]_D^{25}$ +5.5 (c, 2.9 in $CHCl_3$) (Me ester). λ_{max} 221 (MeOH).

7,8ξ-Dihydro: ***11,12-Didehydroplakortide Q***
$C_{21}H_{38}O_4$ 354.529
Isol. from *Plakortis zyggompha*. Oil (as Me ester). $[\alpha]_D^{22}$ -123 (c, 0.1 in $CHCl_3$) (Me ester).

11,12-Dihydro: ***Plakortide I***
[309965-93-3]
$C_{21}H_{38}O_4$ 354.529
Isol. from *Plakortis simplex*. Oil (as Me ester). $[\alpha]_D$ -42 (c, 0.01 in $CHCl_3$) (Me ester).

7,8ξ,11,12-Tetrahydro: ***Plakortide Q***†
$C_{21}H_{40}O_4$ 356.545
Isol. from *Plakortis zyggompha*. Oil. $[\alpha]_D^{22}$ -143 (c, 0.1 in $CHCl_3$).

4-Epimer: [214843-12-6]
Isol. from the sponge *Plakortis* sp.
Pale yellow oil (as Me ester). $[\alpha]_D^{23}$ +19 (c, 0.1 in $CHCl_3$) (Me ester).

4-Epimer, 7,8ξ-dihydro: [214843-22-8]
$C_{21}H_{38}O_4$ 354.529
Isol. from *Plakortis* sp. Pale yellow oil (as Me ester). $[\alpha]_D^{23}$ +40 (c, 0.17 in $CHCl_3$) (Me ester).

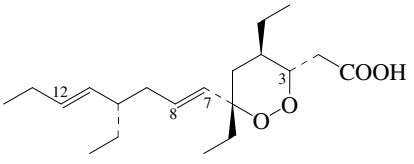
Stereoisomer, 4,5-didehydro, 7,8ξ-dihydro: ***4,6-Diethyl-6-(4-ethyl-2-methyl-5-octenyl)-3,6-dihydro-1,2-dioxin-3-acetic acid, 9CI***. *3,6-Epidioxy-4,6,10-triethyl-8-methyl-4,11-tetradecadienoic acid*
[131835-94-4]
$C_{21}H_{36}O_4$ 352.513
Isol. from the sponge *Plakortis angulospiculatus*. Antifungal and cytotoxic agent. $[\alpha]_D$ -34.6 (c, 0.2 in $CHCl_3$).

Stereoisomer, 4,5-didehydro, 7,8ξ,11,12-tetrahydro: 4,6-Diethyl-6-(4-ethyl-2-methyloctyl)-3,6-dihydro-1,2-dioxin-3-acetic acid. 3,6-Epidioxy-4,6,10-triethyl-8-methyl-4-tetradecenoic acid
[131835-96-6]
$C_{21}H_{38}O_4$ 354.529
From *Plakortis angulospiculatus*. Antifungal and cytotoxic agent. $[\alpha]_D$ -36 (c, 0.2 in $CHCl_3$).

Gunasekera, S.P. *et al., J. Nat. Prod.*, 1990, **53**, 669 (*Plakortis angulospiculatus constits*)
Patil, A.D. *et al., J. Nat. Prod.*, 1996, **59**, 219-223 (*Plakortide H*)
Fontana, A. *et al., J. Nat. Prod.*, 1998, **61**, 1427-1429 (*isol, pmr, cmr*)
Fattorusso, E. *et al., Tetrahedron*, 2000, **56**, 7959-7967 (*Plakortides H,I*)
Berrué, F. *et al., Tetrahedron*, 2005, **61**, 11843-11849 (*Plakortide Q, Didehydroplakortide Q*)

Plakortide J P-475

3,6-Epidioxy-4,6,10-triethyl-7,11-tetradecadienoic acid
[309965-94-4]



Relative Configuration

$C_{20}H_{34}O_4$ 338.486
Some of the Plakortide names have been duplicated. Isol. from the sponges *Plakortis simplex* and *Plakortis halichondrioides*. Oil. $[\alpha]_D^{24}$ -78 (c, 0.001 in $CHCl_3$).

3-Epimer: ***Plakortide O***. *Plakortide M (obsol.)*†
[552323-74-7]
[856426-48-7]
$C_{20}H_{34}O_4$ 338.486
Isol. from *Plakortis halichondrioides*. Oil. $[\alpha]_D^{24}$ -249 (c, 1.4 in $CHCl_3$). Synonym code letter changed from M to avoid duplication.

3-Epimer, 7,8-dihydro: ***Plakortide F***. *Trishomoplakortic acid*
[173240-53-4]
[152821-46-0]
Isol. from *Plakortis halichondrioides*.
Oil (as Me ester). $[\alpha]_D$ -161.6 (c, 0.04 in $CHCl_3$). CAS no. refers to Me ester.

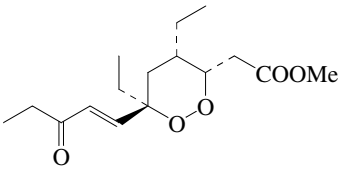
4-Epimer, 7,8-dihydro: ***Plakortide G***
[173240-54-5]
$C_{20}H_{36}O_4$ 340.502
Isol. from *Plakortis halichondrioides*. Oil (as Me ester). $[\alpha]_D^{25}$ +67.2 (Me ester). CAS no. refers to Me ester.

3-Epimer, 13-oxo, 7,8-dihydro: ***13-Oxoplakortide F***
[856426-47-6]
$C_{20}H_{34}O_5$ 354.486
Isol. from a *Plakortis* sp.

Rudi, A. *et al., J. Nat. Prod.*, 1993, **56**, 1827-1830 (*Trishomoplakortic acid*)
Patil, A.D. *et al., J. Nat. Prod.*, 1996, **59**, 219-223 (*Plakortides F,G*)
Fattorusso, E. *et al., Tetrahedron*, 2000, **56**, 7959-7967 (*Plakortide J*)
Gochfield, D.J. *et al., J. Nat. Prod.*, 2001, **64**, 1477-1479 (*Plakortide F, isol, activity*)
Chen, Y. *et al., J. Nat. Prod.*, 2002, **65**, 1509-1512 (*isol, pmr, cmr*)
Jiménez, M. de S. *et al., J. Nat. Prod.*, 2003, **66**, 655-661; 1404 (*Plakortide O*)
Lim, C.W. *et al., CA*, 2005, **143**, 94081y (*13-Oxoplakortide F*)

Plakortide M P-476

[397033-53-3]

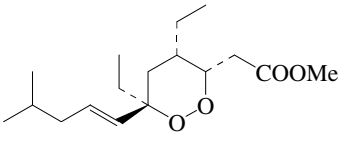


$C_{16}H_{26}O_5$
Originally called Plakortide I but name changed so as not to be confused with. Isol. from a *Plakortis* sp. Pale yellowish oil. $[\alpha]_D^{25}$ -131 (c, 0.2 in $CHCl_3$). λ_{max} 238 (log ϵ 4.27) (MeOH).

Hu, J.-F. *et al., Tetrahedron*, 2001, **57**, 9379-9383; 2002, **58**, 1233

Plakortide N P-477

[397033-58-8]

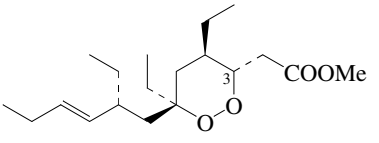


$C_{17}H_{30}O_4$ 298.422
Originally named Plakortide J but name changed so as not to be confused with Plakortide J, P-475. Isol. from a *Plakortis* sp. Oil. $[\alpha]_D^{25}$ -93 (c, 0.1 in $CHCl_3$).

Hu, J.-F. *et al., Tetrahedron*, 2001, **57**, 9379-9383 (*isol, pmr, cmr, ms*)

Plakortide Q† P-478

[874190-09-7]



Absolute Configuration

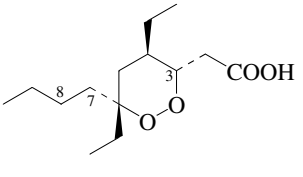
$C_{19}H_{34}O_4$ 326.475
Constit. of *Plakortis simplex*. Oil. $[\alpha]_D^{25}$ +10.3 (c, 2.5 in $CHCl_3$).

3-Epimer: [78104-04-8]
$C_{19}H_{34}O_4$ 326.475
Constit. of *Plakortis halichondrioides*. Abs. config. not determined.

Faulkner, D.J. *et al., CA*, 1981, **95**, 21538h (*3-epimer*)
Campagnuolo, C. *et al., Eur. J. Org. Chem.*, 2005, 5077-5083 (*Plakortide Q*)

Plakortide Z P-479

6-Butyl-4,6-diethyl-1,2-dioxan-3-acetic acid. 3,6-Epidioxy-4,6-diethyldecanoic acid



Absolute Configuration

$C_{14}H_{26}O_4$ 258.357

Et ester: ***Ethyl plakortide Z***
[211632-51-8]
$C_{16}H_{30}O_4$ 286.411
Isol. from the sponge *Plakortis lita*. Cytotoxic agent. Yellow oil. $[\alpha]_D^{25}$ +58.8 (c, 6.8 in CH_2Cl_2).

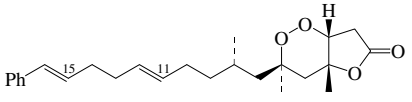
7,8-Didehydro, Me ester: ***Methyl didehydroplakortide Z***
[211632-55-2]
$C_{15}H_{26}O_4$ 270.368
Isol. from the sponge *Plakortis lita*. Yellow oil. $[\alpha]_D^{25}$ +67.3 (c, 0.4 in CH_2Cl_2).

7,8-Didehydro, Et ester: ***Ethyl didehydroplakortide Z***
[211632-53-0]
$C_{16}H_{28}O_4$ 284.395
Isol. from the sponge *Plakortis lita*. Yellow oil. $[\alpha]_D^{25}$ +81.5 (c, 1.7 in CH_2Cl_2).

Harrison, B. *et al., J. Nat. Prod.*, 1998, **61**, 1033-1037

Plakortolide P-480

[138949-85-6]



Absolute Configuration

$C_{25}H_{34}O_4$ 398.541
Isol. from the sponges *Plakortis* sp. and *Plakinastrella onkodes*. Cytotoxic. Shows strong anti-toxoplasma effect. Light orange oil. $[\alpha]_D$ +5.6 (c, 0.014 in $CHCl_3$). λ_{max} 250 (ϵ 15000); 282; 292 (MeOH) (Berdy).

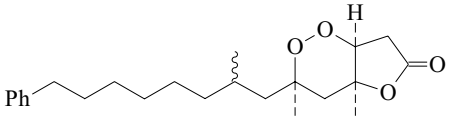
11,12,15,16-Tetrahydro: ***Plakortolide B***
[159985-01-0]
$C_{25}H_{38}O_4$ 402.573
Isol. from the sponge *Plakinastrella onkodes*. Cytotoxic agent. Oil. $[\alpha]_D$ -4.7 (c, 0.1 in $CDCl_3$).

*$\Delta^{10,11}$-Isomer, 8*E*,9-didehydro:* ***Plakortolide H***
$C_{25}H_{32}O_4$ 396.525
Isol. from *Plakortis* aff. *simplex*. Oil. $[\alpha]_D$ -17.3 (c, 0.01 in $CHCl_3$). Abs. config. not confirmed.

Davidson, B.S. *et al., Tet. Lett.*, 1991, **32**, 7167 (*isol*)
Horton, P.A. *et al., J. Nat. Prod.*, 1994, **57**, 1374 (*Plakortolide B*)
Perry, T.L. *et al., Tetrahedron*, 2001, **57**, 1483-1487 (*isol, abs config, activity*)
Rudi, A. *et al., J. Nat. Prod.*, 2003, **66**, 682-685 (*Plakortolide H*)

Plakortolide C P-481

[159985-02-1]

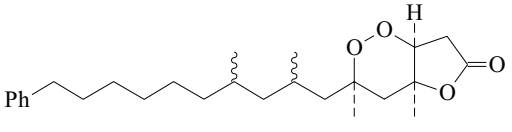


$C_{23}H_{34}O_4$ 374.519
Peroxylactone isol. from the sponge *Plakinastrella onkodes*. Cytotoxic agent. Oil. $[\alpha]_D$ -5.3 (c, 0.05 in $CDCl_3$).

Horton, P.A. *et al., J. Nat. Prod.*, 1994, **57**, 1374 (*isol, pmr, cmr*)

Plakortolide D P-482

[160016-20-6]

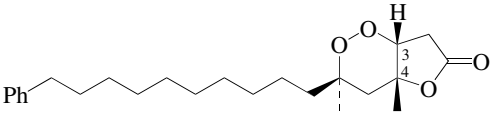


$C_{26}H_{40}O_4$ 416.6
Peroxylactone isol. from the sponge *Plakinastrella onkodes*. Cytotoxic agent. Oil. $[\alpha]_D$ +61.1 (c, 0.04 in $CDCl_3$).

Horton, P.A. *et al., J. Nat. Prod.*, 1994, **57**, 1374 (*isol, pmr, cmr*)

Plakortolide E P-483

*Tetrahydro-3,4*a*-dimethyl-3-(10-phenyldecyl)furo[3,2-*c*]-1,2-dioxin-6(3*H*)-one, 9CI*
[162559-02-6]



Absolute Configuration

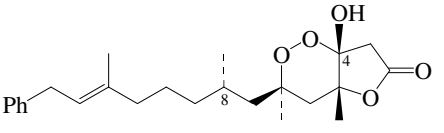
$C_{24}H_{36}O_4$ 388.546
Isol. from the sponge *Plakortis* sp. Cytotoxic agent. Brown waxy solid. $[\alpha]_D$ +10 (c, 0.1 in CH_2Cl_2).

3,4-Diepimer:
$C_{24}H_{36}O_4$ 388.546
Isol. from the sponge *Plakinastrella* sp. Oil. $[\alpha]_D$ -8 (c, 0.05 in $CHCl_3$). λ_{max} 260 (ϵ 3400) (MeOH).

6-Epimer: ***Plakortolide I***
$C_{24}H_{36}O_4$ 388.546
Isol. from *Plakortis* aff. *simplex*.
$[\alpha]_D$ +8 (c, 0.017 in $CHCl_3$).

Varoglu, M. *et al., J. Nat. Prod.*, 1995, **58**, 27-36 (*isol, pmr, cmr*)
Qureshi, A. *et al., J. Nat. Prod.*, 1998, **61**, 1539-1542 (*isol, pmr, cmr*)
Rudi, A. *et al., J. Nat. Prod.*, 2003, **66**, 682-685 (*Plakortolide I*)

Plakortolide F† P-484

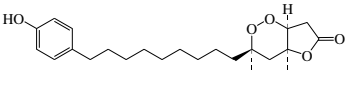


$C_{24}H_{34}O_5$ 402.53
Isol. from *Plakinastrella onkodes*. Active against *Toxoplasma* sp. Oil. $[\alpha]_D$ -59.2 (c, 0.025 in $CHCl_3$). C-8 config. not confirmed. λ_{max} 202 (ϵ 50360); 246 (ϵ 20510); 360 (ϵ 1660) (EtOH).

4-Deoxy: ***Plakortolide G***
$C_{24}H_{34}O_4$ 386.53
Isol. from *Plakinastrella onkodes*. Oil. $[\alpha]_D$ +6 (c, 0.01 in $CHCl_3$). λ_{max} 202 (ϵ 92220); 250 (ϵ 36390); 368 (ϵ 2770) (EtOH).

Perry, T.L. *et al., Tetrahedron*, 2001, **57**, 1483-1487

Plakortolide F† P-485



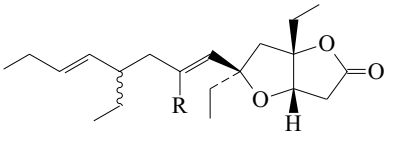
Relative Configuration

$C_{23}H_{34}O_5$ 390.519
Isol. from the sponge *Plakinastrella* sp.

Chen, Y. *et al., J. Nat. Prod.*, 2001, **64**, 262-264 (*isol, pmr, cmr*)

Plakortone A P-486

[172705-53-2]



R = CH_2CH_3

$C_{22}H_{36}O_3$ 348.525

Isol. from the sponge *Plakortis halichondrioides*. Oil. Sol. MeOH, EtOAc, Me_2CO; poorly sol. hexane, H_2O. $[\alpha]_D$ -21.1 (c, 0.04 in $CHCl_3$). λ_{max} 217; 228; 240 ($CHCl_3$). λ_{max} 217; 228; 240 (MeOH) (Berdy).

Patil, A.D. *et al., Tetrahedron*, 1996, **52**, 377 (*isol, uv, ir, pmr, cmr*)

Plakortone B P-487

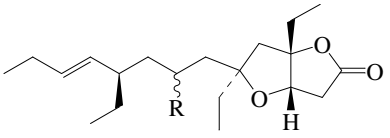
[172705-54-3]
As Plakortone A, P-486 with
R = CH_3
$C_{21}H_{34}O_3$ 334.498
Isol. from the sponge *Plakortis halichondrioides*. Oil. Sol. MeOH, Me_2CO, EtOAc; poorly sol. hexane, H_2O. $[\alpha]_D^{25}$ -9.2 (c, 0.7 in $CHCl_3$). λ_{max} 229; 241 ($CHCl_3$). λ_{max} 229; 241 (MeOH) (Berdy).

7,8,11,12-Tetrahydro: ***Plakortone F***
$C_{21}H_{38}O_3$ 338.529
Isol. from the sponge *Plakortis simplex*. Cytotoxic agent. Oil. $[\alpha]_D^{25}$ -11 (c, 0.001 in $CHCl_3$). λ_{max} 220; 227 (MeCN).

Patil, A.D. *et al., Tetrahedron*, 1996, **52**, 377 (*isol, uv, ir, pmr, cmr*)
Cafieri, F. *et al., Tetrahedron*, 1999, **55**, 13831-13840 (*Plakortone F*)
Semmelhack, M.F. *et al., Org. Lett.*, 2006, **8**, 5203-5206 (*synth*)

Plakortone C P-488

[172705-55-4]



R = CH_3

$C_{21}H_{36}O_3$ 336.514
Abs. config. prob. as indicated. The abs config. of the homologue Plakortone D, P-489 has been determined. Isol. from the sponge *Plakortis halichondrioides*. Oil. Sol. MeOH, Me_2CO, EtOAc; poorly sol. hexane, H_2O. $[\alpha]_D^{25}$ -24.9 (c, 1.2 in $CHCl_3$). λ_{max} 223; 227; 241 ($CHCl_3$). λ_{max} 223; 227; 241 (MeOH) (Berdy).

Patil, A.D. *et al., Tetrahedron*, 1996, **52**, 377 (*isol, uv, ir, pmr, cmr*)

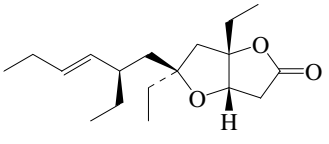
Plakortone D P-489

[172705-56-5]
As Plakortone C, P-488 with
R = H
$C_{20}H_{34}O_3$ 322.487
Isol. from the sponge *Plakortis halichondrioides*. Oil. Sol. MeOH, EtOAc, Me_2CO; poorly sol. hexane, H_2O. $[\alpha]_D^{25}$ -26.3 (c, 1.3 in $CHCl_3$). λ_{max} 219; 227; 241 ($CHCl_3$). λ_{max} 219; 227; 241 (MeOH) (Berdy).

Patil, A.D. *et al., Tetrahedron*, 1996, **52**, 377 (*isol, uv, ir, pmr, cmr*)
Hayes, P.Y. *et al., J.A.C.S.*, 2002, **124**, 9718-9719 (*synth, abs config*)

Plakortone E P-490

[252722-12-6]



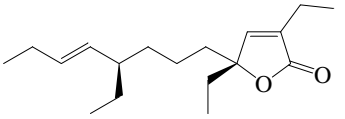
Absolute Configuration

$C_{18}H_{30}O_3$ 294.433
Isol. from the sponge *Plakortis simplex*. Cytotoxic agent. Oil. $[\alpha]_D^{25}$ -10 (c, 0.001 in $CHCl_3$). λ_{max} 214; 230 (MeCN).

Cafieri, F. *et al., Tetrahedron*, 1999, **55**, 13831-13840 (*isol, pmr, cmr*)
Hayes, P.Y. *et al., Heterocycles*, 2004, **62**, 173-177 (*synth, pmr, cmr*)
Akiyama, M. *et al., Tet. Lett.*, 2006, **47**, 2287-2290 (*synth, abs config*)

Plakortone G P-491

*3,5-Diethyl-5-(4-ethyl-5-octenyl)-2(5*H*)-furanone*



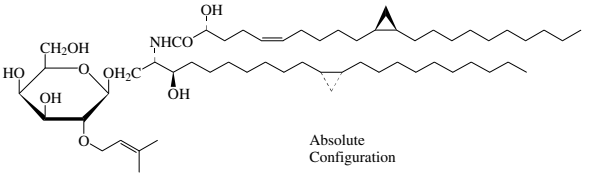
Absolute Configuration

$C_{18}H_{30}O_2$ 278.434
Constit. of a Caribbean sponge *Plakortis* sp. Oil. $[\alpha]_D$ -25.9 (c, 0.008 in $CHCl_3$). λ_{max} 246 (ϵ 410) ($CHCl_3$).

Gochfeld, D.J. *et al., J. Nat. Prod.*, 2001, **64**, 1477-1479 (*isol, pmr, cmr*)
Kowashi, S. *et al., Tet. Lett.*, 2004, **45**, 4393-4396 (*abs config*)

Plakoside A P-492

[199480-72-3]



Absolute Configuration

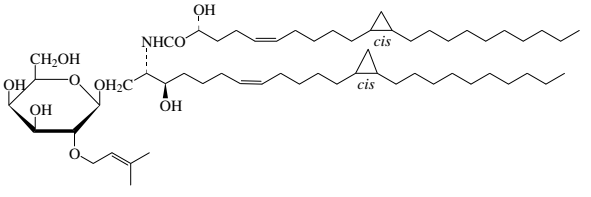
$C_{57}H_{105}NO_9$ 948.458
Isol. from the sponge *Plakortis simplex*. Immunosuppressant. Amorph. solid. $[\alpha]_D^{25}$ +7 (c, 0.5 in MeOH).

6′-O-β-D-Glucopyranosyl: ***Plakoside C***
$C_{63}H_{115}NO_{14}$ 1110.6
Isol. from the sponge *Ectyoplasia ferox*. Amorph. solid. $[\alpha]_D^{25}$ +4 (c, 0.2 in MeOH).

Costantino, V. *et al., J.A.C.S.*, 1997, **119**, 12465-12470 (*isol, pmr, cmr*)
Nicolaou, K.C. *et al., Helv. Chim. Acta*, 2000, **83**, 1977-2006 (*synth*)
Costantino, V. *et al., Tetrahedron*, 2000, **56**, 5953-5957 (*Plakoside C*)
Seki, M. *et al., Eur. J. Org. Chem.*, 2001, 3797-3809 (*synth*)
Tashiro, T. *et al., Eur. J. Org. Chem.*, 2002, 3659-3665 (*synth, abs config*)

Plakoside B P-493

[199480-73-4]

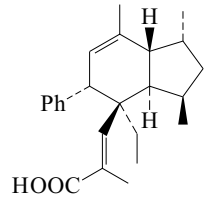


$C_{59}H_{107}NO_9$ 974.496
Isol. from the sponge *Plakortis simplex*. Immunosuppressant. Amorph. solid. $[\alpha]_D^{25}$ +7 (c, 0.2 in MeOH).

6′-O-β-D-Glucopyranosyl: ***Plakoside D***
$C_{65}H_{117}NO_{14}$ 1136.638
Isol. from the sponge *Ectyoplasia ferox*. Amorph. solid. $[\alpha]_D^{25}$ +4 (c, 0.1 in MeOH).

Nicolaou, K.C. *et al., Helv. Chim. Acta*, 2000, **83**, 1977-2006 (*synth*)
Costantino, V. *et al., J.A.C.S.*, 2000, **48**, 1190-1195 (*isol, pmr, cmr*)
Costantino, V. *et al., Tetrahedron*, 2000, **56**, 5953-5957 (*Plakoside D*)

Plakotenin P-494

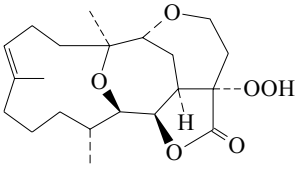


$C_{24}H_{32}O_2$ 352.516
Constit. of *Plakortis lita*. Oil. λ_{max} 217 (ϵ 8000) (MeOH).

Kobayashi, J. *et al., Tet. Lett.*, 1992, **33**, 2579 (*isol, pmr, cmr*)
Ishizaki, M. *et al., Heterocycles*, 1999, **50**, 779-790 (*synth*)

Planaxool P-495

[149204-43-3]



$C_{21}H_{32}O_6$ 380.48
Constit. of *Planaxis sulcatus*. Solid.
Mp 58°. $[\alpha]_D$ +219 (c, 0.621 in $CHCl_3$). Related to 4,13-Epoxy-3-hydroxy-7,15(17)-cembradien-16,14-olide, E-368.

Alam, M. *et al., J. Nat. Prod.*, 1993, **56**, 774-779 (*isol, pmr, cmr*)

Plancitoxins P-496

Two peptides (Plancitoxins I and II) containing 2 subunits (10 and 27 kDa) bridged by a disulfide bond. Isol. from spines of the crown-of-thorns starfish *Acanthaster planci*. Hepatotoxic DNases II.

Shiomi, K. *et al., Toxicon*, 2004, **44**, 499-506 (*isol*)

Plantaricin P-497

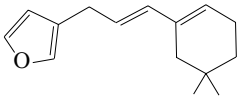
Polypeptides. Prod. by *Lactobacillus plantarum*. Bacteriocins.

Plantaricin F [159605-63-7]
Prod. by *Lactobacillus plantarum* isol. from catfish.

Fricourt, B.W. *et al., J. Food Prot.*, 1994, **57**, 698-702 (*Plantaricin F*)

Pleraplysillin 1 P-498

[41060-03-1]

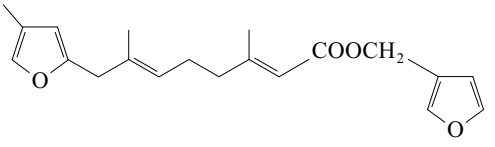


$C_{15}H_{20}O$ 216.322
Constit. of *Pleraplysilla spinifera* and mollusc *Cadlina luteomarginata*. Oil.

Cimino, G. *et al., Tetrahedron*, 1972, **28**, 4761 (*isol*)
Thompson, J.E. *et al., Tetrahedron*, 1982, **38**, 1865 (*isol*)
Masaki, Y. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 3476 (*synth*)

Pleraplysillin 2 P-499

[53492-34-5]



$C_{20}H_{24}O_4$ 328.407
Constit. of *Pleraplysilla spinifera*. Liq.

Cimino, G. *et al., Experientia*, 1974, **30**, 846
Cimino, G. *et al., Tet. Lett.*, 1975, 3727
Knight, D.W. *et al., J.C.S. Perkin 1*, 1981, 1557 (*synth*)

Pleurocidin P-500

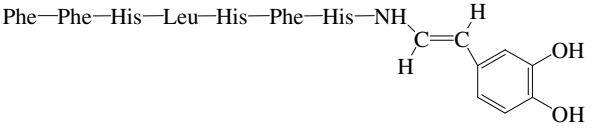
[190324-47-1]

$C_{129}H_{192}N_{36}O_{29}$ 2711.16

Peptide containing 25 amino acid residues. Isol. from skin mucous secretions of the winter flounder *Pleuronectes americanus*. Shows antimicrobial activity. Three pleurocidin-like peptides (23-26 amino acid residues) also isol.

Cole, A.M. *et al., J. Biol. Chem.*, 1997, **272**, 12008-12013 (*isol*)
Douglas, S.E. *et al., Dev. Comp. Immunol.*, 2001, **25**, 137-147 (*pleurocidin-like peptides*)
Syvitski, R.T. *et al., Biochemistry*, 2005, **44**, 7282-7293 (*struct*)

Plicatamide P-501



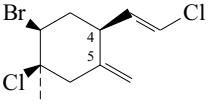
$C_{59}H_{68}N_{14}O_9$ 1117.275

A modified octapeptide. Isol. from the ascidian *Styela plicata*. Shows antimicrobial activity. Not indexed by CAS.

Tincu, J.A. *et al., Biochem. Biophys. Res. Commun.*, 2000, **270**, 421-424 (*isol, pmr, struct*)
Tincu, J.A. *et al., J. Biol. Chem.*, 2003, **278**, 13546-13553 (*isol, activity*)

Plocamadiene A P-502

2-Bromo-1-chloro-4-(2-chloroethenyl)-1-methyl-5-methylenecyclohexane
[66321-25-3]

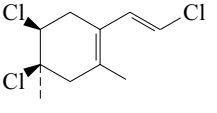


$C_{10}H_{13}BrCl_2$ 284.022
Constit. of *Plocamium mertensii* and *Plocamium cartilagineum*. Cryst. (MeOH aq.). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 46.5-47°. $[\alpha]_D$ -120 (c, 0.7 in $CHCl_3$).

Higgs, M.D. *et al., Tetrahedron*, 1977, **33**, 2775
Capon, R.J. *et al., Aust. J. Chem.*, 1984, **37**, 537

Plocamene B P-503

4,5-Dichloro-1-(2-chloroethenyl)-2,4-dimethylcyclohexene, 9CI
[58207-70-8]



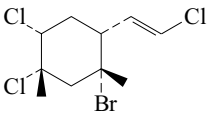
$C_{10}H_{13}Cl_3$ 239.571

Constit. of *Plocamium cartilagineum*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 100-101°. $[\alpha]_D$ -48.

Crews, P. *et al., J.O.C.*, 1975, **40**, 2568; 1978, **43**, 116 (*isol, struct, pmr, cmr, abs config*)

Plocamene C P-504

1-Bromo-4,5-dichloro-2-(2-chloroethenyl)-1,5-dimethylcyclohexane. Violacene 2
[57566-88-8]

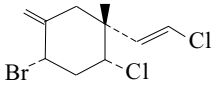


$C_{10}H_{14}BrCl_3$ 320.483
Constit. of *Microcladia* spp. and *Plocamium violaceum*. Cryst. (EtOH).
Mp 43.5-44.5° Mp 78.5-79°. $[\alpha]_D^{20}$ -84 (c, 0.32 in $CHCl_3$).

Mynderse, J.S. *et al., Tet. Lett.*, 1975, 2175 (*cryst struct*)
Crews, P. *et al., J.O.C.*, 1978, **43**, 116 (*struct, pmr, cmr*)
Mynderse, J.S. *et al., Phytochemistry*, 1978, **17**, 237 (*isol*)

Plocamene D′ P-505

4-Bromo-2-chloro-1-(2-chloroethenyl)-1-methyl-5-methylenecyclohexane
[63883-43-2]



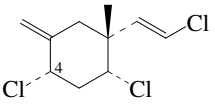
Absolute configuration

$C_{10}H_{13}BrCl_2$ 284.022
Constit. of *Plocamium cartilagineum* and *Plocamium violaceum*. Antifungal agent. Oil. $[\alpha]_D$ +31.3 (c, 0.86 in $CHCl_3$).

Crews, P. *et al., J.O.C.*, 1978, **43**, 116
Stierle, D.B. *et al., Tetrahedron*, 1979, **35**, 1261 (*isol, abs config*)

Plocamene D P-506

2,4-Dichloro-1-(2-chloroethenyl)-1-methyl-5-methylenecyclohexane
[62560-51-4]



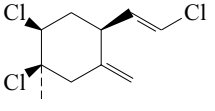
$C_{10}H_{13}Cl_3$ 239.571
Constit. of *Microcladia* spp. Oil. $[\alpha]_D^{20}$ -4.1 (c, 0.73 in $CHCl_3$).

4-Epimer: epi-*Plocamene D*
[73191-60-3]
$C_{10}H_{13}Cl_3$ 239.571
Constit. of *Plocamium violaceum* and *Plocamium cartilagineum*. Shows antifungal props. Oil. $[\alpha]_D$ -63.3 (c, 0.98 in $CHCl_3$).

Crews, P. *et al., Phytochemistry*, 1976, **15**, 1707
Crews, P. *et al., J.O.C.*, 1978, **43**, 116; 1984, **49**, 1371 (*isol, struct, pmr, cmr*)
Stierle, D.B. *et al., Tetrahedron*, 1979, **35**, 1261 (*epimer*)

Plocamene E P-507

1,2-Dichloro-4-(2-chloroethenyl)-1-methyl-5-methylenecyclohexane, 9CI
[63866-51-3]

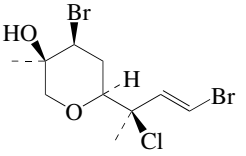


$C_{10}H_{13}Cl_3$ 239.571
Constit. of *Plocamium violaceum*. Oil. $[\alpha]_D^{20}$ -105 (c, 4.57 in $CHCl_3$).

Crews, P. *et al., J.O.C.*, 1978, **43**, 116

Plocamiopyranoid P-508

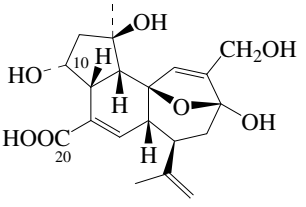
[218603-34-0]



$C_{10}H_{15}Br_2ClO_2$ 362.488
Constit. of *Plocamium cartilagineum*. Oil. $[\alpha]_D^{25}$ -33 (c, 1.05 in $CHCl_3$).

Cuerto, M. *et al., J. Nat. Prod.*, 1998, **61**, 1466-1468 (*isol, pmr, cmr*)

Plumarellic acid P-509

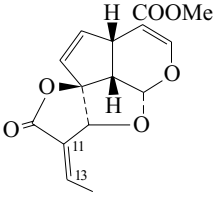


$C_{20}H_{26}O_7$ 378.421
Related to Mandapamate, M-78.
Et ester: ***Ethyl plumarellate***
[405274-17-1]
$C_{22}H_{30}O_7$ 406.475
Constit. of a *Plumarella* sp. Cryst.
Mp 136-138°. $[\alpha]_D^{25}$ +84.1 (c, 0.27 in EtOAc/EtOH).
20→10 Lactone: ***Plumarellide***
[405274-15-9]
$C_{20}H_{24}O_6$ 360.406
Constit. of a *Plumarella* sp. Cryst. (MeOH).
Mp 223-225°. $[\alpha]_D^{25}$ +109.6 (c, 0.23 in $CHCl_3$/MeOH).

Stonik, V.A. *et al., Tet. Lett.*, 2002, **43**, 315-317 (*isol, pmr, cmr*)

Plumericin P-510

[77-16-7]



$C_{15}H_{14}O_6$ 290.272
The abs. config. is proposed to be the opposite as drawn based on quantum-mechanical calculations of CD. This is still to be confirmed. Isol. from *Plumeria* spp. and from *Cliona caribboea*. Shows antibiotic, antifungal and antineoplastic activity. Plate-like needles (C_6H_6). Sol. $CHCl_3$; fairly sol. MeOH, C_6H_6, bases, Me_2CO, EtOH, Et_2O; poorly sol. H_2O, acids, hexane.
Mp 212.5-213.5° sl. dec. $[\alpha]_D^{30}$ +204 ($CHCl_3$). Log P -0.34 (uncertain value) (calc). Related to Plumieride. λ_{max} 215 (ϵ 17400); 240 (sh) (ϵ 15800) (EtOH) (Derep). λ_{max} 215 (ϵ 17380) (MeOH) (Berdy). λ_{max} 212 (ϵ 32600) (EtOH) (Berdy).

(11Z)-Isomer: ***Isoplumericin***
[31298-76-7]
$C_{15}H_{14}O_6$ 290.272
Isol. from roots of *Plumeria rubra*. Antifungal and antineoplastic agent. Cryst. (CH_2Cl_2/toluene).
Mp 200.5-201.5°. $[\alpha]_D^{25}$ +216.4 (c, 1.01 in $CHCl_3$). Log P -0.34 (uncertain value) (calc). λ_{max} 215 (ϵ 17400); 240 (sh) (ϵ 15800) (EtOH) (Derep). λ_{max} 215 (ϵ 16980) (EtOH) (Berdy).

11S,13-Dihydro: ***β-Dihydroplumericin***
$C_{15}H_{16}O_6$ 292.288
Isol. from roots of *Plumeria rubra*. Cryst. (Et_2O/pentane or by subl.).
Mp 150-151°. $[\alpha]_D^{22.5}$ +275.5 ($CHCl_3$).

11S,13-Dihydro, parent acid: ***β-Dihydroplumericinic acid***
$C_{14}H_{14}O_6$ 278.261
Isol. from roots of *Plumeria rubra*.
Mp 189-190° dec.

Parent acid: ***Plumericinic acid****. Desmethylplumericin*
$C_{14}H_{12}O_6$ 276.245
Isol. from *Allamanda cathartica*. Cryst.
Mp 231-232°.

Little, J.E. *et al., Arch. Biochem.*, 1951, **30**, 445 (*isol*)
Albers-Schonberg, G. *et al., Helv. Chim. Acta*, 1961, **44**, 1447 (*isol, uv, pmr*)
Kupchan, S.M. *et al., J.O.C.*, 1977, **39**, 2477 (*isol*)
Trost, B.M. *et al., J.A.C.S.*, 1983, **105**, 6755 (*synth*)
Martin, G.E. *et al., J.O.C.*, 1985, **50**, 2383 (*pmr*)
Parkes, K.E.B. *et al., J.C.S. Perkin 1*, 1988, 1119 (*synth*)
De Melo, S.J. *et al., Fitoterapia*, 1997, **68**, 478 (*Plumericinic acid*)
Bolzani, V. da S. *et al., Ann. Acad. Bras. Cienc.*, 1999, **71**, 131 (*activity*)
Elgässer, B. *et al., Chem. Biodiversity*, 2005, **2**, 799-808 (*cryst struct, abs config*)

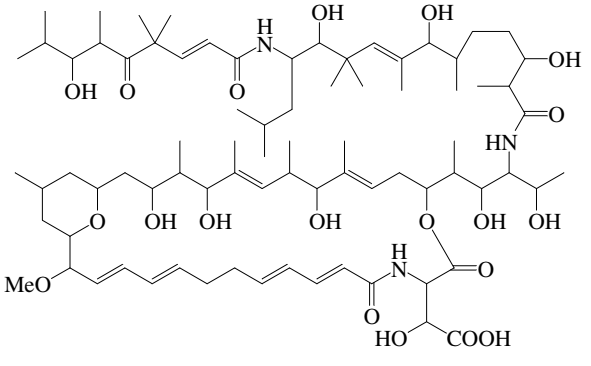
Poecillanosine P-511

2-Acetoxy-1-(hydroxynitrosoamino)heptadecane
[200564-72-3]
$H_3C(CH_2)_{14}CH(OAc)CH_2N(OH)NO$
$C_{19}H_{38}N_2O_4$ 358.52
Isol. from the sponge *Poecillastra* spec. aff. *tenuilaminaris*. Cytotoxic agent and free radical scavenger. Solid. $[\alpha]_D^{25}$ -20.2 (c, 0.1 in MeOH). Ref. states abs. config. as (*R*)- in text but shows (*S*)- in diag. λ_{max} 232 (ϵ 5700) (MeOH).

Natori, T. *et al., Tet. Lett.*, 1997, **38**, 8349-8350 (*isol, uv, ir, pmr, cmr*)

Poecillastrin A P-512

NSC 726108
[471913-55-0]

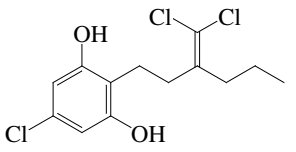


$C_{79}H_{131}N_3O_{20}$ 1442.912
Related to Chondropsin B, C-641. Isol. from the sponge *Poecillastra* sp.
$[\alpha]_D^{27}$ -8.3 (c, 0.056 in MeOH). λ_{max} 229 (ϵ 10800); 235 (ϵ 10900); 263 (ϵ 10200) (MeOH).

Rashid, M.A. *et al., Org. Lett.*, 2002, **4**, 3293-3296 (*isol, pmr, cmr*)

Poipuol P-513

5-Chloro-2-(3-dichloromethylenehexyl)-1,3-benzenediol

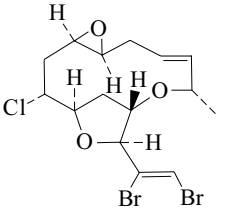


$C_{13}H_{15}Cl_3O_2$ 309.618
Isol. from a sponge *Hyrtios* sp. Amorph. solid. λ_{max} 211 (ϵ 28000) (MeOH).

Sata, N. *et al., J. Nat. Prod.*, 2005, **68**, 262-263 (*isol, pmr, cmr*)

Poitediene P-514

[88428-87-9]



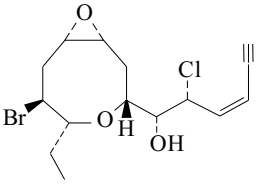
Absolute configuration

$C_{15}H_{19}Br_2ClO_3$ 442.574
Metab. of the marine alga *Laurencia poitei*. Cryst. (CCl_4).
Mp 140-140.5°. $[\alpha]_D$ +60.3 (c, 0.055 in CH_2Cl_2). λ_{max} 214 (ϵ 6670) (EtOH) (Derep).

Wright, G.E. *et al., Tet. Lett.*, 1983, **24**, 4649 (*cryst struct*)

Poiteol P-515

[75921-98-1]

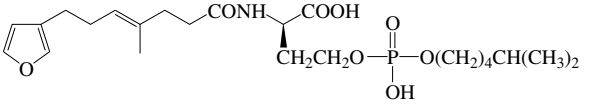


$C_{15}H_{20}BrClO_3$ 363.678
Constit. of *Laurencia* spp. Cryst. (Et_2O).
Mp 151-154°. $[\alpha]_D^{20}$ +116.7 (c, 1.0 in $CHCl_3$).

Howard, B.M. *et al., Tetrahedron*, 1980, **36**, 1747

Pokepola ester P-516

[157446-77-0]



$C_{23}H_{38}NO_8P$ 487.529
Constit. of *Spongia oceania*. Oil. $[\alpha]_D$ -4.5 (c, 0.5 in MeOH).

Kalidindi, R.S. *et al., Tet. Lett.*, 1994, **35**, 5579-5582 (*isol, ir, pmr, cmr, ms*)

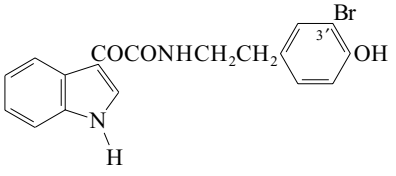
Pol-RF amide P-517

[119116-89-1]
H-5-OxoPro-Leu-Leu-Gly-Gly-Arg-Phe-NH_2
$C_{36}H_{57}N_{11}O_8$ 771.915
Isol. from the hydromedusa *Polyorchis penicillatus*. Neuropeptide.

2-Tryptophan-4-lysine analogue: Pol-RF amide II
[140908-91-4]
$C_{45}H_{65}N_{13}O_8$ 916.091
Isol. from the hydromedusa *Polyorchis penicillatus*.
Grimmelikhiujzen, C.J.P. *et al., Brain Res.*, 1988, **475**, 198-203 (*isol, activity, struct*)
Grimmelikhiujzen, C.J. *et al., Biochem. Biophys. Res. Commun.*, 1992, **183**, 375-382 (*Pol-RF amide II*)

Polyandrocarpamide A P-518

N-*[2-(3-Bromo-4-hydroxyphenyl)ethyl]-α-oxo-1*H-*indole-3-acetamide, 9CI*
[129369-41-1]



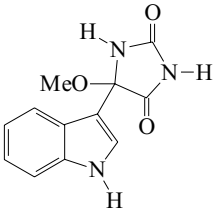
$C_{18}H_{15}BrN_2O_3$ 387.232
Alkaloid from the marine ascidian *Polyandrocarpa* sp. Needles. Mp 178-179°. λ_{max} 207 (ϵ 58500); 247 (ϵ 1600); 266 (ϵ 9900); 272 (ϵ 8600); 309 (ϵ 9800) (MeOH/NaOH) (Derep). λ_{max} 205 (ϵ 41400); 255 (ϵ 10300); 267 (ϵ 9900); 274 (ϵ 9600); 290 (ϵ 5000); 324 (ϵ 8400) (MeOH) (Derep).

Debromo: ***Polyandrocarpamide C***
[107610-00-4]
$C_{18}H_{16}N_2O_3$ 308.336
Alkaloid from *Polyandrocarpa* sp. Amorph. solid. λ_{max} 205 (ϵ 21400); 246 (ϵ 8300); 266 (ϵ 6100); 272 (ϵ 5300); 318 (ϵ 4600) (MeOH/NaOH) (Derep). λ_{max} 205 (ϵ 19200); 254 (ϵ 6400); 266 (ϵ 6100); 272 (ϵ 5700); 285 (sh); 324 (ϵ 4600) (MeOH) (Derep).

3′-Debromo, 3′-iodo: ***Polyandrocarpamide B***
[129369-42-2]
$C_{18}H_{15}IN_2O_3$ 434.233
Alkaloid from *Polyandrocarpa* sp. λ_{max} 203 (ϵ 79100); 247 (ϵ 13200); 267 (sh); 274 (ϵ 7600); 311 (ϵ 8200) (MeOH/NaOH) (Derep). λ_{max} 205 (ϵ 50000); 230 (sh); 254 (ϵ 9100); 267 (sh); 274 (ϵ 8200); 325 (ϵ 6600) (MeOH) (Derep).
Da Settimo, A. *et al., Farmaco, Ed. Sci.*, 1987, **42**, 17-26 (*synth*)
Lindquist, N. *et al., Tet. Lett.*, 1990, **31**, 2521-2524 (*isol, uv, ir, pmr, cmr, struct*)

Polyandrocarpamide D P-519

*5-(1*H-*Indol-3-yl)-5-methoxy-2,4-imidazolidinedione, 9CI*

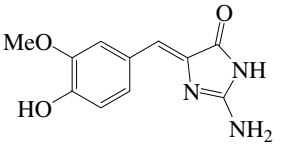


$C_{12}H_{11}N_3O_3$ 245.237

(±)-form [129369-43-3]
Alkaloid from the marine ascidian *Polyandrocarpa* sp. and from the sponge *Zyzza massalis*. Exhibits antibacterial and antifungal activity. Yellow amorph. solid. Artifact. λ_{max} 212 (ϵ 27500); 268 (ϵ 5000); 276 (ϵ 400); 287 (ϵ 3800) (MeOH) (Derep). λ_{max} 204 (ϵ 44800); 217 (sh); 268 (ϵ 4600); 277 (ϵ 4600); 289 (ϵ 3700) (MeOH/NaOH) (Derep).
Lindquist, N. *et al., Tet. Lett.*, 1990, **31**, 2521-2524 (*isol, uv, ir, pmr, cmr, struct*)
Mancini, I. *et al., Helv. Chim. Acta*, 1994, **77**, 1886-1894 (*isol, pmr, cmr*)

Polyandrocarpamine A P-520

[444106-74-5]

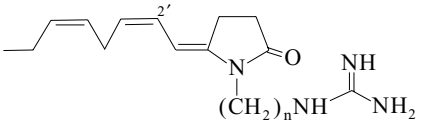


$C_{11}H_{11}N_3O_3$ 233.226
Isol. from the Fijian ascidian *Polyandrocarpa* sp. Yellow solid. λ_{max} 246 (ϵ 2000); 352 (ϵ 2000) (MeOH).

O-*De-Me:* ***Polyandrocarpamine B***
[444106-75-6]
$C_{10}H_9N_3O_3$ 219.199
Isol. from *Polyandrocarpa* sp. Yellow solid. λ_{max} 248 (ϵ 2000); 352 (ϵ 2000) (MeOH).
Davis, R.A. *et al., Tetrahedron*, 2002, **58**, 3263-3269 (*isol, synth, uv, ir, pmr, cmr*)

Polyandrocarpidine A P-521

[5-[2-(2,5-Octadienylidene)-5-oxo-1-pyrrolidinyl]pentyl]guanidine, 9CI
[68838-36-8]



n = 5

$C_{18}H_{30}N_4O$ 318.461
The polyandrocarpidines constitute a 9:1 mixt. of homologues, each homologue being a mixt. of isomers with isomer ratios varying from 4:1 to 1:1. Polyandrocarpidines A and B correspond to the former Polyandrocarpidine I, and the minor polyandrocarpidines C and D to the former Polyandrocarpidine II. Isol. from a marine tunicate *Polyandrocarpa* sp. Shows antimicrobial and cytotoxic props. λ_{max} 275 (MeOH) (Berdy).

*(2′*E*)-Isomer:* ***Polyandrocarpidine B***
[84453-26-9]
$C_{18}H_{30}N_4O$ 318.461
From *Polyandrocarpa* sp. Shows antimicrobial and cytotoxic props. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 276 (ϵ 1000) (MeOH) (Berdy).
Cheng, M.T. *et al., J.A.C.S.*, 1978, **100**, 7409-7411 (*isol*)
Carté, B. *et al., Tet. Lett.*, 1982, **23**, 3863-3866 (*isol, uv, pmr, cmr, struct*)
Rinehart, K.L. *et al., Tet. Lett.*, 1983, **24**, 1593-1596 (*struct*)

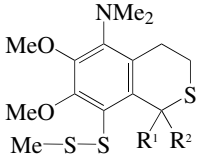
Polyandrocarpidine C P-522

[4-[2-(2,5-Octadienylidene)-5-oxo-1-pyrrolidinyl]butyl]guanidine, 9CI
[68838-37-9]
As Polyandrocarpidine A, P-521 with
n = 4
$C_{17}H_{28}N_4O$ 304.434
See note under Polyandrocarpidine A, P-521. Constit. of a marine tunicate *Polyandrocarpa* sp. Shows antimicrobial and cytotoxic props. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 275 (MeOH) (Berdy).

*(2′*E*)-Isomer:* ***Polyandrocarpidine D***
[84453-27-0]
$C_{17}H_{28}N_4O$ 304.434
From *Polyandrocarpa* sp. Shows antimicrobial and cytotoxic props. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 275 (MeOH) (Berdy).
Cheng, M.T. *et al., J.A.C.S.*, 1978, **100**, 7409-7411 (*isol*)
Carté, B. *et al., Tet. Lett.*, 1982, **23**, 3863-3866 (*isol, uv, pmr, cmr, struct*)
Rinehart, K.L. *et al., Tet. Lett.*, 1983, **24**, 1593-1596 (*struct*)

Polycarpamine A P-523

*3,4-Dihydro-1,6,7-trimethoxy-*N,N*-dimethyl-8-(methyldithio)-1*H*-2-benzothiopyran-5-amine, 9CI. 5-(Dimethylamino)-3,4-dihydro-1,6,7-trimethoxy-8-(methyldithio)-1*H*-2-benzothiopyran*
[128420-43-9]



R^1 = OMe, R^2 = H

$C_{15}H_{23}NO_3S_3$ 361.55
Isol. from the marine ascidian *Polycarpa auzata*. Antifungal agent. Yellow oil. Racemic. λ_{max} 236 (ϵ 17400); 256 (sh); 278 (ϵ 4400); 305 (sh); 375 (ϵ 13200) (MeOH) (Derep).

Lindquist, N. *et al., Tet. Lett.*, 1990, **31**, 2389 (*isol, uv, ir, pmr, cmr, struct*)

Polycarpamine B P-524

*5-(Dimethylamino)-3,4-dihydro-6,7-dimethoxy-8-(methyldithio)-1*H*-2-benzothiopyran-1-one, 9CI*
[128397-81-9]
As Polycarpamine A, P-523 with
R^1, R^2 = O

$C_{14}H_{19}NO_3S_3$ 345.507
Isol. from the marine ascidian *Polycarpa auzata*. Antifungal agent. Yellow oil. λ_{max} 228 (ϵ 22600); 240 (sh); 270 (ϵ 5200); 305 (sh) (MeOH). λ_{max} 228 (ϵ 12000); 270 (ϵ 5200); 305 (MeOH) (Berdy).

Lindquist, N. *et al., Tet. Lett.*, 1990, **31**, 2389-2392 (*isol, uv, ir, pmr, cmr*)

Polycarpamine C P-525

*5-(Dimethylamino)-3,4-dihydro-6,7-dimethoxy-8-(methyldithio)-1*H*-2-benzothiopyran-1-thione, 9CI*
[128397-82-0]
As Polycarpamine A, P-523 with
R^1, R^2 = S

$C_{14}H_{19}NO_2S_4$ 361.574
Isol. from the marine ascidian *Polycarpa auzata*. Yellow oil. λ_{max} 236 (ϵ 17400); 256 (sh); 278 (ϵ 4400); 305 (sh); 375 (ϵ 13200) (MeOH).

Lindquist, N. *et al., Tet. Lett.*, 1990, **31**, 2389-2392 (*isol, uv, ir, pmr, cmr*)

Polycarpamine D P-526

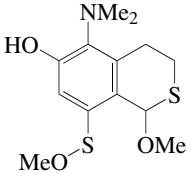
[128397-83-1]
As Polycarpamine A, P-523 with
R^1 = OMe, R^2 = $COCH_3$

$C_{17}H_{25}NO_4S_3$ 403.587
Isol. from the marine ascidian *Polycarpa auzata*. Yellow oil. Racemic. λ_{max} 238 (ϵ 32900); 277 (ϵ 6100) (MeOH).

Lindquist, N. *et al., Tet. Lett.*, 1990, **31**, 2389-2392 (*isol, uv, ir, pmr, cmr*)

Polycarpamine E P-527

[128397-84-2]

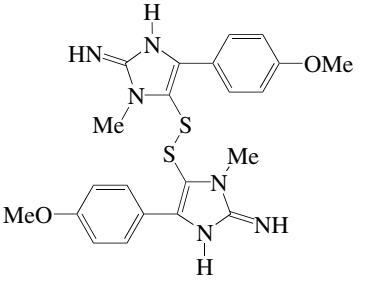


$C_{13}H_{19}NO_3S_2$ 301.43
Isol. from the marine ascidian *Polycarpa auzata*. Yellow oil. λ_{max} 207 (ϵ 11000); 230 (ϵ 10800); 255 (sh) (MeOH). λ_{max} 204 (ϵ 54200); 233 (ϵ 8700); 313 (ϵ 40) (MeOH/NaOH) (Berdy).

Lindquist, N. *et al., Tet. Lett.*, 1990, **31**, 2389-2392 (*isol, uv, ir, pmr, cmr*)

Polycarpine P-528

[175669-17-7]



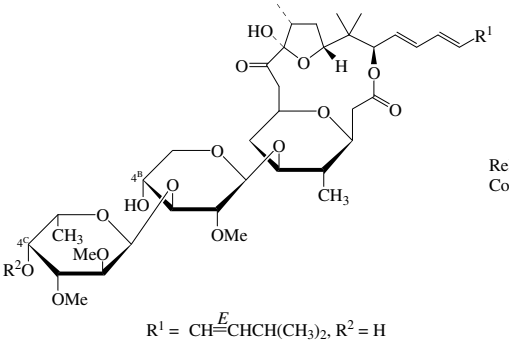
$C_{22}H_{24}N_6O_2S_2$ 468.603
Neutral form illus. The nat. prod. appears to be the dication. Alkaloid from the ascidians *Polycarpa clavata* and *Polycarpa aurata*. Cytotoxic against the human colon tumour cell line HCT-116. Red rods (MeOH/CH_2Cl_2) or orange amorph. solid. Mp 201-204°. λ_{max} 226 (ϵ 21820); 264 (ϵ 23708); 364 (ϵ 9323) (no solvent reported).

Hydrochloride (1:2): [175669-29-1]
Orange rods. Mp 201-203°. Delocalised charges within the two iminoimidazole residues. λ_{max} 202 (log ϵ 4.45); 259 (log ϵ 4.28); 394 (log ϵ 3.58) (MeOH).

Abbas, S.A. *et al., J.O.C.*, 1996, **61**, 2709-2712 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Kang, H. *et al., Tet. Lett.*, 1996, **37**, 2369-2372 (*isol, uv, ir, pmr, cmr, struct*)
Radchenko, O.S. *et al., Tet. Lett.*, 1997, **38**, 3581-3584 (*synth*)

Polycavernoside A_2 P-529

[167613-49-2]



Relative Configuration

R^1 = $CH\overset{E}{=}CHCH(CH_3)_2$, R^2 = H

$C_{42}H_{66}O_{15}$ 810.974
Isol. from the red alga *Polycavernosa tsudai* (*Gracilaria edulis*). Toxin. Oil. λ_{max} 259 (ϵ 25000); 270 (ϵ 32000); 280 (ϵ 26000) (MeCN) (Berdy).

4^B-Me ether: ***Polycavernoside A***
[146644-24-8]
$C_{43}H_{68}O_{15}$ 825.001
Isol. from *Polycavernosa tsudai*. Toxin. Amorph. solid. λ_{max} 259 (ϵ 25000); 270 (ϵ 32000); 280 (ϵ 26000) (MeCN) (Derep). λ_{max} 259 (ϵ 25000); 270 (ϵ 32000); 280 (ϵ 26000) (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 0.2 mg/kg.

4^B,4^C-Di-Me ether: ***Polycavernoside A_3***
[167613-48-1]
$C_{44}H_{70}O_{15}$ 839.028
Isol. from *Polycavernosa tsudai*. Toxin. Oil. λ_{max} 259; 270; 280 (MeCN).

Yotsu-Yamashita, M. *et al., J.A.C.S.*, 1993, **115**, 1147 (*isol, pmr, cmr*)
Hayashi, N. *et al., Chem. Lett.*, 1994, 2143; 2147 (*synth*)
Fujiwara, K. *et al., Chem. Lett.*, 1995, 855 (*pmr, config*)
Yotsu-Yamashita, M. *et al., Tet. Lett.*, 1995, **36**, 5563 (*isol, pmr, ms*)
Fujiwara, K. *et al., J.A.C.S.*, 1998, **120**, 10770-10771 (*synth, abs config*)
Paquette, L.A. *et al., J.A.C.S.*, 2000, **122**, 619-631 (*synth*)
Blakemore, P.R. *et al., J.O.C.*, 2005, **70**, 5449-5460 (*synth*)

Polycavernoside B_2 P-530

[167504-54-3]
As Polycavernoside A_2, P-529 with
$R^1 = CH(CH_3)_2$, $R^2 = CH_3$
$C_{41}H_{66}O_{15}$ 798.963
Isol. from the red alga *Polycavernosa tsudai* (*Gracilaria edulis*). Phycotoxin. Oil. λ_{max} 228 (MeCN).

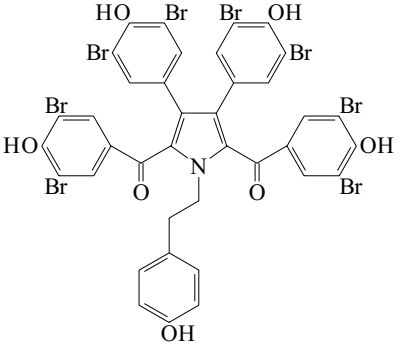
4^B-Ac: ***Polycavernoside B***
[146586-41-6]
$C_{43}H_{68}O_{16}$ 841.001
Isol. from *Polycavernosa tsudai*. Phycotoxin. Oil. λ_{max} 259 (ϵ 25000); 270 (ϵ 32000); 280 (ϵ 26000) (MeCN) (Derep). λ_{max} 220 (MeCN).
▶ LD_{50} (mus, ipr) .2 mg/kg.
Yotsu-Yamashita, M. *et al., Tet. Lett.*, 1995, **36**, 5563 (*isol, pmr, ms*)

Polychaete excitatory peptide P-531

[488822-81-7]
KCTGPWAIHACGGGN
$C_{62}H_{93}N_{21}O_{17}S_2$ 1468.679
Struct. of reduced form shown. Isol. from the marine polychaete *Perinereis vancaurica*. Myoactive agent.
Matsushima, O. *et al., Peptides (N.Y.)*, 2002, **23**, 1379-1390 (*isol*)

Polycitone A P-532

[153212-84-1]

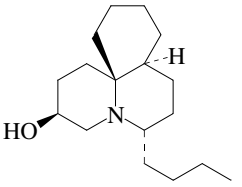


$C_{38}H_{21}Br_8NO_7$ 1242.818
Alkaloid from the marine ascidian *Polycitor* sp. Inhibits retroviral reverse transcriptase and DNA polymerase. Fibroblast inhibitor.
Yellowish needles + $1Me_2CO$ (Me_2CO).
Mp 285°. λ_{max} 285 (ϵ 13500) (MeOH) (Berdy).

N-*Dealkyl:* ***Polycitone B***
[272118-06-6]
$C_{30}H_{13}Br_8NO_6$ 1122.668
Alkaloid from *Polycitor africanus*. Yellow oil.

Rudi, A. *et al., J.O.C.*, 1994, **59**, 999-1003 (*isol, uv, ir, pmr, cmr, cryst struct*)
Loya, S. *et al., Biochem. J.*, 1999, **344**, 85-92 (*activity*)
Rudi, A. *et al., J. Nat. Prod.*, 2000, **63**, 832-833 (*Polycitone B*)
Kreipl, A.T. *et al., Org. Lett.*, 2002, **4**, 3287-3288 (*synth*)
Gupton, J.T. *et al., Tetrahedron*, 2005, **61**, 1845-1854 (*synth*)

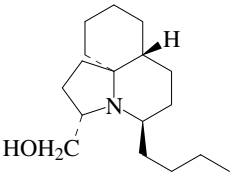
Polycitorol A P-533



Relative Configuration

$C_{17}H_{31}NO$ 265.438
Alkaloid from an ascidian of the family Polycitoridae. Oil.
$[\alpha]_D^{25}$ +15.3 (c, 0.2 in $CHCl_3$).
Issa, H.H. *et al., Mar. Drugs*, 2005, **3**, 78-85 (*isol, pmr, cmr*)

Polycitorol B P-534

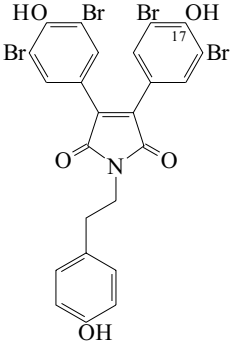


Relative Configuration

$C_{17}H_{31}NO$ 265.438
Alkaloid from an ascidian of the family Polycitoridae. Oil.
$[\alpha]_D^{25}$ -10.3 (c, 0.6 in $CHCl_3$).
Issa, H.H. *et al., Mar. Drugs*, 2005, **3**, 78-85 (*isol, pmr, cmr*)

Polycitrin A P-535

[153212-85-2]



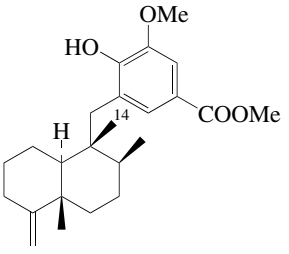
$C_{24}H_{15}Br_4NO_5$ 717.002
Alkaloid from the marine ascidian *Polycitor* sp. Yellowish oil or red cryst.
Mp 180-181°.

17-Me ether: ***Polycitrin B***
[153212-86-3]
$C_{25}H_{17}Br_4NO_5$ 731.029
From *Polycitor* sp. Cryst. (CH_2Cl_2/pentane) (synthetic).
Mp 140-142° (synthetic).

Rudi, A. *et al., J.O.C.*, 1994, **59**, 999 (*isol, uv, ir, pmr, cmr, struct*)
Terpin, A. *et al., Tetrahedron*, 1995, **51**, 9941-9946 (*synth*)
Beccalli, E.M. *et al., Tetrahedron*, 2000, **56**, 2699-2702 (*synth, Polycitrin B*)

Polyfibrospongol A P-536

[185618-01-3]



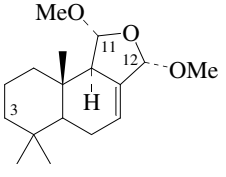
$C_{24}H_{34}O_4$ 386.53
Constit. of *Polyfibrospongia australis*. Amorph. solid. $[\alpha]_D^{25}$ +5.3 (c, 0.3 in $CHCl_3$). λ_{max} 227 (log ϵ 4.51); 269 (log ϵ 4.22); 297 (log ϵ 3.88) (MeOH).

14-Hydroxy: ***Polyfibrospongol B***
[185618-02-4]
$C_{24}H_{34}O_5$ 402.53
Constit. of *Polyfibrospongia australis*. Amorph. solid. $[\alpha]_D^{25}$ +1.8 (c, 0.18 in $CHCl_3$). λ_{max} 227 (log ϵ 4.58); 270 (log ϵ 4.23); 301 (log ϵ 3.85) (MeOH).

Shen, Y.-C. *et al., J. Nat. Prod.*, 1997, **60**, 93 (*isol, pmr, cmr*)

Polygodial acetal P-537

[98204-88-7]



$C_{17}H_{28}O_3$ 280.406
From *Polygonum hydropiper* and *Casella winterana*. Yellow oil.

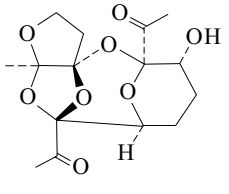
*11-*O*-De-Me, 11-Ac:* ***11-O-Acetyl-11-de-O-methylpolygodial acetal***
[85356-03-2]
$C_{18}H_{28}O_4$ 308.417
Constit. of *Doriopsilla albopunctata*.
$[\alpha]_D$ -17.2 (c, 0.25 in $CHCl_3$).

3β-Acetoxy: ***3β-Acetoxypolygodial 12α-acetal***
[160668-36-0]
$C_{19}H_{30}O_5$ 338.443
Constit. of *Casella winterana*. Oil.

12-Epimer, 3β-acetoxy: ***3β-Acetoxypolygodial 12β-acetal***
[160708-98-5]
$C_{19}H_{30}O_5$ 338.443
Constit. of *Casella winterana*. Cryst.
Mp 110-113°.

Okuda, R.K. *et al., J.O.C.*, 1983, **48**, 1866-1869 (*11-de-Me 11-Ac*)
Fukuyama, Y. *et al., Phytochemistry*, 1985, **24**, 1521-1524 (*isol, pmr, ms*)
Ying, B.-P. *et al., Phytochemistry*, 1995, **38**, 909-915 (*isol, pmr, cmr, ms*)

Laurencia Polyketal P-538

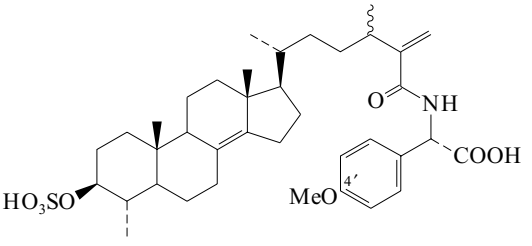


$C_{15}H_{20}O_8$ 328.318
Not named in the paper. Constit. of red alga *Laurencia chilensis*.
Cryst. (EtOAc).
Mp 182-185°. Racemate.

Bittner, M. *et al., Tet. Lett.*, 1987, **28**, 4031 (*cryst struct*)

Polymastiamide A P-539

[151606-40-5]



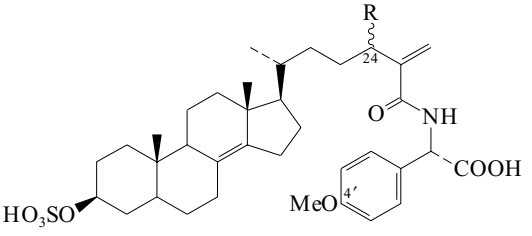
$C_{38}H_{55}NO_8S$ 685.92
Constit. of *Polymastia boletiformis*. Amorph. solid (as Na salt). $[\alpha]_D^{21}$ +67.4 (c, 1.1 in MeOH). λ_{max} 224 (ϵ 8840); 272 (ϵ 1520); 278 (ϵ 1270) (MeOH) (Derep).

4′-Demethoxy: ***Polymastiamide E***
$C_{37}H_{53}NO_7S$ 655.894
Constit. of *Polymastia boletiformis*. λ_{max} 224; 272; 278 (MeOH) (Berdy).

Kong, F. *et al., J.O.C.*, 1993, **58**, 6924-6927 (*Polymastiamide A*)
Kong, F. *et al., J. Nat. Prod.*, 1996, **59**, 379-385 (*Polymastiamide B*)

Polymastiamide B P-540

[174630-07-0]



R = CH_3

$C_{37}H_{53}NO_8S$ 671.894
Isol. from *Polymastia boletiformis*. λ_{max} 224; 272; 278 (MeOH) (Berdy).

Δ^{24}-Isomer: ***Polymastiamide C***
[174630-08-1]
$C_{37}H_{53}NO_8S$ 671.894
Constit. of *Polymastia boletiformis*. λ_{max} 224; 272; 278 (MeOH) (Berdy).

4′-Demethoxy, Δ^{24}-isomer: ***Polymastiamide F***
[174630-11-6]
$C_{36}H_{51}NO_7S$ 641.867
Constit. of *Polymastia boletiformis*. λ_{max} 224; 272; 278 (MeOH) (Berdy).

Kong, F. *et al., J. Nat. Prod.*, 1996, **59**, 379-385 (*isol*)

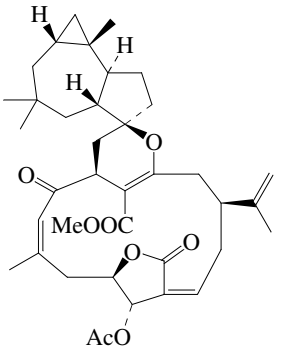
Polymastiamide D P-541

[174630-09-2]
As Polymastiamide B, P-540 with
R = H, Δ^{24}-isomer
$C_{36}H_{51}NO_8S$ 657.867
Constit. of *Polymastia boletiformis*. λ_{max} 224; 272; 278 (MeOH) (Berdy).

Kong, F. *et al., J. Nat. Prod.*, 1996, **59**, 379-385 (*isol*)

Polymaxenolide P-542

[679395-09-6]

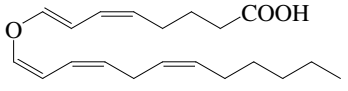


$C_{38}H_{50}O_8$ 634.808
Constit. of *Sinularia maxima* x *Sinularia polydactyla*. Cryst. Mp 189-191°. $[\alpha]_D^{25}$ +83.9.

Kamel, H.N. *et al., Tet. Lett.*, 2004, **45**, 1995-1997 (*isol, pmr, cmr, cryst struct*)

Polyneuric acid P-543

8-(1,3,6-Dodecatrienyloxy)-5,7-octadienoic acid
[189082-69-7]



$C_{20}H_{30}O_3$ 318.455

Me ester: [189082-70-0]
$C_{21}H_{32}O_3$ 332.482
Isol. from the red alga *Polyneura latissima*.

Jiang, Z.-D. *et al., Lipids*, 1997, **32**, 231-235 (*isol, pmr, cmr*)

Polyphemusin I P-544

[125139-67-5]

H-Arg-Arg-Trp-Cys-Phe-Arg-Val-Cys-Tyr-Arg-Gly-Phe-Cys-Tyr-Arg-Lys-Cys-Arg-NH_2
Isol. from the haemocytes of the horseshoe crab *Limulus polyphemus*. Antimicrobial agent.

Akaji, K. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2661 (*synth*)
Miyata, T. *et al., J. Biochem. (Tokyo)*, 1989, **106**, 663 (*isol, props*)
Ohta, M. *et al., Antimicrob. Agents Chemother.*, 1992, **36**, 1460 (*props*)

Polyphemusin II P-545

[125139-68-6]

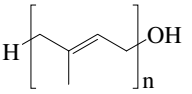
H-Arg-Arg-Trp-Cys-^{5}Phe-Arg-^{7}Val-Cys-Tyr-Lys-Gly-^{12}Phe-Cys-Tyr-Arg-Lys-Cys-Arg-NH_2
Isol. from the haemocytes of the horseshoe crab *Limulus polyphemus*. Antimicrobial agent.

5,12-Dityrosine, 7-lysine analogue: [Tyr^{5,12},Lys^{7}]Polyphemusin II. T22
[142960-16-5]
$C_{109}H_{168}N_{38}O_{22}S_4$ 2491.032
Chemokine CXCR4 receptor antagonist. Anti-HIV agent.

Miyata, T. *et al., J. Biochem. (Tokyo)*, 1989, **106**, 663 (*isol, props*)
Ohta, M. *et al., Antimicrob. Agents Chemother.*, 1992, **36**, 1460 (*props*)
Masuda, M. *et al., Biochem. Biophys. Res. Commun.*, 1992, **189**, 845-850 (*T22, synth, pharmacol*)
Tamamura, H. *et al., Biochem. Biophys. Res. Commun.*, 1996, **229**, 648-652 (*T22, pharmacol*)

Polyprenol P-546

Betulaprenol. Castaprenol. Albizziaprenol. Cleomeprenol. Cappaprenol. Ficaprenol. Malloprenol. Polyisoprenol. Polyprenyl alcohol. Polyisoprenyl alcohol. Moraprenol
[10589-57-8]



The betulaprenol number indicates the no. of isoprene units. Various geom. isomers isol., although most isolates are of undetd. isomers or mixts. Synonyms for most isolates are given here together regardless of geom. isomerism; Cleomeprenols (Malloprenols, Ficaprenols) appear to be the 3*Z*-isomers. Isol. from birch (*Betula verrucosa*). Also (n = 13-15) isol. as Albizziaprenol from leaves of *Albizzia zygia* and from other biol. sources.

Dihydro: See Dolichols in *The Combined Chemical Dictionary.*

Betulaprenol 6

Betulahexaprenol. Hexaisoprenol
[5915-64-0]
$C_{30}H_{50}O$ 426.724
Oil.

Betulaprenol 7

Betulaheptaprenol. Heptaisoprenol
[5905-41-9]
$C_{35}H_{58}O$ 494.843
Oil.

O-*[β-D-Xylopyranosyl-(1→4)-β-D-xylopyranoside]:* ***Plakopolyprenoside***
[265658-62-6]
$C_{45}H_{74}O_9$ 759.074
Isol. from the sponge *Plakortis simplex*. Cytotoxic agent. Amorph. solid. $[\alpha]_D$ -9.

O-*[β-D-Xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-xylopyranoside]:* ***Plaxyloside***
[394657-64-8]
$C_{65}H_{106}O_{25}$ 1287.537
Constit. of *Plakortis simplex*. Amorph. solid. $[\alpha]_D^{25}$ +21 (c, 0.3 in MeOH).

Betulaprenol 8

Betulaoctaprenol. Octaisoprenol
[5905-42-0]
$C_{40}H_{66}O$ 562.961
Oil.

Betulaprenol 9

Solanesol*. Betulanonaprenol. Nonaisoprenol*
[13190-97-1]
$C_{45}H_{74}O$ 631.079
Also from tobacco (*Nicotiana tabacum*). Oil or cryst. Mp 41.5-42.5°.

Betulaprenol 10

Decaprenol. Betuladecaprenol. Decaisoprenol
[15575-04-9]
$C_{50}H_{82}O$ 699.197
Found also in the spadix of *Arum maculatum*. Oil.

(2Z,6Z,10Z,14Z,18Z,22Z,26Z,30Z)-isomer: Arachisprenol 10
$C_{50}H_{82}O$ 699.197
Constit. of *Arachis hypogaea* (peanut). Oil.

Betulaprenol 11

Undecaprenol. Betulaundecaprenol. Undecaisoprenol
[15575-14-1]
$C_{55}H_{90}O$ 767.315
Found in faeces of silkworm grown on mulberry leaves and from *Staphylococcus aureus*. Oil.
Mp 9-10°.

(2Z,6Z,10Z,14Z,18Z,22Z,26Z,30Z,34Z)-isomer: ***Arachisprenol 11***
$C_{55}H_{90}O$ 767.315
Constit. of *Arachis hypogaea* (peanut). Oil.

Betulaprenol 12
Dodecaprenol. Betuladodecaprenol. Dodecaisoprenol
[15575-05-0]
$C_{60}H_{98}O$ 835.434
Isol. from faeces of silkworm grown on mulberry leaves, also from *Betula verrucosa*, *Quercus* spp. and others. Oil.
Mp 15-16°.

Ac: [99936-79-5]
$C_{62}H_{100}O_2$ 877.471
Isol. from *Abies alba* and *Picea abies.*

(2Z,6Z,10Z,14Z,18Z,22Z,26Z,30Z,34Z,38Z)-isomer: ***Arachisprenol 12***
$C_{60}H_{98}O$ 835.434
Constit. of *Arachis hypogaea* (peanut). Oil.

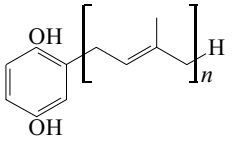
Betulaprenol 13
Betulatridecaprenol. Tridecaprenol. Tridecaisoprenol
[20741-08-6]
$C_{65}H_{106}O$ 903.552
Oil.

[17093-81-1, 26296-50-4, 28973-73-1, 56453-70-4, 56453-71-5, 59684-99-0, 72690-19-8, 86903-50-6, 96647-64-2]

Rüegg, R. *et al., Helv. Chim. Acta*, 1960, **43**, 1745 (*synth*)
Carruthers, W. *et al., Chem. Ind. (London)*, 1962, 1020 (*ms, Solanesol*)
Wellburn, A.R. *et al., Biochem. J.*, 1966, **102**, 313; 325 (*isol*)
Wellburn, A.B. *et al., Nature (London)*, 1966, **212**, 1364 (*isol*)
Fukawa, H. *et al., Tet. Lett.*, 1966, 6209 (*isol*)
Tabacik-Wlotzku, C. *et al., Phytochemistry*, 1967, **6**, 597 (*isol*)
Gough, D.P. *et al., Biochem. J.*, 1970, **117**, 309 (*biosynth*)
Higashi, Y. *et al., J. Biol. Chem.*, 1970, **245**, 3697 (*isol*)
Morton, R.A. *et al., Biochem. J.*, 1972, **128**, 11P (*rev*)
Suga, T. *et al., J.C.S. Perkin 1*, 1980, 2098 (*Cleomeprenol 12*)
Suga, T. *et al., Phytochemistry*, 1980, **19**, 2327 (*Malloprenol 12*)
Pachaly, P. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1983, **316**, 615 (*Albizziaprenol*)
Monaco, P. *et al., J. Nat. Prod.*, 1983, **46**, 174
Sato, K. *et al., Chem. Lett.*, 1984, 1105 (*synth*)
Sato, K. *et al., Chem. Comm.*, 1986, 1761 (*synth*)
Suga, T. *et al., J.A.C.S.*, 1986, **108**, 2366 (*biosynth*)
Novikova, M.A. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1987, 356 (*synth*)
Tanaka, Y. *et al., Chem. Phys. Lipids*, 1989, **51**, 183 (*pmr*)
Suga, T. *et al., J.O.C.*, 1989, **54**, 3390 (*isol, bibl*)
Desoky, E.K. *et al., Phytochemistry*, 1995, **39**, 1383 (*isol, pmr*)
Barrero, A.F. *et al., J. Nat. Prod.*, 1997, **60**, 65 (*Betulaprenol 6, pmr, cmr*)
Aoki, T. *et al., Phytochemistry*, 1997, **46**, 715-720 (*Arachisprenols, Glycinoprenols 7 and 8*)
Costantino, V. *et al., Tetrahedron*, 2000, **56**, 1393-1395 (*Plakopolyprenoside*)
Costantino, V. *et al., Eur. J. Org. Chem.*, 2001, 4457-4462 (*Plaxyloside*)
Fukusaki, E. *et al., Biosci., Biotechnol., Biochem.*, 2004, **68**, 19 8-1990 (*Solanesol, synth*)

2-Polyprenyl-1,4-benzenediol P-547

Polyprenylhydroquinone



For lower homologues see 2-(3-Methyl-2-butenyl)-1,4-benzenediol, M-216, 2-(3,7-Dimethyl-2,6-octadienyl)-1,4-benzenediol, D-974 and Farnesylhydroquinone, F-13. The polyprenyl side chains are numbered here with the prenyl unit adjoining the aryl ring numbered (1′-5′) and so down the chain. Shows analgesic props.

2-Tetraprenyl-1,4-benzenediol
2-(3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraenyl)-1,4-benzenediol. Tetraprenylhydroquinone. Geranylgeranylhydroquinone
[39703-09-8]
$C_{26}H_{38}O_2$ 382.585
Obt. from trichomes of *Phacelia minor* and *Phacelia parryi* and from the marine sponge *Ircinia* sp. Constit. of *Lactarius lignyotus.* Cryst. Mp 35-36°. n = 4.
► Potent contact allergen.

Quinone: Geranylgeranylbenzoquinone. Tetraprenylbenzoquinone
[39703-08-7]
$C_{26}H_{36}O_2$ 380.569
Isol. from sponges *Ircinia muscarum* and *Ircinia ramosa*. Yellow oil.

2-Pentaprenyl-1,4-benzenediol
Pentaprenylhydroquinone
[123086-34-0]
$C_{31}H_{46}O_2$ 450.703
Constit. of the sponges *Sarcotragus* sp. and *Dysidea pallescens.* Cytotoxic.

1-Sulfate: [160210-20-8]
$C_{31}H_{46}O_5S$ 530.767
Constit. of *Sarcotragus* sp. HIV-1 and HIV-2 transcriptase inhibitor.

4-Sulfate: [170661-38-8]
[170661-36-6]
$C_{31}H_{46}O_5S$ 530.767
Isol. from an *Ircinia* sp.

Quinone: 2-(3,7,11,15,19-Pentamethyl-2,6,10,14,18-eicosapentaenyl)-1,4-benzoquinone. 2-Pentaprenyl-1,4-benzoquinone
[56111-39-8]
$C_{31}H_{44}O_2$ 448.687
Isol. from sponge *Dysidea pallescens.* Yellow oil. λ_{max} 246 (ϵ 10470); 311 (ϵ 316) (MeOH) (Derep).

2-Hexaprenyl-1,4-benzenediol
2-(3,7,11,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaenyl)-1,4-benzenediol, 9CI. Hexaprenylhydroquinone
[119980-00-6]
$C_{36}H_{54}O_2$ 518.821
Constit. of the sponges *Hippospongia communis*, *Sarcotragus* sp. and *Dysidea* sp. Shows analgesic props. ATP inhibitor. n = 6.

1-Sulfate: [179822-86-7]
$C_{36}H_{54}O_5S$ 598.886
Isol. from *Dysidea* sp. and *Ircinia muscarum*. CAS no. refers to Na salt.

4-Sulfate: [170661-39-9]
[144861-49-4]
$C_{36}H_{54}O_5S$ 598.886
Isol. from *Ircinia* sp. and *Sarcotragus spinulosus.* Amorph. λ_{max} 283 (ϵ 2700) (EtOH).

2-Heptaprenyl-1,4-benzenediol
2-(3,7,11,15,19,23,27-Heptamethyl-2,6,10,14,18,22,26-octacosaheptaenyl)-1,4-benzenediol, 9CI. Heptaprenylhydroquinone. Heptaprenyl p-*quinol*
[113714-90-2]
$C_{41}H_{62}O_2$ 586.94
Constit. of the sponge *Hippospongia communis.* Shows antibacterial activity; exhibits analgesic props. n = 7.

1-Sulfate: [159154-49-1]
$C_{41}H_{62}O_5S$ 667.004
Isol. from *Ircinia fasciculata*. CAS no. refers to Na salt.

4-Sulfate: [170244-21-0]
$C_{41}H_{62}O_5S$ 667.004
Isol. from *Ircinia spinulosa*. CAS no. refers to Na salt.

Disulfate: [144861-50-7]
$C_{41}H_{62}O_8S_2$ 747.068
Isol. from *Sarcotragus spinulosus.* Amorph. CAS no. refers to Na salt. λ_{max} 283 (ϵ 2700) (EtOH).

Quinone: Heptaprenylbenzoquinone
[113714-92-4]
$C_{41}H_{60}O_2$ 584.924
Artifact.

5′-Hydroxy: 2-(3-Hydroxymethyl-7,11,15,19,23,27-hexamethyl-2,6,10,14,18,22,26-octacosaheptaenyl)-1,4-benzenediol
[170661-42-4]
$C_{41}H_{62}O_3$ 602.939
Isol. from an *Ircinia* sp.

25′-Hydroxy: 2-(19-Hydroxymethyl-3,7,11,15,23,27-hexamethyl-2,6,10,14,18,22,26-octacosaheptaenyl)-1,4-benzenediol
[868843-79-2]
$C_{41}H_{62}O_3$ 602.939
Constit. of *Ircinia spinulosa*. λ_{max} 203 (ϵ 6800); 275 (ϵ 850) (hexane).

2-Octaprenyl-1,4-benzenediol
2-(3,7,11,15,19,23,27,31-Octamethyl-2,6,10,14,18,22,26,30-dotriacontaoctaenyl)-1,4-benzenediol, 9CI. Octaprenylhydroquinone
[113714-91-3]
$C_{46}H_{70}O_2$ 655.058
Constit. of sponges *Hippospongia communis*, *Ircinia spinulosa* and *Ircinia fasciculata*. Shows analgesic props. Muscle relaxant. n = 8. λ_{max} 293 (ϵ 3110) (cyclohexane) (Derep). λ_{max} 294 (MeOH) (Berdy). λ_{max} 211 (ϵ 10400); 291 (ϵ 2600) (hexane) (Berdy).

1-Sulfate: [224169-48-6]
$C_{46}H_{70}O_5S$ 735.122
Isol. from *Sarcotragus* sp. Yellow solid. CAS no. refers to Na salt. λ_{max} 280 (ϵ 2500) (MeOH).

4-Sulfate: [144861-51-8]
$C_{46}H_{70}O_5S$ 735.122
Isol. from *Ircinia spinulosa* and *Sarcotragus spinulosus*. Amorph. CAS no. refers to Na salt.

Quinone: Octaprenylbenzoquinone
[113714-93-5]
$C_{46}H_{68}O_2$ 653.042
Artifact. λ_{max} 245 (ϵ 15800); 315 (ϵ 1580); 440 (ϵ 46) (cyclohexane) (Derep).

15′-Hydroxy: 2-(11-Hydroxymethyl-3,7,15,19,23,27,31-heptamethyl-2,6,10,14,18,22,26,30-dotriacontaoctaenyl)-1,4-benzenediol, 9CI
[261713-57-9]
$C_{46}H_{70}O_3$ 671.057
Constit. of an *Ircinia* sponge.

25′-Hydroxy, 4-sulfate: 2-(19-Hydroxymethyl-3,7,11,15,23,27,31-heptamethyl-2,6,10,14,18,22,26,30-dotriacontaoctaenyl)-1,4-benzenediol, 4-sulfate
[170244-22-1]
$C_{46}H_{70}O_6S$ 751.121
Isol. from *Ircinia spinulosa*. CAS no. refers to Na salt.

2-Nonaprenyl-1,4-benzenediol
2-(3,7,11,15,19,23,27,31,35-Nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl)-1,4-benzenediol, 9CI. Nonaprenylhydroquinone
[126832-53-9]
$C_{51}H_{78}O_2$ 723.176

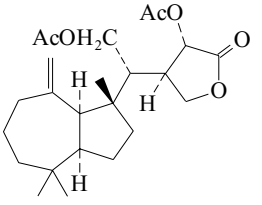
1-Sulfate: [224169-49-7]
$C_{51}H_{78}O_5S$ 803.24
Isol. from *Sarcotragus* sp. Yellow solid. λ_{max} 278 (ϵ 2500) (MeOH).

[119979-99-6]

Cimino, G. *et al., Experientia*, 1972, **28**, 1401-1402 (*Ircinia muscarum constits*)
Cimino, G. *et al., Tetrahedron*, 1972, **28**, 1315-1324 (*Ircinia spinulosa constits*)
Cimino, G. *et al., Tetrahedron*, 1975, **31**, 271-275 (*Pentaprenylbenzoquinone*)
Reynolds, G.W. *et al., Phytochemistry*, 1981, **20**, 1365-1366 (*Tetraprenylhydroquinone*)
Fusetani, N. *et al., Experientia*, 1987, **43**, 1233-1234 (*isol, Dysidea*)
Pouchus, Y.F. *et al., J. Nat. Prod.*, 1988, **51**, 188-189 (*Heptaprenylhydroquinone, Octaprenylhydroquinone*)
De Pasquale, R. *et al., Pharmacol. Res. Commun.*, *Suppl.* 5, 1988, **20**, 23-26 (*Hexaprenylhydroquinone, activity*)
Stonik, V.A. *et al., J. Nat. Prod.*, 1992, **55**, 1256-1260 (*isol, pmr, cmr, ms*)
Venkateswarlu, Y. *et al., J. Nat. Prod.*, 1994, **57**, 1286-1289 (*isol, pmr, cmr*)
Fuller, R.W. *et al., Nat. Prod. Lett.*, 1994, **5**, 179-181 (*Sarcotragus constits*)
Vidari, G. *et al., J. Nat. Prod.*, 1995, **58**, 893-896 (*Lactarius lignyotus constits*)
Bifulco, G. *et al., J. Nat. Prod.*, 1995, **58**, 1444-1449 (*Ircinia sulfates*)
De Rosa, S. *et al., J. Nat. Prod.*, 1995, **58**, 1450-1454 (*Ircinia sulfates*)
Perez Baz, J. *et al., J. Nat. Prod.*, 1996, **59**, 960-961 (*Ircinia muscarum constits*)
Wakimoto, T. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 727-730 (*Sarcotragus 2-sulfates*)
Erdogan, I. *et al., Nat. Prod. Sci.*, 1999, **5**, 177-180; *CA*, **132**, 234468 (*Hydroxyoctaprenylhydroquinone*)
Erdogan, I. *et al., J. Fac. Pharm. Gazi Univ.*, 2000, **17**, 1-7; *CA*, **133**, 249569h (*activity*)
Tziveleka, L.A. *et al., Chem. Biodiversity*, 2005, **2**, 901-909, (*25′-Hydroxyheptaprenylhydroquinone*)

Polyrhaphin A P-548

[121442-22-6]

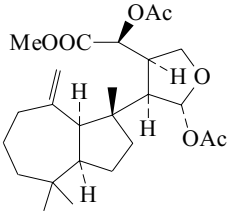


$C_{24}H_{36}O_6$ 420.545
Constit. of *Chromodoris norrisi* and *Aplysilla polyrhaphis*. Oil. $[\alpha]_D$ -23 (c, 0.8 in $CHCl_3$).

Bobzin, S.C. *et al., J.O.C.*, 1989, **54**, 3902-3907 (*isol, pmr, cmr*)

Polyrhaphin B P-549

[121442-23-7]

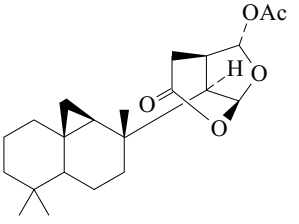


$C_{25}H_{38}O_7$ 450.571
Constit. of *Aplysilla polyrhaphis*. Feeding inhibitor. Oil. $[\alpha]_D$ +54.2 (c, 0.4 in $CHCl_3$).

Bobzin, S.C. *et al., J.O.C.*, 1989, **54**, 3902-3907 (*isol, pmr, cmr*)

Polyrhaphin C P-550

[121442-24-8]

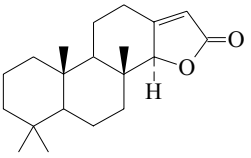


$C_{22}H_{32}O_5$ 376.492
Constit. of *Aplysilla polyrhaphis* and *Chromodoris norrisi*. Feeding inhibitor. Ichthyotoxic agent. Oil. $[\alpha]_D$ -25.3 (c, 0.3 in $CHCl_3$).

Bobzin, S.C. *et al., J.O.C.*, 1989, **54**, 3902-3907 (*isol, pmr, cmr*)

Polyrhaphin D P-551

[121442-25-9]



$C_{20}H_{30}O_2$ 302.456

Constit. of *Aplysilla polyrhaphis* and *Chromodoris norrisi*. Feeding inhibitor. Solid. $[\alpha]_D$ +6.7 (c, 0.12 in $CHCl_3$). λ_{max} 217 (ϵ 6700) (MeOH).

Bobzin, S.C. *et al., J.O.C.*, 1989, **54**, 3902-3907 (*isol, pmr, cmr*)

Polytheonamide P-552

A complex of linear 48-residue polypeptides with *N*-terminus blocked by a carbamoyl group. See ref. for structs. Isol. from the marine sponge *Theonella swinhoei*. Cytotoxic agent.

Polytheonamide A [157856-58-1]
[154530-64-0 (tripropylamine salt)]
$C_{211}H_{363}N_{61}O_{71}$ 4890.555

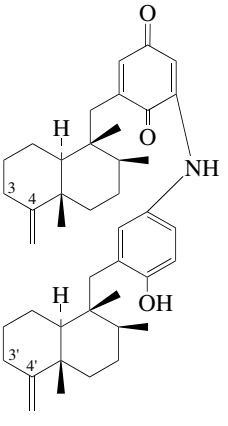
Polytheonamide B [157856-59-2]
[154530-65-1 (tripropylamine salt)]
$C_{211}H_{363}N_{61}O_{71}$ 4890.555
Stereoisomer of Polytheonamide A.

Polytheonamide C [157856-60-5]
[154530-66-2 (tripropylamine salt)]
$C_{212}H_{365}N_{61}O_{71}$ 4904.582

Hamada, T. *et al., Tet. Lett.*, 1994, **35**, 609-612; 719-720 (*isol, pmr*)
Hamada, T. *et al., J.A.C.S.*, 2005, **127**, 110-118 (*isol*)

Popolohuanone A P-553

[133056-07-2]



$C_{42}H_{57}NO_3$ 623.917

Terpenoid (clerodane) numbering shown; different numbering given in the lit. Isol. from the sponge *Dysidea* sp. Intense purple-blue powder. λ_{max} 222 (log ϵ 4.28); 266 (log ϵ 4.21); 512 (log ϵ 3.58) (hexane).

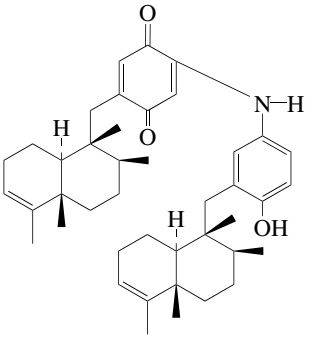
$\Delta^{3,4}$-Isomer: ***Popolohuanone B***
[133056-09-4]
$C_{42}H_{57}NO_3$ 623.917
Isol. from *Dysidea* sp. Purple-blue powder. λ_{max} 222 (log ϵ 4.08); 266 (log ϵ 3.98); 512 (log ϵ 3.36) (hexane).

$\Delta^{3,4;3',4'}$-Isomer: ***Popolohuanone C***
[144587-57-5]
$C_{42}H_{57}NO_3$ 623.917
Isol. from *Dysidea avara*. Dark violet amorph. solid. Mp 125-135°. $[\alpha]_D^{20}$ -9 (c, 0.08 in CH_2Cl_2). λ_{max} 232; 275; 532 (MeOH).

Rodriguez, A.D. *et al., Tetrahedron*, 1990, **46**, 8025-8030 (*isol, uv, ir, pmr, cmr, ms*)
Alvi, K.A. *et al., J.O.C.*, 1992, **57**, 6604-6607 (*Popolohuanone C, isol, uv, pmr, cmr, ms*)

Popolohuanone D P-554

[144587-58-6]



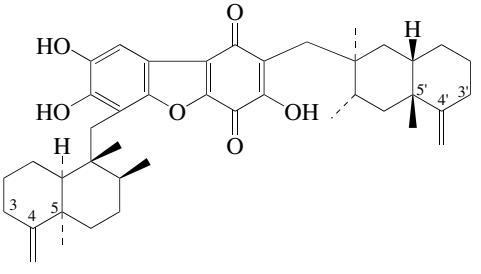
$C_{42}H_{57}NO_3$ 623.917

Isol. from the sponge *Dysidea avara*. Dark violet amorph. solid. Mp 113-120°. $[\alpha]_D$ -15 (c, 0.06 in $CHCl_3$). λ_{max} 234; 275; 533 (MeOH).

Alvi, K.A. *et al., J.O.C.*, 1992, **57**, 6604-6607 (*isol, uv, pmr, cmr, ms*)

Popolohuanone E P-555

[149992-95-0]



$C_{42}H_{54}O_6$ 654.885

Constit. of a *Dysidea* sp. A topoisomerase II inhibitor. Cytotoxic agent. Dark purple solid. Sol. MeOH. λ_{max} 222 (log ϵ 4.5); 254 (log ϵ 4.3); 284 (log ϵ 4); 364 (log ϵ 3.7); 530 (log ϵ 3.5) (MeOH).

$\Delta^{3},\Delta^{3'}$-Isomer, 5,5′-diepimer: [193157-89-0]
$C_{42}H_{54}O_6$ 654.885
Constit. of a *Dysidea* sp. Deep purple amorph. solid. λ_{max} 236; 254; 283; 371; 550 ($CHCl_3$).

Carney, J.R. *et al., Tet. Lett.*, 1993, **34**, 3727-3730 (*isol, pmr, cmr, uv, ir*)
Stewart, M. *et al., Aust. J. Chem.*, 1997, **50**, 341-347 (*isomer*)
Forsyth, C.J. *et al., J.A.C.S.*, 1998, **120**, 5597-5598 (*synth*)
Anderson, J.C. *et al., J.C.S. Perkin 1*, 1998, 2023-2030 (*synth*)

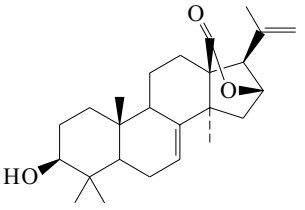
Porphyropsin P-556

[9009-58-9]

Visual pigment found in the rods of retina of fish and amphibians, contains Vitamin A_2 aldehyde.

Sebrell, W.H. *et al., The Vitamins*, Academic Press, 1967,

Posietogenin P-557



$C_{25}H_{36}O_3$ 384.558

3-O-*[3-Methyl-β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)-4-sulfato-β-D-xylopyranoside]:* ***Cucumarioside G₂***
[139307-93-0]
$C_{48}H_{74}O_{23}S$ 1051.165
Constit. of *Eupentacta fraudatrix* and *Pentamera calcigera*. Cryst. Mp 234-235°. $[\alpha]_D^{20}$ -46 (c, 0.1 in Py).

3-O-*[3*-O-*Methyl-β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfato-β-D-xylopyranoside]:* ***Calcigeroside B***
[253678-32-9]
$C_{54}H_{84}O_{27}S$ 1197.307
Constit. of *Pentamera calcigera*. Cryst. Mp 234-236°. $[\alpha]_D^{20}$ -49 (c, 0.1 in Py).

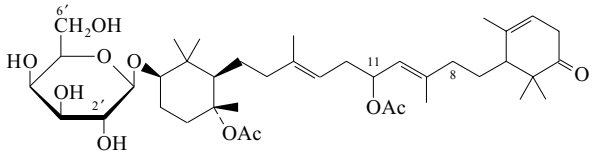
3-O-*[3*-O-*Methyl-β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfato-β-D-xylopyranoside]:* ***Calcigeroside C₁***
[253678-33-0]
$C_{54}H_{84}O_{28}S$ 1213.307
Constit. of *Pentamera calcigera*. Cryst. Mp 204-206°. $[\alpha]_D^{20}$ -60 (c, 0.1 in Py).

3-O-*[3*-O-*Methyl-β-D-xylopyranosyl-(1→3)-6*-O-*sulfo-β-D-glucopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside]:* ***Calcigeroside D₁***
[298693-51-3]
$C_{54}H_{84}O_{31}S_2$ 1293.371
Isol. from *Pentamera calcigera*. Mp 218-220° (as di-Na salt). $[\alpha]_D^{20}$ -49 (c, 0.1 in 50% Py aq.) (di-Na salt).

Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*biosynth*)
Avilov, S.A. *et al., J. Nat. Prod.*, 1994, **57**, 1166-1171 (*Cucumarioside G₂*)
Avilov, S.A. *et al., J. Nat. Prod.*, 2000, **63**, 65-71; 1349-1355 (*Calcigerosides*)

Pouoside C P-558

[114944-00-2]



$C_{40}H_{64}O_{11}$ 720.939
Constit. of a sponge of *Asteropus* sp. Oil.

8-Acetoxy: ***Pouoside A***
[114943-98-5]
$C_{42}H_{66}O_{13}$ 778.976
Constit. of *Asteropus* sp.

8-Acetoxy, 11-O-*de-Ac:* ***Pouoside B***
[114943-99-6]
$C_{40}H_{64}O_{12}$ 736.938
Constit. of *Asteropus* sp. Oil.

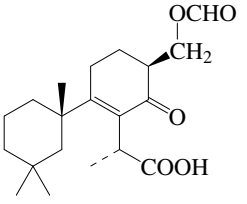
8-Acetoxy, 2′-Ac: ***Pouoside D***
[114944-01-3]
$C_{44}H_{68}O_{14}$ 821.013
Constit. of *Asteropus* sp. Oil.

8-Acetoxy, 6′-Ac: ***Pouoside E***
[114944-02-4]
$C_{44}H_{68}O_{14}$ 821.013
Constit. of *Asteropus* sp. Oil.

Ksebati, M.B. *et al., J.O.C.*, 1988, **53**, 3917-3921 (*isol, pmr, cmr*)

Pourewanone P-559

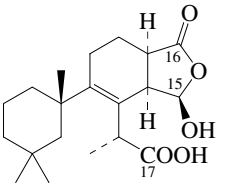
[676154-26-0]



$C_{20}H_{30}O_5$ 350.454
Constit. of *Chelonaplysilla violacea*. Solid. $[\alpha]_D^{20}$ +22.6 (c, 0.35 in CH_2Cl_2). λ_{max} 248 (ϵ 14425) (CH_2Cl_2).

Keyzers, R.A. *et al., Eur. J. Org. Chem.*, 2004, 419-425 (*isol, pmr, cmr*)

Pourewic acid B P-560



$C_{20}H_{30}O_5$ 350.454

Me ester: ***Methyl pourewate B***
[676154-30-6]
$C_{21}H_{32}O_5$ 364.481
Constit. of *Chelonaplysilla violacea*. Solid. $[\alpha]_D^{20}$ -81.8 (c, 0.7 in CH_2Cl_2).

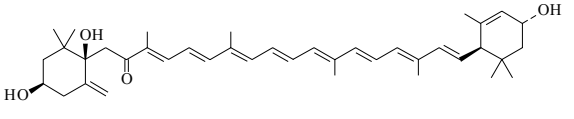
Me ether: ***15-O-Methylpourewic acid B****. 15-Methoxypourewic acid B (incorr.)*
[676154-29-3]
$C_{21}H_{32}O_5$ 364.481
Constit. of *Chelonaplysilla violacea*. Solid. $[\alpha]_D^{20}$ -368.6 (c, 0.23 in CH_2Cl_2).

16-Deoxo, Me ether: ***Pourewic acid A***
[676154-28-2]
$C_{21}H_{34}O_4$ 350.497
Constit. of *Chelonaplysilla violacea*. Solid. $[\alpha]_D^{20}$ -10.8 (c, 0.86 in CH_2Cl_2).

Keyzers, R.A. *et al., Eur. J. Org. Chem.*, 2004, 419-425 (*isol, pmr, cmr*)

Prasinoxanthin P-561

7,8-Dihydro-3,3′,6-trihydroxy-γ,ϵ-caroten-8-one
[94705-97-2]



$C_{40}H_{56}O_4$ 600.88
Constit. of algae within the Prasinophyceae. Useful as a chemosystematic marker for algae.

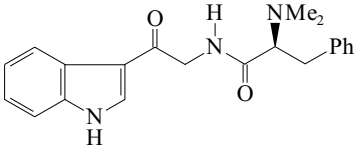
3′-Deoxy, 3′,4′-didehydro: ***Anhydroprasinoxanthin***
$C_{40}H_{54}O_3$ 582.865
Constit. of *Mantoniella squamata*.

7′,8′-Dihydro, 4′,5′-epoxide: 4′,5′-Epoxy-3,3′,6-trihydroxy-4′,5′,7,7′,8,8′-hexahydro-γ,ε-caroten-8-one. ***Dihydroprasinoxanthin epoxide***
[101527-80-4]
$C_{40}H_{58}O_5$ 618.895
Isol. from eucaryotic ultraplankon clones (Prasinophyceae). Stereochem. not firmly assigned. CAS name appears defective.
λ_{max} 430; 448 (Me_2CO).

Foss, P. *et al., Phytochemistry*, 1984, **23**, 1629 (*isol*)
Foss, P. *et al., Acta Chem. Scand., Ser. B*, 1986, **40**, 172
Foss, P. *et al., Phytochemistry*, 1986, **25**, 119 (*Dihydroprasinoxanthin epoxide*)
Egeland, E.S. *et al., Phytochemistry*, 1995, **40**, 515 (*deriv*)

Prealmazole C P-562

[161068-70-8]

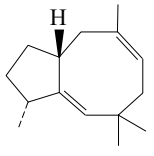


$C_{21}H_{23}N_3O_2$ 349.432
Alkaloid from an unidentified red Senegalese seaweed of the family Delesseriaceae.
$[\alpha]_D^{20}$ +38 (c, 0.25 in MeOH).

Guella, G. *et al., Helv. Chim. Acta*, 1994, **77**, 1999-2006 (*isol, pmr, cmr, ms, struct, synth*)

3,10-Precapnelladiene P-563

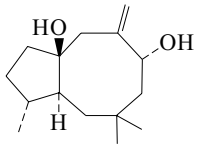
Precapnelladiene
[72715-05-0]



$C_{15}H_{24}$ 204.355
Constit. of *Capnella imbricata*. Oil.

Ayanoglu, E. *et al., Tetrahedron*, 1979, **35**, 1035 (*isol, struct*)
Mehta, G. *et al., J.O.C.*, 1987, **52**, 2875 (*synth*)
Petasis, N.A. *et al., Tet. Lett.*, 1990, **31**, 6799 (*synth*)
Inouye, Y. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 324 (*synth*)
MacDougall, J.M. *et al., J.O.C.*, 1997, **62**, 3792-3793; 1998, **63**, 6905-6913 (*synth*)

4(13)-Precapnellene-3,6-diol P-564

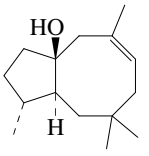


$C_{15}H_{26}O_2$ 238.369

(3α,6β,9βH)-form
Poitediol
[67382-31-4]
Constit. of *Laurencia poitei*.
Mp 40°. $[\alpha]_D$ -62.6 (c, 4.3 in $CHCl_3$).

Fenical, W. *et al., J.O.C.*, 1978, **43**, 3628 (*isol, struct*)
Gadwood, R.C. *et al., J.A.C.S.*, 1984, **106**, 3869 (*synth*)

3-Precapnellen-6-ol P-565



6β-*form*

$C_{15}H_{26}O$ 222.37

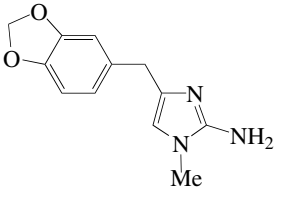
6β-form
Dactylol
[58542-75-9]
Constit. of *Aplysia dactylomela*.
Cryst. (hexane).
Mp 50.3-51.5°. $[\alpha]_D$ +22.5 (c, 1.76 in $CHCl_3$).

(ent-6β)-form
(-)-Dactylol
[244005-85-4]
Constit. of *Conocephalum conicum*.

Schmitz, F.J. *et al., Tetrahedron*, 1978, **34**, 2719 (*isol*)
Gadwood, R.C. *et al., Chem. Comm.*, 1985, 123 (*synth*)
Hayasaka, K. *et al., Tet. Lett.*, 1985, **26**, 873 (*synth*)
Feldman, K.S. *et al., J.A.C.S.*, 1990, **112**, 8490 (*synth*)
Molander, G.A. *et al., J.O.C.*, 1995, **60**, 4559 (*synth*)
Fürstner, A. *et al., J.O.C.*, 1996, **61**, 8746 (*synth*)
Melching, S. *et al., Phytochemistry*, 1999, **51**, 517-523 (*(-)-Dactylol*)

Preclathridine A P-566

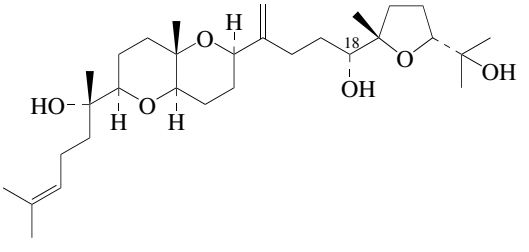
*4-(1,3-Benzodioxol-5-ylmethyl)-1-methyl-1*H*-imidazole-2-amine, 9CI. 2-Amino-1-methyl-4-(3,4-methylenedioxybenzyl)-1*H*-imidazole*
[146556-27-6]



$C_{12}H_{13}N_3O_2$ 231.254
Metab. from the nudibranch *Notodoris gardineri*. Anthelminthic. Yellow oil. λ_{max} 208; 285 (MeOH).

Alvi, K.A. *et al., Tetrahedron*, 1993, **49**, 329-336 (*isol, uv, pmr, cmr, ms, struct*)
Kawasaki, I. *et al., Heterocycles*, 1996, **43**, 1375 (*synth*)
Molina, P. *et al., J.O.C.*, 1999, **64**, 2540-2544 (*synth, pmr, cmr*)

Predehydrovenustatriol P-567

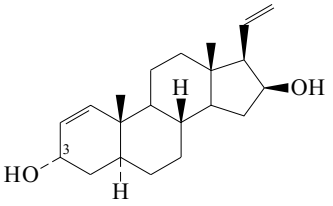


$C_{30}H_{52}O_6$ 508.737

18-Ac: ***Predehydrovenustatriol acetate***
[189453-24-5]
$C_{32}H_{54}O_7$ 550.774
Constit. of *Laurencia viridis*. Oil. $[\alpha]_D^{25}$ +20.6 (c, 0.33 in $CHCl_3$).

Norte, M. *et al., Tetrahedron*, 1997, **53**, 4649-4654 (*isol, pmr, cmr*)

Pregna-1,20-diene-3,16-diol P-568



$C_{21}H_{32}O_2$ 316.483

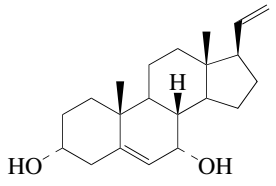
(3α,5α,16β)-*form*
Solid. $[\alpha]_D^{17}$ -63 (c, 0.2 in $CHCl_3$).

Di-Ac: [168004-86-2]
$C_{25}H_{36}O_4$ 400.557
Constit. of *Capnella thyrsoidea*. Oil. $[\alpha]_D^{21}$ +133 (c, 0.53 in $CHCl_3$).

3-Ketone: 16β-Hydroxypregna-1,20-dien-3-one
$C_{21}H_{30}O_2$ 314.467
Yellow oil. $[\alpha]_D^{17}$ +12 (c, 0.24 in $CHCl_3$).

3-Ketone, 16-Ac: [168004-85-1]
$C_{23}H_{32}O_3$ 356.504
Constit. of *Capnella thyrsoidea*. Oil. $[\alpha]_D^{21}$ +91 (c, 0.58 in $CHCl_3$).
Hooper, G.J. *et al., Tetrahedron*, 1995, **51**, 9973 (*isol, pmr, cmr*)

Pregna-5,20-diene-3,7-diol P-569



$C_{21}H_{32}O_2$ 316.483

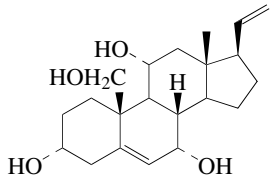
(3α,7α)-*form*

3-Ac: [190451-04-8]
$C_{23}H_{34}O_3$ 358.52
Constit. of *Pieterfaurea unilobata*. Plates (EtOAc/hexane).
Mp 156-159°. $[\alpha]_D^{25}$ -84 (c, 0.02 in $CHCl_3$).

(3β,7α)-*form*

7-Ac: [190451-05-9]
$C_{23}H_{34}O_3$ 358.52
Constit. of *Pieterfaurea unilobata*. Yellow oil. $[\alpha]_D^{25}$ -198 (c, 0.17 in $CHCl_3$).
Beukes, D.R. *et al., J. Nat. Prod.*, 1997, **60**, 573-577 (*isol, pmr, cmr, cryst struct*)

Pregna-5,20-diene-3,7,11,19-tetrol P-570

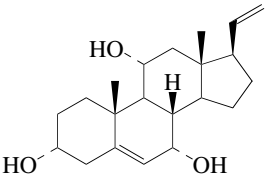


$C_{21}H_{32}O_4$ 348.481

(3α,7α,11α)-*form*

3,7,19-Tri-Ac: [190451-09-3]
$C_{27}H_{38}O_7$ 474.593
Constit. of *Pieterfaurea unilobata*. Yellow oil. $[\alpha]_D^{25}$ -114 (c, 0.013 in $CHCl_3$).
Beukes, D.R. *et al., J. Nat. Prod.*, 1997, **60**, 573-577 (*isol, pmr, cmr*)

Pregna-5,20-diene-3,7,11-triol P-571



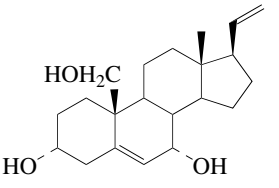
$C_{21}H_{32}O_3$ 332.482

(3α,7α,11α)-*form*

3-Ac: [190451-06-0]
$C_{23}H_{34}O_4$ 374.519
Constit. of *Pieterfaurea unilobata*. Powder.
Mp 226-229° (dec.). $[\alpha]_D^{25}$ -65 (c, 0.08 in $CHCl_3$).

3,7-Di-Ac: [190451-07-1]
$C_{25}H_{36}O_5$ 416.556
Constit. of *Pieterfaurea unilobata*. Oil. $[\alpha]_D^{25}$ -113 (c, 0.09 in $CHCl_3$).
Beukes, D.R. *et al., J. Nat. Prod.*, 1997, **60**, 573-577 (*isol, pmr, cmr*)

Pregna-5,20-diene-3,7,19-triol P-572

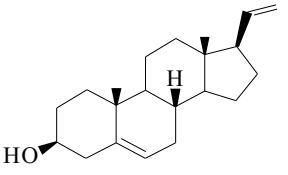


$C_{21}H_{32}O_3$ 332.482

(3α,7α)-*form*

3,19-Di-Ac: [190451-08-2]
$C_{25}H_{36}O_5$ 416.556
Constit. of *Pieterfaurea unilobata*.
$[\alpha]_D^{25}$ -82 (c, 0.04 in $CHCl_3$).
Beukes, D.R. *et al., J. Nat. Prod.*, 1997, **60**, 573-577 (*isol, pmr, cmr*)

Pregna-5,20-dien-3-ol P-573



$C_{21}H_{32}O$ 300.483

3β-*form* [21321-88-0]
Constit. of *Gersemia rubiformis*, *Pieterfaurea unilobata* and the gorgonian *Muricea fruticosa*. Also from sponge *Damiriana hawaiiana*.
Noncryst. $[\alpha]_D^{26}$ -58 (c, 0.05 iin $CHCl_3$).

3-O-β-D-Arabinopyranoside: [654074-73-4]
$C_{26}H_{40}O_5$ 432.599
Constit. of *Cladiella krempfi*.

3-O-β-D-Xylopyranoside: [460060-22-4]
$C_{26}H_{40}O_5$ 432.599
Constit. of *Eunicea pinta*. Cryst.
Mp 210°. $[\alpha]_D^{25}$ -57.3 (c, 0.75 in MeOH).

3-O-α-L-Fucopyranoside: ***Swiftiapregnene***
[746655-95-8]
$C_{27}H_{42}O_5$ 446.626
Constit. of a *Cladiella* sp. Cryst. (MeOH).
Mp 206-208°.

3-O-*(3*-O-*Acetyl-α-L-fucopyranoside):* ***Stereonsteroid H***
[876756-54-6]
$C_{29}H_{44}O_6$ 488.663
Constit. of *Stereonephthya crystalliana*.
$[\alpha]_D^{25}$ -41.5 (c, 0.3 in $CHCl_3$).

3-O-*(4*-O-*Acetyl-α-L-fucopyranoside):* [198274-25-8]
$C_{29}H_{44}O_6$ 488.663
Constit. of a *Eunicea* sp. Oil. $[\alpha]_D^{24}$ -150 (c, 0.3 in $CHCl_3$). λ_{max} 216 (log ϵ 3.34) (MeOH).

3-O-*β-D-Galactopyranoside:* [115952-25-5]
$C_{27}H_{42}O_6$ 462.625
Constit. of *Pseudoplexaura wagenaari*. Cryst. (CH_2Cl_2/MeOH). Mp 268-270°.

3-O-*(6*-O-*Acetyl-α-L-galactopyranoside):* [798575-31-2]
$C_{29}H_{44}O_7$ 504.662
Constit. of *Muricea* cf. *purpurea*. Glass. $[\alpha]_D$ -115 (c, 0.6 in $CHCl_3$).

3-O-*(6*-O-*Acetyl-β-D-galactopyranoside):* [656250-28-1]
$C_{29}H_{44}O_7$ 504.662
Constit. of *Eunicea laciniata*. Semi-solid. $[\alpha]_D$ -193.7 (c, 0.09 in $CHCl_3$).

3-O-*(2-Acetamido-3,4,6-tri*-O-*acetyl-2-deoxy-β-D-galactopyranoside):* ***Muricin 1***
[97564-92-6]
$C_{35}H_{51}NO_9$ 629.789
Isol. from *Muricea fruticosa*. Antifouling factor. $[\alpha]_D^{26}$ +26.3 (c, 1.6 in $CHCl_3$).

3-O-*(2-Acetamido-3,4-di*-O-*acetyl-2-deoxy-6*-O-*butanoyl-β-D-galactopyranoside):* ***Muricin 2***
[97564-93-7]
$C_{37}H_{55}NO_9$ 657.843
From *Muricea fruticosa*. Antifouling factor. $[\alpha]_D^{27}$ -29.7 (c, 1.4 in $CHCl_3$).

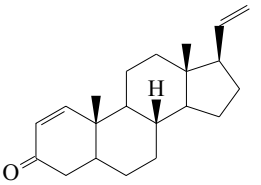
3-O-*(2-Acetamido-3,6-di*-O-*acetyl-2-deoxy-4*-O-*butanoyl-β-D-galactopyranoside):* ***Muricin 3***
[97564-94-8]
$C_{37}H_{55}NO_9$ 657.843
From *Muricea fruticosa*. Antifouling factor. $[\alpha]_D^{27}$ -30.3 (c,1.2 in $CHCl_3$).

3-O-*(2-Acetamido-3*-O-*acetyl-2-deoxy-4,6-di*-O-*butanoyl-β-D-galactopyranoside):* ***Muricin 4***
[97564-95-9]
$C_{39}H_{59}NO_9$ 685.896
From *Muricea fruticosa*. Antifouling factor.
Mp 119-121°. $[\alpha]_D^{27}$ +35.8 (c, 0.8 in $CHCl_3$).

Ac: [72560-37-3]
$C_{23}H_{34}O_2$ 342.52
Constit. of a *Scleronephthya* sp. Cryst.
Mp 134-136°. $[\alpha]_D$ +78 (c, 0.66 in $CHCl_3$).

Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476 (*isol, sponge*)
Kingston, J.F. *et al., J.C.S. Perkin 1*, 1979, 2064 (*isol*)
Bandurraga, M.M. *et al., Tetrahedron*, 1985, **41**, 1057-1065 (*Muricins*)
Dawe, R.D. *et al., Can. J. Chem.*, 1987, **65**, 661 (*synth, pmr, cmr*)
Wasylyk, J.M. *et al., J. Nat. Prod.*, 1989, **52**, 391-394 (*galactopyranoside, cryst struct, pmr, cmr*)
Kirk, D.N. *et al., J.C.S. Perkin 2*, 1990, 1567 (*pmr*)
Beukes, D.R. *et al., J. Nat. Prod.*, 1997, **60**, 573-577 (*isol, pmr, cmr*)
Cóbar, O.M. *et al., J. Nat. Prod.*, 1997, **60**, 1186-1188 (*acetylfucopyranoside*)
Shi, Y.-P. *et al., J. Nat. Prod.*, 2002, **65**, 1232-1241 (*xylopyranoside, cryst struct*)
Lan, W.J. *et al., Gaodeng Xuexiao Huaxue Xuebao*, 2003, **24**, 2019-2021; *CA*, **140**, 160637a (*arabinoside*)
Marville, K.I. *et al., Heterocycles*, 2004, **63**, 107-113 (*6-acetylgalactoside*)
Gutiérrez, M. *et al., Tet. Lett.*, 2004, **45**, 7833-7836 (*6-acetylgalactoside*)
Yan, X.-H. *et al., Youji Huaxue*, 2004, **24**, 1233-1238; *CA*, **142**, 71702 (*Ac*)
Zhang, G.-W. *et al., Gaodeng Xuexiao Huaxue Xuebao*, 2005, **26**, 81-83; *CA*, **142**, 444768k (*Swiftiapregnene*)
Wang, S.-K. *et al., J. Nat. Prod.*, 2006, **69**, 103-106 (*Stereonsteroid H*)

Pregna-1,20-dien-3-one P-574



$C_{21}H_{30}O$ 298.467

5α-form [65754-62-3]
Constit. of *Capnella thyrsoidea*, *Capnella erecta* and a *Scleronephthya* sp. Also isol. from an unidentified soft coral from Canton Island.
Needles.
Mp 125-126°. $[\alpha]_D^{17}$ +45 (c, 1.11 in $CHCl_3$). λ_{max} 229 (ϵ 9630) (EtOH).

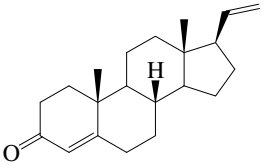
1α,2α-Epoxide: ***1,2-Epoxypregn-20-en-3-one***
[65754-67-8]
$C_{21}H_{30}O_2$ 314.467
Constit. of a *Scleronephthya* sp. Cryst.
Mp 153-156°. $[\alpha]_D$ +80 (c, 0.64 in $CHCl_3$).

[161816-76-8]

Higgs, M.D. *et al., Steroids*, 1977, **30**, 379-388 (*isol*)
Blackman, A.J. *et al., Aust. J. Chem.*, 1985, **38**, 565 (*isol, pmr*)
Hooper, G.J. *et al., Tetrahedron*, 1995, **51**, 9973 (*isol, pmr, cmr*)
Yan, X.-H. *et al., Youji Huaxue*, 2004, **24**, 1233-1238; *CA*, **142**, 71702, (*isol, pmr*)

Pregna-4,20-dien-3-one P-575

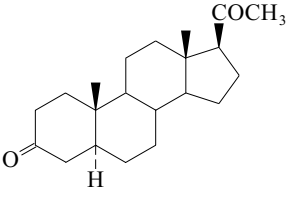
[21317-81-7]



$C_{21}H_{30}O$ 298.467
Constit. of *Subergorgia mollis*. Cryst.
Mp 72-73°. $[\alpha]_D^{27}$ +57 (c, 2.1 in $CHCl_3$). λ_{max} 241 (log ϵ 4.09) (MeOH).

Wu, S.-L. *et al., J. Chin. Chem. Soc. (Taipei)*, 2004, **51**, 205-208; *CA*, **141**, 103421x (*isol, pmr, cmr*)

Pregnane-3,20-dione P-576



$C_{21}H_{32}O_2$ 316.483

5α-form [566-65-4]
Semisynthetic steroid prod. from pregn-4-ene-3,20-dione by incubating with *Cortinarius evernius, Mycobacterium smegmatis, Ophiobolus herpotrichus* or *Penicillium urticae*.
Cryst. (Me_2CO). Mp 198-201°. $[\alpha]_D^{28}$ +121 (c, 1.038 in $CHCl_3$).
▶ TU4157150

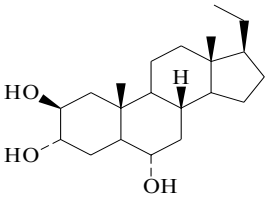
3-Di-Me acetal: ***3,3-Dimethoxypregnan-20-one***
[18603-79-7]
$C_{23}H_{38}O_3$ 362.551

Constit. of *Subergorgia suberosa*.

[14957-73-4, 51154-66-6, 51154-68-8, 76094-56-9, 76094-57-0, 98301-13-4]

Subrahmanyam, C. *et al., Indian J. Chem., Sect. B*, 2003, **42**, 219-220 (*dimethyl acetal*)

Pregnane-2,3,6-triol P-577

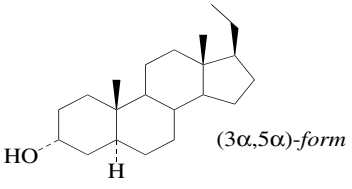


$C_{21}H_{36}O_3$ 336.514

(2β,3α,5α,6α)-*form*

Trisulfate: [163815-28-9]
$C_{21}H_{36}O_{12}S_3$ 576.706
Constit. of *Trachyopsis halichondroides*.
Makarieva, T.N. *et al., Steroids*, 1995, **60**, 316-320 (*isol, pmr, ms*)

Pregnan-3-ol P-578



(3α,5α)-*form*

$C_{21}H_{36}O$ 304.515

(3α,5α)-*form* [13164-12-0]
Cryst. (petrol). Mp 144-146°. Subl.$_{0.001}$ 110°. $[\alpha]_D^{20}$ +37.7 (c, 0.835 in $CHCl_3$).

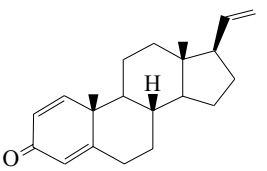
(3α,5β)-*form* [4352-07-2]
Isol. from urine of pregnant women.
Needles (Me_2CO).
Mp 148-149°. $[\alpha]_D^{26}$ +32.3 (c, 1 in $CHCl_3$).
Ac: [16054-60-7]
$C_{23}H_{38}O_2$ 346.552
Plates (MeOH). Mp 106°. $[\alpha]_D^{26}$ +52 (c, 1 in $CHCl_3$).

(3β,5α)-*form* [4352-06-1]
Isol. from Black Sea sponges *Haliclona* spp.
Flakes (MeOH).
Mp 138-139.5°. $[\alpha]_D^{30}$ +18 ($CHCl_3$).
Ac: [1242-01-9]
Cryst. (Me_2CO). Mp 114-116°. $[\alpha]_D^{30}$ +5.5 ($CHCl_3$).

(3β,5β)-*form* [3090-81-1]
Cryst. (MeOH). Mp 144°.
Ac: Mp 87°.
Marker, R.E. *et al., J.A.C.S.*, 1938, **60**, 2438 (*synth, 3β,5β-form*)
Ruzicka, L. *et al., Helv. Chim. Acta*, 1947, **30**, 867 (*synth, 3α,5α-form*)
Ruff, A. *et al., Helv. Chim. Acta*, 1951, **34**, 70 (*synth, 3β,5α-form*)
Cole, A.R.H. *et al., J.A.C.S.*, 1952, **74**, 5571 (*ir*)
Pierce, J.H. *et al., J.C.S.*, 1955, 694 (*synth, 3β,5β-form*)
Cummings, E.G. *et al., J.C.S.*, 1957, 3847 (*ir*)
Jones, R.N. *et al., J.A.C.S.*, 1958, **80**, 6121 (*ir*)
Waters, J.A. *et al., J.O.C.*, 1964, **29**, 428 (*synth, ir, 3β,5α-form*)
Benn, W.R. *et al., J.O.C.*, 1964, **29**, 1142 (*synth, 3β,5α-form*)
Gyermek, L. *et al., J. Med. Chem.*, 1968, **11**, 117 (*synth, uv, pmr*)
Lewbart, M.L. *et al., J.O.C.*, 1968, **33**, 1707 (*synth, 3α,5β-form*)
Kohli, J.M. *et al., Phytochemistry*, 1971, **10**, 442 (*synth, 3α,5α-form*)
Elenkov, I. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1999, **123**, 357-360 (*isol*)

Pregna-1,4,20-trien-3-one P-579

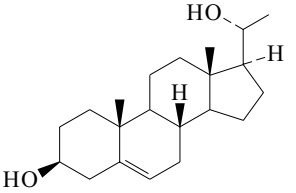
[65754-63-4]



$C_{21}H_{28}O$ 296.452
Constit. of sea raspberry *Gersemia rubiformis* and from an unidentified soft coral from Canton Island. Cryst. (MeOH); needles (MeOH aq.). Mp 166-167°. $[\alpha]_D^{20}$ +36.9 (c, 1.0 in $CHCl_3$). λ_{max} 244 (ϵ 12770) (EtOH).

Higgs, M.D. *et al., Steroids*, 1977, **30**, 379-388
Kingston, J.F. *et al., J.C.S. Perkin 1*, 1979, 2064 (*isol, synth*)

Pregn-5-ene-3,20-diol P-580



(3β,20*R*)–*form*

$C_{21}H_{34}O_2$ 318.498

(3β,20*R*)-*form* [901-57-5]
Occurs in the sponge *Haliclona rubens*. Cryst. (MeOH).
Mp 208-209° (200-205.5°). $[\alpha]_D$ -73 ($CHCl_3$).

(3β,20*S*)-*form*
3β,20α-form
[901-56-4]
Occurs in *Haliclona rubens*. Cryst. (EtOAc). Mp 183-184°.
$[\alpha]_D$ -53.3 (c, 1.12 in $CHCl_3$).

[10148-89-7, 32469-80-0, 59042-34-1, 76984-91-3]

Ballantine, J.A. *et al., Tet. Lett.*, 1977, **18**, 1547-1550 (*Haliclona rubens constits*)

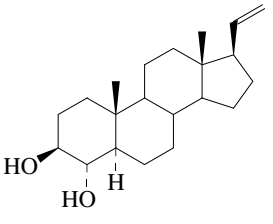
Pregn-20-ene-1,3-diol, 9CI P-581

$C_{21}H_{34}O_2$ 318.498

(1α,3α,5α)-*form*

3-Ac: [65754-65-6]
$C_{23}H_{36}O_3$ 360.536
Minor sterol from an unidentified soft coral from Canton Island. Cryst. (Me_2CO aq.). Mp 104-105°. $[\alpha]_D^{20}$ +51.1 (c, 1.06 in $CHCl_3$).
Higgs, M.D. *et al., Steroids*, 1977, **30**, 379

Pregn-20-ene-3,4-diol P-582



(3β,4α,5α)-*form*

$C_{21}H_{34}O_2$ 318.498

(3β,4α,5α)-*form* [92679-07-7]
Cryst. Mp 205°.

4-O-*β*-D-*Arabinopyranoside:* ***Pregnedioside A***
[92679-02-2]
$C_{26}H_{42}O_6$ 450.614
Constit. of the soft coral *Alcyonium* sp. Needles.
Mp 279°. $[\alpha]_D$ -92 (Py).

4-O-(*3*-O-*Acetyl*-*β*-D-*arabinopyranoside):* ***3′*-O-*Acetylpregnedioside A***
$C_{28}H_{44}O_7$ 492.651
Constit. of *Alcyonium* sp. Cryst. Mp 126°. $[\alpha]_D$ -148 ($CHCl_3$).

4-O-(*4*-O-*Acetyl*-*β*-D-*arabinopyranoside):* ***4′*-O-*Acetylpregnedioside A***
$C_{28}H_{44}O_7$ 492.651
Constit. of *Alcyonium* sp. Cryst. Mp 199°. $[\alpha]_D$ -96 ($CHCl_3$).

4-O-*β*-D-*Xylopyranoside:* ***Pregnedioside B***
[92679-03-3]
$C_{26}H_{42}O_6$ 450.614
Constit. of *Alcyonium* sp. Cryst. Mp 260°. $[\alpha]_D$ +2.6 (Py).

4-O-(*3*-O-*Acetyl*-*β*-D-*xylopyranoside):* ***3′*-O-*Acetylpregnedioside B***
[419572-94-4]
$C_{28}H_{44}O_7$ 492.651
Constit. of a *Lobophytum* sp. Cryst.
Mp 212-214°. $[\alpha]_D^{20}$ +150.6 (c, 0.02 in MeOH).

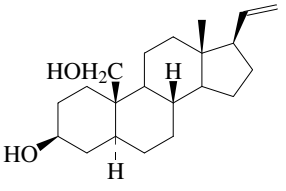
4-O-(*4*-O-*Acetyl*-*β*-D-*xylopyranoside):* ***4′*-O-*Acetylpregnedioside B***
$C_{28}H_{44}O_7$ 492.651
Constit. of *Alcyonium* sp. Cryst. Mp 193°. $[\alpha]_D$ -2.2 ($CHCl_3$).

(3β,4β,5β)-*form*
Cryst. Mp 125°.

4-O-(*2*-O-*Acetyl*-*6*-*deoxy*-*3*-O-*methyl*-*α*-L-*galactopyranoside):* ***Verrucoside***
[141544-59-4]
$C_{30}H_{48}O_7$ 520.705
Constit. of *Eunicella verrucosa*. Amorph. powder. $[\alpha]_D$ -30 (c, 2 in $CHCl_3$).

Kobayashi, M. *et al., Tet. Lett.*, 1984, **25**, 3731
Kashman, Y. *et al., J. Nat. Prod.*, 1991, **54**, 1651-1655 (*Verrucoside*)
He, X.-X. *et al., Huaxue Xuebao*, 2002, **60**, 334-337; *CA*, **136**, 337925p (*3′-Acetylpregnedioside B*)

Pregn-20-ene-3,19-diol P-583



$C_{21}H_{34}O_2$ 318.498

(3β,5α)-*form*
Stereonsteroid A
[876754-76-6]
Constit. of *Stereonephthya crystalliana*.
$[\alpha]_D^{25}$ +18.6 (c, 0.3 in $CHCl_3$).

3-O-(*4*-O-*Acetyl*-*α*-L-*fucopyranoside):* ***Stereonsteroid C***
[876754-78-8]
$C_{29}H_{46}O_7$ 506.678
Constit. of *Stereonephthya crystalliana*.
$[\alpha]_D^{25}$ -22 (c, 0.2 in $CHCl_3$).

19-Ac, 3-O-(*4*-O-*acetyl*-*α*-L-*fucopyranoside):* ***Stereonsteroid D***
[876756-88-6]
$C_{31}H_{48}O_8$ 548.715
Constit. of *Stereonephthya crystalliana*.
$[\alpha]_D^{25}$ -30.3 (c, 0.1 in $CHCl_3$).

19-Aldehyde: 3-Hydroxypregn-20-en-19-al
$C_{21}H_{32}O_2$ 316.483

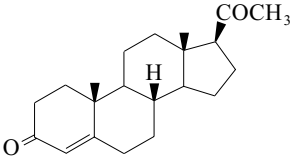
19-Aldehyde, 3-O-(*4*-O-*acetyl*-*α*-L-*fucopyranoside):* ***Stereonsteroid E***
[876756-57-9]
$C_{29}H_{44}O_7$ 504.662
Constit. of *Stereonephthya crystalliana*.
$[\alpha]_D^{25}$ -21.8 (c, 0.2 in $CHCl_3$).

19-Aldehyde, 3-Ac: ***Stereonsteroid B***
[876754-77-7]
$C_{23}H_{34}O_3$ 358.52
Constit. of *Stereonephthya crystalliana*.
$[\alpha]_D^{25}$ +15.4 (c, 0.3 in $CHCl_3$).

Wang, S.-K. *et al., J. Nat. Prod.*, 2006, **69**, 103-106 (*Stereonsteroids*)

Pregn-4-ene-3,20-dione, 9CI P-584

Progesterone, BAN, INN, USAN*. Agolutin. Corlutin. Gesterol. Glanducorpin. Luteohormone. Nalutron. Progestone. Syngesterone. Utrogestan. Vitarrine. Many other names*
[57-83-0]



$C_{21}H_{30}O_2$ 314.467
Progestational hormone secreted by corpus luteum during menstrual cycle. Also found in the gonads and haemolymph of crustaceans. Progestogen. Cryst. (petrol) in two forms.
Mp 121-122° Mp 127-131° (dimorph.). $[\alpha]_D^{20}$ +192 (c, 2 in dioxan).
Log P 3.77 (uncertain value) (calc).

▶ Adverse effects reported when used therapeutically incl. human (male and female) reprod. effects. Human teratogen. Exp. neoplastic agent. TW0175000

Dioxime:
$C_{21}H_{32}N_2O_2$ 344.496
Mp 243°.

(±)-*form* [14546-13-5]
Prisms (MeOH or hexane). Mp 183.5-185.5°.

17α-*form*
17-Isoprogesterone
[2000-66-0]
Cryst. (Et_2O/petrol). Mp 138-142°. $[\alpha]_D^{10}$ 0 (c, 0.9 in $CHCl_3$).

(8α,10α)-*form*
Cryst. (hexane). Mp 118-119°.

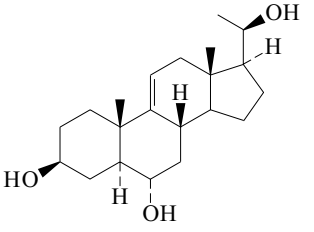
(9β,10α)-*form*
Retroprogesterone
[2755-10-4]
Cryst. (EtOH). Mp 163-164°. $[\alpha]_D^{20}$ -62 ($CHCl_3$).

[5750-05-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1052B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 578A (*nmr*)
Rushig, H. *et al., Chem. Ber.*, 1955, **88**, 883 (*synth*)
Beyer, K.F. *et al., J. Biol. Chem.*, 1956, **219**, 69 (*biosynth*)
Reerink, E.H. *et al., Nature (London)*, 1960, **186**, 168
Westerhof, P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1960, **79**, 771 (*synth, 9β,10α-form*)
Tsuda, K. *et al., Chem. Pharm. Bull.*, 1961, **9**, 925 (*synth*)
Westerhof, P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1961, **80**, 1048 (*synth, 8α10α-form*)
Rothchild, I. *et al., Vitam. Horm. (N.Y.)*, 1965, **23**, 209 (*physiology*)
Campsteyn, H. *et al., Acta Cryst. B*, 1972, **28**, 3032 (*cryst struct*)
Hammerum, S. *et al., Tetrahedron*, 1975, **31**, 2391 (*ms*)
Kim, D.J. *et al., Can. J. Chem.*, 1976, **54**, 3766 (*cmr*)
Raggio, M.L. *et al., J.O.C.*, 1976, **41**, 1873 (*synth*)
Gravestock, M.B. *et al., J.A.C.S.*, 1978, **100**, 4274 (*synth*)
IARC Monog., 1979, **21**, 491 (*tox, rev*)

Mauvais-Jarvis, P. *et al., Progesterone Progestins, [Int. Symp.], 1981 (1983)*, 1981, 1 (*rev*)
McCarty, K.S. *et al., Clin. Endocrinol. Metab.*, 1983, **12**, 133 (*rev*)
Johnson, W.S. *et al., J.A.C.S.*, 1983, **105**, 6653 (*synth*)
Boar, R.B. *et al., J.C.S. Perkin 1*, 1985, **6**, 1201 (*synth*)
Maggi, A. *et al., Life Sci.*, 1985, **37**, 893 (*rev*)
Silva, C.M. *et al., Mol. Mech. Steroid Horm. Action*, 1985, 141; 471; 659 (*rev*)
Wei, L.L. *et al., Steroids*, 1985, **46**, 678 (*rev*)
Numazawa, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3722 (*synth*)
Marat, K. *et al., Magn. Reson. Chem.*, 1987, **25**, 25 (*conformn, pmr*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 6332
Lemos, T.L.G. *et al., J. Nat. Prod.*, 1990, **53**, 152 (*synth*)
Kirk, D.N. *et al.,* T*J.C.S. Perkin 2*, 1990, 1567 (*pmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1194
Nicolaou, K.C. *et al., Classics in Total Synthesis, Targets, Strategies, Methods*, VCH, 1996, 83 (*bibl, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PMH500

Pregn-9(11)-ene-3,6,20-triol P-585



$C_{21}H_{34}O_3$ 334.498

(3β,5α,6α,20*R*)-*form*
Asterogenol
[75921-90-3]
Constit. of the starfish *Asterias forbesi*.
Cryst. (MeOH).
Mp 263-266°. $[\alpha]_D^{20}$ +8 (c, 0.124 in EtOH).

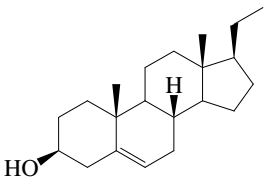
6-O-*(6-Deoxy-β-D-glucopyranoside), 3*-O-*sulfate:* ***Forbeside E1***
[129602-17-1]
$C_{27}H_{44}O_{10}S$ 560.705
Isol. from *Asterias forbesi*. Powder (as Na salt).
Mp 218° (Na salt). $[\alpha]_D^{28}$ +4.2 (c, 0.005 in H_2O).

6-O-*(6-Deoxy-β-D-glucopyranoside), 4′*-O-*sulfate:* ***Forbeside E2***
[129602-18-2]
$C_{27}H_{44}O_{10}S$ 560.705
Isol. from *Asterias forbesi*. Powder (as Na salt).
Mp 204° (Na salt). $[\alpha]_D^{28}$ +8 (c, 0.002 in H_2O).

6-O-*(6-Deoxy-β-D-glucopyranoside), 3,4′-di*-O-*sulfate:* ***Forbeside E***
[125127-57-3]
$C_{27}H_{44}O_{13}S_2$ 640.769
Isol. from *Asterias forbesi*. Powder (as di-Na salt).
Mp 238° dec. (di-Na salt). $[\alpha]_D$ +9.5 (c, 0.004 in H_2O).

ApSimon, J.W. *et al., Can. J. Chem.*, 1980, **58**, 2703-2708 (*Asterogenol*)
Findlay, J.A. *et al., Can. J. Chem.*, 1987, **65**, 1384-1391; 1989, **67**, 2078-2080 (*Forbesides*)
Findlay, J.A. *et al., J. Nat. Prod.*, 1990, **53**, 710-712 (*Forbesides*)

Pregn-5-en-3-ol P-586

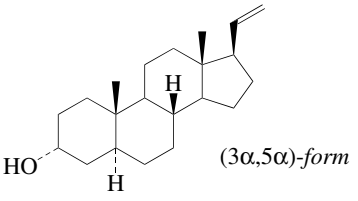


$C_{21}H_{34}O$ 302.499

3β-*form* [2862-58-0]
Trace sterol from the sponge *Damiriana hawaiiana* and from the termite *Nasutitermes rippertii*.
Cryst.
Mp 136.5-137.5°. Prob. artifact; derived from a sponge sample long stored in air and prob. derived by hydroperoxidation.

Ubik, K. *et al., Insect Biochem.*, 1974, **4**, 281-285 (*Nasutitermes rippertii constit*)
Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476 (*Damiriana hawaiiana constit*)

Pregn-20-en-3-ol P-587



$C_{21}H_{34}O$ 302.499

(3α,5α)-*form*
Ac: [65754-64-5]
$C_{23}H_{36}O_2$ 344.536
Minor sterol from an unidentified soft coral from Canton Island.
Needles (MeOH).
Mp 129-130°. $[\alpha]_D^{20}$ +9.4 (c, 0.8 in $CHCl_3$).

(3β,5α)-*form* [33300-02-6]
Constit. of a *Muricea* sp.
Powder. $[\alpha]_D^{25}$ -20 (c, 0.2 in CH_2Cl_2).

3-O-*β-D-Xylopyranoside:* ***Stereonsteroid I***
[876756-50-2]
$C_{26}H_{42}O_5$ 434.615
Constit. of *Stereonephthya crystalliana*.
$[\alpha]_D^{25}$ -52.6 (c, 0.2 in $CHCl_3$).

3-O-*(3*-O-*Acetyl-α-L-fucopyranoside):* ***Stereonsteroid G***
[876756-55-7]
$C_{29}H_{46}O_6$ 490.679
Constit. of *Stereonephthya crystalliana*.
$[\alpha]_D^{25}$ -31.4 (c, 0.2 in $CHCl_3$).

3-O-*(4*-O-*Acetyl-α-L-fucopyranoside):* ***Stereonsteroid F***
[876756-56-8]
$C_{29}H_{46}O_6$ 490.679
Constit. of *Stereonephthya crystalliana*.
$[\alpha]_D^{25}$ -30.6 (c, 0.1 in $CHCl_3$).

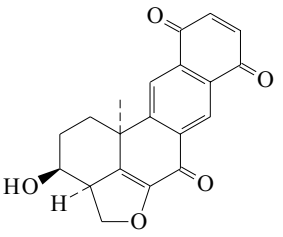
Ac: [22831-64-7]
$C_{23}H_{36}O_2$ 344.536
Constit. of a *Scleronephthya* sp. Cryst.
Mp 78-80°. $[\alpha]_D$ +73 (c, 0.42 in $CHCl_3$).

3-Ketone: ***Pregn-20-en-3-one***
[65754-69-0]
$C_{21}H_{32}O$ 300.483
Constit. of a *Scleronephthya* sp. Cryst.
Mp 115-117°. $[\alpha]_D$ +37 (c, 1 in $CHCl_3$).

Higgs, M.D. *et al., Steroids*, 1977, **30**, 379-388 (*3α,5α-form Ac*)
Yan, X.-H. *et al., Youji Huaxue*, 2004, **24**, 1233-1238; *CA*, **142**, 71702 (*Scleronephthya constits*)
Lorenzo, M. *et al., Eur. J. Org. Chem.*, 2006, 582-585 (*Muricea constit*)
Wang, S.-K. *et al., J. Nat. Prod.*, 2006, **69**, 103-106 (*Stereonsteroids*)

Prehalenaquinone P-588

[158786-75-5]



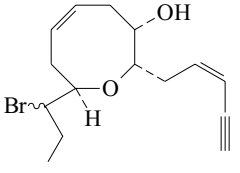
$C_{20}H_{16}O_5$ 336.343
Constit. of *Xestospongia sapra*. Putative biosynthetic precursor to Halenaquinol, H-9 and Xestoquinone, X-52. Cryst.
Mp 207° (synthetic). $[\alpha]_D$ -47.5 (c, 0.747 in $CHCl_3$) (synthetic).

Hydroquinone: Prehalenaquinol
$C_{20}H_{18}O_5$ 338.359
Powder.

Harada, N. *et al., J.O.C.*, 1994, **59**, 6606 (*isol, pmr, cmr, uv, synth*)

Prelaureatin P-589

2-(1-Bromopropyl)-8-(2-penten-4-ynyl)oxacyclooct-4-en-7-ol. 13-Bromo-6,12-epoxy-3,9-pentadecadien-1-yn-7-ol
[139610-22-3]



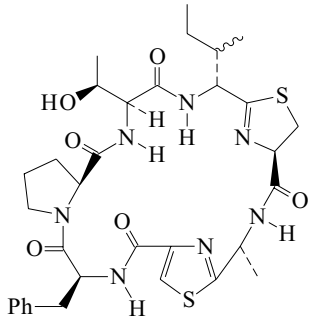
$C_{15}H_{21}BrO_2$ 313.234
Constit. of *Laurencia nipponica*. Oil. $[\alpha]_D^{25}$ +75.8 (c, 0.29 in $CHCl_3$).

Ac:
$C_{17}H_{23}BrO_3$ 355.271
Isol. from *Laurencia obtusa*. Stereochem. homology with prelaureatin not certain (ref. inaccessible).

Fukuzawa, A. *et al., Tet. Lett.*, 1991, **32**, 5597 (*isol, pmr*)
Aydogmus, Z. *et al., Acta Pharm. Turc.*, 1999, **41**, 93-95; *CA*, **132**, 178047 (*Ac*)
Crimmins, M.T. *et al., J.A.C.S.*, 2000, **122**, 5473-5476 (*synth*)

Prelissoclinamide 2 P-590

[104928-31-6]

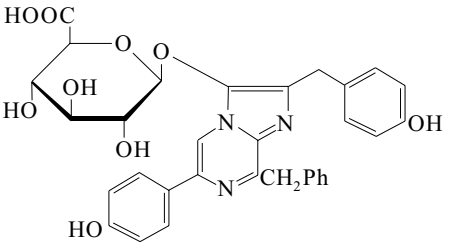


$C_{33}H_{43}N_7O_6S_2$ 697.878
Isol. from the tunicate *Lissoclinum patella*.
$[\alpha]_D$ +18.1 (c, 2.24 in $CHCl_3$).

Sesin, D.F. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 853

Watasenia Preluciferyl glucopyranosiduronic acid P-591

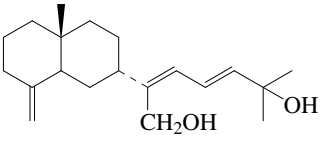
[107503-09-3]



$C_{32}H_{29}N_3O_9$ 599.596
Bioluminescent subst. from the liver of the myctophina fish *Diaphus elucens*. Also found in *Diaphus coeruleus, Diaphus suborbitalis, Benthosema fibulata* and *Myctophum asperum*.

Inoue, S. *et al., Chem. Lett.*, 1987, 417 (*isol, uv, pmr, struct*)

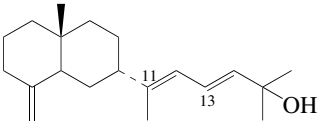
4(20),11,13-Prenyleudesmatriene-15,18-diol P-592



$C_{20}H_{32}O_2$ 304.472
Tentative identification.

(7β*H*,11*E*,13*E*)-*form* [65557-81-5]
Minor component of soft coral *Lobophytum hedleyi*.
Bowden, B.F. *et al., Aust. J. Chem.*, 1978, **31**, 163-170

4(20),11,13-Prenyleudesmatrien-15-ol P-593



(7β*H*,11*E*,13*E*)-*form*

$C_{20}H_{32}O$ 288.472

(7β*H*,11*E*,13*E*)-*form* [202922-91-6]
Constit. of *Lobophytum hedleyi* and *Lobophytum crassum*.
Oil. $[\alpha]_D$ +102 (c, 0.009 in $CHCl_3$). λ_{max} 241 (log ϵ 4.5) (EtOH).

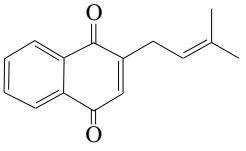
(7β*H*,11*E*,13*Z*)-*form* [202983-57-1]
Constit. of *Lobophytum crassum*.
Oil. $[\alpha]_D$ +70 (c, 0.0014 in $CHCl_3$). λ_{max} 243 (log ϵ 4.1) (EtOH).

(7β*H*,11*Z*,13*E*)-*form* [202983-58-2]
Constit. of *Lobophytum crassum*.
Oil. $[\alpha]_D$ +51 (c, 0.00041 in $CHCl_3$). λ_{max} 241 (log ϵ 4.5) (EtOH).

Bowden, B.F. *et al., Aust. J. Chem.*, 1978, **31**, 163-170 (*isol, pmr, cmr*)
Matthée, G.F. *et al., J. Nat. Prod.*, 1998, **61**, 237-240 (*isol, pmr, cmr*)

2-Prenyl-1,4-naphthoquinone P-594

2-(3-Methyl-2-butenyl)-1,4-naphthoquinone. ***Deoxylapachol***
[3568-90-9]



$C_{15}H_{14}O_2$ 226.274
Obt. from teak and other heartwoods. Also isol. from the brown alga *Landsburgia quercifolia*. Cytotoxic agent. Bright-yellow prisms (petrol).
Mp 60-61°. Steam-volatile. λ_{max} 246 (ϵ 15100); 250 (ϵ 15500); 257 (ϵ 14100); 325 (ϵ 2400) (MeOH) (Derep).

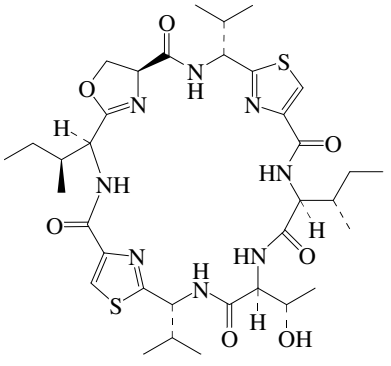
▶ Skin irritant.

*$\Delta^{1',2'}$-Isomer (*E-*), 3′-hydroxy: 2-(3-Hydroxy-3-methyl-1-butenyl)-1,4-benzoquinone. F 11263*
[177345-01-6]
$C_{15}H_{14}O_3$ 242.274
Prod. by *Acremonium* sp. (Sank11894). Sphingomyelinase inhibitor. Antidiabetic and antiosteoporotic agent. λ_{max} 230 (ϵ 7400); 372 (ϵ 1200) (MeOH) (Berdy).

Sandermann, H. *et al., Angew. Chem., Int. Ed.*, 1962, **1**, 599 (*isol*)
Burnett, A.R. *et al., J.C.S.(C)*, 1967, 2100; 1968, 850 (*isol, synth*)
Jacobsen, N. *et al., Acta Chem. Scand.*, 1973, **27**, 3211 (*synth*)
Inouye, H. *et al., Chem. Pharm. Bull.*, 1975, **23**, 392 (*synth*)
Evans, D.A. *et al., J.A.C.S.*, 1976, **98**, 1983 (*synth*)
Kapoor, N.K. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 189 (*synth*)
Perry, N.B. *et al., J. Nat. Prod.*, 1991, **54**, 978 (*isol, pmr, cmr*)
Japan. Pat., 1996, 96 53 387; *CA*, **125**, 8705d (*deriv*)

Prepatellamide A P-595

[350593-23-6]



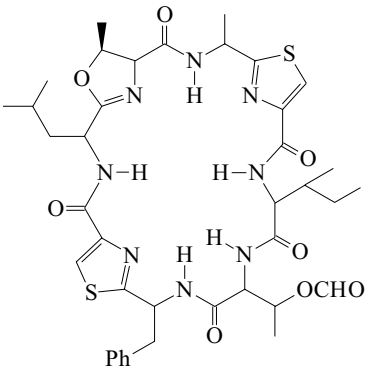
Absolute Configuration

$C_{35}H_{52}N_8O_7S_2$ 760.977
Isol. from *Lissoclinum patella*.

Fu, X. *et al., Sci. China, Ser. B*, 2000, **43**, 643-648; *CA*, **135**, 105198e (*isol*)

Prepatellamide B formate P-596

[104928-32-7]

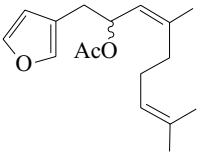


$C_{39}H_{50}N_8O_8S_2$ 823.005
Cyclic peptide antibiotic. Isol. from the tunicate *Lissoclinum patella*.
$[\alpha]_D$ +36.5 (c, 0.3 in $CHCl_3$).

Sesin, D.F. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 853 (*isol, pmr, cmr*)

Prepenlanfuran P-597

[95653-78-4]

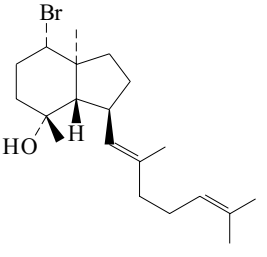


$C_{17}H_{24}O_3$ 276.375
Constit. of *Dysidea fragilis*. Oil. $[\alpha]_D^{20}$ -8.5 (c, 0.64 in $CHCl_3$).

Guella, G. *et al., Helv. Chim. Acta*, 1985, **68**, 39

Prepinnaterpene P-598

[98649-84-4]

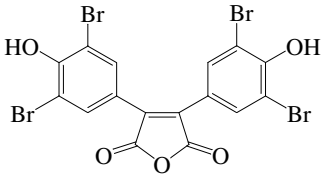


$C_{20}H_{33}BrO$ 369.384
Constit. of *Laurencia pinnata*. Oil. $[\alpha]_D$ -25.2 ($CHCl_3$).

Fukuzawa, A. *et al., Chem. Lett.*, 1985, 1263 (*isol*)
Fukuzawa, A. *et al., Tet. Lett.*, 1987, **28**, 4303 (*synth*)
Sato, Y. *et al., Tetrahedron: Asymmetry*, 1995, **6**, 757 (*synth*)

Prepolycitrin A P-599

3,4-Bis(3,5-dibromo-4-hydroxyphenyl)-2,5-furandione, 9CI
[168422-39-7]



$C_{16}H_6Br_4O_5$ 597.836
Isol. from the ascidian *Polycitor africanus*. Red cryst. ($CHCl_3$/hexane).
Mp 148-149°. Data given is for synthetic prod. λ_{max} 216 (ϵ 15520); 280 (ϵ 8380); 346 (ϵ 6210); 390 (ϵ 5590) (MeOH).

Terpin, A. *et al., Tetrahedron*, 1995, **51**, 9941-9946 (*synth, uv, ir, pmr, cmr*)
Rudi, A. *et al., J. Nat. Prod.*, 2000, **63**, 832-833 (*isol, pmr, cmr*)

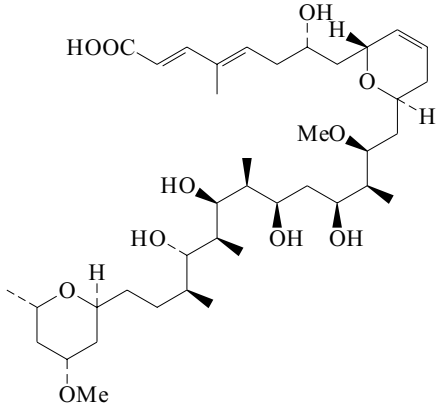
Prepsammaplin A P-600

Methyl 3-oxo-2-oxa-7,8-dithia-4,11-diazadodecan-12-oate, 9CI. Dimethyl (dithiodiethylene)dicarbamate, 8CI
[28138-84-3]
$MeOOCNHCH_2CH_2$-S-S-$CH_2CH_2NHCOOMe$
$C_8H_{16}N_2O_4S_2$ 268.357
Isol. from the marine sponge *Psammaplysilla purpurea*. Oil.

Jimenez, C. *et al., Tetrahedron*, 1991, **47**, 2097 (*isol, pmr, cmr, ms*)

Preswinholide A P-601

[131701-98-9]

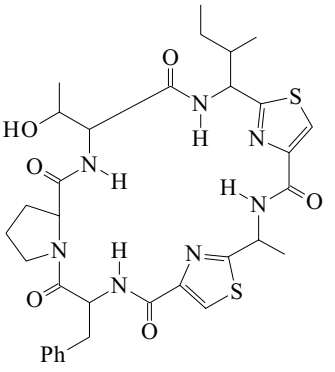


$C_{39}H_{68}O_{11}$ 712.96
Isol. from the sponge *Theonella swinhoei*. Biosynth. precursor of Swinholide A, S-548. $[\alpha]_D^{25}$ -32 (c, 0.14 in MeOH). λ_{max} 269 (ϵ 7000) (MeOH).

Todd, J.S. *et al., Tet. Lett.*, 1992, **33**, 441 (*isol*)
Paterson, I. *et al., J.A.C.S.*, 1994, **116**, 2615 (*synth*)
Paterson, I. *et al., Tet. Lett.*, 1994, **35**, 3405 (*synth*)
Nicolaou, K.C. *et al., Chem. Eur. J.*, 1996, **2**, 847 (*synth*)
Nagasawa, K. *et al., Tet. Lett.*, 1996, **37**, 6881; 6885 (*synth*)

Preulicyclamide P-602

[104928-30-5]

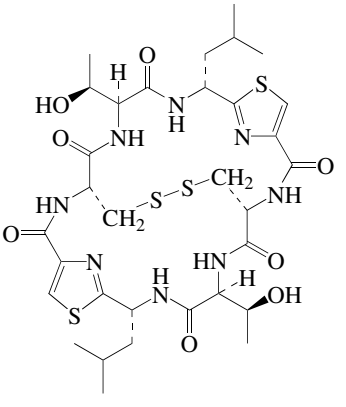


$C_{33}H_{41}N_7O_6S_2$ 695.862
Isol. from the tunicate *Lissoclinum patella*.
$[\alpha]_D$ +5.4 (c, 0.24 in $CHCl_3$).

Sesin, D.F. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 853 (*isol, pmr, cmr*)
Sugiura, T. *et al., Tet. Lett.*, 1987, **28**, 2251 (*synth*)

Preulithiacyclamide P-603

[105637-44-3]

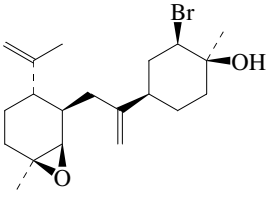


$C_{32}H_{46}N_8O_8S_4$ 799.028
Isol. from the ascidian *Lissoclinum patella*. Amorph. powder.
Mp 178-181° Mp 260-263° (synthetic). $[\alpha]_D^{22}$ +65 (c, 0.5 in DMF) (synthetic). λ_{max} 211; 241 (no solvent reported).

Kato, S. *et al., Tet. Lett.*, 1986, **27**, 2653-2656 (*synth*)
Schmidt, U. *et al., Tet. Lett.*, 1986, **27**, 3495-3496 (*synth*)
Patil, A.D. *et al., Nat. Prod. Lett.*, 1997, **9**, 181-187 (*isol, ir, pmr, cmr*)

Prevezol A P-604

[353796-21-1]

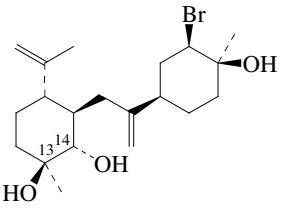


$C_{20}H_{31}BrO_2$ 383.368
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D^{20}$ -32.5 (c, 0.16 in $CHCl_3$). λ_{max} 205 (log ϵ 3.31) (hexane).

Mihopoulos, N. *et al., Tet. Lett.*, 2001, **42**, 3749-3752 (*isol, pmr, cmr*)

Prevezol B P-605

[353796-22-2]



$C_{20}H_{33}BrO_3$ 401.383

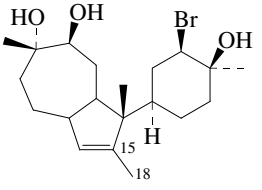
Struct. revised in 2003. Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D^{20}$ +33.33 (c, 0.09 in $CHCl_3$). λ_{max} 208 (log ϵ 3.6) (hexane).

14,15-Diepimer: ***Prevezol C***
[615285-30-8]
$C_{20}H_{33}BrO_3$ 401.383
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ -13.57 (c, 0.28 in $CHCl_3$).

Mihopoulos, N. *et al., Tet. Lett.*, 2001, **42**, 3749-3752 (*isol, pmr, cmr*)
Iliopoulou, D. *et al., J.O.C.*, 2003, **68**, 7667-7674 (*Prevezol C, struct*)

Prevezol D P-606

[615285-31-9]



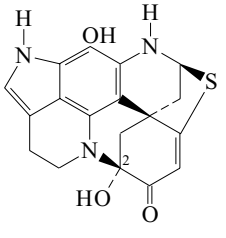
$C_{20}H_{33}BrO_3$ 401.383
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ +17.95 (c, 0.39 in $CHCl_3$). λ_{max} 211 (log ϵ 3.25) (hexane).

$\Delta^{15(18)}$-Isomer: ***Prevezol E***
[615285-32-0]
$C_{20}H_{33}BrO_3$ 401.383
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ +8 (c, 0.2 in $CHCl_3$). λ_{max} 230 (log ϵ 3.12) (hexane).

Iliopoulou, D. *et al., J.O.C.*, 2003, **68**, 7667-7674 (*isol, pmr, cmr*)

Prianosin C P-607

[116302-36-4]

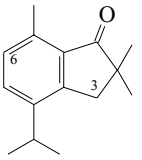


$C_{18}H_{15}N_3O_3S$ 353.401
Alkaloid from the Okinawan marine sponge *Prianos melanos*. Exhibits potent antineoplastic activity. Green solid. Fairly sol. DMF; poorly sol. MeOH, hexane.
Mp 300°. $[\alpha]_D^{22}$ +358 (c, 0.01 in MeOH). Unstable in soln. λ_{max} 231 (ϵ 12300); 263 (ϵ 3900); 292 (ϵ 2100); 370 (ϵ 1280) (MeOH) (Derep).

O^2,N,N-*Tri-Ac:*
Yellow cryst. Mp 200-201° dec. $[\alpha]_D^{23}$ +384 (c, 0.1 in $CHCl_3$).

Cheng, J.F. *et al., J.O.C.*, 1988, **53**, 4621 (*isol, uv, ir, pmr, cmr, ms, cd*)
Kobayashi, J. *et al., Tet. Lett.*, 1991, **32**, 1227 (*struct*)

Primnatrienone P-608



$C_{15}H_{20}O$ 216.322

6-Hydroxy: ***6-Hydroxyprimnatrienone***
[116173-40-1]
$C_{15}H_{20}O_2$ 232.322
Constit. of a *Primnoeides* sp. Cryst. (CH_2Cl_2/hexane). Mp 137-138°.

6-Methoxy: ***6-Methoxyprimnatrienone***
[116173-41-2]
$C_{16}H_{22}O_2$ 246.349
Constit. of a *Primnoeides* sp. Oil.

6-Methoxy, 3-hydroxy: ***3-Hydroxy-6-methoxyprimnatrienone***
[116173-38-7]
$C_{16}H_{22}O_3$ 262.348
Constit. of *Primnoeides* sp. Cryst. (EtOAc/hexane). Mp 122-124°.

6-Methoxy, 3-acetoxy: ***3-Acetoxy-6-methoxyprimnatrienone***
[116173-39-8]
$C_{18}H_{24}O_4$ 304.385
Constit. of a *Primnoeides* sp. Oil. $[\alpha]_D^{20}$ +1.5 (c, 0.3 in $CHCl_3$).

6-Methoxy, 3-oxo: ***6-Methoxy-1,3-primnatrienedione***
[116173-37-6]
$C_{16}H_{20}O_3$ 260.332
Pale yellow microcryst. Mp 92-93°.

Cambie, R.C. *et al., Aust. J. Chem.*, 1988, **41**, 365

Proctolin P-609

Arginyltyrosylleucylprolylthreonine, 9CI. Pea-proctolin. RYLPT
[57966-42-4]
H-Arg-Tyr-Leu-Pro-Thr
$C_{30}H_{48}N_8O_8$ 648.758
Pentapeptide of neural origin found in insects and other invertebrates. There is evidence of some activity in vertebrates. Also present in the pericardial organs of the shore crab *Cancer maenas*. Functions as an excitatory neuromuscular transmitter in visceral muscle of insects and other invertebrates. Is also a potent inhibitor of aminoenkephalase.

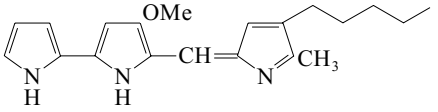
1-L-Alanine analogue: Alanyltyrosylleucylprolylthreonine. ***Ala^1-proctolin****. AYLPT*
[72273-81-5]
$C_{27}H_{41}N_5O_8$ 563.65
Isol. from the brain of the Colorado beetle *Leptinotarsa decemlineata*.

Starratt, A.N. *et al., Can. J. Chem.*, 1977, **55**, 4238 (*synth*)
Brown, B.E. *et al., J. Insect Physiol.*, 1977, **23**, 879 (*occur*)
Jaffe, H. *et al., J. Liq. Chromatogr.*, 1983, **6**, 993 (*hplc*)
Holmann, G.M. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1984, **77C**, 1 (*isol, hplc*)
Hui, K.S. *et al., Life Sci.*, 1985, **36**, 2309 (*enzyme inhibition*)
O'Shea, M. *et al., Adv. Insect Physiol.*, 1986, **19**, 1 (*rev, isol, chem, pharmacol*)
Stangier, J. *et al., Peptides (N.Y.)*, 1986, **7**, 67-72 (*isol, Cancer*)
Adams, M.E. *et al., Am. Zool.*, 1989, **29**, 1321 (*rev, biol activity*)
Orchard, I. *et al., J. Neurobiol.*, 1989, **20**, 470 (*rev, biol activity*)
Spittaels, K. *et al., Mol. Cell. Endocrinol.*, 1995, **110**, 119 (*Ala-proctolin*)
Konopinska, D. *et al., J. Pept. Res.*, 1997, **49**, 457-466 (*rev*)
Konopinska, D. *et al., J. Pept. Sci.*, 1999, **5**, 533-546 (*rev*)

Prodigiosin P-610

*4-Methoxy-5-[(5-methyl-4-pentyl-2*H*-pyrrol-2-ylidene)methyl]-2,2′-bi-1*H*-pyrrole, 9CI*

[82-89-3]



$C_{20}H_{25}N_3O$ 323.437

Pyrrole antibiotic. Pigment from *Serratia*, *Streptomyces*, marine *Beneckea gazogenes* and *Cladophora* spp. Shows antileukaemic and antifungal props. Active against plant-pathogenic fungi; insecticide enhancer. Shows antimalarial activity but too toxic for clinical use. Shows strong immunosuppressive activity. Lustrous dark red square pyramids. Sol. MeOH, acids, Et_2O; poorly sol. H_2O.

Mp 151-152°. Sinters at 70-80°. λ_{max} 216 (ϵ 8660); 275 (sh) (ϵ 6440); 296 (ϵ 12200); 371 (ϵ 7750); 382 (sh) (ϵ 7240); 510 (sh) (ϵ 54400); 541 (ϵ 132000) (EtOH at pH 2.9) (Derep). λ_{max} 257 (ϵ 7950); 281 (ϵ 9520); 336 (ϵ 7860); 469 (ϵ 42400) (EtOH at pH 11) (Derep). λ_{max} 226 (ϵ 10800); 289 (ϵ 9820); 337 (ϵ 7590); 471 (ϵ 41600); 539 (ϵ 17200) (EtOH at pH 7.4) (Derep). λ_{max} 222; 288; 337; 471; 534 (EtOH) (Berdy). λ_{max} 280; 336; 466 (ϵ 43000) (2-propanol) (Berdy).

▶ LD_{50} (mus, ipr) 18 mg/kg; LD_{50} (mus, ivn) 10 mg/kg. DW2977000

Hydrochloride:

Magenta cryst. (C_6H_6/petrol). Mp 148.5-150° dec.

Perchlorate:

Deep red cryst. (EtOH). Mp 228°.

Demethoxy: ***Demethoxyprodigiosin***. *2-Methyl-3-pentylprodigiosiene*

[112373-41-8]

$C_{19}H_{23}N_3$ 293.411

From *Serratia marcescens*. Purple solid (as hydrobromide). λ_{max} 568 (EtOH/HCl) (Berdy).

Wrede, F. *et al., Ber.*, 1929, **62**, 2678
Rapoport, H. *et al., J.A.C.S.*, 1962, **84**, 635 (*synth*)
Williams, R.P. *et al., Antibiotics (N.Y.)*, 1967, **2**, 410; 449 (*rev*)
Jackson, A.H. *et al., Tetrahedron*, 1967, **23**, 603 (*ms*)
Hearn, W.R. *et al., J.O.C.*, 1970, **35**, 142 (*synth*)
Lim, D.V. *et al., J. Bacteriol.*, 1977, **129**, 124 (*biosynth*)
Sveshnikova, M.A. *et al., Antibiotiki (Moscow)*, 1983, **28**, 723 (*isol*)
Boger, D.L. *et al., J.O.C.*, 1988, **53**, 1405-1415 (*synth, biosynth*)
Wasserman, H.H. *et al., Tet. Lett.*, 1989, **30**, 1725; 1999, **40**, 7587-7589 (*synth*)
Okamoto, H. *et al., CA*, 1999, **130**, 207057x; 2000, **132**, 47317 (*activity*)
Fürstner, A. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 3582-3603 (*rev*)

Propanal, 9CI P-611

Propionaldehyde. FEMA 2923

[123-38-6]

H_3CCH_2CHO

C_3H_6O 58.08

Isol. from various plant sources, e.g. hops, banana, sweet or sour cherry, blackcurrants, melon, pineapple, coffee, brown algae (*Laminaria* sp.) and strawberry or apple aroma. Flavouring agent. Liq. with suffocating odour. Mod. sol. H_2O. d_{25}^{25} 0.8.

Fp -81 Mp 131°. Bp 47.5-49°. n_D^{20} 1.3636.

▶ Eye, skin and respiratory tract irritant. LD_{50} (rat, orl) 1410 mg/kg. Highly flammable, fl. p. -30/-9°, autoignition temp. 207°. Peroxidizable. UE0350000

Trimer: See 2,4,6-Triethyl-1,3,5-trioxane in *The Combined Chemical Dictionary.*

Polymer: Metapropanal

[25722-18-3]

Cryst. Insol. H_2O. Mp 180°. Subl.

Oxime: [627-39-4]

C_3H_7NO 73.094

Colorimetric reagent for Pd(*II*). Cryst. (EtOH). Sol. EtOH, H_2O. Mp 40°. Bp 130-132° Bp_{100} 77°.

Phenylhydrazone: [5311-88-6]

$C_9H_{10}N_2$ 146.191

Yellow cryst. Mp 149°.

2,4-Dinitrophenylhydrazone: [725-00-8]

Mp 142-148°.

Semicarbazone: [628-07-9]

Needles (C_6H_6/petrol) or plates (H_2O). Sol. H_2O. Mp 88-90° (needles) Mp 154° (plates).

Di-Me acetal: 1,1-Dimethoxypropane, 9CI

[4744-10-9]

$C_5H_{12}O_2$ 104.149

Liq. Bp 89°.

Di-Et acetal: 1,1-Diethoxypropane

[4744-08-5]

$C_7H_{16}O_2$ 132.202

Bp 123°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 215B; 465C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 349B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 283C; 551B (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 541 (*synth*)
Frankiss, S.G. *et al., Spectrochim. Acta A*, 1972, **28**, 2149 (*ir, Raman*)
Stetsenko, A.I. *et al., Zh. Neorg. Khim.*, 1972, **17**, 2724; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1972, **17**, 1428 (*oxime*)
Miyajima, G. *et al., Org. Magn. Reson.*, 1974, **6**, 313 (*cmr*)
Bowen, R.D. *et al., Org. Mass Spectrom.*, 1981, **16**, 159 (*ms*)
Randell, J. *et al., Z. Naturforsch., A*, 1987, **42**, 957 (*microwave, struct*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PMT750
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 926 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2331-2332 (*use, occur*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1150
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1067
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DOM200; PMT750

2-Propanol, 9CI P-612

Isopropanol. 2-Hydroxypropane. Isopropyl alcohol, USAN. Alcojel. Avantin. Bowsteral. Hartasol. Petrohol. Propol. Takineocol. FEMA 2929

[67-63-0]

[62309-51-7]

$H_3CCH(OH)CH_3$

C_3H_8O 60.096

Manuf. by catalytic hydration of propylene. Present in fruit aromas, e.g. papaya (*Carica papaya*). Widely used solvent for creosote, resins, gums, inks, oil, lotions etc. Used in antifreeze mixt. and as extraction solvent in food preparation. Used to prepare isopropyl esters of carboxylic acids for gc anal. Important industrial chemical, USA production in 1999 0.73 million tons. Topical antiinfective. Pharmaceutic aid (solvent). Liq. Sol. H_2O. d_4^{20} 0.79.

Fp -89.5 Mp -88.5°. Bp 82.5°. n_D^{20} 1.3776. pK_a 17.1. pK_a -4.7 (base). Log P 0.07 (calc). Forms azeotropic mixt. with H_2O ctg. 12.1% H_2O. Can be salted out from aq. solns. Component of Hibistat.

▶ Highly flammable, fl. p. 12°, autoignition temp. 399°. Peroxidisable. Eye, skin and respiratory tract irritant. Contact of the liquid with eyes can cause corneal burns and severe eye damage. Potentiates CCl_4 toxicity. CNS depressant. OES: long-term 400 ppm; short-term 500 ppm (sk). NT8050000

O-α-D-*Glucopyranoside: Isopropyl* α-D-*glucoside*

[25320-92-7]

$C_9H_{18}O_6$ 222.238

Constit. of the coral *Sclerophytum capitalis*. Powder or syrup. Mp 32°. $[\alpha]_D$ +140 (Py).

O-α-D-*Glucopyranoside, tetra-Ac:* [20226-73-7]

Cryst. (EtOH aq.). Mp 86°. $[\alpha]_D^{20}$ +145.2 (c, 2 in $CHCl_3$).

O-β-D-*Glucopyranoside: Isopropyl* β-D-*glucoside*

[5391-17-3]

$C_9H_{18}O_6$ 222.238

Constit. of *Anoectochilus formosanus* and *Foeniculum vulgare*.

Needles (MeOH).
Mp 129-131°. $[\alpha]_D^{25}$ -54.9 (Py). $[\alpha]_D^{23}$ -35.6 (c, 1.1 in MeOH).

O-*β-D-Glucopyranoside, tetra-Ac:* [6586-70-5]
Cryst. Mp 140°. $[\alpha]_D$ -23.3 ($CHCl_3$).

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]: Isopropyl primeveroside*
[178117-37-8]
$C_{14}H_{26}O_{10}$ 354.353
Constit. of *Passiflora morifolia* shoots. Amorph.

O-*[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:* [147742-24-3]
$C_{14}H_{26}O_{10}$ 354.353
Constit. of the roots of cassava (*Manihot esculenta*). Solid + $\frac{1}{2}H_2O$.
Mp 119-120°. $[\alpha]_D^{25}$ -82.7 (c, 0.6 in H_2O).

O-*[3,4-Dihydroxy*-E-*cinnamoyl-(→5)-β-D-apiofuranosyl-(1→6)-β-D-glucopyranoside]:* ***Dracunculifoside G***
$C_{23}H_{32}O_{13}$ 516.498
Constit. of *Baccharis dracunculifolia*. Amorph. powder. $[\alpha]_D^{26}$ -51.8 (c, 0.46 in MeOH). λ_{max} 218 (log ϵ 4.1); 245 (log ϵ 3.96); 302 (log ϵ 4.08); 330 (log ϵ 4.21) (MeOH).

O-*[2*-O-*Methyl-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:*
$C_{16}H_{30}O_{10}$ 382.407
Constit. of the root bark of *Pseudolarix kaempferi*. Powder. $[\alpha]_D^{20}$ -36 (c, 0.45 in MeOH).

Formyl: Isopropyl formate. FEMA 2944
[625-55-8]
Constit. of various mushrooms and dwarf quince (*Chaenomeles japonica*).
Liq. Bp 67.5-68°.
▶ LQ8750000

Ac: See Isopropyl acetate in *The Combined Chemical Dictionary.*

Benzoyl: See Benzoic acid, B-58

Methanesulfonyl: [926-06-7]
$C_4H_{10}O_3S$ 138.187
Liq. Bp_{12} 86-88°. n_D^{20} 1.4172.
▶ Mutagenic. Exp. teratogen. PB2275000

Me ether: See 2-Methoxypropane in *The Combined Chemical Dictionary.*

Et ether: See 2-Ethoxypropane in *The Combined Chemical Dictionary.*

Ph ether: See Isopropyl phenyl ether in *The Combined Chemical Dictionary.*

[3979-51-9, 6831-82-9, 15520-32-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 117D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 175B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 166A (*ir*)
Brooks, B.T. *et al., Chem. Rev.*, 1926, **2**, 382 (*rev*)
Brooks, B.T. *et al., J.A.C.S.*, 1934, **56**, 1998 (*synth*)
Ross, W.C.J. *et al., J.C.S.*, 1957, 2420-2422 (*methanesulfonyl*)
Hatch, L.F. *et al., Isopropyl Alcohol*, McGraw-Hill, N.Y., 1961, (*bibl*)
Katague, D.B. *et al., J. Pharm. Sci.*, 1965, **54**, 891 (*isol*)
Wing, R.E. *et al., Carbohydr. Res.*, 1969, **10**, 441-448 (*synth, glucoside*)
Helferich, B. *et al., Chem. Ber.*, 1971, **104**, 671-673 (*synth, glucosides*)
Harrison, A.G. *et al., Org. Mass Spectrom.*, 1974, **9**, 221 (*ms*)
Biondi, P.A. *et al., J. Chromatogr.*, 1975, **109**, 389 (*use*)
Hikino, H. *et al., Tetrahedron*, 1976, **32**, 325 (*cmr*)
IARC Monog., 1977, **15**, 223; *Suppl.* 7, 229; *Suppl.* 6, 351 (*rev, tox*)
Seo, S. *et al., J.A.C.S.*, 1978, **100**, 3331-3339 (*glucosides*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **19**, 198, (*rev, bibl*)
Kasai, R. *et al., Tetrahedron*, 1979, **35**, 1427-1432 (*cmr, glucosides*)
Food Chemicals Codex, 3rd Ed., 1981, 155 (*anal*)
Kolodziejczyk, A.M. *et al., J.O.C.*, 1981, **46**, 1944-1946 (*methanesulfonyl*)
Slusarska, E. *et al., Synthesis*, 1981, 155-156 (*methanesulfonyl*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, INJ000
Sharma, P. *et al., J. Nat. Prod.*, 1989, **52**, 395-397 (*α-D-glucoside*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 241-242
Prawat, H. *et al., Phytochemistry*, 1995, **40**, 1167 (*6-apiosylglucoside*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1144
Jaroszewski, J.W. *et al., Phytochemistry*, 1996, **42**, 649 (*primeveroside*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1483-1496 (*use, esters*)
Kitajima, J. *et al., Chem. Pharm. Bull.1998,* **46**, 1643-1646 (*β-D-glucoside*)
Du, X.M. *et al., Phytochemistry*, 1998, **49**, 1925-1928 (*isol, pmr, cmr, glucosides*)
Nagatani, Y. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1388-1394 (*Dracunculifoside G*)
Yang, S.-P. *et al., Nat. Prod. Res.*, 2004, **18**, 439-446 (*2-O-Methylrhamnosylglucoside*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4561
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 291
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1203
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 31
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, INJ000; IPC000; IPY000

2-Propenoic acid, 9CI P-613

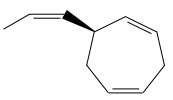
Acrylic acid
[79-10-7]
$H_2C{=}CHCOOH$
$C_3H_4O_2$ 72.063
Manuf. by oxidn. of 1-Propene or by reaction of $Ni(CO)_4$ with Acetylene and H_2O. Found in green algae. Prod. by *Phaeocystis* sp., *Phaeocystis pouchetii*, *Enteromorpha* sp., *Ulva* sp. , *Codium* sp., *Patinopecten yessonensis*, *Protogonyaulax* sp. Undergoes free-radical polym. in aq. soln. to give polyacrylates, acrylic resins etc. USA production in 1999 1.39 million tons. Corrosive liq. with acrid odour and fumes. Misc. H_2O, EtOH, Et_2O; sol. Me_2CO. d_4^{16} 1.06.
Mp 13°. Bp 141° (polymerises). n_D^{20} 1.4424. pK_a 4.25 (25°). Vp 4 mmHg (25°). Polym. readily in the presence of O_2. Acrylic acid and its esters usually contain hydroquinone monomethyl ether as polym. inhibitor. Q/e values for copolym., Q 0.83, e +0.88. Copolym. with vinyl chloride: r_{AA} 6.8; r_{VC} 0.107 (typical values, 60°); Q 1.15; e 0.77.
▶ Flammable, fl. p. 52°, autoignition temp. 438°. May polym. exothermically (possibly violently). Irritant to all tissues. LD_{50} (rat, orl) 33.5 mg/kg. LD_{50} (rbt, skn) 280 mg/kg. Exp. teratogen (ipr route). OES: long-term 10 ppm; short-term 20 ppm (Sk).
AS4375000

[6292-01-9, 7446-81-3, 9003-05-8, 9003-06-9, 10192-85-5, 10344-93-1, 14643-87-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 498B; 638B; 638C; 642A; 732A; 749B; 842D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 776A; 973B; 973C; 974A; 974B; 1199A; 1221A; 1244C; 1358B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 583A; 674A; 674B; 674C; 674D; 770D; 778B; 784B; 802B
Wohlk, A. *et al., J. Prakt. Chem.*, 1900, **61**, 200-214 (*synth*)
Van der Burg, J.H.N. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1922, **41**, 21-23 (*synth*)
Ratchford, W.P. *et al., J.A.C.S.*, 1944, **66**, 1864 (*synth*)
Sieburth, J.M. *et al., Science (Washington, D.C.)*, 1960, **132**, 676 (*isol*)
Katayama, T. *et al., CA*, 1966, **65**, 5924 (*isol*)
Bowles, A.J. *et al., Org. Mass Spectrom.*, 1969, **2**, 809 (*ms*)
Katritzky, A.R. *et al., J.A.C.S.*, 1970, **92**, 6861 (*ir*)
Austin, G.T. *et al., Chem. Eng. (N.Y.)*, 1974, **81**, 86 (*rev, manuf*)
Miyajima, G. *et al., Org. Magn. Reson.*, 1974, **6**, 413 (*cmr*)
IARC Monog., 1979, **19**, 47; 73; 1986, **39**, 41; *Suppl.* 6, 27, 41; *Suppl.* 7, 56, 63, 66, 79, 41; 81; 99 (*rev, tox*)
Ullmann's Encycl. Ind. Chem., 5th edn., VCH-Weinheim, 1985, **A1**, 161 (*rev*)
Charles, S.W. *et al., J. Mol. Struct.*, 1987, **157**, 17 (*ir*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 251; 287; 352 (*rev*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4954
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 55; 57; 58; 234; 318
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1039; 1079; 1109; 1433; 1794
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 19; 20; 21; 584; 824

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADS250; ADZ000; EFT000; BPW100; ADX500; MGA500; ADS750; DOP800

6-(1-Propenyl)-1,4-cycloheptadiene P-614



(*S*)–(*Z*)–*form*

$C_{10}H_{14}$ 134.221

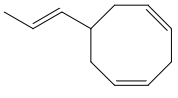
(*S*)-(*Z*)-*form* [142864-29-7]
Constit. of the brown alga *Ectocarpus siliculosus.*

(±)-(*E*)-*form* [50265-65-1]
Bp_{17} 54-55°.

[92340-52-8]

Jaenicke, L. *et al., Annalen*, 1973, 1252 (*synth, pmr*)
Stratmann, K. *et al., Angew. Chem., Int. Ed.*, 1992, **31**, 1246 (*isol*)

7-(1-Propenyl)-1,4-cyclooctadiene P-615



(*E*)-*form*

$C_{11}H_{16}$ 148.247

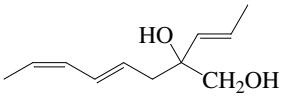
(*E*)-*form* [132636-41-0]
Constit. of the brown alga *Cutleria multifida.*
Oil.

(*Z*)-*form* [132746-14-6]
Constit. of *Cutleria multifida.*
Oil.

Keitel, J. *et al., Helv. Chim. Acta*, 1990, **73**, 2101-2112 (*isol, synth, pmr, cmr, ms*)

2-(1-Propenyl)-4,6-octadiene-1,2-diol, 9CI P-616

4-Hydroxymethyl-2,6,8-decatrien-4-ol



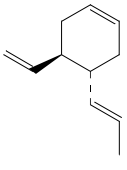
$C_{11}H_{18}O_2$ 182.262

(1′*E*,2ξ,4*E*,6*Z*)-*form* [218166-81-5]
Prod. by a *Coniothyrium* sp. from the sponge *Ectyoplasia ferox*. Oil. $[\alpha]_D^{20}$ -13.8 (c, 0.13 in $CHCl_3$). λ_{max} 235 (ϵ 12600) (EtOH).

Höller, U. *et al., J. Nat. Prod.*, 1999, **62**, 114-118 (*isol, uv, ir, pmr, cmr, ms*)

4-(1-Propenyl)-5-vinylcyclohexene P-617

4-Ethenyl-5-(1-propenyl)cyclohexene, 9CI. ***Aucantene***



(4*S*,5*R*)-*form*

$C_{11}H_{16}$ 148.247

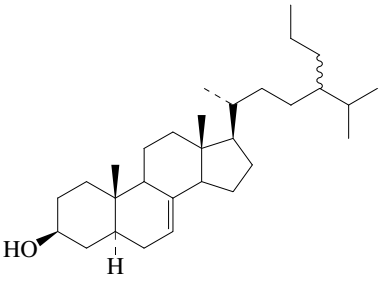
(4*S*,5*R*)-*form*
(+)-trans-*form*
[52811-30-0]
Constit. of *Cutleria multifida.*
$[\alpha]_D^{23.5}$ +105 (c, 0.002 in CCl_4). Biol. inactive.

(4*RS*,5*SR*)-*form*
(±)-trans-*form*
[66965-85-3]
Oil.

Jaenicke, L. *et al., J.A.C.S.*, 1974, **96**, 3324 (*isol*)
Marner, F.J. *et al., Chem. Ber.*, 1975, **108**, 2202 (*synth*)
Liu, H.J. *et al., Can. J. Chem.*, 1978, **56**, 306 (*synth*)
Jaenicke, L. *et al., Angew. Chem., Int. Ed.*, 1982, **21**, 643 (*rev*)
Boland, W. *et al., Helv. Chim. Acta*, 1985, **68**, 2062 (*synth, abs config*)

24-Propylcholest-7-en-3-ol P-618

29-Methylstigmast-7-en-3-ol



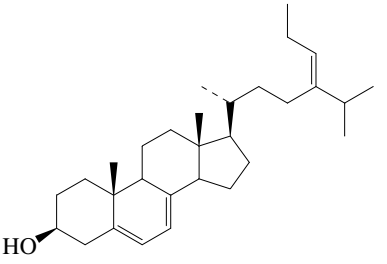
$C_{30}H_{52}O$ 428.74

(3β,5α,24ξ)-*form* [83728-81-8]
Constit. of *Asterias vulgaris.*

Burnell, D.J. *et al., Steroids*, 1982, **39**, 357-369 (*isol*)

24-Propylidenecholesta-5,7-dien-3-ol P-619

28-Ethylergosta-5,7,24(28)-trien-3-ol. 29-Methylstigmasta-5,7,24(28)-trien-3-ol



(3β,24(28)*E*)-*form*

$C_{30}H_{48}O$ 424.709

(3β,24(28)*E*)-*form* [85482-77-5]
Constit. of *Tethya amamensis.*

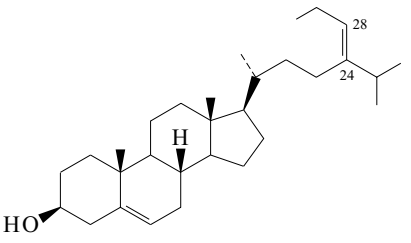
(3β,24(28)*Z*)-*form* [85482-78-6]
Constit. of *Dysidea avara*, *Ircinia pipetta*, *Tethya amamensis* and *Spongionella gracilis.*

(3β,24(28)ξ)-*form* [92345-34-1]
Constit. of *Ircinia foetida* and *Ircinia variabilis.* Double bond stereochem. not established.

Teshima, S. *et al., Lipids*, 1983, **18**, 193-197 (*Tethya amamensis constits*)
Dini, A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1984, **78**, 741-744 (*Ircinia variabilis constit*)
Sica, D. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **81**, 115-118; *Chem. Pharm. Bull.*, 1987, **88**, 293-296 (*Spongionella gracilis constit*)

24-Propylidenecholest-5-en-3-ol P-620

28-Ethylergosta-5,24(28)-dien-3-ol



(3β,24(28)*E*)–*form*

$C_{30}H_{50}O$ 426.724

(3β,24*E*)-*form*

24-Propylidenecholesterol

[59168-99-9]

Constit. of a cultured marine chrysophyte. Also present in sponge *Tethya amamensis*.

Cryst. (MeOH).

Mp 108-110°. $[\alpha]_D^{20}$ -40 (c, 0.29 in $CHCl_3$).

5α,6-Dihydro: ***24-Propylidenecholestan-3-ol***

[75373-62-5]

$C_{30}H_{52}O$ 428.74

Constit. of *Holothuria nobilis*.

*24*R*,28-Dihydro: 24-Propylcholest-5-en-3-ol.* ***24-Propylcholesterol***

[64997-52-0]

$C_{30}H_{52}O$ 428.74

From a marine chrysophyte and *Aureoumbra lagunensis* that causes "Texas brown tide".

5α,6,24ξ,28-Tetrahydro: ***24-Propylcholestan-3-ol***

[117675-19-1]

$C_{30}H_{54}O$ 430.756

Constit. of the edible scallop *Trochostoma orientale* and from *Bathyplotes natans*.

(3β,24*Z*)-*form*

29-Methylisofucosterol

[35339-71-0]

Isol. from scallops *Placopecten magellanicus* and *Patinopecten yessoensis* and sponges *Tethya aurantia* and *Tethya amamensis*.

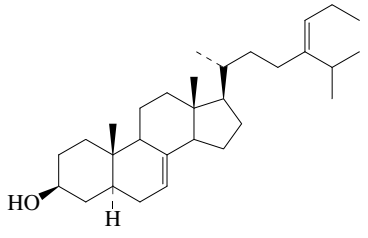
Cryst. (EtOH).

Mp 111-112°. $[\alpha]_D^{20}$ -27 ($CHCl_3$).

Idler, D.R. *et al., Steroids*, 1971, **18**, 545; 1976, **27**, 155 (*isol*)
Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*isol, ms*)
Kobayashi, M. *et al., Steroids*, 1975, **26**, 605 (*isol*)
Rohmer, M. *et al., Steroids*, 1980, **35**, 219 (*isol*)
Teshima, S. *et al., Lipids*, 1983, **18**, 193-197 (*occur, Tethya*)
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*occur, biosynth*)
Giner, J.-L. *et al., J.A.C.S.*, 1991, **113**, 1386 (*biosynth*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*24-Propylcholestan-3-ol, isol, ms*)
Giner, J.-L. *et al., Tetrahedron*, 2000, **56**, 9575-9580 (*synth, abs config*)

24-Propylidenecholest-7-en-3-ol P-621

24-Ethylergosta-7,24(28)-dien-3-ol



(3β,5α,24*Z*)-*form*

$C_{30}H_{50}O$ 426.724

(3β,5α,24*Z*)-*form* [82468-96-0]

Constit. of the chiton *Liolophura japonica*.

(3β,5α,24ξ)-*form* [41398-72-5]

Constit. of *Asterias rubens, Ctenodiscus crispatus, Cucumaria lactea* and a *Pachychalina* sp.

Sulfate: [88341-78-0]

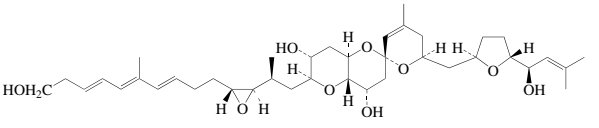
$C_{30}H_{50}O_4S$ 506.789

Constit. of *Asterias rubens*.

Grossert, J.S. *et al., Experientia*, 1973, **29**, 258-259 (*Ctenodiscus constit*)
Teshima, S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **71**, 373-378 (*Lilophiura constit, ms*)
Goodfellow, R.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **76**, 575-578 (*sulfate*)
Zeng, Z. *et al., CA*, 1996, **125**, 190994 (*Pachychalina constit*)

Prorocentin P-622

[865536-64-7]



$C_{39}H_{60}O_9$ 672.898

Isol. from the marine dinoflagellate *Prorocentrum lima*. Amorph. solid. $[\alpha]_D^{25}$ -12.7 (c, 0.2 in MeOH). λ_{max} 274 (ε 25300) (MeOH).

Lu, C.-K. *et al., Org. Lett.*, 2005, **7**, 3893-3896 (*isol, pmr, cmr*)

Prorocentrin P-623

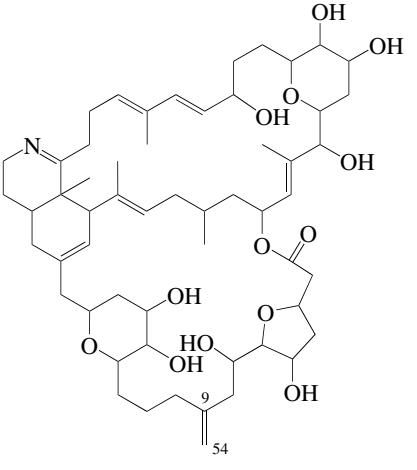
[84861-99-4]

Isol. from the marine dinoflagellate *Prorocentrum minimum*. Siderophore.

Trick, C.G. *et al., Science (Washington, D.C.)*, 1983, **219**, 306-308 (*isol*)

Prorocentrolide P-624

[117120-34-0]



$C_{56}H_{85}NO_{13}$ 980.286

Isol. from the marine dinoflagellate *Prorocentrum lima*. Phycotoxin. Amorph. solid. Sol. MeOH, butanol; fairly sol. $CHCl_3$; poorly sol. Et_2O. $[\alpha]_D^{23}$ +136.5 (c, 0.147 in MeOH). λ_{max} 235 (ε 13600) (MeOH) (Berdy).

▶ Toxic.

9,54-Dihydro: ***Dihydroprorocentrolide***

[123072-68-4]

$C_{56}H_{87}NO_{13}$ 982.302

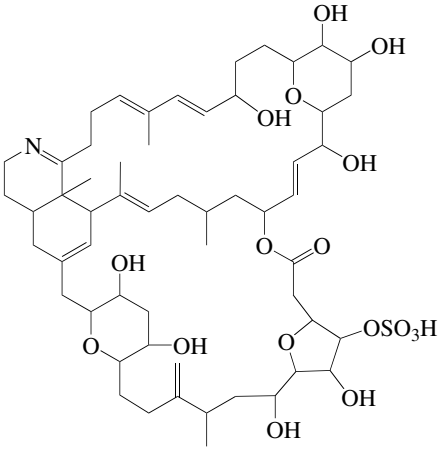
Isol. from *Prorocentrum lima*. Paralytic phycotoxin. Sol. MeOH, butanol; poorly sol. H_2O. Hydrogenated at the exocyclic methylene group.

▶ LD_{50} (mus, ipr) 0.14 mg/kg.

Torigoe, K. *et al., J.A.C.S.*, 1988, **110**, 7876
Torigoe, K. *et al., CA*, 1989, **111**, 173876d

Prorocentrolide B P-625

[184296-31-9]



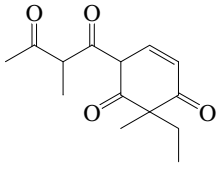
$C_{56}H_{85}NO_{17}S$ 1076.35

Macrolide antibiotic. Isol. from the marine dinoflagellates *Prorocentrum maculosum* and *Prorocentrum concavum*. Fast-acting toxin. Solid.

Mp 199-201°. $[\alpha]_D^{25}$ +76.7 (c, 0.2 in MeOH). λ_{max} 235 (MeCN).

Hu, T. *et al., J. Nat. Prod.*, 1996, **59**, 1010-1014 (*isol, uv, ir, pmr, cmr, ms*)

Prospiciferone P-626



$C_{14}H_{18}O_4$ 250.294

Prod. by the marine-derived *Microsphaeropsis* sp. strain 6288. Yellow solid.

Mp 85°. λ_{max} 318 (log ϵ 2.71); 401 (log ϵ 2.7) (MeOH). λ_{max} 285 (log ϵ 2.03) (MeOH/HCl). λ_{max} 318 (log ϵ 2.83); 400 (log ϵ 2.81) (MeOH/NaOH).

Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*isol, uv, cd, pmr, cmr, ms*)

Protamines P-627

[9012-00-4]

Group of simple proteins that yield basic amino acids on hydrolysis. Occur combined with nucleic acid mainly in the sperm of fish. Inhibits inflammation and certain immune reactions.

▶ UK9440000

Sulfate: ***Protamine sulfate, BAN, INN, JAN, USAN***
[9009-65-8] Heparin antidote. Haemostatic.

▶ UK9450000

Kossel, A. *et al., The Protamines and Histones*, Longmans, N.Y., 1928, (*isoln*)
Felix, K. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1963, **330**, 205 (*struct*)
Vendrely, R. *et al., Protoplasmatologia*, 1966, **5**, 88 (*rev, struct, synth, metab*)
Bradburg, E.M. *et al., J. Mol. Biol.*, 1967, **29**, 507 (*conformn, ir, pmr*)
Ando, T. *et al., Int. J. Protein Res.*, 1969, **1**, 221
Jaques, L.B. *et al., Can. Med. Assoc. J.*, 1973, **108**, 1291 (*rev*)
Ando, T. *et al., Protamines*, Springer-Verlag, Berlin, 1973, (*book*)
Taylor, S. *et al., Nature (London)*, 1982, **297**, 307 (*activity*)
Speckert, W. *et al., Eur. J. Biochem.*, 1983, **136**, 283 (*struct*)
Ammer, H. *et al., Biol. Chem. Hoppe-Seyler*, 1986, **367**, 515 (*isoln, struct*)
McKay, D.J. *et al., Eur. J. Biochem.*, 1986, **156**, 5 (*isol, struct*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 692
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, POD750

Protein prenyltransferases P-628

A family of enzymes. Isol. from mammals, fungi and plants.

Protein farnesyltransferase

E.C. 2.5.1.58. Farnesyl-diphosphate:protein-cysteine farnesyltransferase. FTase

Catalyses the reaction of farnesyl diphosphate with a cysteine residue in a protein to give diphosphate and a *S*-farnesylcysteine unit. A Zn metalloenzyme requiring $Mg^{2\oplus}$ for activity. Substrates include Ras, Rho, Rab, other Ras-related small GTP-binding proteins, γ-subunits of heterotrimeric G-proteins, nuclear lamins, centromeric proteins and many proteins involved in visual signal transduction.

Protein geranylgeranyltransferase type I

E.C. 2.5.1.59. Geranylgeranyl-diphosphate:protein-cysteine geranyltransferase. GGTase-I

Catalyses the reaction of geranylgeranyl diphosphate with a cysteine residue in a protein to give diphosphate and a *S*-geranylgeranylcysteine unit. A Zn metalloenzyme. Substrates incl. most γ-subunits of heterotrimeric G proteins and Ras-related GTPases such as members of the Ras and Ras/Rho families.

Protein geranylgeranyltransferase type II

E.C. 2.5.1.60. Geranylgeranyl-diphosphate, geranylgeranyl-diphosphate:protein-cysteine geranyltransferase. GGTase-II. Rab geranylgeranyltransferase

Catalyses the reaction of 2 mols. of geranylgeranyl diphosphate with cysteine residues in a protein to give diphosphate and *S*-geranylgeranylcysteine residues. Attaches geranylgeranyl groups to 2 *C*-terminal cysteines in Ras-related GTPases of a single family, the Rab family.

Clarke, S. *et al., Annu. Rev. Biochem.*, 1992, **61**, 355-386 (*rev*)
Yokoyama, K. *et al., Biochem. Soc. Trans.*, 1992, **20**, 489-494 (*rev*)
Moomaw, J.F. *et al., Methods Enzymol.*, 1995, **250**, 12-21 (*E.C. 2.5.1.59, bovine brain*)
Jiang, Y. *et al., Methods Enzymol.*, 1995, **257**, 21-29 (*E.C. 2.5.1.60, yeast*)
Zhang, F.L. *et al., Annu. Rev. Biochem.*, 1996, **65**, 241-269 (*rev*)
Casey, P.J. *et al., J. Biol. Chem.*, 1996, **271**, 5289-5292 (*rev*)
Park, H.W. *et al., Curr. Opin. Struct. Biol.*, 1997, **7**, 873-880 (*rev*)
Lane, K.T. *et al., J. Lipid Res.*, 2006, **47**, 681-695 (*rev*)

Urticina piscivora Protein UpI P-629

Basic protein, MW *ca*. 28 kDa. Isol. from the sea anemone *Urticina piscivora*. Potent cardiac stimulatory protein.

Cline, E.A. *et al., Pharmacol. Res.*, 1995, **32**, 309-314 (*isol*)

Protein-arginine *N*-methyltransferases P-630

E.C. 2.1.1.23 (deleted)

[9055-07-6]

Enzymes. Catalyse the reaction of *S*-adenosyl-L-methionine with an L-arginine residue in a protein to give *S*-adenosyl-L-homocysteine and a N^{ω}-methyl-L-arginine residue. E.C. 2.1.1.23 has been replaced by E.C. 2.1.1.124, E.C. 2.1.1.125 and E.C. 2.1.1.126.

[Cytochrome *c*]-arginine *N*-methyltransferase

E.C. 2.1.1.124. S-*Adenosyl-L-methionine:[cytochrome c]-arginine* N^{ω}*-methyltransferase*

Isol. from *Euglena gracilis*. Acts on an arginine residue in cytochrome *c*.

Histone-arginine *N*-methyltransferase

E.C. 2.1.1.125. S-*Adenosyl-L-methionine:histone-arginine* N^{ω}*-methyltransferase. Histone protein methylase I*

Isol. from rat liver. Acts on an arginine residue in a histone.

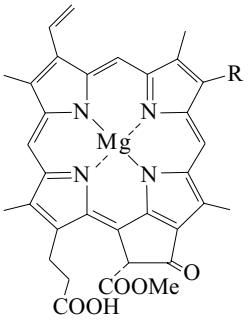
[Myelin basic protein]-arginine *N*-methyltransferase

E.C. 2.1.1.126. S-*Adenosyl-L-methionine:[myelin-basic-protein]-arginine* N^{ω}*-methyltransferase. Myelin basic protein methylase I*
Isol. from bovine brain. Acts on an arginine residue in myelin basic protein.

Farooqui, J.Z. *et al., J. Biol. Chem.*, 1985, **260**, 527-545 (*E.C. 2.1.1.124*)
Kim, S. *et al., Adv. Exp. Med. Biol.*, 1988, **231**, 327-340 (*E.C. 2.1.1.126, rev*)
Young, P.R. *et al., Biochem. J.*, 1988, **250**, 221-226 (*E.C. 2.1.1.126*)
Ghosh, S.K. *et al., J. Biol. Chem.*, 1988, **263**, 19024-19033 (*E.C. 2.1.1.126*)
Rawal, N. *et al., Biochem. J.*, 1994, **300**, 483-489 (*E.C. 2.1.1.125*)
Bedford, M.T. *et al., Mol. Cell*, 2005, **18**, 263-272 (*rev*)

Protochlorophyllide **P-631**

Magnesium 2,4-divinylphaeoporphyrin a_5 *monomethyl ester. Divinyl protochlorophyllide. Monovinyl protochlorophyllide*
[14751-08-7]



R = $CH{=}CH_2$ or CH_2CH_3

$C_{35}H_{30}MgN_4O_5$ 610.951

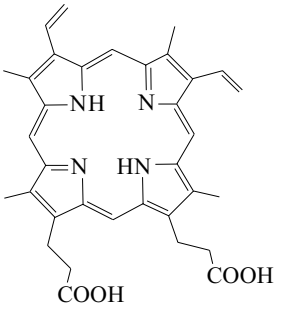
Mol. formula given is for divinyl compd., R = $CH{=}CH_2$. Isol. from photosynthetic bacteria, e.g. *Rhodopseudomonas spheroides*. Also from marine flagellates and reported from the seed husks of *Cucurbita pepo*. Intermed. in Chlorophyll biosynth. Two distinct pathways exist via mono- and divinyl protochlorophyllides. Protochlorophyllides accumulate in dark-grown plant seedlings as the enzymic redn. to chlorophyllides is a photochemical step. Esters with e.g. geranylgeraniol or phytol (protochlorophylls) also occur in lesser amounts. Violet-red solid.

Phytyl ester: Protochlorophyll a. Trichosanthin†
$C_{55}H_{68}MgN_4O_5$ 889.471
Present with the unesterified form in various plants. Thought to have been isol. in 1890 as Trichosanthin from *Trichosanthes palmata*. Dark green substance.

Fischer, F.G. *et al., Annalen*, 1959, **627**, 35
Jones, O.T.G. *et al., Biochem. J.*, 1963, **88**, 335; **89**, 182; 1966, **101**, 153
Ricketts, T.R. *et al., Phytochemistry*, 1966, **5**, 223 (*isol*)
Shioi, Y. *et al., Arch. Biochem. Biophys.*, 1983, **220**, 286
Shioi, Y. *et al., Biochim. Biophys. Acta*, 1983, **722**, 72
Wu, S.M. *et al., Tetrahedron*, 1984, **40**, 659 (*nmr, ms*)
Wong, Y.S. *et al., Plant Physiol.*, 1985, **79**, 725; 730 (*biosynth*)

Protoporphyrin **P-632**

Protoporphyrin IX. Ooporphyrin. Lebersdan. Many other names
[553-12-8]



$C_{34}H_{34}N_4O_4$ 562.667

Obt. by demetallation of Haemin, occurs in small amounts in faeces. Brown pigment (Ooporphyrin) of birds' eggs. Isol. from *Atolla wyvillei*. Branch point in the biosynthetic pathway leading to Haem (by insertion of iron) and chlorophylls (by insertion of Mg and further side-chain transformation). Used to treat liver disorders, mainly as Na salt. Shows anti-HIV activity. Reddish-purple cryst. Sol. EtOH, EtOAc, AcOH, Py; fairly sol. Et_2O, hexane; poorly sol. H_2O.
Mp 300°. λ_{max} 557; 582; 602 (dication, aq. HCl).

▶ LD_{50} (mus, ipr) 1029 mg/kg (di-Na salt).

Zn complex: Zinc protoporphyrin
[15442-64-5]
$C_{34}H_{30}N_4O_4Zn$ 624.025
Prod. by patients with Pb poisoning.

Co complex: Cobalt protoporphyrin
[14325-03-2]
$C_{34}H_{30}CoN_4O_4$ 617.569
Haem oxygenase inhibitor.

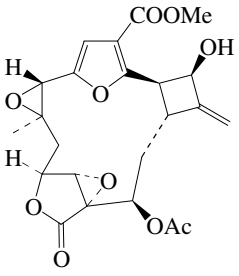
Sn complex: Tin protoporphyrin
[14325-05-4]
$C_{34}H_{30}N_4O_4Sn$ 677.345
Haem oxygenase inhibitor.

Di-Me ester: [5522-66-7]
Violet cryst. ($CHCl_3$/MeOH). Mp 233°. λ_{max} 508; 542; 573; 603; 631 ($CHCl_3$). λ_{max} 407; 506; 541; 576; 631 ($CHCl_3$). λ_{max} 409; 556; 601 (25% HCl).

[50865-01-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 575A (*ir*)
Fischer, H. *et al., Die Chemie des Pyrrols*, Akademische Verlag, Leipzig, Vol. II, (i), 1937, 396-405 (*struct, synth*)
Ramsey, V.G. *et al., Biochem. Prep.*, 1953, **3**, 39-43 (*isol, di-Me ester, uv*)
Sano, S. *et al., Biochem. J.*, 1965, **97**, 250-256; 1966, **98**, 641 (*pmr*)
Jackson, A.H. *et al., Tetrahedron*, 1965, **21**, 2913-2924 (*ms*)
Carr, R.P. *et al., J.C.S.(C)*, 1971, 487-502 (*synth*)
Herring, P.J. *et al., Nature (London)*, 1972, **238**, 276 (*isol*)
Kennedy, G.Y. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **55**, 117-123 (*isol*)
Smith, K.M. *et al., Acc. Chem. Res.*, 1979, **12**, 374-381 (*rev*)
Dinello, R.K. *et al., The Porphyrins*, (Dolphin, D., Ed.), Academic Press, N.Y., Vol. I, 1979, 290
Clezy, P.S. *et al., Aust. J. Chem.*, 1980, **33**, 557-573 (*di-Me ester*)
Kappas, A. *et al., BioEssays*, 1985, **3**, 256-259 (*rev, Sn complex, Co complex*)
Mohinder, K. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1987, **84**, 2464-2468 (*Sn complex*)
Asanaka, M. *et al., AIDS*, 1989, **3**, 403 (*anti-HIV activity*)
Drummond, G.S. *et al., Semin. Hematol.*, 1989, **26**, 24-26 (*rev, Sn complex*)
DeVito, V.L. *et al., J. Phys. Chem.*, 1992, **96**, 6917-6922 (*uv, Raman*)
Dennis, M. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1992, **89**, 5306-5310 (*Co complex*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1622
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, DXF700

Providencin P-633



$C_{23}H_{24}O_{10}$ 460.437
Constit. of *Pseudopterogorgia kallos*. Cryst. (MeOH/$CHCl_3$). $[\alpha]_D^{20}$ +7.9 (c, 1.2 in $CHCl_3$). λ_{max} 203 (ϵ 11500); 251 (ϵ 4900) (MeOH).

Marrero, J. *et al., Org. Lett.*, 2003, **5**, 2551-2554 (*isol, pmr, cmr, cryst struct*)

PRQFV amide P-634

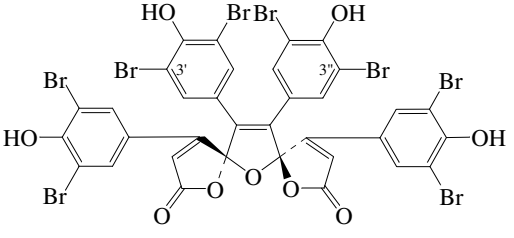
H-Pro-Arg-Gln-Phe-Val-NH_2

$C_{30}H_{48}N_{10}O_6$ 644.773
Isol. from the CNS and gut of *Aplysia* sp.

Furukawa, Y. *et al., J. Neurophysiol.*, 2003, **89**, 3114-3127 (*isol*)

Prunolide A P-635

[225779-74-8]



$C_{34}H_{14}Br_8O_9$ 1205.711
Isol. from the Australian ascidian *Synoicum prunum*. Yellow plates (DMSO).
Mp 212-214°. Racemic.

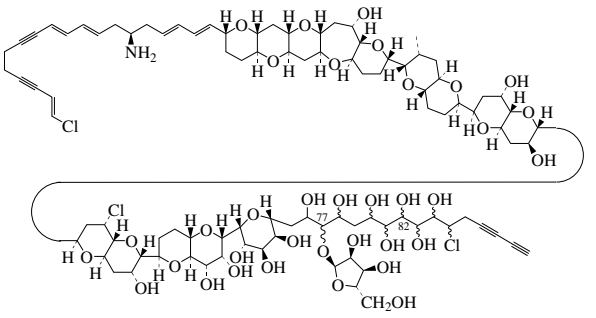
3′,3″-Bis(debromo): ***Prunolide B***
[225779-76-0]
$C_{34}H_{16}Br_6O_9$ 1047.919
Isol. from *Synoicum prunum*. Yellow gum. Racemic. λ_{max} 215 (ϵ 273500); 309 (ϵ 70700); 394 (ϵ 59600) (MeOH).

Octakis(debromo): ***Prunolide C***
[225779-77-1]
$C_{34}H_{22}O_9$ 574.542
Isol. from *Synoicum prunum*. Yellow gum. Racemic. λ_{max} 210 (ϵ 308500); 314 (ϵ 37400) (MeOH).

Carroll, A.R. *et al., J.O.C.*, 1999, **64**, 2680-2682 (*isol*)

Prymnesin 2 P-636

[168010-52-4]



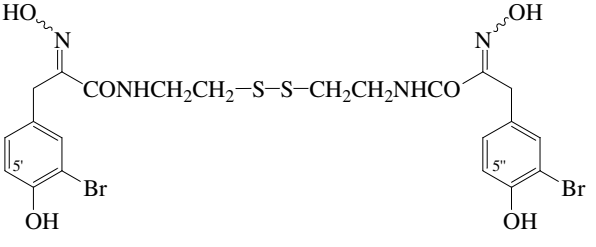
$C_{96}H_{136}Cl_3NO_{35}$ 1970.474
Polyether antibiotic. Isol. from the red tide alga *Prymnesium parvum*. Ichthyotoxic and haemolytic agent. Pale yellow solid. Sol. dioxan, acids. $[\alpha]_D^{23}$ +21.2 (c, 0.1 in dioxan/AcOH). λ_{max} 244 (ϵ 20800); 267 (ϵ 24500); 278 (ϵ 19800) (dioxan/AcOH). λ_{max} 244 (ϵ 20800); 267 (ϵ 24500); 278 (ϵ 19800) (dioxan) (Berdy).

*77-De-*O*-glycosyl, 77-*O*-α-D-ribofuranoside, 78-*O*-α-L-arabinopyranoside, 82-*O*-β-D-galactofuranoside:* ***Prymnesin 1***
[168180-17-4]
$C_{107}H_{154}Cl_3NO_{44}$ 2264.732
Isol. from the alga *Prymnesium parvum*. Ichthyotoxic and haemolytic agent. Pale yellow solid. $[\alpha]_D^{23}$ +9 (c, 0.12 in 1-propanol/AcOH aq.).

Glendenning, L. *et al., Bull. Chem. Soc. Jpn.*, 1996, **69**, 2253-2263 (*conformn*)
Igarashi, T. *et al., J.A.C.S.*, 1996, **118**, 479-480; 1999, **121**, 8499-8511 (*isol, uv, ir, pmr, ms*)
Murata, M. *et al., Nat. Prod. Rep.*, 2000, **17**, 293-314 (*rev*)
Sasaki, M. *et al., Tet. Lett.*, 2001, **42**, 5725-5728 (*synth, config*)
Sasaki, M. *et al., Org. Lett.*, 2004, **6**, 1501-1504 (*config*)

Psammaplin A P-638

N,N′-Bis[3-(3-bromo-4-hydroxyphenyl)-2-oximidopropanoyl]cystamine
[110659-91-1]
[109152-27-4, 109152-30-9]



$C_{22}H_{24}Br_2N_4O_6S_2$ 664.395
Both the (*E,E*)- (Mp 172-174°) and (*E,Z*)-isomers have been isol. and characterised. See Park *et al* (2003). Major metab. from a sponge tentatively identified as *Thorectopsamma xana*. Also from the sponge *Pseudoceratina purpurea* and isol. from another unidentified sponge. Inhibitor of chitinase, histone deacetylase and DNA methyltransferase. Antifungal agent. Exhibits farnesyl protein transferase and leucine aminopeptidase inhibitory activity. Shows cytotoxic and antimicrobial activity. Semicryst. solid.
Mp 67-75°. λ_{max} 219 (ϵ 64600); 277 (ϵ 4875); 286 (sh); 290 (ϵ 10000) (MeOH) (Derep).

*4′-*O*-Sulfate:* ***Psammaplin A$_1$****. Psammaplin A 11′-sulfate*
[263009-15-0]
$C_{22}H_{24}Br_2N_4O_9S_3$ 744.459
Isol. from the sponge *Aplysinella rhax*. Oil; amorph. pale yellow solid (as *N,N*-dimethylguanidine salt).
Mp 76-80° (*N,N*-dimethylguanidine salt). λ_{max} 206 (ϵ 33000);

283 (ϵ 3000); 324 (ϵ 750) (MeOH). λ_{max} 204 (log ϵ 4.73); 280 (log ϵ 3.88) (MeOH) (*N,N*-dimethylguanidine).

4′,4″-Di-O-*sulfate:* ***Psammaplin A₂***
$C_{22}H_{24}Br_2N_4O_{12}S_4$ 824.523
Isol. from the sponge *Aplysinella rhax*. Amorph. pale yellow solid (as *N,N*-dimethylguanidine salt).
Mp 155-160° (*N,N*-dimethylguanidine salt). λ_{max} 204 (log ϵ 4.6); 281 (log ϵ 3.98) (MeOH) (*N,N*-dimethylguanidine).

S-*Oxide:* ***Psammaplin J***
$C_{22}H_{24}Br_2N_4O_7S_2$ 680.394
Alkaloid from the sponge *Pseudoceratina purpurea*.

5′-Hydroxy: ***Psammaplin K***
$C_{22}H_{24}Br_2N_4O_7S_2$ 680.394
Isol. from the sponge *Aplysinella rhax*. Light pinkish oil.
λ_{max} 290 (ϵ 3438) (MeOH).

5′,5″-Dihydroxy: ***Psammaplin L***
$C_{22}H_{24}Br_2N_4O_8S_2$ 696.394
Isol. from the sponge *Aplysinella rhax*. Light pinkish oil.
λ_{max} 291 (ϵ 3139) (MeOH).

5′,5″-Dimer: ***Bisaprasin***
[112514-43-9]
$C_{44}H_{46}Br_4N_8O_{12}S_4$ 1326.774
Minor metab. of a sponge tentatively identified as *Thorectopsamma xana*. Also isol. from *Pseudoceratina purpurea* and *Aplysinella rhax*. Inhibitor of DNA methyltransferase and histone deacetylase. Exhibits farnesyl protein transferase and leucine aminopeptidase inhibitory activity. Shows cytotoxic and antimicrobial activity. Foam. Sol. EtOH, butanol; poorly sol. H_2O, EtOAc. λ_{max} 204 (ϵ 77000); 284 (ϵ 16000) (MeOH) (Berdy).

5′,5″-Dimer, 4′-O-*sulfate:* ***Bisaprasin 11′-sulfate***
[263009-16-1]
$C_{44}H_{46}Br_4N_8O_{15}S_5$ 1406.838
Isol. from *Aplysinella rhax*. Oil. λ_{max} 203 (ϵ 83000); 283 (ϵ 7900); 324 (ϵ 5300) (MeOH).

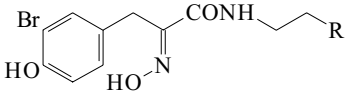
5′-Bromo: ***5-Bromopsammaplin A***
[612089-85-7]
$C_{22}H_{23}Br_3N_4O_6S_2$ 743.291
Isol. from an association of the sponges *Jaspis wondoensis* and *Poecillastra wondoensis*. Amorph. solid. Possesses (*E,E*)-config.

Trisulfide: ***Psammaplin A trisulfide***
$C_{22}H_{24}Br_2N_4O_6S_3$ 696.461
Isol. from an association of the sponges *Jaspis wondoensis* and *Poecillastra wondoensis*. Amorph. solid. Possesses (*E,E*)-config.

Arabshahi, L. *et al., J.O.C.*, 1987, **52**, 3584-3586 (*isol, struct*)
Rodriguez, A.D. *et al., Tet. Lett.*, 1987, **28**, 4989-4992 (*isol, uv, ir, pmr, cmr, activity*)
Jimenez, C. *et al., Tetrahedron*, 1991, **47**, 2097-2102 (*activity*)
Hoshino, O. *et al., Bioorg. Med. Chem. Lett.*, 1992, **2**, 1561-1562 (*synth*)
Pham, N.B. *et al., J. Nat. Prod.*, 2000, **63**, 393-395 (*11′-sulfates*)
Shin, J. *et al., Tetrahedron*, 2000, **56**, 9071-9077 (*Psammaplins A_1,A_2, activity*)
Tabudravu, J.N. *et al., Bioorg. Med. Chem.*, 2002, **10**, 1123-1128 (*pmr, cmr, Psammaplins K,L*)
Park, Y. *et al., J. Nat. Prod.*, 2003, **66**, 1495-1498 (*isol, pmr, cmr*)
Piña, I.C. *et al., J.O.C.*, 2003, **68**, 3866-3873 (*isol, pmr, cmr*)
Godert, A.M. *et al., Bioorg. Med. Chem. Lett.*, 2006, **16**, 3330-3333 (*synth*)
Mora, F.D. *et al., J. Nat. Prod.*, 2006, **69**, 547-552 (*Psammaplin A, activity*)

Psammaplin B P-639

2-[[3-(3-Bromo-4-hydroxyphenyl)-2-(hydroxyimino)-1-oxopropyl]amino]ethyl thiocyanate, 9CI
[133991-67-0]



R = SCN

$C_{12}H_{12}BrN_3O_3S$ 358.215
Isol. from the marine sponge *Pseudoceratina purpurea*. Oil.
λ_{max} 280 (ϵ 5450) (MeOH) (Berdy).

Jimenez, C. *et al., Tetrahedron*, 1991, **47**, 2097-2102 (*isol, pmr, cmr*)
Piña, I.C. *et al., J.O.C.*, 2003, **68**, 3866-3873 (*isol, activity*)

Psammaplin C P-640

N-*[2-(Aminosulfonyl)ethyl]-3-bromo-4-hydroxy-α-(hydroxyimino)benzenepropanamide, 9CI*
[133991-68-1]
As Psammaplin B, P-639 with
R = $-SO_2NH_2$
$C_{11}H_{14}BrN_3O_5S$ 380.219
Isol. from the marine sponge *Pseudoceratina purpurea*. Oil.
λ_{max} 282 (ϵ 2200) (MeOH) (Berdy).

Jimenez, C. *et al., Tetrahedron*, 1991, **47**, 2097-2102 (*isol, pmr, cmr*)
Piña, I.C. *et al., J.O.C.*, 2003, **68**, 3866-3873 (*isol, activity*)

Psammaplin D P-641

[133991-69-2]
As Psammaplin B, P-639 with
R = $-SSCH_2CH_2NHCOOMe$
$C_{15}H_{20}BrN_3O_5S_2$ 466.376
Isol. from the marine sponge *Pseudoceratina purpurea*. Exhibits antimicrobial and mild tyrosine kinase inhibitory activities. Oil.
λ_{max} 280 (ϵ 17733) (MeOH) (Berdy).

Jimenez, C. *et al., Tetrahedron*, 1991, **47**, 2097-2102 (*isol, pmr, cmr*)
Park, Y. *et al., J. Nat. Prod.*, 2003, **66**, 1495-1498 (*isol, pmr, cmr*)
Piña, I.C. *et al., J.O.C.*, 2003, **68**, 3866-3873 (*isol, cmr, activity*)

Psammaplin E P-642

As Psammaplin B, P-639 with
R = -S-S-$CH_2CH_2NHCOCONH_2$
$C_{15}H_{19}BrN_4O_5S_2$ 479.375
Alkaloid from the sponge *Pseudoceratina purpurea*. λ_{max} 206 (ϵ 18070); 284 (ϵ 1860) (MeOH).

Piña, I.C. *et al., J.O.C.*, 2003, **68**, 3866-3873 (*isol, pmr, cmr*)

Psammaplin F P-643

As Psammaplin B, P-639 with
R = -S-S-$CH_2CH_2NHCOCOOH$
$C_{15}H_{18}BrN_3O_6S_2$ 480.36
Alkaloid from the sponge *Pseudoceratina purpurea*. Potent histone deacetylase inhibitor. λ_{max} 206 (ϵ 25935); 280 (ϵ 2060) (MeOH).

Piña, I.C. *et al., J.O.C.*, 2003, **68**, 3866-3873 (*isol, pmr, cmr*)

Psammaplin G P-644

As Psammaplin B, P-639 with
R = -S-S-$CH_2CH_2NHC(COOH){=}NNH_2$
$C_{15}H_{20}BrN_5O_5S_2$ 494.39
Alkaloid from the sponge *Pseudoceratina purpurea*. Potent DNA methyltransferase inhibitor.

Piña, I.C. *et al., J.O.C.*, 2003, **68**, 3866-3873 (*isol, pmr, cmr*)

Psammaplin H P-645

As Psammaplin B, P-639 with
R = -S-S-$CH_2CH_2NHCOOEt$
$C_{16}H_{22}BrN_3O_5S_2$ 480.403
Alkaloid from the sponge *Pseudoceratina purpurea*.

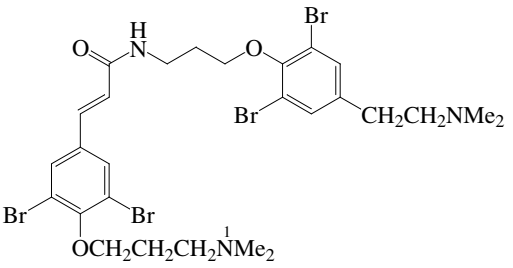
Piña, I.C. *et al., J.O.C.*, 2003, **68**, 3866-3873 (*isol, pmr, cmr*)

Psammaplin I P-645a

As Psammaplin B, P-639 with
R = $-SO_2Me$
$C_{12}H_{15}BrN_2O_5S$ 379.231
Alkaloid from the sponge *Pseudoceratina purpurea*.

Piña, I.C. *et al.,* IJ.O.C., 2003, **68**, 3866-3873 (*isol, pmr, cmr*)

Psammaplysene A P-646



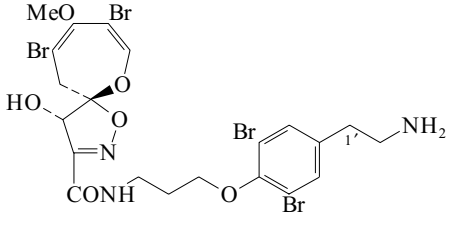
$C_{27}H_{35}Br_4N_3O_3$ 769.208
Isol. from the sponge *Psammaplysilla* sp. Specific inhibitor of FOXO1a nuclear export.

N^1-*De-Me:* ***Psammaplysene B***
$C_{26}H_{33}Br_4N_3O_3$ 755.181
Isol. from *Psammaplysilla* sp.

Schroeder, F.C. *et al., J. Nat. Prod.*, 2005, **68**, 574-576 (*isol, pmr, cmr, ms*)
Georgiades, S.N. *et al., Org. Lett.*, 2005, **7**, 4091-4094 (*synth*)

Psammaplysin A P-647

[85819-66-5]



$C_{21}H_{23}Br_4N_3O_6$ 733.045
Isol. from Red Sea sponge *Psammaplysilla purpurea*. Shows antibiotic props.; active against gram-positive bacteria. Exhibits moderate *in vitro* cytotoxicity towards the human colon tumour cell-line HCT116. Also shows antifouling activity. Foam. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{22}$ -65.2 (c, 0.52 in MeOH). λ_{max} 229 (ϵ 12700); 262 (sh) (ϵ 7100); 276 (ϵ 2500); 283 (sh) (ϵ 3200) (MeOH) (Derep). λ_{max} 228 (ϵ 9000); 256 (ϵ 4000); 272 (ϵ 2800); 276 (ϵ 2500) (MeOH) (Berdy). λ_{max} 229 (ϵ 12500); 276 (ϵ 7100); 283 (ϵ 3200) (MeOH/HCl) (Berdy). λ_{max} 229 (ϵ 12500) (EtOH) (Berdy).

Di-Ac: [95739-54-1]
Needles (MeOH). Mp 140°.

N-*Formyl:* ***Ceratinamide A***. N-*Formylpsammaplysin A*
[178214-21-6]
$C_{22}H_{23}Br_4N_3O_7$ 761.056
Metab. from the marine sponge *Pseudoceratina purpurea*. Shows potent antifouling activity. Solid. Sol. MeOH. $[\alpha]_D^{24}$ -89.7 (c, 0.146 in MeOH). λ_{max} 207 (ϵ 64200) (MeOH) (Berdy).

N-*(13-Methyltetradecanoyl):* ***Ceratinamide B***. *1′-Deoxypsammaplysin D*
[178214-22-7]
$C_{36}H_{51}Br_4N_3O_7$ 957.431
Metab. from the marine sponge *Pseudoceratina purpurea*. Shows antifouling activity. Solid. Sol. MeOH. $[\alpha]_D^{24}$ -53.5 (c, 0.263 in Me_2CO). λ_{max} 207 (ϵ 51100) (MeOH) (Berdy).

N-*Me:* ***Psammaplysin F***
[190510-86-2]
$C_{22}H_{25}Br_4N_3O_6$ 747.072
Alkaloid from *Aplysinella* sp.
$[\alpha]_D$ -62.3 (c, 1.2 in MeOH/CH_2Cl_2).

1′-Hydroxy: ***Psammaplysin B***
[85819-67-6]
$C_{21}H_{23}Br_4N_3O_7$ 749.045
Isol. from *Psammaplysilla purpurea*. Active against gram-positive bacteria. Shows moderate *in vivo* cytotoxicity *vs* human colon tumour cells. Foam. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -60.2 (c, 0.632 in MeOH). λ_{max} 218 (ϵ 28600); 256 (sh) (ϵ 7000); 262 (sh) (ϵ 6400); 277 (sh) (ϵ 4000); 282 (ϵ 3000) (MeOH) (Derep). λ_{max} 218 (ϵ 28600); 282 (ϵ 3000) (MeOH/HCl) (Berdy).

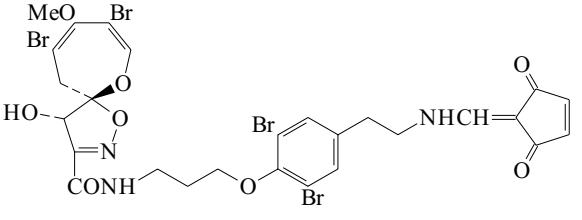
1′-Hydroxy, N-*Me:* ***Psammaplysin C***
[142449-78-3]
$C_{22}H_{25}Br_4N_3O_7$ 763.071
Metab. from the marine sponge *Druinella purpurea* (*Psammaplysilla purpurea*). Exhibits moderate *in vitro* cytotoxicity towards the human colon tumour cell-line HCT116. Glass. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{23}$ -57.1 (c, 0.014 in MeOH). λ_{max} 218 (ϵ 17600); 255 (ϵ 6700); 279 (ϵ 3000) (MeOH) (Berdy).

1′-Hydroxy, N-*(13-methyltetradecanoyl):* ***Psammaplysin D***
[149415-75-8]
$C_{36}H_{51}Br_4N_3O_8$ 973.43
Alkaloid from the sponge *Aplysinella* sp. Immunosuppressant. Oil. $[\alpha]_D^{18}$ -71.4 (c, 2.8 in Me_2CO). λ_{max} 210 (ϵ 50900); 224; 298 (MeOH) (Berdy).

Rotem, M. *et al., Tetrahedron*, 1983, **39**, 667 (*isol, uv, ir, pmr, cmr, ms, struct*)
Roll, D.M. *et al., J.A.C.S.*, 1985, **107**, 2916 (*uv, ir, pmr, cmr, ms, struct*)
Copp, B.R. *et al., J. Nat. Prod.*, 1992, **55**, 822 (*Psammaplysin C*)
Ichiba, T. *et al., J.O.C.*, 1993, **58**, 4149 (*Psammaplysin D*)
Tsukamoto, S. *et al., Tetrahedron*, 1996, **52**, 8181 (*Ceratinamide A, Ceratinamide B*)
Liu, S. *et al., J. Nat. Prod.*, 1997, **60**, 614 (*Psammaplysin F*)

Psammaplysin E P-648

[149415-76-9]

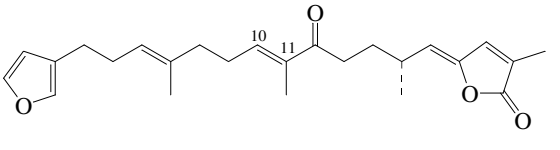


$C_{27}H_{25}Br_4N_3O_8$ 839.126
Alkaloid from the sponge *Aplysinella* sp. and *Pseudoceratina purpurea*. Immunosuppressive, antifouling agent. Bright yellow oil. $[\alpha]_D^{18}$ -80.3 (c, 0.3 in Me_2CO). λ_{max} 208 (ϵ 53400); 224; 298 (ϵ 25000) (MeOH) (Berdy).

Ichiba, T. *et al., J.O.C.*, 1993, **58**, 4149 (*isol, uv, ir, pmr, cmr, struct*)

Psammocinin A_1 P-649

[745819-27-6]



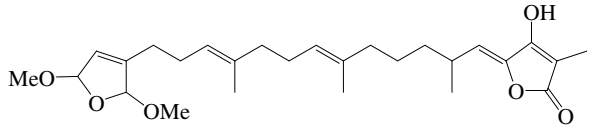
$C_{25}H_{32}O_4$ 396.525
Constit. of a *Psammocinia* sp. Oil. $[\alpha]_D^{21}$ +26.9 (c, 0.12 in MeOH).

10,11-Dihydro: ***Psammocinin A_2***
[745819-28-7]
$C_{25}H_{34}O_4$ 398.541
Constit. of a *Psammocinia* sp. Oil. $[\alpha]_D^{21}$ +42.1 (c, 0.18 in MeOH).

Choi, K. *et al., J. Nat. Prod.*, 2004, **67**, 1186-1189 (*isol, pmr, cmr*)

Psammocinin A_3 P-650

[745819-29-8]



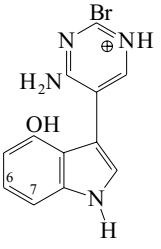
$C_{27}H_{40}O_6$ 460.609

Constit. of a *Psammocinia* sp. Oil. $[\alpha]_D^{21}$ +16.3 (c, 0.1 in MeOH).

Choi, K. *et al., J. Nat. Prod.*, 2004, **67**, 1186-1189 (*isol, pmr, cmr*)

Psammopemmin A P-651

[145940-63-2]



$C_{12}H_{10}BrN_4O^{\oplus}$ 306.141

Counterion unknown (prob. chloride). Attempts to produce free base resulted in dec. CAS Reg. No. refers to free base. Alkaloid from an Antarctic sponge *Psammopemma* sp. Yellow solid. λ_{max} 220 (ϵ 24000); 287 (ϵ 4300); 362 (ϵ 9800) (EtOH) (Berdy).

6-Bromo: ***Psammopemmin C***

[145940-65-4]

$C_{12}H_9Br_2N_4O^{\oplus}$ 385.037

From *Psammopemma* sp. Yellow solid. CAS Reg. No. refers to free base. λ_{max} 228 (ϵ 33000); 292 (ϵ 2800); 362 (ϵ 15400) (EtOH) (Berdy).

7-Bromo: ***Psammopemmin B***

[145940-64-3]

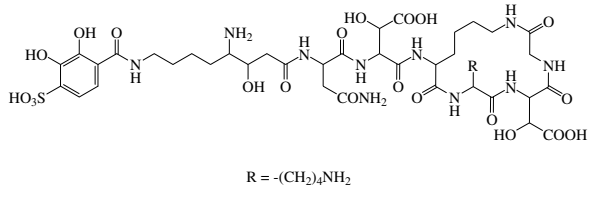
$C_{12}H_9Br_2N_4O^{\oplus}$ 385.037

From *Psammopemma* sp. CAS Reg. No. refers to free base. λ_{max} 227 (ϵ 34500); 292 (ϵ 2800); 361 (ϵ 15200) (EtOH) (Berdy).

Butler, M.S. *et al., Aust. J. Chem.*, 1992, **45**, 1871 (*isol, uv, pmr, cmr, ms, struct*)

Pseudoalterobactin A P-652

[691850-60-9]



R = $-(CH_2)_4NH_2$

$C_{41}H_{63}N_{11}O_{21}S$ 1078.076

Prod. by the marine bacterium *Pseudoalteromonas* sp. KP20-4. Siderophore.

Kanoh, K. *et al., J. Antibiot.*, 2003, **56**, 871-875 (*isol, pmr, cmr, ms*)

Pseudoalterobactin B P-653

As Pseudoalterobactin A, P-652 with

R = $-(CH_2)_3NHC(NH_2)=NH$

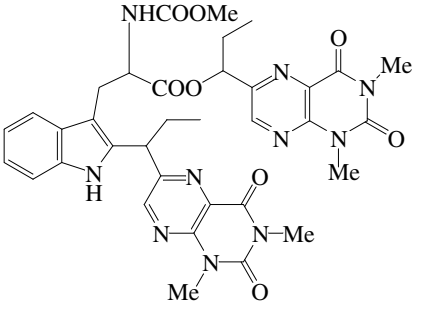
$C_{41}H_{63}N_{13}O_{21}S$ 1106.089

Prod. by the marine bacterium *Pseudoalteromonas* sp. KP20-4. Siderophore.

Kanoh, K. *et al., J. Antibiot.*, 2003, **56**, 871-875 (*isol, pmr, cmr, ms*)

Pseudoanchynazine A P-654

[445430-63-7]



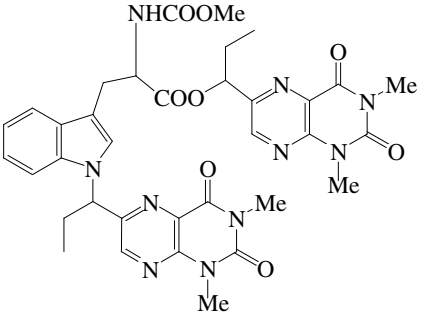
$C_{35}H_{38}N_{10}O_8$ 726.747

Alkaloid from the sponge *Clathria* sp. Yellow powder. $[\alpha]_D^{25}$ -60.7 (c, 0.83 in MeOH). λ_{max} 248 (ϵ 9700) (MeOH).

Zuleta, I.A. *et al., Tetrahedron*, 2002, **58**, 4481-4486 (*isol, pmr, cmr*)

Pseudoanchynazine B P-655

[445430-64-8]



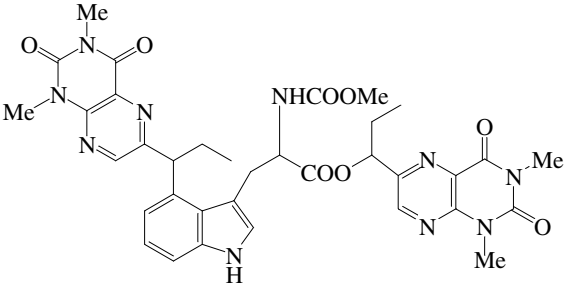
$C_{35}H_{38}N_{10}O_8$ 726.747

Alkaloid from the sponge *Clathria* sp. Yellow powder. $[\alpha]_D^{25}$ +81.2 (c, 0.42 in MeOH). λ_{max} 242 (ϵ 11300) (MeOH).

Zuleta, I.A. *et al., Tetrahedron*, 2002, **58**, 4481-4486 (*isol, pmr, cmr*)

Pseudoanchynazine C P-656

[445430-65-9]



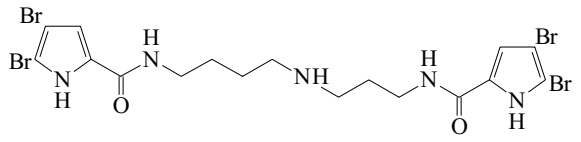
$C_{35}H_{38}N_{10}O_8$ 726.747

Alkaloid from the sponge *Clathria* sp. Yellow powder. $[\alpha]_D^{25}$ +96.6 (c, 2.21 in MeOH). λ_{max} 253 (ϵ 10900) (MeOH).

Zuleta, I.A. *et al., Tetrahedron*, 2002, **58**, 4481-4486 (*isol, pmr, cmr*)

Pseudoceratidine P-657

[174545-78-9]



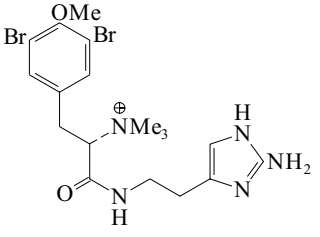
$C_{17}H_{21}Br_4N_5O_2$ 647.001

Metab. from the marine sponge *Pseudoceratina purpurea*. Antifouling agent; larval settlement and development inhibitor. Solid. λ_{max} 275 (ϵ 18400) (MeOH) (Berdy).

Tsukamoto, S. *et al., Tet. Lett.*, 1996, **37**, 1439 (*isol, uv, ir, pmr, cmr, struct*)
Behrens, C. *et al., Bioorg. Med. Chem. Lett.*, 1997, **7**, 321 (*synth*)
Ponasik, J.A. *et al., Tetrahedron*, 1998, **54**, 6977-6986 (*synth*)

Pseudoceratinine B P-658

[172670-15-4]



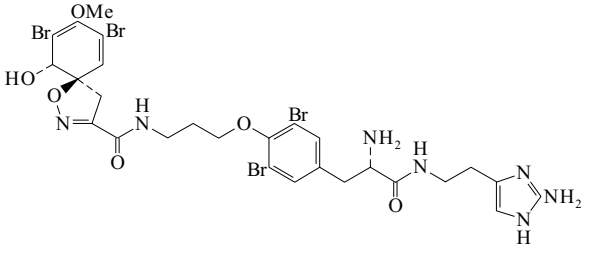
$C_{18}H_{26}Br_2N_5O_2^{\oplus}$ 504.244

Alkaloid from the sponge *Pseudoceratina verrucosa*. Sol. MeOH, CH_2Cl_2; poorly sol. H_2O. $[\alpha]_D$ +17 (c, 1 in MeOH) (as hydrochloride). λ_{max} 285 (ϵ 1480); 330 (ϵ 490) (MeOH) (Berdy).

Benharref, A. *et al., J. Nat. Prod.*, 1996, **59**, 177 (*isol, uv, ir, pmr, cmr, cd, struct*)

Pseudoceratinine C P-659

[172617-97-9]



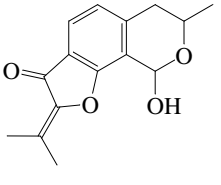
$C_{27}H_{31}Br_4N_7O_6$ 869.201

Alkaloid from the sponge *Pseudoceratina verrucosa*. Sol. MeOH, CH_2Cl_2; poorly sol. H_2O. $[\alpha]_D$ -10 (c, 1 in MeOH) (as hydrochloride). Closely related to Purealine, P-721. λ_{max} 220 (ϵ 34670); 228 (ϵ 12880) (MeOH) (Berdy).

Benharref, A. *et al., J. Nat. Prod.*, 1996, **59**, 177 (*isol, uv, ir, cd, pmr, cmr, struct*)

Pseudodeflectusin P-660

*6,9-Dihydro-9-hydroxy-7-methyl-2-(1-methylethylidene)-7*H*-furo[3,2-*h*][2]benzopyran-3(2*H*)-one*



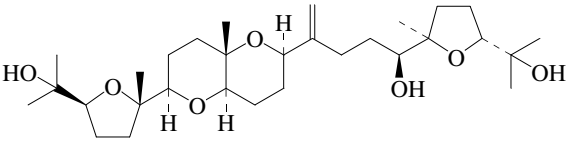
$C_{15}H_{16}O_4$ 260.289

Prod. by *Aspergillus pseudodeflectus* isol. from *Sargassum fusiform*. Cytotoxic. Needles (THF/hexane).
Mp 179-180°. $[\alpha]_D^{23}$ +11 (c, 0.18 in MeOH).

Ogawa, A. *et al., Bioorg. Med. Chem. Lett.*, 2004, **14**, 3539-3543 (*isol, pmr, cmr*)

Pseudodehydrothyrsiferol P-661

[346583-58-2]



$C_{30}H_{52}O_7$ 524.737

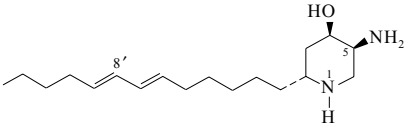
Constit. of *Laurencia viridis*. Amorph. solid. $[\alpha]_D^{25}$ -13.1 (c, 0.13 in $CHCl_3$).

Manriquez, C.P. *et al., Tetrahedron*, 2001, **57**, 3117-3123 (*isol, pmr, cmr*)

Pseudodistomin B P-662

5-Amino-2-(6,8-tridecadienyl)-4-piperidinol, 9CI

[106293-83-8]



$C_{18}H_{34}N_2O$ 294.479

Struct. revised in 1992. Originally assigned as the 3′,5′-diene. Metab. from the Okinawan tunicate *Pseudodistoma kanoko* and *Pseudodistoma megalarva*. Exhibits antineoplastic activity; phosphodiesterase inhibitor; calmodulin antagonist. Oil (as *N,N′*-di-Ac). Sol. $CHCl_3$, MeOH; poorly sol. H_2O, toluene. $[\alpha]_D^{24}$ +35 (c, 1 in MeOH) (di-Ac). λ_{max} 233 (ϵ 17500) (MeOH) (Derep).

8′Z-Isomer: ***Pseudodistomin A***

[106231-30-5]

Metab. from *Pseudodistoma kanoko*. Exhibits antineoplastic activity; phosphodiesterase inhibitor; calmodulin antagonist. Oil (as *N,N′*-di-Ac). Sol. $CHCl_3$, MeOH; poorly sol. H_2O, toluene. $[\alpha]_D^{24}$ +36 (c, 1 in MeOH) (di-Ac). λ_{max} 233 (ϵ 17500) (MeOH) (Derep).

4-Epimer: ***Pseudodistomin D***

[196099-42-0]

$C_{18}H_{34}N_2O$ 294.479

Isol. from *Pseudodistoma megalarva*. Gum. $[\alpha]_D^{25}$ +5 (c, 0.3 in MeOH). λ_{max} 240 (MeOH).

4,5-Diepimer: ***Pseudodistomin E***

[196099-44-2]

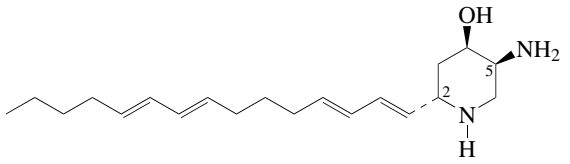
$C_{18}H_{34}N_2O$ 294.479

Isol. from *Pseudodistoma megalarva*. Gum. $[\alpha]_D^{25}$ -20.8 (c, 0.4 in MeOH). λ_{max} 239 (MeOH).

Ishibashi, M. *et al., J.O.C.*, 1987, **52**, 450-453 (*Pseudodistomins A,B, isol, uv, ir, pmr, cmr, ms*)
Kiguchi, T. *et al., Tet. Lett.*, 1992, **33**, 7389-7390 (*synth, struct*)
Ishibashi, M. *et al., J. Nat. Prod.*, 1995, **58**, 804-806 (*struct*)
Naito, T. *et al., J.C.S. Perkin 1*, 1996, 281-288 (*synth, struct, bibl*)
Kiguchi, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1212-1215 (*synth*)
Freyer, A.J. *et al., J. Nat. Prod.*, 1997, **60**, 986-990 (*Pseudodistomins D,E, isol, uv, ir, pmr, cmr*)
Ninomiya, I. *et al., Alkaloids (N.Y.)*, 1998, **50**, 317-342 (*rev*)
Trost, B.M. *et al., Org. Lett.*, 2005, **7**, 823-826 (*synth*)

Pseudodistomin F P-663

5-Amino-2-(1,3,8,10-pentadecatetraenyl)-4-piperidinol
[196099-46-4]

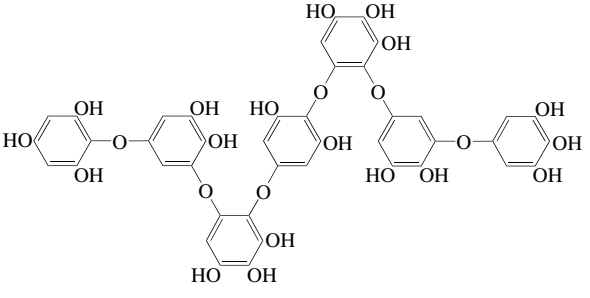


$C_{20}H_{34}N_2O$ 318.501
Isol. from the ascidian *Pseudodistoma megalarva*. Gum. $[\alpha]_D^{25}$ -13.9 (c, 0.4 in MeOH). λ_{max} 233 (MeOH).

4,5-Diepimer: ***Pseudodistomin C***
[169626-36-2]
$C_{20}H_{34}N_2O$ 318.501
Isol. from *Pseudodistoma kanoko* and *Pseudodistoma megalarva*. Cytotoxic agent. Oil (as N^1,N^5,*O*-tri-Ac). $[\alpha]_D^{22}$ +85 (c, 1 in $CHCl_3$) (tri-Ac). λ_{max} 235 (ϵ 37000) (MeOH) (tri-Ac).

Kobayashi, J. *et al., J.O.C.*, 1995, **60**, 6941-6945 (*Pseudodistomin C*)
Doi, Y. *et al., Tetrahedron*, 1996, **52**, 4573-4580 (*Pseudodistomin C, synth*)
Freyer, A.J. *et al., J. Nat. Prod.*, 1997, **60**, 986-990 (*Pseudodistomin F*)
Langlois, N. *et al., Org. Lett.*, 2002, **4**, 185-187 (*Pseudodistomin C, synth*)
Tanaka, K. *et al., Heterocycles*, 2006, **68**, 183-192 (*Pseudodistomin C, synth*)

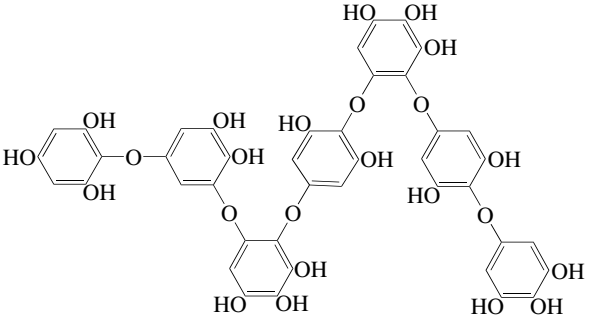
Pseudoheptafuhalol A P-664



$C_{42}H_{30}O_{24}$ 918.685
Constit. of the alga *Sargassum spinuligerum*. Isol. as octadeca-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)

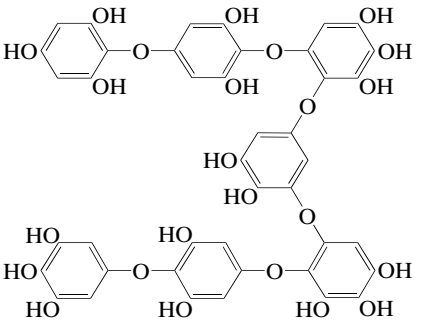
Pseudoheptafuhalol B P-665



$C_{42}H_{30}O_{24}$ 918.685
Constit. of the brown algae *Sargassum spinuligerum* and *Carpophyllum angustifolium*. Isol. as octadeca-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

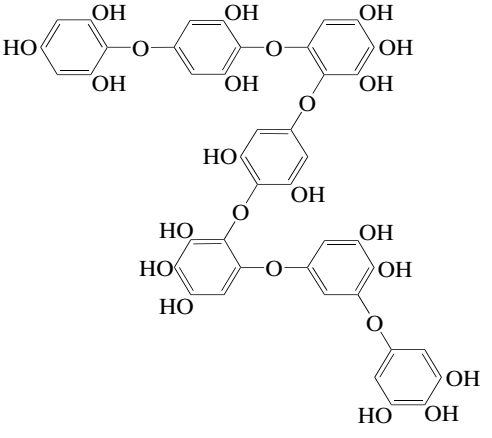
Pseudoheptafuhalol C P-666



$C_{42}H_{30}O_{24}$ 918.685
Constit. of brown algae *Sargassum spinuligerum* and *Carpophyllum angustifolium*. Isol. as octadeca-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

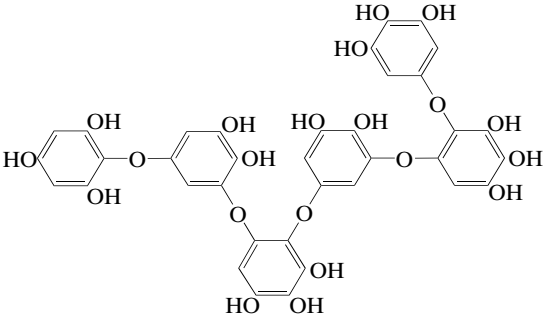
Pseudoheptafuhalol D P-667



$C_{42}H_{30}O_{24}$ 918.685
Constit. of brown algae *Sargassum spinuligerum* and *Carpophyllum angustifolium*. Isol. as octadeca-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

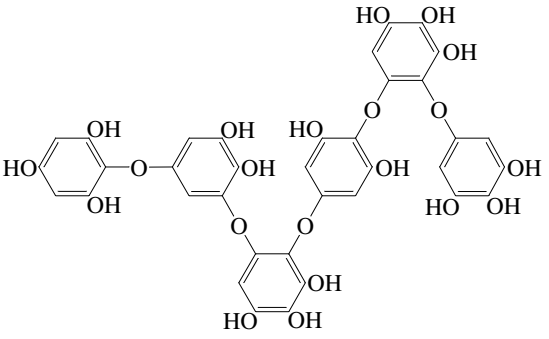
Pseudohexafuhalol A P-668



$C_{36}H_{26}O_{21}$ 794.589
Constit. of the brown algae *Sargassum spinuligerum* and *Carpophyllum angustifolium*. Isol. as hexadeca-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

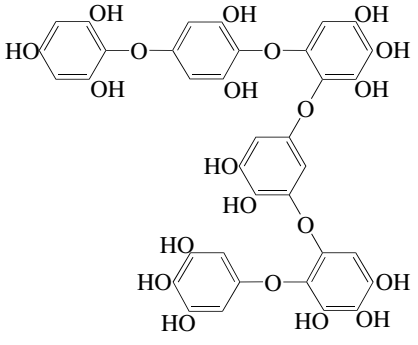
Pseudohexafuhalol B P-669



$C_{36}H_{26}O_{21}$ 794.589
Constit. of the brown algae *Sargassum spinuligerum* and *Carpophyllum angustifolium*. Isol. as hexadeca-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1418 (*isol, pmr, cmr*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

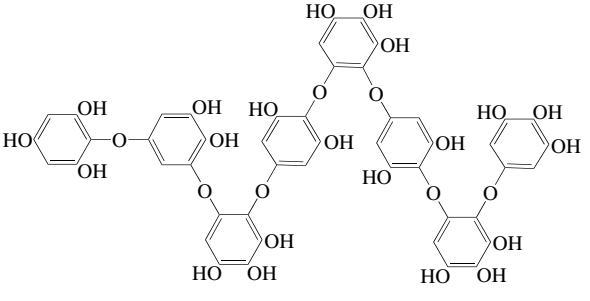
Pseudohexafuhalol C P-670



$C_{36}H_{26}O_{21}$ 794.589
Constit. of the brown algae *Sargassum spinuligerum* and *Carpophyllum angustifolium*. Isol. as hexadeca-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1328-1240 (*isol*)

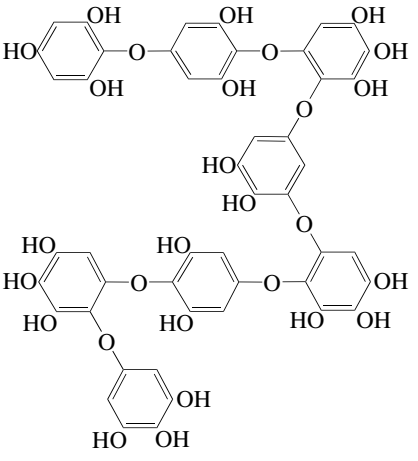
Pseudooctafuhalol B P-671



$C_{48}H_{34}O_{28}$ 1058.78
Constit. of the alga *Sargassum spinuligerum*. Isol. as heneicosa-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)

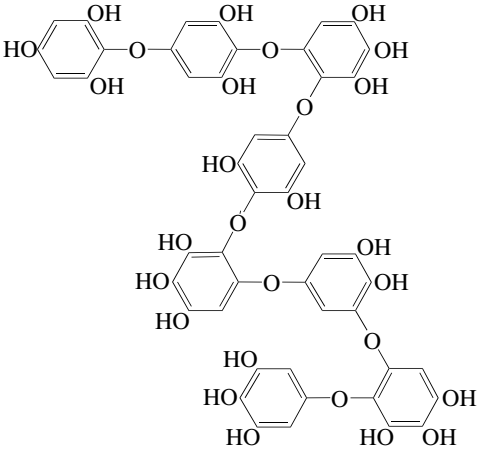
Pseudooctafuhalol C P-672



$C_{48}H_{34}O_{28}$ 1058.78
Constit. of the alga *Sargassum spinuligerum*. Isol. as heneicosa-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)

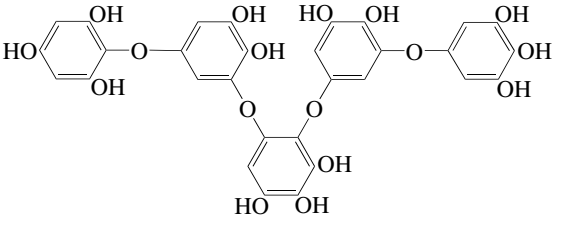
Pseudooctafuhalol D P-673



$C_{48}H_{34}O_{28}$ 1058.78
Constit. of the alga *Sargassum spinuligerum*. Isol. as heneicosa-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)

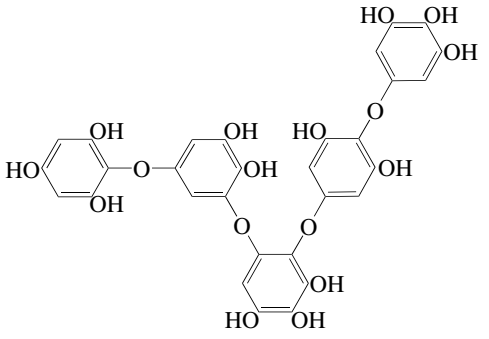
Pseudopentafuhalol A P-674



$C_{30}H_{22}O_{17}$ 654.494
Constit. of the alga *Sargassum spinuligerum*. Isol. as trideca-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)

Pseudopentafuhalol B P-675

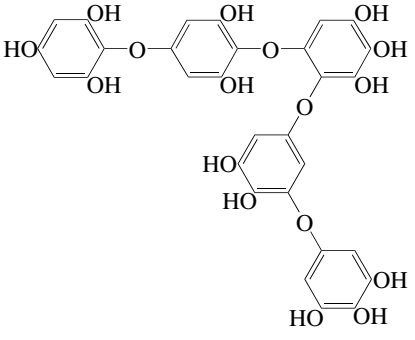


$C_{30}H_{22}O_{17}$ 654.494
Constit. of the alga *Sargassum spinuligerum*. Isol. as trideca-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)

Pseudopentafuhalol C P-676

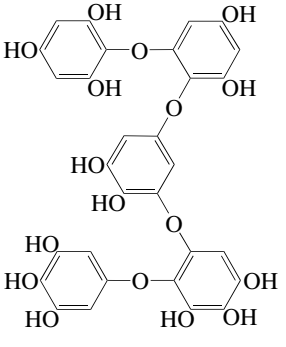
[202211-82-3]



$C_{30}H_{22}O_{17}$ 654.494
Constit. of the alga *Sargassum spinuligerum*. Isol. as trideca-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)

Pseudopentafuhalol D P-677

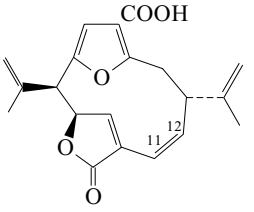


$C_{30}H_{22}O_{17}$ 654.494
Constit. of the alga *Sargassum spinuligerum*. Isol. as trideca-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)

Pseudopteradienoic acid P-678

[173357-05-6]



$C_{20}H_{20}O_5$ 340.375
Isol. from coelenterate *Pseudopterogorgia acerosa*. Antiinflammatory agent. Pale yellow oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ +14.2 (c, 0.2 in $CHCl_3$). λ_{max} 250 (ϵ 10200) (MeOH) (Berdy).

Me ester: ***Pseudopteradiene***
[173357-04-5]
$C_{21}H_{22}O_5$ 354.402
Constit. of *Pseudopterogorgia acerosa*. Antiinflammatory agent. Pale yellow oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ +17.5 (c, 0.2 in $CHCl_3$). λ_{max} 248 (ϵ 10050) (MeOH) (Berdy).

11,12-Dihydro: ***Pseudopteranoic acid***
[173357-07-8]
$C_{20}H_{22}O_5$ 342.391
Constit. of *Pseudopterogorgia acerosa*. Antiinflammatory agent. Pale yellow oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ +5 (c, 4.5 in $CHCl_3$). λ_{max} 252 (ϵ 4000) (MeOH) (Berdy).

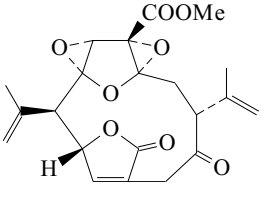
11,12-Dihydro, Me ester: ***Deoxypseudopterolide***
[132235-60-0]
$C_{21}H_{24}O_5$ 356.418
Constit. of *Pseudopterogorgia acerosa*. Pale yellow oil.

11,12-Dihydro, 11β-hydroxy, Me ester: ***11-Pseudopteronol***
[173357-06-7]
$C_{21}H_{24}O_6$ 372.417
Constit. of *Pseudopterogorgia acerosa*. Antiinflammatory agent. Pale yellow oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ +5 (c, 0.2 in $CHCl_3$). λ_{max} 248 (ϵ 2880) (MeOH) (Berdy).

Chan, W.R. *et al., J.O.C.*, 1993, **58**, 186-191 (*isol*)
Rodrigúez, A.D. *et al., Chem. Pharm. Bull.*, 1996, **44**, 91-94 (*isol, pmr, cmr*)

Pseudopterogorgia lactone P-679

[137605-13-1]

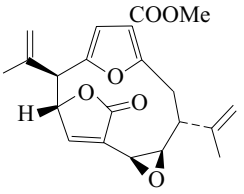


$C_{21}H_{22}O_8$ 402.4
Compd. not named in reference. Constit. of *Pseudopterogorgia acerosa*. Cryst.
Mp 180-181°. $[\alpha]_D$ -319 (c, 0.27 in $CHCl_3$).

Tinto, W.F. *et al., Tet. Lett.*, 1991, **31**, 4661 (*isol, pmr, cmr, cryst struct*)

Pseudopterolide P-680

[83560-98-9]



$C_{21}H_{22}O_6$ 370.401

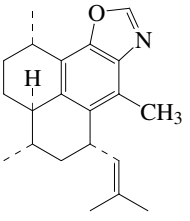
Terpene antibiotic. Prod. by *Pseudopterogorgia acerosa*. Inhibits cell cleavage. Acts similarly to Cytochalasin D. Amorph. solid. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{26}$ +96.3 (c, 1.9 in $CHCl_3$). λ_{max} 223 (ϵ 8000) (Et_2O) (Derep).

MeOH adduct:
Amorph. $[\alpha]_D^{26}$ -115.4 (c, 2.4 in $CHCl_3$). λ_{max} 235; 275 (MeOH).

Bandurraga, M.M. *et al., J.A.C.S.*, 1982, **104**, 6463-6465 (*isol, struct*)

Pseudopteroxazole P-681

[242150-01-2]



Absolute Configuration

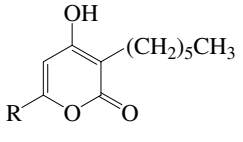
$C_{21}H_{27}NO$ 309.45

Struct. revised in 2001. Isol. from *Pseudopterogorgia elisabethae*. Active against *Mycobacterium tuberculosis*. Yellowish oil. $[\alpha]_D^{25}$ +101 (c, 1 in $CHCl_3$). λ_{max} 220 (ϵ 15400); 250 (ϵ 5000); 284 (ϵ 2000) (MeOH).

Rodriguez, A.D. *et al., Org. Lett.*, 1999, **1**, 527-530 (*isol*)
Johnson, T.W. *et al., J.A.C.S.*, 2001, **123**, 4475-4479 (*struct*)
Davidson, J.P. *et al., J.A.C.S.*, 2003, **125**, 13486-13489 (*synth, abs config*)
Harmata, M. *et al., Org. Lett.*, 2005, **7**, 3581-3583 (*synth*)

Pseudopyronine A P-682

*3-Hexyl-4-hydroxy-6-pentyl-2*H*-pyran-2-one*



R = $-(CH_2)_4CH_3$

$C_{16}H_{26}O_3$ 266.38

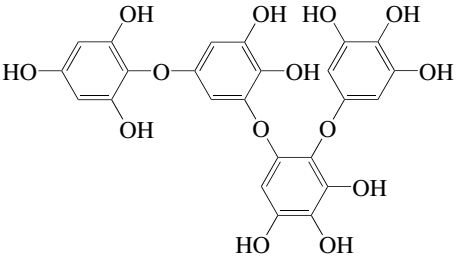
Prod. by a marine *Pseudomonas* sp. F92S91. Powder.

Kong, F.-M. *et al., J. Nat. Prod.*, 2005, **68**, 920-923 (*isol, uv, pmr, cmr, ms*)

Pseudotetrafuhalol A P-683

Tetrafuhalol C

[137809-88-2]



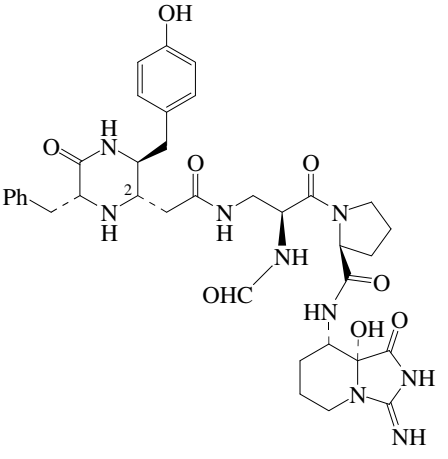
$C_{24}H_{18}O_{14}$ 530.398

Revised struct. (1997). The name was changed on structure revision from Tetrafuhalol C to Pseudotetrafuhalol A. Constit. of the algae *Carpophyllum maschalocarpum* and *Sargassum spinuligerum*. Isol. as undeca-Ac.

Glombitza, K.-W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1981, **314**, 602 (*isol, pmr*)
Glombitza, K.-W. *et al., Phytochemistry*, 1991, **30**, 2741 (*isol*)
Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)

Pseudotheonamide A_1 P-684

[224577-31-5]



$C_{36}H_{45}N_9O_8$ 731.807

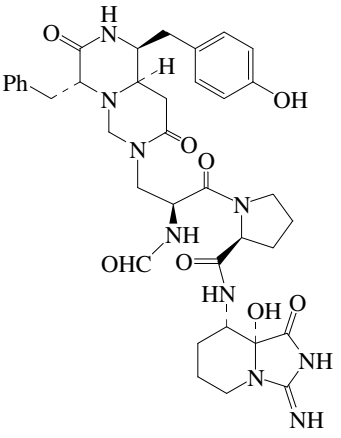
The pseudotheonamides were initially named as Pseudocyclotheonamides. Isol. from the sponge *Theonella swinhoei*. Serine protease inhibitor. Amorph. solid. $[\alpha]_D^{29}$ -28 (c, 0.08 in MeOH). λ_{max} 227 (sh) (ϵ 14000); 243 (sh) (ϵ 4500); 278 (sh) (ϵ 2000) (MeOH).

2-Epimer: ***Pseudotheonamide A_2***
[224577-33-7]
$C_{36}H_{45}N_9O_8$ 731.807
Isol. from *Theonella swinhoei*. Serine protease inhibitor. Amorph. solid. $[\alpha]_D^{29}$ -34 (c, 0.06 in MeOH). λ_{max} 227 (sh) (ϵ 17000); 243 (sh) (ϵ 7100); 278 (sh) (ϵ 2300) (MeOH).

Nakao, Y. *et al., J.A.C.S.*, 1999, **121**, 2425-2431

Pseudotheonamide B_2 P-685

[224577-34-8]



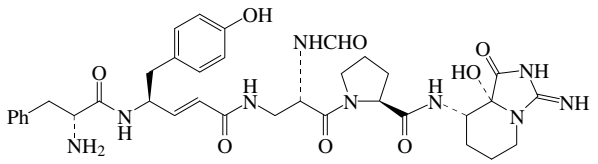
$C_{37}H_{45}N_9O_8$ 743.818

Isol. from the sponge *Theonella swinhoei*. Serine protease inhibitor. Amorph. solid. $[\alpha]_D^{29}$ -17 (c, 0.05 in MeOH). Pseudotheonamide B not isolated. λ_{max} 226 (sh) (ϵ 15000); 243 (sh) (ϵ 4500); 278 (sh) (ϵ 1800) (MeOH).

Nakao, Y. *et al., J.A.C.S.*, 1999, **121**, 2425-2431

Pseudotheonamide C P-686

[224577-35-9]



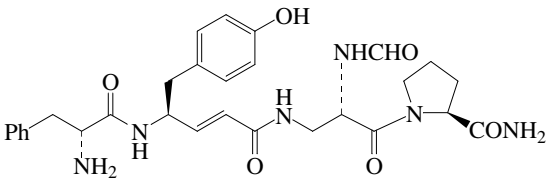
$C_{36}H_{45}N_9O_8$ 731.807

Isol. from the sponge *Theonella swinhoei*. Serine protease inhibitor. Amorph. solid. $[\alpha]_D^{29}$ -16 (c, 0.47 in MeOH). λ_{max} 227 (sh) (ϵ 19000); 242 (sh) (ϵ 11000); 278 (sh) (ϵ 2300) (MeOH).

Nakao, Y. *et al., J.A.C.S.*, 1999, **121**, 2425-2431

Pseudotheonamide D P-687

[224577-36-0]



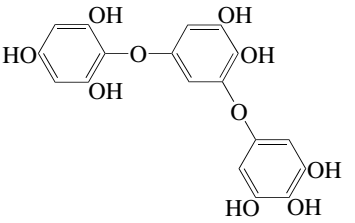
$C_{29}H_{36}N_6O_6$ 564.64

Isol. from the sponge *Theonella swinhoei*. Serine protease inhibitor. Amorph. solid. $[\alpha]_D^{29}$ -11 (c, 0.085 in MeOH). λ_{max} 225 (sh) (ϵ 15000); 243 (sh) (ϵ 5100); 278 (sh) (ϵ 1600) (MeOH).

Nakao, Y. *et al., J.A.C.S.*, 1999, **121**, 2425-2431

Pseudotrifuhalol A P-688

[202211-78-7]

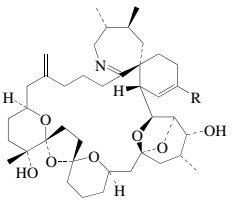


$C_{18}H_{14}O_{10}$ 390.303

Constit. of the alga *Sargassum spinuligerum*. Isol. as octa-Ac.

Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*isol, pmr, cmr*)

Pteriatoxin A P-690



R = -^{34}CH(OH)CH_2SCH_2-$^{2'}$CH(NH_2)COOH (34*S*,2′*R*-)

$C_{45}H_{70}N_2O_{10}S$ 831.121

Exists as a zwitterion. Neutral form shown. Related to Pinnatoxin A, P-428. Toxin from the bivalve *Pteria penguin*.

Takada, N. *et al., Tet. Lett.*, 2001, **42**, 3495-3497 (*isol*)
Matsuura, F. *et al., J.A.C.S.*, 2006, **128**, 7463-7465; 7742-7743 (*synth, abs config*)

Pteriatoxin B P-691

As Pteriatoxin A, P-690 with
R = ^{34}CH(CH_2OH)SCH$_2^{2'}$CH(NH_2)COOH (34*R*,2′,*R*-)

$C_{45}H_{70}N_2O_{10}S$ 831.121

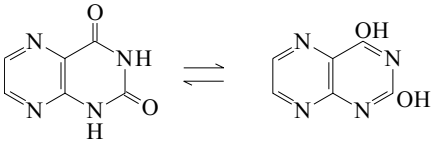
Exists as a zwitterion. Neutral form shown. Toxin from the bivalve *Pteria penguin*.

34-Epimer: ***Pteriatoxin C***
$C_{45}H_{70}N_2O_{10}S$ 831.121
Toxin from *Pteria penguin*.

Takada, N. *et al., Tet. Lett.*, 2001, **42**, 3495-3497 (*isol*)
Matsuura, F. *et al., J.A.C.S.*, 2006, **128**, 7463-7465; 7742-7743 (*synth, abs config*)

2,4(1*H*,3*H*)-Pteridinedione, 9CI P-692

Lumazine, 8CI. 2,4-Pteridinediol. 2,4-Dihydroxypteridine



Di–*NH–form* Di–*OH–form*

$C_6H_4N_4O_2$ 164.123

Di-*NH*-form occurs in aq. soln. Intermediate tautomers also possible. Yellow cryst. (H_2O). Mp 350°. Subl.0.05 145. pK_{a1} 7.95 (20°). Bluish-green fluor. in aq. soln., green in alkali, blue in acid.

1-Me: ***1-Methyl-2,4-pteridinedione***
[50256-18-3]
$C_7H_6N_4O_2$ 178.15
Isol. from the New Caledonian sponge *Corallistes fulvodesmus*.

Needles (H_2O).
Mp 290-291° (271°).

3-Me: [50256-19-4]
$C_7H_6N_4O_2$ 178.15
Cryst. (H_2O). Mp 332°.

1-Ph: [32433-26-4]
$C_{12}H_8N_4O_2$ 240.221
Cryst. Mp 307-308°.

3-Ph:
$C_{12}H_8N_4O_2$ 240.221
Cryst. (MeOH). Mp 359-360°.

Di-*NH-form* [487-21-8]
▶ UO3416000

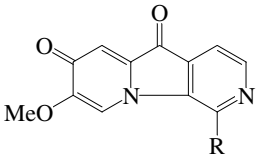
1,3-Di-Me: [13401-18-8]
$C_8H_8N_4O_2$ 192.177
Cryst. (H_2O). Mp 200°.

1,3-Di-Et: [94591-34-1]
$C_{10}H_{12}N_4O_2$ 220.23
Cryst. (Et_2O/petrol). Mp 87-88°.

1,3-Dibenzyl: [94591-35-2]
$C_{20}H_{16}N_4O_2$ 344.372
Needles (EtOH aq.). Mp 140°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 768A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 894B (*ir*)
Pfleiderer, W. *et al., Chem. Ber.*, 1957, **90**, 2582 (*Me derivs, uv*)
Brown, D.J. *et al., J.C.S.*, 1961, 4413 (*synth*)
Pfleiderer, W. *et al., Chem. Ber.*, 1973, **106**, 3149 (*synth*)
Ewers, J. *et al., Chem. Ber.*, 1974, **107**, 3275 (*cmr*)
Pfleiderer, W. *et al., Annalen*, 1984, 1798 (*derivs, synth*)
Tsuzuki, K. *et al., J. Het. Chem.*, 1986, **23**, 1299 (*1-Me*)
Klein, R. *et al., Photochem. Photobiol.*, 1987, **45**, 55 (*tautom, uv*)
Debitus, C. *et al., Tet. Lett.*, 1989, **30**, 1534-1538 (*1-Methylpteridine-2,4-dione, isol*)

Pterocellin A P-693



R = $CH_2CH(CH_3)_2$

$C_{16}H_{16}N_2O_3$ 284.314
Isol. from the marine bryozoan *Pterocella vesiculosa*. Cytotoxic. Dark red needles (toluene).
Mp 172-173°. λ_{max} 202 (log ϵ 3.83); 256 (log ϵ 3.7); 280 (log ϵ 3.87); 483 (log ϵ 2.93) (MeOH).

Yao, B. *et al., J. Nat. Prod.*, 2003, **66**, 1074-1077 (*isol, pmr, cmr, N-15 nmr, cryst struct*)
O'Malley, M.M. *et al., Org. Lett.*, 2006, **8**, 2651-2652 (*synth*)

Pterocellin B P-694

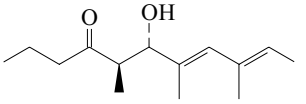
As Pterocellin A, P-693 with
R = CH_2Ph

$C_{19}H_{14}N_2O_3$ 318.331
Isol. from the marine bryozoan *Pterocella vesiculosa*. Cytotoxic. Amorph. red solid. λ_{max} 202 (log ϵ 4.08); 287 (log ϵ 3.63); 485 (log ϵ 2.63) (MeOH).

Yao, B. *et al., J. Nat. Prod.*, 2003, **66**, 1074-1077 (*isol, pmr, cmr, N-15 nmr*)

Pteroenone P-695

6-Hydroxy-5,7,9-trimethyl-7,9-undecadien-4-one, 9CI
[160791-63-9]

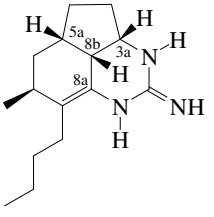


$C_{14}H_{24}O_2$ 224.342
Defensive metab. of the pteropod *Clione antarctica*. Feeding deterrent. $[\alpha]_D$ +48 (c, 0.6 in hexane). λ_{max} 234 (ϵ 11600) (hexane) (Derep).

Yoshida, W.Y. *et al., J.O.C.*, 1995, **60**, 780-782 (*isol, uv, ir, pmr, cmr, ms*)

Ptilocaulin P-696

[78777-02-3]



(+)-*form*

$C_{15}H_{25}N_3$ 247.383
Isol. from the Caribbean sponge *Ptilocaulis* aff. *Ptilocaulis spiculifer*, may be a symbiont metab. Also from *Batzella* sp., *Monanchora arbuscula* and *Hemimycale* sp. Active against gram-positive bacteria and leukaemia cells. Cryst. (as nitrate). Sol. MeOH, $CHCl_3$; poorly sol. hexane.
Mp 183-185° (nitrate). $[\alpha]_D$ +74.4 (MeOH). λ_{max} 225 (ϵ 10000) (MeOH).

*8*b-*Hydroxy:* ***8b-Hydroxyptilocaulin***
[167499-84-5]
$C_{15}H_{25}N_3O$ 263.382
Alkaloid from the marine sponge *Monanchora arbuscula*. Oil (as hydrochloride). $[\alpha]_D$ +77.5 (c, 0.12 in MeOH) (hydrochloride).

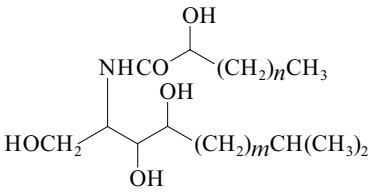
*3*a,*5*a-*Diepimer, $\Delta^{8a,8b}$-isomer(8*βH*):* ***8a,8b-Dehydroptilocaulin***
$C_{15}H_{25}N_3$ 247.383
Isol. from the sponge *Batzella* sp. Oil. $[\alpha]_D$ +13.3 (c, 1.2 in MeOH). The synonym is misleading. λ_{max} 228; 242; 306 (MeOH).

*3*a,*5*a-*Diepimer, $\Delta^{8a,8b}$-isomer, 8*β*-hydroxy:* ***8a,8b-Dehydro-8-hydroxyptilocaulin***
$C_{15}H_{25}N_3O$ 263.382
Isol. from the sponge *Batzella* sp. Gum. $[\alpha]_D$ +24.2 (c, 0.33 in MeOH). Misleading synonym. λ_{max} 237; 299 (MeOH).

[86594-30-1, 88154-76-1]

Harbour, G.C. *et al., J.A.C.S.*, 1981, **103**, 5604 (*isol, uv, pmr, cmr, ms, struct*)
Roush, M.R. *et al., J.A.C.S.*, 1984, **106**, 721 (*synth*)
Snider, B.B. *et al., J.A.C.S.*, 1984, **106**, 1443 (*synth, ir, pmr, cmr, ms, cd*)
Watts, A.E. *et al., Tetrahedron*, 1985, **41**, 3463 (*synth*)
Uyehara, T. *et al., Chem. Comm.*, 1986, 539 (*synth*)
Murthy, K.S.K. *et al., Isr. J. Chem.*, 1991, **31**, 239 (*synth*)
Tavares, R. *et al., J. Nat. Prod.*, 1995, **58**, 1139 (*8b-Hydroxyptilocaulin*)
Patil, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 704-707 (*isol, uv, pmr, cmr, derivs*)

Ptiloceramide P-697



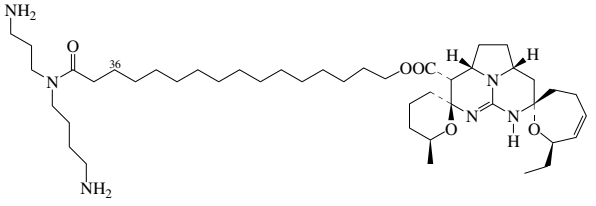
m = 10, 11, 12
n = 20, 21, 22

A complex of five homologues. Isol. from *Ptilocaulis spiculifer*. Antifungal agent.

Hirsch, S. *et al., Tetrahedron*, 1989, **45**, 3897 (*isol, struct*)

Ptilomycalin A P-698

[124512-47-6]



$C_{45}H_{80}N_6O_5$ 785.164
Alkaloid from the Caribbean sponge *Ptilocaulis spiculifer*, the Red Sea sponge *Hemimycale* sp., the New Caledonian starfish *Celerina heffernani* and the Caribbean sponge *Batzella* sp. Exhibits remarkable antifungal, antiviral and antitumour activities.
$[\alpha]_D^{25}$ -2.5 (c, 0.70 in $CHCl_3$).

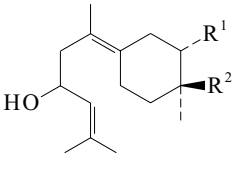
*36*R-*Hydroxy:* ***Celeromycalin***
[163597-72-6]
$C_{45}H_{80}N_6O_6$ 801.164
Alkaloid from the starfish *Celerina heffernani*. Highly cytotoxic.
$[\alpha]_D$ -4.5.

38-Parent acid: ***Crambescidic acid***
$C_{38}H_{63}N_3O_6$ 657.932
Isol. from the sponge *Monanchora unguifera*.
$[\alpha]_D^{25}$ +4.4 (c, 0.2 in MeOH).

Kashman, Y. *et al., J.A.C.S.*, 1989, **111**, 8925-8926 (*isol, ir, pmr, cmr, struct*)
Ohtani, I. *et al., J.A.C.S.*, 1992, **114**, 8472-8479 (*isol, ir, pmr, cmr, struct*)
Overman, L.E. *et al., J.A.C.S.*, 1995, **117**, 2657-2658 (*synth*)
Patil, A.D. *et al., J.O.C.*, 1995, **60**, 1182-1188 (*isol*)
Palagiano, E. *et al., Tetrahedron*, 1995, **51**, 3675-3682 (*Celeromycalin*)
Coffey, D.S. *et al., J.A.C.S.*, 2000, **122**, 4893-4903 (*synth*)
Gallimore, W.A. *et al., J. Nat. Prod.*, 2005, **68**, 1420-1423 (*Crambescidic acid*)

Puertitol A P-699

2-Bromo-3-chloro-6,10-bisaboladien-9-ol
[119736-67-3]



R^1 = Br, R^2 = Cl

$C_{15}H_{24}BrClO$ 335.711
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ -37 (c, 1.62 in $CHCl_3$).

Vazquez, J.T. *et al., J. Nat. Prod.*, 1988, **51**, 1257 (*isol, pmr, cmr, cd*)

Puertitol B P-700

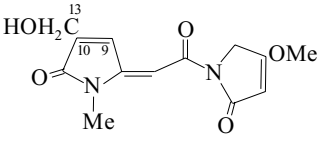
3-Bromo-2-chloro-6,10-bisaboladien-9-ol
[119736-69-5]
As Puertitol A, P-699 with
R^1 = Cl, R^2 = Br
$C_{15}H_{24}BrClO$ 335.711
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ +66 (c, 0.25 in $CHCl_3$).

Ac: ***Puertitol B acetate***
[119736-70-8]
$C_{17}H_{26}BrClO_2$ 377.748
Constit. of *Aplysia dactylomela*.
$[\alpha]_D$ +35.6 (c, 0.23 in $CHCl_3$).

Vazquez, J.T. *et al., J. Nat. Prod.*, 1988, **51**, 1257-1260 (*isol, pmr, cmr, cd*)
Wessels, M. *et al., J. Nat. Prod.*, 2000, **63**, 920-928 (*Ac*)

Pukeleimide P-701

*1-[[1,5-Dihydro-4-(hydroxymethyl)-1-methyl-5-oxo-2*H*-pyrrol-2-ylidene]acetyl]-1,5-dihydro-4-methoxy-2*H*-pyrrol-2-one, 9CI*



(*E*)*–form*

$C_{13}H_{14}N_2O_5$ 278.264

(E)-form

Pukeleimide A
[72362-15-3]
Metab. from the marine cyanophyte *Lyngbya majuscula*.
Solid. λ_{max} 224 (ϵ 11200); 287 (ϵ 25200) (MeOH) (Derep).

Me ether: ***Pukeleimide G***
[72362-23-3]
$C_{14}H_{16}N_2O_5$ 292.291
Metab. from *Lyngbya majuscula*. Solid.

9,10-Dihydro, 10-hydroxy: ***Pukeleimide D***
[72362-20-0]
$C_{13}H_{16}N_2O_6$ 296.279
Metab. from *Lyngbya majuscula*. Solid.

9,10-Dihydro, 10-methoxy: ***Pukeleimide C***
[72362-19-7]
$C_{14}H_{18}N_2O_6$ 310.306
Metab. from *Lyngbya majuscula*. Cryst. ($CHCl_3$/hexane or Me_2CO/hexane).
Mp 186° (part. subl.). Racemic. λ_{max} 224 (ϵ 11200); 287 (ϵ 25200) (MeOH) (Derep).

$\Delta^{10,13}$-Isomer, 13-deoxy: ***Pukeleimide E***
[72362-21-1]
$C_{13}H_{14}N_2O_4$ 262.265
Metab. from *Lyngbya majuscula*. Solid.

(Z)-form

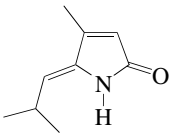
Pukeleimide B
[72362-17-5]
Metab. from *Lyngbya majuscula*.
Solid.

Me ether: ***Pukeleimide F***
[72362-22-2]
$C_{14}H_{16}N_2O_5$ 292.291
Metab. from *Lyngbya majuscula*. Solid.

Cardellina, J.H. *et al., Tet. Lett.*, 1979, 2003; 2007 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
James, G.D. *et al., Tet. Lett.*, 1985, **26**, 3617 (*synth, Pukeleimide A*)

Pulchellalactam P-702

*1,5-Dihydro-4-methyl-5-(2-methylpropylidene)-2*H*-pyrrol-2-one*



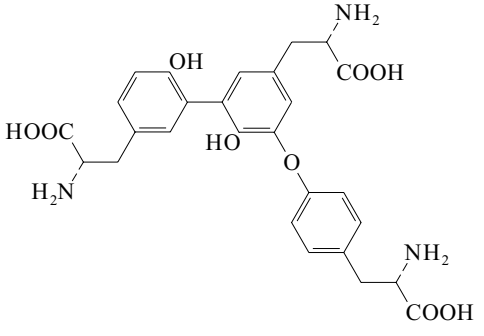
$C_9H_{13}NO$ 151.208

Isol. from the marine-derived fungus *Corollospora pulchella*. Inhibitor of CD45 protein tyrosine phosphatase. Oil. λ_{max} 276 (no solent reported). λ_{max} 275 (MeOH) (Berdy).

Alvi, K.A. *et al., J. Antibiot.*, 1998, **51**, 515-517 (*isol, pmr, cmr*)
Li, W.-R. *et al., J.O.C.*, 2002, **67**, 4702-4706 (*synth*)
Bessho, J. *et al., Heterocycles*, 2004, **63**, 1013-1016 (*synth*)

Pulcherosine P-703

5-[4-(2-Amino-2-carboxyethyl)phenoxy]-3,3′-dityrosine
[126723-16-8]



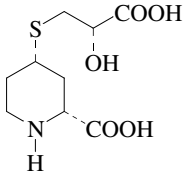
$C_{27}H_{29}N_3O_9$ 539.541

Tyrosine trimer. Constit. of the embryo fertilisation envelope of the sea urchin *Hemicentrotus pulcherrimus* and other *Hemicentrotus* spp. Also found in the primary cell walls of tomato cell cultures. No phys. props. reported.

Nomura, K. *et al., Biochemistry*, 1990, **29**, 4525-4534 (*isol, uv, pmr, cmr*)
Brady, J.D. *et al., Phytochemistry*, 1998, **47**, 349-353 (*isol, uv, pmr*)
Skaff, O. *et al., J.O.C.*, 2005, **70**, 7353-7363 (*synth*)

Pulcherrimine P-704

4-[(2-Carboxy-2-hydroxyethyl)thio]-2-piperidinecarboxylic acid
[309946-45-0]



Absolute Configuration

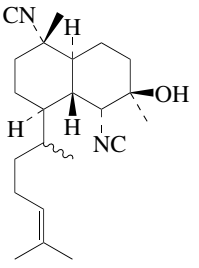
$C_9H_{15}NO_5S$ 249.287

Abs. config. revised in 2002. Isol. from the ovaries of the sea urchin, *Hemicentrotus pulcherrimus*. Amorph. powder. $[\alpha]_D^{24}$ -16.5 (c, 0.2 in H_2O). All 8 stereoisomers have been synthesised.

Murata, Y. *et al., J. Agric. Food Chem.*, 2000, **48**, 5557-5560 (*isol, pmr, cmr, ms*)
Sata, N.U. *et al., Tet. Lett.*, 2002, **43**, 115-118 (*synth, abs config*)

Pulcherrimol P-705

[216973-08-9]



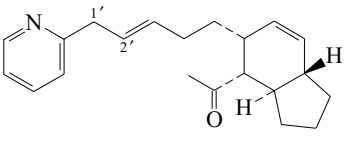
$C_{22}H_{34}N_2O$ 342.523

Constit. of *Phakellia pulcherrima*.
$[\alpha]_D^{20}$ +18 (c, 0.03 in $CHCl_3$).

Wolf, D. *et al., J. Nat. Prod.*, 1998, **61**, 1524-1527 (*isol, pmr, cmr*)

Puloupone P-706

[97190-30-2]



$C_{21}H_{27}NO$ 309.45

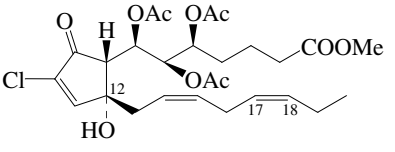
Probable abs. config. shown based on the tentative assignment to Isopuloupone. A minor metab. of the cephalaspidean mollusc *Philinopsis speciosa*. Oil. Sol. MeOH, hexane; poorly sol. H_2O. $[\alpha]_D$ -10 (c, 0.20 in hexane). λ_{max} 206 (ϵ 10700); 257 (ϵ 3870); 263 (ϵ 4200); 269 (ϵ 3130) (EtOH) (Derep).

$\Delta^{1',2'}$-Isomer: ***Isopuloupone***
[149155-21-5]
$C_{21}H_{27}NO$ 309.45
Isol. from the mollusc *Navanax inermis* and its prey *Bulla gouldiana*. Ichthyotoxin. $[\alpha]_D^{20}$ -119 (c, 0.4 in hexane). λ_{max} 242 (ϵ 11400); 281 (ϵ 5400) (MeOH) (Berdy).

Coval, S.J. *et al., J.O.C.*, 1985, **50**, 3024-3025 (*isol, uv, ir, pmr, ms, struct*)
Sugahara, T. *et al., Tet. Lett.*, 1989, **30**, 1821 (*synth, abs config*)
Spinella, A. *et al., Tetrahedron*, 1993, **49**, 3203 (*Isopulo'upone*)

Punaglandin 1 P-707

Methyl 5,6,7-tris(acetyloxy)-10-chloro-12-hydroxy-9-oxoprosta-10,14,17-trien-1-oate, 9CI
[96055-63-9]



$C_{27}H_{37}ClO_{10}$ 557.036

Isol. from Japanese octocoral *Telesto riisei*. Possesses potent antitumour props. Antiinflammatory. Sol. MeOH, hexane; poorly sol. H_2O. $[\alpha]_D$ +10.6 (2.4 in MeOH). λ_{max} 228 (ϵ 7900) (MeOH) (Derep).

12-Ac: ***Punaglandin 1 acetate***
$C_{29}H_{39}ClO_{11}$ 599.073
From *Telesto riisei*. Antiinflammatory.

17,18-Dihydro: ***Punaglandin 2***
[96055-64-0]
$C_{27}H_{39}ClO_{10}$ 559.052
From *Telesto riisei*. Possesses potent antitumour props. Antiinflammatory. Sol. MeOH, hexane; poorly sol. H_2O. $[\alpha]_D$ +8.8

(c, 1.9 in MeOH). λ_{max} 228 (ϵ 7900) (MeOH) (Derep). λ_{max} 227 (ϵ 7500) (MeOH) (Berdy).

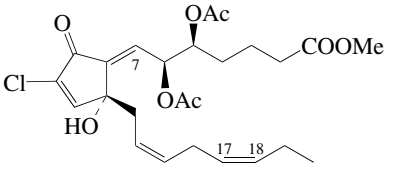
17,18-Dihydro, 12-Ac: ***Punaglandin 2 acetate***
$C_{29}H_{41}ClO_{11}$ 601.089
From *Telesto riisei*. Antiinflammatory. $[\alpha]_D$ +10 (c, 0.6 in MeOH). λ_{max} 242 (ϵ 5600) ($CHCl_3$) (Berdy).

*Bromo analogue, tri-*O*-de-Ac:* ***Bromopunaglandin 1***
$C_{21}H_{31}BrO_7$ 475.376
Isol. from the coral *Tubipora musica*. Oil. $[\alpha]_D^{22}$ +11.3 (c, 0.12 in MeOH).

Baker, B.J. *et al., J.A.C.S.*, 1985, **107**, 2976 (*isol, struct*)
Sasai, H. *et al., Tet. Lett.*, 1987, **28**, 333
Baker, B.J. *et al., J. Nat. Prod.*, 1994, **57**, 1346 (*isol, pmr, cmr*)
Rezanka, T. *et al., Eur. J. Org. Chem.*, 2003, 309-316 (*Bromopunaglandin 1*)

Punaglandin 3 P-708

Methyl 5,6-bis(acetyloxy)-10-chloro-12-hydroxy-9-oxoprosta-7,10,14,17-tetraen-1-oate, 9CI
[96055-65-1]



$C_{25}H_{33}ClO_8$ 496.984
The 12-config. in Punaglandins 3 and 4 is the opposite of that originally assigned and the opposite of that in Punaglandin 1, P-707. Isol. from Japanese octocoral *Telesto riisei*. Shows potent antitumour props. Antiinflammatory. Oil. Sol. MeOH, hexane; poorly sol. H_2O. $[\alpha]_D$ +66.8 (c, 0.5 in MeOH). λ_{max} 239 (ϵ 8600) (MeOH) (Derep). λ_{max} 238 (ϵ 8600) (MeOH) (Berdy).

12-Ac: ***Punaglandin 3 acetate***
[160561-43-3]
$C_{27}H_{35}ClO_9$ 539.021
From *Telesto riisei*.
$[\alpha]_D$ +31 (c, 2.7 in $CHCl_3$). λ_{max} 251 (ϵ 8000) ($CHCl_3$) (Berdy).

10β,11β-Epoxide: ***Punaglandin 3 epoxide***
[160561-47-7]
$C_{25}H_{33}ClO_9$ 512.983
From *Telesto riisei*. Antiinflammatory. $[\alpha]_D$ +16 (c, 3 in MeOH). λ_{max} 245 (ϵ 7400) (MeOH) (Berdy).

17,18-Dihydro: ***Punaglandin 4***
[96055-66-2]
$C_{25}H_{35}ClO_8$ 498.999
From *Telesto riisei*. Possesses potent antitumour props. Antiinflammatory. Oil. Sol. MeOH, hexane; poorly sol. H_2O. $[\alpha]_D^{24}$ +72.3 (c, 0.52 in $CHCl_3$) (synthetic). n_D^{24} 1.4967. λ_{max} 239 (ϵ 8600) (MeOH) (Derep). λ_{max} 240 (ϵ 6900) (MeOH) (Berdy).

17,18-Dihydro, 12-Ac: ***Punaglandin 4 acetate***
[160561-44-4]
$C_{27}H_{37}ClO_9$ 541.037
From *Telesto riisei*. Aniinflammatory. $[\alpha]_D$ +9.4 (c, 3.6 in $CHCl_3$). λ_{max} 249 (ϵ 6700) ($CHCl_3$) (Berdy).

17,18-Dihydro, 10β,11β-epoxide: ***Punaglandin 4 epoxide***
[160561-48-8]
$C_{25}H_{35}ClO_9$ 514.999
From *Telesto riisei*. Antiinflammatory. $[\alpha]_D$ +22.5 (c, 0.8 in MeOH).

7Z-Isomer: ***(Z)-Punaglandin 3***
[96055-67-3]
$C_{25}H_{33}ClO_8$ 496.984
From *Telesto riisei*. Aniinflammatory.

7Z-Isomer, 12-Ac: ***(Z)-Punaglandin 3 acetate***
[160561-45-5]
$C_{27}H_{35}ClO_9$ 539.021
From *Telesto riisei*. Antiinflammatory. $[\alpha]_D$ +19 (c, 1.8 in $CHCl_3$). λ_{max} 255 (ϵ 9000) ($CHCl_3$). λ_{max} 242 (ϵ 7900); 255 (ϵ 9000) ($CHCl_3$) (Berdy).

7Z-Isomer, 17,18-dihydro: ***(Z)-Punaglandin 4***
[96055-68-4]
Isol. from *Telesto riisei*. Antiinflammatory. Oil.

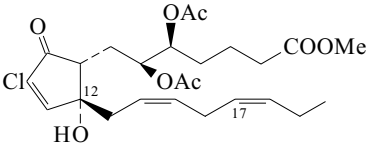
7Z-Isomer, 17,18-dihydro, 12-Ac: ***(Z)-Punaglandin 4 acetate***
[160561-46-6]
$C_{27}H_{37}ClO_9$ 541.037
Prod. by *Telesto riesii*. Antiinflammatory. $[\alpha]_D$ +11 (c, 1.8 in $CHCl_3$). λ_{max} 241 (ϵ 5100); 254 (ϵ 5300) ($CHCl_3$) (Berdy).

Bromo analogue, 5-epimer, 7Z-isomer, di-de-Ac: ***Bromo-5-epi-Z-punaglandin 3***
$C_{21}H_{29}BrO_6$ 457.361
Isol. from the coral *Tubipora musica*. Oil. $[\alpha]_D^{22}$ +37.4 (c, 0.14 in MeOH). λ_{max} 240 (log ϵ 3.91) (MeOH).

Baker, B.J. *et al., J.A.C.S.*, 1985, **107**, 2976 (*isol*)
Nagaoka, H. *et al., J.A.C.S.*, 1986, **108**, 5019; 5021 (*synth, struct*)
Sasai, H. *et al., Tet. Lett.*, 1987, **28**, 333 (*synth*)
Suzuki, M. *et al., J.O.C.*, 1988, **53**, 286 (*synth, uv, pmr, ms, abs config, bibl*)
Mori, K. *et al., Tetrahedron*, 1988, **44**, 333 (*synth, ir, pmr, ms, cd*)
Baker, B.J. *et al., J. Nat. Prod.*, 1994, **57**, 1346-1353 (*isol, pmr, cmr*)
Rezanka, T. *et al., Eur. J. Org. Chem.*, 2003, 309-316 (*Bromo-5-epi-Z-punaglandin 3*)

Punaglandin 5 P-709

[160791-06-0]



$C_{25}H_{35}ClO_8$ 498.999
Isol. from the Japanese octocoral *Telesto riisei*. Antitumour agent. $[\alpha]_D$ +10.2 (c, 4.7 in $CHCl_3$). λ_{max} 244 (ϵ 5000) (MeOH) (Berdy).

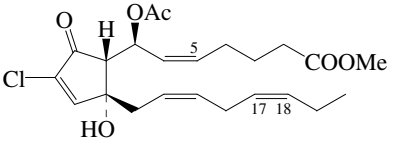
12-Ac: ***Punaglandin 5 acetate***
[160561-49-9]
$C_{27}H_{37}ClO_9$ 541.037
From *Telesto riisei*.
$[\alpha]_D$ +8 (c, 1.2 in MeOH). λ_{max} 240 (ϵ 4500) ($CHCl_3$) (Berdy).

17,18-Dihydro: ***Punaglandin 6***
[160791-07-1]
$C_{25}H_{37}ClO_8$ 501.015
From *Telesto riisei*.
$[\alpha]_D$ +14 (c, 0.9 in $CHCl_3$). λ_{max} 231 (ϵ 5300) (MeOH) (Berdy).

Baker, B.J. *et al., J. Nat. Prod.*, 1994, **57**, 1346 (*isol, pmr, cmr*)

Punaglandin 7 P-710

[160791-08-2]



$C_{23}H_{31}ClO_6$ 438.947
Isol. from the Japanese octocoral *Telesto riisei*. Antitumour and antiinflammatory agent.

17,18-Dihydro: 7-Acetoxy-7,8-dihydrochlorovulone I. ***Punaglandin 8***
[160791-09-3]
$C_{23}H_{33}ClO_6$ 440.963
From *Telesto riisei* and *Clavularia viridis*. Antitumour and antiinflammatory agent. Oil. $[\alpha]_D$ +43.9 (c, 0.04 in $CHCl_3$). λ_{max} 227 (ϵ 6900) (MeOH) (Berdy).

*5*E*-Isomer, 17,18-dihydro: 7-Acetoxy-7,8-dihydrochlorovulone II.* ***(5E)-Punaglandin 8***
$C_{23}H_{33}ClO_6$ 440.963
Isol. from the soft coral *Clavularia viridis*. Oil. $[\alpha]_D$ +45.5 (c, 0.01 in $CHCl_3$).

Bromo analogue, 17,18-dihydro: 7-Acetoxy-7,8-dihydrobromovulone I. ***Bromopunaglandin 8***
$C_{23}H_{33}BrO_6$ 485.414
Isol. from the coral *Clavularia viridis*. Oil. $[\alpha]_D$ +37 (c, 0.17 in $CHCl_3$). λ_{max} 236 (ϵ 5900) (MeOH).

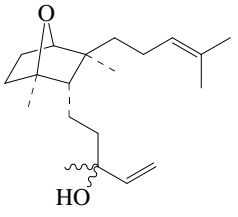
*Bromo analogue, 5*E*-isomer, 17,18-dihydro: 7-Acetoxy-7,8-dihydrobromovulone II.* ***(5E)-Bromopunaglandin 8***
$C_{23}H_{33}BrO_6$ 485.414
Isol. from *Clavularia viridis*. Oil. $[\alpha]_D$ +40 (c. 0.02 in $CHCl_3$). λ_{max} 233 (ϵ 6300) (MeOH).

Iodo analogue, 17,18-dihydro: 7-Acetoxy-7,8-dihydroiodovulone I. ***Iodopunaglandin 8***
$C_{23}H_{33}IO_6$ 532.415
Isol. from the coral *Clavularia viridis*. Cytotoxic. Oil. $[\alpha]_D$ +22.7 (c, 0.67 in $CHCl_3$). λ_{max} 251 (ϵ 3500) (no solvent reported).

*Iodo analogue, 5*E*-isomer, 17,18-dihydro: 7-Acetoxy-7,8-dihydroiodovulone II.* ***(5E)-Iodopunaglandin 8***
$C_{23}H_{33}IO_6$ 532.415
Isol. from *Clavularia viridis*. Oil. $[\alpha]_D$ +38.7 (c, 0.07 in $CHCl_3$). λ_{max} 245 (ϵ 4500) (MeOH).

Baker, B.J. *et al., J. Nat. Prod.*, 1994, **57**, 1346-1353 (*isol, pmr, cmr*)
Watanabe, K. *et al., J. Nat. Prod.*, 2001, **64**, 1421-1425 (*Clavularia viridis derivs*)

Punctatene P-711



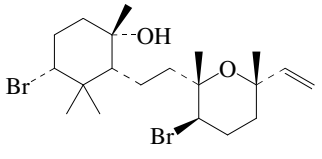
$C_{20}H_{34}O_2$ 306.487
Parent not isol.

Ac: ***Punctatene acetate***
[539824-88-9]
$C_{22}H_{36}O_3$ 348.525
Isol. from the sea hare *Aplysia punctata*. Oil. $[\alpha]_D$ -14.5 (c, 0.002 in $CHCl_3$).

Findlay, J.A. *et al., Can. J. Chem.*, 2002, **80**, 1697-1707 (*isol, pmr, cmr, ms*)

Punctatol P-712

[539824-89-0]



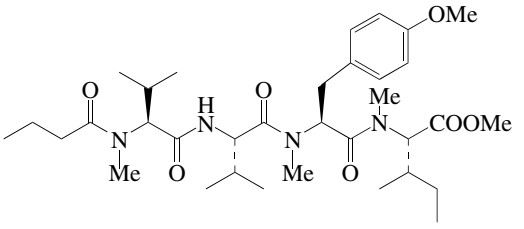
Relative Configuration

$C_{20}H_{34}Br_2O_2$ 466.295
Isol. from the sea hare *Aplysia punctata*. Solid.
Mp 101-103°. $[\alpha]_D$ +40 (c, 0.0001 in $CHCl_3$).

Findlay, J.A. *et al., Can. J. Chem.*, 2002, **80**, 1697-1707 (*isol, pmr, cmr, ms*)

Pupukeamide P-713

[185446-70-2]

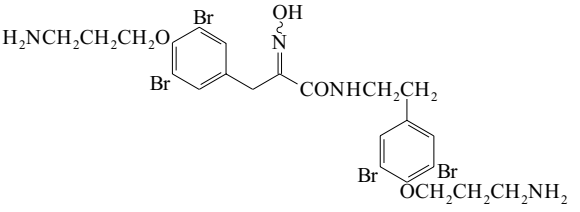


$C_{34}H_{56}N_4O_7$ 632.839
Isol. from the mollusc *Philinopsis speciosa*. λ_{max} 261 (ϵ 1100) (MeOH) (Berdy).

Nakao, Y. *et al., Tet. Lett.*, 1996, **37**, 8993-8996 (*isol, pmr, cmr*)

Purealidin C P-714

[138590-56-4]

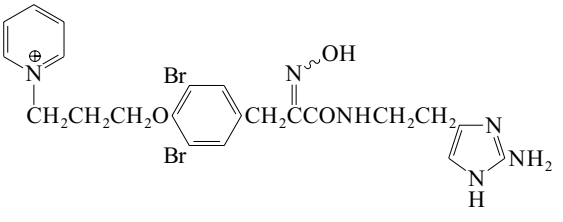


$C_{23}H_{28}Br_4N_4O_4$ 744.115
Alkaloid from the marine sponge *Psammaplysilla purea*. Antifungal agent. Cytotoxic. Amorph. λ_{max} 210 (ϵ 23000); 285 (ϵ 1600) (MeOH) (Berdy).

Kobayashi, J. *et al., Tetrahedron*, 1991, **47**, 6617 (*isol, uv, ir, pmr, cmr, ms, struct*)

Purealidin D P-715

[143052-17-9]

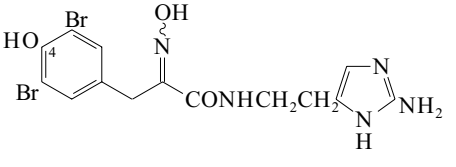


$C_{22}H_{25}Br_2N_6O_3^{\oplus}$ 581.286
Alkaloid from the sponge *Psammaplysilla purea*. $Na^{\oplus}$ and $K^{\oplus}$-ATPase inhibitor. Isol. as the bis(trifluoroacetate) salt. λ_{max} 217 (ϵ 15300); 260 (ϵ 2900); 269 (sh); 286 (ϵ 800) (MeOH) (Derep).

Tsuda, M. *et al., Tet. Lett.*, 1992, **33**, 2597 (*isol, pmr, cmr*)

Purealidin H P-716

[164301-30-8]



$C_{14}H_{15}Br_2N_5O_3$ 461.112
Alkaloid from the Okinawan sponge *Psammaplysilla purea*. Oil. λ_{max} 277 (ϵ 1700); 284 (ϵ 1400) (MeOH).

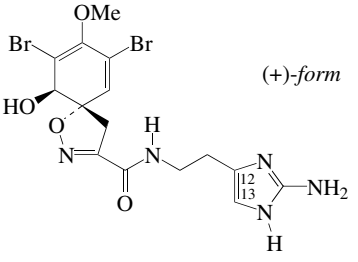
O^4-*(3-Aminopropyl):* ***Purealidin A***
[134850-51-4]
$C_{17}H_{22}Br_2N_6O_3$ 518.207
Alkaloid from *Psammaplysilla purea* and *Pseudoceratina verrucosa*. Cytotoxic, inhibitor of $Na^{\oplus}/K^{\oplus}$ ATPase. Ichthyotoxic agent. Amorph. solid.

O^4-*(3-Trimethylaminopropyl):* ***Purealidin E***
[145205-26-1]
[145205-28-3]
$C_{20}H_{29}Br_2N_6O_3^{\oplus}$ 561.296
Alkaloid from *Psammaplysilla purea*. $Na^{\oplus}/K^{\oplus}$ ATPase inhibitor. Amorph. solid (as bis(trifluoroacetate)). Sol. MeOH. λ_{max} 218 (ϵ 13600); 287 (ϵ 1000) (MeOH).

Ishibashi, M. *et al., Experientia*, 1991, **47**, 299 (*Purealidin A*)
Tsuda, M. *et al., J. Nat. Prod.*, 1992, **55**, 1325-1327 (*Purealidin E*)
Kobayashi, J. *et al., J. Nat. Prod.*, 1995, **58**, 467 (*Purealidin H*)

Purealidin J P-717

Pseudoceratinine A



$C_{15}H_{17}Br_2N_5O_4$ 491.138
Pseudoceratinine A was the (-)-form.

(+)-*form*
Alkaloid from the Okinawan marine sponge *Psammaplysilla purea*. Shows moderate inhibitory activity against epidermal growth factor receptor kinase. Oil (as trifluoroacetate). Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{21}$ +24 (c, 0.98 in MeOH) (trifluoroacetate). λ_{max} 277 (ϵ 1700); 284 (ϵ 1400) (MeOH) (Berdy).

*12,13-Dihydro, 13-oxo (12*RS-*):* ***Purealidin K***
[167394-76-5]
$C_{15}H_{17}Br_2N_5O_5$ 507.138
Alkaloid from *Psammaplysilla purea*. Shows mod. inhibition of epidermal growth factor receptor kinase. Oil (as trifluoroacetate). Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{24}$ +26 (c, 0.38 in MeOH) (trifluoroacetate). λ_{max} 231 (ϵ 6300); 284 (ϵ 2400) (MeOH) (Berdy).

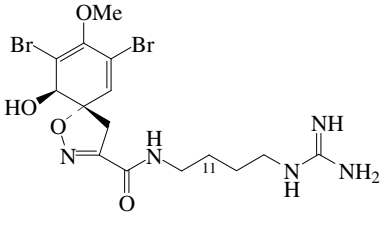
Deamino: See Aerophobin 1, A-124

(-)-*form* [172723-35-2]
Alkaloid from the sponge *Pseudoceratina verrucosa*. $[\alpha]_D$ -158 (c, 1 in MeOH) (as hydrochloride). Incorrect struct. assigned in CA. λ_{max} 220 (log ϵ 4.47); 284 (log ϵ 4.08) (MeOH).

Kobayashi, J. *et al., Chem. Pharm. Bull.*, 1995, **43**, 403 (*isol, uv, ir, pmr, cmr, cd, struct*)
Benharref, A. *et al., J. Nat. Prod.*, 1996, **59**, 177-180 (*Pseudoceratinine A*)

Purealidin L P-718

[167394-77-6]



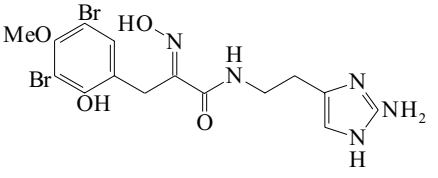
$C_{15}H_{21}Br_2N_5O_4$ 495.17
Alkaloid from the Okinawan marine sponge *Psammaplysilla purea* and from *Aiolochroia crassa*. Oil (as trifluoroacetate). $[\alpha]_D^{24}$ +27 (c, 0.18 in MeOH) (trifluoroacetate). Genus name sometimes misspelt Ailochroia.

11ξ-Hydroxy: ***Caissarine A***
[439132-04-4]
$C_{15}H_{21}Br_2N_5O_5$ 511.169
Isol. from the Brazilian sponge *Aplysina caissara*. Glassy solid. λ_{max} 232 (ϵ 9100); 283 (ϵ 4250) (MeOH).

Kobayashi, J. *et al., Chem. Pharm. Bull.*, 1995, **43**, 403-407 (*isol, uv, ir, pmr, cmr, cd, struct*)
Saeki, B.M. *et al., J. Nat. Prod.*, 2002, **65**, 796-799; 2003, **66**, 1039 (*Caissarine A*)

Purealidin M P-719

N-*[2-(2-Amino-1*H*-imidazol-4-yl)ethyl]-3,5-dibromo-2-hydroxy-α-(hydroxyimino)-4-methoxybenzenepropanamide, 9CI*
[167394-78-7]



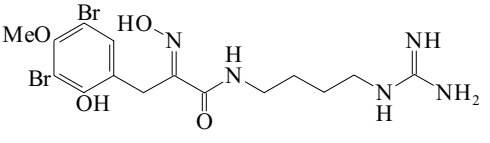
$C_{15}H_{17}Br_2N_5O_4$ 491.138
Alkaloid from the Okinawan marine sponge *Psammaplysilla purea*. Oil (as trifluoroacetate).

Deamino: ***Purealidin N***
[167394-79-8]
$C_{15}H_{16}Br_2N_4O_4$ 476.124
From *Psammaplysilla purea*. Exhibits cytotoxicity against murine lymphoma L1210 cells and human epidermoid carcinoma KB cells *in vitro*. Oil. Sol. MeOH, EtOAc; poorly sol. H_2O. λ_{max} 235 (ϵ 2600); 290 (ϵ 2800) (MeOH) (Berdy).

Kobayashi, J. *et al., Chem. Pharm. Bull.*, 1995, **43**, 403 (*isol, uv, ir, pmr, cmr, struct*)
Boehlow, T.R. *et al., J.O.C.*, 2001, **66**, 3111-3118 (*Purealidin N, synth*)

Purealidin O P-720

N-*[4-[(Aminoiminomethyl)amino]butyl]-3,5-dibromo-2-hydroxy-α-(hydroxyimino)-4-methoxybenzenepropanamide*
[167394-80-1]

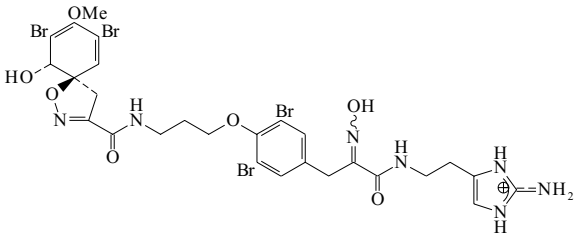


$C_{15}H_{21}Br_2N_5O_4$ 495.17
Alkaloid from the Okinawan marine sponge *Psammaplysilla purea*. Oil (as trifluoroacetate).

Kobayashi, J. *et al., Chem. Pharm. Bull.*, 1995, **43**, 403 (*isol, uv, ir, pmr, cmr, struct*)

Purealine P-721

[100101-28-8]



$C_{27}H_{30}Br_4N_7O_7^{\oplus}$ 884.193

Isol. from the Okinawan marine sponge *Psammaplysilla purea*. Na/K-ATPase inhibitor. Sol. MeOH, EtOAc; poorly sol. H_2O. λ_{max} 276 (sh); 284; 292 (sh) (MeOH) (Derep).

Chloride:

$C_{27}H_{30}Br_4ClN_7O_7$ 919.645

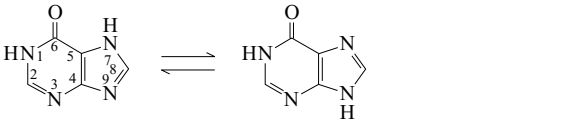
Amorph. solid. Mp 142-145°. $[\alpha]_D$ -85 (c, 2.1 in MeOH).

Nakamura, H. *et al., Tet. Lett.*, 1985, **26**, 4517 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)

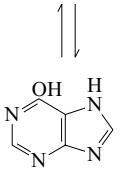
6-Purinol P-722

*1,7-Dihydro-6*H*-purin-6-one, 9CI.* ***Hypoxanthine****. Sarcine. Sarkine. 6-Hydroxypurine. 6(1*H*)-Purinone*

[68-94-0]



1,7−Dihydro−*form* 1,9−Dihydro−*form*



OH−form

$C_5H_4N_4O$ 136.113

Many alternative tautomeric forms possible. Occurs widely in plant and animal tissue. Used as a 0.8% soln. in DMF for pptn. detn. of Ag, Bi, Pd. Needles.

Mp 360°. pK_{a1} 1.91; pK_{a2} 8.96; pK_{a3} 12.18 (20°).

▶ Exp. teratogen (large does). LD_{50} (mus, ipr) 750 mg/kg.

UP0791000

1,9-Dihydro-*form* [51953-23-2]

*1,9-Di-Me: 1,9-Dihydro-1,9-dimethyl-6*H*-purin-6-one, 9CI. 1,9-Dimethylhypoxanthine*

[20535-82-4]

$C_7H_8N_4O$ 164.166

Isol. from the sponge *Spongosorites* sp. Cryst. (EtOH).

Mp 255-256°. λ_{max} 209 (log ϵ 3.7); 260 (log ϵ 3.4) (H_2O).

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 584A (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 709A (*ir*)

Krebs, E.G. *et al., Arch. Biochem. Biophys.*, 1949, **24**, 49 (*1,9-di-Me*)

Bullock, F.J. *et al., J.O.C.*, 1964, **29**, 1988 (*pmr*)

Bergmann, F. *et al., J.C.S.(C)*, 1966, 10 (*synth*)

Lister, J.H. *et al., Chem. Heterocycl. Compd.*, (Weissberger, A. etal, Ed.), Part II, 1971, (*rev*)

Sekiya, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 209; 1975, **23**, 2401 (*synth, deriv*)

Chenon, M.T. *et al., J.A.C.S.*, 1975, **97**, 4627; 4636 (*cmr, tautom*)

Raurez, G. *et al., Quim. Anal. (Madrid)*, 1975, **29**, 216 (*use*)

Scheiner, P. *et al., J. Het. Chem.*, 1985, **22**, 1435 (*synth, pmr, uv*)

Schmalle, H.W. *et al., Acta Cryst. C*, 1988, **44**, 732 (*cryst struct*)

Capon, R.J. *et al., J. Nat. Prod.*, 2000, **63**, 261-262 (*isol, 1,9-Dimethylhypoxanthine*)

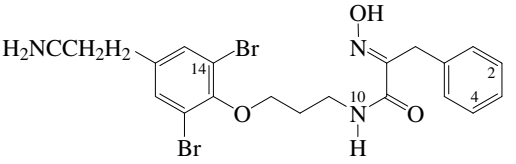
Lagoja, I.M. *et al., Chem. Biodiversity*, 2004, **1**, 106-111 (*synth*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DMC000

Purpuramine A P-723

N-*[3-[4-(2-Aminoethyl)-2,6-dibromophenoxy]propyl]-α-(hydroxyimino)benzenepropanamide, 9CI*

[149636-92-0]



$C_{20}H_{23}Br_2N_3O_3$ 513.228

Isol. from the sponge *Psammaplysilla purpurea*. λ_{max} 280 (ϵ 834) (MeOH).

2-Bromo, 4-methoxy, N^{10}*-Me:* ***Purpuramine L***

$C_{22}H_{26}Br_3N_3O_4$ 636.177

Isol. from *Psammaplysilla purpurea*. Amorph. solid.

Mp 175-178°. λ_{max} 214 (log ϵ 5.12); 280 (log ϵ 4.02) (MeOH).

14-Debromo: ***Purpuramine B***

[149636-93-1]

$C_{20}H_{24}BrN_3O_3$ 434.332

Isol. from *Psammaplysilla purpurea*. λ_{max} 280 (ϵ 641) (MeOH).

14-Debromo, 2,4-dibromo, 3-methoxy: ***14-Debromoprearaplysillin I***

[136685-30-8]

$C_{21}H_{24}Br_3N_3O_4$ 622.15

Alkaloid from the sponge *Psammaplysilla purpurea*. Glass.

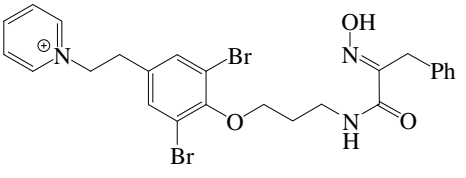
James, D.M. *et al., J. Nat. Prod.*, 1991, **54**, 1137 (*14-Debromoprearaplysillin I*)

Yagi, H. *et al., Tetrahedron*, 1993, **49**, 3749-3754 (*Purpuramines A,B*)

Goud, T.V. *et al., Chem. Pharm. Bull.*, 2003, **51**, 990-993 (*Purpuramine L*)

Purpuramine C P-724

[149636-94-2]



$C_{25}H_{26}Br_2N_3O_3^{\oplus}$ 576.307

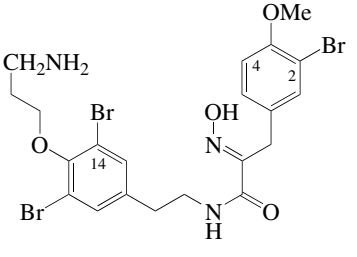
Isol. from the sponge *Psammaplysilla purpurea*. λ_{max} 250 (ϵ 5600) (MeOH).

Yagi, H. *et al., Tetrahedron*, 1993, **49**, 3749-3754 (*isol*)

Purpuramine H P-725

Aplysamine 3

[149636-99-7]



$C_{21}H_{24}Br_3N_3O_4$ 622.15

Metab. from the sponge *Psammaplysilla purpurea*. Cytotoxic agent. Amorph. or semicryst. solid. Isol. as a salt, counterion not specified. λ_{max} 214 (ϵ 17000); 222 (ϵ 16700); 280 (ϵ 3100) (MeOH).

N^{20}-*(13-Methyltetradecanoyl):* ***Aplysamine 5***
[152606-62-7]
$C_{36}H_{52}Br_3N_3O_5$ 846.536
Isol. from sponge *Psammaplysilla purpurea*. Cytotoxic agent. Gum. λ_{max} 214 (ϵ 18500); 222 (ϵ 17200); 282 (ϵ 2700) (MeOH).

N^{20}-*Me:* ***Purpuramine I***
[149637-00-3]
$C_{22}H_{26}Br_3N_3O_4$ 636.177
Isol. from *Psammaplysilla purpurea* and *Suberea* sp. λ_{max} 280 (ϵ 1800) (MeOH).

N^{20}-*Me,* N^{20}-*(methoxycarbonyl):* ***Purpuramine K***
[627544-34-7]
$C_{24}H_{28}Br_3N_3O_6$ 694.214
Isol. from *Psammaplysilla purpurea*. Amorph. solid.
Mp 190-195°. λ_{max} 218 (log ϵ 3.65); 280 (log ϵ 4.78) (MeOH).

N^{20},N^{20}-*Di-Me:* ***Aplysamine 2***
[172486-24-7]
[125547-39-9]
$C_{23}H_{28}Br_3N_3O_4$ 650.204
Isol. from *Aplysina* sp., *Psammaplysilla purpurea* and *Pseudoceratina purpurea*. Pale tan semicryst. solid (as hydrochloride).
Mp 87-88.5° (hydrochloride). λ_{max} 214 (ϵ 17000); 222 (ϵ 16700); 280 (ϵ 3100) (MeOH).

N^{20},N^{20}-*Di-Me,* N^{20}-*oxide:* ***Purpuramine J***
[478487-88-6]
$C_{23}H_{28}Br_3N_3O_5$ 666.203
Isol. from the Fijian sponge *Druinella* sp. Cytotoxic. Oil. λ_{max} 280 (log ϵ 3.26) (MeOH).

O-*De-Me:* ***Purpuramine F***
[149636-97-5]
$C_{20}H_{22}Br_3N_3O_4$ 608.124
Isol. from *Psammaplysilla purpurea*. λ_{max} 282 (ϵ 2600) (MeOH).

O-*De-Me,* N^{20}-*Me:* ***Purpuramine G***
[149636-98-6]
$C_{21}H_{24}Br_3N_3O_4$ 622.15
Isol. from *Psammaplysilla purpurea*. λ_{max} 282 (ϵ 2800) (MeOH).

4-Bromo: ***Aplysamine 4***
[152606-61-6]
$C_{21}H_{23}Br_4N_3O_4$ 701.046
From *Psammaplysilla purpurea*. Cytotoxic agent. Semicryst. solid. Isol. as a salt, counterion not specified. λ_{max} 218 (ϵ 17600); 222 (ϵ 17400); 274 (ϵ 2100) (MeOH).

2-Debromo, 3-demethoxy: ***Purpuramine D***
[149636-95-3]
$C_{20}H_{23}Br_2N_3O_3$ 513.228
Isol. from *Psammaplysilla purpurea*. λ_{max} 282 (ϵ 512) (MeOH).

2-Debromo, 3-demethoxy, N^{20}-*Me:* ***Purpuramine E***
[149636-96-4]
$C_{21}H_{25}Br_2N_3O_3$ 527.255
Isol. from *Psammaplysilla purpurea*. λ_{max} 282 (ϵ 600) (MeOH).

14-Debromo: [159157-29-6]
$C_{21}H_{25}Br_2N_3O_4$ 543.254
Isol. from *Psammaplysilla purpurea*.

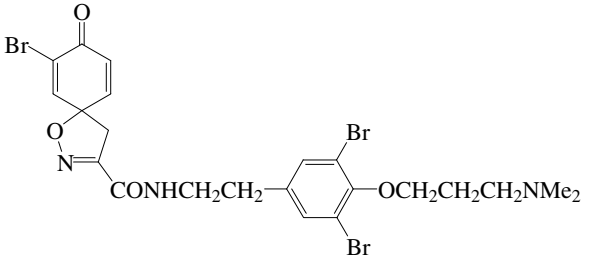
14-Debromo, 4-bromo: ***14-Debromoaplysamine 4***
[159157-30-9]
$C_{21}H_{24}Br_3N_3O_4$ 622.15
Isol. from *Psammaplysilla purpurea*.

14-Debromo, 4-bromo, N^{20}-*Me:* ***Purpurealidin H***
[799246-92-7]
$C_{22}H_{26}Br_3N_3O_4$ 636.177
Isol. from *Psammaplysilla purpurea*. Amorph. solid (MeOH). λ_{max} 218 (ϵ 12675); 280 (ϵ 2675) (MeOH).

Xynas, R. *et al., Aust. J. Chem.*, 1989, **42**, 1427-1433 (*Aplysamine 2*)
Yagi, H. *et al., Tetrahedron*, 1989, **49**, 3749-3754 (*Purpuramines*)
Pakrashi, S.C. *et al., Tetrahedron*, 1990, **50**, 12009-12014; 12783 (*isol*)
Jurek, J. *et al., J. Nat. Prod.*, 1993, **56**, 1609-1612 (*Aplysamines 3-5*)
Rao, M.R. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 1301-1303 (*Aplysamine 2*)
Tabudravu, J.N. *et al., J. Nat. Prod.*, 2002, **65**, 1798-1801 (*Purpuramine J*)
Goud, T.V. *et al., Chem. Pharm. Bull.*, 2003, **51**, 990-993 (*Purpuramine K*)
Tilvi, S. *et al., Tetrahedron*, 2004, **60**, 10207-10215 (*Purpurealidin H, 14-Debromoaplysamine 4*)
Kijjoa, A. *et al., Z. Naturforsch., B*, 2005, **60**, 904-908 (*Aplysamine 2*)

Purpurealidin B P-726

[799246-87-0]

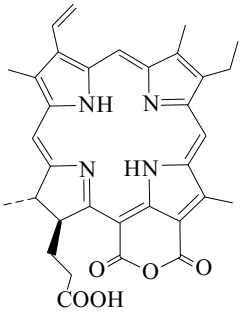


$C_{22}H_{24}Br_3N_3O_4$ 634.161
Isol. from the sponge *Psammaplysilla purpurea*. Amorph. solid.
Mp 175.8°. λ_{max} 283 (ϵ 1320) (MeOH).

Tilvi, S. *et al., Tetrahedron*, 2004, **60**, 10207-10215 (*isol, pmr, cmr, ms*)

Purpurin 18 P-727

[25465-77-4]



$C_{33}H_{32}N_4O_5$ 564.64
Oxidn. prod. from Phaeophorbide a, P-295. Isol. from *Ruditapes philippinarum* and constit. of various marine sediments. Photosensitiser. Green-brown solid.

Me ester: ***Phellophyll a***
[51744-55-9]
$C_{34}H_{34}N_4O_5$ 578.666
Isol. from the clam *Ruditapes philippinarum*. Constit. of the leaves of *Phellodendron amurense* var. *wilsonii*. Greenish-black cryst. ($CHCl_3$/MeOH).
Mp 270° (141-142°). $[\alpha]_D^{25}$ +298 (c, 0.007 in MeOH). λ_{max} 212 (log ϵ 2.99); 279 (log ϵ 2.82); 360 (log ϵ 3.25); 407 (log ϵ 3.6); 508 (log ϵ 2.53); 546 (log ϵ 2.9); 697 (log ϵ 3.14) (MeOH). λ_{max} 362 (ϵ 48900); 412 (ϵ 126100); 480 (ϵ 4800); 508 (ϵ 7200); 548 (ϵ 25500); 644 (ϵ 9400); 702 (ϵ 52100) ($CHCl_3$).

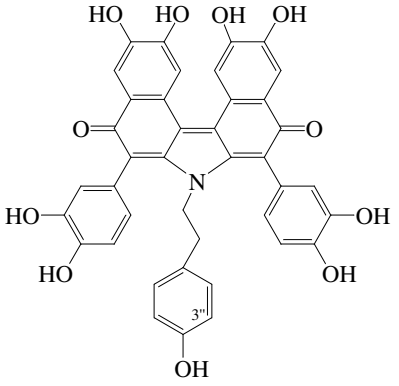
*2,6,10,14-Tetramethylhexadec-2*E*-enyl ester:* ***Aristophyll C***
[236734-78-4]
$C_{53}H_{70}N_4O_5$ 843.16
Constit. of the leaves of *Aristolochia heterophylla*. Grey-green solid.
Mp 247-249°. λ_{max} 225 (sh) (log ϵ 4.36); 277 (log ϵ 4.05); 361 (log ϵ 4.45); 408 (log ϵ 4.8); 480 (log ϵ 3.54); 508 (log ϵ 3.68); 546 (log ϵ 4.12); 642 (log ϵ 3.77); 698 (log ϵ 4.4) (MeOH).

Fischer, H. *et al., Die Chemie des Pyrrols*, Akademische Verlag, Leipzig, Vol. II, (ii), 1940, 116
Hoffman, D.R. *et al., J.O.C.*, 1965, **30**, 3512 (*ms*)
Inhoffen, H.H. *et al., Annalen*, 1967, **704**, 188

Hynninen, P.H. *et al., Acta Chem. Scand.*, 1973, **27**, 1771 (*synth, uv*)
Kenner, G.W. *et al., J.C.S. Perkin 1*, 1973, 2517
Smith, K.M. *et al., Porphyrins and Metalloporphyrins*, (ed. Smith, K.M.), Elsevier Elsevier, Amsterdam, 1975, 776
Watanabe, N. *et al., J. Nat. Prod.*, 1993, **56**, 305-317 (*isol, pmr, cmr*)
Sakata, K. *et al., ACS Symp. Ser.*, 1994, **547**, 164
Ma, L. *et al., J.O.C.*, 1996, **61**, 2501-2510 (*synth, uv, pmr, cmr*)
Chan, Y.-Y. *et al., Chem. Pharm. Bull.*, 1999, **47**, 887-889 (*Aristophyll C*)
Di Stefano, A. *et al., Photochem. Photobiol.*, 2001, **73**, 290-296 (*pharmacol*)
Wu, T.-S. *et al., J. Nat. Prod.*, 2003, **66**, 1207-1211 (*Phellophyll a*)
Sharma, S. *et al., Cancer Chemother. Pharmacol.*, 2006, **57**, 500-506 (*pharmacol*)

Purpurone P-728

[147362-37-6]



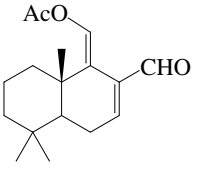
$C_{40}H_{27}NO_{11}$ 697.653
Alkaloid from the marine sponge *Iotrochota* sp. Exhibits ATP-citrate lyase inhibitory activity. Lipogenesis inhibitor. Purple glass. λ_{max} 215 (ϵ 30400); 315 (ϵ 16400); 511 (ϵ 8500) (MeOH/KOH) (Derep). λ_{max} 216 (ϵ 28100); 296 (ϵ 15100); 500 (ϵ 11400) (MeOH) (Derep).

3''-Hydroxy: ***Ningalin D***
[188111-70-8]
$C_{40}H_{27}NO_{12}$ 713.653
Alkaloid from the ascidian *Didemnum* sp. Dark red solid. λ_{max} 206 (ϵ 41000); 276 (ϵ 18000); 294 (ϵ 17000); 404 (sh); 508 (ϵ 9900) (MeOH).

Chan, G.W. *et al., J.O.C.*, 1993, **58**, 2544-2546 (*isol, uv, ir, pmr, cmr*)
Kang, H. *et al., J.O.C.*, 1997, **62**, 3254-3262 (*Ningalin D*)
Peschko, C. *et al., Tet. Lett.*, 2000, **41**, 9477-9481 (*synth*)
Hamasaki, A. *et al., J.A.C.S.*, 2005, **127**, 10767-10770 (*Ningalin D, synth*)

Puulenal P-729

11-Acetoxy-7,9(11)-drimadien-12-al
[83630-99-3]

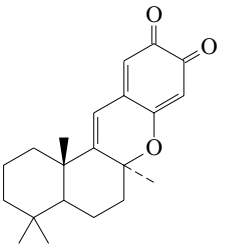


$C_{17}H_{24}O_3$ 276.375
Enol acetate of, 11,12-Dialdehyde. Isol. from the nudibranch *Chromodoris albonotato*. Cryst.
Mp 97-99°. $[\alpha]_D$ -14.7 (c, 0.15 in $CHCl_3$). λ_{max} 227 (ϵ 5560); 262 (ϵ 2340) (MeOH).

Schulte, G.R. *et al., Tetrahedron*, 1982, **38**, 1857-1863

Puupehedione P-730

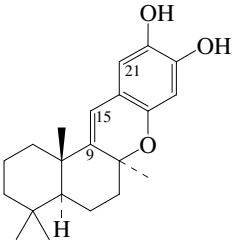
[151345-10-7]



$C_{21}H_{26}O_3$ 326.435
Constit. of a Verongid sponge.
$[\alpha]_D$ +208 (c, 0.087 in MeOH). λ_{max} 204 (ϵ 12000); 250 (ϵ 20000); 356 (ϵ 11000); 436 (ϵ 1670) (MeOH) (Derep).

Hamann, N.T. *et al., J.O.C.*, 1993, **58**, 6505 (*isol, pmr, cmr*)
Urban, S. *et al., J. Nat. Prod.*, 1996, **59**, 900 (*abs config*)
Barrero, A.F. *et al., Tetrahedron*, 1999, **55**, 15181-15208 (*synth*)
Maiti, S. *et al., Tet. Lett.*, 2001, **42**, 2389-2392 (*synth*)
Armstrong, V. *et al., J. Nat. Prod.*, 2003, **66**, 1382-1383 (*synth*)
Ishibashi, H. *et al., J.A.C.S.*, 2004, **126**, 11122-11123 (*synth*)

Puupehenol P-731



Absolute Configuration

$C_{21}H_{28}O_3$ 328.45
Parent not known.

20-Me ether: [479637-05-3]
$C_{22}H_{30}O_3$ 342.477
Constit. of a *Hyrtios* sp. Pink powder. $[\alpha]_D^{24}$ +41 (c, 4.68 in MeOH). λ_{max} 234 (ϵ 6700); 324 (ϵ 9500) (CH_2Cl_2).

9α,15-Dihydro, 15-oxo: ***15-Oxopuupehenol***
[168781-80-4]
$C_{21}H_{28}O_4$ 344.45
Isol. from sponge *Hyrtios* spp. Antitumour and antimalarial agent. Glass. $[\alpha]_D$ -106 (c, 0.52 in MeOH). λ_{max} 212 (ϵ 10870); 246 (ϵ 6040); 284 (ϵ 5595); 354 (ϵ 3060) (MeOH).

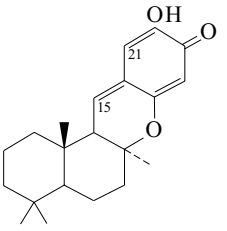
9α,15-Dihydro, 15α-methoxy, 20-Me ether: ***15,20-Dimethoxypuupehenol (incorr.)***
[479637-06-4]
$C_{23}H_{34}O_4$ 374.519
Constit. of a *Hyrtios* sp. Oil.

21-Chloro: ***21-Chloropuupehenol***
[168781-79-1]
$C_{21}H_{27}ClO_3$ 362.895
Isol. from the sponges *Hyrtios* and *Dysidea* spp. Red glass. $[\alpha]_D$ +112 (c, 0.35 in MeOH). λ_{max} 202 (ϵ 14215); 224 (sh) (ϵ 6790); 248 (ϵ 6850); 332 (ϵ 3050); 368 (sh) (ϵ 1985); 458 (ϵ 300) (MeOH).

Nasu, S.S. *et al., J.O.C.*, 1995, **60**, 7290-7292 (*isol, uv, ir, pmr, cmr, ms*)
Urban, S. *et al., J. Nat. Prod.*, 1996, **59**, 900-901 (*abs config*)
Piña, I.C. *et al., J. Nat. Prod.*, 2003, **66**, 2-6 (*20-Me ether, 15,20-Dimethoxypuupehenol*)
Hua, D.H. *et al., J.O.C.*, 2004, **69**, 6065-6078 (*synth*)
Alvarez-Manzaneda, E.J. *et al., Org. Lett.*, 2005, **7**, 1477-1480, (*15-Oxopuupehenol, synth*)

Puupehenone P-732

[73573-17-8]



$C_{21}H_{28}O_3$ 328.45
Constit. of sponges and other marine organisms, *Heteronema* sp., *Strongylophora hartmanii*, *Hyrtios eubamma*, *Psammaplysilla* sp., *Dysidea* sp., *Chondrosia chuculla*. Enzyme inhibitor, shows insecticidal props. Cryst. (hexane).
Mp 129-130°. $[\alpha]_D$ +315 (c, 1.64 in CCl_4). λ_{max} 308 (sh) (ϵ 21600); 317 (ϵ 24300); 328 (sh) (ϵ 16000) (cyclohexane) (Derep).

20-Me ether: ***20-Methoxypuupehenone (incorr.)***
[479637-04-2]
$C_{22}H_{30}O_3$ 342.477
Constit. of a *Hyrtios* sponge. Yellow oil. $[\alpha]_D^{24}$ +37 (c, 1.52 in MeOH). λ_{max} 232 (ϵ 8800); 322 (ϵ 9500) (CH_2Cl_2).

15-Cyano: ***15-Cyanopuupehenone***
[151029-41-3]
$C_{22}H_{27}NO_3$ 353.46
Constit. of a Verongid sponge. Immunomodulator. Yellow glass. $[\alpha]_D$ +168 (c, 0.082 in MeOH). λ_{max} 204 (ϵ 10700); 348 (ϵ 13300); 530 (ϵ 540) (MeOH) (Derep).

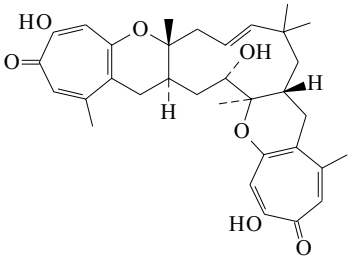
21-Chloro: ***21-Chloropuupehenone***
[73516-53-7]
$C_{21}H_{27}ClO_3$ 362.895
Constit. of a Verongid sponge.

21-Bromo: ***21-Bromopuupehenone***
[73516-54-8]
$C_{21}H_{27}BrO_3$ 407.347
Isol. from a *Hyrtios*, *Heteronema* and *Dysidea* spp.

Trammell, G.L. *et al., Tet. Lett.*, 1978, **19**, 1525-1528 (*Puupehenone, synth*)
Ravi, B.N. *et al., Pure Appl. Chem.*, 1979, **51**, 1893-1900 (*21-chloro, 21-bromo, isol*)
Hamann, M.T. *et al., J.O.C.*, 1993, **58**, 6565-6569 (*Verongid sponge isolates*)
Urban, S. *et al., J. Nat. Prod.*, 1996, **59**, 900-901 (*abs config*)
Barrero, A.F. *et al., Tet. Lett.*, 1997, **38**, 2325-2328 (*synth*)
Quideau, S. *et al., Org. Lett.*, 2002, **4**, 3975-3978 (*synth*)
Piña, I.C. *et al., J. Nat. Prod.*, 2003, **66**, 2-6 (*20-Me ether*)
Hua, D.H. *et al., J.O.C.*, 2004, **69**, 6065-6078 (*synth*)

Pycnidione P-733

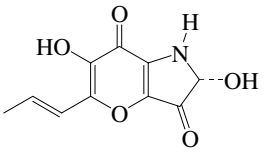
[149064-34-6]



$C_{33}H_{40}O_7$ 548.675
Metab. of a *Phoma* sp. Erythropoietin inducer. Cryst. (EtOH). Mp 216-219° dec. $[\alpha]_D^{25}$ +278 (c, 0.23 in CH_2Cl_2). λ_{max} 255 (ϵ 67000); 324; 365 (ϵ 24000) (MeOH) (Berdy). λ_{max} 255 (ϵ 67600); 362 (ϵ 24300); 366 (ϵ 24400) (EtOH) (Berdy).

Harris, G.H. *et al., Tetrahedron*, 1993, **49**, 2139 (*isol, pmr, cmr, cryst struct*)
Cai, P. *et al., J. Nat. Prod.*, 1998, **61**, 791-795 (*activity, isol*)
Höller, U. *et al., Dissertation*, Univ. of Braunschweig, 1999, (*marine isol*)

Pyranonigrin A P-734

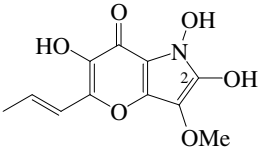


Absolute Configuration

$C_{10}H_9NO_5$ 223.185
Prod. by *Aspergillus niger* isol. from the sponge *Axinella damicornis*. Amorph. solid. $[\alpha]_D^{20}$ +59.9 (c, 1 in DMSO).

Hiort, J. *et al., J. Nat. Prod.*, 2004, **67**, 1532-1543 (*isol, pmr, cmr*)

Pyranonigrin B P-735

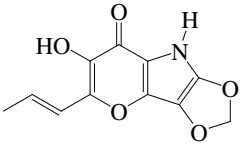


$C_{11}H_{11}NO_6$ 253.211
Prod. by *Aspergillus niger* isol. from the sponge *Axinella damicornis*. Amorph. solid.

O-*De-Me, 2-Me ether:* ***Pyranonigrin C***
$C_{11}H_{11}NO_6$ 253.211
Prod. by *Aspergillus niger* from *Axinella damicornis*. Amorph. solid.

Hiort, J. *et al., J. Nat. Prod.*, 2004, **67**, 1532-1543 (*isol, pmr, cmr*)

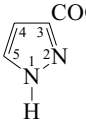
Pyranonigrin D P-736



$C_{11}H_9NO_5$ 235.196
Prod. by *Aspergillus niger* isol. from the sponge *Axinella damicornis*. Amorph. solid.

Hiort, J. *et al., J. Nat. Prod.*, 2004, **67**, 1532-1543 (*isol, pmr, cmr*)

3(5)-Pyrazolecarboxylic acid, 9CI P-737



1H–form

$C_4H_4N_2O_2$ 112.088
Prisms (H_2O). Sol. EtOH; mod. sol. Et_2O, AcOH; insol. $CHCl_3$, C_6H_6. Mp 293° dec. A claimed isolation in 1997 from a marine sponge was shown to be incorr. (2003).

Me ester: [15366-34-4]
$C_5H_6N_2O_2$ 126.115
Cryst. (C_6H_6). Sol. MeOH; spar. sol. petrol. Mp 139-140°.

Et ester: [5932-27-4]
$C_6H_8N_2O_2$ 140.141
Cryst. (hexane/EtOAc). Mp 158-159°.

Amide: [33064-36-7]
$C_4H_5N_3O$ 111.103
Mp 203-204°.

Nitrile: 3-Cyanopyrazole
[33064-34-5]
$C_4H_3N_3$ 93.088
Cryst. (C_6H_6). Mp 76-77°.

1*H-form* [1621-91-6]

N-*Me: 1-Methyl-1*H-*pyrazole-3-carboxylic acid, 9CI*
[25016-20-0]
$C_5H_6N_2O_2$ 126.115
Cryst. Mod. sol. hot H_2O. Mp 155-155.5° (146°) Mp 222°.

N-*Me, Me ester:* [17827-61-1]
$C_6H_8N_2O_2$ 140.141
Liq. Bp_9 120°.

N-*Me, Et ester:*
$C_7H_{10}N_2O_2$ 154.168
Liq. Mp 9-11°. Bp_{13} 140-143°.

N-*Ph: 1-Phenyl-1*H-*pyrazole-3-carboxylic acid, 9CI*
[4747-46-0]
$C_{10}H_8N_2O_2$ 188.185
Needles (H_2O). Mp 146°. pK_{a1} 3.6 (20°).

N-*Ph, Me ester:*
$C_{11}H_{10}N_2O_2$ 202.212
Needles. Mp 77°.

N-*Ph, nitrile: 3-Cyano-1-phenyl-1*H-*pyrazole*
[18093-85-1]
$C_{10}H_7N_3$ 169.185
Cryst. (Et_2O/petrol).

2H-form

N-*Me: 1-Methyl-1*H-*pyrazole-5-carboxylic acid, 9CI*
[16034-46-1]
[17827-60-0, 25832-41-1]
$C_5H_6N_2O_2$ 126.115
Isol. from the gorgonian *Echinomuraceae splendens*. Cryst. (H_2O).
Mp 223-224° (219-220°).

N-*Me, Et ester:*
Liq. Bp_{18} 95°.

N-*Ph: 1-Phenyl-1*H-*pyrazole-5-carboxylic acid, 9CI*
[1133-77-3]
$C_{10}H_8N_2O_2$ 188.185
Needles (H_2O). Mp 183°. pK_{a1} 2.7 (20°).

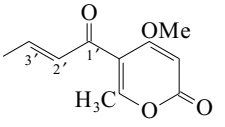
N-*Ph, Me ester:* [55115-07-6]
Needles. Mp 67°.

N-*Ph, nitrile: 5-Cyano-1-phenyl-1*H-*pyrazole*
$C_{10}H_7N_3$ 169.185
Liq. $Bp_{0.625}$ 95-100° (lit. gives a pressure range).

Claisen, L. *et al., Annalen*, 1894, **278**, 292 (*N-Ph*)
v. Pechmann, H. *et al., Ber.*, 1900, **33**, 3594 (*synth*)
Buchner, E. *et al., Ber.*, 1902, **35**, 37 (*synth*)
Rojahn, C.A. *et al., Annalen*, 1924, **437**, 303 (*N-Ph*)
v. Auwers, K. *et al., J. Prakt. Chem.*, 1935, **143**, 259 (*ester*)
Cusmano, S. *et al., Gazz. Chim. Ital.*, 1940, **70**, 227 (*N-Ph*)
Panizzi, L. *et al., Gazz. Chim. Ital.*, 1947, **77**, 556 (*N-Ph*)
Roedig, A. *et al., Annalen*, 1955, **597**, 214 (*N-Ph*)
Hüttel, R. *et al., Annalen*, 1959, **625**, 55 (*synth*)
Gundermann, K. *et al., Chem. Ber.*, 1960, **93**, 883 (*synth*)
Wijnberger, C. *et al., J. Het. Chem.*, 1969, **6**, 545 (*N-Me*)
Manecke, G. *et al., Tet. Lett.*, 1969, 617 (*synth*)
Sasaki, T. *et al., J.C.S.(C)*, 1971, 2147 (*derivs*)
Akhrem, A.A. *et al., Tet. Lett.*, 1973, 2655 (*pmr, ir, uv*)
Scherowsky, G. *et al., Annalen*, 1977, 1235 (*N-Ph*)
Beck, J.R. *et al., J. Het. Chem.*, 1988, **25**, 555 (*N-Ph*)
Pavlik, J.W. *et al., J. Het. Chem.*, 1992, **29**, 1357 (*N-Me*)
Martins, M.A.P. *et al., Synthesis*, 1995, 1491 (*Et ester*)
Parameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 2002, **41**, 1093-1096 (*isol, N-Me*)
Rao, K.V. *et al., J. Nat. Prod.*, 1993, **66**, 823-828 (*claimed isol*)

Pyrenocine A P-738

*4-Methoxy-6-methyl-5-(1-oxo-2-butenyl)-2*H-*pyran-2-one, 9CI. Citreopyrone*
[76868-97-8]



$C_{11}H_{12}O_4$ 208.213

Formerly assigned furanoid struct. Isol. from *Pyrenochaeta terrestris*, a marine-derived *Penicillium waksmanii* and *Penicillium citreo-viride* and *Alternaria* sp. nov. Plant growth inhibitor. Cytotoxic agent. Cryst. (MeOH). Sol. MeOH, C_6H_6, Et_2O. Mp 110.9-111.6°. λ_{max} 228 (ϵ 10200); 274 (ϵ 5550) (EtOH) (Derep).

1′-Alcohol: ***Pyrenocine C***
[94474-69-8]
$C_{11}H_{14}O_4$ 210.229
From *Penicillium terrestris*. Weak phytotoxin. Needles (Et_2O). Sol. MeOH, EtOAc.
Mp 81.5-82°. $[\alpha]_D^{20}$ +0.3 (c, 0.37 in $CHCl_3$). Virtually racemic.
λ_{max} 284 (ϵ 7940) (MeOH) (Berdy).

2′,3′-Dihydro, 3′-hydroxy: ***Pyrenocine B***
[72674-29-4]
$C_{11}H_{14}O_5$ 226.229
Metab. of *Penicillium terrestris*, *Penicillium citreo-viride*, a marine-derived *Penicillium waksmanii* and *Alternaria* sp. nov. Phytotoxin. Cytotoxic agent. Cryst. (Et_2O/hexane). Sol. MeOH, Et_2O, C_6H_6. Mp 103-103.5°. $[\alpha]_D^{20}$ +0.03 (c, 0.56 in $CHCl_3$). Formerly assigned furanoid struct. λ_{max} 216 (sh) (ϵ 8200); 258 (ϵ 6100); 282 (ϵ 4600) (EtOH) (Derep).

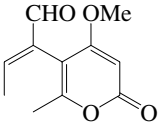
2′,3′-Dihydro, 3′-methoxy: ***Pyrenocine E***
[208390-05-0]
$C_{12}H_{16}O_5$ 240.255
Prod. by a marine algal derived strain of *Penicillium waksmanii*. Cytotoxic agent. Powder. Sol. DMSO, EtOAc, $CHCl_3$, Me_2CO, MeOH; poorly sol. H_2O.
Mp 82-84°. Racemic. λ_{max} 215 (sh) (log ϵ 3.63); 250 (log ϵ 3.29); 280 (sh) (log ϵ 3.06) (EtOH). λ_{max} 250 (ϵ 1950) (MeOH) (Berdy).

[72674-30-7]

Sato, H. *et al., Agric. Biol. Chem.*, 1979, **43**, 2409; 1981, **45**, 795 (*isol, cryst struct*)
Niwa, M. *et al., Tet. Lett.*, 1980, 4483 (*isol*)
Sparace, S.A. *et al., Phytochemistry*, 1984, **23**, 2693 (*deriv*)
Shizuri, Y. *et al., Tet. Lett.*, 1984, **25**, 1583 (*biosynth*)
Tal, B. *et al., Z. Naturforsch., C*, 1986, **41**, 1032 (*isol*)
Sparace, S.A. *et al., Can. J. Microbiol.*, 1987, **33**, 327 (*props*)
Ichihara, A. *et al., Tetrahedron*, 1987, **43**, 5245 (*synth*)
Amagata, T. *et al., J. Antibiot.*, 1998, **51**, 432-434 (*Pyrenocines A,B,E, activity*)

Pyrenocine D P-739

[208390-04-9]

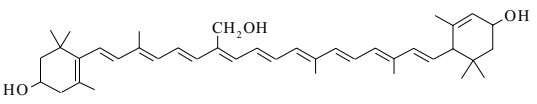


$C_{11}H_{12}O_4$ 208.213
Prod. by a marine algal derived strain of *Penicillium waksmanii*. Cytotoxic agent. Needles. Sol. DMSO, Me_2CO, $CHCl_3$, EtOAc, MeOH; poorly sol. H_2O.
Mp 112-114°. λ_{max} 220 (sh) (log ϵ 4.14); 282 (log ϵ 3.62) (EtOH). λ_{max} 282 (ϵ 4168) (MeOH) (Berdy).

Amagata, T. *et al., J. Antibiot.*, 1998, **51**, 432-434 (*isol, uv, ir, pmr, cmr*)

Pyrenoxanthin P-740

β,ε-Carotene-3,3′,20-triol
[28392-44-1]

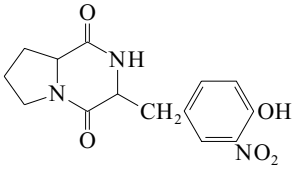


$C_{40}H_{56}O_3$ 584.881
Constit. of *Chlorella pyrenoidosa*. Cryst. (petrol).
Mp 148-149°. May be identical with Loroxanthin, L-236.

Yamamoto, H.Y. *et al., J.O.C.*, 1969, **34**, 4207

Pyriculamide P-741

Hexahydro-3-[(4-hydroxy-3-nitrophenyl)methyl]pyrrolo[1,2-a]pyrazine-1,4-dione, 9CI. Cyclo(prolyl-3-nitrotyrosyl)
[134876-76-9]



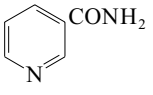
$C_{14}H_{15}N_3O_5$ 305.29
Isol. from *Pyricularia oryzae* and the marine-derived *Flavobacterium* sp. T436. Plant growth inhibitor. Bright yellow needles (Me_2CO).
Mp 183-185° dec. $[\alpha]_D$ -84.4 (c, 0.66 in MeOH).

[125034-08-4]

Boldyrev, A.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **94**, 237 (*pharmacol*)
Sviridov, S.I. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 691-696 (*isol*)
Bavykina, N.I. *et al., Zh. Obshch. Khim.*, 1990, **60**, 170 (*synth*)
Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

3-Pyridinecarboxamide, 9CI P-742

Nicotinamide, 8CI, INN. *Niacinamide. Nicotinic acid amide. Antipellagra factor. Nicosan 2. PP-Factor. Vitamin B_3. Many other names*
[98-92-0]



$C_6H_6N_2O$ 122.126
Widespread in plants, e.g. rice, yeast and fungi. Prod. by the marine bacterium strain He159b. Enzyme cofactor, used in treatment of pellagra, low mammalian toxicity. Needles (C_6H_6).
Mp 129-130°. $Bp_{0.0005}$ 150-160°. pK_a 3.33 (20°). Log P -0.21 (calc).

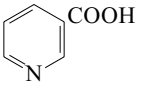
▶ QS3675000

[6485-44-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 796B; 917A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 338B; 342B (*nmr*)
La Forge, F.B. *et al., J.A.C.S.*, 1928, **50**, 2477 (*synth*)
Georg, A. *et al., Helv. Chim. Acta*, 1943, **26**, 358 (*synth*)
Rohrlich, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1950, **283**, 122 (*synth*)
Birdsall, B. *et al., J.C.S. Perkin 2*, 1972, 1643; 1973, 2145 (*cmr, pmr*)
Auerbach, J. *et al., J.O.C.*, 1976, **41**, 725 (*synth*)
Chen, P.H. *et al., J.O.C.*, 1976, **41**, 2973 (*ms*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **24**, 59 (*rev*)
Oppenheimer, N.J. *et al., Org. Magn. Reson.*, 1980, **13**, 14 (*N-15 nmr*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 410
El-Shahawy, A.S. *et al., Spectrochim. Acta A*, 1987, **43A**, 1371 (*uv*)
Abdel Moety, E.M. *et al., Anal. Profiles Drug Subst.*, 1991, **20**, 475 (*rev*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NCR000

3-Pyridinecarboxylic acid P-743

Nicotinic acid, INN. *Niacin, USAN. Nicamin. Nicobid. Nyclin. Pelonin. Wampocap. Many other names*
[59-67-6]



$C_6H_5NO_2$ 123.111
Present in fruits and other plant materials. Used as 2.5% aq. soln. for extraction-photometric detn. of U(*VI*) (λ_{max} 556 nm, ε 120000). Vitamin, enzyme cofactor, vasodilator. Antihyperglycaemic agent. Used to treat lipid disorders. Approved for clinical use in the UK (1999). Needles (H_2O or EtOH). Sol. hot H_2O; spar. sol. Et_2O.
Mp 236° (225-227°). pK_{a1} 2; pK_{a2} 4.82 (25°). Log P 0.8 (calc). Sublimes.

▶ Can cause dermal and gastrointestinal reactions and hepatic effects at high therapeutic doses. Low acute mammalian toxicity. QT0525000

Hydrochloride: [636-79-3]
Prisms or plates (H_2O). Mp 274°.

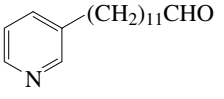
N-*(2-Hydroxyethyl), betaine: 3-Carboxy-1-(2-hydroxyethyl)pyridinium betaine.* ***Pyridinebetaine A***
$C_8H_9NO_3$ 167.164
Isol. from the sponge *Agelas dispar*. Amorph. solid. λ_{max} 220 (ε 3000); 266 (ε 2500) (MeOH).

[1976-28-9]

Cafieri, F. *et al., J. Nat. Prod.*, 1998, **61**, 1171-1173 (*Pyridinebetaine A*)

3-Pyridinedodecanal P-744

12-(3-Pyridinyl)dodecanal



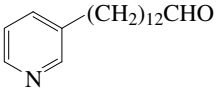
$C_{17}H_{27}NO$ 261.406

Oxime: [291775-86-5]
$C_{17}H_{28}N_2O$ 276.421
Isol. from *Amphimedon* sp. Config. not determined. λ_{max} 264 (ε 3200) (MeOH).

Hirano, K. *et al., Chem. Pharm. Bull.*, 2000, **48**, 974-977 (*isol, pmr, cmr, uv*)

3-Pyridinetridecanal P-745

13-(3-Pyridinyl)tridecanal



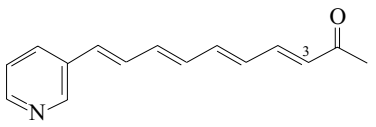
$C_{18}H_{29}NO$ 275.433

Oxime: [291775-85-4]
$C_{18}H_{30}N_2O$ 290.448
Isol. from *Amphimedon* sp. Config. not determined. λ_{max} 264 (ε 3100) (MeOH).

Hirano, K. *et al., Chem. Pharm. Bull.*, 2000, **48**, 974-977 (*isol, pmr, cmr, uv*)

10-(3-Pyridinyl)-3,5,7,9-decatetraen-2-one, 9CI P-746

3-(9-Oxo-1,3,5,7-decatetraenyl)pyridine



(all–*E*)–*form*

$C_{15}H_{15}NO$ 225.29

(all-*E*)-*form*

Navenone A

[62695-67-4]

Major constit. of the alarm pheromone of the marine opisthobranch mollusc *Navanax inermis (Chelidonura inermis)*.

Yellow cryst. (C_6H_6).

Mp 144-145°. λ_{max} 399 (ϵ 14400) (MeOH) (Berdy).

3-Methyl: ***3-Methylnavenone A***

[73414-53-6]

$C_{16}H_{17}NO$ 239.316

Minor constit. of the alarm pheromone of *Navanax inermis*.

(3*Z*,5*E*,7*E*,9*E*)-*form* [73465-89-1]

Minor constit. of the alarm pheromone of *Navanax inermis*.

(3*Z*,5*Z*,7*E*,9*E*)-*form* [73952-89-3]

Minor constit. of the alarm pheromone of *Navanax inermis*.

Sleeper, H.L. *et al., J.A.C.S.*, 1977, **99**, 2367-2368 (*isol, uv, ir, pmr, cmr, ms, struct*)

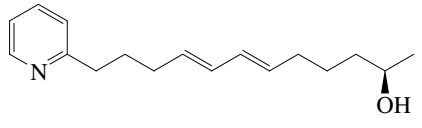
Sakakibara, M. *et al., Agric. Biol. Chem.*, 1979, **43**, 117 (*synth*)

Fenical, W. *et al., Pure Appl. Chem.*, 1979, **51**, 1865 (*derivs*)

Sleeper, H.L. *et al., J. Chem. Ecol.*, 1980, **6**, 57 (*isol*)

Soullez, D. *et al., Nat. Prod. Lett.*, 1994, **4**, 203 (*synth*)

12-(2-Pyridinyl)-6,8-dodecadien-2-ol P-747



$C_{17}H_{25}NO$ 259.391

(2*R*,6*E*,8*E*)-*form*

Phormidinine A

Alkaloid from the cyanobacterium *Phormidium* sp.

Oil. $[\alpha]_D^{20}$ -4 (c, 0.09 in $CHCl_3$). λ_{max} 232 (ϵ 17100); 262 (ϵ 3900); 268 (ϵ 1700) (MeOH).

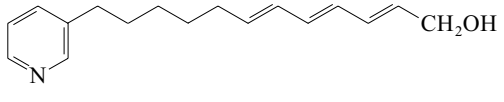
Ac: ***Phormidinine B***

$C_{19}H_{27}NO_2$ 301.428

Isol. from *Phormidium* sp. Oil.

Teruya, T. *et al., Tet. Lett.*, 2005, **46**, 4001-4003 (*isol, pmr, cmr*)

12-(3-Pyridinyl)-2,4,6-dodecatrien-1-ol, 9CI P-748



$C_{17}H_{23}NO$ 257.375

(2*E*,4*E*,6*E*)-*form*

Ac: ***Haminol C***

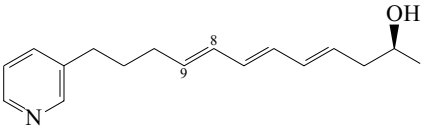
[147362-36-5]

$C_{19}H_{25}NO_2$ 299.412

Alkaloid from the mollusc *Haminoea orteai*. Alarm pheromone.

Spinella, A. *et al., Tetrahedron*, 1993, **49**, 1307-1314 (*isol, struct*)

12-(3-Pyridinyl)-4,6,8-dodecatrien-2-ol, 9CI P-749



$C_{17}H_{23}NO$ 257.375

(2*S*,4*E*,6*E*,8*E*)-*form*

Haminol 1

[147391-85-3]

Alkaloid from the molluscs *Haminoea orbignyana* and *Haminoea fusari*. Alarm pheromone.

Ac: ***Haminol 2***

[147391-84-2]

$C_{19}H_{25}NO_2$ 299.412

From *Haminoea orbignyana* and *Haminoea fusari*. Alarm pheromone. $[\alpha]_D^{20}$ -19 (c, 1.3 in MeOH).

8,9-Dihydro: 12-(3-Pyridinyl)-4,6-dodecadien-2-ol, 9CI. ***Haminol 3***

[147362-30-9]

$C_{17}H_{25}NO$ 259.391

From *Haminoea fusari*. Alarm pheromone.

8,9-Dihydro, Ac: ***Haminol 4***

[147362-25-2]

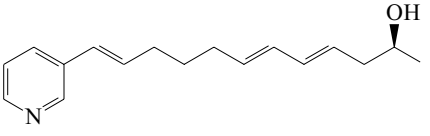
$C_{19}H_{27}NO_2$ 301.428

From *Haminoea fusari*. Alarm pheromone. $[\alpha]_D^{20}$ -12.5 (c, 0.7 in MeOH).

Spinella, A. *et al., Tetrahedron*, 1993, **49**, 1307 (*isol, uv, ir, pmr, cmr, ms, struct*)

Solladie, G. *et al., Tetrahedron: Asymmetry*, 1997, **8**, 801-810 (*synth, Haminol 1*)

12-(3-Pyridinyl)-4,6,11-dodecatrien-2-ol P-750



$C_{17}H_{23}NO$ 257.375

(2*S*,4*E*,6*E*,11*E*)-*form*

Haminol A

[133412-13-2]

Alkaloid from the molluscs *Haminoea navicula* and *Haminoea orteai*. Alarm pheromone. Oil. $[\alpha]_D$ +5 (c, 0.3 in MeOH). λ_{max} 232 (ϵ 30200); 282 (ϵ 4340) (MeOH) (Derep).

Ac: ***Haminol B***

[133412-14-3]

$C_{19}H_{25}NO_2$ 299.412

From *Haminoea navicula*. Alarm pheromone. Oil. $[\alpha]_D$ -24 (c, 0.4 in MeOH). λ_{max} 230 (ϵ 23400); 282 (ϵ 3440) (MeOH) (Derep).

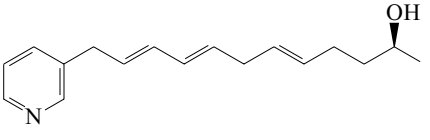
Cimino, G. *et al., Experientia*, 1991, **47**, 61-63 (*isol, uv, ir, pmr, cmr, ms, struct*)

Spinella, A. *et al., Tetrahedron*, 1993, **49**, 1307

Matikainen, J. *et al., J. Nat. Prod.*, 1995, **58**, 1622 (*synth*)

Alvarez, R. *et al., Tetrahedron: Asymmetry*, 1998, **9**, 3065-3072 (*Haminol B*)

12-(3-Pyridinyl)-5,8,10-dodecatrien-2-ol, 9CI P-751



$C_{17}H_{23}NO$ 257.375

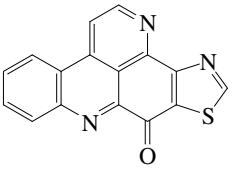
(2*S*,5*E*,8*E*,10*E*)-*form*
Haminol 5
[147391-86-4]
Alkaloid from the mollusc *Haminoea fusari*. Alarm pheromone.

Ac: ***Haminol 6***
[147362-35-4]
$C_{19}H_{25}NO_2$ 299.412
From *Haminoea fusari*. Alarm pheromone. $[\alpha]_D^{20}$ -4.2 (c, 0.2 in MeOH).

Spinella, A. *et al., Tetrahedron*, 1993, **49**, 1307-1314 (*isol, uv, ir, pmr, cmr, ms, struct*)

9*H*-Pyrido[4,3,2-*mn*]thiazolo[4,5-*b*]acridin-9-one, 9CI P-752

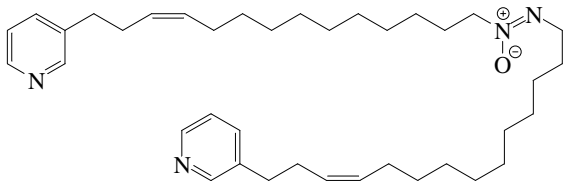
Kuanoniamine A
[133401-10-2]



$C_{16}H_7N_3OS$ 289.317
Alkaloid from a tunicate and its predator mollusc *Chelynotus semperi*. Cytotoxic. Yellow needles ($CHCl_3$).
Mp 255-258° dec. λ_{max} 214 (ϵ 18200); 224 (ϵ 19100); 250 (ϵ 15800); 258 (ϵ 15500); 295 (ϵ 6310); 354 (ϵ 5750); 394 (ϵ 4070) (MeOH) (Derep). λ_{max} 208 (ϵ 17200); 226 (ϵ 17780); 292 (ϵ 15000); 382 (ϵ 5150); 430 (MeOH/NaOH) (Berdy). λ_{max} 480 (MeOH/HCl) (Berdy).

Carroll, A.R. *et al., J.O.C.*, 1990, **55**, 4426-4431 (*isol, uv, ir, pmr, cmr, ms, struct*)
Kitahara, Y. *et al., Tetrahedron*, 1997, **53**, 17029-17038 (*synth*)

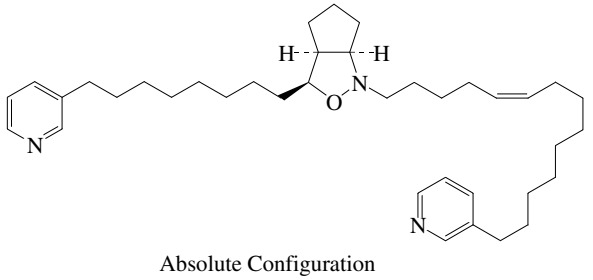
Pyrinadine A P-753



$C_{38}H_{60}N_4O$ 588.918
Alkaloid from *Cribrochalina* sp. (SS-1115). Cytotoxic. Oil.
λ_{max} 213 (ϵ 10600); 251 (ϵ 3600); 257 (ϵ 4200); 262 (ϵ 4700); 269 (ϵ 3700) (MeOH).

Kariya, Y. *et al., Tet. Lett.*, 2006, **47**, 997-998 (*isol, pmr, cmr*)

Pyrinodemin A P-754



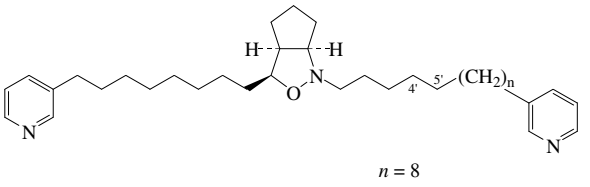
Absolute Configuration

$C_{38}H_{59}N_3O$ 573.904
Isol. from the sponge *Amphimedon* sp. Cytotoxic agent. Oil.
$[\alpha]_D^{25}$ -9 (c, 1 in $CHCl_3$). λ_{max} 264 (ϵ 6300) (MeOH).

Tsuda, M. *et al., Tet. Lett.*, 1999, **40**, 4819-4820 (*isol, uv, ir, pmr, cmr, ms*)
Snider, B.B. *et al., Tet. Lett.*, 2001, **42**, 1639-1642 (*synth*)
Romeril, S.P. *et al., Tet. Lett.*, 2002, **43**, 327-329; 2003, **44**, 7757-7761 (*synth, abs config*)
Mormoto, Y. *et al., Org. Lett.*, 2003, **5**, 2611-2614 (*synth, abs config*)
Ishiyama, H. *et al., Molecules*, 2005, **10**, 312-316 (*synth, struct*)

Pyrinodemin B P-755

[292041-81-7]



n = 8

$C_{37}H_{59}N_3O$ 561.893
Isol. from *Amphimedon* sp. Cytotoxic agent. λ_{max} 264 (ϵ 6000) (MeOH).

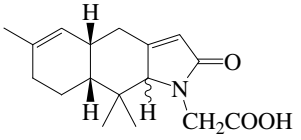
4′,5′-Didehydro(Z-): ***Pyrinodemin C***
[292041-82-8]
$C_{37}H_{57}N_3O$ 559.877
Isol. from *Amphimedon* sp. Cytotoxic agent. λ_{max} 263 (ϵ 5800) (MeOH).

Lower homologue (n = 7): ***Pyrinodemin D***
[292041-83-9]
$C_{36}H_{57}N_3O$ 547.866
Isol. from *Amphimedon* sp. Cytotoxic agent. λ_{max} 264 (ϵ 3300) (MeOH).

Hirano, K. *et al., Chem. Pharm. Bull.*, 2000, **48**, 974-977 (*Pyrinodemins B-D, isol, pmr, cmr, uv*)
Snider, B.B. *et al., Tet. Lett.*, 2001, **42**, 1639-1642 (*synth*)
Romeril, S.P. *et al., Tet. Lett.*, 2003, **44**, 7757-7761 (*config*)

Pyrodysinoic acid P-756

[385801-57-0]



Relative Configuration

$C_{17}H_{23}NO_3$ 289.374
Isol. from a *Dysidea* sp. Pale yellow oil. $[\alpha]_D^{23}$ +9.1 (c, 0.07 in MeOH). λ_{max} 204 (log ϵ 1.46) (MeOH).

Goetz, G.H. *et al., J. Nat. Prod.*, 2001, **64**, 1486-1488 (*isol, pmr, cmr*)

Pyroglutamylglycylargininylphenylalaninamide P-757

H-5-Oxo-Pro-Gly-Arg-Phe-NH_2
$C_{22}H_{32}N_8O_5$ 488.545

L-L-L-L-*form*
Antho-RF amide. CP1. Peptide CP1
[107535-01-3]
Neuropeptide isol. from *Anthopleura elegantissima, Callinectes sapidus* and *Renilla koellikeri*. Neurotransmitter. No phys. props. reported.

Grimmelikhuijzen, C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1986, **83**, 9817 (*isol*)
Grimmelikhuijzen, C. *et al., FEBS Lett.*, 1987, **211**, 105 (*isol*)
Yasuda, A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1993, **104**, 235 (*isol*)

Pyroglutamylglycylleucylargininyltryptophanamide P-758

H-5-Oxo-Pro-Gly-Leu-Arg-Trp-NH_2
$C_{30}H_{44}N_{10}O_6$ 640.741

L-L-L-L-L-*form*
Antho-RW amide II
[118904-15-7]
Neuropeptide isol. from sea anemones.
No phys. props. reported.
Graff, D. *et al., FEBS Lett.*, 1988, **239**, 137 (*isol*)

Pyroglutamylleucylglycylargininylphenylalanina-mide **P-759**
CP2. Peptide CP2
[148297-92-1]
H-5-OxoPro-Leu-Gly-Arg-Phe-NH_2
$C_{28}H_{43}N_9O_6$ 601.704
Isol. from the eyestalks of *Callinectes sapidus*. Similar to Pyroglutamylglycylargininylphenylalaninamide, P-757.
Yasuda, A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1993, **104**, 235 (*isol, struct*)

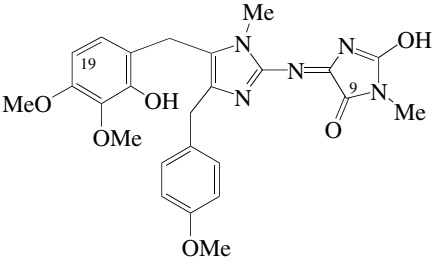
Pyroglutamylserylleucylarginyltryptophanamide **P-760**
H-5-OxoPro-Ser-Leu-Arg-Trp-NH_2
$C_{31}H_{46}N_{10}O_7$ 670.767

L-L-L-L-*form*
Antho-RW amide I
[114056-25-6]
Neuropeptide isol. from sea anemones.
No phys. props. reported.
Graff, D. *et al., Brain Res.*, 1988, **442**, 354 (*isol*)

***Penaeus vannamei* Pyrokinin 1** **P-761**
Pev-Pk 1
[329897-07-6]
H-^{1}Asp-Phe-Ala-Phe-^{5}Ser-Pro-Arg-Leu-NH_2
$C_{45}H_{66}N_{12}O_{11}$ 951.09
Isol. from the CNS of the female white shrimp, *Penaeus vannamei*. Neuropeptide.

5-L-Asparagine analogue, 1-L-alanyl: Penaeus vannamei *Pyrokinin 2. Pev-Pk 2*
[329897-08-7]
$C_{49}H_{72}N_{14}O_{12}$ 1049.194
Isol. from the female of *Penaeus vannamei*. Neuropeptide.
Torfs, P. *et al., Eur. J. Biochem.*, 2001, **268**, 149-154 (*isol, synth, activity*)

Pyronaamidine **P-762**
[124535-77-9]

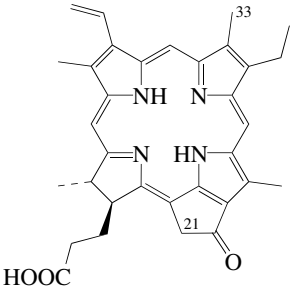


$C_{25}H_{27}N_5O_6$ 493.518
Alkaloid from a Micronesian sponge, *Leucetta* sp. Cytotoxic against KB cells (MIC 5 μg/mL). Yellow feathery cryst.
Mp 185-187°. λ_{max} 208 (ϵ 49000); 224 (ϵ 34700); 276 (ϵ 6030); 388 (ϵ 16600) (MeOH) (Derep).

19-Hydroxy: ***Naamidine E***
[152273-84-2]
$C_{25}H_{27}N_5O_7$ 509.518
Alkaloid from *Leucetta* sp. and *Notodoris gardineri*. Yellow amorph. solid.
Mp 115-118°.

*9-(*N*-Methylimide):* ***Pyronaamidine 9*-N-*methylimide***
[191362-11-5]
$C_{26}H_{30}N_6O_5$ 506.56
Alkaloid from *Leucetta* sp. cf. *chagosensis*. Yellow cryst. (CH_2Cl_2/MeOH).
Mp 222-225°. λ_{max} 211 (5.14); 274 (4.78); 388 (4.96) (MeOH).
Akee, R.K. *et al., J.O.C.*, 1990, **55**, 1944 (*isol, uv, ir, pmr, cmr, ms, struct*)
Carroll, A.R. *et al., Aust. J. Chem.*, 1993, **46**, 1229 (*Naamidine E*)
Plubrukarn, A. *et al., J. Nat. Prod.*, 1997, **60**, 712 (*9-methylimide*)
Nakamura, S. *et al., J.C.S. Perkin 1*, 2002, 1061-1066 (*synth, pmr*)

Pyrophaeophorbide a **P-763**
9-Ethenyl-14-ethyl-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoic acid, 9CI. Pyropheophorbide a
[24533-72-0]



$C_{33}H_{34}N_4O_3$ 534.657
Formed on mild hydrol. and decarboxylation of Phaeophorbide a, P-295. Isol. from *Ruditapes philippinarum*., leaves of *Atalantia monophylla*, alga *Pterocladia tennis*, tunicate *Trididemnum solidum* and other sources incl. tea and aquatic sediments. Shows antiviral and antitumour props. Antioxidant. Cryst. (Et_2O).
Mp 210°. $[\alpha]_D^{20}$ -342 (c, 1.12 in Me_2CO) (white light). λ_{max} 410; 509; 538; 608; 667 (MeOH). λ_{max} 273; 324; 410; 508; 539; 609; 666 (MeOH) (Berdy).

Me ester: [6453-67-4]
$C_{34}H_{36}N_4O_3$ 548.683
Constit. of *Atalantia monophylla*. Dark blue needles (Et_2O).
Mp 220-225° (217-219°). $[\alpha]_D^{20}$ -388 (c, 1.39 in Me_2CO) (white light). λ_{max} 409; 507; 538; 608; 665 (MeOH).

*3,7*R*,5,11*R*-Tetramethyl-2*E*-hexadecenyl ester:* ***Pyropheophytin a***
[14409-87-1]
$C_{53}H_{72}N_4O_3$ 813.177
Isol. from various plants including the alga *Eisenia bicyclis*, *Euglena gracilis* and from the tunicate *Trididemnum solidum*. Antioxidant.
Dark green oil. λ_{max} 415; 510; 540; 611; 668 ($CHCl_3$).

33-Oxo: Pyrophaeophorbide b. Pyropheophorbide b
[82040-65-1]
$C_{33}H_{32}N_4O_4$ 548.64
Cryst. (CH_2Cl_2) (as Me ester). Mp 245-246° (Me ester).

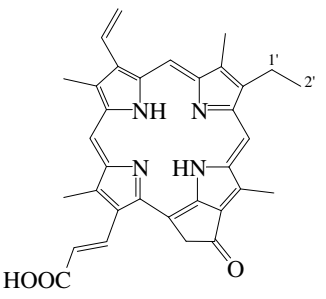
*33-Oxo, 3,7*R*,5,11*R*-tetramethyl-2*E*-hexadecenyl ester:* ***Pyropheophytin b***
[77331-75-0]
$C_{53}H_{70}N_4O_4$ 827.16
Constit. of various plants incl. spinach.

[25145-41-9]

Fischer, H. *et al., Die Chemie des Pyrrols*, Akademische Verlag, Leipzig, Vol. II, (ii), 1940, 73-75 (*rev*)
Pennington, F.C. *et al., J.A.C.S.*, 1964, **86**, 1418-1426 (*synth*)
Smith, K.M. *et al., Tetrahedron*, 1975, **31**, 367-375 (*cmr*)
Kenner, G.W. *et al., J.C.S. Perkin 1*, 1978, 845-852 (*synth*)
Wasielewski, M.R. *et al., J.O.C.*, 1980, **45**, 1969-1974 (*synth, uv, pmr*)
Smith, K.M. *et al., J.A.C.S.*, 1985, **107**, 4946-4954; 1988, **110**, 2854-2861 (*synth, uv, pmr*)
Risch, N. *et al., Annalen*, 1988, 343-347 (*synth, uv*)
Cahyana, A.H. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1533-1535 (*Pyropheophytin A*)
Watanabe, N. *et al., J. Nat. Prod.*, 1993, **56**, 305-317 (*isol*)
Chansakaow, S. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1415-1417 (*isol, uv, ir, pmr, cmr, cd*)

Pyrophaeoporphyrin c_1 P-764

Pyropheoporphyrin c_1
[207397-30-6]

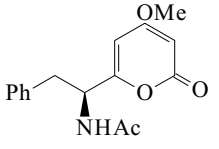


$C_{33}H_{30}N_4O_3$ 530.625
Occurs in the sediment of a small eutrophic lake and in the products from feeding the diatom *Thalassiosira weissflogii* to the copepod *Calanus helgolandicus*.

1′,2′-Didehydro: ***Pyrophaeoporphyrin c_2***. *Pyropheoporphyrin c_2*
[207397-31-7]
$C_{33}H_{28}N_4O_3$ 528.609
Occurs in the sediment of a small eutrophic lake and in the products from feeding the diatom *Thalassiosira weissflogii* to the copepod *Calanus helgolandicus*.
Harradine, P.J. *et al., Org. Geochem.*, 1998, **28**, 111-117 (*isol*)

Pyrophen P-765

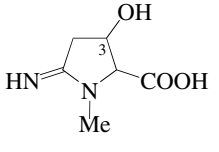
N-*[1-(4-Methoxy-2-oxo-2*H*-pyran-6-yl)-2-phenylethyl]acetamide, 9CI. 6-(1-(Acetylamino)-2-phenylethyl)-4-methoxy-2*H*-pyran-2-one*
[131190-56-2]



$C_{16}H_{17}NO_4$ 287.315
Prod. by *Aspergillus niger*.
Barnes, C.L. *et al., Int. J. Pept. Protein Res.*, 1990, **36**, 292-296 (*isol, cryst struct*)
Varoglu, M. *et al., J. Nat. Prod.*, 2000, **63**, 41-43 (*isol, pmr, cmr*)

Pyrostatin A P-766

3-Hydroxy-5-imino-1-methylproline, 9CI. 3-Hydroxy-5-imino-1-methyl-2-pyrrolidinecarboxylic acid
[162763-50-0]

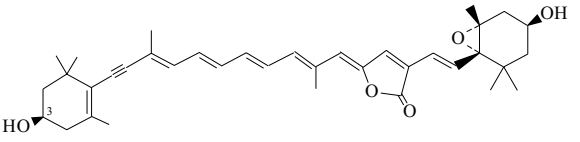


$C_6H_{10}N_2O_3$ 158.157
Prod. by *Streptomyces* sp. SA-3501. Inhibitor of *N*-acetyl-β-D-glucosaminidase. Powder. $[\alpha]_D$ +125.4 (H_2O). λ_{max} 200 (H_2O).

3-Deoxy: 5-Imino-1-methylproline, 9CI. 5-Imino-1-methyl-2-pyrrolidinecarboxylic acid. ***Pyrostatin B***
[162763-51-1]
$C_6H_{10}N_2O_2$ 142.157
From *Streptomyces* sp. SA-3501. Inhibitor of *N*-acetyl-β-D-glucosaminidase. Powder. $[\alpha]_D$ +98.4 (H_2O).
Aoyami, T. *et al., J. Enzyme Inhib.*, 1995, **8**, 223-232

Pyrrhoxanthinol P-767

[54369-11-8]

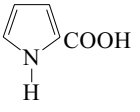


$C_{37}H_{46}O_5$ 570.767
Constit. of the Dinophyceae and *Mytilus edulis*. Oil.

3-Ac: ***Pyrrhoxanthin***
[54369-13-0]
$C_{39}H_{48}O_6$ 612.805
Constit. of the Dinophyceae. Oil. λ_{max} 466 (EtOH). λ_{max} 487 (hexane).
Johansen, J.E. *et al., Phytochemistry*, 1974, **13**, 2261 (*isol*)
Fiksdahl, A. *et al., Biochem. Syst. Ecol.*, 1979, **7**, 173 (*isol*)
Skjenstad, T. *et al., Biochem. Syst. Ecol.*, 1984, **12**, 149 (*Pyrrhoxanthin, isol, pmr, cmr*)
Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495 (*isol, pmr, uv, ms*)
Ito, M. *et al., J.C.S. Perkin 1*, 1990, 197 (*Pyrrhoxanthin, synth*)
Aakermann, T. *et al., Phytochemistry*, 1992, **31**, 1779 (*isol, synth, abs config*)
Yamano, Y. *et al., J.C.S. Perkin 1*, 1993, 1599 (*Pyrrhoxanthin, synth*)
Vaz, B. *et al., J.O.C.*, 2006, **71**, 5914-5920 (*synth*)

1*H*-Pyrrole-2-carboxylic acid, 9CI P-768

Minaline
[634-97-9]



$C_5H_5NO_2$ 111.1
Occurs in various microorganisms, e.g. *Streptomyces griseoflavus*. Imino-acid occurring in diastase, prob. resulting from dehydration of hydroxyprolines. Esters possess local anaesthetic props. Protein racemase inhibitor. Platelet aggregation inhibitor. Leaflets (H_2O). Sol. H_2O, EtOH, Et_2O.
Mp 208.5° dec. pK_{a1} 1.48; pK_{a2} 4.5 (25°). Decarboxylates at Mp. Isoelectric point 2.9. λ_{max} 263 (MeOH) (Berdy).

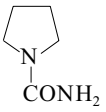
Me ester: [1193-62-0]
$C_6H_7NO_2$ 125.127
Isol. from an *Agelas* sp. Needles (petrol). Sol. EtOH, Et_2O.
Mp 73°. Bp_{740} 220-223° Bp_{14} 115-120° (lit. gives a pressure range).

*Amide: 1*H*-Pyrrole-2-carboxamide*
[4551-72-8]
$C_5H_6N_2O$ 110.115
Alkaloid from the sponge *Agelas oroides*. Plates (H_2O or EtOH). Mp 176°. Sweet taste. λ_{max} 262 (ε 3700) (MeOH) (Berdy).

N-*Formylamide:* N-*Formyl-1*H*-pyrrole-2-carboxamide, 9CI*
[160156-23-0]
$C_6H_6N_2O_2$ 138.126
Alkaloid from the sponge *Agelas oroides*. Powder. λ_{max} 284 (ε 8140) (MeOH).
Barnett, G.H. *et al., Can. J. Chem.*, 1980, **58**, 409 (*amide, nitrile*)
Koenig, G.M. *et al., Nat. Prod. Lett.*, 1994, **5**, 141-146 (*isol, amides*)
Assman, M. *et al., Marine Ecol.: Progr. Ser.*, 2000, **207**, 255-262 (*Agelas constit*)

1-Pyrrolidinecarboxamide, 9CI P-769

N-*Carbamoylpyrrolidine. 1-(Aminocarbonyl)pyrrolidine*
[4736-71-4]

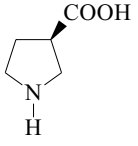


$C_5H_{10}N_2O$ 114.147
Metab. of the Mediterranean sponge *Aplysina (Verongia) cavernicola*. Cryst. (H_2O).
Mp 148-152° (nat.) Mp 218° (synth.).

Reppe, W. *et al., Annalen*, 1955, **596**, 80 (*synth*)
D'Ambrosio, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **83**, 309 (*isol, ir, pmr, cmr, ms*)

3-Pyrrolidinecarboxylic acid P-770

β-Proline
[59378-87-9]



(R)–form

$C_5H_9NO_2$ 115.132

N-*Me:* ***Achyranthine***
$C_6H_{11}NO_2$ 129.158
Alkaloid from *Achyranthes aspera*. Vasodilator, diuretic, purgative, antihypertensive agent. Monohydrate.
Mp 292-293° dec. $[\alpha]_D^{25}$ -6.5. Log P -2.23 (calc). Struct. proof not convincing. Abs. config. not detd.

N-*Me; hydroiodide:* Mp 204-205°.

Dimethylbetaine: 3-Carboxy-1,1-dimethylpyrrolidinium hydroxide inner salt, 9CI. ***β-Stachydrine***
[86849-51-6]
$C_7H_{13}NO_2$ 143.185
Alkaloid from the marine red alga *Griffithsia flosculosa*.
Mp 238°. Natural β-Stachydrine was characterised as the hydrochloride. The Mp given here is for semisynthetic material obt. by methylation of Achyranthine. Abs. config. not detd.

Dimethylbetaine; hydrochloride: Mp 236-238° dec. $[\alpha]_D^{23}$ -5.5 (c ,0.27 in MeOH). Deriv. of β-Stachydrine.

Dimethylbetaine; hydroiodide: Mp 267°. Derived from Achyranthine.

(*R*)-*form* [72580-54-2]
Synthetic.
Cryst. (EtOH). Mp 188-190°. $[\alpha]_D^{25}$ -18.9 (c, 2.0 in H_2O).

(*S*)-*form* [72580-53-1]
Mp 186-188.5°. $[\alpha]_D^{25}$ +19.1 (c, 2 in H_2O). Struct. incorr. drawn by Flešet *al* (1964).

Me ester:
$C_6H_{11}NO_2$ 129.158
Volatile oil. $[\alpha]_D^{23}$ +7.2 (c, 1.0 in $CHCl_3$).

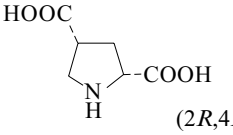
(±)-*form* [68464-02-8]
Plates. Mp 186°.

Et ester: [72925-15-6]
$C_7H_{13}NO_2$ 143.185
Bp_4 70-74°.

Basu, N.K. *et al., J. Proc. Inst. Chem. (India)*, 1957, **29**, 55; 73 (*Achyranthine*)
Miyamoto, M. *et al., Yakugaku Zasshi*, 1957, **77**, 568; *CA*, **51**, 16422h (*synth*)
Fleš, D. *et al., Croat. Chem. Acta*, 1964, **36**, 27-32; *CA*, **61**, 10644b (*S-form, synth, abs config.*)
Yuki, H. *et al., J. Polym. Sci., Polym. Chem. Ed.*, 1979, **17**, 3867-3878, (*R-form, synth, resoln, pmr*)
Blunden, G. *et al., Phytochemistry*, 1983, **22**, 293 (*β-Stachydrine*)
Mazzini, C. *et al., J.O.C.*, 1997, **62**, 5215-5218 (*R-form, S-form, synth, pmr, cmr*)
Thomas, C. *et al., Synthesis*, 1998, 1491-1496 (*R-form, S-form, synth, ir, pmr*)

2,4-Pyrrolidinedicarboxylic acid P-771

4-Carboxyproline



(2R,4R)–form

$C_6H_9NO_4$ 159.141

(2*R*,4*R*)-*form*
D-cis-*form*
[130830-78-3]
Prisms. Mp 224-225°. $[\alpha]_D^{21}$ +41.5 (c, 1.01 in H_2O) (+37).

N-*Benzoyl:* [188345-79-1]
$C_{13}H_{13}NO_5$ 263.249
Mp 164-165°. $[\alpha]_D^{20}$ +82 (c, 1.04 in EtOH).

(2*R*,4*S*)-*form*
D-trans-*form*
[130830-77-2]
Prisms. Mp 219-220°. $[\alpha]_D^{25}$ +51 (c, 1.04 in H_2O).

(2*S*,4*R*)-*form*
L-trans-*form*
[64769-66-0]
Constit. of the Mediterranean red algae *Chondria coerulescens, Chondria dasiphylla* and *Ceramium rubrum*; found in the seeds of *Afzelia bella* (Leguminosae).
Cryst. (MeOH aq.).
Mp 223-225°. $[\alpha]_D$ -54 (c, 1.04 in H_2O).

4-Me ester:
$C_7H_{11}NO_4$ 173.168
No phys. props. reported. $[\alpha]_D$ -11 (c, 1.5 in $CHCl_3$).

N-*Benzyl:* [627100-87-2]
$C_{13}H_{15}NO_4$ 249.266
Mp 60-62° (as hydrochloride). $[\alpha]_D^{20}$ +29.4 (c, 0.78 in MeOH) (hydrochloride). CAS no. refers to the hydrochloride.

2-Et ester, 4-nitrile, N-*benzyl:* [627100-83-8]
$C_{15}H_{18}N_2O_2$ 258.319
Oil. $[\alpha]_D^{20}$ +64.8 (c, 1 in $CHCl_3$).

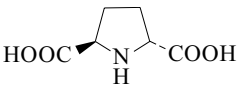
(2*S*,4*S*)-*form*
L-cis-*form*
[64927-38-4]
Prisms (EtOH aq./Me_2CO). Mp 225-256°. $[\alpha]_D^{25}$ -40 (c, 1.02 in H_2O).

(2*RS*,4*RS*)-*form*
(±)-cis-*form*
[136033-11-9]
Prisms (EtOH). Mp 226-230°.

Impellizzeri, G. *et al., Phytochemistry*, 1977, **16**, 1601-1602 (*isol, pmr, ms, struct*)
Dupont, L. *et al., Acta Cryst. B*, 1978, **34**, 850-854 (*cryst struct*)
Welter, A. *et al., Phytochemistry*, 1978, **17**, 131-134 (*isol, ir, pmr, cmr, ms, cd, struct*)
Bridges, R.J. *et al., J. Med. Chem.*, 1991, **34**, 717-725 (*synth, pmr, cmr, ir*)
Arakawa, Y. *et al., Chem. Pharm. Bull.*, 1997, **45**, 255-259 (*2R,3R-form, 2S,3S-form, 2RS,3RS-form, synth, pmr, cmr*)
Wang, Q. *et al., Tetrahedron*, 1998, **54**, 15759-15780 (*2S,4R-form, synth, ir, nmr, 4-Me ester*)
Heindl, C. *et al., Tetrahedron: Asymmetry*, 2003, **14**, 3141-3152 (*2S,4R-form, benzyl derivs*)

2,5-Pyrrolidinedicarboxylic acid P-772

[72000-65-8]



(2*R*,5*R*)–*form*

$C_6H_9NO_4$ 159.141

(2*R*,5*R*)-*form*

(+)-trans-*form*
[93713-35-0]
Used in synth. of chiral auxiliaries.
Cryst. Mp 274°. $[\alpha]_D^{25}$ +106 (c, 1.02 in H_2O).

Di-Me ester: [115413-67-7]
$C_8H_{13}NO_4$ 187.195
Oil. $Bp_{0.1}$ 100-103°. $[\alpha]_D^{20}$ +47.2 (c, 1.2 in $CHCl_3$).

N-*Benzyl:*
$C_{13}H_{15}NO_4$ 249.266
Cryst. (H_2O). Mp 239°. $[\alpha]_D^{25}$ +93 (c, 1.00 in H_2O).

N-*Me, di-Me ester:*
$C_9H_{15}NO_4$ 201.222
Oil. $[\alpha]_D^{20}$ +100.3 (c, 1.0 in $CHCl_3$).

(2*S*,5*S*)-*form*

(-)-trans-*form*
[81702-31-0]
Reported from red algae *Schizymenia dubyi* and/or *Haematocelis rubens*.
Mp 272-277°. $[\alpha]_D^{20}$ -108 (c, 1 in H_2O).

Di-Me ester: [111071-93-3]
Oil. $Bp_{0.1}$ 100-103°. $[\alpha]_D^{20}$ -47 (c, 1.3 in $CHCl_3$).

(2*RS*,5*SR*)-*form*

(±)-cis-*form*

Di-Et ester: [90514-00-4]
$C_{10}H_{17}NO_4$ 215.249
Bp_2 127-130°.

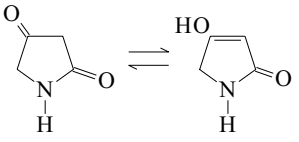
N-*Benzyl, di-Et ester:* [52321-06-9]
$C_{17}H_{23}NO_4$ 305.373
Liq. Bp_2 170-174°.

[35634-41-4, 49653-02-3, 97275-65-5, 97275-67-7]

Impellizzeri, G. *et al., Phytochemistry*, 1975, **14**, 1549-1557 (*2S,5S-form, isol, ir, pmr, ms, struct*)
Kawanami, Y. *et al., Tet. Lett.*, 1984, **25**, 857-860 (*synth, use*)
Yamamoto, Y. *et al., Synthesis*, 1993, 298 (*synth, pmr, cmr*)
Sasaki, N.A. *et al., Tetrahedron*, 1994, **50**, 7093-7108 (*synth, cmr*)
Collado, I. *et al., J.O.C.*, 1995, **60**, 5011-5015 (*pmr, cmr*)
Shi, M. *et al., J.C.S. Perkin 1*, 1998, 2547-2552 (*N-Me, di-Me ester*)
Fraenkel, G. *et al., J.A.C.S.*, 1999, **121**, 432-443 (*cis-form, di-Et ester*)
Sunilkumar, G. *et al., Synthesis*, 2003, 2304-2306 (*2S,5S-form, synth, pmr, cmr*)

2,4-Pyrrolidinedione, 9CI P-773

*1,5-Dihydro-4-hydroxy-2*H*-pyrrol-2-one. Tetramic acid*
[37772-90-0]



$C_4H_5NO_2$ 99.089
Pale yellow solid. Mp 360°.

N-*Ac:* [182352-40-5]
$C_6H_7NO_3$ 141.126
Cryst. solid (MeOH). Mp 165-168°.

N-*Benzoyl:* [68661-20-1]
$C_{11}H_9NO_3$ 203.197
Solid. Mp 180° dec.

N-*Ethoxycarbonyl:*
$C_7H_9NO_4$ 171.152
Solid. Mp 105-108° (96-102°).

N-tert-*Butyloxycarbonyl:*
$C_9H_{13}NO_4$ 199.206
Cryst. solid (EtOAc). Mp 130-132° dec.

N-*Benzyloxycarbonyl:*
$C_{12}H_{11}NO_4$ 233.223
Cryst. solid. Mp 151-153° dec.

Enol-form

*Me ether: 1,5-Dihydro-4-methoxy-2*H*-pyrrol-2-one, 9CI*
[69778-83-2]
$C_5H_7NO_2$ 113.116
Constit. of the marine cyanophyte *Lyngbya majuscula*. Hydrol. prod. of Malyngamide A, M-57. Needles (C_6H_6).
Mp 128-129°.

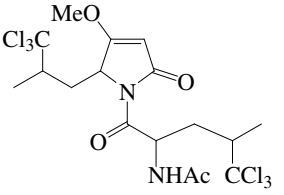
Me ether, N-*Ac: 1-Acetyl-1,5-dihydro-4-methoxy-2*H*-pyrrol-2-one*
$C_7H_9NO_3$ 155.153
Minor constit. of *Lyngbya majuscula*.
Mp 89-90°.

*Benzyl ether: 4-Benzyloxy-1,5-dihydro-2*H*-pyrrol-2-one*
[113896-95-0]
$C_{11}H_{11}NO_2$ 189.213
Mp 150-153°.

N^1*,4-Di-Me: 1,5-Dihydro-4-methoxy-1-methyl-2*H*-pyrrol-2-one, 9CI*
[90968-33-5]
$C_6H_9NO_2$ 127.143
Prisms (C_6H_6/hexane). Mp 86-87°.

Cram, D.J. *et al., J.A.C.S.*, 1963, **85**, 1430 (*deriv, synth*)
Mulholland, T.P.C. *et al., J.C.S. Perkin 1*, 1972, 2121 (*synth*)
Lowe, G. *et al., J.C.S. Perkin 1*, 1973, 2907 (*synth, nmr*)
Cardellina, J.H. *et al., J.A.C.S.*, 1979, **101**, 240 (*occur, derivs*)
Kochhar, K.S. *et al., Tet. Lett.*, 1984, **25**, 1871 (*synth*)
Gill, G.B. *et al., J.C.S. Perkin 1*, 1993, 2567 (*deriv, synth, ir, pmr, cmr*)
James, G.D. *et al., J.C.S. Perkin 1*, 1993, 2581 (*deriv, synth, ir, pmr, cmr*)
Hamilakis, S. *et al., J. Het. Chem.*, 1996, **33**, 825 (*acyl derivs*)
Parsons, A.F. *et al., Tet. Lett.*, 1996, **37**, 1667 (*benzyl ether, synth*)
Lu, Z. *et al., Bioorg. Med. Chem. Lett.*, 2003, **13**, 2505-2507 (*synth*)

Asteronotus cespitosus Pyrrolidone P-774

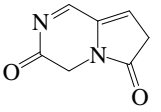


$C_{17}H_{22}Cl_6N_2O_4$ 531.088
Related to Dysideapyrrolidone, D-1277. Alkaloid from the dorid nudibranch *Asteronotus cespitosus*.
$[\alpha]_D$ +4.8 (c, 0.0004 in $CHCl_3$).

Fahey, S.J. *et al., J. Chem. Ecol.*, 2002, **28**, 1773-1785 (*isol, pmr, cmr*)

Pyrrolo[1,2-*a*]pyrazine-3,6(4*H*,7*H*)-dione, 9CI P-775

[870136-68-8]



$C_7H_6N_2O_2$ 150.137
Prod. by a marine-derived *Bacillus* sp.

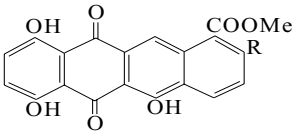
Zhang, H.-L. *et al., Zhongguo Yaowu Huaxue Zazhi*, 2003, **13**, 294-296; *CA*, **144**, 2926x (*isol*)

Pyrromycin P-776

Aclacinomycin T_2. Ciclamycin 6. 1-Hydroxyaklavine. MA 144T2. Antibiotic MA 144T2

[668-17-7]

As η_1-Pyrromycinone, P-777 with



R = CH_2CH_3

$C_{30}H_{35}NO_{11}$ 585.607

Anthracycline antibiotic. Prod. by *Streptomyces* sp. DOA 1205 and *Streptomyces capoamus*. Active against gram-positive bacteria. Bright red cryst. (as hydrochloride). Sol. MeOH, C_6H_6, acids, bases; poorly sol. H_2O, hexane.

Mp 162-165° (hydrochloride). $[\alpha]_D$ +132 (MeOH). λ_{max} 234 (ϵ 43100); 257 (ϵ 18100); 293 (ϵ 7250); 495 (ϵ 10600); 525 (ϵ 8400) (EtOH). λ_{max} 288; 297; 498; 518; 533 ($CHCl_3$) (Berdy).

▶ QI9279200

7-Epimer: ***ϵ-Pyrromycin***. *R 578A. Antibiotic R 578A*

[91050-37-2]

$C_{30}H_{35}NO_{11}$ 585.607

Prod. by a *Streptomyces* sp. Red cryst. Sol. MeOH, $CHCl_3$, acids; poorly sol. H_2O, hexane. λ_{max} 234; 258; 290; 470; 485; 496 (MeOH). λ_{max} 498; 519; 534 (cyclohexane).

9-Epimer:

$C_{30}H_{35}NO_{11}$ 585.607

Prod. by a marine-derived *Streptomyces* sp. (CANU Fox 21-2-6a). Cytotoxic. Deep red solid. $[\alpha]_D^{20}$ +128 (c, 0.25 in MeOH). λ_{max} 202; 234; 258; 290; 492 (MeOH).

7,9-Diepimer:

$C_{30}H_{35}NO_{11}$ 585.607

Prod. by a marine-derived *Streptomyces* sp. (CANU Fox 21-2-6a). Cytotoxic. Deep red solid. $[\alpha]_D^{20}$ +224 (c, 0.12 in MeOH).

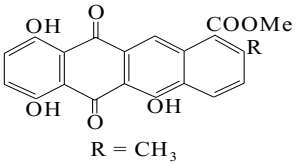
1-Deoxy: See Aklavine in *The Combined Chemical Dictionary.*

Brockmann, H. *et al., Chem. Ber.*, 1959, **92**, 1904 (*isol, uv*)
Keller-Schierlein, W. *et al., Antimicrob. Agents Chemother.*, 1970, 68 (*struct*)
Doyle, T.W. *et al., J.A.C.S.*, 1979, **101**, 7041 (*cmr*)
Qi, C. *et al., CA*, 1984, **101**, 53217 (ϵ-*Pyrromycin*)
Bieber, L.W. *et al., J. Antibiot.*, 1987, **40**, 1335
Phipps, R.K. *et al., ARKIVOC*, 2004, **x**, 94-100 (*marine, epimers*)

η_1-Pyrromycinone P-777

Methyl 6,11-dihydro-5,7,10-trihydroxy-2-methyl-6,11-dioxo-naphthacene-1-carboxylate, 8CI

[19383-86-9]



R = CH_3

$C_{21}H_{14}O_7$ 378.337

Anthracyclinone pigment from *Streptomyces* spp. Orange cryst. (C_6H_6/hexane or dioxan aq.). Spar. sol. org. solvs. Mp 290-292°.

Tri-Ac: [19383-87-0]

Yellow. Mp 224-226°.

Tri-Me ether: Mp 254-265°.

Parent acid: Bisanhydronogalamycinonecarboxylic acid

[19574-30-2] Degradn. prod. of Nogalamycin. Mp 328-330°.

Parent acid, tri-Ac: [19383-88-1]

Yellow cryst. Mp 197-198°.

10-Deoxy: ***Resomycin C***. *Methyl 6,11-dihydro-5,7-dihydroxy-2-methyl-6,11-dioxo-1-naphthacenecarboxylate*

$C_{21}H_{14}O_6$ 362.338

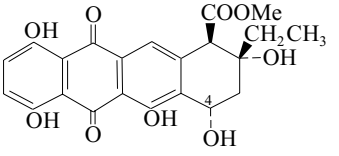
Anthracyclinone antibiotic. Prod. by *Streptomyces* sp. GW71/2497. Orange solid. λ_{max} 245 (log ϵ 4.27); 263 (log ϵ 4.36); 292 (log ϵ 4.07); 451 (log ϵ 3.97) ($CHCl_3$).

Hegyi, J.R. *et al., Tet. Lett.*, 1968, 1587 (*isol, struct, uv, pmr*)
Wiley, P.F. *et al., J.A.C.S.*, 1977, **99**, 542
Maskey, R.P. *et al., J. Antibiot.*, 2003, **56**, 795-800 (*Resomycin C*)

ϵ-Pyrromycinone P-778

Rutilantinone. Rutilantone. MA 144D_2. Antibiotic MA 144D_2

[21288-61-9]



$C_{22}H_{20}O_9$ 428.395

Anthraquinone antibiotic. Pigment from *Streptomyces* spp. Shows some anticoccidial activity. Metab. of Aclacinomycin, Musettamycin and Marcellomycin. Orange-red needles.

Mp 213-214°. $[\alpha]_{Hg}^{20}$ +143 (c, 1.0 in $CHCl_3$). pK_a 9.9. λ_{max} 234 (ϵ 42660); 257 (ϵ 18200); 293 (ϵ 7240); 494 (ϵ 10470); 525 (ϵ 8310) (MeOH) (Berdy). λ_{max} 498; 518; 533 (cyclohexane) (Berdy).

▶ QI9289000

Tetra-Ac:

Yellow cryst. Mp 219-221° (250°). $[\alpha]_D^{20}$ -10.3 (c, 1.0 in $CHCl_3$).

4-Deoxy: ***Galirubinone C***. *ζ-Pyrromycinone. Ryemycin A_1. Tavromycetin component II. MA 144C_2. Antibiotic MA 144C_2*

[21179-18-0]

$C_{22}H_{20}O_8$ 412.395

Prod. by many *Streptomyces* spp. Orange-red needles (EtOH). Mp 224-226° dec. $[\alpha]_D^{24}$ +121.5. $[\alpha]_D^{20}$ +74 (c, 1.0 in $CHCl_3$) (cadmium light). Forms fluorescent solns. Subl. *in vacuo.*

4-Deoxy, tetra-Ac:

Yellow cryst. Mp 195-196°. $[\alpha]_D$ +15 ($CHCl_3$).

10-Deoxy: See Aklavinone in *The Combined Chemical Dictionary.*

Brockmann, H. *et al., Chem. Ber.*, 1959, **92**, 1880-1903 (*isol, 4-deoxy, struct, uv*)
Eckardt, K. *et al., Chem. Ber.*, 1967, **100**, 2561-2568 (*isol, 4-deoxy*)
Brockmann, H. *et al., Tet. Lett.*, 1968, 4719-4724 (*abs config*)
Kralovcova, E. *et al., Coll. Czech. Chem. Comm.*, 1980, **45**, 2558-2565 (*isol, uv, nmr, struct*)
Hauser, F.M. *et al., J.A.C.S.*, 1984, **106**, 1098-1104 (*synth*)
Krohn, K. *et al., Tetrahedron*, 1984, **40**, 3677-3694 (*synth*)
Dodion, P. *et al., Cancer Chemother. Pharmacol.*, 1985, **15**, 153-160 (*metab*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)

η-Pyrromycinone P-779

6,11-Dihydro-2-ethyl-5,7,10-trihydroxy-6,11-dioxonaphthacene-1-carboxylic acid, methyl ester, 8CI. Bisanhydrorutilantinone. Ciclacidine. Cyclacidin. Galirubinone B_2

[749-18-8]

As η_1-Pyrromycinone, P-777 with R=CH_2CH_3

$C_{22}H_{16}O_7$ 392.364

Metab. of *Streptomyces* spp., incl. marine *Streptomyces* sp. B8904. Aclacinomycin metab. Red needles (C_6H_6 or $CHCl_3$).

Mp 242°.

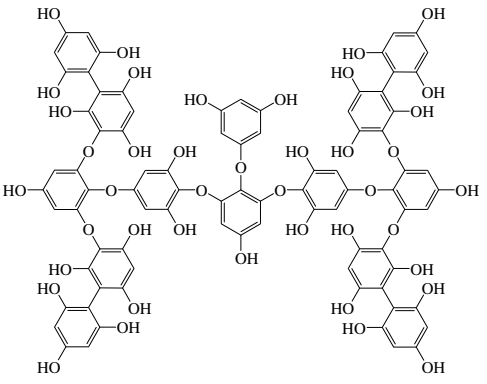
▶ QJ1956730

Tri-Ac: [20465-90-1]

Yellow cryst. (MeOH). Mp 212-213°.

Eckardt, K. *et al., Chem. Ber.*, 1967, **100**, 2561-2568 (*isol*)
Goncalves da Lima, O. *et al., Tet. Lett.*, 1968, 471 (*isol, pmr, uv, bibl*)
Nikitina, N.A. *et al., CA*, 1982, **100**, 144866 (*isol, purifn*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)

Quaterfucononaphlorethol Q-1



$C_{84}H_{58}O_{42}$ 1739.357

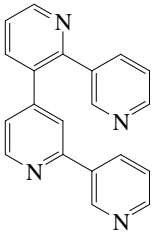
Isol. from brown alga *Carpophyllum maschalocarpum.*

Glombitza, K.W. *et al., Phytochemistry*, 1991, **30**, 3423-3427 (*isol, pmr, ms*)

3,2′:3′,4″:2″,3‴-Quaterpyridine, 9CI Q-2

Nemertelline

[59697-14-2]

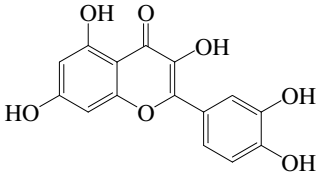


$C_{20}H_{14}N_4$ 310.357

Struct. revised in 1995. Alkaloid from the marine hoplonomertine *Amphiporus angulatus.* Neurotoxin. Cryst. (Et_2O).
Mp 154-156°.

Kem, W.R. *et al., Experientia*, 1976, **32**, 684-686 (*isol*)
Cruskie, M.P. *et al., J.O.C.*, 1995, **60**, 7491-7495 (*synth, pmr, cmr, cryst struct*)
Zoltewicz, J.A. *et al., Tetrahedron*, 1995, **51**, 11401-11410 (*synth*)
Bouillon, A. *et al., J.O.C.*, 2003, **68**, 10178-10180 (*synth, pmr, cmr*)

Quercetin 3-glycosides Q-3



Glycosides of 3,3′,4′,5,7-Pentahydroxyflavone substituted at O^3 only.

Monosaccharides

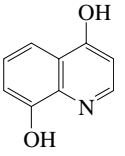
3-O-α-L-Fucopyranoside: Quercetin 3-α-L-fucopyranoside.
Acanthophorin B
[200860-89-5]
$C_{21}H_{20}O_{11}$ 448.382
Isol. from the red alga *Acanthophora spicifera*. Yellow solid ($MeOH/CHCl_3$).
Mp 180-182°. $[\alpha]_D$ -175 (c, 0.35 in MeOH). λ_{max} 257 (log ϵ 4.23); 349 (log ϵ 3.89) (MeOH).

Zeng, L.-M. *et al., Chin. J. Chem.*, 2001, **19**, 1097-1100 (*Acanthophorin B*)

4,8-Quinolinediol Q-4

8-Hydroxy-4(1H)-quinolinone, 9CI. 4,8-Dihydroxyquinoline

[53846-46-1]



$C_9H_7NO_2$ 161.16

Alkaloid from octopus ink (*Octopus dofleini martini*) and the urine of silkworm pupae. Cryst. (CH_2Cl_2).
Mp 305-308° dec.

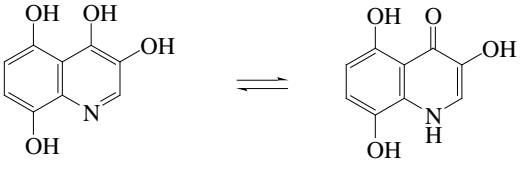
Hydrochloride:
Needles + ½H_2O (Me_2CO/EtOH). Mp 295-298° dec.

Inagami, K. *et al., CA*, 1956, **50**, 8077a (*isol*)
Matsuura, Y. *et al., CA*, 1959, **53**, 8373b (*synth*)
Siuda, J.F. *et al., J. Nat. Prod.*, 1974, **37**, 501-503 (*isol, synth, pmr*)
Grandjean, D. *et al., Bull. Soc. Chim. Fr.*, 1989, 657-660 (*synth, pmr*)

3,4,5,8-Quinolinetetrol Q-5

3,5,8-Trihydroxy-4(1H)-quinolinone, 9CI. 3,4,5,8-Tetrahydroxyquinoline. ***Uranidine***

[92264-09-0]



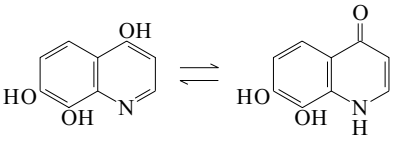
$C_9H_7NO_4$ 193.159

Yellow zoochrome of the sponge *Verongia aerophoba*. Also from *Tylodina perversa*. HIV reverse transcriptase (HIV-rt) inhibitor. Very unstable; rapidly turns blue, then purple, and finally black on exposure to air. λ_{max} 240 (ϵ 15000); 321 (ϵ 2600); 368 (ϵ 2900) (pH 1 H_2O) (Derep). λ_{max} 236 (ϵ 14700); 315 (ϵ 2900); 604 (ϵ 3000); 641 (ϵ 3100) (pH 13 H_2O) (Derep). λ_{max} 239 (ϵ 15000); 319 (ϵ 2600); 365 (ϵ 2900) (H_2O pH 7) (Derep).

Cimino, G. *et al., Tet. Lett.*, 1984, **25**, 2925-2928 (*isol, uv, pmr, cmr*)
Loya, S. *et al., Arch. Biochem. Biophys.*, 1994, **309**, 315-322 (*activity*)

4,7,8-Quinolinetriol Q-6

4,7,8-Trihydroxyquinoline. 7,8-Dihydroxy-4(1H)-quinolinone



$C_9H_7NO_3$ 177.159

8-Me ether: 4,7-Dihydroxy-8-methoxyquinoline. 8-Methoxy-4,7-quinolinediol. 7-Hydroxy-8-methoxy-4(1H)-quinolinone
[98267-21-1]
$C_{10}H_9NO_3$ 191.186
Isol. from the soft corals *Sinularia polydactyla* and *Sinularia microclavate.* Cardiovascular agent.

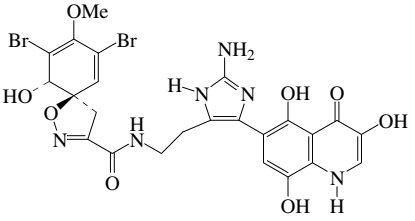
7,8-Di-Me ether: 4-Hydroxy-7,8-dimethoxyquinoline. 7,8-Dimethoxy-4(1H)-quinolinone. 7,8-Dimethoxy-4-quinolinol
[99878-76-9]
$C_{11}H_{11}NO_3$ 205.213
Cryst. (EtOAc/MeOH). Mp 187-190°.

[108915-16-8]

Long, K. *et al., CA*, 1985, **103**, 128867; 1990, **112**, 118619; 1991, **115**, 71358 (*synth, isol, pharmacol*)

Kelly, T.R. *et al., Tetrahedron*, 1985, **41**, 3033 (*deriv*)
Huang, S. *et al., Jiegou Huaxue*, 1986, **5**, 1; *CA*, **107**, 39495 (*cryst struct*)

Oceanapia Quinolone alkaloid Q-7



Absolute Configuration

$C_{24}H_{22}Br_2N_6O_8$ 682.281

Isol. from the sponge *Oceanapia* sp. Inhibitor of mycothiol S-conjugate amidase. $[\alpha]_D^{20}$ -150 (c, 0.19 in MeOH).

Nicholas, G.M. *et al., Org. Lett.*, 2001, **3**, 1543-1545 (*isol, cd, pmr, cmr*)

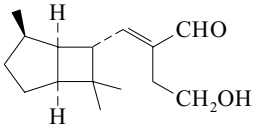
Rhopilema esculentum Radical scavenging protein R-1

Protein. Isol. from the jellyfish *Rhopilema esculentum*. Radical scavenger.

Yu, H. *et al., Bioorg. Med. Chem. Lett.*, 2005, **15**, 2659-2664 (*isol, activity*)

Raikovenal R-2

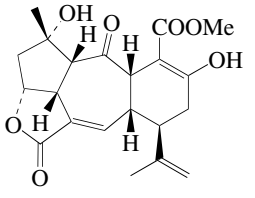
[159736-48-8]



$C_{15}H_{24}O_2$ 236.353
Constit. of *Euplotes raikovi*. Cytotoxic to ciliates. Oil. $[\alpha]_D^{20}$ -40 (c, 0.1 in MeOH). λ_{max} 245 (ϵ 7000) (MeOH) (Derep).

Guella, G. *et al., Chem. Comm.*, 1994, 2585 (*isol, pmr, cmr*)
Snider, B.B. *et al., Synth. Commun.*, 1997, **27**, 1583-1600 (*synth, pmr, cmr*)
Rosini, G. *et al., J.O.C.*, 1998, **63**, 2389-2392 (*synth*)

Rameswaralide R-3

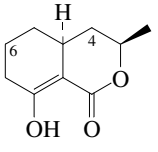


$C_{21}H_{24}O_7$ 388.416
Constit. of *Sinularia dissecta*. Cryst.
Mp 169-171°. $[\alpha]_D$ -20.5 (c, 0.22 in $CHCl_3$). λ_{max} 205 (ϵ 14700); 222 (ϵ 15700); 229 (sh) (ϵ 15500); 250 (sh) (ϵ 11700) (no solvent reported).

Ramesh, P. *et al., Tet. Lett.*, 1998, **39**, 8217-8220 (*isol, pmr, cmr*)

Ramulosin R-4

*3,4,4*a,*5,6,7-Hexahydro-8-hydroxy-3-methyl-1*H-*2-benzopyran-1-one, 9CI*
[29914-01-0]



$C_{10}H_{14}O_3$ 182.219
Enolised β-ketolactone. Metab. of *Pestalotia ramulosa*. Phytotoxin. Plates (Me_2CO aq.).
Mp 120-121°. $[\alpha]_D^{28}$ +18 (c, 2.8 in EtOH). λ_{max} 264 (ϵ 10000) (MeOH) (Berdy). λ_{max} 265 (ϵ 10250) (EtOH) (Berdy).

Benzoyl:
Needles (EtOH aq.). Mp 82-83°.

*8α,8*aα*-Dihydro: 3,4,4*a,*5,6,7,8,8*a-*Octahydro-8-hydroxy-3-methyl-1*H-*2-benzopyran-1-one.* ***8,8*a*-Dihydroramulosin***
[172926-10-2]
$C_{10}H_{16}O_3$ 184.235
Isol. from the conifer endophytic fungus *Canoplea elegantula* and from a *Botrytis* sp. Toxic to spruce budworm larvae. Yellow oil (*Canoplea* sp.).
Mp 142-144° (*Botrytis* sp.). $[\alpha]_D^{20}$ -244 (c, 0.007 in $CHCl_3$) (*Canoplea* sp.). $[\alpha]_D^{23}$ +18.6 (c, 0.6 in MeOH) (*Botrytis* sp.). The two apparently different isolates are given the same stereochem. by Findley, *et al*, (1995) and Stierle, *et al* (1998).

*4α-Hydroxy: 3,4,4*a,*5,6,7-Hexahydro-4,8-dihydroxy-3-methyl-1*H-*2-benzopyran-1-one.* ***4-Hydroxyramulosin***
[172806-93-8]
$C_{10}H_{14}O_4$ 198.218
Isol. from *Canoplea elegantula*. Needles.
Mp 140-143°. $[\alpha]_D^{20}$ +16.7 (c, 0.001 in $CHCl_3$).

4α-Hydroxy, 6,7-didehydro: ***3,4,4*a,*5-Tetrahydro-4,8-dihydroxy-3-methyl-1*H-*2-benzopyran-1-one***
[172806-92-7]
$C_{10}H_{12}O_4$ 196.202
Isol. from *Canoplea elegantula*. Cryst.
Mp 120-123°. $[\alpha]_D^{20}$ +164 (c, 0.01 in $CHCl_3$). λ_{max} 295 (ϵ 12400) (EtOH).

4β-Hydroxy, 6,7-didehydro: [172926-09-9]
$C_{10}H_{12}O_4$ 196.202
Isol. from *Canoplea elegantula*. Amorph.

4β-Hydroxy, 6α,7α-epoxy: ***6,7-Epoxy-3,4,4*a,*5,6,7-hexahydro-4,8-dihydroxy-3-methyl-1*H-*2-benzopyran-1-one***
[172806-94-9]
$C_{10}H_{12}O_5$ 212.202
Isol. from *Canoplea elegantula*. Oil. $[\alpha]_D$ +47.3 (c, 0.0003 in $CHCl_3$).

5β-Hydroxy: ***5-Hydroxyramulosin***
$C_{10}H_{14}O_4$ 198.218
Prod. by the marine *Phoma tropica* isol. from the alga *Fucus spiralis*. Cryst. (Me_2CO/petrol).
Mp 191°. $[\alpha]_D^{20}$ +17.1 (c, 0.2 in EtOH). λ_{max} 264 (log ϵ 3.62) (EtOH).

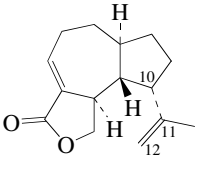
6α-Hydroxy: ***6-Hydroxyramulosin***
[29913-85-7]
$C_{10}H_{14}O_4$ 198.218
Isol. from a *Botrytis* sp., *Canoplea elegantula* and *Pestalotia ramulosa*. Needles ($CHCl_3$/hexane).
Mp 132-133°. $[\alpha]_D^{25}$ +91.6 (c, 1 in MeOH).

*3,4*a-*Diepimer, 8β,8*aα*-dihydro:* **ent-*8,8*a-*Dihydroramulosin***
$C_{10}H_{16}O_3$ 184.235
Prod. by the fungus sp. GT 46045. Oil.
Mp 121-122°. $[\alpha]_D^{20}$ +36 (c, 0.8 in $CHCl_3$). λ_{max} 204 (ϵ 2100); 222 (ϵ 2000); 268 (ϵ 500) (MeOH).

Stodola, F.H. *et al., Biochem. J.*, 1964, **93**, 92 (*isol, struct*)
Tanenbaum, S.W. *et al., Tet. Lett.*, 1970, 2377-2380 (*pmr*)
Findlay, J.A. *et al., Can. J. Chem.*, 1976, **54**, 3419 (*abs config*)
Mori, K. *et al., Tetrahedron*, 1985, **41**, 5295 (*synth*)
Takano, S. *et al., Heterocycles*, 1989, **29**, 2101 (*synth, bibl*)
Asaoka, M. *et al., Tetrahedron*, 1990, **46**, 1541 (*synth*)
Findlay, J.A. *et al., J. Nat. Prod.*, 1995, **58**, 1759-1766 (*isol, derivs, pmr, cmr*)
Enders, D. *et al., Synthesis*, 1996, 209 (*synth*)
Schultz, A.G. *et al., Tet. Lett.*, 1997, **38**, 2071 (*synth*)
Stierle, D.B. *et al., J. Nat. Prod.*, 1998, **61**, 1277-1278 (*isol, pmr, cmr*)
Maul, C. *et al., J. Antibiot.*, 1999, **52**, 1124-1134 (*ent-Dihydroramulosin*)
Uchida, K. *et al., Heterocycles*, 2000, **53**, 539-542 (*synth, deriv*)
Osterhage, C. *et al., Planta Med.*, 2002, 1052-1054 (*5-Hydroxyramulosin*)

Rarisetenolide R-5

[188253-45-4]



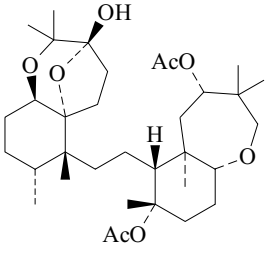
$C_{15}H_{20}O_2$ 232.322
Constit. of *Euplotes rariseta*. Defensive agent. $[\alpha]_D^{20}$ -54 (c, 0.28 in MeOH). λ_{max} 225 (ϵ 8200) (MeOH).

10-Epimer: ***Epirarisetenolide***
[188253-43-2]
$C_{15}H_{20}O_2$ 232.322
Constit. of *Euplotes rariseta*. Defensive agent. λ_{max} 226 (ϵ 9000) (MeOH).

11β,12-Epoxide: ***Epoxyrarisetenolide***
[188253-44-3]
$C_{15}H_{20}O_3$ 248.321
Constit. of *Euplotes rariseta*. Defensive agent. $[\alpha]_D^{20}$ -52 (c, 0.24 in MeOH). λ_{max} 226 (ϵ 8000) (MeOH).
Guella, G. *et al., Helv. Chim. Acta*, 1996, **79**, 2180-2189 (*isol, pmr, cmr*)

Raspacionin A R-6

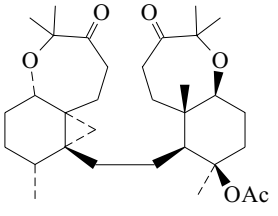
[145458-07-7]



$C_{34}H_{56}O_8$ 592.812
Constit. of *Raspaciona aculeata*. Oil. $[\alpha]_D$ -3.95 (c, 1.17 in $CHCl_3$).
Cimino, G. *et al., Tetrahedron*, 1992, **48**, 9013 (*isol, pmr, cmr, cryst struct*)

Raspacionin B R-7

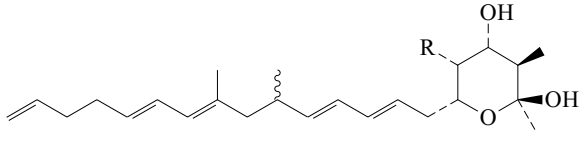
[148371-08-8]



$C_{32}H_{50}O_6$ 530.743
Constit. of *Raspaciona aculeata*. Amorph. powder. $[\alpha]_D^{25}$ +10.8 (c, 0.21 in $CHCl_3$).
Cimino, G. *et al., J. Nat. Prod.*, 1993, **56**, 534 (*isol, pmr, cmr*)

Raspailol A R-8

*6-(6,8-Dimethyl-2,4,8,10,14-pentadecapentaenyl)tetrahydro-2,3-dimethyl-2*H*-pyran-2,4-diol, 9CI*
[162341-07-3]



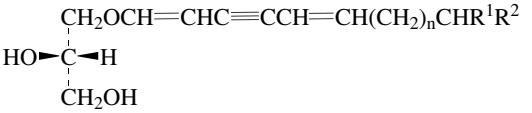
R = H

$C_{24}H_{38}O_3$ 374.562
Isol. from a Palauan sponge *Raspailia* sp. (*Raspaxilla* sp.). Oil. $[\alpha]_D$ +62 (c, 0.5 in C_6H_6). λ_{max} 234 (ϵ 45710); 241 (ϵ 46770) (hexane).
Cerda-Garcia-Rojas, C.M. *et al., Tetrahedron*, 1995, **51**, 1087 (*isol, pmr, cmr*)
Czuba, I.R. *et al., Org. Biomol. Chem.*, 2003, 2044-2056 (*synth*)

Raspailol B R-9

*6-(6,8-Dimethyl-2,4,8,10,14-pentadecapentaenyl)tetrahydro-2,3,5-trimethyl-2*H*-pyran-2,4-diol, 9CI*
[162341-08-4]
As Raspailol A, R-8 with
R = CH_3
$C_{25}H_{40}O_3$ 388.589
Isol. from the Palauan sponge *Raspailia* sp. (*Raspaxilla* sp.). Oil. $[\alpha]_D$ +111 (c, 0.1 in C_6H_6). λ_{max} 234 (ϵ 45710); 241 (ϵ 45710) (hexane).
Cerda-Garcia-Rojas, C.M. *et al., Tetrahedron*, 1995, **51**, 1087 (*isol, pmr, cmr*)
Czuba, I.R. *et al., Org. Biomol. Chem.*, 2003, 2044-2056 (*synth*)

Raspailynes R-10



Isol. from the sponges *Raspailia pumila* and *Raspailia ramosa*.

Raspailyne A
3-(18-Hydroxy-1,5-octadecadien-3-ynyl)oxy-1,2-propanediol
[102629-91-4]
$C_{21}H_{36}O_4$ 352.513
Herbicide. Amorph. solid (MeOH). Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 54-55°. $[\alpha]_D^{25}$ +5.6 (c, 0.9 in MeOH). n = 11, R^1 = OH, R^2 = H (1*Z*,5*Z*)-isomer. λ_{max} 261 (sh) (ϵ 14200); 273 (ϵ 18300); 288 (ϵ 15000) (MeOH). λ_{max} 273 (ϵ 18300); 288 (ϵ 15000) (MeOH) (Berdy).

Raspailyne A_1
3-(16-Hydroxy-1,5-hexadecadien-3-ynyl)oxy-1,2-propanediol
[110600-69-6]
$C_{19}H_{32}O_4$ 324.459
$[\alpha]_D^{22}$ +1 (c, 0.3 in $CHCl_3$). n = 9, R^1 = OH, R^2 = H, (1*Z*,5*Z*)-isomer.

Raspailyne B
3-(1,5-Pentadecadien-3-ynyl)oxy-1,2-propanediol
[110600-73-2]
$C_{18}H_{30}O_3$ 294.433
n = 8, R^1 = R^2 = H, (1*Z*,5*Z*)-isomer.

Raspailyne B_1
3-(1,5-Tetradecadien-3-ynyl)oxy-1,2-propanediol
[110600-72-1]
$C_{17}H_{28}O_3$ 280.406
$[\alpha]_D^{22}$ -4.9 (c, 0.5 in $CHCl_3$). n = 7, R^1 = R^2 = H (1*Z*,5*Z*)-isomer.

*(1*E*)-Isomer:* ***Isoraspailyne B_{1b}***
[110659-90-0]
$C_{17}H_{28}O_3$ 280.406

*(5*E*)-Isomer:* ***Isoraspailyne B_{1a}***
[110659-89-7]
$C_{17}H_{28}O_3$ 280.406

Raspailyne B_2
3-(1,5-Tridecadien-3-ynyl)oxy-1,2-propanediol
[110600-71-0]
$C_{16}H_{26}O_3$ 266.38
$[\alpha]_D^{22}$ -10.8 (c, 0.06 in $CHCl_3$). n = 6, R^1 = R^2 = H, (1*Z*,5*Z*)-isomer.

Isoraspailyne A
3-(17-Hydroxy-1,5-octadecadien-3-ynyl)oxy-1,2-propanediol
[110600-70-9]
$C_{21}H_{36}O_4$ 352.513
$[\alpha]_D^{22}$ +2.1 (c, 0.2 in $CHCl_3$). n = 10, R^1 = OH, R^2 = CH_3, (1*Z*,5*Z*)-isomer.

Isoraspailyne B
3-(13-Methyl-1,5-tetradecadien-3-ynyl)oxy-1,2-propanediol
[110660-59-8]
$C_{18}H_{30}O_3$ 294.433
n = 6, R^1 = R^2 = CH_3, (1*Z*,5*Z*)-isomer.

*(5*E*)-Isomer: Isoraspailyne B_a*
[110600-74-3]
$C_{18}H_{30}O_3$ 294.433

Isoraspailyne B_1

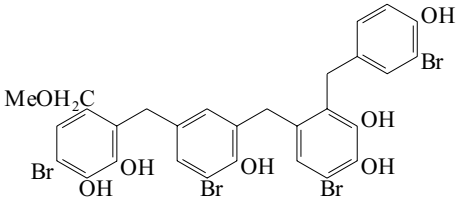
3-(12-Methyl-1,5-tridecadien-3-ynyl)oxy-1,2-propanediol
[110619-09-5]

$C_{17}H_{28}O_3$ 280.406
n = 5, $R^1 = R^2 = CH_3$, (1*Z*,5*Z*)-isomer.

Guella, G. *et al., Chem. Comm.*, 1986, 77 (*isol, uv, pmr, cmr*)
Guella, G. *et al., Helv. Chim. Acta*, 1987, **70**, 1050 (*isol, cmr, ms*)

Rawsonol **R-11**

[125111-69-5]



$C_{29}H_{24}Br_4O_7$ 804.12
Constit. of *Avrainvillea rawsoni*. HMG-CoA reductase inhibitor. λ_{max} 285 (ϵ 3200) (MeOH) (Berdy). λ_{max} 300 (ϵ 3900) (MeOH/NaOH) (Berdy).

Corte, B.K. *et al., Phytochemistry*, 1989, **28**, 2917-2919 (*Rawsonol*)

Red pigment-concentrating hormone **R-12**

Erythrocyte-concentrating hormone. Blanching hormone. RPCH. Pab-RPCH
[37933-92-9]
H-5-oxoPro-Leu-Asn-Phe-Ser-Pro-Gly-Trp-NH_2
$C_{45}H_{59}N_{11}O_{11}$ 930.028
Peptide structurally related to insect adipokinetic hormones. Isol. from eyestalks of the shrimp *Pandalus borealis* and other crustaceans.

[56092-80-9]

Fernlund, P. *et al., Biochim. Biophys. Acta*, 1974, **371**, 304-311; 312-322 (*isol, synth*)
Josefsson, L. *et al., Am. Zool.*, 1983, **23**, 507-515 (*rev*)
Rao, K.R. *et al., Prog. Clin. Biol. Res.*, 1988, **256**, 407-422 (*rev*)
Graus, G. *et al., J. Comp. Physiol., B*, 1990, **160**, 373-379 (*isol*)

Relaxins **R-13**

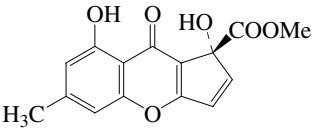
[9002-69-1]
Peptide hormones. All relaxins have a two chain, disulfide-linked insulin-like struct. and two arginine residues in the midregion of the B chain. The primary structs. of relaxins from apparently closely related species can differ significantly in their AA compositions. Present in mammals and other species, e.g. sharks and chickens. Hormones of reproduction which appear to affect parturition, uterine accommodation and sperm motility in varying degrees in many species.
▶ VG0720000

[64339-45-3, 75627-11-1, 75639-98-4, 75639-99-5, 77467-85-7, 77614-15-4, 77640-64-3, 79005-81-5, 82120-04-5, 82611-45-8, 82658-27-3, 82658-28-4, 105231-40-1, 105231-41-2, 105286-99-5, 107628-11-5, 107712-70-9, 107720-74-1, 117697-87-7, 117697-88-8, 119370-85-3, 119397-12-5, 127664-25-9, 135644-72-3, 135644-80-3, 140683-99-4]

Anderson, R.R. *et al., Adv. Exp. Med. Biol.*, 1982, **143**, 1 (*rev*)
Steinetz, B.G. *et al., Ann. N.Y. Acad. Sci.*, 1982, **380**, 1 (*rev*)
Schwabe, C. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1990, **96**, 15 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1408
Sherwood, O.D. *et al., Oxford Rev. Reprod. Biol.*, 1993, **15**, 143 (*rev*)
Bryant-Greenwood, G.D. *et al., Endocr. Rev.*, 1994, **15**, 5 (*rev*)
Wade, J.D. *et al., J. Protein Chem.*, 1994, **13**, 315 (*synth*)

Remisporine A **R-14**

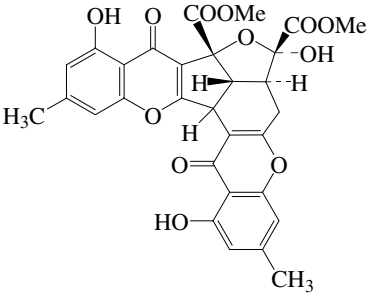
*Methyl 1,8-dihydroxy-6-methyl-9-oxo-1*H*-cyclopenta[*b*][1]benzopyran-1-carboxylate*



$C_{15}H_{12}O_6$ 288.256
Similar to Coniochaetone B. Isol. from the marine fungus *Remispora maritima*. Unstable under normal conditions and dimerises to give Remisporine B, R-15.

Kong, F. *et al., Tet. Lett.*, 2003, **44**, 3119-3122 (*isol*)

Remisporine B **R-15**

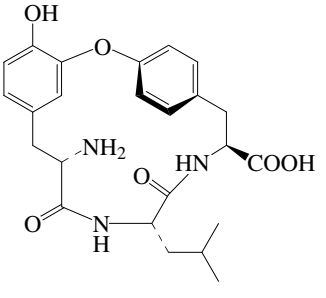


Relative Configuration

$C_{30}H_{24}O_{12}$ 576.512
Diels-Alder dimer of Remisporine A, R-14. Isol. from the marine fungus *Remispora maritima*. λ_{max} 228 (sh); 240; 260 (sh); 325 (no solvent reported).

Kong, F. *et al., Tet. Lett.*, 2003, **44**, 3119-3122 (*isol, cd, pmr, cmr*)

Renieramide **R-16**

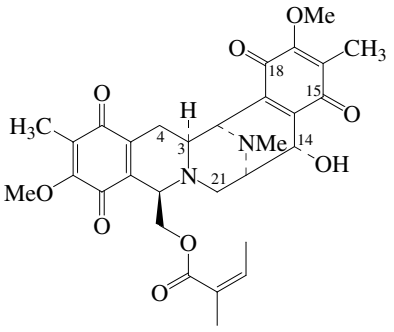


$C_{24}H_{29}N_3O_6$ 455.51
Similar to Eurypamide A, E-897 and Antibiotic OF 4949. Isol. from the Vanuatu sponge *Reniera* n. sp. Powder. $[\alpha]_D$ -31 (c, 1 in MeOH). λ_{max} 203 (ϵ 4000); 230 (ϵ 8900); 278 (ϵ 2000) (MeOH).

Ciasullo, L. *et al., J. Nat. Prod.*, 2002, **65**, 407-410 (*isol, pmr, cmr, ms*)

Renieramycin A R-17

[79664-60-1]



$C_{30}H_{34}N_2O_9$ 566.607

Metab. from the marine sponge *Reniera* sp. Shows antimicrobial and antitumour props.; active against *Staphylococcus aureus* and *Bacillus subtilis*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{20}$ -36.3 (c, 0.16 in MeOH). λ_{max} 267 (ϵ 15800); 363 (ϵ 1400) (MeOH) (Derep). λ_{max} 268 (ϵ 15800); 365 (ϵ 1370) (MeOH) (Berdy).

Et ether: ***Renieramycin B***
[79664-61-2]
$C_{32}H_{38}N_2O_9$ 594.66
Prod. by *Reniera* sp. Shows antimicrobial and antitumour props. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{20}$ -32.2 (c, 0.15 in MeOH). Prob. an artifact. λ_{max} 265 (ϵ 16100); 370 (ϵ 1450) (MeOH) (Derep). λ_{max} 268 (ϵ 17400); 365 (ϵ 1460) (MeOH) (Berdy).

21α-Hydroxy, Me ether: ***Renieramycin F***
[123641-96-3]
$C_{31}H_{36}N_2O_{10}$ 596.633
From *Reniera* sp. Yellow powder. λ_{max} 265 (ϵ 16100); 370 (ϵ 1450) (MeOH) (Derep). λ_{max} 265 (ϵ 12000) (MeOH) (Berdy).

21-Oxo: ***Renieramycin C***
[79664-62-3]
$C_{30}H_{32}N_2O_{10}$ 580.59
Prod. by *Reniera* sp. Shows antimicrobial and antitumour props. Poorly sol. hexane. $[\alpha]_D^{20}$ -89.2 (c, 0.065 in MeOH). λ_{max} 267 (ϵ 15800); 363 (ϵ 1400) (MeOH) (Derep). λ_{max} 266 (ϵ 14900); 360 (ϵ 21600) (MeOH) (Berdy).

21-Oxo, Et ether: ***Renieramycin D***
[79664-63-4]
$C_{32}H_{36}N_2O_{10}$ 608.644
Prod. by *Reniera* sp. Shows antimicrobial and antitumour props. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{20}$ -100.7 (c, 0.092 in MeOH). λ_{max} 265 (ϵ 16100); 370 (ϵ 1450) (MeOH) (Derep).

14-Deoxy, 21α-hydroxy: ***Renieramycin E***
[123641-95-2]
$C_{30}H_{34}N_2O_9$ 566.607
From *Reniera* sp. Yellow powder. λ_{max} 267 (ϵ 15800); 363 (ϵ 1400) (MeOH) (Derep). λ_{max} 266 (ϵ 17000) (MeOH) (Berdy).

14-Deoxy, 21-oxo: ***Renieramycin G***
[143458-75-7]
$C_{30}H_{32}N_2O_9$ 564.591
Major metab. from the Fijian sponge *Xestospongia caycedoi*. Exhibits moderate cytotoxicity. Unstable. λ_{max} 267 (ϵ 15800); 363 (ϵ 1400) (MeOH) (Derep). λ_{max} 269 (ϵ 20000) (MeOH) (Berdy).

8a,9-Didehydro, 21-oxo, Me ether: ***Renieramycin I***
[224566-79-4]
$C_{31}H_{32}N_2O_{10}$ 592.601
Isol. from the sponge *Haliclona cribricutis*. λ_{max} 220 (log ϵ 4.4); 260 (log ϵ 4.1); 340 (log ϵ 3.5); 520 (log ϵ 3.1) (MeOH).

21α-Cyano: ***Renieramycin O***
[631913-68-3]
$C_{31}H_{33}N_3O_9$ 591.616
Isol. from a *Xestospongia* sp. pre-treated with KCN. Oxidn. prod. of Renieramycin N. Pale yellow powder. $[\alpha]_D^{20}$ -134.4 (c, 0.7 in $CHCl_3$). λ_{max} 269 (log ϵ 4.62); 370 (log ϵ 3.1) (no solvent reported).

21α-Cyano, Me ether: ***Renieramycin R***
$C_{32}H_{35}N_3O_9$ 605.643
Isol. from a *Xestospongia* sp. pre-treated with KCN. Pale yellow solid. $[\alpha]_D^{18}$ -17.6 (c, 0.1 in $CHCl_3$). λ_{max} 269 (log ϵ 4.62); 370 (log ϵ 3.12) (no solvent reported).

21α-Cyano, 14-ketone, 15,18-hydroquinone: ***Renieramycin Q***
$C_{31}H_{33}N_3O_9$ 591.616
Isol. from a *Xestospongia* sp. pre-treated with KCN. Pale yellow solid. $[\alpha]_D^{18}$ -69.8 (c, 0.1 in $CHCl_3$). λ_{max} 224 (log ϵ 4.02); 276 (log ϵ 4.07); 374 (log ϵ 3.61) (no solvent reported).

21α-Cyano, 14-deoxy: ***Renieramycin M***
[631913-64-9]
$C_{31}H_{33}N_3O_8$ 575.617
Isol. from a *Xestospongia* sp. pre-treated with KCN. Cytotoxic. Dark yellow prisms (EtOAc).
Mp 194.5-197°. $[\alpha]_D^{20}$ -49.5 (c, 1 in $CHCl_3$). λ_{max} 269 (log ϵ 4.63); 370 (log ϵ 3.11) (no solvent reported).

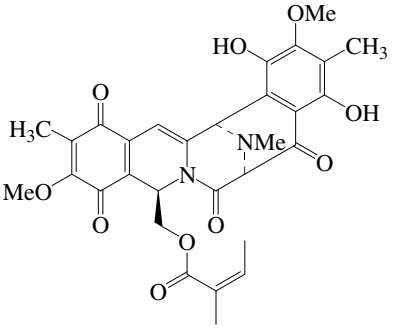
*21α-Cyano, 14-deoxy, 7-*O*-de-Me:* ***Renieramycin S***
$C_{30}H_{31}N_3O_8$ 561.59
Isol. from a *Xestospongia* sp. pre-treated with KCN. Pale yellow needles (EtOAc/petrol).
Mp 179-180°. $[\alpha]_D^{20}$ -38.8 (c, 0.1 in $CHCl_3$). λ_{max} 269 (log ϵ 4.62); 370 (log ϵ 3.12) (no solvent reported).

21α-Cyano, 15,18-hydroquinone: ***Renieramycin N***
[631913-65-0]
$C_{31}H_{35}N_3O_9$ 593.632
Isol. from a *Xestospongia* sp. pre-treated with KCN. Cytotoxic. Pale yellow prisms (EtOH).
Mp 162.5-164°. $[\alpha]_D^{20}$ -24.7 (c, 0.01 in MeOH). λ_{max} 273 (log ϵ 3.99); 370 (log ϵ 2.7) (no solvent reported).

Frincke, J.M. *et al., J.A.C.S.*, 1982, **104**, 265-269 (*Renieramycins A-D, isol, uv, ir, pmr, cmr, ms, struct*)
He, H. *et al., J.O.C.*, 1989, **54**, 5822-5824 (*Renieramycins E,F*)
Fukuyama, T. *et al., Tet. Lett.*, 1990, **31**, 5989-5992 (*synth, struct*)
Davidson, B.S. *et al., Tet. Lett.*, 1992, **33**, 3721-3724 (*Renieramycin G*)
Parameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 1258-1263 (*Renieramycin I*)
Suwanborirux, K. *et al., J. Nat. Prod.*, 2003, **66**, 1441-1446; 2004, **67**, 1023-1028 (*Renieramycins M,N,O,Q,R,S*)
Magnus, P. *et al., J.A.C.S.*, 2005, **127**, 12476-12477 (*Renieramycin G, synth*)
Lane, J.W. *et al., J.A.C.S.*, 2005, **127**, 12684-12690 (*Renieramycin G, synth*)

Renieramycin H R-18

Cribrostatin 4
[276682-85-0]
[224566-78-3]



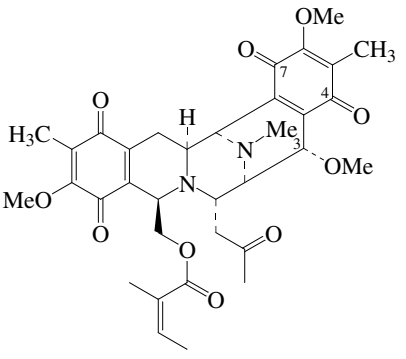
$C_{30}H_{30}N_2O_{10}$ 578.574

Struct. revised in 2001. Isol. from sponges *Cribrochalina* sp. and *Haliclona cribicutis*. Cytotoxic agent. Red prisms (MeOH). Mp 190-192° dec. λ_{max} 209 (ϵ 40770); 274 (ϵ 13680); 359 (ϵ 8070); 507 (ϵ 3420) (MeOH).

Pasameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 1258-1263 (*isol*)
Pettit, G.R. *et al., J. Nat. Prod.*, 2000, **63**, 793-798 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Saito, N. *et al., Heterocycles*, 2001, **55**, 21-28 (*pmr, cmr, struct*)
Chan, C. *et al., J.A.C.S.*, 2005, **127**, 4596-4598; 7262 (*synth*)

Renieramycin K R-19

[631913-66-1]



$C_{34}H_{40}N_2O_{10}$ 636.697

Isol. from a Thai sponge *Xestospongia* sp. Amorph. yellow powder. λ_{max} 271 (log ϵ 4.4); 372 (log ϵ 3.11) (no solvent reported).

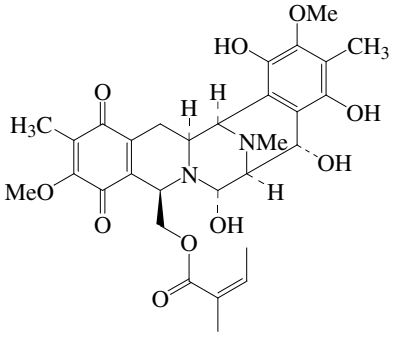
3-Demethoxy: ***Renieramycin J***
[500111-59-1]
$C_{33}H_{38}N_2O_9$ 606.671
Isol. from *Xestospongia* sp. Amorph. yellow powder. λ_{max} 273 (log ϵ 4.32); 370 (log ϵ 3) (no solvent reported).

4,7-Hydroquinone, O^3-de-Me, 3-ketone: ***Renieramycin L***
[631913-67-2]
$C_{33}H_{38}N_2O_{10}$ 622.671
Isol. from a *Xestospongia* sp. Pale yellow powder. λ_{max} 244 (log ϵ 4.02); 276 (log ϵ 4.07); 375 (log ϵ 3.75) (no solvent reported).

Suwanborirux, K. *et al., J. Nat. Prod.*, 2003, **66**, 1441-1446 (*isol, pmr, cmr*)

Renieramycin P R-20

Reneiramycin J (obsol.)†
[593280-18-3]



Absolute Configuration

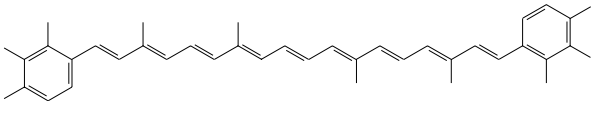
$C_{30}H_{36}N_2O_{10}$ 584.622

Originally called Reneiramycin J; renamed to avoid duplication. Isol. from the sponge *Neopetrosia* sp. Brownish solid. $[\alpha]_D^{21}$ +1.2 (c, 0.02 in MeOH). λ_{max} 203 (ϵ 39000); 273 (ϵ 12000) (MeOH).

Oku, N. *et al., J. Nat. Prod.*, 2003, **66**, 1136-1139 (*isol, pmr, cmr*)
Suwanborirux, K. *et al., J. Nat. Prod.*, 2003, **66**, 1441-1446 (*nomencl*)

Renierapurpurin R-21

χ,χ-Carotene
[6805-08-9]



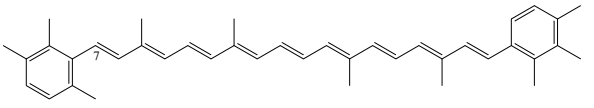
$C_{40}H_{48}$ 528.819

Constit. of *Reniera japonica* and of sediments. Purple plates ($CHCl_3$/EtOH).
Mp 161° (237-238°).

Yamaguchi, M. *et al., Bull. Chem. Soc. Jpn.*, 1957, **30**, 111; 1960, **33**, 1560
Cooper, R.D.G. *et al., J.C.S.*, 1963, 5637 (*synth*)
Schaeflé, J. *et al., Tet. Lett.*, 1977, 3673-3676 (*isol, pmr, cmr*)

Renieratene R-22

ϕ,χ-Carotene. Renieratane
[550-29-8]



$C_{40}H_{48}$ 528.819

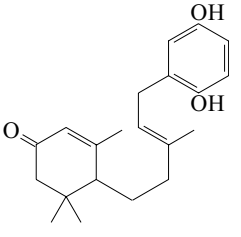
Constit. of *Reniera japonica* and *Tethya auranthium* and of sediments. Purplish red needles (C_6H_6/EtOH).
Mp 187-188°.

(7Z)-Isomer: ***Renieracistene***
[84773-17-1]
$C_{40}H_{48}$ 528.819
Constit. of *Tethya amamensis.*

Yamaguchi, M. *et al., Bull. Chem. Soc. Jpn.*, 1957, **30**, 111; 979; 1960, **33**, 1560
Schaeflé, J. *et al., Tet. Lett.*, 1977, 3673-3676 (*isol, pmr, cmr*)
Shimada, A. *et al., Tet. Lett.*, 1981, **22**, 773 (*synth*)
Tanaka, Y. *et al., Nippon Shashin Gakkaishi*, 1982, **48**, 1651-1655; *CA*, **98**, 86548t (*Renieracistene*)
Czeczuga, B. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1984, **78**, 259 (*occur*)

Renierin A R-23

[157047-58-0]



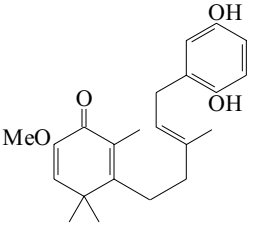
$C_{21}H_{28}O_3$ 328.45

Constit. of *Reniera mucosa*. Yellow oil. $[\alpha]_D$ -12.5 (c, 0.2 in $CHCl_3$).

Zubía, E. *et al., Tetrahedron*, 1994, **50**, 8153 (*isol, pmr, cmr*)

Renierin B R-24

[157002-39-6]



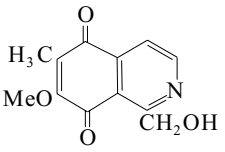
$C_{22}H_{28}O_4$ 356.461

Constit. of *Reniera mucosa*. Yellow oil.

Zubía, E. *et al., Tetrahedron*, 1994, **50**, 8153 (*isol, pmr, cmr*)

Renierol† R-25

1-(Hydroxymethyl)-7-methoxy-6-methyl-5,8-isoquinolinedione, 9CI
[77640-19-8]



$C_{12}H_{11}NO_4$ 233.223
Alkaloid from the Fijian sponge *Xestospongia caycedoi*; also from *Oceanapia* sp. Shows antibiotic activity. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 205 (ϵ 15000); 241 (ϵ 13000); 314 (ϵ 4100) (MeOH) (Berdy).

O-*Ac:* ***Renierol acetate***
[97603-18-4]
$C_{14}H_{13}NO_5$ 275.26
Metab. from the marine sponge *Xestospongia* sp. and its associated nudibranch *Jorunna funebris*. Cryst. (MeOH). Mp 118-119°. λ_{max} 246 (ϵ 17780); 318 (ϵ 5011) (MeOH) (Berdy). λ_{max} 206; 237; 296; 315 (EtOH) (Berdy).

O-*Propanoyl:* ***Renierol propionate***
[124909-65-5]
$C_{15}H_{15}NO_5$ 289.287
Isol. from the sponge *Xestospongia* sp. and its associated nudibranch *Jorunna funebris*. Yellow needles (MeOH). Mp 89-90°.

O-*Angeloyl:* ***Renierone***
[73777-65-8]
$C_{17}H_{17}NO_5$ 315.325
Major metab. from an intense blue sponge *Reniera* sp., possibly prod. by symbiotic microorganism. Active against gram-positive bacteria, fungi and tumours.
Mp 91.5-92.5°. Related to Mimocin. λ_{max} 214 (ϵ 20000); 312 (ϵ 4000) (MeOH) (Derep).

O^7-*De-Me,* $O^{1'}$-*Ac:* **O-*Demethylrenierol acetate***
[149022-06-0]
$C_{13}H_{11}NO_5$ 261.234
Isol. from a bright blue sponge *Petrosia* sp. Shows antibacterial activity. Yellow oil. λ_{max} 226 (ϵ 19400); 300 (ϵ 4094) (MeOH).

O^7-*De-Me,* O-*angeloyl:* **O-*Demethylrenierone***
[77515-81-2]
$C_{16}H_{15}NO_5$ 301.298
Isol. from an unidentified *Reniera* sp. and a *Cribrochalina* sp. Shows antibacterial props. Orange solid.
Mp 135-136°. λ_{max} 208 (ϵ 12500); 248 (ϵ 7640); 290 (ϵ 3260); 316 (ϵ 1610) (MeOH) (Derep). λ_{max} 228 (log ϵ 3.92); 298 (log ϵ 3.31) (MeOH).

1,2-Dihydro, O-*Ac,* N-*formyl:* **N-*Formyl-1,2-dihydrorenierol acetate***
[124909-71-3]
$C_{15}H_{15}NO_6$ 305.287
Isol. from the sponge *Xestospongia* sp. and its associated nudibranch *Jorunna funebris*. Dark red oil. Sol. MeOH. λ_{max} 269 (ϵ 9772); 340 (ϵ 3467); 500 (ϵ 1550) (MeOH) (Berdy). λ_{max} 204; 217; 269; 344 (EtOH) (Berdy).

1,2-Dihydro, O-*propanoyl,* N-*formyl:* **N-*Formyl-1,2-dihydrorenierol propionate***
[124909-72-4]
$C_{16}H_{17}NO_6$ 319.313
Isol. from the sponge *Xestospongia* sp. and its associated nudibranch *Jorunna funebris*. Dark red oil. λ_{max} 268 (ϵ 10000); 340 (ϵ 3715); 500 (ϵ 1737) (MeOH) (Berdy).

*1,2*R-*Dihydro,* O-*angeloyl,* N-*formyl:* ***(-)*-N-*Formyl-1,2-dihydrorenierone***
[79664-57-6]
$C_{18}H_{19}NO_6$ 345.351
Isol. from a *Reniera* sp. Active against tumours. Red non-cryst. solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{20}$ -227 (c, 0.023 in MeOH). Shown to be a 2:1 mixt. of two rotamers by pmr and cmr. λ_{max} 216 (ϵ 31000); 265 (ϵ 16500); 340 (ϵ 6000); 515 (ϵ 3500) (MeOH) (Derep).

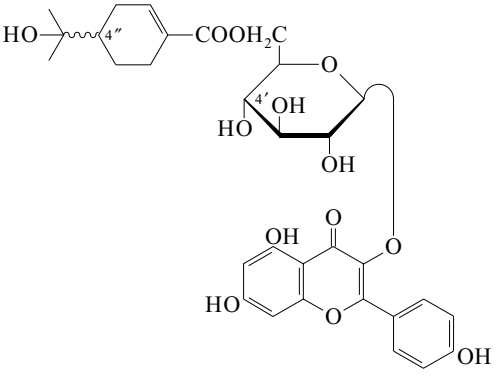
*1,2*S-*Dihydro,* O-*angeloyl,* N-*formyl:* ***(+)*-N-*Formyl-1,2-dihydrorenierone***
[80108-30-1]
$C_{18}H_{19}NO_6$ 345.351
Isol. from a *Cribrochalina* sp. and a *Reniera* sp. Dark red solid. $[\alpha]_D$ +230 (c, 0.04 in MeOH). λ_{max} 218 (log ϵ 4.35); 268 (log ϵ 3.96); 344 (log ϵ 3.53) (MeOH).

1,2-Dihydro, O-*angeloyl,* N-*(3-oxo-1-butenyl):* **N-*(3-Oxo-1-butenyl)-1,2-dihydrorenierone***
[182293-46-5]
$C_{21}H_{23}NO_6$ 385.416
Isol. from the Philippine marine sponge *Xestospongia* sp. Active against gram-positive bacteria. Shows weak insecticidal activity. Blue gum. λ_{max} 223 (ϵ 27000); 312 (ϵ 23000); 330 (ϵ 21000) (MeOH).

McIntyre, D.E. *et al., Tet. Lett.*, 1979, 4163-4166 (*Renierone, isol, uv, ir, cmr, pmr, cryst struct*)
Danishefsky, S. *et al., Tet. Lett.*, 1980, 4819-4822 (*Renierone, synth*)
Kubo, A. *et al., Chem. Pharm. Bull.*, 1981, **29**, 595-596; 1983, **31**, 341-343; 1986, **34**, 4056-4068; 1989, **37**, 1384-1386 (*synth, ir, derivs*)
Frincke, J.M. *et al., J.A.C.S.*, 1982, **104**, 265-269 (*Renierone, N-formyl-1,2-dihydrorenierone, O-Demethylrenierone*)
Berman, E. *et al., Diss. Abstr. Int., B*, 1984, **45**, 556 (*synth*)
Kitahara, Y. *et al., Chem. Pharm. Bull.*, 1985, **33**, 823-830 (*cmr*)
McKee, T.C. *et al., J. Nat. Prod.*, 1987, **50**, 754-756 (*isol, uv, ir, pmr, cmr, ms, struct*)
Saito, N. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1493-1499 (*Renierone, synth*)
Venkateswarlu, Y. *et al., Indian J. Chem., Sect. B*, 1993, **32**, 704 (*O-Demethylrenierol acetate*)
Edrada, R.A. *et al., J. Nat. Prod.*, 1996, **59**, 973-976 (*N-(3-Oxo-1-butenyl)-1,2-dihydrorenierone*)
Ramesh, P. *et al., J. Nat. Prod.*, 1999, **62**, 780-781 (*activity, isol*)
Fontana, A. *et al., Tetrahedron*, 2000, **56**, 7305-7308 (*isol*)
Plubrukarn, A. *et al., Pharm. Biol.*, 2003, **41**, 439-442 (*(+)-N-Formyl-1,2-dihydrorenierone*)
Kuwabara, N. *et al., Tetrahedron*, 2004, **60**, 2943-2952 (*synth*)

Resinoside A R-26

[144027-78-1]



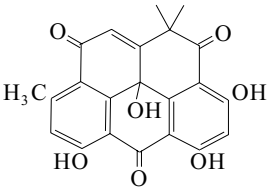
$C_{31}H_{34}O_{13}$ 614.602
Anomeric mixture at the C-4″ posn. Isol. from the leaves of *Eucalyptus resinfera*. Repellent against *Mytilus edulis*. $[\alpha]_D^{28}$ -12.7 (c, 1 in MeOH). λ_{max} 275 (ϵ); 326 (ϵ); 400 (ϵ) (MeOH/NaOMe) (Derep). λ_{max} 266 (ϵ 16000); 350 (ϵ 16000) (MeOH) (Derep).

4′-Epimer: ***Resinoside B***
[144027-79-2]
$C_{31}H_{34}O_{13}$ 614.602
From *Eucalyptus resinfera*. Repellent against *M. edulis*. $[\alpha]_D^{28}$ +7.6 (c, 0.4 in MeOH). λ_{max} 275 (ϵ); 326 (ϵ); 400 (ϵ) (MeOH/NaOMe) (Derep). λ_{max} 266 (ϵ 16000); 350 (ϵ 16000) (MeOH) (Derep).

Hyodo, S. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 138 (*isol, struct*)

Resistoflavin R-27

*3,5,7,11*b-*Tetrahydroxy-1,1,9-trimethyl-2*H-*benzo[*cd*]pyrene-2,6,10(1*H*,11*b*H)-trione, 9CI, 8CI. A 3733Y. Antibiotic A 3733Y*
[29706-96-5]



$C_{22}H_{16}O_7$ 392.364

Structurally related to Resistomycin, R-28. Prod. by *Streptomyces* JA 3733, marine-derived *Streptomyces* sp. B8005 and other *Streptomyces* spp. Shows antibiotic props. Cryst. (EtOAc). Sol. bases, $CHCl_3$, EtOAc; poorly sol. H_2O.
Mp 238-240° dec. $[\alpha]_D^{23}$ -96 (c, 0.5 in Py). λ_{max} 266 (ϵ 44500); 295 (sh) (ϵ 22400); 391 (ϵ 9600) ($CHCl_3$) (Derep).

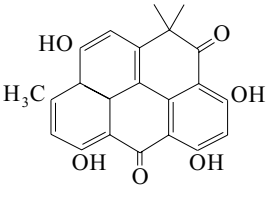
▶ LD_{50} (mus, ivn) 75 mg/kg. DJ8070000

*11*b-*Me ether:* ***11b-O-Methylresistoflavin***
$C_{23}H_{18}O_7$ 406.391
Prod. by the marine-derived *Streptomyces* sp. B4842. Yellow solid. Mp 244-246°. λ_{max} 303; 379; 539; 547 (MeCN).

Eckardt, K. *et al., Tetrahedron*, 1970, **26**, 5875 (*struct, ir, uv, nmr*)
Poltorak, V.A. *et al., Antibiotiki (Moscow)*, 1975, **20**, 206 (*isol, struct*)
Höfle, G. *et al., Annalen*, 1983, 835 (*isol, biosynth, cmr*)
Kock, I. *et al., J. Antibiot.*, 2005, **58**, 530-534 (*11b-O-Methylresistoflavin*)

Resistomycin R-28

*3,5,7,10-Tetrahydroxy-1,1,9-trimethyl-2*H-*benzo[*cd*]pyrene-2,6(1*H*)-dione, 9CI, 8CI. Croceomycin. Geliomycin. Heliomycin, INN. Itamycin. A 3733A. X 340. Antibiotic 11-98. Antibiotic A 3733A. Antibiotic X 340*
[20004-62-0]



$C_{22}H_{16}O_6$ 376.365

Related to Resistoflavin, R-27. Prod. by *Streptomyces resistomycificius* and other *Streptomyces* spp. incl. marine-derived spp. RNA polymerase inhibitor. Shows activity against gram-positive and mycobacteria. Yellow needles (dioxan). Spar. sol. H_2O, $CHCl_3$; sol. dioxan.
Mp 315° dec. Subl.0.0001 200-205. λ_{max} 255 (ϵ); 290 (ϵ); 375 (ϵ); 485 (ϵ) (ph 11.3) (Derep). λ_{max} 234 (sh) (ϵ); 268 (ϵ 24000); 290 (ϵ 23000); 320 (ϵ 14400); 338 (ϵ 13900); 367 (ϵ 11000); 458 (ϵ 15400); 515 (ϵ 10000) (EtOH) (Derep).

▶ LD_{50} (mus, orl) 2000 mg/kg. Exp. carcinogen. DJ6350000

Tetra-Ac:
Amorph. Mp 204-206°.

Tetrabenzoyl:
Needles (C_6H_6/petrol). Mp 244°.

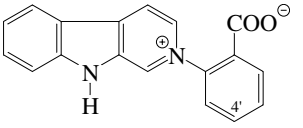
5,7,10-Tri-Me ether:
Red prisms (MeOH). Mp 280° dec.

[11029-70-2]

Brockmann, A. *et al., Chem. Ber.*, 1954, **87**, 1036 (*isol*)
Rosenbrook, W. *et al., J.O.C.*, 1967, **32**, 2924 (*struct, uv, nmr*)
Bailey, N.A. *et al., Chem. Comm.*, 1968, 374 (*cryst struct*)
Brockmann, H. *et al., Chem. Ber.*, 1969, **102**, 1224 (*struct, ir, uv, nmr*)
Eckhardt, K. *et al., Tetrahedron*, 1970, **26**, 5875 (*struct, ir, uv, nmr*)
Kingston, J.F. *et al., Can. J. Chem.*, 1977, **55**, 785 (*synth*)
Keay, B.A. *et al., J.A.C.S.*, 1982, **104**, 4725 (*synth*)
Höfle, G. *et al., Annalen*, 1983, 835 (*isol, biosynth, cmr*)
Arora, S.K. *et al., J. Antibiot.*, 1985, **38**, 113 (*struct*)
Kelly, T.R. *et al., J.A.C.S.*, 1985, **107**, 3879 (*synth*)
Shiono, Y. *et al., Z. Naturforsch., C*, 2002, **57**, 923-929 (*isol, pmr, cmr, activity*)
Kock, I. *et al., J. Antibiot.*, 2005, **58**, 530-534 (*isol, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HAL000

Reticulatate R-29

[552846-52-3]



$C_{18}H_{12}N_2O_2$ 288.305
Alkaloid from the sponges *Fascaplysinopsis reticulata* and *Thorectandra* sp. Light yellow solid. λ_{max} 215 (log ϵ 3.72); 260 (log ϵ 3.71); 312 (log ϵ 3.6); 388 (log ϵ 2.94) (MeOH).

Me ester: ***Reticulatine****. 1-Deoxysecofascaplysin A. Methyl reticulatate*
[552846-51-2]
$C_{19}H_{15}N_2O_2^{\oplus}$ 303.34
Alkaloid from the sponges *Fascaplysinopsis reticulata* and a *Thorectandra* sp. Light yellow solid. Counterion not specified. λ_{max} 218 (log ϵ 3.89); 261 (log ϵ 3.85); 313 (log ϵ 3.71); 348 (log ϵ 3.18); 394 (log ϵ 3.14) (MeOH).

Me ester, salt with Dehydroluffariellolide diacid, D-60: ***Reticulatine B***
[135091-12-2]
$C_{44}H_{52}N_2O_6$ 704.905
Isol. from *Fascaplysinopsis reticulata*. Red amorph. solid. Consists of alkaloid cation with sesterterpenoid anion. λ_{max} 250; 308; 340 (sh); 382 (MeOH) (Derep).

Me ester, salt with, 16-Oxo: ***Reticulatine A***
[135091-11-1]
$C_{44}H_{50}N_2O_7$ 718.888
Alkaloid from the sponge *Fascaplysinopsis reticulata*. Red amorph. solid. Consists of alkaloid cation with sesterterpenoid anion. λ_{max} 250; 308; 340 (sh); 382 (MeOH) (Derep).

4′-Bromo: ***14-Bromoreticulatate***
[548773-66-6]
$C_{18}H_{11}BrN_2O_2$ 367.201
Alkaloid from the sponge *Fascaplysinopsis reticulata*. Yellow solid.

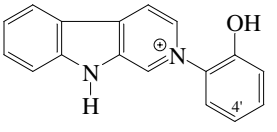
4′-Bromo, Me ester: ***14-Bromoreticulatine***
[693790-76-0]
$C_{19}H_{14}BrN_2O_2^{\oplus}$ 382.236
Alkaloid from the Indo-Pacific sponge *Fascaplysinopsis reticulata*. Yellow solid (as chloride).

4′,7-Dibromo, Me ester: ***Methyl 7,14-dibromoreticulatate***
[693790-77-1]
$C_{18}H_{10}Br_2N_2O_2$ 446.097
Alkaloid from *Fascaplysinopsis reticulata*. Yellow solid. Different numbering systems used. CAS no. not found CA 139-142.

Jiménez, C. *et al., Tet. Lett.*, 1991, **32**, 1843-1846 (*Reticulatines A,B*)
Segraves, N.L. *et al., Tet. Lett.*, 2003, **44**, 3471-3475 (*isol, pmr, cmr*)
Segraves, N.L. *et al., J. Nat. Prod.*, 2004, **67**, 783-792 (*isol, activity*)
Charan, R.D. *et al., Nat. Prod. Res.*, 2004, **18**, 225-229 (*Thorectandra alkaloids*)

Reticulatol R-30

[694436-62-9]

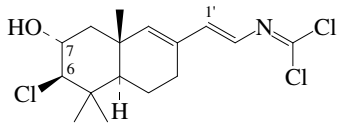


$C_{17}H_{13}N_2O^{\oplus}$ 261.303
Alkaloid from the sponge *Fascaplysinopsis reticulata*. Yellow solid (as chloride).

4′-Bromo: ***14-Bromoreticulatol***
[693790-79-3]
$C_{17}H_{12}BrN_2O^{\oplus}$ 340.199
Alkaloid from *Fascaplysinopsis reticulata*. Yellow solid (as chloride).
Segraves, N.L. *et al., J. Nat. Prod.*, 2004, **67**, 783-792 (*isol, pmr, cmr, 4′-bromo*)

Reticulidin A R-31

*[2-(6-Chloro-3,4,4*a*,5,6,7,8,8*a*-octahydro-7-hydroxy-5,5,8*a*-trimethyl-2-naphthalenyl)ethenyl]carbonimidic dichloride*
[245122-48-9]



$C_{16}H_{22}Cl_3NO$ 350.714
Constit. of *Reticulidia fungia*. Glass. $[\alpha]_D^{26}$ +11 (c, 0.32 in $CHCl_3$). λ_{max} 289 (log ϵ 4.3) (MeOH).

7-Deoxy: 7-Deoxyreticulidin A
[321582-36-9]
$C_{16}H_{22}Cl_3N$ 334.715
Constit. of *Stylotella aurantium*. Oil. $[\alpha]_D^{25}$ +40 (c, 0.13 in $CHCl_3$). λ_{max} 288 (log ϵ 4.2) (MeOH).

7-Deoxy, 1′Z-isomer: [67600-98-0]
$C_{16}H_{22}Cl_3N$ 334.715
Constit. of *Pseudaxinyssa pitys*.

7-Epimer: [67600-96-8]
$C_{16}H_{22}Cl_3NO$ 350.714
Constit. of the sponge *Pseudaxinyssa pitys*.

7-Epimer, 1′Z-isomer: [67600-95-7]
$C_{16}H_{22}Cl_3NO$ 350.714
Constit. of *Pseudaxinyssa pitys*. Cryst.
Mp 171-172°. $[\alpha]_D^{20}$ -15 (c, 0.2 in $CHCl_3$).

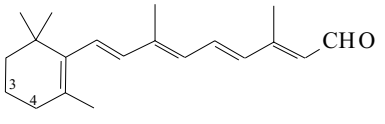
7-Epimer, $\Delta^{2,3}$-isomer: ***Reticulidin B***
$C_{16}H_{22}Cl_3NO$ 350.714
Constit. of *Reticulidia fungia*. Glass. $[\alpha]_D^{26}$ -26 (c, 0.92 in $CHCl_3$).
No CAS no. (CAS error). λ_{max} 291 (log ϵ 4.2) (MeOH).

7-Epimer, $\Delta^{2,3}$-isomer, 1′Z-isomer: [67600-97-9]
$C_{16}H_{22}Cl_3NO$ 350.714
Constit. of *Pseudaxinyssa pitys*.

Wratten, S.J. *et al., Tet. Lett.*, 1978, 1391-1394; 1395-1398 (*isol, pmr, cryst struct*)
Tanaka, J. *et al., J. Nat. Prod.*, 1999, **62**, 1339-1340 (*Reticulidins A,B*)
Musman, M. *et al., J. Nat. Prod.*, 2001, **64**, 111-113 (*7-deoxy*)

Retinal, 9CI R-32

10,15-Cyclo-2,4,6,8,10-phytapentaen-1-al. Retinene 1. Retinaldehyde. Vitamin A_1 aldehyde



$C_{20}H_{28}O$ 284.441

(all-E)-form [116-31-4]
Forms part of the Rhodopsin complex in the mammalian eye.
Cryst. Sol. EtOH, hexane; poorly sol. H_2O.
Mp 64-65°. λ_{max} 373 (E1%/1cm 1548) (cyclohexane).
▶VH6407000

Semicarbazone:
Yellow cryst. ($CHCl_3/Et_2O$). Mp 199-201°.

3,4-Didehydro: 10,15-Cyclo-2,4,6,8,10-phytahexaen-1-al. ***Vitamin A_2 aldehyde****. Dehydroretinal. Didehydroretinal. Retinene 2*
[472-87-7]
$C_{20}H_{26}O$ 282.425
Constit. fish of liver oils. Orange-red cryst.
Mp 77-78°.

(7E,9E,11E,13Z)-form
*13-*cis*-Retinal*
[472-86-6]
Cryst. (petrol); orange oil. Mp 77°.

(7E,9E,11Z,13E)-form
*11-*cis*-Retinal*
[564-87-4]
Cryst. (petrol). Mp 63.5-64.4°.

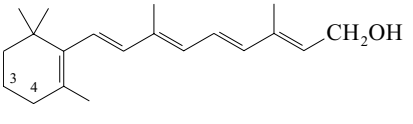
*4*R*-Hydroxy: 10,15-Cyclo-12-hydroxy-2,4,6,8,10-phytapentaen-1-al.* ***4-Hydroxy-11-cis-retinal***
[140387-20-8]
[117305-82-5]
$C_{20}H_{28}O_2$ 300.44
Constit. of the bioluminescent squid, *Watasenia scintillans*. Oil.
$[\alpha]_D$ -76.

(7E,9Z,11E,13E)-form
*9-*cis*-Retinal*
[514-85-2]
Mp 56-58°.
▶VH6406500

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 746B (*nmr*)
Ball, S. *et al., Biochem. J.*, 1948, **42**, 516-523 (*synth*)
Arens, J.F. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1949, **68**, 604-608 (*synth*)
Robeson, C.D. *et al., J.A.C.S.*, 1955, **77**, 4120-4125 (*isomers, synth*)
Brown, P.K. *et al., J. Biol. Chem.*, 1956, **222**, 865-877 (*11Z-form, 13Z-form, synth, uv*)
Von Plouta, C. *et al., Helv. Chim. Acta*, 1962, **45**, 548-561 (*isomers, synth*)
Sebrell, W.H. *et al., The Vitamins*, Academic Press, Vol. 1, 1967, (*rev*)
Patel, D.J. *et al., Nature (London)*, 1969, **221**, 825-828 (*pmr*)
Hamanaka, T. *et al., Acta Cryst. B*, 1972, **28**, 214-222 (*all-E form, cryst struct*)
Gilardi, R.G. *et al., Acta Cryst. B*, 1972, **28**, 2605-2612 (*11Z-form, cryst struct*)
Yasaka, W.J. *et al., J. Nutr. Sci. Vitaminol.*, 1973, **19**, 369-373 (*isol*)
Honig, B. *et al., Annu. Rev. Biophys. Bioeng.*, 1974, **3**, 151-177 (*rev*)
Englert, G. *et al., Helv. Chim. Acta*, 1975, **58**, 2367-2390 (*cmr*)
Shriver, J. *et al., J.A.C.S.*, 1976, **98**, 2407-2409 (*cmr*)
Simmons, C.J. *et al., Acta Cryst. B*, 1981, **37**, 2197-2205 (*13Z-form, synth, cryst struct*)
Asato, A.E. *et al., J.A.C.S.*, 1983, **105**, 2923-2924 (*synth*)
Liu, R.S.H. *et al., Tetrahedron*, 1984, **40**, 1931-1969 (*rev*)
Matsui, S. *et al., Biochim. Biophys. Acta*, 1988, **966**, 370-374 (*4-Hydroxy-11-cis-retinal*)
Zhu, Y. *et al., Tetrahedron*, 1992, **48**, 10061-10078 (*ir, uv, pmr*)
Duhamel, L. *et al., Tet. Lett.*, 1993, **34**, 319-322; 1994, **35**, 1209-1210 (*synth*)
Katsuta, Y. *et al., J.O.C.*, 1994, **59**, 6917-6921 (*4-Hydroxyretinal, synth*)
Bienayme, H. *et al., Tetrahedron*, 1994, **50**, 3389-3396 (*synth*)
Taylor, R.J.K. *et al., J.C.S. Perkin 1*, 1995, 2385-2392 (*13Z-form, synth, ir, pmr, cmr, ms*)
Uenishi, J. *et al., Angew. Chem., Int. Ed.*, 1998, **37**, 320-322 (*11Z-form, synth*)
Wada, A. *et al., J.O.C.*, 2000, **65**, 2438-2443 (*synth*)
Leuenberger, M.G. *et al., Angew. Chem., Int. Ed.*, 2001, **40**, 2614-2617 (*biosynth*)
van Wijk, A.A.C. *et al., Eur. J. Org. Chem.*, 2003, 863-868 (*4-Hydroxyretinal, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VSK975

Retinol, 9CI, BAN, INN R-33

3,7-Dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4,6,8-nonatetraen-1-ol. 15-Apo-β-caroten-15-ol. Afaxin. Axerol. Axerophthol. Gadol. Prepalin. Testavol. Vitamin A. Vitamin A alcohol. Vitamin A_1 alcohol
[68-26-8]



$C_{20}H_{30}O$ 286.456
Constit. of many fish-liver oils, milk, egg-yolk, etc. Nutrient, dietary supplement. Yellow cryst. Sol. MeOH, Et_2O; poorly sol. H_2O.

Mp 63-64°. $Bp_{0.000001}$ 137-138°. Log P 6.2 (calc). λ_{max} 328 (E1%/1cm 1780) (EtOH) (Berdy).

▶ Acute and chronic toxic effects in humans (large doses). Exp. and human teratogen. Exp. reprod. effects. LD_{50} (rat, orl) 2000 mg/kg. VH6750000

Ac: Retinol acetate. Vitamin A acetate. Many other names
[127-47-9]
$C_{22}H_{32}O_2$ 328.494
Dietary supplement. Cryst. (MeOH). Mp 57-58°.

▶ LD_{50} (mus, orl) 4100 mg/kg. Exp. reprod. and teratogenic effects. VH6825000

Propanoyl: Retinol propanoate. Axerofluid. Axerophthol propionate. Vitamin A propionate
[7069-42-3]
$C_{23}H_{34}O_2$ 342.52
n_D^{25} 1.6042. Fluid to -10°.

Hexadecanoyl: Retinol palmitate. Vitamin A palmitate. Arovit. Many other names
[79-81-2]
$C_{36}H_{60}O_2$ 524.869
Found in fish liver oils. Dietary supplement, permitted in infant formulas. Dietary supplement.
Mp 28-29°.

▶ LD_{50} (mus, orl) 4760 mg/kg. Exp. reprod. and teratogenic effects. VH6860000

3,4-Didehydro: ***3,4-Didehydroretinol****. Dehydroretinol. 3-Dehydroretinol. Vitamin A_2*
[79-80-1]
$C_{20}H_{28}O$ 284.441
Constit. of fresh-water fish oils. Golden-yellow oil. Mixt. of stereoisomers. Has 40% biological activity of Vit. A_1.

15-Aldehyde: See Retinal, R-32

15-Carboxylic acid: See Retinoic acid in *The Combined Chemical Dictionary.*

(11*Z*)-*form* [22737-96-8]
Shows about 25% of the biological potency of vitamin A in the rat growth test. Viscous yellow oil.

4-Nitrobenzoyl: Mp 67°.

(13*Z*)-*form*
Neovitamin A
[2052-63-3]
Shows about 75% of the biological potency of vitamin A in the rat growth test. Constit. of cod liver oil.
Mp 58-59°.

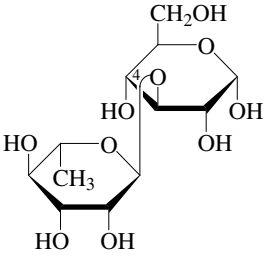
4-Nitrobenzoyl: Mp 94-95°.

[631-87-8, 631-88-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 149C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 262C (*nmr*)
Robeson, C.D. *et al., J.A.C.S.*, 1955, **77**, 4111-4119 (*13Z-form, synth, uv, ir*)
Oroshnik, W. *et al., J.A.C.S.*, 1956, **78**, 2651-2652 (*11Z-form, synth, uv, props*)
Isler, O. *et al., Adv. Org. Chem.*, 1963, **4**, 115 (*synth, rev*)
Fr. Pat., 1966, 1 452 791; *CA*, **66**, 105072r (*synth, propanoate*)
Isler, O. *et al., Chim. Ind. (Milan)*, 1967, **49**, 1317 (*rev*)
Sebrell, W.H. *et al., The Vitamins*, Academic Press, Vol. 1, 1967, (*rev*)
Westermann, F.H. *et al., Int. J. Vitam. Nutr. Res.*, 1972, **42**, 104 (*metab, palmitate*)
Oberhänsli, W.E. *et al., Acta Cryst. B*, 1974, **30**, 161 (*cryst struct*)
Mukaiyama, T. *et al., Chem. Lett.*, 1975, 1201 (*synth*)
Englert, G. *et al., Helv. Chim. Acta*, 1975, **58**, 2367 (*cmr*)
Baumann, C. *et al., Method. Chim.*, 1978, **11**, 200 (*rev, Vitamin A_2*)
Cardillo, G. *et al., J.C.S. Perkin 1*, 1979, 1729 (*synth*)
Mehta, R.R. *et al., J.C.S. Perkin 1*, 1982, **12**, 2921 (*synth, acetate*)
Pitt, G.A. *et al., Proc. Nutr. Soc.*, 1983, **42**, 43 (*struct, activity, rev*)
Pure Appl. Chem., 1983, **55**, 722 (*nomencl*)
Williams, J.B. *et al., J. Lipid Res.*, 1984, **25**, 638 (*metab, acetate*)
Goodman, D.S. *et al., Retinoids*, 1984, **2**, 1; 177 (*metab, biosynth, rev*)
Liu, R.S.H. *et al., Tetrahedron*, 1984, **40**, 1931 (*rev*)
Otera, J. *et al., Chem. Lett.*, 1985, 1883-1886 (*13Z-form*)
Harbison, G.S. *et al., J.A.C.S.*, 1985, **107**, 4809 (*cmr, acetate*)
Ajima, A. *et al., Biotechnol. Lett.*, 1986, **8**, 547 (*synth, hexadecanoate*)
Otera, J. *et al., J.O.C.*, 1986, **51**, 3834 (*synth*)
Sundaresan, P. *et al., J. Sci. Ind. Res.*, 1987, **46**, 105 (*rev, metab*)
Vaezi, H.F. *et al., Org. Prep. Proced. Int.*, 1987, **19**, 187 (*synth, Vitamin A_2*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 5941; 6719; 8103
Hosoda, A. *et al., Tet. Lett.*, 1987, **28**, 65 (*synth*)
Solladie, G. *et al., Tet. Lett.*, 1988, **29**, 209-212 (*13Z-form*)
Vogt, P. *et al., Tet. Lett.*, 1991, **32**, 4115 (*synth*)
Soukup, M. *et al., Tet. Lett.*, 1991, **32**, 4117 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1051
Vitamin A in Health and Disease, (ed. Blomhoff, R.), M. Dekker, 1994, (*book*)
Biesalski, H.-K. *et al., Annalen*, 1995, 717 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2920-2926 (*use, esters*)
Rauchschwalbe, G. *et al., Eur. J. Org. Chem.*, 2001, 3903-3909 (*synth*)
Jeong, Y.C. *et al., Tetrahedron*, 2004, **60**, 10181-10185 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VSK600; VSP000; VSK900

3-*O*-α-L-Rhamnopyranosyl-D-glucose R-34

3-O-*(6-Deoxy-α-L-mannopyranosyl)-D-glucose, 9CI.* ***Rungiose***
[36506-90-8]



α-D-Pyranose-*form*

$C_{12}H_{22}O_{10}$ 326.3
$[\alpha]_D^{20}$ -15.1 (c, 1.25 in H_2O).

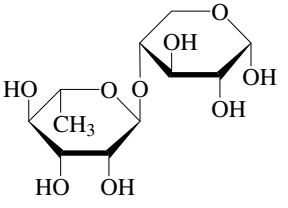
4-O-*(4-Hydroxy*-E-*cinnamoyl):* ***Cistanoside I***
[104806-91-9]
$C_{21}H_{28}O_{12}$ 472.445
Isol. from *Cistanche salsa* (crude drug Cistanche herba). The crude drug is a tonic in oriental medicine. Hemihydrate. $[\alpha]_D^{20}$ -82.2 (c, 1.5 in MeOH).

4-O-*(3,4-Dihydroxy*-E-*cinnamoyl):* ***Cistanoside F***
[97411-47-7]
$C_{21}H_{28}O_{13}$ 488.444
Isol. from *Cistanche salsa*. Amorph. powder. $[\alpha]_D^{25}$ -83.5 (c, 0.9 in MeOH).

6-O-*(3,4-Dihydroxy*-E-*cinnamoyl):* ***Isocistanoside F***
$C_{21}H_{28}O_{13}$ 488.444
Constit. of *Acanthus ilicifolius*. Amorph. powder. $[\alpha]_D^{25}$ -85 (c, 0.8 in H_2O).

Birkofer, L. *et al., Annalen*, 1973, 731-739 (*synth*)
Imperato, F. *et al., J.O.C.*, 1976, **41**, 3478-3479 (*synth*)
Kobayashi, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1452-1457 (*Cistanoside F*)
Karasawa, H. *et al., Yakugaku Zasshi*, 1986, **106**, 562-566 (*Cistanoside I*)
Wu, J. *et al., Magn. Reson. Chem.*, 2004, **42**, 659-662 (*Cistanoside F, Isocistanoside F*)

4-*O*-α-L-Rhamnopyranosyl-D-xylose R-35



α-Pyranose-*form*

$C_{11}H_{20}O_9$ 296.274
Autohydrolytic product from the mucilage of the green seaweed alga *Urospora penicilliformis.*

α-Pyranose-*form*

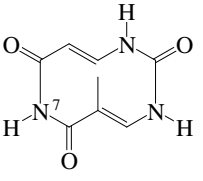
Me glycoside: Methyl 4-O-α-L-rhamnopyranosyl-α-D-xylopyranoside, 9CI
[99104-71-9]
$C_{12}H_{22}O_9$ 310.3
Monohydrate. $[\alpha]_D^{10}$ +47 (c, 3.5 in MeOH).

Me glycoside, 2,3-dibenzoyl, tri-Ac: Methyl 2,3-dibenzoyl-4-O-(2,3,4-tri-O-acetyl-α-L-rhamnopyranosyl)-α-D-xylopyranoside
[99104-82-2]
$C_{32}H_{36}O_{14}$ 644.628
Amorph. $[\alpha]_D^{15}$ -40 (c, 1.2 in $CHCl_3$).

Bourne, E.J. *et al., J. Carbohydr., Nucleosides, Nucleotides*, 1974, **1**, 235 (*occur*)
Kamiya, S. *et al., Agric. Biol. Chem.*, 1985, **49**, 2351 (*Me gly*)

Rhapallin A R-36

5-Methyl-1,3,7-triazecine-2,6,8(1H,3H,7H)-trione, 9CI. 5-Methyl-1,3,7-triazacyclodeca-4,9-diene-2,6,8-trione



(*E,E*)-*form*

$C_8H_9N_3O_3$ 195.177

(*E,E*)-*form*
Isol. from the sponge *Rhaphisia pallida*.

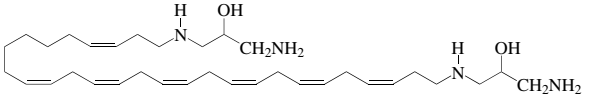
(*Z,Z*)-*form* [193224-03-2]
Alkaloid from the sponge *Rhaphisia pallida*.

N^7-*Bromo: 7-Bromo-5-methyl-1,3,7-triazecine-2,6,8(1H,3H,7H)-trione*
[193224-05-4]
$C_8H_8BrN_3O_3$ 274.074
Alkaloid from the sponge *Rhaphisia pallida*.

Cen, Y.Z. *et al., CA*, 1997, **127**, 147229f (*isol, uv, pmr, cmr, ms*)
Zeng, L. *et al., Pure Appl. Chem.*, 1999, **71**, 1147-1151

Rhapsamine R-37

1,28-Bis[(3-amino-2-hydroxypropyl)amino]-3,6,9,12,15,18,25-octacosaheptaene
[198826-15-2]

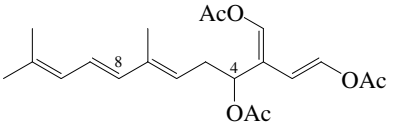


$C_{34}H_{60}N_4O_2$ 556.874
Alkaloid from the sponge *Leucetta leptorhapsis*. Amorph. solid. Racemic. λ_{max} 232 (ε 6340) (MeOH).

Jayatilake, G.S. *et al., Tet. Lett.*, 1997, **38**, 7507-7510 (*isol, uv, pmr, cmr*)

Rhipocephalin R-38

[71135-78-9]



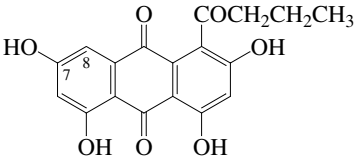
$C_{21}H_{28}O_6$ 376.449
Constit. of *Rhipocephalus phoenix*. Fish antifeedant. Phospholipase A2 inhibitor. Oil. $[\alpha]_D$ 0. λ_{max} 257 (ε 30000); 266 (ε 33000); 277 (ε 35000); 287 (ε 27000) (MeOH) (Berdy).

8,9-Dihydro: ***Dihydrorhipocephalin***. *4-Acetoxyflexilin*
[93888-65-4]
$C_{21}H_{30}O_6$ 378.464
Isol. from *Penicillus capitatus* and *Udotea cyathiformis*. Antibacterial agent and ichthyotoxin. $[\alpha]_D^{25}$ +18 (c, 1.2 in $CHCl_3$). λ_{max} 241 (ε 1300) (MeOH).

Sun, H.H. *et al., Tet. Lett.*, 1979, **20**, 685-688 (*isol*)
Paul, V.J. *et al., Tetrahedron*, 1984, **40**, 2913-2918 (*Dihydrorhipocephalin*)
Commeiras, L. *et al., Synlett*, 2003, 1719-1721 (*Dihydrorhipocephalin, synth*)

Rhodocomatulin R-39

2,4,5,7-Tetrahydroxy-1-(1-oxobutyl)-9,10-anthracenedione, 9CI. 1-Butanoyl-2,4,5,7-tetrahydroxyanthraquinone
[15478-53-2]



$C_{18}H_{14}O_7$ 342.304
The trivial names of the derivs. derive from nonsystematic numbering.

7-Me ether: Rhodocomatulin 6-methyl ether
[15979-72-3]
$C_{19}H_{16}O_7$ 356.331
Constit. of the crinoids *Comatula pectinata* and *Comatula cratera*. Orange-red cryst. (EtOH).
Mp 250-252° dec.

7-Me ether, 2-O-sulfate: [72241-34-0]
$C_{19}H_{16}O_{10}S$ 436.395
Isol. from *Comatula pectinata*.

5,7-Di-Me ether: Rhodocomatulin 6,8-dimethyl ether
[15979-71-2]
$C_{20}H_{18}O_7$ 370.358
Major pigment of *Comatula pectinata* and *Comatula cratera*. Orange-yellow cryst. (Me_2CO).
Mp 208.5-209.5°.

5,7-Di-Me ether, 2-O-sulfate: [72241-35-1]
[80604-81-5 (Na salt)]
$C_{20}H_{18}O_{10}S$ 450.422
Constit. of *Comatula pectinata*. Orange cryst. + $5H_2O$ (MeOH/EtOAc) (as Na salt). Dec. on heating.

Tetra-Me ether:
Yellow cryst. (C_6H_6). Mp 211-212° (203.5-204°).

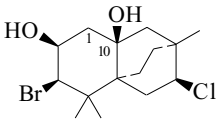
8-Hydroxy, 7-Me ether: 1-Butanoyl-2,4,5,8-tetrahydroxy-7-methoxyanthraquinone. Rubrocomatulin monomethyl ether
[15979-73-4]
$C_{19}H_{16}O_8$ 372.331
Constit. of *Comatula pectinata* and *Comatula cratera*. Scarlet prisms (AcOH).
Mp 298-299° dec.

8-Hydroxy, 7-Me ether, 2-O-sulfate: [72241-36-2]
$C_{19}H_{16}O_{11}S$ 452.395
Isol. from *Comatula pectinata*.

Sutherland, M.D. *et al., Aust. J. Chem.*, 1967, **20**, 515-533; 535-540 (*isol, struct*)
Banville, J. *et al., J.C.S. Perkin 1*, 1976, 1852-1856 (*tetra-Me ether, synth, pmr*)
Grandimaison, J.-L. *et al., J.O.C.*, 1978, **43**, 1435-1438 (*synth*)
Rideout, J.A. *et al., Experientia*, 1979, **35**, 1273-1274 (*sulfates, isol*)
Rideout, J.A. *et al., Aust. J. Chem.*, 1981, **34**, 2385-2392 (*isol*)
Simoneau, B. *et al., J. Nat. Prod.*, 1987, **50**, 1080-1082 (*7-Me ether, 5,7-di-Me ether, synth*)

Rhodolauradiol R-40

[83108-35-4]

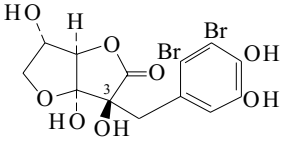


$C_{15}H_{24}BrClO_2$ 351.71
Constit. of a *Laurencia* sp. Oil.

10-Deoxy, 1,10-didehydro: ***Rhodolaureol***
[83108-36-5]
$C_{15}H_{22}BrClO$ 333.695
Constit. of a *Laurencia* sp. Cryst. (hexane).
Mp 57-58°. $[\alpha]_D$ +139 (c, 1.2 in $CHCl_3$).
González, A.G. *et al., Chem. Comm.*, 1985, 260

Rhodomelol R-41

[100676-10-6]

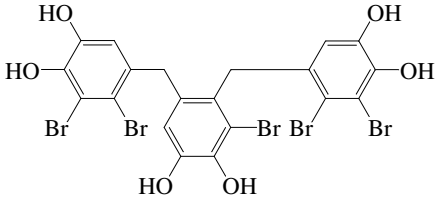


$C_{13}H_{12}Br_2O_8$ 456.041
Constit. of *Polysiphonia lanosa*.

3-Me ether: ***Methylrhodomelol***
[100676-08-2]
$C_{14}H_{14}Br_2O_8$ 470.068
From *Polysiphonia lanosa*.
Glambitza, K.-W. *et al., Planta Med.*, 1985, 437

Rhodomevoidin R-42

3-Bromo-4,5-bis(2,3-dibromo-4,5-dihydroxybenzyl)-1,2-benzenediol

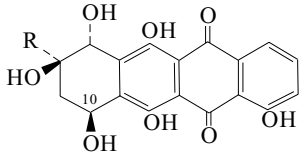


$C_{20}H_{13}Br_5O_6$ 748.839
Constit. of *Rhodomela confervoides*. Needles (Me_2CO).
Mp 237-238°.

Xu, N.J. *et al., Chin. Chem. Lett.*, 2003, **14**, 807-809 (*isol, pmr, cmr*)

α_1-Rhodomycinone R-43

7,8,9,10-Tetrahydro-1,6,7,8,10,11-hexahydroxy-8-methyl-5,12-naphthacenedione, 9CI
[21204-31-9]



R = CH_3

$C_{19}H_{16}O_8$ 372.331
Isol. from *Streptomyces* sp.

*10-*O*-(3-Amino-2,3,6-trideoxy-α-L-*lyxo*-hexopyranoside):* ***Antibiotic R 20X10***. *R 20X10*
$C_{25}H_{27}NO_{10}$ 501.489
Prod. by *Actinomadura roseoviolacae*.

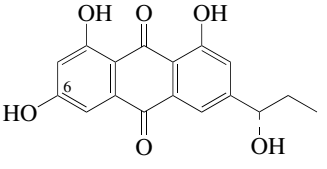
7-Deoxy: 7,8,9,10-Tetrahydro-1,6,8,10,11-pentahydroxy-8-methyl-5,12-naphthacenedione, 9CI. ***Komodoquinone B***
$C_{19}H_{16}O_7$ 356.331
Isol. from marine *Streptomyces* sp. KS3. Red solid. $[\alpha]_D^{25}$ +6 (c, 0.05 in $CHCl_3$). λ_{max} 234 (ε 15600); 245 (ε 1200); 292 (ε 3700); 492 (ε 6200); 526 (ε 4500) (MeOH).

*7-Deoxy, 10-*O*-[3-dimethylamino-3,6-dideoxy-α-L-galactopyranoside]:* ***Komodoquinone A***
$C_{27}H_{31}NO_{10}$ 529.543
Isol. from marine *Streptomyces* sp. KS3. Neuritogenic agent. Red solid. $[\alpha]_D^{25}$ +30 (c, 0.05 in MeOH). λ_{max} 233 (ε 19200); 252 (ε 18800); 289 (ε 9600); 492 (ε 5300); 525 (ε 3200) (MeOH).

Brockmann, H. *et al., Tet. Lett.*, 1968, 4719 (*abs config*)
Kende, A.S. *et al., Chem. Comm.*, 1977, 140 (*synth*)
Pandey, R.C. *et al., J. Chromatogr.*, 1980, **198**, 407 (*hplc*)
Krohn, K. *et al., Tetrahedron*, 1984, **40**, 4609-4616 (*synth*)
Japan. Pat., 1986, 86 152 693; *CA*, **106**, 17031 (*R 20X10*)
Itoh, T. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1402-1404 (*Komodoquinones, abs config*)
Itoh, T. *et al., J. Nat. Prod.*, 2003, **66**, 1373-1377 (*Komodoquinones*)

Rhodoptilometrin R-44

1,3,8-Trihydroxy-6-(1-hydroxypropyl)anthraquinone. 1′-Hydroxycrinemodin



$C_{17}H_{14}O_6$ 314.294

(*S*)-*form* [15979-74-5]
Constit. of the crinoids *Ptilometra australis* and *Comanthus bennetti*.
Orange-red needles (AcOH).
Mp 217-218°.

*6-*O*-Sulfate:* [172173-99-8]
$C_{17}H_{14}O_9S$ 394.358
Constit. of *Ptilometra* sp. Cytotoxic agent. Cryst. (as Na salt).

Tetra-Ac:
Yellow cryst. (MeOH). Mp 156-157°.

1′-Ketone: 1,3,8-Trihydroxy-6-(1-oxopropyl)-9,10-anthracenedione. 1,3,8-Trihydroxy-6-propanoylanthraquinone
[52422-01-2]
$C_{17}H_{12}O_6$ 312.278
Pigment from *Comanthus bennetti*. Orange needles (EtOH).
Mp 265-266°.

1′-Ketone, tri-Me ether: 1,3,8-Trimethoxy-6-propanoylanthraquinone
[77761-54-7]
$C_{20}H_{18}O_6$ 354.359
Isol. from flowers of *Antigonon leptopus*. Orange cryst.
Mp 182°.

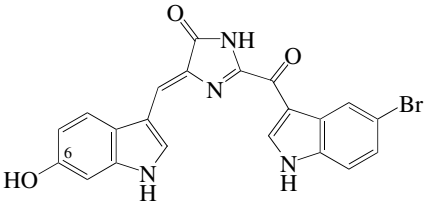
1′-Deoxy: 1,3,8-Trihydroxy-6-propylanthraquinone. ***Crinemodin***. *1′-Deoxyrhodoptilometrin*
[52421-99-5]
$C_{17}H_{14}O_5$ 298.295
Pigment from *Comanthus bennetti, Echinaster echinophorus, Ptilometra australis* and *Henricia leviuscula*. Orange plates ($MeOH/CHCl_3$).
Mp 219.5-221.5°.

*1′-Deoxy, 6-*O*-sulfate: Crinemodin 6-sulfate*
[172173-98-7]
$C_{17}H_{14}O_8S$ 378.359
Constit. of *Ptilometra* sp.
Powell, V.H. *et al., Aust. J. Chem.*, 1967, **20**, 541-553 (*isol, struct*)

Bartolini, G.L. *et al., Tetrahedron*, 1973, **29**, 3699-3702 (*Rhodoptilometrin, Crinemodin, 1′-ketone, isol, uv, ir, pmr, ms, struct*)
Banville, J. *et al., J.C.S. Perkin 1*, 1976, 613-619 (*synth*)
Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1977, **13**, 636; 1979, **15**, 148; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 528; 1979, **15**, 124 (*Crinemodin, sol*)
Rideout, J.A. *et al., Experientia*, 1979, **35**, 1273 (*Crinemodin, isol*)
Minocha, P.K. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 251 (*1′-ketone tri-Me ether*)
Lee, N.K. *et al., Bull. Korean Chem. Soc.*, 1995, **16**, 1011-1013 (*sulfates*)

Rhopaladin A R-45

[212069-48-2]



$C_{21}H_{13}BrN_4O_3$ 449.263
Alkaloid from the marine tunicate *Rhopalaea* sp. Amorph. red solid. λ_{max} 218 (ϵ 29000); 268 (ϵ 10000); 280 (ϵ 9700); 291 (ϵ 9600); 344 (ϵ 6700); 488 (ϵ 13000) (MeOH).

Debromo: ***Rhopaladin B***
[212069-49-3]
$C_{21}H_{14}N_4O_3$ 370.367
Alkaloid from *Rhopalaea* sp. Amorph. red solid. λ_{max} 213 (ϵ 19000); 267 (ϵ 6900); 281 (ϵ 5800); 293 (ϵ 5100); 350 (ϵ 4400); 485 (ϵ 8900) (MeOH).

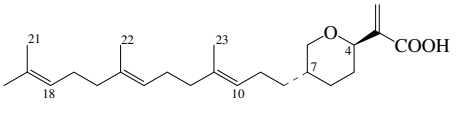
6-Deoxy: ***Rhopaladin C***
[212069-50-6]
$C_{21}H_{13}BrN_4O_2$ 433.263
Alkaloid from *Rhopalaea* sp. Amorph. red solid. λ_{max} 212 (ϵ 56000); 258 (sh); 282 (ϵ 4900); 291 (sh); 471 (ϵ 5600) (MeOH).

Debromo, 6-deoxy: ***Rhopaladin D***
[212069-51-7]
$C_{21}H_{14}N_4O_2$ 354.367
Alkaloid from *Rhopalaea* sp. Amorph. red solid. λ_{max} 211 (ϵ 22000); 259 (sh); 276 (ϵ 5400); 281 (sh); 468 (ϵ 4800) (MeOH).

Sato, H. *et al., Tetrahedron*, 1998, **54**, 8687-8690 (*Rhopaladings A-D, isol, uv, ir, pmr, cmr, ms*)
Janosik, T. *et al., Tetrahedron*, 2002, **58**, 2813-2819 (*synth*)

Rhopaloic acid A R-46

[175097-29-7]



Relative Configuration

$C_{24}H_{38}O_3$ 374.562
Constit. of *Hippospongia* sp. and *Rhopaloeides* sp. Oil. $[\alpha]_D^{25}$ +40 (c, 0.47 in $CHCl_3$).

6,7-Didehydro: ***Rhopaloic acid C***
[220080-95-5]
$C_{24}H_{36}O_3$ 372.547
Constit. of *Hippospongia* sp. and *Rhopaloeides* sp. Oil. $[\alpha]_D^{25}$ +84 (c, 0.03 in $CHCl_3$). λ_{max} 203 (log ϵ 4.23) (MeCN).

10,11-Dihydro, 10ξ,11ξ-dihydroxy: ***Rhopaloic acid G***
[457938-84-0]
$C_{24}H_{40}O_5$ 408.577
Constit. of a *Hippospongia* sp.

$\Delta^{11(23)}$-Isomer, 10ξ-hydroxy: ***Rhopaloic acid F***
[457938-83-9]
$C_{24}H_{38}O_4$ 390.562
Constit. of a *Hippospongia* sp.

$\Delta^{15(22)}$-Isomer, 14ξ-hydroxy: ***Rhopaloic acid E***
[457938-82-8]
$C_{24}H_{38}O_4$ 390.562
Constit. of a *Hippospongia* sp.

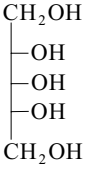
$\Delta^{19(21)}$-Isomer, 18ξ-hydroxy: ***Rhopaloic acid D***
[457938-81-7]
$C_{24}H_{38}O_4$ 390.562
Constit. of a *Hippospongia* sp.

4-Epimer: ***Rhopaloic acid B***
[220080-91-1]
$C_{24}H_{38}O_3$ 374.562
Constit. of *Hippospongia* sp. and *Rhopaloeides* sp. Oil. $[\alpha]_D^{25}$ +55 (c, 0.23 in $CHCl_3$). λ_{max} 202 (log ϵ 4.32) (MeCN).

Ohta, S. *et al., Tet. Lett.*, 1996, **37**, 2265-2266 (*isol, pmr, cmr*)
Snider, B.B. *et al., Tet. Lett.*, 1997, **38**, 5453-5454 (*synth*)
Takagi, R. *et al., J.C.S. Perkin 1*, 1998, 925-934 (*synth, abs config*)
Yanai, M. *et al., Tetrahedron*, 1998, **54**, 15607-15612 (*Rhopaloic acids B,C*)
Craig, K.S. *et al., Tet. Lett.*, 2002, **43**, 4801-4804 (*Rhopaloic acids D-G*)
Kadota, K. *et al., Heterocycles*, 2003, **59**, 485-490 (*synth*)

Ribitol, 9CI, 8CI R-47

Adonitol
[488-81-3]



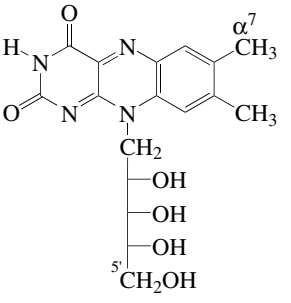
$C_5H_{12}O_5$ 152.147
A *meso* compd. but chiral derivs. (e.g. isopropylidene derivs.) have been prepd. The abs. config. of these is given by the numbering scheme for the D-ribitol skeleton. Occurs free in the plants *Adonis vernalis* and *Bupleurum falcatum* and in bound form in bacterial cell wall teichoic acids and in Riboflavine, R-48. Cryst. (EtOH). Mp 102°.
▶ VJ0800000

Pentakis(4-hydroxybenzoyl): ***Buccinulin***. *Kelletinin A*
[112727-22-7]
$C_{40}H_{32}O_{15}$ 752.684
Metab. of the marine mollusc *Buccinulum corneum*. HIV reverse transcriptase (HIV-rt) inhibitor. Exhibits antibacterial props.

Cimino, G. *et al., J. Nat. Prod.*, 1987, **50**, 1171-1173 (*Buccinulin*)
Ciminiello, P. *et al., Gazz. Chim. Ital.*, 1988, **118**, 105-107 (*Buccinulin, synth*)

Riboflavine, 9CI, BAN, INN R-48

1-Deoxy-1-(3,4-dihydro-7,8-dimethyl-2,4-dioxobenzo[g]pteridin-10(2H)-yl)-D-ribitol, 9CI. Flavaxin. Lactoflavine. Ovoflavine. Vitamin B_2. Vitamin G. Russupteridine yellow III. E101. Many other names
[83-88-5]



$C_{17}H_{20}N_4O_6$ 376.368
Widely distributed, but occurs naturally in free form only in the retina, in whey and in urine. Main forms occurring in tissues and cells are flavine mononucleotide and flavine-adenine dinucleotide.

Colour additive in food. Used as adsorption indicator in titrimetric detn. of Ag. Nutrient supplement. Vitamin cofactor. Orange needles. Sol. EtOH; spar. sol. H_2O.
Mp 280° dec. $[\alpha]_D$ -9.8 (H_2O). $[\alpha]_D$ -125 (20*N* NaOH). pK_{a1} 1.9; pK_{a2} 10.2 (25°). Green fluor. in soln. λ_{max} 220; 265; 365; 455 (H_2O).

▶ LD_{50} (rat, ipr) 560 mg/kg. VJ1400000

5′-Phosphate: Riboflavine 5′-(dihydrogen phosphate), 9CI. Flavin mononucleotide. Lactoflavin phosphate. Monophosphoriboflavin. Riboflavin monophosphate. Vitamin B_2 phosphate. FMN. Bisulase
[146-17-8]
[130-40-5]
$C_{17}H_{20}N_4O_9P$ 455.34
The prosthetic group of various flavine enzymes. Enzyme co-factor, vitamin. Sodium salt used as dietary and nutrient supplement. Yellow cryst. + $2H_2O$. Tends to isomerise to isomeric phosphates.

▶ LD_{50} (mus, ivn) 365 mg/kg. VJ1350000

4′,5′-Cyclic phosphate: ***Riboflavine 4′,5′-cyclic phosphate***
[986-54-9]
$C_{17}H_{19}N_4O_8P$ 438.333
Isol. from the brown alga *Scytosiphon lomentaria*. Autofluorescent agent.

5′-Adenosine diphosphate: See Flavine adenine dinucleotide in *The Combined Chemical Dictionary.*

5′-α-D-Ribofuranoside: ***Lampteroflavin***
[114590-52-2]
$C_{22}H_{28}N_4O_{10}$ 508.484
Isol. from the toxic luminous mushroom *Lampteromyces japonicus*. Fluorescent. λ_{max} 265 (ϵ); 368 (ϵ); 445 (ϵ) (H_2O) (Derep).

2′,3′,4′,5′-Tetra-Ac: [752-13-6]
Mp 250-252°.

2′,3′,4′,5′-Tetrabutanoyl: Riboflavine 2′,3′,4′,5′-tetrabutanoate, 9CI. Riboflavine butyrate. Riboflavine tetrabutyrate. Vitamin B_2 tetrabutyrate. Many other names
[752-56-7]
$C_{33}H_{44}N_4O_{10}$ 656.731
Widely used food additive. Antiatherosclerotic and antihyperlipidaemic agent. Transparent red plates (MeOH). Mp 149° (142-146°).

▶ VJ1755000

2′,3′-Bis(3-pyridinecarbonyl), 4′(5′)-phosphate: Riboflavine 2′,3′-di-3-pyridinecarboxylate monodihydrogen phosphate (ester), 9CI. FMN-dinicotinate
[36119-03-6]
$C_{29}H_{27}N_6O_{11}P$ 666.54
Used in treatment of diabetic neuropathy.

2′,3′,4′,5′-Tetrakis(3-pyridinecarbonyl): Riboflavine 2′,3′,4′,5′-tetra-3-pyridinecarboxylate, 9CI. Riboflavine nicotinate. RN-4
[14984-66-8]
$C_{41}H_{32}N_8O_{10}$ 796.751
Antilipidaemic agent. Mp 154-155°.

*3*N*-Me, tetra-Ac:* [21066-33-1]
Mp 189-191°.

5′-Carboxylic acid: ***Schizoflavin 1****. Vitamin B_2 acid*
[59224-03-2]
$C_{17}H_{18}N_4O_7$ 390.352
Metab. of *Schizophyllum commune* and other basidiomycetes. Shows antialgal activity vs. *Chartonella antigua* in red tides. Yellow needles (EtOH).
Mp 250° dec.

5′-Aldehyde: Vitamin B_2 aldehyde. ***Schizoflavin 2***
[59224-04-3]
$C_{17}H_{18}N_4O_6$ 374.352
Prod. by *Schizophyllum commune.*

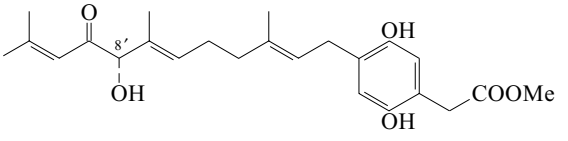
α^7-Hydroxy: α^7-Hydroxyriboflavine, 9CI. ***Nekoflavin***
[86073-07-6]
$C_{17}H_{20}N_4O_7$ 392.368
Isol. from the choroids of cats eye. Fine yellow cryst. (EtOH).
Mp 196.5-198°.

[6184-17-4, 129569-92-2, 129569-93-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 895B (*ir*)
Viscontini, M. *et al., Helv. Chim. Acta*, 1952, **35**, 457 (*synth, phosphate*)
Forrest, H.S. *et al., J.C.S.*, 1952, 2530 (*synth, 4′,5′-cyclic phosphate*)
Kotaki, A. *et al., J. Vitaminol.*, 1968, **14**, 247 (*synth, tetranicotinate*)
Tanaka, N. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 1546 (*cryst struct*)
Paterson, T. *et al., Chem. Comm.*, 1969, 290 (*biosynth*)
Beach, R. *et al., Tet. Lett.*, 1969, 3489 (*synth*)
Mayhew, S.S. *et al., Biochim. Biophys. Acta*, 1971, **235**, 289-302 (*synth, uv, 1,5-dihydro 5′-phosphate*)
Kainosho, M. *et al., Biochemistry*, 1972, **11**, 741 (*P-31 nmr, phosphate*)
Bishop, E. *et al., Indicators*, Pergamon, Oxford, 1972, (*use*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 2610 (*occur*)
McCormick, D.A. *et al., J. Het. Chem.*, 1974, **11**, 969
Tachibana, S. *et al., J. Nutr. Sci. Vitaminol.*, 1975, **21**, 347; 1979, **25**, 361; 1980, **66**, 333 (*Schizoflavins*)
Yagi, K. *et al., Biochemistry*, 1976, **15**, 2877 (*N-15 nmr*)
Yoneda, F. *et al., J.A.C.S.*, 1976, **98**, 830 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **24**, 108 (*rev, synth*)
Holmgren, A. *et al., Experientia*, 1980, **36**, 149 (*rev, FAD*)
Walt, D.R. *et al., J.A.C.S.*, 1980, **102**, 7805 (*synth, 5′-phosphate*)
Merrill, A.H. *et al., Methods Enzymol.*, 1980, **66**, 287 (*phosphate, synth*)
Tachibana, S. *et al., Methods Enzymol.*, 1980, **66**, 333 (*Schizoflavin 1*)
Van Schagen, C.G *et al., Eur. J. Biochem.*, 1981, **120**, 33-39 (*synth, cmr, 1,5-dihydro 5′-phosphate*)
Brown, G.M. *et al., Adv. Enzymol. Relat. Areas Mol. Biol.*, 1982, **53**, 345 (*rev, biosynth*)
Bacher, A. *et al., J.A.C.S.*, 1982, **104**, 3754 (*biosynth*)
Tachibana, S. *et al., Mol. Cell. Biochem.*, 1983, **51**, 149-160 (*Schizoflavins, isol, struct*)
Ulrich, E.L. *et al., Tet. Lett.*, 1983, **24**, 473 (*pmr*)
Keller, P.J. *et al., Tetrahedron*, 1983, **39**, 3471 (*biosynth*)
Moonem, C.T.W. *et al., Biochemistry*, 1984, **23**, 4859-4867 (*pmr, cmr, conformn, tetra-Ac, 5′-phosphate, 1,5-dihydro 5′-phosphate*)
Cooperman, J.M. *et al., Food Sci. Technol.*, 1984, **13**, 299 (*rev, metab, props*)
Nielsen, P. *et al., Methods Enzymol.*, 1986, **122**, 209 (*synth, phosphates*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 4425; 4473; 7551
Ebitani, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2273 (*cryst struct, tetrabutyrate*)
Al-Shammary, F.J. *et al., Anal. Profiles Drug Subst.*, 1990, **19**, 429 (*rev*)
Isobe, M. *et al., Tet. Lett.*, 1990, **31**, 717 (*Lampteroflavin*)
Uyakul, D. *et al., Tetrahedron*, 1990, **46**, 1367 (*Lampteroflavin*)
Takahashi, H. *et al., Tetrahedron*, 1991, **47**, 6215 (*Lampteroflavin*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1054
Matsui, K. *et al., J. Biochem. (Tokyo)*, 1996, **119**, 441-447 (*Nekoflavin*)
Yamano, K. *et al., Z. Naturforsch., C*, 1996, **51**, 155 (*4′,5′-cyclic phosphate*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2431-2435 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, RIF500; RIK000

Rietone R-49

[163597-23-7]



$C_{24}H_{32}O_6$ 416.513
Constit. of *Alcyonium fauri*. Orange oil. $[\alpha]_D^{19}$ +95 (c, 0.8 in $CHCl_3$). λ_{max} 209; 235; 297 (MeOH) (Berdy).

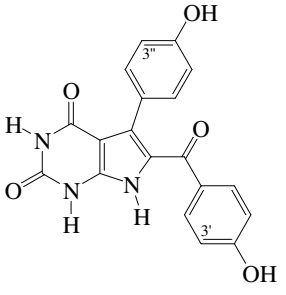
8-Ac: ***8′-Acetylrietone****. 8′-Acetoxyrietone (incorr.)*
[163498-09-7]
$C_{26}H_{34}O_7$ 458.55
Constit. of *Alcyonium fauri*.
$[\alpha]_D^{21}$ +133 (c, 0.9 in $CHCl_3$).

8′-Deoxy: ***8′-Deoxyrietone***
[163498-10-0]
$C_{24}H_{32}O_5$ 400.514
Constit. of *Alcyonium fauri*.

Hooper, G.J. *et al., Tet. Lett.*, 1995, **36**, 3265 (*isol, pmr, cmr*)

Rigidin A R-50

*6-(4-Hydroxybenzoyl)-5-(4-hydroxyphenyl)-1*H*-pyrrolo[2,3-*d*]pyrimidine-2,4(3*H*,7*H*)-dione, 9CI. Rigidin*
[132160-44-2]



$C_{19}H_{13}N_3O_5$ 363.329
Alkaloid from the marine tunicate *Eudistoma* cf. *rigida* and *Cystodytes* sp. Calmodulin antagonist. Purple solid.
Mp 300°. λ_{max} 232 (sh); 276 (ϵ 4500); 356 (ϵ 2500); 552 (ϵ 200) (MeOH/HCl) (Derep). λ_{max} 240 (sh); 285 (ϵ 4300); 346 (ϵ 4500); 401 (ϵ 2500) (MeOH/KOH) (Derep). λ_{max} 240 (sh); 285 (ϵ 4300); 346 (ϵ 2500); 401 (ϵ 2500) (MeOH) (Derep). λ_{max} 206 (ϵ 39780); 278 (ϵ 21070); 285 (ϵ 4300); 308 (ϵ 14860); 346 (ϵ 2500); 356 (ϵ 14110); 401 (ϵ 2500) (MeOH) (Berdy).

3-N-*Me:* ***Rigidin E***
$C_{20}H_{15}N_3O_5$ 377.356
Alkaloid from a *Eudistoma* sp. Dark green film. λ_{max} 276 (ϵ 7000); 362 (ϵ 4000) (MeOH).

3′-Methoxy: ***Rigidin B***
$C_{20}H_{15}N_3O_6$ 393.355
Alkaloid from the marine tunicate *Cystodytes* sp. Amorph. yellow solid. λ_{max} 236 (sh); 278 (ϵ 13200); 304 (sh); 319 (ϵ 9600); 364 (ϵ 9400) (MeOH).

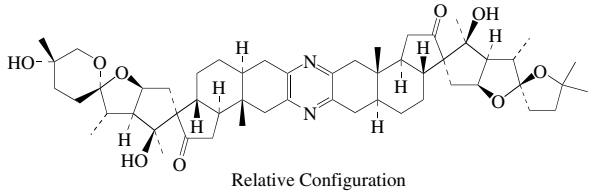
3″-Methoxy: ***Rigidin C***
$C_{20}H_{15}N_3O_6$ 393.355
Alkaloid from *Cystodytes* sp. Amorph. yellow solid. λ_{max} 236 (sh); 272 (ϵ 14400); 304 (sh); 317 (ϵ 11600); 352 (ϵ 9400) (MeOH).

3′,3″-Dimethoxy: ***Rigidin D***
$C_{21}H_{17}N_3O_7$ 423.381
Alkaloid from *Cystodytes* sp. Amorph. yellow solid. λ_{max} 238 (sh); 270 (ϵ 12000); 304 (sh); 322 (ϵ 11000); 352 (ϵ 9300) (MeOH).

Kobayashi, J. *et al., Tet. Lett.*, 1990, **31**, 4617-4620 (*isol, uv, ir, pmr, cmr, struct*)
Edstrom, E.D. *et al., J.O.C.*, 1993, **58**, 403-407 (*synth*)
Sakamoto, T. *et al., J.C.S. Perkin 1*, 1996, 459-464 (*synth*)
Tsuda, M. *et al., J. Nat. Prod.*, 2003, **66**, 292-294 (*Rigidins B,C,D*)
Davis, R.A. *et al., Mar. Drugs*, 2003, **1**, 27-33 (*Rigidin E*)

Ritterazine V R-51

[184770-01-2]



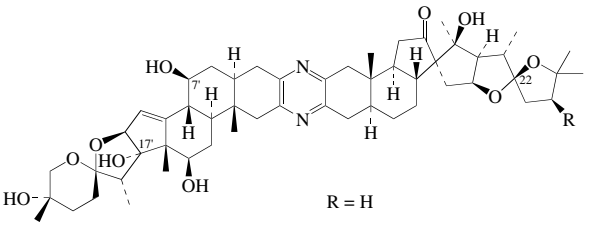
Relative Configuration

$C_{54}H_{76}N_2O_9$ 897.202
Alkaloid from the tunicate *Ritterella tokioka*.
$[\alpha]_D$ +109.2 (c, 0.05 in $CHCl_3$). λ_{max} 290 (ϵ 9209); 308 (sh) ($CHCl_3$).

Fukuzawa, S. *et al., J.O.C.*, 1997, **62**, 4484-4491 (*isol, uv, pmr, cmr*)

Ritterazine A R-52

[160391-62-8]



R = H

$C_{54}H_{76}N_2O_{10}$ 913.202
Alkaloid from the tunicate *Ritterella tokioka*. Shows potent cytotoxicity against P388 murine leukaemia cells. Glassy solid.
$[\alpha]_D$ +112 (c, 0.1 in MeOH). λ_{max} 287 (ϵ 8580); 308 (sh) (MeOH) (Derep).

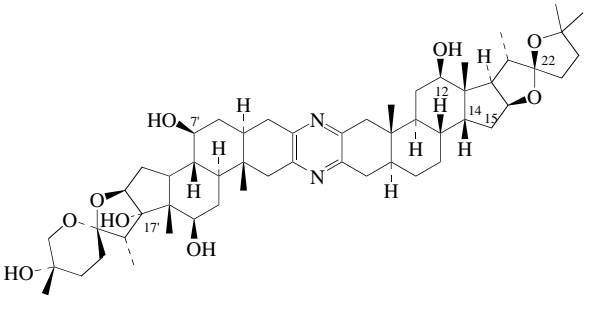
22-Epimer: ***Ritterazine D***
[165172-44-1]
$C_{54}H_{76}N_2O_{10}$ 913.202
From *Ritterella tokioka*. Shows potent cytotoxicity against P388 murine leukaemia cells. Glassy solid. $[\alpha]_D$ +81.4 (c, 0.1 in MeOH). λ_{max} 286 (ϵ 9200) (MeOH) (Berdy).

7′,17′-Dideoxy: ***Ritterazine T***
[184768-89-6]
$C_{54}H_{76}N_2O_8$ 881.203
Alkaloid from *Ritterella tokioka*.
$[\alpha]_D$ +106.6 (c, 0.1 in $CHCl_3$). λ_{max} 290 (ϵ 9870); 308 (sh) ($CHCl_3$).

Fukuzawa, S. *et al., J.O.C.*, 1994, **59**, 6164-6166; 1997, **62**, 4484-4491 (*isol, uv, ir, pmr, cmr, struct*)
Fukuzawa, S. *et al., Tetrahedron*, 1995, **51**, 6707-6716 (*Ritterazine D*)

Ritterazine B R-53

[160568-10-5]



$C_{54}H_{78}N_2O_9$ 899.218
Alkaloid from the tunicate *Ritterella tokioka*. Shows potent cytotoxicity against P388 murine leukaemia cells. Glassy solid.
$[\alpha]_D$ +43 (c, 0.1 in MeOH). λ_{max} 287 (ϵ 6880); 308 (sh) (MeOH) (Derep).

12-Ketone: ***Ritterazine H***
[165074-71-5]
$C_{54}H_{76}N_2O_9$ 897.202
From *Ritterella tokioka*. Shows potent cytotoxicity against P388 murine leukaemia cells. Glassy solid. $[\alpha]_D$ +96 (c, 0.1 in MeOH). λ_{max} 287 (ϵ 8920) (MeOH) (Berdy).

22-Epimer: ***Ritterazine F***
[165172-45-2]
$C_{54}H_{78}N_2O_9$ 899.218
From *Ritterella tokioka*. Shows potent cytotoxicity against P388 murine leukaemia cells. Glassy solid. $[\alpha]_D$ +59 (c, 0.1 in MeOH). λ_{max} 288 (ϵ 7900) (MeOH) (Berdy).

7′,17′-Dideoxy: ***Ritterazine Y***
[184770-06-7]
$C_{54}H_{78}N_2O_7$ 867.219
Alkaloid from *Ritterella tokioka*. Cytotoxic agent. $[\alpha]_D$ +57.4 (c, 0.1 in $CHCl_3$). λ_{max} 289 (ϵ 9156); 308 (sh) ($CHCl_3$).

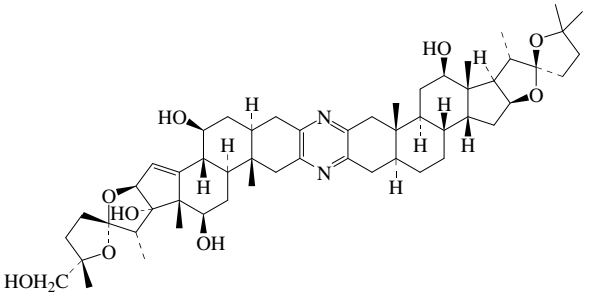
14,15-Didehydro, 22-epimer: ***Ritterazine G***
[164991-70-2]
$C_{54}H_{76}N_2O_9$ 897.202
From *Ritterella tokioka*. Shows potent cytotoxicity against P388 murine leukaemia cells. Glassy solid. $[\alpha]_D$ +91.4 (c, 0.1 in MeOH). λ_{max} 288 (ϵ 11200) (MeOH) (Berdy).

12-Ketone, 14-hydroxy, 22-epimer: ***Ritterazine I***
[164991-71-3]
$C_{54}H_{76}N_2O_{10}$ 913.202
From *Ritterella tokioka*. Shows potent cytotoxicity against P388 murine leukaemia cells. Glassy solid. $[\alpha]_D$ +74.5 (c, 0.1 in MeOH). λ_{max} 286 (ϵ 9120) (MeOH) (Berdy).

Fukuzawa, S. *et al., J.O.C.*, 1995, **60**, 608-614; 1997, **62**, 4484-4491 (*isol, uv, ir, pmr, cmr, struct*)
Fukuzawa, S. *et al., Tetrahedron*, 1995, **51**, 6707-6716 (*Ritterazines F-I*)

Ritterazine C R-54

[160604-68-2]



$C_{54}H_{78}N_2O_9$ 899.218
Alkaloid from the tunicate *Ritterella tokioka*. Shows potent cytotoxicity against P388 murine leukaemia cells. Glassy solid. $[\alpha]_D$ +72 (c, 0.1 in MeOH). λ_{max} 287 (ϵ 6880); 308 (sh) (MeOH) (Derep). λ_{max} 285 (ϵ 8720); 303 (MeOH) (Berdy).

Fukuzawa, S. *et al., J.O.C.*, 1995, **60**, 608-614 (*isol, uv, ir, pmr, cmr, struct*)

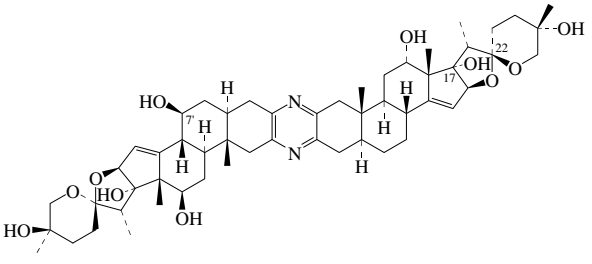
Ritterazine E R-55

24-Methylritterazine D
[164991-69-9]
As Ritterazine A, R-52 with
R = CH_3, 22-epimer
$C_{55}H_{78}N_2O_{10}$ 927.229
Alkaloid from the tunicate *Ritterella tokioka*. Shows potent cytotoxicity against P388 murine leukaemia cells. Glassy solid. $[\alpha]_D$ +70.8 (c, 0.1 in MeOH). λ_{max} 288 (ϵ 10100) (MeOH) (Berdy).

Fukuzawa, S. *et al., Tetrahedron*, 1995, **51**, 6707-6716 (*isol, uv, ir, pmr, cmr, struct*)

Ritterazine J R-56

[164991-72-4]



$C_{54}H_{76}N_2O_{11}$ 929.201
Stereochem. revised in 2001. Alkaloid from the tunicate *Ritterella tokioka*. Shows potent cytotoxicity against P388 murine leukaemia cells. Glassy solid. $[\alpha]_D$ +66.1 (c, 0.1 in MeOH). λ_{max} 289 (ϵ 8420) (MeOH) (Berdy).

7′-Deoxy: ***Ritterazine K***
[164991-73-5]
$C_{54}H_{76}N_2O_{10}$ 913.202
From *Ritterella tokioka*. Shows potent cytotoxicity against P388 murine leukaemia cells. Glassy solid. $[\alpha]_D$ +74 (c, 0.1 in MeOH). λ_{max} 288 (ϵ 7100) (MeOH) (Berdy).

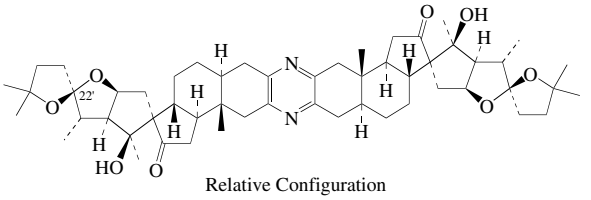
7′,17-Dideoxy: ***Ritterazine L***
[164991-74-6]
$C_{54}H_{76}N_2O_9$ 897.202
From *Ritterella tokioka*. Shows potent cytotoxicity against P388 murine leukaemia cells. Glassy solid. $[\alpha]_D$ +85.5 (c, 0.1 in MeOH). λ_{max} 288 (ϵ 11000) (MeOH) (Berdy).

7′,17-Dideoxy, 25-epimer: ***Ritterazine M***
[165172-46-3]
$C_{54}H_{76}N_2O_9$ 897.202
From *Ritterella tokioka*. Shows potent cytotoxicity against P388 murine leukaemia cells. Glassy solid. $[\alpha]_D$ +95.1 (c, 0.1 in MeOH). Struct. revised in 2002. λ_{max} 289 (ϵ 11900) (MeOH) (Berdy).

Fukuzawa, S. *et al., Tetrahedron*, 1995, **51**, 6707-6716 (*isol, uv, ir, pmr, cmr, struct*)
Jeong, J.U. *et al., J.A.C.S.*, 1999, **121**, 2071-2084 (*synth, Ritterazine K*)
Lee, S. *et al., Org. Lett.*, 2002, **4**, 313-316; 317-318 (*Ritterazine M, synth, struct*)

Ritterazine N R-57

[184764-19-0]



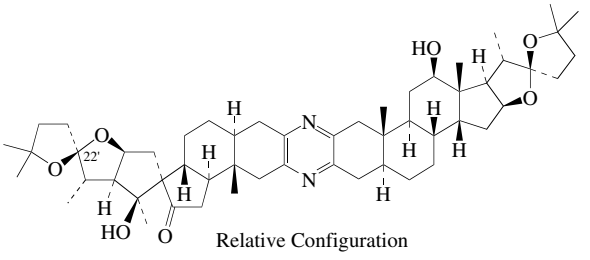
Relative Configuration

$C_{54}H_{76}N_2O_8$ 881.203
Alkaloid from the tunicate *Ritterella tokioka*. Cytotoxic agent. $[\alpha]_D$ +121.7 (c, 0.05 in $CHCl_3$). λ_{max} 289 (ϵ 9388); 309 (sh) ($CHCl_3$).

22′-Epimer: ***Ritterazine O***
[184971-68-4]
$C_{54}H_{76}N_2O_8$ 881.203
From *Ritterella tokioka*.
$[\alpha]_D$ +108.6 (c, 0.1 in $CHCl_3$). λ_{max} 289 (ϵ 9379); 308 (sh) ($CHCl_3$).
Fukuzawa, S. *et al., J.O.C.*, 1997, **62**, 4484-4491 (*isol, uv, pmr, cmr*)

Ritterazine P R-58

[184765-85-3]



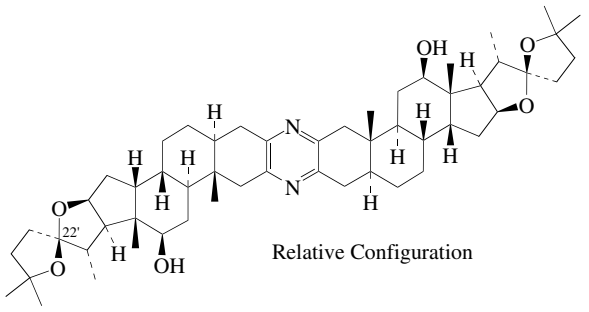
Relative Configuration

$C_{54}H_{78}N_2O_7$ 867.219
Alkaloid from the tunicate *Ritterella tokioka*. Cytotoxic agent. $[\alpha]_D$ +42.5 (c, 0.05 in $CHCl_3$). λ_{max} 289 (ϵ 10618); 309 (sh) ($CHCl_3$).

22′-Epimer: ***Ritterazine Q***
[184971-69-5]
$C_{54}H_{78}N_2O_7$ 867.219
From *Ritterella tokioka*. Cytotoxic agent. $[\alpha]_D$ +57.8 (c, 0.05 in $CHCl_3$). λ_{max} 289 (11225); 309 (sh) ($CHCl_3$).
Fukuzawa, S. *et al., J.O.C.*, 1997, **62**, 4484-4491 (*isol, uv, pmr, cmr*)

Ritterazine R R-59

[184766-99-2]

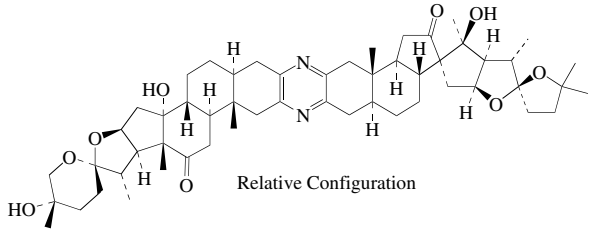


$C_{54}H_{80}N_2O_6$ 853.236
Alkaloid from the tunicate *Ritterella tokioka*.
$[\alpha]_D$ +26.3 (c, 0.05 in $CHCl_3$). λ_{max} 288 (9557); 309 (sh) ($CHCl_3$).

22′-Epimer: ***Ritterazine S***
[184971-73-1]
From *Ritterella tokioka*. Cytotoxic agent. $[\alpha]_D$ +43.3 (c, 0.05 in $CHCl_3$). λ_{max} 290 (ϵ 10480); 308 (sh) ($CHCl_3$).
Fukuzawa, S. *et al., J.O.C.*, 1997, **62**, 4484-4491 (*isol, uv, pmr, cmr*)

Ritterazine U R-60

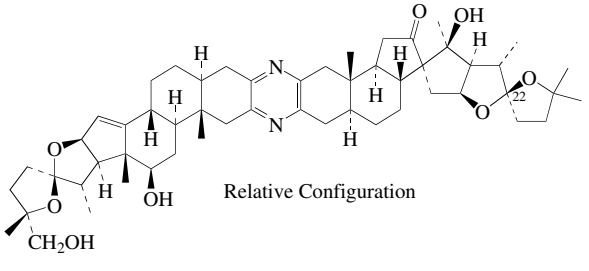
[184769-28-6]



$C_{54}H_{76}N_2O_9$ 897.202
Alkaloid from the tunicate *Ritterella tokioka*.
$[\alpha]_D$ +89 (c, 0.1 in $CHCl_3$). λ_{max} 290 (9424); 308 (sh) ($CHCl_3$).
Fukuzawa, S. *et al., J.O.C.*, 1997, **62**, 4484-4491 (*isol, uv, pmr, cmr*)

Ritterazine W R-61

[184770-05-6]

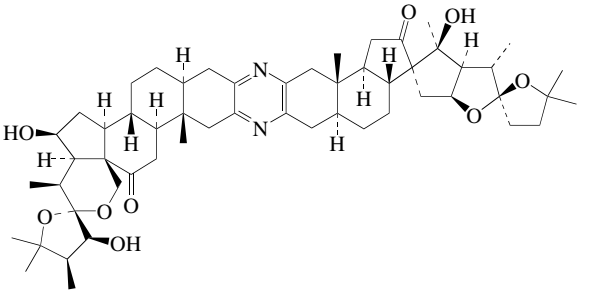


$C_{54}H_{76}N_2O_8$ 881.203
Alkaloid from the tunicate *Ritterella tokioka*.
$[\alpha]_D$ +120.4 (c, 0.05 in $CHCl_3$). λ_{max} 290 (ϵ 8155); 308 (sh) ($CHCl_3$).

22-Epimer: ***Ritterazine X***
[184971-98-0]
$C_{54}H_{76}N_2O_8$ 881.203
From *Ritterella tokioka*.
$[\alpha]_D$ +108 (c, 0.05 in $CHCl_3$). λ_{max} 290 (ϵ 8816); 308 (sh) ($CHCl_3$).
Fukuzawa, S. *et al., J.O.C.*, 1997, **62**, 4484-4491 (*isol, uv, pmr, cmr*)

Ritterazine Z R-62

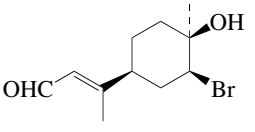
[184770-08-9]



$C_{55}H_{78}N_2O_9$ 911.229
Alkaloid from the tunicate *Ritterella tokioka*.
$[\alpha]_D$ +105.8 (c, 0.1 in $CHCl_3$). λ_{max} 289 (8958); 308 (sh) ($CHCl_3$).
Fukuzawa, S. *et al., J.O.C.*, 1997, **62**, 4484-4491 (*isol, uv, pmr, cmr*)

Rogiolal R-63

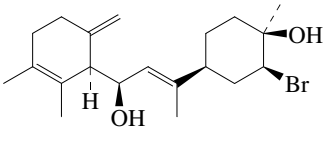
[193540-56-6]



$C_{11}H_{17}BrO_2$ 261.158
Constit. of *Laurencia microcladia*. Biodegradation product of 2-Bromo-7,11(18),13-obtusatriene-3,9-diol, B-492.
Guella, G. *et al., Helv. Chim. Acta*, 1997, **80**, 684-694 (*isol, pmr, cmr, cryst struct*)

Rogioldiol B R-64

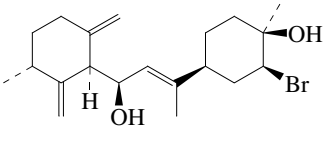
[215035-81-7]



$C_{20}H_{31}BrO_2$ 383.368
Constit. of *Laurencia microcladia*.
$[\alpha]_D^{20}$ -195 (c, 0.45 in MeOH).
Guella, G. *et al., Chem. Eur. J.*, 1998, **4**, 1692-1697 (*isol, pmr, cmr*)

Rogioldiol C R-65

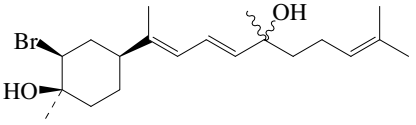
[215035-82-8]



$C_{20}H_{31}BrO_2$ 383.368
Constit. of *Laurencia microcladia*.
$[\alpha]_D^{20}$ -61 (c, 0.18 in MeOH).
Guella, G. *et al., Chem. Eur. J.*, 1998, **4**, 1692-1697 (*isol, pmr, cmr*)

Rogioldiol D R-66

[321847-11-4]

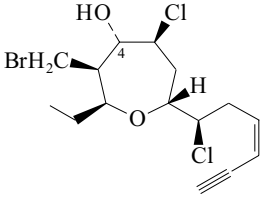


$C_{20}H_{33}BrO_2$ 385.384
Constit. of *Laurencia microcladia*.

Guella, G. *et al., Helv. Chim. Acta*, 2000, **83**, 2946-2952 (*isol, pmr, cmr*)

Rogiolenyne B R-67

3-(Bromomethyl)-5-chloro-7-(1-chloro-3-hexen-5-ynyl)-2-ethyl-4-oxepanol
[133352-30-4]

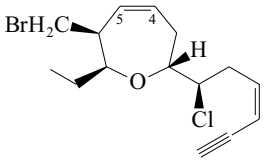


$C_{15}H_{21}BrCl_2O_2$ 384.139
Constit. of the sponge *Spongia zimocca*. Oil. $[\alpha]_D$ -5 (c, 0.1 in MeOH).

4-Ac: ***Rogiolenyne C***
[133376-41-7]
$C_{17}H_{23}BrCl_2O_3$ 426.176
From *Spongia zimocca*. Oil. $[\alpha]_D$ -4 (c, 0.12 in MeOH).

Guella, G. *et al., Helv. Chim. Acta*, 1991, **74**, 47; 1992, **75**, 303 (*isol, pmr, cmr, abs config*)

Rogiolenyne D R-68



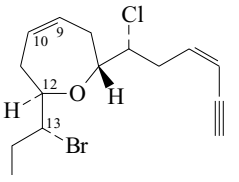
$C_{15}H_{20}BrClO$ 331.679
Isol. from the red seaweed *Laurencia microcladia*. Oil. $[\alpha]_D^{20}$ +91 (c, 0.28 in $CHCl_4$).

4β,5β-Epoxide: ***Rogiolenyne A***
[133352-29-1]
$C_{15}H_{20}BrClO_2$ 347.678
Isol. from *Laurencia microcladia*. Oil. $[\alpha]_D^{24}$ -22.8 (c, 0.18 in MeOH).

Guella, G. *et al., Helv. Chim. Acta*, 1991, **74**, 47; 1992; 1992, **75**, 303 (*isol, pmr, cmr, abs config*)

Rogioloxepane A R-69

2-(1-Bromopropyl)-7-(1-chloro-3-hexen-5-ynyl)-2,3,6,7-tetrahydrooxepin, 9CI. 13-Bromo-6-chloro-7,12-epoxy-3,9-pentadecadien-1-yne
[143120-38-1]



$C_{15}H_{20}BrClO$ 331.679
Constit. of *Laurencia microcladia*. Oil. $[\alpha]_D$ +21 (c, 0.2 in CCl_4).

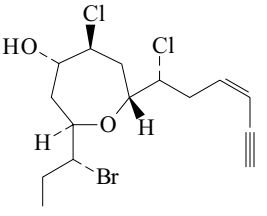
9α,10α-Epoxide: ***Rogioloxepane B***
[143051-65-4]
$C_{15}H_{20}BrClO_2$ 347.678
Constit. of *Laurencia microcladia*. Oil. $[\alpha]_D$ +8 (c, 0.04 in CCl_4).

12,13-Diepimer: ***Isolaurepinnacin***
[81053-29-4]
$C_{15}H_{20}BrClO$ 331.679
Constit. of *Laurencia pinnata*. Oil. Sol. MeOH, Et_2O. $[\alpha]_D$ -6.2 ($CHCl_3$).

Kotsuki, H. *et al., J.O.C.*, 1989, **54**, 5153-5161 (*Isolaurepinnacin*)
Guella, G. *et al., Helv. Chim. Acta*, 1992, **75**, 310 (*isol, pmr, cmr*)
Berger, D. *et al., J.A.C.S.*, 1997, **119**, 2446-2452 (*synth, Isolaurepinnacin*)
Suzuki, T. *et al., Tet. Lett.*, 2001, **42**, 65-67 (*synth, Isolaurepinnacin*)
Matsumara, R. *et al., Tet. Lett.*, 2001, **42**, 1543 (*synth*)
Crimmins, M.T. *et al., Org. Lett.*, 2003, **5**, 3009-3011 (*synth*)

Rogioloxepane C R-70

3-Bromo-7,10-dichloro-4,9-epoxy-12-pentadecen-14-yn-6-ol

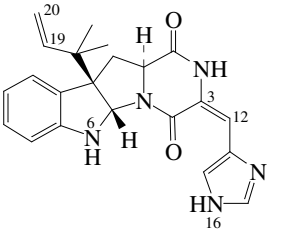


$C_{15}H_{21}BrCl_2O_2$ 384.139
Constit. of *Laurencia microcladia*. Oil. $[\alpha]_D$ +23 (c, 0.11 in CCl_4).

Guella, G. *et al., Helv. Chim. Acta*, 1992, **75**, 303 (*isol, pmr, cmr*)

Roquefortine R-71

Roquefortine C
[58735-64-1]



Absolute Configuration

$C_{22}H_{23}N_5O_2$ 389.456
CAS numbering shown. The abs. config. ref. is inaccessible but the results are given in the 1998 Synthesis ref. Metab. of *Penicillium roquefortii* ATCC 10110, *Penicillium commune*, *Penicillium cyclopium* NRRL 6093, *Penicillium farinosum* and many other *Penicillium* spp. incl. a marine -derived sp. Common constit. of blue cheese. Neurotoxin. Needles + 1MeOH (MeOH aq.). Mp 195-200° dec Mp 225-228° dec. $[\alpha]_D^{22}$ -703 (c, 1 in $CHCl_3$).

$[\alpha]_D^{15}$ -764 (c, 0.5 in Py). λ_{max} 210 (ϵ 31620); 243 (ϵ 18200); 325 (ϵ 28800) (EtOH).

▶ LD_{50} (mus, ipr) 15 mg/kg. UQ4730500

N^6-*Formyl:* **N^6-*Formylroquefortine C***
[158200-10-3]
$C_{23}H_{23}N_5O_3$ 417.466
Metab. of *Penicillium verrucosum* var. *cyclopium* AV 67718. Mycotoxin. Solid (MeOH aq.).
Mp 216-219° dec. λ_{max} 207; 242; 326 (MeOH) (Berdy).

N^{16}-*Et:* **N^{16}-*Ethylroquefortine***
[174792-02-0]
$C_{24}H_{27}N_5O_2$ 417.51
Prod. by *Penicillium janczewskii*.

3α,12-Dihydro: 3,12-Dihydroroquefortine. ***Roquefortine D****. Alkaloid Z*
[58735-66-3]
$C_{22}H_{25}N_5O_2$ 391.472
Prod. by *Penicillium* sp. incl. *Penicillium roquefortii* ATCC 10110. Neurotoxin. Prisms (MeCN).
Mp 153-154°. $[\alpha]_D^{15}$ -370 (c, 0.23 in Py). λ_{max} 208 (ϵ 195000); 244 (ϵ 35480); 298 (ϵ 15140) (EtOH).

▶ Toxic.

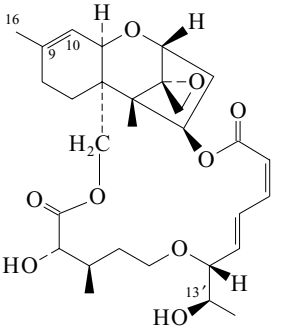
3α,12-Dihydro, N^{16}*-ethoxycarbonyl:* N^{16}*-Ethoxycarbonylroquefortine D.* **N^{16}-*Carboxyethyldihydroroquefortine***
$C_{25}H_{29}N_5O_4$ 463.535
Prod. by *Penicillium aureovirens* VKM FW-766. Wax. $[\alpha]_D^{22}$ -66.8 (c, 10.1 in MeOH). λ_{max} 210; 239; 300 (MeOH).

19,20-Dihydro: Mp 185-187°. $[\alpha]_D^{22}$ -740 (c, 0.15 in $CHCl_3$).

Ohmomo, S. *et al., Agric. Biol. Chem.*, 1975, **39**, 1333-1334; 1977, **41**, 2097-2098; 1978, **42**, 2387-2389; 1979, **43**, 2035-2038; 1980, **44**, 1929-1930 (*isol, uv, ir, pmr, ms, biosynth, Roquefortine D*)
Scott, P.M. *et al., Experientia*, 1976, **32**, 140-142 (*isol, uv, ir, pmr, cmr, struct*)
Barrow, K.D. *et al., Chem. Comm.*, 1979, 225-226 (*biosynth*)
Scott, P.M. *et al., J. Agric. Food Chem.*, 1979, **27**, 201-202 (*config*)
Engel, G. *et al., J. Chromatogr.*, 1979, **170**, 288-291 (*tlc, uv*)
Wagener, R.E. *et al., Appl. Environ. Microbiol.*, 1980, **39**, 882-887 (*isol, uv, ir, ms*)
Vesonder, R.F. *et al., Experientia*, 1980, **36**, 1308 (*isol, uv, ir*)
Kozlovsky, A.G. *et al., Experientia*, 1981, **37**, 472-473 (*Roquefortine D, isol, biosynth*)
Gorst-Allman, C.P. *et al., Chem. Comm.*, 1982, 652-653 (*biosynth, cmr*)
Scott, P.M. *et al., Dev. Food Sci.*, 1984, **8**, 463-468 (*rev*)
Yamaguchi, T. *et al., Proc. Jpn. Assoc. Mycotoxicol.*, 1991, **34**, 29-32 (*abs config*)
Bhat, B. *et al., Tetrahedron*, 1993, **49**, 10663-10669 (*biosynth*)
Musuku, A. *et al., J. Nat. Prod.*, 1994, **57**, 983-987 (*N^9-Formylroquefortine C*)
Kozlovsky, A.G. *et al., Prikl. Biokhim. Mikrobiol.*, 1997, **33**, 70-74 (*N-Ethylroquefortine*)
Chen, W.-C. *et al., Tet. Lett.*, 1998, **39**, 8401-8404 (*Roquefortine D, synth*)
Kozlovsky, A.G. *et al., Heterocycles*, 2003, **60**, 1639-1644 (*Ethoxycarbonylroquefortine D*)
Bringmann, G. *et al., Tetrahedron*, 2005, **61**, 7252-7265 (*marine isol*)

Roridin A R-72

7′-Deoxo-7′-(1-hydroxyethyl)verrucarin A, 9CI
[14729-29-4]



$C_{29}H_{40}O_9$ 532.63
Metab. of *Myrothecium* spp. Shows platelet aggregation inhibitory activity. Exhibits antifungal and cytostatic activity. Short needles (Me_2CO/Et_2O). Sol. MeOH, Et_2O; poorly sol. H_2O, hexane.
Mp 198-204°. $[\alpha]_D^{22}$ +130 (c, 1.36 in $CHCl_3$). λ_{max} 262 (ϵ 19900) (EtOH) (Derep).

▶ Skin irritant. LD_{50} (mus, orl) 9 mg/kg; LD_{50} (mus, ivn) 1 mg/kg. VL0355000

9β,10β-Epoxide: 9,10-Epoxyroridin A
[74516-67-9]
$C_{29}H_{40}O_{10}$ 548.629
Semisynthetic. Antileukaemic agent.

8β-Hydroxy: 8-Hydroxyroridin A
[87583-91-3]
$C_{29}H_{40}O_{10}$ 548.629
Semisynthetic. Antileukaemic agent.
Mp 237-239°.

16-Hydroxy: 16-Hydroxyroridin A
[87532-28-3]
$C_{29}H_{40}O_{10}$ 548.629
Semisynthetic. Antileukaemic agent.
Mp 206-207°.

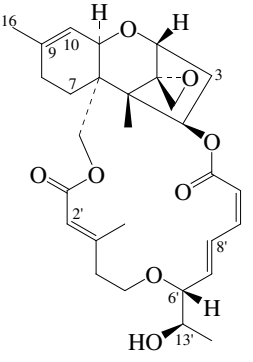
16-Hydroxy, 9β,10β-epoxide: 9,10-Epoxy-16-hydroxyroridin A
[87532-33-0]
$C_{29}H_{40}O_{11}$ 564.628
Semisynthetic. Antileukaemic agent.
Mp 138-142°.

13′-Epimer: ***Isororidin A***
[84773-08-0]
$C_{29}H_{40}O_9$ 532.63
Metab. of *Myrothecium verrucaria* and the marine-derived *Acremonium neo-caledoniae*. Cryst. (CH_2Cl_2/hexane). Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane.
Mp 183-185°. $[\alpha]_D^{25}$ +6.7 (c, 3.3 in $CHCl_3$). λ_{max} 260 (MeOH) (Berdy).

Härri, E. *et al., Helv. Chim. Acta*, 1962, **45**, 839 (*isol*)
Muller, B. *et al., Helv. Chim. Acta*, 1975, **58**, 453; 471 (*biosynth*)
Breitenstein, W. *et al., Helv. Chim. Acta*, 1975, **58**, 1172 (*cmr*)
Eppley, R. *et al., J.O.C.*, 1977, **42**, 240 (*nmr*)
Jarvis, B.B. *et al., J. Med. Chem.*, 1980, **23**, 1054; 1984, **27**, 239 (*derivs, props*)
Jarvis, B.B. *et al., J. Nat. Prod.*, 1982, **45**, 440 (*cryst struct, isol*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2220 (*uv, ir, pmr, ms, cd*)
Trichothecenes - Chemical, Biological and Toxicological Aspects, (ed. Ueno, Y.), Elsevier, 1983, (*book*)
Mizutani, Y. *et al., Cereal Res. Commun.*, 1997, **25**, 501-502; *CA*, **128**, 31292n (*activity*)
Laurent, D. *et al., Planta Med.*, 2000, **66**, 63-66 (*Acremonium, isol*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 230

Roridin E R-73

2′,3′-Didehydro-7′-deoxo-2′-deoxy-7′-(1-hydroxyethyl)verrucarin A, 9CI. Satratoxin D
[16891-85-3]



$C_{29}H_{38}O_8$ 514.614
Isol. from *Myrothecium verrucaria* and *Myrothecium roridum*. Antibiotic. Cryst. Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 183-184° Mp 220-222° (dimorph.). $[\alpha]_D^{23}$ -16 ($CHCl_3$). λ_{max} 218 (ϵ 17800); 262 (ϵ 9550) (MeOH or EtOH) (Derep). λ_{max} 221 (E1%/1cm 370); 263 (E1%/1cm 330) (MeOH) (Berdy).

▶ YX9821500

13′-Ac: ***Roridin E acetate***
[32656-18-1]
$C_{31}H_{40}O_9$ 556.652
Constit. of *Myrothecium verrucaria*. Amorph. solid. $[\alpha]_D^{27}$ +43 (c, 0.06 in $CHCl_3$).

Deepoxy (12,13-didehydro): ***12,13-Deoxyroridin E***
[333977-86-9]
$C_{29}H_{38}O_7$ 498.615
Metab. of a marine-derived *Myrothecium roridum*.
$[\alpha]_D$ -204 (c, 0.025 in $CHCl_3$). λ_{max} 263 (ϵ 15700) (MeOH).

3ξ-Hydroxy: 3-Hydroxyroridin E. ***Roridin L***
$C_{29}H_{38}O_9$ 530.614
Prod. by *Myrothecium verrucaria*. Powder.
Mp 138-140° dec. λ_{max} 224 (ϵ 25000); 263 (ϵ 19500) (MeOH).

16-Hydroxy: ***16-Hydroxyroridin E***
[436144-43-3]
$C_{29}H_{38}O_9$ 530.614
Metab. of *Myrothecium roridum*. Powder.
Mp 190-195°. $[\alpha]_D^{25}$ -29 (c, 0.001 in $CHCl_3$). λ_{max} 218 (log ϵ 4.28); 258 (log ϵ 4.31) (MeOH).

8α-Acetoxy: ***8-Acetoxyroridin E***
$C_{31}H_{40}O_{10}$ 572.651
Prod. by *Myrothecium* sp.

6′-Epimer: ***Epiisororidin E***
[249744-12-5]
$C_{29}H_{38}O_8$ 514.614
Metab. of *Myrothecium verrucaria*. Amorph. solid. $[\alpha]_D^{30}$ -29.2 (c, 1.5 in $CHCl_3$).

13′-Epimer: ***Epiroridin E***
[249744-08-9]
$C_{29}H_{38}O_8$ 514.614
Metab. of *Myrothecium verrucaria*. Amorph. solid. $[\alpha]_D^{30}$ +0.7 (c, 1.8 in $CHCl_3$).

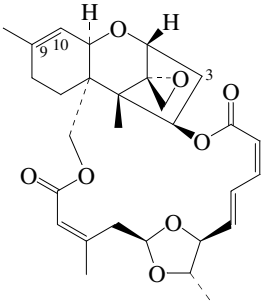
6′,13′-Diepimer: ***Isororidin E***
[64726-84-7]
$C_{29}H_{38}O_8$ 514.614
Metab. of *Cylindrocarpon* spp. and *Myrothecium verrucaria*.
Prisms (EtOAc).
Mp 200-202°. $[\alpha]_D^{24}$ -65.1 ($CHCl_3$). Stereochem. finalised in 1999.
λ_{max} 223 (ϵ 24000); 262 (ϵ 16000) (EtOH) (Berdy).

6′,13′-Diepimer, 7β,8β-epoxide: ***7,8-Epoxyisororidin E***
[64687-83-8]
$C_{29}H_{36}O_9$ 528.598
Metab. of *Cylindrocarpon* spp. and *Myrothecium verrucaria*.
Prisms (Me_2CO).
Mp 216-219°. $[\alpha]_D^{24}$ -69.9 ($CHCl_3$). Stereochem. finalised in 1999.
λ_{max} 221 (ϵ 76300); 262 (ϵ 16700) (EtOH) (Berdy).

Böhner, B. *et al., Helv. Chim. Acta*, 1965, **48**, 1079 (*isol*)
Traxler, P. *et al., Helv. Chim. Acta*, 1970, **53**, 2071 (*struct*)
Eppley, R.M. *et al., Science (Washington, D.C.)*, 1973, **181**, 758 (*stereochem*)
Matsumoto, M. *et al., J. Antibiot.*, 1977, **30**, 681 (*derivs*)
Matsumoto, M. *et al., Tet. Lett.*, 1977, 4093 (*cmr, struct*)
Still, W.C. *et al., J.A.C.S.*, 1984, **106**, 260 (*synth*)
Jarvis, B.B. *et al., J. Nat. Prod.*, 1996, **59**, 254-261 (*config*)
Isaka, M. *et al., J. Nat. Prod.*, 1999, **62**, 329-331 (*13′-Ac*)
Jarvis, B.B. *et al., J. Nat. Prod.*, 1999, **62**, 1284-1289 (*isol, pmr, cmr, stereochem, cryst struct*)
Wagenaar, M.M. *et al., J. Antibiot.*, 2001, **54**, 517-520 (*8-Acetoxyroridin E*)
Murakami, Y. *et al., J. Antibiot.*, 2001, **54**, 980-983 (*Roridin L*)
Namikoshi, M. *et al., J. Nat. Prod.*, 2001, **64**, 396-398 (*12,13-Deoxyroridin E, Roridin E, cmr*)
Saikawa, Y. *et al., Tetrahedron*, 2001, **57**, 8277-8281 (*Roridin E, isol, uv, ir, pmr, cmr*)
Alvi, K.A. *et al., J. Nat. Prod.*, 2002, **65**, 742-744 (*16-Hydroxyroridin E*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 237; 242; 243

Roridin H R-74

2′,3′-Didehydro-7′-deoxo-2′-deoxy-7′,5′-(ethylideneoxy)verrucarin A, 9CI. Verrucarin H
[29953-50-2]



$C_{29}H_{36}O_8$ 512.599
Isol. from *Myrothecium verrucaria*. Shows antileukaemic activity.
Needles. Sol. MeOH, C_6H_6; poorly sol. H_2O, Et_2O, hexane.
Mp 325°. $[\alpha]_D^{23}$ +31 (c, 1.16 in $CHCl_3$). λ_{max} 218 (ϵ 17800); 262 (ϵ 9550) (MeOH or EtOH) (Derep). λ_{max} 224 (ϵ 24550); 260 (ϵ 18200) (EtOH) (Berdy).

▶ LD_{50} (mus, ivn) 3 mg/kg. YX9828000

7β,8β-Epoxide: ***7,8-Epoxyroridin H***
[64687-85-0]
$C_{29}H_{34}O_9$ 526.582
Metab. of *Cylindrocarpon* spp. Amorph. powder.

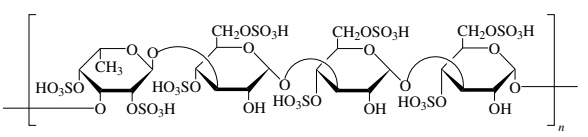
9β,10β-Epoxide: 9,10-Epoxyroridin H
[87532-26-1]
$C_{29}H_{36}O_9$ 528.598
Semisynthetic. Shows antileukaemic activity.

3ξ-Hydroxy: ***Roridin M****. 3-Hydroxyroridin H*
$C_{29}H_{36}O_9$ 528.598
Prod. by *Myrothecium verrucaria*. Powder.
Mp 180-182° dec. λ_{max} 224 (ϵ 24200); 263 (ϵ 19100) (MeOH).

8α-Acetoxy: ***8-Acetoxyroridin H****. Calcarisporin B_1*
[361544-63-0]
$C_{31}H_{38}O_{10}$ 570.635
Prod. by a marine-derived *Myrothecium* sp. Z16 and *Calcarisporium arbuscula*. Amorph. powder. $[\alpha]_D^{20}$ +70 (c, 0.95 in $CHCl_3$). λ_{max} 210 (log ϵ 4.45); 246 (log ϵ 4.23) (MeOH).

Bohner, B. *et al., Helv. Chim. Acta*, 1965, **48**, 1079 (*isol*)
Traxler, P. *et al., Helv. Chim. Acta*, 1970, **53**, 1846 (*struct*)
Breitenstein, W. *et al., Helv. Chim. Acta*, 1975, **58**, 1172 (*nmr*)
Matsumoto, M. *et al., J. Antibiot.*, 1977, **30**, 681 (*deriv*)
Matsumoto, M. *et al., Tet. Lett.*, 1977, 4093 (*stereochem*)
Jarvis, B.B. *et al., J.O.C.*, 1982, **47**, 1117 (*isol, struct*)
Jarvis, B.B. *et al., J. Med. Chem.*, 1984, **27**, 239 (*epoxide*)
Wagenaar, M.M. *et al., J. Antibiot.*, 2001, **54**, 517-520 (*8-Acetoxyroridin H*)
Murakami, Y. *et al., J. Antibiot.*, 2001, **54**, 980-983 (*Roridin M*)
Yu, N.-J. *et al., J. Asian Nat. Prod. Res.*, 2002, **4**, 179-183 (*Calcarisporin B_1*)
Liu, J.Y. *et al., J. Appl. Microbiol.*, 2006, **100**, 195-202 (*marine, isol*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, ; 244

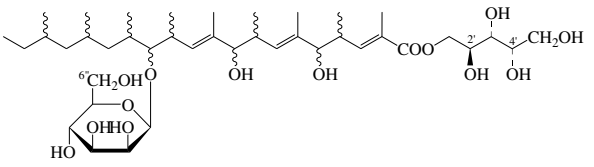
Rosacelose R-75



Polymer of sulfated D-glucose/L-fucose in approx. 3:1 ratio. Idealised struct. shown. Isol. from the marine sponge *Myxilla rosacea*. Shows anti-HIV props. Genus name misspelt as Mixylla.

Cimino, P. *et al., Carbohydr. Res.*, 2001, **334**, 39-47 (*isol, pmr, cmr, struct*)

Roselipin 1A R-76



$C_{40}H_{72}O_{14}$ 777
Prod. by the marine fungus *Gliocladium roseum* KF-1040. Diacylglycerol acyltransferase (DGAT) inhibitor. Powder. Mp 36-37°. $[\alpha]_D^{24}$ +12 (c, 0.1 in MeOH). λ_{max} 203 (ϵ 45800); 222 (ϵ 33100) (MeOH).

2′,4′-Diepimer: ***Roselipin 1B***
$C_{40}H_{72}O_{14}$ 777
Prod. by *Gliocladium roseum* KF-1040. DGAT inhibitor. Powder.
Mp 35-36°. $[\alpha]_D^{24}$ +8 (c, 0.1 in MeOH). λ_{max} 203 (ϵ 25800); 222 (ϵ 17800) (MeOH).

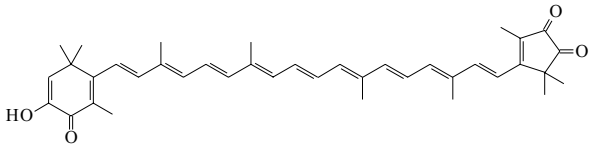
6′′-Ac: ***Roselipin 2A***
$C_{42}H_{74}O_{15}$ 819.038
Prod. by *Gliocladium roseum* KF-1040. DGAT inhibitor. $[\alpha]_D^{24}$ +22 (c, 0.1 in MeOH). λ_{max} 203 (ϵ 27000); 222 (ϵ 20900) (MeOH).

2′,4′-Diepimer, 6′′-Ac: ***Roselipin 2B***
$C_{42}H_{74}O_{15}$ 819.038
Prod. by *Gliocladium roseum* KF-1040. DGAT inhibitor. $[\alpha]_D^{24}$ +10 (c, 0.1 in MeOH). λ_{max} 203 (ϵ 41600); 222 (ϵ 32000) (MeOH).

Omura, S. *et al., J. Antibiot.*, 1999, **52**, 586-589; 689-694; 815-826

Roserythrin R-77

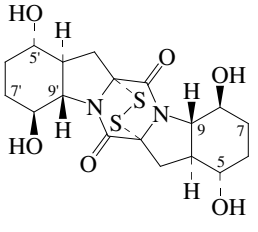
[38310-08-6]



$C_{39}H_{46}O_4$ 578.79
Constit. of *Actinia equina*. Blue-black needles (Me_2CO/petrol). Mp 200°.

Francis, G.W. *et al., Acta Chem. Scand.*, 1972, **26**, 1097

Rostratin A R-78



Absolute Configuration

$C_{18}H_{24}N_2O_6S_2$ 428.529
Related to Exserohilone, E-905. Isol. from the marine-derived *Exserohilum rostratum*. Cytotoxic. Gum. $[\alpha]_D^{20}$ -185 (c, 0.004 in $MeOH/CH_2Cl_2$). CAS no. not found in CA 141.

9,9′-Diepimer, 5,5′-diketone: ***Rostratin B***
$C_{18}H_{20}N_2O_6S_2$ 424.498
Isol. from *Exserohilum rostratum*. Cytotoxic. Gum. $[\alpha]_D^{20}$ -210 (c, 0.0004 in $MeOH/CH_2Cl_2$). CAS no. not found in CA 141.

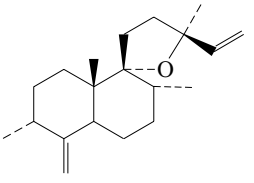
*9,9′-Diepimer, 7*S*,7′*S*-dimethoxy, 5,5′-diketone:* ***Rostratin C***
$C_{20}H_{24}N_2O_8S_2$ 484.55
Isol. from *Exserohilum rostratum*. Cytotoxic. Gum. $[\alpha]_D^{20}$ -167 (c, 0.002 in $MeOH/CH_2Cl_2$). CAS no. not found in CA 141.

*9,9′-Diepimer, 7*R*,7′*R*-dimercapto, 5,5′-diketone:* ***Rostratin D***
$C_{18}H_{20}N_2O_6S_4$ 488.63
Isol. from *Exserohilum rostratum*. Cytotoxic. Gum. $[\alpha]_D^{20}$ +108 (c, 0.007 in $MeOH/CH_2Cl_2$). CAS no. not found in CA 141.

Tan, R.-X. *et al., J. Nat. Prod.*, 2004, **67**, 1374-1382 (*isol, pmr, cmr, cryst struct*)

Rotalin A R-79

[119979-81-6]

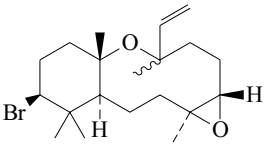


$C_{20}H_{32}O$ 288.472
Metab. of sponge *Mycale rotalis*. Oil. $[\alpha]_D$ -1.8 (c, 2.8 in $CHCl_3$).

Corriero, G. *et al., Tetrahedron*, 1989, **45**, 277

Rotalin B R-80

[119979-80-5]

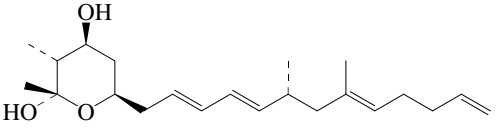


$C_{20}H_{33}BrO_2$ 385.383
Metab. of sponge *Mycale rotalis*. Amorph. solid. $[\alpha]_D$ +13.9 (c, 0.43 in $CHCl_3$).

Corriero, G. *et al., Tetrahedron*, 1989, **45**, 277

Rottnestol R-81

*6-(6,8-Dimethyl-2,4,8,12-tridecatetraenyl)tetrahydro-2,3-dimethyl-2*H*-pyran-2,4-diol, 9CI*
[170311-43-0]



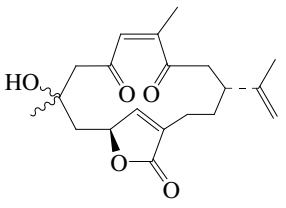
Absolute Configuration

$C_{22}H_{36}O_3$ 348.525
Isol. from the sponge *Haliclona* sp. Oil. $[\alpha]_D$ +67.4 (c, 0.4 in $CHCl_3$). λ_{max} 227 (sh) (ϵ 31620); 232 (ϵ 33100) (2-propanol).

Erickson, K.L. *et al., Tetrahedron*, 1995, **51**, 11953 (*isol, uv, ir, pmr, cmr, ms*)
Czuba, I.R. *et al., Org. Biomol. Chem.*, 2003, 2044-2056 (*synth, abs config*)

Rubifol R-82

8-Hydroxy-3,6-dioxo-4,11,15-cembratrien-20,10-olide
[118025-71-1]

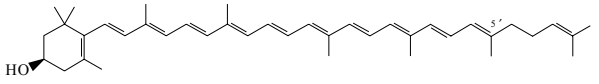


$C_{20}H_{26}O_5$ 346.422
Metab. of *Gersemia rubiformis*. Needles (MeOH).
Mp 127-130°. $[\alpha]_D^{25}$ -41 (c, 0.38 in CH_2Cl_2). λ_{max} 207 (ϵ 10300); 230 (ϵ 6700) (MeOH) (Derep).

Williams, D.E. *et al., Can. J. Chem.*, 1988, **66**, 2928-2934 (*Rubifol*)

Rubixanthin R-83

β,ψ-Caroten-3-ol. γ-Caroten-3-ol. 3-Hydroxy-γ-carotene
[3763-55-1]



$C_{40}H_{56}O$ 552.882

(all-*E*)-*form*
Constit. of ripe fruit of *Rosa rubiginosa*, *Rubus chamaemorus* (cloudberry), *Butea capitata* and other plants. Main pigment of *Astragalus petersii* and other *Astragalus* spp. Also prod. by microorganisms e.g. *Staphylococcus aureus*.
Dark red cryst. (C_6H_6/MeOH).
Mp 160°.

O-*Hexadecanoyl:* ***Rubixanthin palmitate***
[11001-80-2]
$C_{56}H_{86}O_2$ 791.294
Isol. from flowers of *Astragalus petersii* (Leguminosae).

5,6-Epoxide: 5,6-Epoxy-5,6-dihydro-β,ψ-caroten-3-ol. ***Rubixanthin 5,6-epoxide***
[29706-95-4]
$C_{40}H_{56}O_2$ 568.881
A possible nat. prod. Orange-red needles (Et_2O/Me_2CO). Mp 170-171°. Not definitely known to occur naturally.

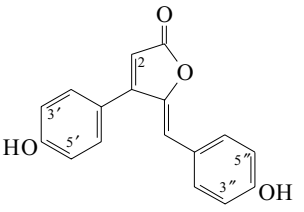
7′,8′-Dihydro: 7′,8′-Dihydro-β,ψ-caroten-3-ol. 3-Hydroxy-β-zeacarotene. β-Zeacaroten-3-ol
[62667-76-9]
$C_{40}H_{58}O$ 554.898
Isol. from a *Flavobacterium* sp. and the green alga *Scenedesmus obliqus*. λ_{max} 405; 428; 453 (EtOH).

(5*Z*)-*form*
Gazaniaxanthin
[19603-65-7]
Constit. of flowers of *Gazania rigens*.
Red platelets (C_6H_6/MeOH).
Mp 133-137°. $[\alpha]_D^{25}$ +65 (c, 0.09 in $CHCl_3$) (cd).

Zechmeister, L. *et al., J.A.C.S.*, 1943, **65**, 1535-1540 (*Gazaniaxanthin*)
Karrer, P. *et al., Helv. Chim. Acta*, 1947, **30**, 531-535 (*epoxide*)
Neamtu, G. *et al., Stud. Cercet. Biochim.*, 1965, **8**, 67; *CA*, **63**, 10317c (*palmitate*)
Brown, B.O. *et al., Chem. Comm.*, 1968, 382-384 (*Gazaniaxanthin*)
de Ville, T.E. *et al., Chem. Comm.*, 1969, 1311-1312 (*struct*)
Bartlett, L. *et al., J.C.S.(C)*, 1969, 2527-2544 (*ord, abs config*)
Arpin, N. *et al., Phytochemistry*, 1969, **8**, 185-193 (*ir*)
Arpin, N. *et al., Acta Chem. Scand.*, 1973, **27**, 2321-2334 (*pmr, ms, uv*)
McDermott, J.C.B. *et al., Biochem. J.*, 1973, **134**, 1115-1117 (*biosynth*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1983, **66**, 494-513 (*isol, synth*)

Rubrolide E R-84

[136762-97-5]



$C_{17}H_{12}O_4$ 280.279
Constit. of *Ritterella rubra* and *Synoicum blochmanni*.

4″-Me ether: ***Rubrolide F***
[136762-98-6]
$C_{18}H_{14}O_4$ 294.306
Constit. of *Ritterella rubra*. Yellow solid.

3″-Bromo, 2-chloro: ***Rubrolide M***
[287965-28-0]
$C_{17}H_{10}BrClO_4$ 393.62
Constit. of *Synoicum blochmanni*. Amorph. orange solid. λ_{max} 252 (ϵ 10000); 366 (ϵ 19000); 446 (ϵ 3200) (MeOH).

2,3″-Dibromo, 3′-chloro: ***Rubrolide N***
[287965-29-1]
$C_{17}H_9Br_2ClO_4$ 472.516
Constit. of *Synoicum blochmanni*. Amorph. yellow solid. λ_{max} 259 (ϵ 8100); 378 (ϵ 13200) (MeOH).

3′,3″-Dibromo, 2-chloro: ***Rubrolide K***
[287965-20-2]
$C_{17}H_9Br_2ClO_4$ 472.516
Constit. of *Synoicum blochmanni*. Amorph. orange powder. λ_{max} 257 (ϵ 9900); 371 (ϵ 16000) (MeOH).

3′,5′-Dibromo: ***Rubrolide D***
[136762-96-4]
$C_{17}H_{10}Br_2O_4$ 438.072
Constit. of *Ritterella rubra*.

3″,5″-Dibromo: ***Rubrolide C***
[136762-95-3]
$C_{17}H_{10}Br_2O_4$ 438.072
Constit. of *Ritterella rubra* and *Synoicum blochmanni*. Red amorph. solid (Me_2CO).

3″,5″-Dibromo, 2-chloro: ***Rubrolide L***
[287965-27-9]
$C_{17}H_9Br_2ClO_4$ 472.516
Constit. of *Synoicum blochmanni*. Amorph. red-orange solid. λ_{max} 265 (ϵ 8400); 353 (ϵ 11000) (MeOH).

3′,3″,5″-Tribromo: ***Rubrolide J***
[287964-86-7]
$C_{17}H_9Br_3O_4$ 516.968
Constit. of *Synoicum blochmanni*. Amorph. orange solid. λ_{max} 257 (ϵ 4400); 358 (ϵ 5000); 446 (ϵ 3500) (MeOH).

3′,3″,5″-Tribromo, 2-chloro: ***Rubrolide I***
[287964-85-6]
$C_{17}H_8Br_3ClO_4$ 551.413
Constit. of *Synoicum blochmanni*. Orange-yellow powder. λ_{max} 262 (ϵ 8800); 358 (ϵ 11800); 459 (ϵ 9000) (MeOH).

3′,3″,5′,5″-Tetrabromo: ***Rubrolide A***
[136762-94-2]
$C_{17}H_8Br_4O_4$ 595.864
Constit. of *Ritterella rubra* and *Synoicum blochmanni*. Red amorph. solid (Me_2CO). λ_{max} 257 (ϵ 23000); 324 (sh) (ϵ 17000); 355 (ϵ 19000); 439 (ϵ 14000) (MeOH) (Derep).

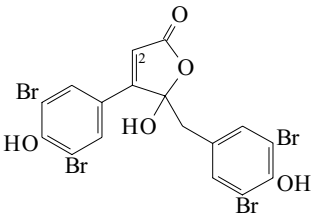
3′,3″,5′,5″-Tetrabromo, 2-chloro: ***Rubrolide B***
[136781-95-8]
$C_{17}H_7Br_4ClO_4$ 630.309
Constit. of *Ritterella rubra* and *Synoicum blochmanni*. Red amorph. solid (Me_2CO).

Miao, S. *et al., J.O.C.*, 1991, **56**, 6275-6280 (*Rubrolides A-H, isol, pmr, cmr*)
Kotora, M. *et al., Synthesis*, 1997, 121-128 (*diacetates, Rubrolide C*)

Boukouvalas, J. *et al., Tet. Lett.*, 1998, **39**, 7665-7668 (*synth*)
Ortega, M.J. *et al., Tetrahedron*, 2000, **56**, 3963-3967 (*Rubrolides I-N*)
Bellina, F. *et al., Tet. Lett.*, 2002, **43**, 2023-2027 (*Rubrolide M, synth*)
Kar, A. *et al., Synthesis*, 2005, 2284-2286 (*synth, ir, uv, pmr, cmr*)

Rubrolide G R-85

[136762-99-7]

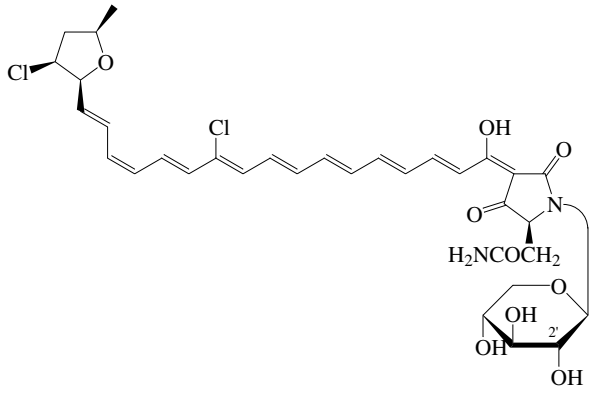


$C_{17}H_{10}Br_4O_5$ 613.879
Constit. of *Ritterella rubra*.

2-Chloro: ***Rubrolide H***
[136763-00-3]
$C_{17}H_9Br_4ClO_5$ 648.324
Constit. of *Ritterella rubra*.
Miao, S. *et al., J.O.C.*, 1991, **56**, 6275-6280 (*isol, pmr, cmr*)

Rubroside G R-86

[227597-42-4]



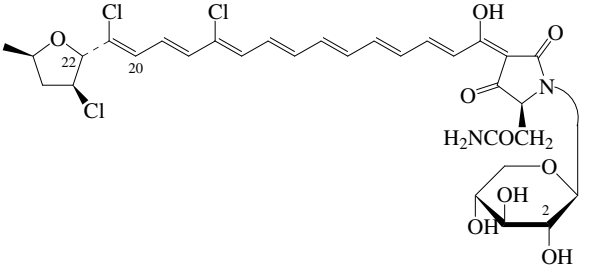
$C_{33}H_{38}Cl_2N_2O_9$ 677.577
Similar to Aurantoside A, A-748. Isol. from the marine sponge *Siliquariaspongia japonica*. Antifungal agent. Amorph. red solid. $[\alpha]_D^{24}$ -1212 (c, 0.001 in MeOH). λ_{max} 248 (ϵ 32400); 435 (ϵ 154400); 460 (ϵ 175500) (MeOH).

*2′-*O*-[5-Deoxy-β-D-arabinofuranosyl-(1→4)-β-D-xylopyranosyl]:* ***Rubroside B***
[227597-37-7]
$C_{43}H_{54}Cl_2N_2O_{16}$ 925.809
Isol. from *Siliquariaspongia japonica*. Amorph. red solid. $[\alpha]_D^{24}$ -1460 (c, 0.001 in MeOH). λ_{max} 250 (ϵ 18900); 432 (ϵ 71300); 457 (ϵ 69700) (MeOH).

*2′-*O*-[5-Deoxy-2-*O*-methyl-β-D-arabinofuranosyl-(1→4)-β-D-xylopyranosyl]:* ***Rubroside D***
[227597-39-9]
$C_{44}H_{56}Cl_2N_2O_{16}$ 939.836
Isol. from *Siliquariaspongia japonica*. Amorph. red solid. $[\alpha]_D^{24}$ -1024 (c, 0.001 in MeOH). λ_{max} 251 (ϵ 16400); 432 (ϵ 109100) (MeOH).
Sata, N.U. *et al., J.O.C.*, 1999, **64**, 2331-2339 (*Rubrosides B,D,G*)

Rubroside H R-87

[227597-43-5]



$C_{31}H_{35}Cl_3N_2O_9$ 685.984
Similar to Aurantoside A, A-748. Isol. from the marine sponge *Siliquariaspongia japonica*. Antifungal agent. Amorph. red solid. $[\alpha]_D^{24}$ -1308 (c, 0.001 in MeOH). λ_{max} 245 (ϵ 13700); 440 (ϵ 44700) (MeOH).

*2′-*O*-[5-Deoxy-β-D-arabinofuranosyl-(1→4)-β-D-xylopyranosyl]:* ***Rubroside E***
[227597-40-2]
$C_{41}H_{51}Cl_3N_2O_{16}$ 934.216
Isol. from *Siliquariaspongia japonica*. Amorph. red solid. $[\alpha]_D^{24}$ -1424 (c, 0.001 in MeOH). λ_{max} 243 (ϵ 17000); 450 (ϵ 61700) (MeOH).

*2′-*O*-[5-Deoxy-2-*O*-methyl-β-D-arabinofuranosyl-(1→4)-β-D-xylopyranosyl]:* ***Rubroside F***
[227597-41-3]
$C_{42}H_{53}Cl_3N_2O_{16}$ 948.243
Isol. from *Siliquariaspongia japonica*. Amorph. red solid. $[\alpha]_D^{24}$ -490 (c, 0.001 in MeOH). λ_{max} 250 (ϵ 9100); 425 (ϵ 80000) (MeOH).

*21-Dechloro, 2′-*O*-[5-deoxy-2-*O*-methyl-β-D-arabinofuranosyl-(1→4)-β-D-xylopyranosyl]:* ***Rubroside C***
[227597-38-8]
$C_{42}H_{54}Cl_2N_2O_{16}$ 913.798
Isol. from *Siliquariaspongia japonica*. Amorph. red solid. $[\alpha]_D^{24}$ -1088 (c, 0.001 in MeOH). λ_{max} 240 (ϵ 18600); 450 (ϵ 60600) (MeOH).

*21-Dechloro, 20Z-isomer, 22-epimer, 2′-*O*-[5-deoxy-2-*O*-methyl-β-D-arabinofuranosyl-(1→4)-β-D-xylopyranosyl]:* ***Rubroside A***
[227597-36-6]
$C_{42}H_{54}Cl_2N_2O_{16}$ 913.798
Isol. from *Siliquariaspongia japonica*. Amorph. red solid. $[\alpha]_D^{24}$ -1824 (c, 0.001 in MeOH). λ_{max} 246 (ϵ 29100); 418 (ϵ 110400); 430 (ϵ 110200) (MeOH).
Sata, N.U. *et al., J.O.C.*, 1999, **64**, 2331-2339 (*Rubrosides A,C,E,F,H*)

RYIRF amide R-88

[153919-56-3]
H-Arg-Tyr-Ile-Arg-Phe-NH_2
$C_{36}H_{56}N_{12}O_6$ 752.915
Isol. from the turbellarian *Artioposthia triangulata*. Related to *Macrocallista nimbosa* Neuropeptide C, N-97.
Maule, A.G. *et al., Regul. Pept.*, 1994, **50**, 37 (*isol*)

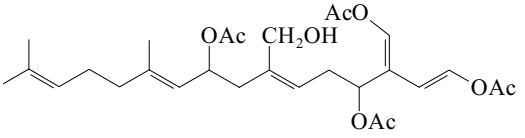
SAI II S-1

Isol. from *Anemonia sulcata*. Proteinase inhibitor.

Beress, L. *et al., Chem. Pept. Proteins*, 1993, **5-6**, 327-335; *CA*, **122**, 183480 (*isol*)

Sacoglossan S-2

[94393-09-6]



$C_{28}H_{40}O_9$ 520.619

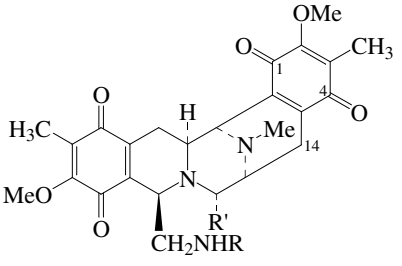
Metab. of seaweed *Halimeda macroloba* excreted by ascolossan marine mollusc *Elysia halimedae*. Feeding deterrent. Oil. $[\alpha]_D$ -25.1 (c, 0.14 in $CHCl_3$).

[116560-99-7]

Schmitz, F.J. *et al., Phytochemistry*, 1984, **23**, 1331-1332 (*cmr, pmr*)
Paul, K.J. *et al., J. Exp. Mar. Biol. Ecol.*, 1988, **119**, 15-29 (*isol, ir, uv, pmr, cmr, props*)

Saframycin A S-3

[66082-27-7]



R = -CO[25]COCH$_3$, R' = CN

$C_{29}H_{30}N_4O_8$ 562.578

CAS numbering shown. Isol. from *Streptomyces lavendulae*. Shows antibiotic and antineoplastic props. Yellow powder. Sol. MeOH, $CHCl_3$; fairly sol. Et_2O; poorly sol. hexane, H_2O. Mp 122-126°. $[\alpha]_D^{20}$ +18.2 (c, 0.9 in MeOH). λ_{max} 268 (ϵ 21880); 368 (ϵ 1450) (MeOH) (Derep).

▶ LD_{50} (mus, ipr) 4.9 mg/kg; LD_{50} (mus, ivn) 3.3 mg/kg. VN2265000

25-Alcohol (1): Saframycin AR$_1$. 25-Dihydrosaframycin A. Saframycin AH$_2$
[81382-09-4]
$C_{29}H_{32}N_4O_8$ 564.594
Prod. by microbial conversion of Saframycin A. Active against gram-positive bacteria, weakly active against gram-negative bacteria. Weak antineoplastic agent. Yellow powder + $^1/_3H_2O$. Sol. EtOAc. Mp 142-145°. $[\alpha]_D^{25}$ +21.4 (MeOH). Log P -0.42 (calc). λ_{max} 268 (ϵ 10500) (MeOH) (Berdy).

25-Alcohol (2): Saframycin AH$_1$
[92621-76-6]
$C_{29}H_{32}N_4O_8$ 564.594
Semisynthetic, prod. by redn. of Saframycin A. Potent antineoplastic agent. Log P -0.42 (calc). C-25 Epimer of Saframycin AR$_1$.

5α-Hydroxy: ***Saframycin G***
[92569-02-3]
$C_{29}H_{30}N_4O_9$ 578.577
From *Streptomyces lavendulae*. Yellow powder. Sol. MeOH; poorly sol. H_2O.
Mp 134-136°. $[\alpha]_D^{22}$ -28 (c, 1 in MeOH). λ_{max} 268 (ϵ 21880); 368 (ϵ 1450) (MeOH) (Derep). λ_{max} 264 (ϵ 17500); 370 (ϵ 891) (MeOH) (Berdy).

14-Oxo, 1,4-hydroquinone: ***Saframycin F***
[92569-03-4]
$C_{29}H_{30}N_4O_9$ 578.577
Prod. by *Streptomyces lavendulae*. Antineoplastic agent. Light yellow powder. Sol. MeOH; poorly sol. H_2O.
Mp 134-136° dec. $[\alpha]_D^{22}$ +28.4 (c, 0.1 in MeOH). Planar struct. only currently known. λ_{max} 243 (ϵ 13800); 274 (ϵ 17400); 369 (ϵ 5620) (MeOH) (Derep). λ_{max} 231 (ϵ 9550); 277 (ϵ 12880); 375 (ϵ 4466) (MeOH) (Berdy).

Decyano: ***Saframycin B***
[66082-28-8]
$C_{28}H_{31}N_3O_8$ 537.568
From *Streptomyces lavendulae*. Orange-yellow prisms (Et_2O). Sol. MeOH, Py, $CHCl_3$, C_6H_6; fairly sol. Et_2O; poorly sol. hexane, H_2O.
Mp 108-109°. $[\alpha]_D^{20}$ -54.4 (c, 1 in MeOH). λ_{max} 268 (ϵ 21880); 368 (ϵ 1450) (MeOH) (Derep).

▶ LD_{50} (mus, ipr) 250 mg/kg. TX1418200

Decyano, 25-alcohol: Saframycin AR$_3$. 25-Dihydrosaframycin B. 21-Decyano-25-dihydrosaframycin A
[81853-83-0]
$C_{28}H_{33}N_3O_8$ 539.584
Prod. by microbial conversion of Saframycin B. Active against gram-positive and -negative bacteria. Yellow powder + $^1/_2H_2O$. Sol. EtOAc. Mp 123-126°. $[\alpha]_D^{25}$ -76.7 (MeOH). Log P 0.12 (calc). λ_{max} 269 (ϵ 13100) (MeOH) (Berdy).

Decyano, 5α-methoxy: ***Saframycin C***
[66082-29-9]
$C_{29}H_{33}N_3O_9$ 567.594
From *Streptomyces lavendulae*. Orange needles (Et_2O). Sol. MeOH, Py, C_6H_6, $CHCl_3$; fairly sol. Et_2O; poorly sol. H_2O, hexane.
Mp 143-146°. $[\alpha]_D^{20}$ -20.8 (c, 1 in MeOH). λ_{max} 268 (ϵ 21880); 368 (ϵ 1450) (MeOH) (Derep).

▶ LD_{50} (mus, ipr) 250 mg/kg. TX1418300

Decyano, 14-oxo, 1,4-hydroquinone: ***Saframycin D***
[66082-30-2]
$C_{28}H_{31}N_3O_9$ 553.568
Prod. by *Streptomyces lavendulae*. Shows antibiotic and anti-neoplastic props. Yellow needles. Sol. MeOH, $CHCl_3$, Py, C_6H_6; fairly sol. Et_2O, EtOAc, Me_2CO; poorly sol. hexane, H_2O.
Mp 150-154°. $[\alpha]_D^{20}$ +141 (c, 1 in MeOH). λ_{max} 243 (ϵ 13800); 274 (ϵ 17400); 369 (ϵ 5620) (MeOH) (Derep).

▶ LD_{50} (mus, ipr) 250 mg/kg. TX1486750

Decyano, 5α-hydroxy, 1,4-hydroquinone: ***Saframycin E***
[66082-31-3]
$C_{28}H_{33}N_3O_9$ 555.583
Isol. from *Streptomyces lavendulae*. Yellow powder. Sol. MeOH, $CHCl_3$, Py, C_6H_6; fairly sol. Et_2O, Me_2CO, EtOAc, $CHCl_3$; poorly sol. hexane, H_2O.
Mp 146-148°. $[\alpha]_D^{20}$ -37.3 (c, 0.53 in MeOH). λ_{max} 243 (ϵ 13800); 274 (ϵ 17400); 369 (ϵ 5620) (MeOH) (Derep). λ_{max} 272 (ϵ 10700); 368 (ϵ 8500) (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 250 mg/kg. VN2265100

(±)-form

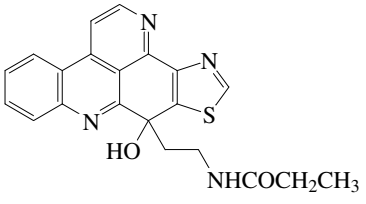
Decyano: [82660-65-9]
$C_{28}H_{31}N_3O_8$ 537.568
Synthetic. Mp 175-180° dec.

Arai, T. *et al., J. Antibiot.*, 1977, **30**, 1015-1018 (*Saframycins A,B,C,D,E, isol, ir, uv, ms, pmr*)
Ger. Pat., 1979, 2 839 668; *CA*, **90**, 166572 (*isol*)
Arai, T. *et al., Tet. Lett.*, 1979, 2355-2358 (*Saframycin C, cryst struct, Saframycin B*)
Arai, T. *et al., Experientia*, 1980, **36**, 1025-1027 (*uv, ir, pmr, cmr, ms, cd, struct*)
Lown, J.W. *et al., Can. J. Chem.*, 1981, **59**, 2945-2952 (*pmr, bibl*)
Takahashi, K. *et al., J. Antibiot.*, 1982, **35**, 196-202 (*25-alcohol, decyano 25-alcohol*)
Yazawa, K. *et al., J. Antibiot.*, 1982, **35**, 915-917 (*biosynth*)

Fukuyama, T. *et al., J.A.C.S.*, 1982, **104**, 4957-4958; 1990, **112**, 3712-3713 (*Saframycin B, synth*)
Arai, T. *et al., Alkaloids (N.Y.)*, 1983, **21**, 89-95 (*biol props*)
Kishi, K. *et al., J. Antibiot.*, 1984, **37**, 847-852 (*struct, props, Saframycins D,F,G*)
Haruyama, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 905-915 (*pmr, abs config*)
Cooper, R. *et al., J. Antibiot.*, 1985, **38**, 24-30 (*ms*)
Mikami, V. *et al., J. Biol. Chem.*, 1985, **260**, 344-348 (*biosynth*)
Sachleben, R.A. *et al., Diss. Abstr. Int., B*, 1986, **46**, 1429 (*synth*)
Kubo, A. *et al., Chem. Pharm. Bull.*, 1987, **35**, 440-442 (*Saframycin D, uv, ir, pmr, cmr, ms, struct*)
Mikami, Y. *et al., J. Antibiot.*, 1988, **41**, 734-740 (*Saframycins F,G*)
Kubo, A. *et al., J.O.C.*, 1988, **53**, 4295-4310 (*Saframycin B, synth*)
Saito, N. *et al., Tetrahedron*, 1990, **46**, 7711-7728 (*Saframycins C,D, synth*)
Shawe, T.T. *et al., Tetrahedron*, 1991, **47**, 5643-5666 (*Saframycin B, synth*)
Saito, N. *et al., Chem. Pharm. Bull.*, 1995, **43**, 777-782 (*Saframycin E, synth*)
Myers, A.G. *et al., J.A.C.S.*, 1999, **121**, 10828-10829 (*synth*)
Martinez, E.J. *et al., Org. Lett.*, 1999, **1**, 75-77 (*Saframycin A, synth*)
Saito, N. *et al., Heterocycles*, 2001, **55**, 21-28 (*Saframycin D, pmr, cmr*)

Sagitol S-4

[185543-92-4]

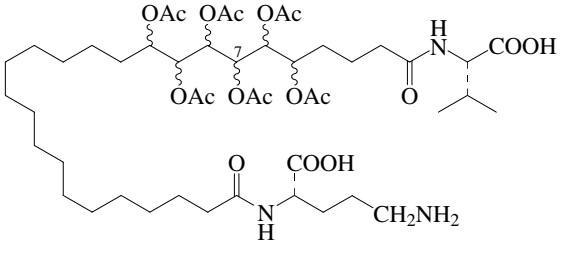


$C_{21}H_{18}N_4O_2S$ 390.465

Minor alkaloid from the sponge *Oceanapia sagittaria*. Yellow glass. Closely related to Kuanoniamine C, in D-30. λ_{max} 260 (ϵ 22810); 318 (ϵ 3430); 335 (ϵ 3920); 351 (ϵ 3430); 396 (ϵ 1470) (MeOH).

Salomon, C.E. *et al., Tet. Lett.*, 1996, **37**, 9147 (*isol, uv, ir, pmr, cmr, struct*)

Sagittamide A S-5



$C_{48}H_{81}N_3O_{18}$ 988.177

Two groups of workers have come to different conclusions regarding the abs. config. of Sagittamide A. Isol. from an unidentified didemnid ascidian from Micronesia. Glass. $[\alpha]_D^{25}$ -22 (c, 0.6 in MeOH). λ_{max} 214; 228; 276 (MeOH).

7-O-*De-Ac:* ***Sagittamide B***

$C_{46}H_{79}N_3O_{17}$ 946.14

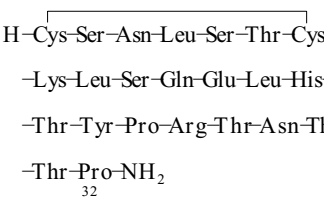
Isol. from an unidentified didemnid ascidian from Micronesia. Glass. $[\alpha]_D^{25}$ -19.7 (c, 0.17 in MeOH). λ_{max} 214 (ϵ 1534); 256 (ϵ 702) (MeOH).

Lievens, S.C. *et al., Org. Lett.*, 2005, **7**, 2281-2284 (*isol, pmr, cmr*)
Lievens, S.C. *et al., J.A.C.S.*, 2006, **128**, 11764-11765 (*abs config*)
Seike, H. *et al., Org. Lett.*, 2006, **8**, 3865-3868 (*synth, abs config*)

Salcatonin, BAN S-6

Calcitonin (salmon), 9CI. Salmon calcitonin. Calcimar. Calcitonin L. Calsynar. Miacalcin. Osteotonina. Prontocalcin. Tonocalcin. SCT 1. SMC 20l051

[47931-85-1]



$C_{145}H_{240}N_{44}O_{48}S_2$ 3431.889

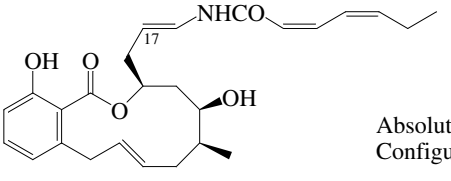
A hormone isol. from the ultimabranchial body of salmon. Differs markedly in struct. from human calcitonin (13 residues differ) see Calcitonin. Used in diagnosis of occult medullary carcinoma of the thyroid and treatment osteoporosis and various hypercalcaemic states. Compared with human calcitonin, has enhanced activity as an inhibitor of bone resorption. It is approx. 25-fold more potent and of 5-fold longer duration. Shows more side-effects. Approved for pharmaceutical use 1991. Recombinant salmon calcitonin (Forcaltonin) approved for use in the EU (1999). Powder. Sol. H_2O.

▶ EV8000000

Guttmann, S. *et al., Helv. Chim. Acta*, 1969, **52**, 1789 (*synth*)
Napoli, J. *et al., Burger's Med. Chem.*, 4th edn., (Ed. Wolff, M.E.), Wiley-Interscience, 1979, 705 (*rev*)
Meienhofer, J. *et al., Burger's Med. Chem.*, 4th edn., (Ed. Wolff, M.E.), Wiley-Interscience, 1979, 806 (*rev*)
U.S. Pat., 1980, 4 212 795; *CA*, **94**, 66084c (*synth*)
Epand, R.M. *et al., Int. J. Pept. Protein Res.*, 1986, **27**, 501 (*conformn, props*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 8392
Wuester, C. *et al., Eur. J. Clin. Pharmacol.*, 1991, **41**, 211 (*pharmacol*)
Lee, I.H. *et al., J. Chromatogr. Sci.*, 1991, **29**, 136 (*hplc*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 655

Salicylihalamide A S-7

[198481-99-1]



Absolute Configuration

$C_{26}H_{33}NO_5$ 439.55

Isol. from the sponge *Haliclona* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D$ -35 (c ,0.7 in MeOH). λ_{max} 280 (ϵ 34000) (MeOH).

17Z-Isomer: ***Salicylihalamide B***

[198482-00-7]

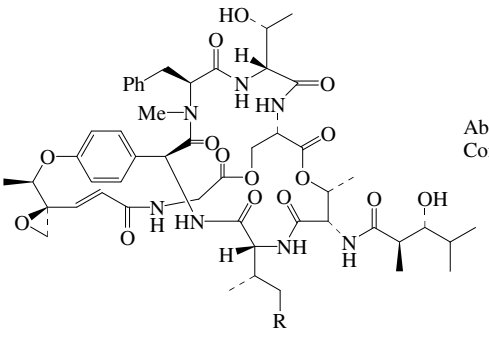
$C_{26}H_{33}NO_5$ 439.55

Isol. from *Haliclona* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D$ -73 (c, 0.3 in MeOH). λ_{max} 280 (ϵ 38000) (MeOH).

Erickson, K.L. *et al., J.O.C.*, 1997, **62**, 8188-8192; 2001, **66**, 1532 (*isol, uv, ir, pmr, cmr, ms*)
Fuerstner, A. *et al., Chem. Eur. J.*, 2001, **7**, 5286-5298 (*synth*)
Snider, B.B. *et al., Org. Lett.*, 2001, **3**, 1817-1820 (*synth*)
Smith III, A.B. *et al., Synlett*, 2001, 1019-1023 (*synth*)
Labrecque, D. *et al., Tet. Lett.*, 2001, **42**, 2645-2648 (*synth*)
Wu, Y. *et al., J.A.C.S.*, 2002, **124**, 3245-3253 (*synth, abs config*)
Smith, A.B. *et al., Tetrahedron*, 2002, **58**, 6455-6471 (*synth*)
Yet, L. *et al., Chem. Rev.*, 2003, **103**, 4283-4306 (*rev*)
Holloway, G.A. *et al., J.O.C.*, 2003, **68**, 2200-2204 (*synth*)
Yang, K. *et al., J.O.C.*, 2003, **68**, 10030-10039 (*synth*)
Herb, C. *et al., Chem. Eur. J.*, 2004, **10**, 5649-5660 (*synth*)
Haack, T. *et al., J.O.C.*, 2005, **70**, 7592-7604 (*synth*)

Salinamide A S-8

[152340-22-2]



Absolute Configuration

R = CH_3

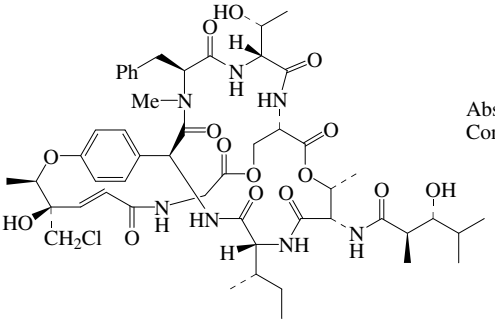
$C_{51}H_{69}N_7O_{15}$ 1020.144

Bicyclic depsipeptide antibiotic. Prod. by a marine *Streptomyces* sp. CNB-091 from a jellyfish. Mod. active against gram-positive bacteria. Pale yellow solid.
Mp 221-225° dec. $[\alpha]_D$ -26 (c, 0.97 in $CDCl_3$). λ_{max} 208; 224; 267; 281 (MeOH). λ_{max} 208; 224; 267; 281 (MeOH) (Berdy).

Miao, S. *et al., J. Nat. Prod.*, 1997, **60**, 858-861 (*isol, activity*)
Moore, B.S. *et al., Tet. Lett.*, 1998, **39**, 3915-3918 (*biosynth*)
Moore, B.S. *et al., J.O.C.*, 1999, **64**, 1145-1150 (*isol, uv, ir, pmr, cmr, ms*)

Salinamide B S-9

[152340-23-3]



Absolute Configuration

$C_{51}H_{70}ClN_7O_{15}$ 1056.605

Bicyclic depsipeptide antibiotic. Prod. by a marine Streptomycete. Mod. active against gram-positive bacteria. Cryst.
Mp 239-241°. $[\alpha]_D$ -65 (c, 0.57 in $CDCl_3$). Probable artifact. λ_{max} 209; 227; 268; 282 (MeOH).

Trischman, J.A. *et al., J.A.C.S.*, 1994, **116**, 757-758 (*cryst struct*)
Moore, B.S. *et al., J.O.C.*, 1999, **64**, 1145-1150 (*isol, uv, ir, pmr, cmr, ms*)

Salinamide D S-10

[221524-55-6]

As Salinamide A, S-8 with

R = H

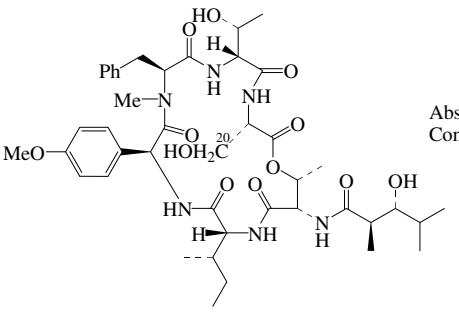
$C_{50}H_{67}N_7O_{15}$ 1006.117

Depsipeptide antibiotic. Prod. by a marine *Streptomyces* sp. CNB-091 from a jellyfish. Pale yellow solid. $[\alpha]_D$ -54.4 (c, 0.85 in $CDCl_3$).

Moore, B.S. *et al., J.O.C.*, 1999, **64**, 1145-1150 (*isol, ir, pmr, cmr*)

Salinamide E S-11

[221524-70-5]



Absolute Configuration

$C_{43}H_{62}N_6O_{12}$ 854.996

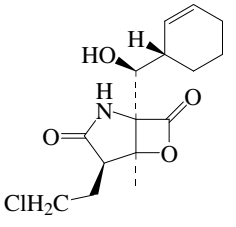
Depsipeptide antibiotic. Prod. by *Streptomyces* sp. CNB-091 from a jellyfish. Off-white solid. $[\alpha]_D$ -93.4 (c, 1.35 in $CDCl_3$).

20-O-[(4-Methyl-2,4-hexadienoylamino)acetyl]: ***Salinamide C***
[221524-63-6]
$C_{52}H_{73}N_7O_{14}$ 1020.187
Prod. by *Streptomyces* sp. CNB-091 from a jellyfish. Off-white solid.

Moore, B.S. *et al., J.O.C.*, 1999, **64**, 1145-1150 (*isol, ir, pmr, cmr, ms*)

Salinosporamide A S-12

NPI 0052. Antibiotic NPI 0052



Absolute Configuration

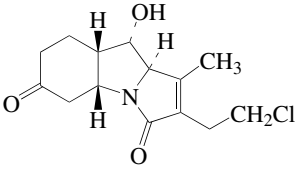
$C_{15}H_{20}ClNO_4$ 313.78

Prod. by the marine bacterium *Salinospora tropica* (strain CNB-392). Proteasome inhibitor. Cytotoxic. Needles (EtOAc/isooctane).
Mp 169-171°. $[\alpha]_D^{25}$ -72.9 (c, 0.55 in MeOH). λ_{max} 205 (log ϵ 4.03); 225 (log ϵ 3.3) (MeOH).

Dechloro: ***Salinosporamide B****. NPI 0047. Antibiotic NPI 0047*
$C_{15}H_{21}NO_4$ 279.335
Prod. by *Salinospora tropica* (strain CNB-392). Amorph. solid.
Mp 143-145°. $[\alpha]_D$ -54.5 (c, 0.29 in MeOH). λ_{max} 256 (log ϵ 3.7) (MeOH).

Feling, R.H. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 355-357 (*isol, pmr, cmr, cryst struct*)
Macherla, V.R. *et al., J. Med. Chem.*, 2005, **48**, 3684-3687 (*sar*)
Endo, A. *et al., J.A.C.S.*, 2005, **127**, 8298-8299 (*synth*)
Williams, P.G. *et al., J.O.C.*, 2005, **70**, 6196-6203 (*Salinosporamide B*)
Reddy, L.R. *et al., Org. Lett.*, 2005, **7**, 2699-2701 (*synth*)
Groll, M. *et al., J.A.C.S.*, 2006, **128**, 5136-5141 (*proteasome complex, struct*)
Mulholland, N.P. *et al., Org. Biomol. Chem.*, 2006, **4**, 2845-2846 (*synth*)

Salinosporamide C S-13



Relative Configuration

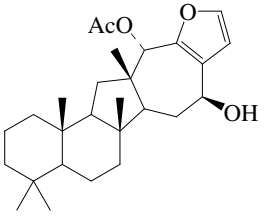
$C_{14}H_{18}ClNO_3$ 283.754

Prod. by the marine bacterium *Salinospora tropica* (strain CNB-392). Cytotoxic. Oil. $[\alpha]_D$ -33.6 (c, 0.27 in MeOH). Possible artifact. λ_{max} 222 (log ϵ 3.9) (MeOH).

Williams, P.G. *et al., J.O.C.*, 2005, **70**, 6196-6203 (*isol, pmr, cmr*)

Salmahyrtisol A S-14

[394248-41-0]



$C_{27}H_{40}O_4$ 428.611
Constit. of *Hyrtios erecta*. Cryst. $[\alpha]_D$ -59.15 (c, 0.64 in CH_2Cl_2). λ_{max} 206 (log ϵ 3.19); 262 (log ϵ 2.57) (MeOH).

Youssef, D.T.A. *et al., J. Nat. Prod.*, 2002, **65**, 2-6 (*isol, pmr, cmr*)

Salmine S-15

Salmon protamine
[9014-82-8]
[53597-25-4]

Protein. Isol. from salmon sperm. Used in the form of its sulfate to reverse the anticoagulant effect of heparin. Shows antimicrobial activity.

Block, R.J. *et al., Proc. Soc. Exp. Biol. Med.*, 1949, **70**, 494-496 (*isol*)
Brock, T.D. *et al., Can. J. Microbiol.*, 1958, **4**, 65-71 (*activity*)
Ando, T. *et al., Int. J. Pept. Protein Res.*, 1969, **1**, 221-234 (*isol*)

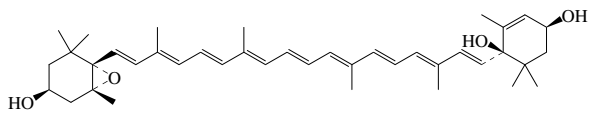
Salmon gonadotrophin-releasing hormone S-16

Salmon GnRH. Sea bream GnRH-III. Rana dybowskii *Gonadotrophin-releasing hormone. [Trp^8]GnRH*
[86073-88-3]
5-OxoPro-His-Trp-Ser-Tyr-Gly-Trp-Leu-Pro-Gly
$C_{60}H_{73}N_{15}O_{13}$ 1212.329
Isol. from brains of salmon (*Oncorhynchus keta*) and Dybowski's brown frog *Rana dybowskii*; also from sea bream (*Sparus aurata*) and Pacific herring (*Clupea harrengus pallasi*).

Sherwood, N. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1983, **80**, 2794-2798 (*isol, salmon*)
Powell, J.F. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1994, **91**, 12081-12085 (*isol, sea bream*)
Carolsfeld, J. *et al., Endocrinology (Baltimore)*, 2000, **141**, 505-512 (*isol, herring*)
Yoo, M.S. *et al., Mol. Cell. Endocrinol.*, 2000, **164**, 197-204 (*isol*)

Salmoxanthin S-17

5,6-Epoxy-5,6-dihydro-β,ϵ-carotene-3,3′,6′-triol
[75138-59-9]

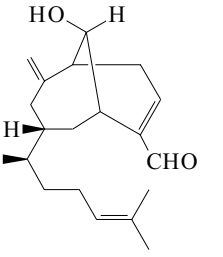


$C_{40}H_{56}O_4$ 600.88
Constit. of *Oncorhynchus keta* and other salmon spp.
Mp 208°. λ_{max} 416; 440; 470 (Et_2O).

Matsuno, T. *et al., Nippon Suisan Gakkaishi*, 1980, **46**, 879; 911 (*occur, struct*)
Matsuno, T. *et al., J. Nat. Prod.*, 2001, **64**, 507-510 (*isol, pmr, uv, cd, abs config*)

Sanadaol S-18

β-Crenulal
[83643-92-9]



Absolute configuration

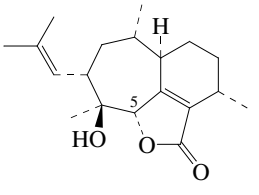
$C_{20}H_{30}O_2$ 302.456
Constit. of brown alga *Pachydictyon coriaceum* and *Dictyota crenulata*. Oil. $[\alpha]_D$ +74.8 (c, 1.33 in $CHCl_3$). May be artifact. λ_{max} 234 (ϵ 7000) (EtOH).

Ac: ***Acetylsanadaol***
[83643-93-0]
$C_{22}H_{32}O_3$ 344.493
Constit. of *Pachydictyon coriaceum* and *Dictyota linearis*. Oil. $[\alpha]_D$ +42.5 (c, 0.89 in $CHCl_3$).

Ishitsuka, M. *et al., Tet. Lett.*, 1982, **23**, 3179 (*isol*)
Kirkup, M.P. *et al., Phytochemistry*, 1983, **22**, 2527-2529 (*β-Crenulal*)
Nagaoka, H. *et al., Tet. Lett.*, 1987, **28**, 2021; 1988, **29**, 5945 (*synth, abs config*)
Siamopoulou, P. *et al., Phytochemistry*, 2004, **65**, 2025-2030 (*Acetylsanadaol, pmr, cmr*)

Sandresolide A S-19

[250726-99-9]



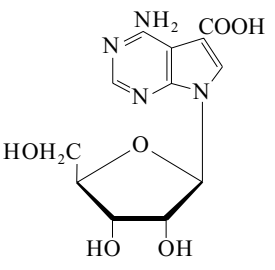
$C_{19}H_{28}O_3$ 304.428
Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{28}$ +23.8 (c, 1.3 in $CHCl_3$). λ_{max} 226 (ϵ 12000) (MeOH).

5β-Hydroxy: ***Sandresolide B***
[250727-01-6]
$C_{19}H_{28}O_4$ 320.428
Constit. of *Pseudopterogorgia elisabethae*. Oil. $[\alpha]_D^{28}$ -18 (c, 1 in $CHCl_3$). λ_{max} 220 (ϵ 10000) (MeOH).

Rodriguez, A.D. *et al., Tet. Lett.*, 1999, **40**, 7627-7631 (*isol, pmr, cmr*)

Sangivamycic acid S-20

*4-Amino-7-β-D-ribofuranosyl-7*H*-pyrrolo[2,3-*d*]pyrimidine-5-carboxylic acid, 8CI*
[18418-00-3]



$C_{12}H_{14}N_4O_6$ 310.266
Cryst. (H_2O). Mp 238° dec.

Hydrochloride: [21090-38-0]
Plates (MeOH). Mp 236-238°.

Me ester: ***5-(Methoxycarbonyl)tubercidin***
[18440-68-1]
$C_{13}H_{16}N_4O_6$ 324.293
Isol. from the sponge *Jaspis johnstoni*. Cytotoxic agent. Cryst. (MeOH/$CHCl_3$). Sol. MeOH, $CHCl_3$; poorly sol. hexane.
Mp 216-218°. λ_{max} 211; 232 (sh); 281 (MeOH).

Me ester, hydrochloride:
Prisms (MeOH). Mp 216-218°.

Amide: ***Sangivamycin***. *B 14437. BA 90912. NSC 65346. OS 1998. Antibiotic B 14437. Antibiotic BA 90912*
[18417-89-5]
$C_{12}H_{15}N_5O_5$ 309.281
Produced by a strain of *Streptomyces rimosus*. Possesses cytotoxicity against HeLa cells and exhibits significant activity against leukaemia 1210 in mice.
Mp 260°. $[\alpha]_D^{26}$ -45.7 (c, 1 in 0.1*M* HCl). λ_{max} 229 (ε 8200); 278 (ε 15100) (EtOH).
▶ LD_{50} (mus, orl) 11 mg/kg. UY9355000

*Nitrile: 4-Amino-7-β-D-ribofuranosyl-7*H*-pyrrolo[2,3-*d*]pyrimidine-5-carbonitrile, 9CI.* ***Toyocamycin***. *Cyanotubercidin. Unamycin B. Vengicide. E 212. Antibiotic 1037. Antibiotic E 212. Anhygroscopin B. Naritheracin*
[606-58-6]
$C_{12}H_{13}N_5O_4$ 291.266
Prod. by *Streptomyces toyocaensis* and *Streptomyces fungicidicus*. Isol. from the sponge *Jaspis johnstoni*. Active against gram-positive organisms; shows some exp. antineoplastic activity.
Needles or prisms + $1H_2O$.
Mp 243°. $[\alpha]_D^{26}$ -55.6 (c, 1 in 0.1*M* HCl). λ_{max} 235 (ε 22100); 273 (ε 16300) (0.1*N* HCl) (Derep). λ_{max} 235 (ε 11600); 280 (ε 16600) (0.1*N* NaOH) (Derep). λ_{max} 207; 232 (ε 11060); 274 (sh); 278 (ε 15700); 289 (sh) (MeOH) (Derep).
▶ LD_{50} (mus, orl) 8 mg/kg. UY9100000

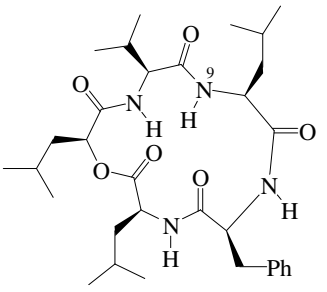
*Nitrile, 5′-*O*-α-D-glucopyranoside:* ***Toyocamycin 5′-α-D-glucopyranose***
[117456-79-8]
$C_{18}H_{23}N_5O_9$ 453.408
Isol. from *Tolypothrix tenuis* and *Plectonema radiosum*. Cytotoxic and antifungal agent. Amorph. Sol. H_2O. $[\alpha]_D^{25}$ +2.1 (c, 0.03 in H_2O). λ_{max} 230 (ε 7400); 278 (ε 10000) (H_2O) (Derep).

5′-Deoxy, nitrile: ***5′-Deoxytoyocamycin***
[65562-55-2]
$C_{12}H_{13}N_5O_3$ 275.266
Prod. by *Streptomyces* sp. A14345. Cryst. + $\frac{1}{2}H_2O$ (H_2O).
Mp 187-188°. λ_{max} 235 (ε 22100); 273 (ε 16300) (0.1*N* HCl) (Derep). λ_{max} 235 (ε 11600); 280 (ε 16600) (0.1*N* NaOH) (Derep). λ_{max} 207; 232 (ε 11060); 274 (sh); 278 (ε 15700); 289 (sh) (MeOH) (Derep).

Suzuki, S. *et al., J. Antibiot., Ser. A*, 1961, **14**, 343
Aszalos, A. *et al., J. Antibiot.*, 1966, **19**, 285
Rao, K.V. *et al., J. Med. Chem.*, 1968, **11**, 939 (*Sangivamycin, isol, struct*)
Tolman, R.L. *et al., J.A.C.S.*, 1968, **90**, 524; 1969, **91**, 2102 (*Sangivamycic acid, Sangivamycin, Toyocamycin, struct, synth*)
U.S. Pat., 1969, 3 423 398; *CA*, **70**, 86268y (*Sangivamycin*)
Uematsu, T. *et al., J. Biol. Chem.*, 1970, **245**, 4365 (*biosynth*)
Japan. Pat., 1970, 70 19 638; *CA*, **73**, 108253f (*isol*)
Nichol, C.A. *et al., Handb. Exp. Pharmacol.*, 1975, **38**, 434 (*rev, pharmacol*)
Chenon, M.-T. *et al., J.A.C.S.*, 1975, **97**, 4627 (*nmr*)
Wang, Y. *et al., Carbohydr. Res.*, 1977, **59**, 449 (*5′-Deoxytoyocamycin*)
Prusiner, P. *et al., Acta Cryst. B*, 1978, **34**, 517 (*cryst struct, deriv*)
Bergstrom, D.E. *et al., J.O.C.*, 1981, **46**, 1423-1431 (*Methoxycarbonyltubercidin, synth*)
Stewart, J.B. *et al., J. Antibiot.*, 1988, **41**, 1048 (*deriv*)
Isono, K. *et al., J. Antibiot.*, 1988, **41**, 1711 (*rev*)
Osada, H. *et al., J. Antibiot.*, 1989, **42**, 102 (*props*)
Zabriskie, T.M. *et al., J. Nat. Prod.*, 1989, **52**, 1353-1356 (*Jaspis johnstoni constits*)
Isaac, B.G. *et al., J. Antibiot.*, 1991, **44**, 729 (*5′-Deoxytoyocamycin*)
Iimori, T. *et al., Tet. Lett.*, 1991, **32**, 7273 (*pmr, conformn*)
Sharma, M. *et al., Nucleosides Nucleotides*, 1993, **12**, 643 (*Toyocamycin, synth*)
Porcari, A.R. *et al., Nucleosides Nucleotides*, 1999, **18**, 153-159 (*Toyocamycin, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SAU000; VGZ000

Sansalvamide S-21

[227084-43-7]



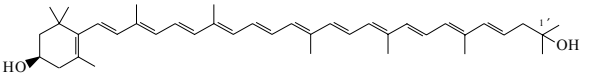
$C_{32}H_{50}N_4O_6$ 586.77
Depsipeptide antibiotic. Prod. by a *Fusarium* sp. collected on *Halodule wrightii*. Cytotoxic. Powder.
Mp 143-152°. $[\alpha]_D$ -115 (c, 0.001 in MeOH). λ_{max} 202 (ε 11690); 214 (ε 6180); 254 (ε 211) (MeOH).

N^9-*Me:* **N-*Methylsansalvamide***
$C_{33}H_{52}N_4O_6$ 600.797
Prod. by a marine *Fusarium* sp., strain CNL-619. Weak cytotoxic agent. Oil. $[\alpha]_D$ -132 (c, 0.41 in CH_2Cl_2). λ_{max} 220 (ε 10120); 256 (ε 1320); 269 (ε 1200) ($CHCl_3$).

Belofsky, G.N. *et al., Tet. Lett.*, 1999, **40**, 2913-2916 (*isol, uv, ir, pmr, cmr, ms*)
Cueto, M. *et al., Phytochemistry*, 2000, **55**, 223-226 (*N-Methylsansalvamide*)
Gu, W. *et al., Org. Lett.*, 2002, **4**, 4171-4174 (*synth*)

Saproxanthin S-22

3′,4′-Didehydro-1′,2′-dihydro-γ-carotene-1′,3-diol. 3′,4′-Didehydro-1′,2′-dihydro-β,ψ-carotene-1′,3-diol
[10153-99-8]



$C_{40}H_{56}O_2$ 568.881
Prod. by the marine flexibacterium *Saprospira grandis*. Cryst. (Et_2O/petrol).
Mp 178-179°. λ_{max} 460, 486 and 518 nm ($CHCl_3$).

*1′-*O*-Rhamnoside:* [36526-61-1]
$C_{46}H_{66}O_6$ 715.024
Prod. by the myxobacterium *Sorangium compositum* isol. from rabbit dung.

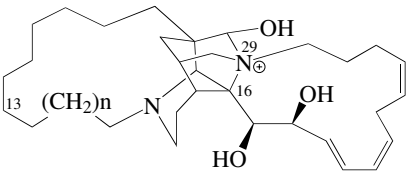
*1′-*O*-Glucoside:* [12742-39-1]
$C_{46}H_{66}O_7$ 731.023
Prod. by the myxobacterium *Sorangium compositum* isol. from rabbit dung.

1′-Me ether: 3′,4-Didehydro-1′,2′-dihydro-1′-methoxy-β,ψ-caroten-3-ol. ***Bacteriorubixanthin***
[119188-86-2]
$C_{41}H_{58}O_2$ 582.908
Prod. by *Erythrobacter longus* isol. from seaweed. λ_{max} 293; 361; 468; 499 (MeOH). λ_{max} 315; 384; 466; 491; 524 (MeOH).

Aasen, A.J. *et al., Acta Chem. Scand.*, 1966, **20**, 811-819 (*isol, uv*)
Liaanen-Jensen, S. *et al., Phytochemistry*, 1969, **8**, 1259-1280; 1970, **9**, 629-635 (*synth, uv*)
Kleinig, H. *et al., Arch. Mikrobiol.*, 1971, **18**, 224-233 (*Sorangium compositum constits*)
Takaichi, S. *et al., Phytochemistry*, 1988, **27**, 3605-3609 (*1′-Me ether*)
Takaichi, S. *et al., Phytochemistry*, 1988, **27**, 3605-3609 (*Bacteriorubixanthin*)
Takaichi, S. *et al., Arch. Microbiol.*, 1990, **153**, 118-122 (*Bacteriorubixanthin*)

Sarain A S-23

[123117-93-1]



n = 1

$C_{32}H_{51}N_2O_3^{\oplus}$ 511.767
Alkaloid from the sponge *Reniera sarai*. Vasodilator, insecticide. Amorph. powder (as acetate salt). $[\alpha]_D$ +66 (c, 1.3 in $CHCl_3$) (acetate). λ_{max} 238 (ϵ 14939) (MeOH).

13,14-Didehydro(Z-), n = 2: ***Sarain B***
[123391-00-4]
$C_{33}H_{51}N_2O_3^{\oplus}$ 523.778
Alkaloid from *Reniera sarai*. Insecticide, acaricide. Toxic to sea urchins. Powder (as acetate salt). $[\alpha]_D$ +76.3 (c, 1.2 in $CHCl_3$) (acetate). λ_{max} 238 (ϵ 13415) (MeOH).

[123117-94-2, 123117-96-4, 123391-01-5]

Cimino, G. *et al., Tetrahedron*, 1989, **45**, 3863 (*isol, uv, ir, pmr, cmr, cryst struct*)
Cimino, G. *et al., J. Nat. Prod.*, 1990, **53**, 1519 (*uv, ir, pmr, cmr, ms*)
Guo, Y. *et al., Tetrahedron*, 1996, **52**, 8341-8348 (*pmr, cmr, abs config*)
Matzanke, N. *et al., Org. Prep. Proced. Int.*, 1998, **30**, 3-51 (*rev*)
Garg, N.K. *et al., Angew. Chem., Int. Ed.*, 2006, **45**, 2912-2915 (*synth*)

Sarain C S-24

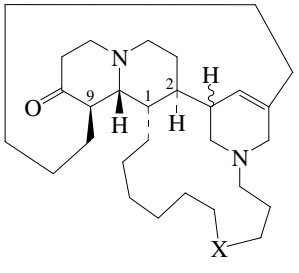
[123089-18-9]
As Sarain A, S-23 with
n = 2
$C_{33}H_{53}N_2O_3^{\oplus}$ 525.793
Alkaloid from the sponge *Reniera sarai*. Insecticide, acaricide, toxic to sea urchins. Amorph. powder. $[\alpha]_D$ +67.4 (c,1 in $CHCl_3$). λ_{max} 238 (ϵ 13582) (MeOH).

[123089-19-0]

Cimino, G. *et al., Tetrahedron*, 1989, **45**, 3863 (*isol, uv, ir, pmr, cmr*)
Caprioli, V. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1992, **103**, 293 (*activity*)
Guo, Y. *et al., Tetrahedron*, 1996, **52**, 8341 (*abs config*)

Saraine 1 S-25

[105418-77-7]



Absolute Configuration

X = —CH=CH—(*Z*-)

$C_{31}H_{50}N_2O$ 466.749
Alkaloid from the marine sponge *Reniera sarai*. Antiarrythmic, ion chelator, insecticide. Amorph. powder. $[\alpha]_D$ -47.8 (c, 1.2 in $CHCl_3$).
▶ LD_{50} (mus, ipr) 200 mg/kg.

1,2,9-Triepimer: ***Isosaraine 1***
[119766-95-9]
$C_{31}H_{50}N_2O$ 466.749
Minor alkaloid from the Mediterranean sponge *Reniera sarai*. Shows insecticidal props. Amorph. solid. $[\alpha]_D$ -23.1 (c, 1.2 in $CHCl_3$).

Cimino, G. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 783-800 (*isol, pmr, cmr, biosynth*)
Cimino, G. *et al., Tet. Lett.*, 1989, **30**, 133-136 (*isol, pmr, cmr, ms, struct*)
Caprioli, V. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1992, **103**, 293-296 (*biochem*)
Guo, Y. *et al., Tetrahedron*, 1996, **52**, 14961-14974 (*cmr*)
Guo, Y. *et al., Tet. Lett.*, 1998, **39**, 463-466 (*abs config*)

Saraine 2 S-26

[105418-80-2]
As Saraine 1, S-25 with
X = –CH_2–
$C_{30}H_{50}N_2O$ 454.738
Alkaloid from the marine sponge *Reniera sarai*. Antiarrythmic, ion-chelator, insecticide. Amorph. powder. $[\alpha]_D$ -117 (c, 1.1 in $CHCl_3$).

1,2,9-Triepimer: ***Isosaraine 2***
[135091-28-0]
$C_{30}H_{50}N_2O$ 454.738
Alkaloid from the marine sponge *Reniera sarai*. Oil. $[\alpha]_D$ -34.6 (c, 2 in $CHCl_3$).

Cimino, G. *et al., Bull. Soc. Chim. Belg.*, 1986, 783-800 (*isol, pmr, cmr, biosynth*)
Cimino, G. *et al., Tet. Lett.*, 1989, **30**, 133-136 (*struct*)
Cimino, G. *et al., Magn. Reson. Chem.*, 1991, **29**, 327-332 (*isol, pmr, cmr, struct*)
Caprioli, V. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1992, **103**, 293-296 (*biochem*)
Guo, Y. *et al., Tetrahedron*, 1996, **52**, 14961-14974 (*abs config, cmr*)
Guo, Y. *et al., Tet. Lett.*, 1998, **39**, 463-466 (*config*)

Saraine 3 S-27

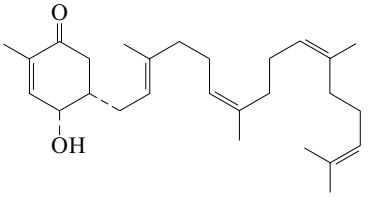
[105305-54-2]
As Saraine 1, S-25 with
X = –CH=CH–CH_2–
$C_{32}H_{52}N_2O$ 480.776
Alkaloid from the marine sponge *Reniera sarai*. Antiarrythmic, ion-chelator , insecticide. Amorph. powder. $[\alpha]_D$ -27.4 (c, 0.8 in $CHCl_3$).

1,2,9-Triepimer: ***Isosaraine 3***
[184429-62-7]
$C_{32}H_{52}N_2O$ 480.776
Alkaloid from the sponge *Reniera sarai*. Amorph. powder. $[\alpha]_D$ -16.3 (c, 1.34 in $CHCl_3$).

Cimino, G. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 783-800 (*isol, pmr, cmr, biosynth*)
Cimino, G. *et al., Tet. Lett.*, 1989, **30**, 133-136 (*struct*)
Caprioli, V. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1992, **103**, 293-296 (*biochem*)
Guo, Y. *et al., Tetrahedron*, 1996, **52**, 14961-14974 (*pmr, cmr, struct*)
Guo, Y. *et al., Tet. Lett.*, 1998, **39**, 463-466 (*abs config*)

Sarcodictyenone S-28

[111074-75-0]

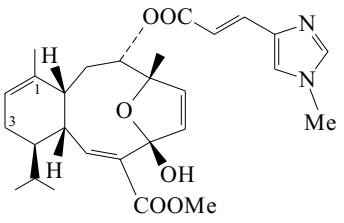


$C_{27}H_{42}O_2$ 398.628
Constit. of *Sarcodictyon roseum*. Viscous oil. $[\alpha]_D^{23}$ +52 (c, 0.17 in EtOH). λ_{max} 203 (ϵ 25000); 229 (ϵ 8500) (EtOH).

D'Abrosio, M. *et al., Helv. Chim. Acta*, 1986, **69**, 1581-1584 (*isol, pmr, cmr, ms*)

Sarcodictyin A S-29

[113540-81-1]



$C_{28}H_{36}N_2O_6$ 496.602
Constit. of *Sarcodictyon roseum*, *Eleutherobia aurea* and *Rolandia rosea*. Histidine decarboxylase inhibitor; shows potent antitumour activity; induces tubulin polymerisation. Powder (MeOH). Mp 219-222°. $[\alpha]_D^{20}$ -15.2 (c, 1.12 in EtOH). λ_{max} 202 (ϵ 12000); 290 (ϵ 2000) (EtOH) (Berdy).

Et ester analogue: ***Sarcodictyin B***
[113555-26-3]
$C_{29}H_{38}N_2O_6$ 510.629
Constit. of *Sarcodictyon roseum* and *Rolandia rosea*. Histidine decarboxylase inhibitor; shows potent antitumour activity; induces tubulin polymerisation. Oil. $[\alpha]_D^{20}$ -4.36 (c, 0.27 in EtOH).

3α-Hydroxy: ***Sarcodictyin C***
[122169-38-4]
$C_{28}H_{36}N_2O_7$ 512.602
Constit. of *Sarcodictyon roseum*. Microcryst. powder (Me_2CO). Mp 225-227°. $[\alpha]_D^{20}$ -16.5 (c, 0.085 in EtOH).

3α-Acetoxy: ***Sarcodictyin D***
[122052-96-4]
$C_{30}H_{38}N_2O_8$ 554.639
Constit. of *Sarcodictyon roseum*. Microcryst. powder (MeOH). Mp 130-132°. $[\alpha]_D^{20}$ -27.2 (c, 0.25 in MeOH).

Z-Urocanic ester isomer: ***Z-Sarcodictyin A***
[514830-04-7]
$C_{28}H_{36}N_2O_6$ 496.602
Constit. of *Bellonella albiflora*. Powder. $[\alpha]_D^{20}$ +40 (c, 0.1 in EtOH). λ_{max} 208 (ϵ 16000); 217 (ϵ 14000); 296 (ϵ 9900) (MeOH).

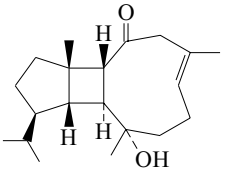
Z-Urocanic ester isomer, 3α-hydroxy: ***Sarcodictyin E***
[122052-94-2]
$C_{28}H_{36}N_2O_7$ 512.602
Constit. of *Sarcodictyon roseum*. Microcryst. powder (MeOH). Mp 212-214°. $[\alpha]_D^{20}$ +15.6 (c, 0.42 in MeOH).

Δ^2-Isomer, 1α-hydroxy: ***Sarcodictyin F***
[122052-95-3]
$C_{28}H_{36}N_2O_7$ 512.602
Constit. of *Sarcodictyon roseum*. Microcryst. powder (MeOH). Mp 228-229°. $[\alpha]_D^{20}$ +2.7 (c, 0.15 in MeOH).

D'Ambrosio, M. *et al., Helv. Chim. Acta*, 1987, **70**, 2019; 1988, **71**, 964 (*isol, pmr, cmr*)
Ketzinel, S. *et al., J. Nat. Prod.*, 1996, **59**, 873 (*isol, pmr, cmr*)
Nicolaou, K.C. *et al., Angew. Chem., Int. Ed.*, 1998, **37**, 1418-1421 (*Sarcodictyins A,B, synth, activity*)
Bernardelli, P. *et al., Heterocycles*, 1998, **49**, 531-556 (*rev*)
Nicolaou, K.C. *et al., J.A.C.S.*, 1998, **120**, 8661-8673 (*Sarcodictyins A,B, synth*)
Nicolaou, K.C. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1199-1213 (*rev*)
Nakao, Y. *et al., J. Nat. Prod.*, 2003, **66**, 524-527 (*Z-Sarcodictyin A*)

Sarcoglane S-30

[181820-13-3]

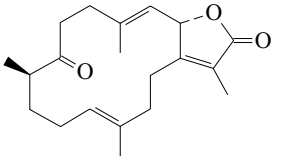


$C_{20}H_{32}O_2$ 304.472
Constit. of *Sarcophyton glaucum*. Cryst. Mp 138°. $[\alpha]_D$ +110.

Fridkovsky, E. *et al., Tet. Lett.*, 1996, **37**, 6909-6910 (*isol, pmr, cmr*)

Sarcophinone S-31

7-Oxo-1(15),3,11-cembratrien-16,2-olide
[99685-17-3]



$C_{20}H_{28}O_3$ 316.439
Constit. of the soft coral *Sarcophyton decaryi*. Mp 141-142°.

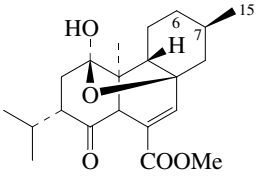
2-Epimer: ***Isosarcophinone***
[392696-43-4]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Sarcophyton molle*.

[99647-41-3]

Yan, Z. *et al., Redai Haiyang*, 1985, **4**, 80; *CA*, **104**, 106609m (*isol, pmr, cmr, ir*)
Czarkie, D. *et al., Tetrahedron*, 1985, **41**, 1049 (*synth*)
Liu, Y.X. *et al., Acta Cryst. C*, 1986, **42**, 373 (*cryst struct*)
Su, J.Y. *et al., Gaodeng Xuexiao Huaxue Xuebao*, 2001, **22**, 1515-1517; *CA*, **136**, 131780d (*Isosarcophinone*)

Sarcophytin S-32

[201740-15-0]



$C_{21}H_{30}O_5$ 362.465
Constit. of coelenterate *Sarcophyton elegans*. Cryst. Mp 162-163°. $[\alpha]_D^{25}$ +0.24 (c, 0.08 in $CHCl_3$). λ_{max} 219 (MeOH) (Berdy).

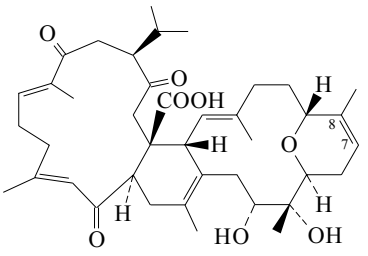
6,7-Didehydro: ***Sarcophytin B***
[256386-54-6]
$C_{21}H_{28}O_5$ 360.449
Constit. of a *Sarcophyton* sp. Cryst. (MeOH). Mp 185-188°. $[\alpha]_D$ +206 (c, 0.43 in $CHCl_3$). λ_{max} 245 (log ϵ 3600) (EtOH).

7,8-Didehydro: ***7,8-Dehydrosarcophytin***
[221455-12-5]
$C_{21}H_{28}O_5$ 360.449
Constit. of *Sarcophyton elegans*. Cryst. Mp 160-162°. $[\alpha]_D^{25}$ +403.6 (c, 0.5 in $CHCl_3$). λ_{max} 238 ($CHCl_3$).

7,15-Didehydro: ***Sarcophytin C****. 7,15-Dehydrosarcophytin*
[221541-48-6]
$C_{21}H_{28}O_5$ 360.449
Constit. of *Sarcophyton elegans*. Needles (hexane/Me_2CO). Mp 160-162°. $[\alpha]_D^{25}$ +0.3 (c, 1 in $CHCl_3$).

Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 1090-1091
Anjaneyulu, A.S.R. *et al., Tet. Lett.*, 1998, **39**, 135-138 (*isol, pmr, cmr, cryst struct*)
Anjaneyulu, A.S.R. *et al., J. Indian Chem. Soc.*, 1999, **76**, 651-659 (*isol*)
Anjaneyulu, V. *et al., J. Nat. Prod.*, 2000, **63**, 109-111 (*Sarcophytins B and C, cryst struct*)

Sarcophytoic acid S-33



$C_{40}H_{56}O_8$ 664.878

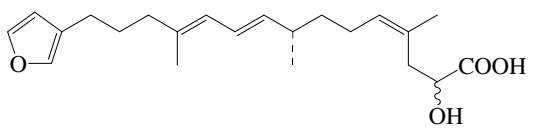
Me ester: ***Methyl sarcophytoate***
[129239-13-0]
$C_{41}H_{58}O_8$ 678.904
Constit. of *Sarcophyton glaucum*. Oil. $[\alpha]_D$ +157 (c, 0.34 in $CHCl_3$). λ_{max} 232 (ϵ 18000) (MeOH) (Derep).

7,8-Dihydro, 8α-chloro, Me ester: ***Methyl chlorosarcophytoate***
[129239-14-1]
$C_{41}H_{59}ClO_8$ 715.365
Constit. of *Sarcophyton glaucum*. Oil. $[\alpha]_D$ +140 (c, 0.38 in $CHCl_3$). λ_{max} 231 (ϵ 17000) (MeOH) (Derep).

Kusumi, T. *et al., J.O.C.*, 1990, **55**, 6286 (*isol, pmr, cmr*)
Ishitsuka, M.O. *et al., Tet. Lett.*, 1991, **32**, 6595 (*abs config*)

Sarcotin I S-34

[472974-64-4]



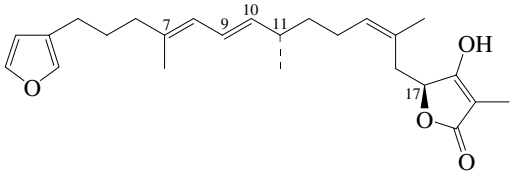
$C_{22}H_{32}O_4$ 360.492
Constit. of a *Sarcotragus* sponge. Oil (as Na salt). $[\alpha]_D^{21}$ +33.1 (c, 0.14 in MeOH) (Na salt).

Me ester: ***Sarcotin J***
[472974-65-5]
$C_{23}H_{34}O_4$ 374.519
Constit. of a *Sarcotragus* sponge. Oil. $[\alpha]_D^{21}$ +115.4 (c, 0.046 in MeOH).

Liu, Y. *et al., J. Nat. Prod.*, 2002, **65**, 1307-1314 (*isol, pmr, cmr*)

Sarcotin A S-35

[369367-31-7]



$C_{25}H_{34}O_4$ 398.541
Struct. revised in 2002. Constit. of a *Sarcotragus* sp. Oil. $[\alpha]_D^{25}$ +67.9 (c, 0.04 in MeOH).

*(7Z,9Z,17*R*)-Isomer:* ***Sarcotin B***
[369367-32-8]
$C_{25}H_{34}O_4$ 398.541
Constit. of a *Sarcotragus* sp. Oil.

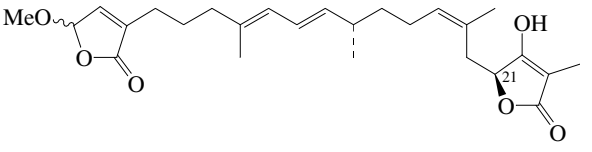
*Δ^6,Δ^{10}-Isomer(6*E*,10*E*):* ***Sarcotin C***
[369383-48-2]
$C_{25}H_{34}O_4$ 398.541
Constit. of a *Sarcotragus* sp. Oil.

17-Epimer: ***Episarcotin A***
[472974-45-1]
$C_{25}H_{34}O_4$ 398.541
Constit. of a *Sarcotragus* sponge. Oil. $[\alpha]_D^{25}$ +37.5 (c, 0.04 in MeOH). λ_{max} 226 (log ϵ 4.76) (MeOH).

Liu, Y. *et al., J. Nat. Prod.*, 2001, **64**, 1301-1304; 2002, **65**, 1307-1314 (*isol, pmr, cmr, struct, Episarcotin A*)

Sarcotin F S-36

[472974-57-5]



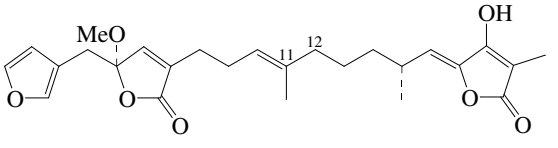
$C_{26}H_{36}O_6$ 444.567
Constit. of a *Sarcotragus* sponge. Oil. $[\alpha]_D^{21}$ +30.8 (c, 0.36 in MeOH). λ_{max} 247 (log ϵ 4.95) (MeOH).

21-Epimer: ***Episarcotin F***
[627895-35-6]
$C_{26}H_{36}O_6$ 444.567
Constit. of a *Sarcotragus* sp. Yellow oil. $[\alpha]_D^{21}$ +57.7 (c, 0.04 in MeOH).

Liu, Y. *et al., J. Nat. Prod.*, 2002, **65**, 1307-1314; 2003, **66**, 1451-1456 (*isol, pmr, cmr*)

Sarcotin G S-37

[472974-58-6]



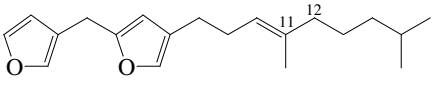
$C_{26}H_{32}O_7$ 456.535
Constit. of a *Sarcotragus* sponge. Oil. $[\alpha]_D^{21}$ +27.9 (c, 0.09 in MeOH). λ_{max} 248 (log ϵ 4.67) (MeOH).

Δ^{11}-Isomer (11Z-): ***Sarcotin H***
[472974-63-3]
$C_{26}H_{32}O_7$ 456.535
Constit. of a *Sarcotragus* sponge. Oil. $[\alpha]_D^{21}$ +35.2 (c, 0.1 in MeOH).

Liu, Y. *et al., J. Nat. Prod.*, 2002, **65**, 1307-1314 (*isol, pmr, cmr*)

Sarcotin K S-38

[472974-66-6]



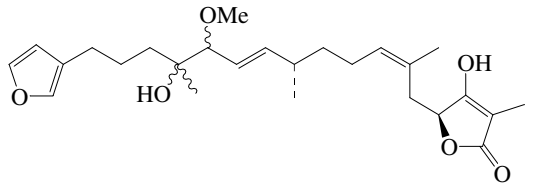
$C_{20}H_{28}O_2$ 300.44
Constit. of a *Sarcotragus* sponge. Oil.

Δ^{11}-Isomer (11Z-): ***Sarcotin L***
[472974-69-9]
$C_{20}H_{28}O_2$ 300.44
Constit. of a *Sarcotragus* sp. Oil.

Liu, Y. *et al., J. Nat. Prod.*, 2002, **65**, 1307-1314 (*isol, pmr, cmr*)

Sarcotin M S-39

[472974-85-9]

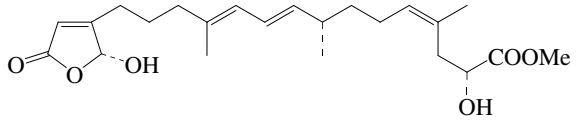


$C_{26}H_{38}O_6$ 446.583
Constit. of a *Sarcotragus* sponge. Oil. $[\alpha]_D^{21}$ +26.8 (c, 0.02 in MeOH).

Liu, Y. *et al., J. Nat. Prod.*, 2002, **65**, 1307-1314 (*isol, pmr, cmr*)

Sarcotin N S-40

[627895-33-4]

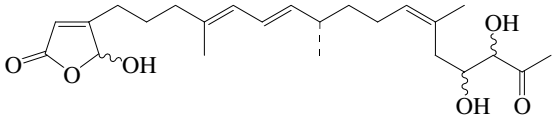


$C_{23}H_{34}O_6$ 406.518
Constit. of a *Sarcotragus* sp. Oil. $[\alpha]_D^{21}$ +66.7 (c, 0.06 in MeOH).

Liu, Y. *et al., J. Nat. Prod.*, 2003, **66**, 1451-1456 (*isol, pmr, cmr*)

Sarcotin O S-41

[627895-34-5]

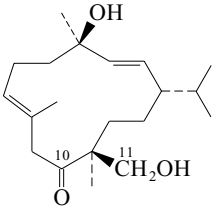


$C_{24}H_{36}O_6$ 420.545
Constit. of a *Sarcotragus* sp. Oil. $[\alpha]_D^{21}$ +13.6 (c, 0.04 in MeOH).

Liu, Y. *et al., J. Nat. Prod.*, 2003, **66**, 1451-1456 (*isol, pmr, cmr*)

Sarcotol S-42

[161897-62-7]



$C_{20}H_{34}O_3$ 322.487
Constit. of a *Sarcophyton* sp. Needles.
Mp 113°. $[\alpha]_D^{27}$ -189.7 (c, 0.01 in MeOH). λ_{max} 208 (ϵ 3500) (MeOH) (Berdy).

11-Ac: ***Sarcotol acetate***
[161897-63-8]
$C_{22}H_{36}O_4$ 364.524
Constit. of a *Sarcophyton* sp. Oil. $[\alpha]_D^{27}$ -182.4 (c, 0.187 in MeOH). λ_{max} 208 (ϵ 2130) (MeOH) (Berdy).

4-Me ether: ***4-O-Methylsarcotol***
[185102-36-7]
$C_{21}H_{36}O_3$ 336.514
Constit. of a *Sarcophyton* sp. Oil. $[\alpha]_D^{27}$ -67.8 (c, 0.15 in MeOH). λ_{max} 207 (ϵ 2800) (MeOH).

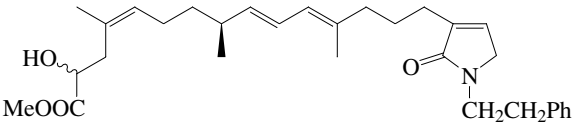
10β-Alcohol, 11-aldehyde, 10-Ac: ***Sarcotal acetate***
[163658-58-0]
$C_{22}H_{36}O_4$ 364.524
Constit. of a *Sarcophyton* sp. Oil. $[\alpha]_D^{27}$ -44 (c, 0.1 in MeOH). λ_{max} 209 (ϵ 3780) (MeOH) (Berdy).

6β-Hydroxy, 11-Ac: ***6-Hydroxysarcotol acetate***
[185102-35-6]
$C_{22}H_{36}O_5$ 380.523
Constit. of a *Sarcophyton* sp. Oil. $[\alpha]_D^{27}$ -80 (c, 0.06 in MeOH). λ_{max} 206 (ϵ 2740) (MeOH).

Iwagawa, T. *et al., Tetrahedron*, 1995, **51**, 5291-5298 (*isol, pmr, cmr, cryst struct*)
Iwagawa, T. *et al., Bull. Chem. Soc. Jpn.*, 1996, **69**, 3543-3549 (*isol, pmr, cmr, derivs*)

Sarcotragin A S-43

[346583-99-1]

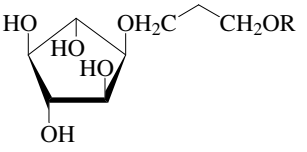


$C_{31}H_{43}NO_4$ 493.685
Alkaloid from the sponge *Sarcotragus* sp. Gum. $[\alpha]_D^{25}$ +16 (c, 0.11 in MeOH). λ_{max} 204 (log ϵ 4.1); 236 (log ϵ 4.07) (MeOH).

N-*De-(2-phenylethyl),* N-*(carboxymethyl):* ***Sarcotragin B***
[346584-00-7]
$C_{25}H_{37}NO_6$ 447.57
Alkaloid from *Sarcotragus* sp. Gum (as Na salt). $[\alpha]_D^{25}$ +17.5 (c, 0.12 in MeOH) (Na salt). λ_{max} 209 (log ϵ 4.12); 232 (log ϵ 4.15) (MeOH) (Na salt).

Shin, J. *et al., Tet. Lett.*, 2001, **42**, 3005-3007 (*isol, pmr, cmr*)

Sarcotride A S-44



R = $-(CH_2)_9CH(CH_3)(CH_2)_5CH_3$

$C_{25}H_{50}O_7$ 462.666
Isol. from a sponges *Petrosia* sp. and *Sarcotragus* sp. Replication inhibitor. Light yellow oil. $[\alpha]_D^{21}$ -6 (c, 0.15 in MeOH).

Kim, D.-K. *et al., J. Nat. Prod.*, 1999, **62**, 773-776 (*isol, pmr, cmr, ms*)
Liu, Y. *et al., Bull. Korean Chem. Soc.*, 2002, **23**, 1467-1469 (*isol, pmr, cmr*)

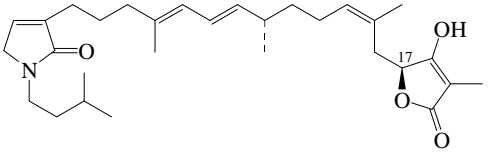
Sarcotride B S-45

As Sarcotride A, S-44 with
R = $-(CH_2)_{10}CH{=}CH(CH_2)_3CH_3$
$C_{24}H_{46}O_7$ 446.623
Isol. from the sponge *Sarcotragus* sp. Light yellow oil. $[\alpha]_D^{21}$ +24 (c, 0.14 in MeOH).

Liu, Y. *et al., Bull. Korean Chem. Soc.*, 2002, **23**, 1467-1469 (*isol, pmr, cmr*)

Sarcotrine A S-46

[472974-46-2]



$C_{30}H_{45}NO_4$ 483.69

Constit. of a *Sarcotragus* sponge. Oil. $[\alpha]_D^{21}$ +36.1 (c, 0.18 in MeOH). λ_{max} 240 (log ϵ 4.81) (MeOH).

N-*Dealkyl,* N-*(2-methylbutyl):* ***Sarcotrine C***
[472974-48-4]
$C_{30}H_{45}NO_4$ 483.69
Constit. of a *Sarcotragus* sponge. Oil. $[\alpha]_D^{21}$ +19.1 (c, 0.18 in MeOH). λ_{max} 245 (log ϵ 4.28) (MeOH).

N-*Dealkyl,* N-*(2-phenylethyl):* ***Sarcotrine B***
[472974-47-3]
$C_{33}H_{43}NO_4$ 517.707
Constit. of a *Sarcotragus* sponge. Oil. $[\alpha]_D^{21}$ +36.9 (c, 0.07 in MeOH).

N-*Dealkyl,* N-*(carboxymethyl):* ***Sarcotrine E***
[627895-36-7]
$C_{27}H_{37}NO_6$ 471.592
Constit. of *Sarcotragus* sp. Oil. $[\alpha]_D^{21}$ +38.8 (c, 0.18 in MeOH).

17-Epimer: ***Episarcotrine A***
[471278-72-5]
$C_{30}H_{45}NO_4$ 483.69
Constit. of a *Sarcotragus* sponge. Oil. $[\alpha]_D^{21}$ +42.8 (c, 0.05 in MeOH). λ_{max} 242 (log ϵ 4.56) (MeOH).

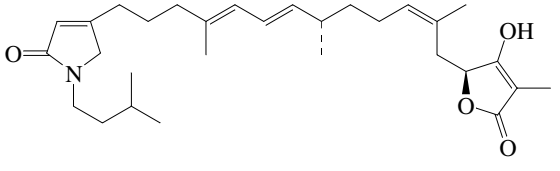
17-Epimer, N-*dealkyl,* N-*(2-methylbutyl):* ***Episarcotrine C***
[472974-54-2]
$C_{30}H_{45}NO_4$ 483.69
Constit. of a *Sarcotragus* sponge. Oil. $[\alpha]_D$ +24 (c, 0.06 in MeOH).

17-Epimer, N-*dealkyl,* N-*(2-phenylethyl):* ***Episarcotrine B***
[471278-73-6]
$C_{33}H_{43}NO_4$ 517.707
Constit. of a *Sarcotragus* sponge. Oil. $[\alpha]_D^{21}$ +42.1 (c, 0.04 in MeOH).

Liu, Y. *et al., J. Nat. Prod.*, 2002, **65**, 1307-1314 (*isol, pmr cmr*)
Liu, Y. *et al., J. Nat. Prod.*, 2003, **66**, 1451-1456 (*Sarcotrine E*)

Sarcotrine D S-47

[472974-56-4]



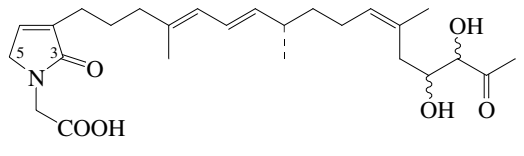
$C_{30}H_{45}NO_4$ 483.69
Constit. of a *Sarcotragus* sponge. Oil. $[\alpha]_D^{21}$ +65.2 (c, 0.01 in MeOH). λ_{max} 239 (log ϵ 4.34) (MeOH).

N-*Dealkyl,* N-*(carboxymethyl):* ***Isosarcotrine E***
[627895-37-8]
$C_{27}H_{37}NO_6$ 471.592
Constit. of a *Sarcotragus* sp. Oil. $[\alpha]_D^{21}$ +33.3 (c, 0.09 in MeOH).

Liu, Y. *et al., J. Nat. Prod.*, 2002, **65**, 1307-1314 (*Sarcotrine D*)
Liu, Y. *et al., J. Nat. Prod.*, 2003, **66**, 1451-1456 (*Isosarcotrine E*)

Sarcotrine F S-48

[627895-38-9]



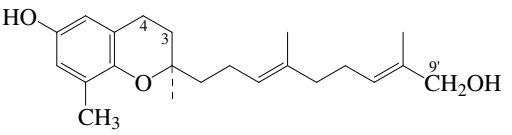
$C_{26}H_{39}NO_6$ 461.597
Constit. of a *Sarcotragus* sp. Oil. Isol. as a mixt. with Isosarcotrine F.

3-Deoxo, 5-oxo: ***Isosarcotrine F***
[627895-39-0]
$C_{26}H_{39}NO_6$ 461.597
Constit. of a *Sarcotragus* sp. Oil. Stereochem. need not necessarily correspond.

Liu, Y. *et al., J. Nat. Prod.*, 2003, **66**, 1451-1456 (*isol, pmr, cmr*)

Sargachromanol B S-49

[856414-51-2]



$C_{22}H_{32}O_3$ 344.493
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ +14.6 (c, 0.1 in MeOH).

9′-Aldehyde: ***Sargachromanol A***
[856414-50-1]
$C_{22}H_{30}O_3$ 342.477
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ +15.8 (c, 0.1 in MeOH). λ_{max} 225 (log ϵ 3.84) (MeOH).

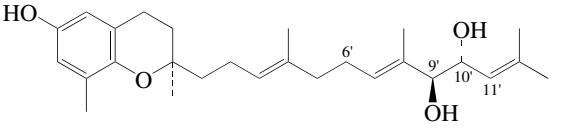
*9′-Deoxy: 2-(4,8-Dimethyl-3,7-nonadienyl)-3,4-dihydro-2,8-dimethyl-2*H*-1-benzopyran-6-ol. 7-Demethylplastochromanol 2.* ***Oligandrol***
[155661-15-7]
$C_{22}H_{32}O_2$ 328.494
Constit. of *Beilschmiedia oligandra* (Lauraceae). Oil. $[\alpha]_D$ -1.04 (c, 0.93 in $CHCl_3$). λ_{max} 298 (ϵ 3360) (no solvent reported).

*9′-Deoxy, 3,4-didehydro: 2-(4,8-Dimethyl-3,7-nonadienyl)-2,8-dimethyl-2*H*-1-benzopyran-6-ol.* ***7-Demethylplastochromenol 2***
[192711-15-2]
$C_{22}H_{30}O_2$ 326.478
Constit. of *Seseli farreynii*. Yellow oil. Racemic.

Banfield, J.E. *et al., Aust. J. Chem.*, 1994, **47**, 587-607 (*Oligandrol*)
Muckensturm, B. *et al., Phytochemistry*, 1997, **45**, 549-550 (*7-Demethylplastochromenol*)
Jang, K.H. *et al., J. Nat. Prod.*, 2005, **68**, 716-723 (*Sargachromanols A,B*)

Sargachromanol D S-50

[856414-53-4]



$C_{27}H_{40}O_4$ 428.611
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ +19.4 (c, 0.16 in MeOH).

9′-Me ether (9′ξ): ***Sargachromanol F***
[856414-55-6]
$C_{28}H_{42}O_4$ 442.637
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ +27 (c, 0.14 in MeOH). 9-Config. not determined.

9′-Ketone: ***Sargachromanol G***
[856414-56-7]
$C_{27}H_{38}O_4$ 426.595
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ -79.2 (c, 0.12 in MeOH). λ_{max} 230 (log ϵ 3.8) (MeOH).

10′-Ketone: ***Sargachromanol K***
[856414-60-3]
$C_{27}H_{38}O_4$ 426.595
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ +175.6 (c, 0.11 in MeOH). λ_{max} 237 (log ϵ 3.77) (MeOH).

7′,8′-Dihydro, 9′-ketone: ***Sargachromanol I***
[856414-58-9]
$C_{27}H_{40}O_4$ 428.611
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ -118.2 (c, 0.11 in MeOH).

7′,8′,11′,12′-Tetrahydro, 9′-ketone: ***Sargachromanol J***
[856414-59-0]
$C_{27}H_{42}O_4$ 430.626
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ +8.2 (c, 0.14 in MeOH).

10′-Deoxy: ***Sargachromanol C***
[856414-52-3]
$C_{27}H_{40}O_3$ 412.611
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ +10.6 (c, 0.09 in MeOH).

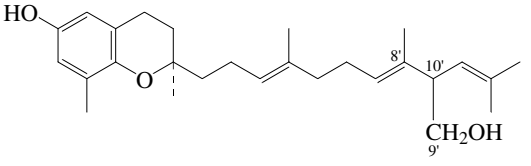
$\Delta^{6'}$-Isomer(Z-), 9′-ketone: ***Sargachromanol H***
[856414-57-8]
$C_{27}H_{38}O_4$ 426.595
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ -143 (c, 0.1 in MeOH).

10′-Epimer: ***Sargachromanol E***
[856414-54-5]
$C_{27}H_{40}O_4$ 428.611
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ +14.4 (c, 0.12 in MeOH).

Jang, K.H. *et al., J. Nat. Prod.*, 2005, **68**, 716-723 (*Sargachromanols C-K*)

Sargachromanol L S-51

[856414-61-4]



$C_{27}H_{40}O_3$ 412.611
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ +17.6 (c, 0.13 in MeOH).

9′-Carboxylic acid: ***Sargachromanol O***
[856414-64-7]
$C_{27}H_{38}O_4$ 426.595
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ +12.9 (c, 0.11 in MeOH).

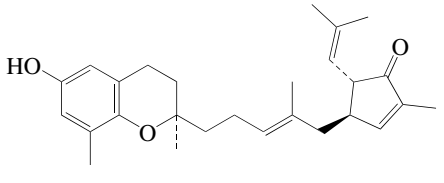
$\Delta^{8'(10')}$-Isomer(E-), 9′-aldehyde: ***Sargachromanol M***
[856414-62-5]
$C_{27}H_{38}O_3$ 410.595
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ +11.8 (c, 0.12 in MeOH). λ_{max} 225 (log ϵ 3.97) (MeOH).

$\Delta^{8'(10')}$-Isomer(Z-), 9′-aldehyde: ***Sargachromanol N***
[856414-63-6]
$C_{27}H_{38}O_3$ 410.595
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ +10 (c, 0.12 in MeOH). λ_{max} 225 (log ϵ 3.95) (MeOH).

Jang, K.H. *et al., J. Nat. Prod.*, 2005, **68**, 716-723 (*Sargachromanols L-O*)

Sargachromanol P S-52

[856414-65-8]

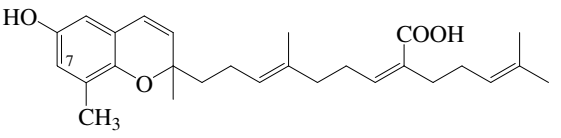


$C_{27}H_{36}O_3$ 408.58
Constit. of *Sargassum siliquastrum*. Gum. $[\alpha]_D^{20}$ +14.7 (c, 0.16 in MeOH). λ_{max} 224 (log ϵ 3.86) (MeOH).

Jang, K.H. *et al., J. Nat. Prod.*, 2005, **68**, 716-723 (*Sargachromanol P*)

Sargachromenol S-53

[70363-89-2]



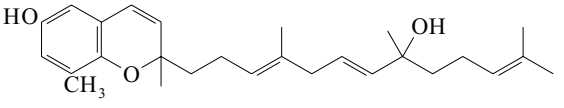
$C_{27}H_{36}O_4$ 424.579
Isol. from *Sargassum serratifolium*. Oil. Artifact. Opt. inactive.

7-Methyl: ***7-Methylsargachromenol***
[351441-18-4]
$C_{28}H_{38}O_4$ 438.606
Constit. of *Iryanthera juruensis* fruits. Brown oil. λ_{max} 326 (ϵ 3800) (MeOH).

Kusumi, T. *et al., Chem. Lett.*, 1979, 277-278 (*isol, pmr*)
Silva, D.H.S. *et al., Phytochemistry*, 2001, **57**, 437-442 (*7-Methylsargachromenol*)

Sargadiol II S-54

[142060-03-5]

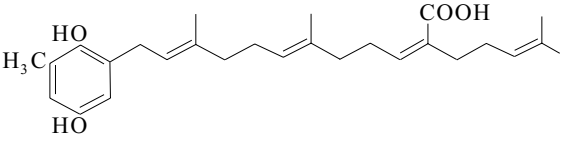


$C_{27}H_{38}O_3$ 410.595
Constit. of *Sargassum tortile*. Pale brown oil. $[\alpha]_D^{23}$ +1.8 (c, 0.98 in $CHCl_3$). λ_{max} 210 (ϵ 21880); 230 (ϵ 21380); 260 (ϵ 6760); 275 (ϵ 6310); 335 (ϵ 3310) (MeOH) (Berdy). λ_{max} 203 (ϵ 2840) (EtOH) (Berdy).

Numata, A. *et al., Phytochemistry*, 1992, **31**, 1209-1213 (*isol, pmr, cmr*)

Sargahydroquinoic acid S-55

[110360-00-4]

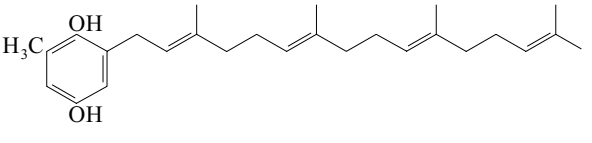


$C_{27}H_{38}O_4$ 426.595
Plastoquinone constit. of brown alga *Sargassum sagamianum* var. *yezoense*. Oil.

Segawa, M. *et al., Chem. Lett.*, 1987, 1365

Sargahydroquinone S-56

2-Methyl-6-(3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)-1,4-benzenediol, 9CI. 2-(Geranylgeranyl)-6-methyl-1,4-benzenediol
[57576-81-5]



$C_{27}H_{40}O_2$ 396.612
Constit. of *Stypopodium zonale*. Oil. λ_{max} 287 (ϵ 2950) (MeOH).

Di-Ac: [75558-34-8]
Cryst. Mp 105-106°.

1,4-Quinone: See Sargaquinone, S-59

Hexahydro: See 2-Methyl-6-phytylhydroquinone, M-455

10′,11′-Dihydro, 10′,11′-dihydroxy: 2-(10,11-Dihydroxygeranylgeranyl)-6-methyl-1,4-benzenediol. 10′,11′-Dihydroxysargaquinol
[82354-25-4]
$C_{27}H_{42}O_4$ 430.626
Constit. of *Cystoseira caespitosa*. Oil. $[\alpha]_D$ +7 (c, 2 in $CHCl_3$). Stereochem. appears to be (*R,S*) but not clear from the lit. Organism previously misidentified as *C. stricta*.

10′,11′-Dihydro, 10′,11′-dihydroxy, 4-Me ether: ***2-(10,11-Dihydroxygeranylgeranyl)-1-hydroxy-4-methoxymethylbenzene***
$C_{28}H_{44}O_4$ 444.653
From *Cystoseira caespitosa*. Oil. $[\alpha]_D^{20}$ -3.3.

*14′,15′-Dihydro, 14′*R*,15′-dihydroxy:* ***14′,15′-Dihydroxysargahydroquinone***
$C_{27}H_{42}O_4$ 430.626
Isol. from *Sargassum micracanthum*. Pale yellow oil. $[\alpha]_D^{25}$ +10.3 (c, 0.53 in $CHCl_3$). λ_{max} 230 (log ϵ 4); 265 (log ϵ 3.6); 334 (log ϵ 3.4) (EtOH).

5′ξ-Hydroxy: ***2-(5-Hydroxy-3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)-6-methyl-1,4-benzenediol***
[115788-01-7]
$C_{27}H_{40}O_3$ 412.611
Constit. of the brown alga *Cystoseira spinosa* var. *squarrosa*. Yellow oil. $[\alpha]_D^{20}$ +1 (c, 2.3 in EtOH).

5′,17′-Dihydroxy: 2-(5,16-Dihydroxy-3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)-6-methyl-1,4-benzenediol
[115788-02-8]
$C_{27}H_{40}O_4$ 428.611
Constit. of *Cystoseira spinosa* var. *squarrosa*.

5′-Oxo: [592533-83-0]
$C_{27}H_{38}O_3$ 410.595
Constit. of *Cystoseira crinita*. Oil. λ_{max} 243 (ϵ 12100); 288 (ϵ 3500) (EtOH).

5′-Oxo, 13′-hydroxy: [592533-81-8]
$C_{27}H_{38}O_4$ 426.595
Constit. of *Cystoseira crinita*. Oil. $[\alpha]_D^{28}$ +4.6 (c, 0.1 in EtOH). λ_{max} 240 (ϵ 11300); 289 (ϵ 2900) (no solvent reported).

5′-Oxo, 17′-hydroxy: [592533-79-4]
$C_{27}H_{38}O_4$ 426.595
Constit. of *Cystoseira crinita*. Oil. λ_{max} 236 (ϵ 12100); 290 (ϵ 3400) (EtOH).

12′-Oxo, 5′-acetoxy: [128718-11-6]
$C_{29}H_{40}O_5$ 468.632
Constit. of *Cystoseira barbatula*. Oil. $[\alpha]_D^{20}$ +14.5 (c, 0.46 in EtOH). λ_{max} 220 (ϵ 19800); 242 (ϵ 10200); 287 (ϵ 5600) (EtOH).

12′-Oxo, 5′-hydroxy, 10′,11′-dihydro: 16-(2,5-Dihydroxy-3-methylphenyl)-12-hydroxy-2,6,10,14-tetramethyl-2,10,14-hexadecatrien-5-one
[128745-98-2]
$C_{27}H_{40}O_4$ 428.611
Constit. of *Cystoseira barbatula*. Oil. λ_{max} 220 (ϵ 10900); 287 (ϵ 4100) (EtOH).

12′-Oxo, 5′-acetoxy, 10′,11′-dihydro: [128718-10-5]
$C_{29}H_{42}O_5$ 470.648
Constit. of *Cystoseira barbatula*. Oil. $[\alpha]_D^{20}$ +5.2 (c, 0.57 in EtOH). λ_{max} 220 (ϵ 12200); 290 (ϵ 4200) (EtOH).

5′,13′-Dioxo: 16-(2,5-Dihydroxy-3-methylphenyl)-2,6,10,14-tetramethyl-2,6,10,14-hexadecatetraene-4,12-dione. 2-(3,7,11,15-Tetramethyl-5,13-dioxo-2,6,10,14-hexadecatetraenyl)-6-methylhydroquinone
[115788-03-9]
$C_{27}H_{36}O_4$ 424.579
Constit. of *Cystoseira spinosa* var. *squarrosa*. Oil.

*6′*Z*-Isomer, 5′-oxo:* [592533-84-1]
$C_{27}H_{38}O_3$ 410.595
Constit. of *Cystoseira crinita*. Oil. λ_{max} 236 (ϵ 18400); 288 (ϵ 5400) (EtOH).

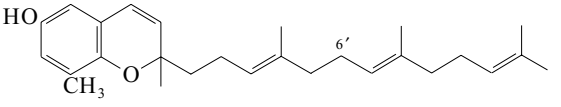
*6′*Z*-Isomer, 5′-oxo, 13′-hydroxy:* [592533-82-9]
$C_{27}H_{38}O_4$ 426.595
Constit. of *Cystoseira crinita*. Oil. $[\alpha]_D^{28}$ -5.4 (c, 0.1 in EtOH). λ_{max} 247 (ϵ 13900); 286 (ϵ 3400) (MeOH).

*6′*Z*-Isomer, 5′-oxo, 17′-hydroxy:* [592533-80-7]
$C_{27}H_{38}O_4$ 426.595
Constit. of *Cystoseira crinita*. Oil. λ_{max} 236 (ϵ 13000); 285 (ϵ 4200) (EtOH).

Ishitsuka, M. *et al., Chem. Lett.*, 1979, 1269-1272 (*Sargassum tortile constits*)
Gerwick, W.H. *et al., J.O.C.*, 1981, **46**, 22-27 (*isol, uv, ir, pmr, ms*)
Amico, V. *et al., J. Chem. Res., Synop.*, 1982, 262 (*Cytoseira caespitosa constits*)
Amico, V. *et al., Phytochemistry*, 1988, **27**, 1327 (*Cytoseira spinosa constits*)
Amico, V. *et al., Gazz. Chim. Ital.*, 1990, **120**, 9 (*Cytoseira barbatula constits*)
Fisch, K.M. *et al., J. Nat. Prod.*, 2003, **66**, 968-975 (*Cytoseira crinata constits*)
Iwashima, M. *et al., Biol. Pharm. Bull.*, 2005, **28**, 374-377 (*14′,15′-Dihydroxysargahydroquinone*)

Sargaol S-57

[142060-00-2]



$C_{27}H_{38}O_2$ 394.596
Constit. of *Sargassum tortile* and *Dimocarpus fumatus*. Pale brown oil. λ_{max} 210 (ϵ 24550); 230 (ϵ 24550); 265 (ϵ 5888); 272 (ϵ 5495); 330 (ϵ 3800) (MeOH). λ_{max} 256 ($CHCl_3$) (Berdy).

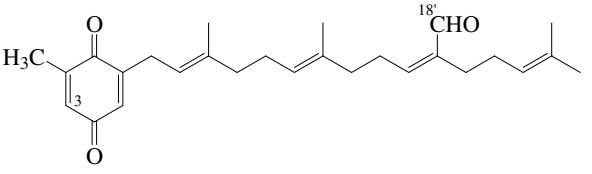
6′-Hydroxy: ***Sargadiol I***
[142060-02-4]
$C_{27}H_{38}O_3$ 410.595
Constit. of *Sargassum tortile* and *Desmarestia menziesii*. Hepatotoxin, anthelmintic agent. Pale brown oil. $[\alpha]_D^{23}$ +1.5 (c, 0.78 in $CHCl_3$). λ_{max} 208 (ϵ 22387); 230 (ϵ 20420); 265 (ϵ 5888); 272 (ϵ 5750); 337 (ϵ 3631) (MeOH) (Berdy).

*11′,12′-Dihydro, 11′*R*,12′-dihydroxy:* ***11′,12′-Dihydro-11′,12′-dihydroxysargaol***
$C_{27}H_{40}O_4$ 428.611
Constit. of *Sargassum micracanthum*. Antiviral agent. $[\alpha]_D^{25}$ +12.5 (c, 0.38 in $CHCl_3$).

Numata, A. *et al., Phytochemistry*, 1992, **31**, 1209-1213 (*isol, pmr, cmr*)
Voutquenne, L. *et al., Phytochemistry*, 1999, **50**, 63-69 (*pmr, cmr*)
Iwashima, M. *et al., Biol. Pharm. Bull.*, 2005, **28**, 374 (*Dihydrodihydroxysargaol*)
Mori, J. *et al., Chem. Pharm. Bull.*, 2006, **54**, 391-396 (*Dihydrodihydroxysargaol, synth, pmr, cmr*)

Sargaquinal S-58

[70363-88-1]



$C_{27}H_{36}O_3$ 408.58
Found in the brown alga *Sargassum serratifolium*. Yellow oil.

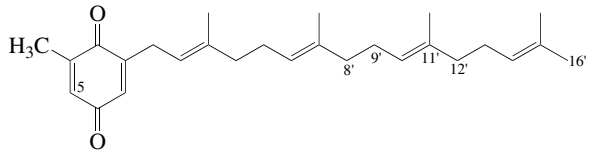
18′-Carboxylic acid: ***Sargaquinoic acid***
[70363-87-0]
$C_{27}H_{36}O_4$ 424.579
From *Sargassum serratifolium*. Yellow oil.

3-Methyl, 18′-carboxylic acid: ***3-Methylsargaquinoic acid***
[351432-35-4]
$C_{28}H_{38}O_4$ 438.606
Constit. of *Iryanthera juruensis* fruits. Brown oil. λ_{max} 257 (ϵ 4400) (MeOH).

Kusumi, T. *et al., Chem. Lett.*, 1979, 277-278 (*isol, pmr*)
Silva, D.H.S. *et al., Phytochemistry*, 2001, **57**, 437-442 (*3-Methylsargaquinoic acid*)

Sargaquinone S-59

6-Methyl-2-(3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)-1,4-benzoquinone. 2-Geranylgeranyl-6-methylbenzoquinone
[57576-82-6]



$C_{27}H_{38}O_2$ 394.596
Constit. of *Sargassum tortile* and *Stypopodium zonale*. Oil. λ_{max} 254 (ϵ 2160) (MeOH).

10′,11′-Dihydro, 10′ξ,11′ξ-dihydroxy: ***10′,11′-Dihydroxysargaquinone***
[82345-59-3]
$C_{27}H_{40}O_4$ 428.611
Isol. from the brown alga *Cystoseira stricta* var. *spicata*. Yellow cryst.
Mp 43-44°. $[\alpha]_D$ +15 (c, 1.38 in $CHCl_3$).

*14′,15′-Dihydro, 14′*R*,15′-dihydroxy:* ***14′,15′-Dihydroxysargaquinone***
$C_{27}H_{40}O_4$ 428.611
Isol. from *Sargassum micracanthum*. Pale yellow oil. $[\alpha]_D^{25}$ +11.3 (c, 0.59 in $CHCl_3$). λ_{max} 234 (log ϵ 3.3); 285 (log ϵ 5.2); 310 (log ϵ 3.9) (EtOH).

9′-Hydroxy: ***9′-Hydroxysargaquinone****. 2-(9-Hydroxygeranylgeranyl)-6-methyl-1,4-benzoquinone*
[130756-37-5]
$C_{27}H_{38}O_3$ 410.595
From *Desmarestia menziesii* and *Sargassum tortile*. Cytotoxic agent. Yellow oil. $[\alpha]_D^{21}$ +2 (c, 1.9 in $CHCl_3$). λ_{max} 212 (ϵ 10715); 253 (ϵ 10965); 295 (ϵ 1023); 325 (ϵ 692) (MeOH) (Berdy).

9′-Methoxy: ***9′-Methoxysargaquinone****. 2-(9-Methoxygeranylgeranyl)-6-methyl-1,4-benzoquinone*
[72239-42-0]
$C_{28}H_{40}O_3$ 424.622
From *Sargassum tortile*. Yellow oil. $[\alpha]_D$ +2.68 ($CHCl_3$). λ_{max} 253 (ϵ 14700) (EtOH).

8′,9′-Dihydroxy: 8′,9′-Dihydroxysargaquinone. 2-(8,9-Dihydroxygeranylgeranyl)-6-methyl-1,4-benzoquinone
[72239-44-2]
$C_{27}H_{38}O_4$ 426.595
From *Sargassum tortile* and *Desmarestia menziesii*. Yellow oil. $[\alpha]_D$ -15 (c, 0.4 in $CHCl_3$). Stereochem. unknown. λ_{max} 253 (ϵ 13100) (EtOH).

8′,9′-Dioxo: ***8′,9′-Dioxosargaquinone***
$C_{27}H_{34}O_4$ 422.563
Isol. from the brown alga *Desmarestia menziesii*.

8′,16′-Dioxo: ***8′,16′-Dioxosargaquinone***
$C_{27}H_{34}O_4$ 422.563
Isol. from the brown alga *Desmarestia menziesii*.

$\Delta^{9'}$-Isomer, 11′-methoxy: ***11′-Methoxysargaquinone****. 2-(11-Methoxygeranylgeranyl)-6-methyl-1,4-benzoquinone*
[72239-43-1]
$C_{28}H_{40}O_3$ 424.622
From *Sargassum tortile*. Yellow oil. $[\alpha]_D$ 0. Postive opt. rotn. at short wavelengths. λ_{max} 253 (ϵ 15800) (EtOH).

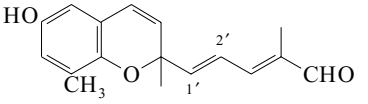
*2′*Z*-Isomer:* ***Z-Sargaquinone***
[868730-07-8]
$C_{27}H_{38}O_2$ 394.596
Constit. of *Taonia atomaria*. Yellow oil. λ_{max} 210 (ϵ 10000); 250 (ϵ 20000) (hexane).

5-Methyl, 8′,9′-dihydroxy: 8′,9′-Dihydroxy-5-methylsargaquinone. 2-(8,9-Dihydroxygeranylgeranyl)-5,6-dimethyl-1,4-benzoquinone
[72239-45-3]
$C_{28}H_{40}O_4$ 440.622
From *Sargassum tortile*. Yellow oil.

Kumarireng, A.S. *et al., Chem. Lett.*, 1973, 1045 (*synth*)
Ishitsuka, M. *et al., Chem. Lett.*, 1979, 1269-1272 (*9′-Methoxysargaquinone, 8′,9′-Dihydroxysargaquinone, 11′-Methoxysargaquinone, 8′,9′-Dihydroxy-5-methylsargaquinone*)
Gerwick, W.H. *et al., J.O.C.*, 1981, **46**, 22 (*isol, uv, ir, pmr, cmr, ms*)
Amico, V. *et al., Phytochemistry*, 1982, **21**, 421 (*10′,11′-Dihydroxysargaquinone*)
Rivera, P. *et al., Can. J. Chem.*, 1990, **68**, 1399 (*9′-Hydroxysargaquinone*)
Numata, A. *et al., Phytochemistry*, 1992, **31**, 1209 (*9′-Hydroxysargaquinone*)
Rivera, L. *et al., Bol. Soc. Chil. Quim.*, 1996, **41**, 103; *CA*, **124**, 283931u (*Dioxosargaquinones*)
Voutquenne, L. *et al., Phytochemistry*, 1999, **50**, 63-69 (*Sargaquinone, pmr, cmr*)
Iwashima, M. *et al., Biol. Pharm. Bull.*, 2005, **28**, 374-377 (*14′,15′-Dihydroxysargaquinone*)
Tziveleka, L.-A. *et al., Chem. Biodiversity*, 2005, **2**, 901-909 (*2′Z-isomer*)

Sargasal II S-60

[142060-01-3]



$C_{17}H_{18}O_3$ 270.327
Constit. of *Sargassum tortile*. Pale brown oil. λ_{max} 215 (ϵ 9332); 228 (ϵ 9330); 275 (ϵ 9330); 322 (ϵ 3550) (MeOH) (Berdy).

1′,2′-Dihydro: ***Sargasal I***
[85872-94-2]
$C_{17}H_{20}O_3$ 272.343
Constit. of *Sargassum tortile*. Pale brown oil. λ_{max} 208 (ϵ 9772); 225 (ϵ 7762); 265 (ϵ 2512); 275 (ϵ 2510); 325 (ϵ 630) (MeOH) (Berdy).

Numata, A. *et al., Phytochemistry*, 1992, **31**, 1209 (*isol, pmr, cmr*)

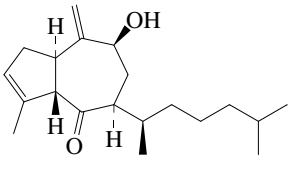
Sargassan, 8CI S-61

[37271-13-9]
Branched sulfated polysaccharide based on a linear glucuronomannan chain. Isol. from the brown alga *Sargassum pallidum*. Anticoagulant. $[\alpha]_D^{20}$ -40 (H_2O).

Ovodov, Y.S. *et al., Khim. Prir. Soedin.*, 1970, **6**, 285; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 285 (*isol*)
Khomenko, V.A. *et al., Khim. Prir. Soedin.*, 1971, **7**, 393; 396; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 375; 378 (*struct*)
Ovodov, Y.S. *et al., Khim. Prir. Soedin.*, 1975, **11**, 300; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 319 (*struct, rev*)
Pavlenko, A.F. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1976, **12**, 515 (*struct*)

Sargassinone S-62

[408306-56-9]

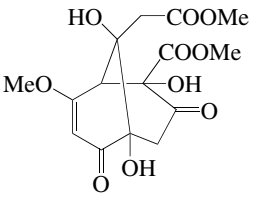


$C_{20}H_{32}O_2$ 304.472
Isol. from the brown alga *Sargassum crispum*. Cytotoxic.

Ayyad, S.E.N. *et al., Boll. Chim. Farm.*, 2001, **140**, 155-159 (*isol*)

Sargassumketone S-63

[163436-59-7]

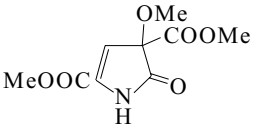


$C_{15}H_{18}O_{10}$ 358.301
Isol. from the brown algae *Sargassum kjellmanianum* and *Sargassum thunbergii*. Cryst.
Mp 189.6-190.4°. Racemic. Biogenesis currently unknown (1995).
λ_{max} 255 (ϵ 7900) (MeOH).

Nozaki, H. *et al., Chem. Lett.*, 1995, 331 (*isol, uv, ir, pmr, cmr, cryst struct*)

Sargassumlactam S-64

[75956-49-9]

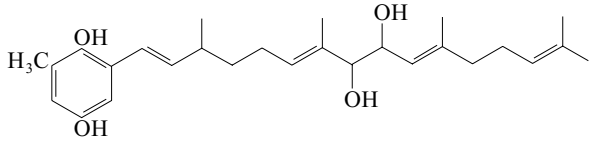


$C_9H_{11}NO_6$ 229.189
Isol. from the marine brown alga *Sargassum kjellmanianum*.
Mp 140-141.5°. $[\alpha]_D$ 0. λ_{max} 208 (ϵ 6100); 293 (ϵ 3400) (EtOH) (Derep).

Nozaki, H. *et al., Chem. Lett.*, 1980, 1453 (*uv, ir, pmr, cmr, cryst struct*)

Sargatetraol S-65

[72239-39-5]

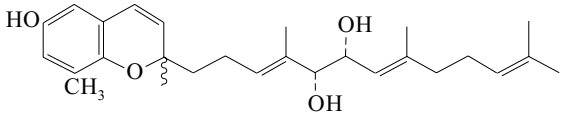


$C_{27}H_{40}O_4$ 428.611
Constit. of *Sargassum tortile*.

Ishitsuka, M. *et al., Chem. Lett.*, 1979, 1269

Sargatriol S-66

[55831-27-1]

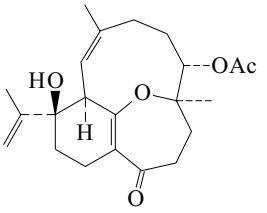


$C_{27}H_{38}O_4$ 426.595
Constit. of *Sargassum tortile*. Pale yellow oil. $[\alpha]_D$ +16 ($CHCl_3$).
λ_{max} 232 (ϵ 24700); 266 (ϵ 5300); 275 (ϵ 4580); 355 (ϵ 2560) (MeOH) (Berdy).

Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1983, **31**, 106
Numata, A. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2129 (*cmr*)

Sarsolenone S-67

[163318-79-4]

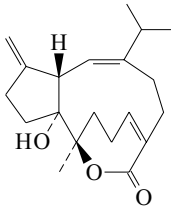


$C_{22}H_{30}O_5$ 374.476
Constit. of *Sarcophyton solidum*. Cryst.
Mp 219.5-221°. $[\alpha]_D^{25}$ +145.8 (c, 0.02 in EtOH).

Zhang, M. *et al., J. Nat. Prod.*, 1995, **58**, 414 (*isol, pmr, cmr*)

Sarsolide A S-68

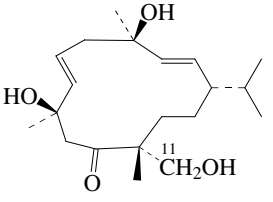
[145757-44-4]



$C_{20}H_{28}O_3$ 316.439
Constit. of *Sarcophyton solidun*. Cryst.
Mp 240.2-242.2°. $[\alpha]_D^{25}$ +142.2 (c, 0.03 in EtOH).

Zhang, M. *et al., J. Nat. Prod.*, 1992, **55**, 1672 (*isol, pmr, cmr, cryst struct*)
Zhang, J. *et al., Tet. Lett.*, 2000, **41**, 941-944 (*synth*)

Sartol B S-69

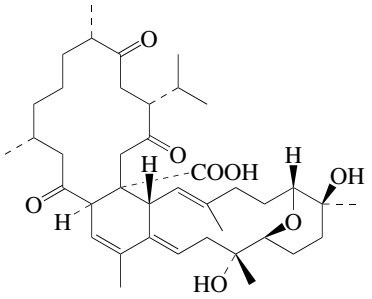


$C_{20}H_{34}O_4$ 338.486
Related to Sarcotol, S-42.

11-Ac: ***Sartol acetate B***
[237755-16-7]
$C_{22}H_{36}O_5$ 380.523
Constit. of a *Sarcophyton* sp. Oil. $[\alpha]_D$ +11.1 (c, 0.19 in MeOH).
λ_{max} 205 (log ϵ 3.4) (MeOH).

Iwagawa, T. *et al., J. Nat. Prod.*, 1999, **62**, 1046-1049 (*isol, pmr, cmr*)

Sartortuic acid S-70



Absolute Configuration

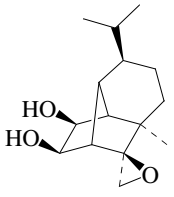
$C_{40}H_{60}O_8$ 668.909
Struct. revised in 1988.

Me ester: ***Methyl sartortuoate***
[102141-25-3]
$C_{41}H_{62}O_8$ 682.936
Constit. of *Sarcophyton tortuosum*. Cryst.
Mp 246-246.5°. $[\alpha]_D^{28}$ +196 (c, 0.05 in EtOH).

Su, J.-Y. *et al., Huaxue Xuebao*, 1985, **43**, 796; *CA*, **104**, 207480t (*isol, pmr, cmr, cryst struct*)
Su, J. *et al., Sci. Sin., Ser. B: (Engl. edn.)*, 1988, **31**, 1172 (*isol, uv, pmr, cmr, cryst struct*)
Lan, W.-J. *et al., Youji Huaxue*, 2005, **25**, 1465-1468 (*Me ester, pmr, cmr, cryst struct*)

Sativene epoxide S-71

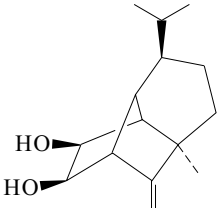
[405157-92-8]



$C_{15}H_{24}O_3$ 252.353
Metab. of *Drechslera dematioidea*. Amorph. powder. $[\alpha]_D^{22}$ -39 (c, 0.1 in EtOH).

Osterhage, C. *et al., J. Nat. Prod.*, 2002, **65**, 306-313 (*isol, pmr, cmr*)

Sativenediol S-72



(±)–*cis–form*

$C_{15}H_{24}O_2$ 236.353

(-)-*cis-form* [55556-01-9]
Metab. of *Cochliobolus setariae*, *Helminthosporium sativum* and *Drechslera dematioidea*. Plant growth promotor.
Oil. $[\alpha]_D^{25}$ -119 (c, 0.94 in $CHCl_3$).

(-)-*trans-form* [55537-09-2]
From *Cochliobolus setariae* and *Helminthosporium sativum*. Plant growth promotor.
Needles.
Mp 176°. $[\alpha]_D^{27}$ -3.4 (c, 1.4 in $CHCl_3$).

(±)-*cis-form* [60426-94-0]
Cryst. (MeCN). Mp 56-57°.

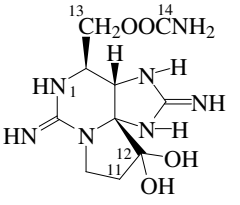
Di-Ac: [72675-81-1]
Mp 87.5-88°.

[59952-94-2, 59952-95-3]

Nukina, H. *et al., J.A.C.S.*, 1975, **97**, 2542 (*isol, struct*)
McMurry, J.E. *et al., J.O.C.*, 1976, **41**, 3953 (*synth, pmr*)
Piers, E. *et al., Can. J. Chem.*, 1977, **55**, 1039 (*synth*)
Yanagiya, M. *et al., Tet. Lett.*, 1979, 1761 (*synth*)
Sigrist, R. *et al., Helv. Chim. Acta*, 1988, **71**, 788 (*synth*)
Wenkert, E. *et al., J.A.C.S.*, 1992, **114**, 644 (*synth*)
Osterhage, C. *et al., J. Nat. Prod.*, 2002, **65**, 306-313 (*isol, pmr, cmr*)

Saxitoxin S-73

STX
[35523-89-8]



$C_{10}H_{17}N_7O_4$ 299.289
Isol. from Alaska butter clams (*Saxidomus giganteus*), toxic mussels (*Mytilus californianus*), the plankton *Gonyaulax catenella*, *Protogonyaulax tamarensis* and other marine organisms. Sodium channel (I, II, III, h1) blocker. Causal agent of paralytic shellfish poisoning. Noncryst. Sol. H_2O, MeOH; fairly sol. EtOH, AcOH; poorly sol. butanol, hexane. $[\alpha]_D$ +130. See also 11-Hydroxysaxitoxin, H-941.

▶ Extremely toxic, among the most toxic substances known. LD_{50} (rat, orl) 0.192 mg/kg. LD_{50} (mus, ipr) 0.005 mg/kg. LD_{50} (mus, ivn) 0.008 mg/kg. UY8708500

N^{14}-*Sulfonic acid:* ***Gonyautoxin V. GTX5. Toxin B_1***
[64296-25-9]
$C_{10}H_{17}N_7O_7S$ 379.353
Present in *Gonyaulax* and *Protogonyaulax* spp. and other marine organisms. Neurotoxin.

▶ Toxic.

N^{14}-*Me:* ***N′-Methylsaxitoxin***
[209856-64-4]
$C_{11}H_{19}N_7O_4$ 313.316
Isol. from the freshwater puffer *Tetraodon cutcutia*.

Decarbamoyl: ***Decarbamoylsaxitoxin***
[58911-04-9]
$C_9H_{16}N_6O_3$ 256.264
Isol. from various shellfish.

Decarbamoyl, 13-Ac: LWTX5
[133144-32-8]
$C_{11}H_{18}N_6O_4$ 298.301
Isol. from *Lyngbya wollei*.

*Decarbamoyl, 13-*O*-(4-hydroxybenzoyl):* ***GC 3***
[603125-82-2]
$C_{16}H_{20}N_6O_5$ 376.371
Isol. from *Gymnodinium catenatum*.

De(carbamoyloxy): ***Decarbamoyloxysaxitoxin***
[143084-69-9]
[164905-60-6]
$C_9H_{16}N_6O_2$ 240.264
Isol. from *Gymnodinium catenatum*.

N^1-*Hydroxy:* ***Neosaxitoxin***
[64296-20-4]
$C_{10}H_{17}N_7O_5$ 315.288
Prod. by *Protogonyaulax* and found in shellfish, marine algae and other organisms incl. *Gonyaulax tamarensis* , *Aphanizomenon flos-aquae*, *Saxidomus giganteus* ,*Vibrio* sp., *Pyrodinium* sp. Neurotoxic neuromuscular blocker.

▶ Potent neurotoxin; LD_{50} (mus, ipr) 5 mg/kg.

N^{1}-*Hydroxy,* N^{14}-*sulfonic acid:* ***Gonyautoxin VI***. *GTX6*. *Toxin* B_2
[82810-44-4]
$C_{10}H_{17}N_7O_8S$ 395.352
Prod. by *Gonyaulax* and *Protogonyaulax* spp., isol. from shellfish. Neurotoxin; causal agent of shellfish poisoning.

▶ Toxic.

N^{1}-*Hydroxy, decarbamoyl:* ***Decarbamoylneosaxitoxin***
[68683-58-9]
$C_9H_{16}N_6O_4$ 272.263
Isol. from the crab *Zosimus aeneus*.

N^{14}-*Hydroxy:* ***N′-Hydroxysaxitoxin***
[153856-77-0]
$C_{10}H_{17}N_7O_5$ 315.288
Isol. from the crab *Zosimus aeneus*. Contains an *N*-hydroxycarbamoyl group.

N^{14},*1-Dihydroxy:* ***N′-Hydroxyneosaxitoxin***
[153856-78-1]
$C_{10}H_{17}N_7O_6$ 331.288
Isol. from the crab *Zosimus aeneus*. Toxic paralytic agent.

*12-Deoxy(12*S-*), decarbamoyl:* ***Decarbamoyl-12-deoxysaxitoxin***. *LWTX4*
[75352-31-7]
[80844-68-4]
$C_9H_{16}N_6O_2$ 240.264
Isol. from *Lyngbya wollei*. Neurotoxin.

*12-Deoxy(12*S-*), decarbamoyl, 13-*O-*Ac: LWTX6*
[200816-98-4]
$C_{11}H_{18}N_6O_3$ 282.302
Isol. from *Lyngbya wollei*.

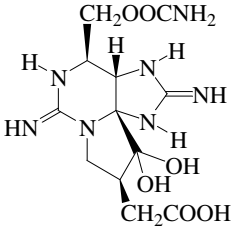
11-Hydroxy: See 11-Hydroxysaxitoxin, H-941

[35554-08-6]

Schantz, E.J. *et al., Biochemistry*, 1966, **5**, 1191-1195 (*isol, bibl*)
Bordner, J. *et al., J.A.C.S.*, 1975, **97**, 6008-6012 (*cryst struct, pmr, cmr*)
Tanino, H. *et al., J.A.C.S.*, 1977, **99**, 2818-2819 (*synth*)
Koehn, F.E. *et al., Bioorg. Chem.*, 1981, **10**, 412-428 (*decarbamoyl, synth*)
Fix Wichman, C. *et al., Tet. Lett.*, 1981, **22**, 1941-1944 (*isol*)
Harada, T. *et al., Agric. Biol. Chem.*, 1982, **46**, 1861-1864 (*Gonyautoxins V,VI*)
Onoue, Y. *et al., J. Agric. Food Chem.*, 1983, **31**, 420-423 (*props*)
Oshima, Y. *et al., Agric. Biol. Chem.*, 1984, **48**, 1707-1711 (*chromatog, struct, bibl*)
Maruyama, J. *et al., Agric. Biol. Chem.*, 1984, **48**, 2783-2788 (*ms*)
Shimizu, Y. *et al., Tetrahedron*, 1984, **40**, 539-544 (*props*)
Kodama, M. *et al., Agric. Biol. Chem.*, 1988, **52**, 1075-1077 (*isol*)
Hall, S. *et al., ACS Symp. Ser.*, 1990, **418**, (*book*)
Arakawa, O. *et al., Toxicon*, 1994, **32**, 175-183 (*Zosimus aeneus constits*)
Onodera, H. *et al., Nat. Toxins*, 1997, **5**, 175-186 (*LWTX toxins*)
Zaman, L. *et al., Toxicon*, 1998, **36**, 627-630 (*N′-Methylsaxitoxin*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 16273
Food Sci. Technol., Seafood and Freshwater Toxins, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*revs*)
Negri, A. *et al., Chem. Res. Toxicol.*, 2003, **16**, 1029-1033 (*GC3*)
Ciminiello, P. *et al., Eur. J. Org. Chem.*, 2004, 2533-2551 (*rev*)
Fleming, J.J. *et al., J.A.C.S.*, 2006, **128**, 3926-3927 (*synth*)
Llewellyn, L.E. *et al., Nat. Prod. Rep.*, 2006, **23**, 200-222 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, SBA500

11-Saxitoxinacetic acid S-74

11-Saxitoxinethanoic acid
[172888-62-9]



Absolute Configuration

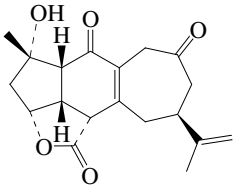
$C_{12}H_{19}N_7O_6$ 357.325

Assumed to exist as a mixt. of 3 tautomers. Isol. from the xanthid crab *Atergatis floridus*.

Arakawa, O. *et al., Toxicon*, 1995, **33**, 1577-1584

Scabrolide A S-75

[479201-56-4]

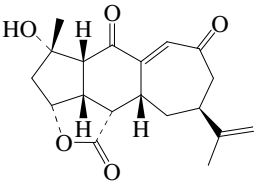


$C_{19}H_{22}O_5$ 330.38
Constit. of *Sinularia scabra*. Cryst.
Mp 92-93°. $[\alpha]_D^{29}$ -104 (c, 0.48 in $CHCl_3$).

Sheu, J.-H. *et al., J. Nat. Prod.*, 2002, **65**, 1904-1908 (*isol, pmr, cmr*)

Scabrolide B S-76

[479201-57-5]

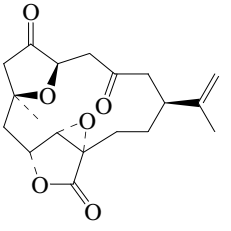


$C_{19}H_{22}O_5$ 330.38
Constit. of *Sinularia scabra*. Cryst.
Mp 110-111°. $[\alpha]_D^{29}$ -80 (c, 0.33 in $CHCl_3$).

Sheu, J.-H. *et al., J. Nat. Prod.*, 2002, **65**, 1904-1908 (*isol, pmr, cmr*)

Scabrolide D S-77

[479201-59-7]

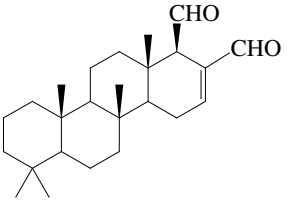


$C_{19}H_{24}O_6$ 348.395
Constit. of *Sinularia scabra*. Cryst.
Mp 83-84°. $[\alpha]_D^{25}$ -58.3 (c, 0.24 in $CHCl_3$).

Sheu, J.-H. *et al., J. Nat. Prod.*, 2002, **65**, 1904-1908 (*isol, pmr, cmr*)

16-Scalarene-24,25-dial S-78

Scalarenedial. *12-Deacetoxyscalaradial*
[154554-90-2]

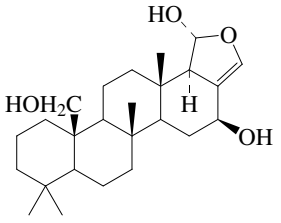


$C_{25}H_{38}O_2$ 370.574

Constit. of *Cacospongia mollior*. Cryst. (EtOH).
Mp 200-203°. $[\alpha]_D^{25}$ -19 (c, 0.7 in $CHCl_3$). λ_{max} 231 (ϵ 14000) (MeOH).

De Rosa, S. *et al., J. Nat. Prod.*, 1994, **57**, 256-262 (*isol, pmr, cmr, cryst struct*)
Soetjipto, H. *et al., Chem. Lett.*, 2000, 1302-1303 (*synth*)

17(24)-Scalarene-16,22,25-triol S-79



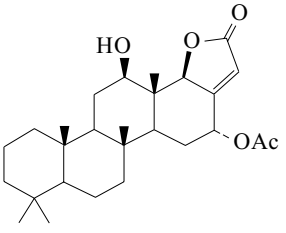
$C_{25}H_{40}O_4$ 404.589

(16β,25α)-*form*

16,25-Di-Ac: [782491-80-9]
$C_{29}H_{44}O_6$ 488.663
Constit. of a *Smenospongia* sp. Amorph. solid. $[\alpha]_D^{25}$ -38.1 (c, 0.25 in MeOH).
Rho, J.-R. *et al., J. Nat. Prod.*, 2004, **67**, 1748-1751 (*isol, pmr, cmr*)

Scalarolbutenolide S-80

[77517-33-0]



$C_{27}H_{40}O_5$ 444.61
Constit. of *Spongia nitens*. Cryst.
Mp 220-222°. $[\alpha]_D$ +1.9 ($CHCl_3$). Derivs. are not named consistently in the lit.

16-Epimer: ***16-Episcalarabutenolide***
[201213-05-0]
$C_{27}H_{40}O_5$ 444.61
Constit. of *Spongia agaricina*. Amorph. powder. $[\alpha]_D^{25}$ -7.3 (c, 0.15 in $CHCl_3$). λ_{max} 206 (ϵ 7510) (MeOH).

16-Epimer, 16-deacetyl:
$C_{25}H_{38}O_4$ 402.573
Constit. of *Hyrtios* cf. *erectus*. Amorph. solid. $[\alpha]_D^{23}$ +19.2 (c, 0.24 in $CHCl_3$). λ_{max} 217 (ϵ 7800) (MeOH) (Berdy).

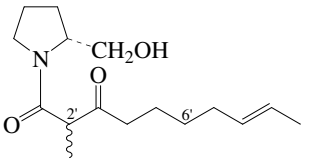
16-Epimer, 16-deacetyl, 12-Ac:
$C_{27}H_{40}O_5$ 444.61
Constit. of *Hyrtios* cf. *erectus*. Amorph. solid. $[\alpha]_D^{23}$ +62 (c, 0.26 in $CHCl_3$). λ_{max} 217 (ϵ 7600) (MeOH) (Berdy).

12,16-Diepimer, 16-deacetyl, 12-Ac: 12α-Acetoxy-16β-hydroxyscalarolbutenolide (incorr.)
$C_{27}H_{40}O_5$ 444.61
Constit. of *Chromodoris inornata* and *Spongia matamata*. Pale yellow needles.
Mp 183-185°. $[\alpha]_D$ +61.4 (c,1 in $CHCl_3$). λ_{max} 229 (ϵ 7800) (CH_2Cl_2).

12,16-Diepimer, 12-Ac: 12α,16β-Diacetoxyscalarolbutenolide (incorr.)
$C_{29}H_{42}O_6$ 486.647
Constit. of *Spongia matamata*. Pale yellow amorph. solid.
Mp 60-62°. $[\alpha]_D$ +51 (c, 0.33 in $CHCl_3$). λ_{max} 229 (ϵ 8400) (CH_2Cl_2).

Cimino, G. *et al., Experientia*, 1981, **37**, 214-216 (*isol*)
Ryu, G. *et al., J. Nat. Prod.*, 1996, **59**, 515 (*isol, pmr, cmr*)
Lu, Q. *et al., J. Nat. Prod.*, 1997, **60**, 195 (*derivs*)
Rueda, A. *et al., J. Nat. Prod.*, 1998, **61**, 258-261 (*16-Episcalarabutenolide*)
Tsuchiya, N. *et al., J. Nat. Prod.*, 1998, **61**, 468-473 (*isol, pmr, cmr*)
Miyamoto, T. *et al., Tetrahedron*, 1999, **55**, 9133-9142 (*Chromodoris inornata constit*)

Scalusamide A S-81



$C_{16}H_{27}NO_3$ 281.394
Prod. by marine-derived *Penicillium citrinum* strain N 055.
Antifungal agent. Amorph. solid. $[\alpha]_D^{22}$ -28 (c, 1 in $CHCl_3$).

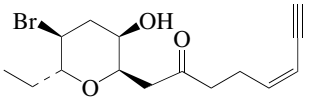
8′,9′-Dihydro: ***Scalusamide C***
$C_{16}H_{29}NO_3$ 283.41
Prod. by *Penicillium citrinum* strain N 055. Amorph. solid.
$[\alpha]_D^{26}$ -13 (c, 0.2 in $CHCl_3$).

*6′,7′-Didehydro(*E-*), 8′,9′-dihydro:* ***Scalusamide B***
$C_{16}H_{27}NO_3$ 281.394
Prod. by *Penicillium citrinum* strain N 055. Amorph. solid.
$[\alpha]_D^{26}$ -13 (c, 0.2 in $CHCl_3$).

Tsuda, M. *et al., J. Nat. Prod.*, 2005, **68**, 273-276 (*isol, pmr, cmr*)

Scanlonenyne S-82

*1-(5-Bromo-6-ethyltetrahydro-3-hydroxy-2*H*-pyran-2-yl)-5-octen-7-yn-2-one, 9CI. 12-Bromo-9,13-epoxy-10-hydroxy-3-pentadecen-1-yn-7-one*
[189308-07-4]

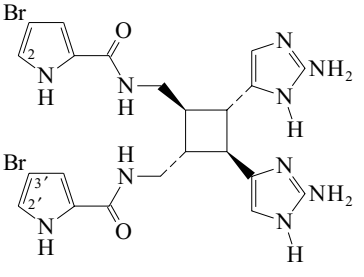


$C_{15}H_{21}BrO_3$ 329.233
Isol. from the red alga *Laurencia obtusa*. Cryst. (pentane).
Mp 80-81°. $[\alpha]_D^{20}$ +40.8 (c, 0.4 in $CHCl_3$).

Suzuki, M. *et al., Tetrahedron*, 1997, **53**, 4271 (*isol, ur, pmr, cmr, ms*)

Sceptrine S-83

[79703-25-6]



$C_{22}H_{24}Br_2N_{10}O_2$ 620.305
Conts. 2 tautomeric aminoimidazole fragments. Isol. from the sponge *Agelas sceptrum, Agelas conifera, Agelas schmidtii, Agelas dispar, Agelas nakamurai, Agelas novaecalendoniae, Agelas longissima, Agelas clathrodes, Axinella* sp., *Hymeniacidon* sp. and from an unidentified Micronesian sponge. Exhibits antimicrobial activity. antiserotonergic, prophage inductio, ichthyotoxic, adrenergic antagonist , serotonin antagonist, antimuscarinic, somatostatin inhibitor, vasoactive intestinal peptide inhibitor, antihistamine. Cryst. + H_2O (H_2O) (as hydrochloride).

Sol. MeOH; poorly sol. Me_2CO, hexane, H_2O, EtOAc. Mp 215-225° dec. (hydrochloride). $[\alpha]_D$ -7.4 (c, 1.2 in MeOH). The elemental anal. of a dried sample of the hydrochloride required $1H_2O$ but the X-ray study indicated $3H_2O$. λ_{max} 265 (ϵ 20900) (MeOH) (Derep). λ_{max} 203 (ϵ 27300); 214 (ϵ 28300); 267 (ϵ 25200) (MeOH) (Berdy).

2-Bromo: ***Bromosceptrine***
$C_{22}H_{23}Br_3N_{10}O_2$ 699.202
Isol. from *Agelas conifera*.

2,2′-Dibromo: ***Dibromosceptrine***
[117417-71-7]
$C_{22}H_{22}Br_4N_{10}O_2$ 778.098
Isol. from *Agelas conifera* and *Agelas clathrodes*. Antifouling agent, neutrotoxin. Sol. MeOH, $CHCl_3$, EtOAc; poorly sol. H_2O. $[\alpha]_D^{25}$ -44 (c, 0.108 in MeOH) (as di-Ac). λ_{max} 202 (ϵ 27300); 215 (ϵ 24800); 273 (ϵ 26300) (MeOH) (Derep).

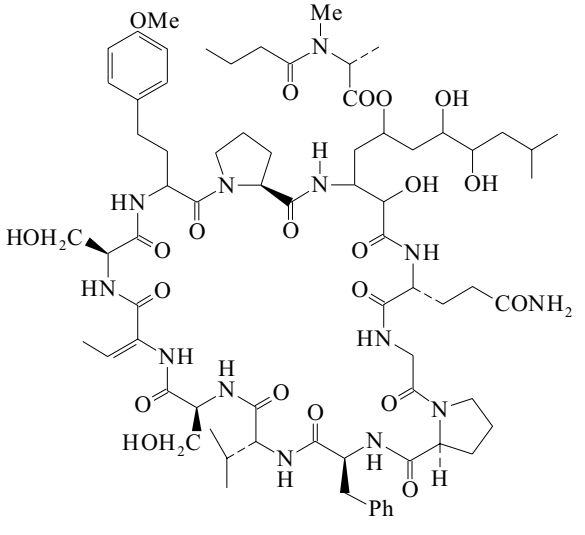
3′-Debromo: ***Debromosceptrine***
[117442-38-3]
$C_{22}H_{25}BrN_{10}O_2$ 541.409
Isol. from *Agelas conifera*.
$[\alpha]_D^{25}$ -30 (c, 1.03 in MeOH) (as di-Ac). λ_{max} 203 (ϵ 25700); 212 (ϵ 26700); 265 (ϵ 25600) (MeOH) (Derep).

Bis(debromo): ***Didebromosceptrine***
$C_{22}H_{26}N_{10}O_2$ 462.513
Isol. from *Agelas conifera*. Amorph. pale yellow powder (as dihydrochloride). $[\alpha]_D$ +53.8 (c, 0.36 in EtOH) (dihydrochloride). λ_{max} 267 (log ϵ 3.5) (EtOH) (dihydrochloride).

Walker, R.P. *et al., J.A.C.S.*, 1981, **103**, 6772 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Albizati, K.F. *et al., J.O.C.*, 1985, **50**, 4163 (*isol*)
Keifer, P.A. *et al., J.O.C.*, 1991, **56**, 2965; 6728 (*isol, pmr, cmr*)
Shen, X. *et al., J. Nat. Prod.*, 1998, **61**, 1302-1303 (*isol, uv, pmr, cmr*)
Assmann, M. *et al., Z. Naturforsch., C*, 2002, **57**, 157-160 (*Bromosceptrine*)
Birman, V.B. *et al., Org. Lett.*, 2004, **6**, 2369-2371 (*synth*)
Baran, P.S. *et al., Angew. Chem., Int. Ed.*, 2006, **45**, 249-252 (*synth*)

Schizothrin A S-84

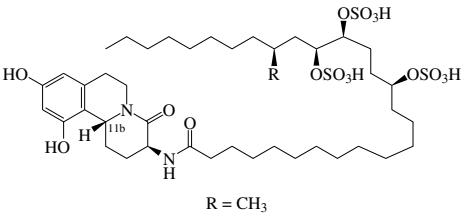
Schizotrin A
[160325-99-5]



$C_{72}H_{107}N_{13}O_{21}$ 1490.712
Cyclic peptide antibiotic. Prod. by *Schizothrix* sp. Antibacterial and antifungal agent. Amorph. powder. $[\alpha]_D^{20}$ -64.7 (c, 0.03 in MeOH). Name misspelt in ref. λ_{max} 224 (ϵ 19800) (MeOH) (Derep).

Pergament, I. *et al., Tet. Lett.*, 1994, **35**, 8473-8476 (*isol, pmr, cmr*)

Schulzeine A S-85



Absolute Configuration

R = CH_3

$C_{42}H_{72}N_2O_{16}S_3$ 957.233
Alkaloid from the marine sponge *Penares schulzei*. α-Glucosidase inhibitor. Powder (as tri-Na salt). $[\alpha]_D^{22}$ +40 (c, 0.1 in MeOH) (tri-Na salt). λ_{max} 209 (ϵ 27500); 284 (ϵ 1390) (MeOH) (tri-Na salt).

Takada, K. *et al., J.A.C.S.*, 2004, **126**, 187-193 (*isol, cd, pmr, cmr, ms*)

Schulzeine C S-86

As Schulzeine A, S-85 with
R = H

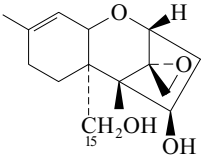
$C_{41}H_{70}N_2O_{16}S_3$ 943.206
Alkaloid from the marine sponge *Penares schulzei*. α-Glucosidase inhibitor. Powder (as tri-Na salt). $[\alpha]_D^{22}$ +33 (c, 0.1 in MeOH) (tri-Na salt). λ_{max} 209 (ϵ 27800); 284 (ϵ 1500) (MeOH) (tri-Na salt).

*11*b*-Epimer:* ***Schulzeine B***
$C_{41}H_{70}N_2O_{16}S_3$ 943.206
Alkaloid from *Penares schulzei*. α-Glucosidase inhibitor. Powder (as tri-Na salt). $[\alpha]_D^{22}$ -23 (c, 0.1 in MeOH) (tri-Na salt). λ_{max} 209 (ϵ 20800); 281 (ϵ 1500) (MeOH) (tri-Na salt).

Takada, K. *et al., J.A.C.S.*, 2004, **126**, 187-193 (*isol, pmr, cmr, ms*)

4,15-Scirpenediol S-87

12,13-Epoxy-9-trichothecene-4,15-diol, 9CI



$C_{15}H_{22}O_4$ 266.336

4β-*form*
Verrucarol
[2198-92-7]
Prod. by *Myrothecium verrucaria*. Shows antifungal activity. Needles (Me_2CO/Et_2O).
Mp 155-158°. $[\alpha]_D^{22}$ -39 (c, 1.069 in $CHCl_3$). λ_{max} 195 (ϵ 7900) (MeOH) (Berdy).

Di-Ac: ***Diacetylverrucarol***. *Antibiotic A2*
[2198-94-9]
$C_{19}H_{26}O_6$ 350.411
From *Myrothecium verrucaria*. Antifungal mycotoxin. Needles (Me_2CO/Et_2O/petrol). Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O.
Mp 148-150°. $[\alpha]_D^{25}$ -17 (c, 1.22 in $CHCl_3$).

Dibenzoyl:
Cryst. (Et_2O/petrol). Mp 151-152°. $[\alpha]_D^{24}$ -64 (c, 1.13 in Me_2CO).

*15-(5-Hydroxy-3-methyl-2*E*-pentenoyl):* ***Verrol***
[84412-91-9]
$C_{21}H_{30}O_6$ 378.464
Prod. by *Myrothecium verrucaria* ATCC 24571. Shows antimicrobial, cytotoxic and mycotoxic props. Oil. $[\alpha]_D^{24}$ -41 (c, 0.572 in $CHCl_3$). λ_{max} 220 (EtOH) (Berdy).

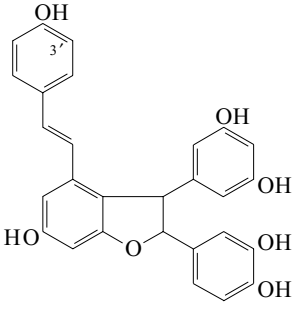
*15-(5-Hydroxy-3-methyl-2*E*-pentenoyl), 4-Ac:* ***4-O-Acetylverrol***. *Verrol 4-acetate*
[263244-91-3]
$C_{23}H_{32}O_7$ 420.502

Prod. by the marine-derived *Acremonium neo-caledoniae*. $[\alpha]_D^{20}$ -30 (c, 0.1 in MeOH). λ_{max} 220 (ϵ 10800) (EtOH).

Härri, E. *et al., Helv. Chim. Acta*, 1962, **45**, 839
Gutzwiller, T. *et al., Helv. Chim. Acta*, 1962, **45**, 1726; 1963, **46**, 1786
McPhail, A.T. *et al., Chem. Comm.*, 1965, 350 (*struct, abs config*)
Fetz, E. *et al., Helv. Chim. Acta*, 1965, **48**, 1669 (*synth, Verrol*)
Achini, R. *et al., Chem. Comm.*, 1971, 404 (*biosynth*)
Breitenstein, W. *et al., Helv. Chim. Acta*, 1975, **58**, 1172 (*nmr*)
White, J.D. *et al., J.O.C.*, 1981, **46**, 3376 (*synth*)
Ong, C.W. *et al., Heterocycles*, 1982, **19**, 1685 (*rev*)
Schlessinger, R.H. *et al., J.A.C.S.*, 1982, **104**, 1116 (*synth*)
Trost, B.M. *et al., J.A.C.S.*, 1982, **104**, 6110; 1984, **106**, 383 (*synth*)
McDougal, P.G. *et al., Diss. Abstr. Int., B*, 1983, **43**, 3245 (*synth, rev*)
Nugent, R.A. *et al., Diss. Abstr. Int., B*, 1983, **44**, 1831 (*synth, rev*)
Roush, W.R. *et al., J.A.C.S.*, 1983, **105**, 1058 (*synth*)
Jarvis, B.B. *et al., J.O.C.*, 1983, **48**, 2576 (*isol, Verrol*)
Trichothecenes - Chemical, Biological and Toxicological Aspects, (ed., Ueno, Y.), Elsevier, 1983, (*tox, rev*)
Koreeda, M. *et al., J.O.C.*, 1988, **53**, 5586 (*synth*)
Ishihara, J. *et al., J.O.C.*, 1998, **63**, 2679-2688 (*synth*)
White, J.D. *et al., Synthesis*, 1998, 619-626 (*Verrucarol, synth*)
Laurent, D. *et al., Planta Med.*, 2000, **66**, 63-66 (*4-Acetylverrol*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 157; 189

Scirpusin A S-88

[69297-51-4]



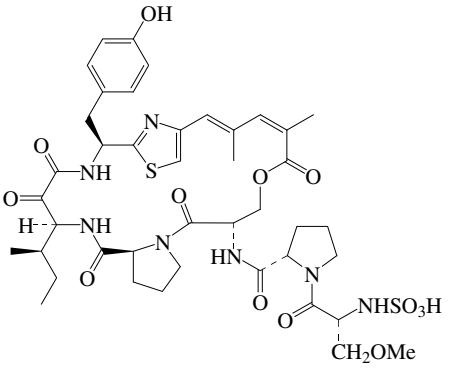
$C_{28}H_{22}O_7$ 470.478
Constit. of *Scirpus fluviatilis*, *Scirpus maritimus* and *Maackia amurensis*. Phytotoxin. Antifeedant. Toxic to brine shrimp. Xanthine oxidase inhibitor. Pale brown amorph. powder. $[\alpha]_D^{23}$ +12.8 (c, 0.25 in MeOH). λ_{max} 224 (ϵ 54200); 286 (sh) (ϵ 15100); 310 (ϵ 22800); 324 (ϵ 24300); 345 (sh) (ϵ 13000) (EtOH) (Derep).

3′-Hydroxy: ***Scirpusin B***
[69297-49-0]
$C_{28}H_{22}O_8$ 486.477
Constit. of *Scirpus fluviatilis*, *Scirpus maritimus* and *Maackia amurensis*. Pale brown amorph. powder. $[\alpha]_D^{23}$ +3.2 (c, 0.63 in Me_2CO). λ_{max} 225 (sh) (ϵ 35500); 290 (ϵ 14800); 308 (sh) (ϵ 16200); 331 (ϵ 20900) (EtOH) (Derep). λ_{max} 331 (ϵ 20900) (MeOH) (Berdy).

Nakajima, K. *et al., Chem. Pharm. Bull.*, 1978, **26**, 3050 (*isol*)
Powell, R.G. *et al., J. Nat. Prod.*, 1987, **50**, 293 (*isol*)

Scleritodermin A S-89

[663597-92-0]



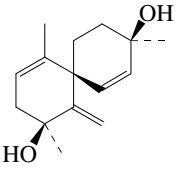
Absolute Configuration

$C_{42}H_{55}N_7O_{13}S_2$ 930.068
Isol. from the sponge *Scleritoderma nodosum*. Cytotoxic. Off-yellow powder (as Na salt). $[\alpha]_D$ -41 (c, 0.1 in MeOH) (Na salt). λ_{max} 200 (ϵ 26500); 305 (ϵ 11300) (MeOH) (Na salt).

Schmidt, E.W. *et al., J. Nat. Prod.*, 2004, **67**, 475-478 (*isol, pmr, cmr*)

Scopariol S-90

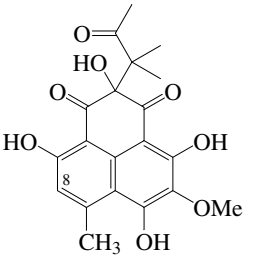
[389064-48-6]



$C_{15}H_{22}O_2$ 234.338
Constit. of *Laurencia scoparia*. Amorph. solid. Mp 188-190°. $[\alpha]_D^{25}$ -8.8 (c, 0.16 in $CHCl_3$).

Davyt, D. *et al., J. Nat. Prod.*, 2001, **64**, 1552-1555 (*isol, pmr, cmr*)

Sculezonone A S-91



$C_{20}H_{20}O_8$ 388.373
Prod. by a marine-derived *Penicillium* sp. Inhibitor of DNA polymerases. Amorph. yellow solid. $[\alpha]_D^{23}$ +45 (c, 0.2 in MeOH). λ_{max} 217 (ϵ 24200); 274 (ϵ 34700); 393 (ϵ 15100) (EtOH).

8-Hydroxy: ***Sculezonone B***
$C_{20}H_{20}O_9$ 404.373
Prod. by a marine-derived *Penicillium* sp. Amorph. yellow solid. $[\alpha]_D^{23}$ +130 (c, 0.2 in MeOH). λ_{max} 214 (ϵ 39300); 276 (ϵ 57800); 412 (ϵ 25500) (EtOH).

Komatsu, K. *et al., J. Nat. Prod.*, 2000, **63**, 408-409 (*isol, pmr, cmr*)
Perpelescu, M. *et al., Biochemistry*, 2002, **41**, 7610-7616 (*activity*)

Scyliorhinin† S-92

H-Ala-Arg-Ser-Arg-Ser-Arg-Arg-Ser-Tyr(SO_3H)-Gly-Arg-Gly-Arg-Arg-Arg-Gly-Gly-Arg-Arg-Arg-Arg-Arg-Arg-Arg-Arg-Arg-Arg-Arg-Gly-Gly-Arg-OH

Struct. of Scyliorhinin Z3 shown. Three other protamines, Z1, Z2 and S4 were also isol. Protamines isol. from mature sperm nuclei of the dogfish *Scyliorhinus caniculus*.

[79215-60-4, 88386-27-0, 88386-28-1, 88386-29-2]

Santiere, P. *et al., Eur. J. Biochem.*, 1981, **119**, 251 (*isol, Z3*)
Gusse, M. *et al., Biochim. Biophys. Acta*, 1983, **748**, 93 (*isol*)
Santiere, P. *et al., Biochim. Biophys. Acta*, 1984, **791**, 82 (*struct, S4*)
Martinage, A. *et al., Biochim. Biophys. Acta*, 1985, **831**, 172 (*struct, Z2*)

Scyliorhinin I S-93

[103425-21-4]

H-Ala-Lys-Phe-Asp-Lys-Phe-Tyr-Gly-Leu-Met-NH_2

$C_{59}H_{87}N_{13}O_{13}S$ 1218.482

Isol. from intestine of the dogfish *Scyliorhinus caniculus*. Has tachykinin-like ability to induce smooth muscle contraction.

Conlan, J.M. *et al., FEBS Lett.*, 1986, **200**, 111-116 (*isol*)
Kiso, Y. *et al., Pept. Chem.*, 1986, 211; 1987, 347 (*synth*)
Qi, X.F. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1997, **71**, 1082-1092 (*pmr, conformn*)

Scyliorhinin II S-94

[103170-36-1]

H-Ser-Pro-Ser-Asn-Ser-Lys-Cys-Pro-Asp-Gly-Pro-Asp-Cys-Phe-Val-Gly-Leu-Met-NH_2

$C_{77}H_{119}N_{21}O_{26}S_3$ 1851.11

Reduced form shown. Isol. from intestine of the dogfish *Scyliorhinus caniculus*. Has tachykinin-like activity to induce smooth muscle contraction.

1-Deseryl-2-deprolyl: [117354-73-1]
$C_{69}H_{107}N_{19}O_{23}S_3$ 1666.916

Isol. from intestine of the ray *Torpedo marmorata*.

Conlan, J.M. *et al., FEBS Lett.*, 1986, **200**, 111-116 (*isol*)
Kiso, Y. *et al., Pept. Chem.*, 1986, 211; 1987, 347 (*synth*)
Conlon, J.M. *et al., Gen. Comp. Endocrinol.*, 1988, **71**, 383-388 (*deriv*)

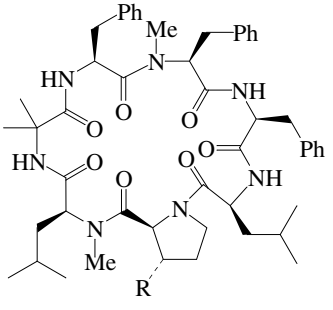
Scyllin S-95

[184378-81-2]

Glycoprotein rich in acidic and neutral amino acids and containing a large amount of mannose; MW 4.8-5 kDa. Isol. from the haemolymph of the crab *Scylla serrata* (Mud crab). Lectin.

Chattopadhyay, T. *et al., Biochem. Mol. Biol. Int.*, 1997, **42**, 183-191 (*isol*)

Scytalidamide A S-96



R = H

$C_{50}H_{67}N_7O_7$ 878.122

Prod. by the marine fungus *Scytalidium* sp. Cytotoxic. Fine cryst. Mp 147-150°. $[\alpha]_D^{25}$ -151.2 (c, 0.6 in MeOH). λ_{max} 202 (log ϵ 0.82) (MeOH).

Tan, L.T. *et al., J.O.C.*, 2003, **68**, 8767-8773 (*isol, pmr, cmr*)
Gu, W. *et al., J.O.C.*, 2003, **68**, 8774-8779 (*synth*)

Scytalidamide B S-97

As Scytalidamide A, S-96 with
R = CH_3

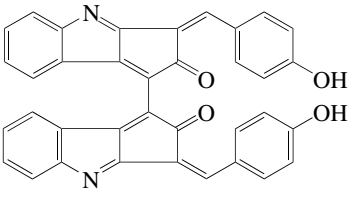
$C_{51}H_{69}N_7O_7$ 892.149

Prod. by the marine fungus *Scytalidium* sp. Cytotoxic. Fine cryst. Mp 141-143°. $[\alpha]_D^{25}$ -156.9 (c, 0.6 in MeOH). λ_{max} 202 (log ϵ 0.63) (MeOH).

Tan, L.T. *et al., J.O.C.*, 2003, **68**, 8767-8773 (*isol, pmr, cmr*)

Scytonemin† S-98

3,3′-Bis[(4-hydroxyphenyl)methylene]-[1,1′-bicyclopent[b]indole]-2,2′(3H,3′H)-dione, 9CI
[152075-98-4]



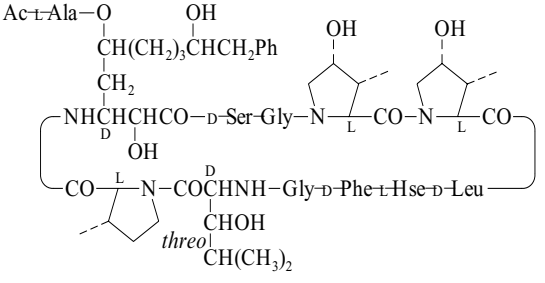
$C_{36}H_{20}N_2O_4$ 544.565

Pigment from the sheaths of cyanobacteria *Calothrix* spp. and *Stigonema* sp. UV sunscreen. Antiproliferative agent. Yellow-green cryst.
Mp >325°.

Proteau, P.J. *et al., Experientia*, 1993, **49**, 825-829 (*isol, pmr, cmr*)
Edwards, H.G. *et al., Spectrochim. Acta A*, 2000, **56**, 193-200 (*Raman*)
Stevenson, C.S. *et al., J. Pharmacol. Exp. Ther.*, 2002, **303**, 858-866 (*activity*)

Scytonemin A† S-99

[112793-66-5]



$C_{71}H_{107}N_{12}O_{21}$ 1464.694

Cyclic peptide antibiotic. Isol. from the cyanobacteria *Scytonema* sp., *Plectonema* sp. and *Oscillatoria agardhii*. Calcium antagonist. Powder. Sol. MeOH. $[\alpha]_D$ +38.8 (c, 0.04 in MeOH). λ_{max} 210 (ϵ 52700); 253; 259 (ϵ 1000); 263 (MeOH) (Derep). λ_{max} 384 (Me_2CO) (Berdy).

Helms, G.L. *et al., J.O.C.*, 1988, **53**, 1298 (*isol, pmr, cmr, struct*)

SDRNFLRF amide S-100

[113611-67-9]

Ser-Asp-Arg-Asn-Phe-Leu-Arg-Phe-NH_2

$C_{42}H_{72}N_{16}O_{12}$ 993.131

FMRF amide-related peptide. Isol. from the nervous system of the crab *Cancer borealis* and the lobster *Homarus americanus*. Neuropeptide.

Trimmer, B.A. *et al., J. Comp. Neurol.*, 1987, **266**, 16-26 (*isol, Homarus*)
Weimann, J.M. *et al., J. Exp. Biol.*, 1993, **181**, 1 (*isol, Cancer*)

Sea bream gonadotrophin-releasing hormone **S-101**

Sea bream GnRH. Gilt head sea bream GnRH. SbGnRH. Sparus aurata *Gonadotrophin-releasing hormone*

[107569-48-2]

5-OxoPro-His-Trp-Ser-Tyr-Gly-Leu-Ser-Pro-Gly-NH_2

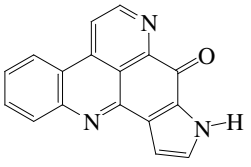
$C_{52}H_{68}N_{14}O_{14}$ 1113.195

Isol. from brain of the sea bream *Sparus aurata*. Sea bream GnRH-II identical to chicken GnRH-II also isol.

Powell, J.F. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1994, **91**, 12081-12085 (*isol*)
Zohar, Y. *et al., Gen. Comp. Endocrinol.*, 1995, **97**, 289-299 (*isol*)

Sebastianine A **S-102**

[448264-64-0]



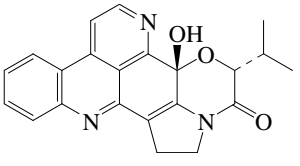
$C_{17}H_9N_3O$ 271.278

Isol. from the Brazilian ascidian *Cystodytes dellechiajei*. Cytotoxic. Amorph. yellow solid. λ_{max} 223 (log ϵ 4.56); 238 (log ϵ 4.49); 265 (log ϵ 4.36); 301 (log ϵ 4.11); 390 (log ϵ 3.85) (MeOH).

Torres, Y.R. *et al., J.O.C.*, 2002, **67**, 5429-5432 (*isol, pmr, cmr*)
Legentil, L. *et al., Tet. Lett.*, 2003, **44**, 2473-2475 (*synth*)

Sebastianine B **S-103**

[448264-65-1]



Relative Configuration

$C_{22}H_{19}N_3O_3$ 373.41

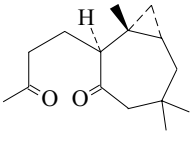
Isol. from the Brazilian ascidian *Cystodytes dellechiajei*. Cytotoxic. Pale yellow solid. λ_{max} 206 (log ϵ 4.57); 252 (log ϵ 4.58); 292 (log ϵ 4.23); 366 (log ϵ 4.19) (MeOH).

Torres, Y.R. *et al., J.O.C.*, 2002, **67**, 5429-5432 (*isol, cd, pmr, cmr*)

2,3-Seco-2,3-africananedione **S-104**

4,5-Seco-4,5-africananedione

[146028-69-5]



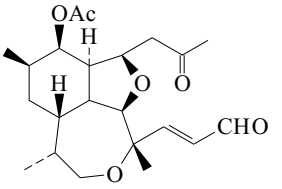
$C_{15}H_{24}O_2$ 236.353

Constit. of *Lippia integrifolia*. Also isol. from the soft coral *Sinularia intacta*. Oil. $[\alpha]_D^{25}$ +120 (c 2 in $CHCl_3$).

Catalan, C.A.N. *et al., Phytochemistry*, 1992, **31**, 4025-4026 (*isol, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 4-7

Secoasbestinin **S-105**

[157469-39-1]



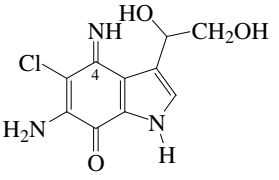
$C_{22}H_{32}O_6$ 392.491

Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{25}$ +21.14 (c, 3.5 in $CHCl_3$). λ_{max} 214 (ϵ 5780) (MeOH) (Derep).

Rodríguez, A.D. *et al., Tet. Lett.*, 1994, **35**, 5793 (*isol, pmr, cmr*)

Secobatzelline A **S-106**

[247590-59-6]



$C_{10}H_{10}ClN_3O_3$ 255.66

Alkaloid from the sponge *Batzella* sp.

Mp 169-170° (as di-Ac) Mp > 300° (blackens at 165-170°). $[\alpha]_D^{24}$ -135 (c, 0.01 in MeOH). λ_{max} 203 (log ϵ 4.19); 233 (log ϵ 4.13); 322 (log ϵ 4) (MeOH).

4-Deimino, 4-oxo: ***Secobatzelline B***

[247590-60-9]

$C_{10}H_9ClN_2O_4$ 256.645

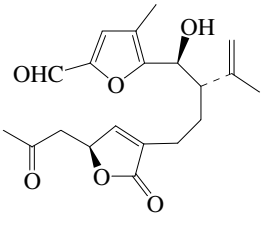
Alkaloid from *Batzella* sp.

Mp 170-171° (as di-Ac) Mp > 300° (blackens at 180-182°). $[\alpha]_D^{24}$ -18 (c, 0.01 in MeOH). Prob. artifact. λ_{max} 203 (log ϵ 4.32); 245 (log ϵ 4); 335 (log ϵ 4.32) (MeOH).

Gunasekera, S.P. *et al., J. Nat. Prod.*, 1999, **62**, 1208-1211 (*Secobatzellines A,B*)

Secobipinnatin J **S-107**

[302924-16-9]



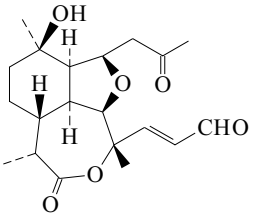
$C_{20}H_{24}O_6$ 360.406

Constit. of *Pseudopterogorgia bipinnata*. Gum. $[\alpha]_D^{24}$ +16.3 (c, 0.86 in $CHCl_3$). λ_{max} 206 (ϵ 14700); 292 (ϵ 10000) (MeOH).

Rodríguez, A.D. *et al., J. Nat. Prod.*, 2000, **63**, 1548-1550 (*isol, pmr, cmr*)

Secobriarellin S-108

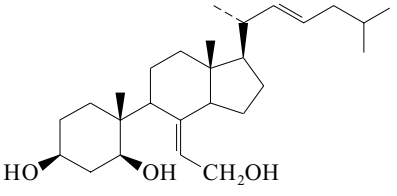
[165127-18-4]



$C_{20}H_{28}O_6$ 364.438
Constit. of *Briareum asbestinum*. Oil. $[\alpha]_D^{26}$ -11.49 (c, 1.56 in $CHCl_3$).

Rodríguez, A.D. *et al., Tetrahedron*, 1995, **51**, 6869 (*isol, pmr, cmr*)

5,6-Secocholesta-7,22-diene-3,5,6-triol S-109

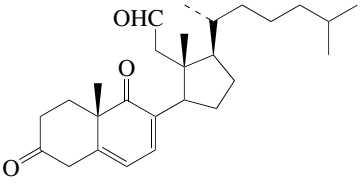


$C_{27}H_{46}O_3$ 418.659

(3β,5β,7*Z*,22*E*)-*form*
Constit. of *Hippospongia communis*.
Madaio, A. *et al., J. Nat. Prod.*, 1990, **53**, 565 (*isol, pmr, ms*)

9,11-Secocholesta-5,7-diene-3,9,11-trione S-110

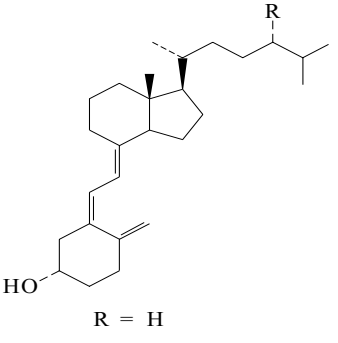
[193266-26-1]



$C_{27}H_{40}O_3$ 412.611
Constit. of *Subergorgia suberosa*. Oil. $[\alpha]_D^{25}$ +15 (c, 0.2 in $CHCl_3$). λ_{max} 303 ($CHCl_3$).

Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 418-423 (*isol, pmr, cmr*)

9,10-Secocholesta-5,7,10(19)-trien-3-ol, 9CI S-111



R = H

$C_{27}H_{44}O$ 384.644

(3*S*,5*Z*,7*E*)-*form*
Vitamin D₃. *Cholecalciferol, BAN. Colecalciferol, INN. Calciol. Delsterol. Provitina. Racumin D. Ricketon. Vigorsan*
[67-97-0]
Produced in humans by the action of sunlight on in the skin. Constit. of fish-liver oil, esp. tuna oil. Antirachitic vitamin with approx. the same potency as vitamin D_2 in humans. Dietary supplement. Rodenticide. Cryst. (Me_2CO).
Mp 87-88°. $[\alpha]_D^{20}$ +84.8 (c, 1.6 in Me_2CO). Log P 9.48 (uncertain value) (calc). A lower-melting form, Mp 63-4° (from MeOH) was also reported.
▶ Excessive intake can cause hypercalcaemia and other effects. LD_{50} (rat, orl) 42 mg/kg. Exp. teratogen. VS2900000

3-O-Sulfate:
$C_{27}H_{44}O_4S$ 464.708
Amorph. solid (as Na salt). Mp 113-120° (Na salt).

Ac: [22350-49-8]
$C_{29}H_{46}O_2$ 426.681
Mp 131-132°. $[\alpha]_D^{18}$ +142 ($CHCl_3$).

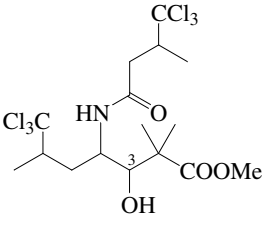
Benzoyl:
$C_{34}H_{48}O_2$ 488.752
Mp 63-64°. $[\alpha]_D$ +39 ($CHCl_3$).

3,5-Dinitrobenzoyl:
Yellow needles. Mp 131°.

[1406-16-2, 2200-64-8, 3844-73-3, 7489-19-2, 10597-47-4, 13083-02-8, 22350-41-0, 57651-82-8, 57651-83-9, 72409-70-2, 72506-00-4, 74512-98-4, 74512-99-5, 77286-64-7, 80666-48-4, 81126-11-6, 81126-44-5, 98744-46-8, 98818-17-8, 118584-54-6, 122958-39-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1049D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 570C (*nmr*)
Inhoffen, M. *et al., Angew. Chem.*, 1960, **72**, 875 (*rev*)
Haussler, M.S. *et al., J. Biol. Chem.*, 1972, **247**, 2328 (*rev*)
Borle, A.B. *et al., Annu. Rev. Physiol.*, 1974, **36**, 361 (*rev, metab*)
Wing, R.M. *et al., J.A.C.S.*, 1975, **97**, 4980 (*pmr, conformn*)
Okamura, W.H. *et al., Tet. Lett.*, 1976, 4807 (*ms*)
Lythgoe, B. *et al., Tet. Lett.*, 1977, 3685 (*synth*)
Fraser, D.R. *et al., Br. Med. Bull.*, 1981, **37**, 37 (*rev, metab*)
Pure Appl. Chem., 1982, **54**, 1511 (*nomencl*)
Koshy, K.T. *et al., Anal. Profiles Drug Subst.*, 1984, **13**, 655 (*rev*)
Wilson, S.R. *et al., Tet. Lett.*, 1984, **25**, 3147 (*synth*)
Nemoto, H. *et al., Heterocycles*, 1985, **23**, 567 (*synth*)
Nemoto, H. *et al., J.O.C.*, 1986, **51**, 5311 (*synth*)
Coldwell, R.D. *et al., Steroids*, 1990, **55**, 418 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1058
Zhu, G.-D. *et al., Chem. Rev.*, 1995, **95**, 1877 (*rev, synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2935-2937 (*props, use*)
Jankowski, P. *et al., Tetrahedron*, 1998, **54**, 12071-12150 (*rev, synth*)
Pesticide Manual, 12th edn., 2000, No. 805
Olsen, R.A. *et al., J.A.C.S.*, 2003, **125**, 11784-11785 (*cmr, conformn*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CMC750; HJV000

1,2-Secodysidamide S-112

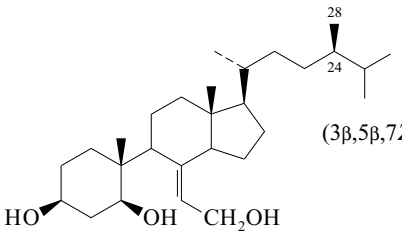


$C_{16}H_{25}Cl_6NO_4$ 508.094
Constit. of the Red Sea sponge *Lamellodysidea herbacea*. Needles. Mp 173-174°. $[\alpha]_D$ -41.8 (c, 1.1 in CH_2Cl_2).

3-Ketone: ***1,2-Secodysidamide H***
$C_{16}H_{23}Cl_6NO_4$ 506.078
Constit. of *Lamellodysidea herbacea*. Needles.
Mp 95-96°. $[\alpha]_D$ -29.6 (c, 0.44 in CH_2Cl_2).
Sauleau, P. *et al., Tetrahedron*, 2005, **61**, 955-963 (*isol, pmr, cmr*)

5,6-Secoergost-7-ene-3,5,6-triol S-113

24-Methyl-5,6-secocholest-7-ene-3,5,6-triol



(3β,5β,7*Z*,24*R*)–*form*

$C_{28}H_{50}O_3$ 434.701

(3β,5β,7*Z*,24*R*)-*form*

5,6-Secocampest-7-ene-3,5,6-triol
Constit. of *Hippospongia communis.*

22,23-Didehydro: 24-Methyl-5,6-secocholesta-7,22-diene-3,5,6-triol
$C_{28}H_{48}O_3$ 432.685
Constit. of *Hippospongia communis.*

(3β,5β,7*Z*,24*S*)-*form*

Constit. of *Hippospongia communis.*

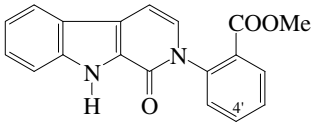
22,23-Didehydro: Constit. of *Hippospongia communis.*

24,28-Didehydro: 24-Methylene-5,6-secocholest-7-ene-3,5,6-triol. 5,6-Secoergosta-7,24(28)-diene-3,5,6-triol
$C_{28}H_{48}O_3$ 432.685
Constit. of *Hippospongia communis.*

Madaio, A. *et al., J. Nat. Prod.*, 1990, **53**, 565 (*isol, synth, pmr, ms*)

Secofascaplysin A S-114

[132911-53-6]



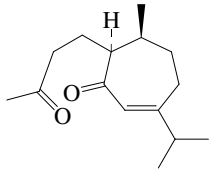
$C_{19}H_{14}N_2O_3$ 318.331
Alkaloid from the sponge *Fascaplysinopsis reticulata*. Pale yellow cryst.; originally isol. as a red oil.
Mp 105-107°. λ_{max} 238 (ϵ 22500); 286 (ϵ); 296 (ϵ 4780); 334 (ϵ 3600); 350 (sh) (ϵ 3000) (MeOH) (Derep).

4′-Bromo: ***3-Bromosecofascaplysin A***
[693790-80-6]
$C_{19}H_{13}BrN_2O_3$ 397.227
Alkaloid from *Fascaplysinopsis reticulata*. Yellow solid.

4′-Bromo, parent acid: ***3-Bromosecofascaplysin B***
[693790-81-7]
$C_{18}H_{11}BrN_2O_3$ 383.201
Alkaloid from *Fascaplysinopsis reticulata*. Yellow solid.

Jimenez, C. *et al., J.O.C.*, 1991, **56**, 3403-3410 (*isol, uv, ir, pmr, cmr, struct*)
Fürster, A. *et al., Tetrahedron*, 1996, **52**, 7329-7344 (*synth, ir, pmr, cmr*)
Segraves, N.L. *et al., J. Nat. Prod.*, 2004, **67**, 783-792 (*3-Bromosecofascaplysins*)

4,5-Seco-6-guaiene-4,5-dione S-115



$C_{15}H_{24}O_2$ 236.353

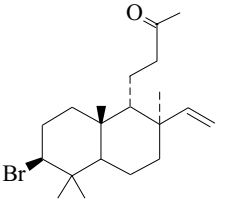
(1α,10β)-*form*

Gibberodione
[864530-16-5]
Constit. of *Sinularia gibberosa*.
Oil. $[\alpha]_D^{25}$ +20.8 (c, 0.72 in $CHCl_3$).

Ahmed, A.F. *et al., J. Nat. Prod.*, 2005, **68**, 1208-1212 (*Gibberodione*)

Secoisoaplysin 20 S-116

[95387-43-2]

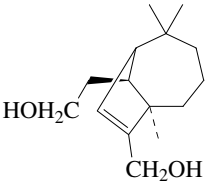


$C_{20}H_{33}BrO$ 369.384
Constit. of *Laurencia perforata*. Oil. $[\alpha]_D$ -112 (c, 0.18 in $CHCl_3$).

Gonzalez, A.G. *et al., J.O.C.*, 1985, **50**, 1261

Secolongifolenediol S-117

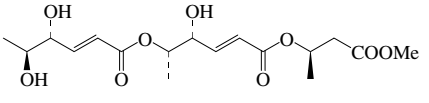
[53587-37-4]



$C_{15}H_{26}O_2$ 238.369
Metab. of *Drechslera dematioidea*. Amorph. powder. $[\alpha]_D^{22}$ +7 (c, 0.08 in EtOH).

Dorn, F. *et al., Experientia*, 1974, **30**, 851-852 (*isol, pmr*)
Yadav, J.S. *et al., Indian J. Chem., Sect. B*, 1983, **22**, 212-214 (*synth*)
Osterhage, C. *et al., J. Nat. Prod.*, 2002, **65**, 306-313 (*isol, pmr, cmr*)

Secomacrosphelide E S-118



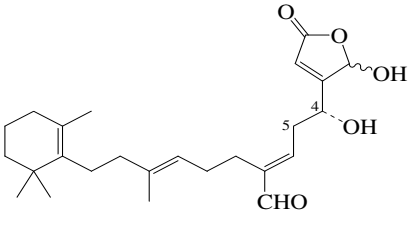
Absolute Configuration

$C_{17}H_{26}O_9$ 374.387
Isol. from a strain of *Periconia byssoides* originally separated from *Aplysia kurodai*. Oil. $[\alpha]_D$ +56 (c, 0.1 in EtOH). λ_{max} 215 (log ϵ 4.21) (EtOH).

Nakamura, H. *et al., Chem. Pharm. Bull.*, 2002, **50**, 303-306 (*isol, pmr, cmr, cd*)

Secomanoalide S-119

[80388-50-7]



$C_{25}H_{36}O_5$ 416.556

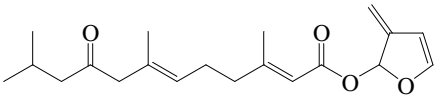
Constit. of *Luffariella variabilis*. Shows cytotoxic and antibacterial activities. Glass. $[\alpha]_D$ +16.2 (c, 0.99 in $CHCl_3$). λ_{max} 228 (ϵ 5000) (MeOH) (Derep).

*4-Deoxy, 4,5*E*-didehydro:* ***Dehydromanoalide***
[98754-59-7]
$C_{25}H_{34}O_4$ 398.541
Constit. of *Luffariella variabilis*. Pale yellow waxy solid. λ_{max} 204 (ϵ 23760); 317 (ϵ 34180) (MeOH) (Berdy). λ_{max} 252 (ϵ 5100); 290 (ϵ 3600); 464 (ϵ 60080) (MeOH/NaOH) (Berdy).

De Silva, E.D. *et al., Tet. Lett.*, 1981, **22**, 3147-3150 (*isol, pmr, cmr*)
Katsumura, S. *et al., Tet. Lett.*, 1985, **26**, 5827-5830 (*synth*)
Potts, B.C.M. *et al., J.O.C.*, 1992, **57**, 2965 (*Dehydromanoalide*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 265-270 (*abs config, pmr, cmr*)
Gauvin, A. *et al., Riv. Ital. EPPOS*, 1998, 622-626 (*activity*)

Secomarislin S-120

[78284-86-3]

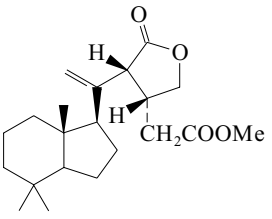


$C_{20}H_{28}O_4$ 332.439
Isol. from the nudibranch *Chromodoris marislae*. Oil.

Hochlowski, J.E. *et al., Tet. Lett.*, 1981, **22**, 271-274 (*isol, pmr*)

Seconorrlandin B S-121

Seconorrisolide B
[129350-19-2]

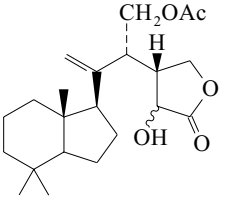


$C_{21}H_{32}O_4$ 348.481
Rearranged spongiane. Constit. of *Dysidea* sp. Oil. $[\alpha]_D$ +3.3 (c, 0.15 in $CHCl_3$). Authors use both names.

Rudi, A. *et al., Tetrahedron*, 1990, **46**, 4019 (*isol, struct*)

Seconorrlandin C S-122

Seconorrisolide C
[129350-20-5]

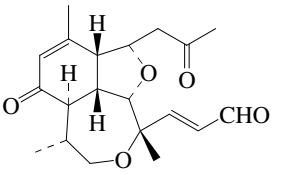


$C_{22}H_{34}O_5$ 378.508
Rearranged spongiane. Constit. of *Dysidea* sp. Oil.

Rudi, A. *et al., Tetrahedron*, 1990, **46**, 4019 (*isol, struct*)

Secopachyclavulariaenone A S-123

[369632-02-0]

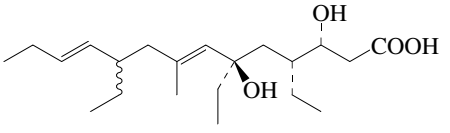


$C_{20}H_{26}O_5$ 346.422
Constit. of *Pachyclavularia violacea*. Oil. $[\alpha]_D^{28}$ -20 (c, 0.02 in $CHCl_3$). λ_{max} 208 (ϵ 6963) (EtOH aq.).

Sheu, J.-H. *et al., Tetrahedron*, 2001, **57**, 7639-7648 (*isol, pmr, cmr*)

Secoplakortide H S-124

4,6,10-Triethyl-3,6-dihydroxy-8-methyl-7,11-tetradecadienoic acid



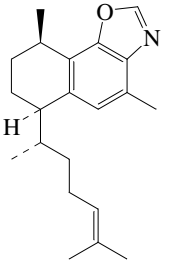
$C_{21}H_{38}O_4$ 354.529
Isol. from the sponge *Plakortis simplex*. Amorph. solid (as Me ester). $[\alpha]_D$ +13 (c, 0.01 in $CHCl_3$) (Me ester).

11,12-Dihydro: 4,6,10-Triethyl-3,6-dihydroxy-8-methyl-7-tetradecenoic acid. ***Secoplakortide I***
$C_{21}H_{40}O_4$ 356.545
Isol. from *Plakortis simplex*. Amorph. solid (as Me ester). $[\alpha]_D$ -4 (c, 0.008 in $CHCl_3$) (Me ester).

Fattorusso, E. *et al., Tetrahedron*, 2000, **56**, 7959-7967

Secopseudopteroxazole S-125

[242150-02-3]

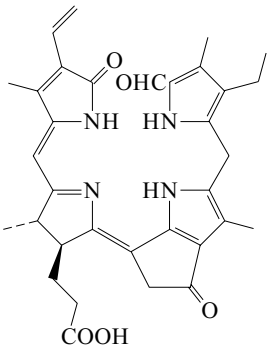


$C_{21}H_{29}NO$ 311.466
Isol. from *Pseudopterogorgia elisabethae*. Active against *Mycobacterium tuberculosis*. Yellowish oil. $[\alpha]_D^{25}$ +28.2 (c, 0.85 in $CHCl_3$). Isolate was contaminated with traces of Elisabethin A, E-72.

Rodriguez, A.D. *et al., Org. Lett.*, 1999, **1**, 527-530

4,5-Secopyrophaeophorbide a S-126

[138530-73-1]

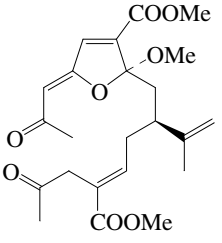


$C_{33}H_{36}N_4O_5$ 568.671
Isol. from the alga *Chlorella protothecoides*. Red pigment.

Engel, N. *et al., FEBS Lett.*, 1991, **293**, 131 (*isol, pmr, struct*)
Engel, N. *et al., Helv. Chim. Acta*, 1993, **76**, 2236 (*cryst struct*)

Secosethukarailin S-127

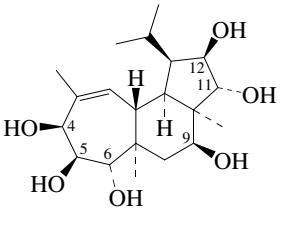
[445394-06-9]



$C_{23}H_{30}O_8$ 434.485
Constit. of *Sinularia dissecta*. Oil. $[\alpha]_D^{25}$ -27.3 (c, 0.25 in $CHCl_3$).
λ_{max} 217 (log ϵ 3.79); 313 (log ϵ 3.53) (MeOH).

Reddy, N.S. *et al., J. Nat. Prod.*, 2002, **65**, 1059-1060 (*isol, pmr, cmr*)

3,4-Seco-2-verrucosene-4,5,6,9,11,12-hexol S-128



$C_{20}H_{34}O_6$ 370.485

(4β,5β,6α,9β,10α,11α,12β,13α*H*)-*form*
10,13-Diepihomoverrucos-2-ene-4,5,6,9,11,12-hexol
[495413-95-1]
Gum.

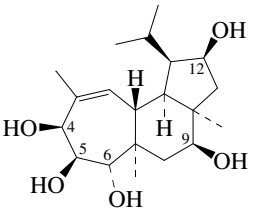
6,9,12-Tributanoyl, 5,11-di-Ac: ***Gagunin C***
[495413-90-6]
$C_{36}H_{56}O_{11}$ 664.832
Constit. of a *Phorbas* sp. Amorph. solid.
Mp 63-66°. $[\alpha]_D^{25}$ +54.1 (c, 0.04 in MeOH).

6,9,11,12-Tetrabutanoyl, 5-Ac: ***Gagunin B***
[495413-89-3]
$C_{38}H_{60}O_{11}$ 692.885
Constit. of a *Phorbas* sp. Amorph. solid.
Mp 76-78°. $[\alpha]_D^{25}$ +55.3 (c, 0.65 in MeOH).

12-(3-Methylbutanoyl), 6,9,11-tributanoyl, 5-Ac: ***Gagunin A***
[495413-88-2]
$C_{39}H_{62}O_{11}$ 706.912
Constit. of a *Phorbas* sp. Amorph. solid.
Mp 88-90°. $[\alpha]_D$ +48.6 (c, 0.71 in MeOH).

Rho, J.-R. *et al., Tetrahedron*, 2002, **58**, 9585-9591 (*isol, pmr, cmr*)

3,4-Seco-2-verrucosene-4,5,6,9,12-pentol S-129



$C_{20}H_{34}O_5$ 354.486

(4β,5β,6α,9β,10α,12β,13α*H*)-*form*
10,13-Diepihomoverrucos-2-ene-4,5,6,9,12-pentol

6,9-Dibutanoyl, 4,12-di-Ac: ***Gagunin G***
[495413-94-0]
$C_{32}H_{50}O_9$ 578.742
Constit. of a *Phorbas* sp. Amorph. solid.
Mp 77-78°. $[\alpha]_D^{25}$ +74.9 (c, 0.18 in MeOH).

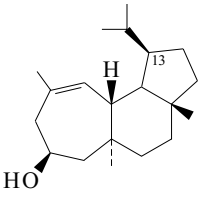
5,9,12-Tributanoyl, 4-Ac: ***Gagunin E***
[495413-92-8]
$C_{34}H_{54}O_9$ 606.795
Constit. of a *Phorbas* sp. Amorph. solid.
Mp 57-59°. $[\alpha]_D^{25}$ +161.6 (c, 0.21 in MeOH).

6,9,12-Tributanoyl, 4-Ac: ***Gagunin F***
[495413-93-9]
$C_{34}H_{54}O_9$ 606.795
Constit. of a *Phorbas* sp. Amorph. solid.
Mp 59-61°. $[\alpha]_D^{25}$ +157.3 (c, 0.14 in MeOH).

6,9,12-Tributanoyl, 5-Ac: ***Gagunin D***
[495413-91-7]
$C_{34}H_{54}O_9$ 606.795
Constit. of a *Phorbas* sp. Amorph. solid.
Mp 73-75°. $[\alpha]_D^{25}$ +51.3 (c, 0.12 in MeOH).

Rho, J.-R. *et al., Tetrahedron*, 2002, **58**, 9585-9591 (*isol, pmr, cmr*)

3,5-Seco-2-verrucosen-5-ol S-130



(5β,13α*H*)–*form*

$C_{20}H_{34}O$ 290.488

(5β,13α*H*)-*form*
13-Epihomoverrucosan-5β-ol
[119242-42-1]
Constit. of *Schistochila nobilis*.
Cryst.
Mp 123-124°. $[\alpha]_D$ +47.1 (c, 0.55 in $CHCl_3$).

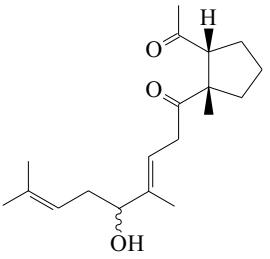
(5β,13β*H*)-*form*
5-Homoverrucosanol. *Homoverrucosanol*
[68420-55-3]
Constit. of *Schistochila rigidula* and *Epipolasis kushimotoensis*.
Cryst. (MeOH).
Mp 135-136°. $[\alpha]_D$ +21 (c, 0.50 in $CHCl_3$).

Asakawa, Y. *et al., Phytochemistry*, 1988, **27**, 3509

Tanaka, J. *et al., Chem. Lett.*, 1997, 489-490 (*isol, pmr, cmr*)
Piers, E. *et al., Tet. Lett.*, 1997, **38**, 8815-8818 (*synth*)

Secoxestenone S-131

[123231-48-1]

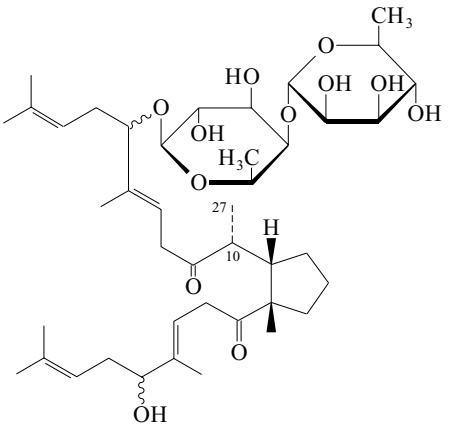


$C_{19}H_{30}O_3$ 306.444
Constit. of *Xestospongia vanilla*. Oil.

Northcote, P.T. *et al., Can. J. Chem.*, 1989, **67**, 1359 (*isol, pmr, cmr*)

Secoxestovanin A S-132

[121541-67-1]



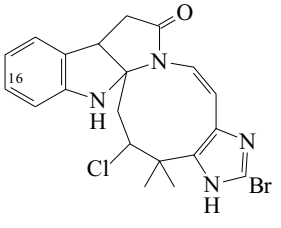
$C_{42}H_{68}O_{12}$ 764.992
Constit. of *Xestospongia vanilla*. Glass.

10,27-Didehydro: ***Secodehydroxestovanin A***
[137415-11-3]
$C_{42}H_{66}O_{12}$ 762.976
Constit. of *Xestospongia vanilla*. Oil.

Northcote, P.T. *et al., J.A.C.S.*, 1989, **111**, 6276-6280 (*isol, pmr, cmr*)
Morris, S.A. *et al., Can. J. Chem.*, 1991, **69**, 1352 (*Secodehydroxestovanin A, isol, pmr, cmr*)

Securamine A S-133

[173220-55-8]



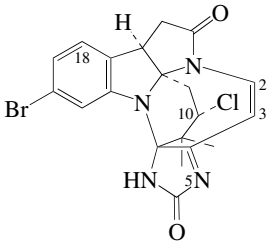
$C_{20}H_{20}BrClN_4O$ 447.761
Exists in equilib. with Securine A. Alkaloid from the marine bryozoan *Securiflustra securifrons*. Cryst.
Mp 200° dec. $[\alpha]_D^{20}$ -87.5 (c, 0.064 in $CHCl_3$).

16-Bromo: ***Securamine B***
[173220-56-9]
$C_{20}H_{19}Br_2ClN_4O$ 526.657
From *Securiflustra securifrons*. Cryst. $[\alpha]_D^{20}$ -316.7 (c, 0.030 in $CHCl_3$). Exists in equilib. with Securine B.

Rahbaek, L. *et al., J.O.C.*, 1996, **61**, 887-889 (*isol, uv, ir, cd, pmr, cmr, struct*)

Securamine C S-134

[173220-57-0]



Relative Configuration

$C_{20}H_{18}BrClN_4O_2$ 461.744
Alkaloid from the marine bryozoan *Securiflustra securifrons*. Amorph. yellow solid. $[\alpha]_D^{20}$ -433.5 (c, 0.033 in $CHCl_3$).

Debromo: ***Securamine D***
[173220-58-1]
$C_{20}H_{19}ClN_4O_2$ 382.848
Isol. from *Securiflustra securifrons*. Amorph. green solid.
$[\alpha]_D^{20}$ -320 (c, 0.069 in $CHCl_3$).

18-Bromo: ***Securamine E***
[185616-44-8]
$C_{20}H_{17}Br_2ClN_4O_2$ 540.641
Isol. from *Securiflustra securifrons*. Amorph. yellow solid.
$[\alpha]_D^{20}$ -115 (c, 0.0078 in $CHCl_3$). λ_{max} 303 (log ϵ 3.82); 327 (log ϵ 3.83) ($CHCl_3$).

10-Epimer: ***Securamine F***
[185616-45-9]
$C_{20}H_{18}BrClN_4O_2$ 461.745
Isol. from *Securiflustra securifrons*. Amorph. orange solid.
$[\alpha]_D^{20}$ -200 (c, 0.0045 in $CHCl_3$). λ_{max} 299 (log ϵ 3.86); 328 (log ϵ 3.88) ($CHCl_3$).

2,3,4,5-Tetrahydro, 3,4-didehydro: ***Securamine G***
[185616-47-1]
$C_{20}H_{20}BrClN_4O_2$ 463.76
Isol. from *Securiflustra securifrons*. Amorph. brown solid.
$[\alpha]_D^{20}$ -15.6 (c, 0.032 in $CHCl_3$). λ_{max} 298 (log ϵ 2.81) ($CHCl_3$).

Rahbaek, L. *et al., J.O.C.*, 1996, **61**, 887-889 (*isol, uv, ir, cd, pmr, cmr, struct*)
Rahbaek, L. *et al., J. Nat. Prod.*, 1997, **60**, 175-177 (*Securamines E-G*)

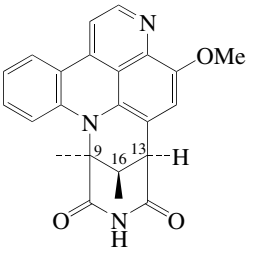
Seductin S-135

Protein. Isol. from albumen gland of *Aplysia californica* and *Aplysia brasiliana*. Waterborne pheromone.

Cummins, S.F. *et al., Peptides (N.Y.)*, 2005, **26**, 351-359 (*isol*)

Segoline A S-136

[117694-96-9]



Absolute Configuration

$C_{23}H_{19}N_3O_3$ 385.421

Alkaloid from the Red Sea tunicate *Eudistoma* sp. Cell proliferation inhibitor. Amorph. powder. Sol. MeOH.
Mp 276°. $[\alpha]_D^{24}$ -322 (c, 1 in $CHCl_3$). λ_{max} 245 (ϵ 7400); 278 (sh) (ϵ 15600); 298 (ϵ 21300); 366 (ϵ 1400); 382 (ϵ 2500); 545 (ϵ 2500) (MeOH/HCl) (Derep). λ_{max} 236 (sh) (ϵ 9000); 270 (ϵ 16200); 308 (ϵ 5100); 320 (ϵ 5600); 368 (ϵ 1600); 383 (ϵ 2600); 460 (ϵ 3100) (MeOH) (Derep).

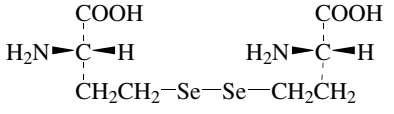
16-Epimer: ***Segoline C***
[340162-11-0]
$C_{23}H_{19}N_3O_3$ 385.421
Alkaloid from *Eudistoma bituminis.*
$[\alpha]_D$ -374 ($CHCl_3$).

9,13-Diepimer: ***Segoline B***
[122795-54-4]
$C_{23}H_{19}N_3O_3$ 385.421
Alkaloid from the Red Sea tunicate *Eudistoma* sp. Amorph. powder. $[\alpha]_D^{24}$ +355 (c, 1 in $CHCl_3$). λ_{max} 245 (ϵ 7400); 278 (sh) (ϵ 15600); 298 (ϵ 21300); 366 (ϵ 1400); 382 (ϵ 2500); 545 (ϵ 2500) (MeOH/HCl) (Derep). λ_{max} 236 (sh) (ϵ 9000); 270 (ϵ 16200); 308 (ϵ 5100); 320 (ϵ 5600); 368 (ϵ 1600); 383 (ϵ 2600); 460 (ϵ 3100) (MeOH) (Derep).

Rudi, A. *et al., J.O.C.*, 1989, **54**, 5331-5337 (*isol, uv, ir, pmr, cmr, cd, struct*)
Viracaoundin, I. *et al., Tet. Lett.*, 2001, **42**, 2669-2671 (*isol, cd, pmr, cmr, abs config*)

Selenohomocystine S-137

4,4′-Diselenobis[2-aminobutanoic acid], 9CI
[7776-33-2]



(*S,S*)-*form*

$C_8H_{16}N_2O_4Se_2$ 362.145

(S,S)-form
L,L-form
[7730-03-2]
Occurs in seleniferous cabbage *Brassica oleracea capitata*.
Mp 214°. $[\alpha]_D^{21}$ +31 (1*M* HCl).

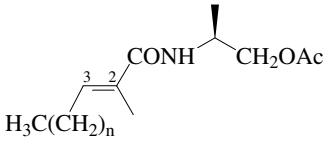
(ξ,ξ)-form
Prod. by a marine bacillus.

[97276-02-3 R,R-form]

Painter, E.P. *et al., J.A.C.S.*, 1947, **69**, 232-234 (*synth*)
Klosterman, H.J. *et al., J.A.C.S.*, 1947, **69**, 2009-2010 (*synth*)
Hamilton, J.W. *et al., J. Agric. Food Chem.*, 1975, **23**, 1150-1152 (*occur*)
Zhou, Z.S. *et al., Bioorg. Med. Chem. Lett.*, 2000, **10**, 2471-2475 (*S,S-form, synth*)
Kotrebai, M. *et al., J. Chromatogr., A*, 2000, **866**, 51-53 (*hplc, ms*)
Imada, C. *et al., J. Antibiot.*, 2002, **55**, 223-226 (*isol, activity*)

Semiplenamide C S-138

[630100-43-5]



Absolute Configuration

n = 12

$C_{22}H_{41}NO_3$ 367.571
Alkaloid from *Lyngbya semiplena*. Amorph. solid. $[\alpha]_D^{26}$ -5 (c, 0.3 in $CHCl_3$). λ_{max} 213 (ϵ 6500) (MeOH).

Han, B. *et al., J. Nat. Prod.*, 2003, **66**, 1364-1368 (*isol, pmr, cmr*)
Davies, I.R. *et al., Tet. Lett.*, 2005, **46**, 5547-5549 (*synth*)

Semiplenamide D S-139

[630100-44-6]
As Semiplenamide C, S-138 with
n = 16
$C_{26}H_{49}NO_3$ 423.678
Alkaloid from *Lyngbya semiplena*. Amorph. solid. $[\alpha]_D^{26}$ -10.6 (c, 0.15 in $CHCl_3$). λ_{max} 207 (ϵ 5200) (MeOH).

Han, B. *et al., J. Nat. Prod.*, 2003, **66**, 1364-1368 (*isol, pmr, cmr*)

Semiplenamide E S-140

[630100-45-7]
As Semiplenamide C, S-138 with
n = 14
$C_{24}H_{45}NO_3$ 395.624
Alkaloid from *Lyngbya semiplena*. Amorph. solid. $[\alpha]_D^{26}$ -7.1 (c, 0.28 in $CHCl_3$). λ_{max} 207 (ϵ 4300) (MeOH).

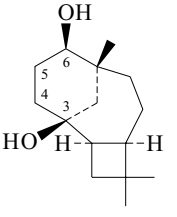
2R,3S*-Epoxide:* ***Semiplenamide G***
[630100-47-9]
$C_{24}H_{45}NO_4$ 411.624
Alkaloid from *Lyngbya semiplena*. Amorph. solid. $[\alpha]_D^{26}$ -3 (c, 0.6 in $CHCl_3$). 1′-Config. not determined. λ_{max} 207 (ϵ 6100) (MeOH).

2R,3S*-Epoxide,* O*-de-Ac:* ***Semiplenamide F***
[630100-46-8]
$C_{22}H_{43}NO_3$ 369.587
Alkaloid from *Lyngbya semiplena*. Amorph. solid. $[\alpha]_D^{26}$ -5 (c, 0.3 in $CHCl_3$). 1′-Config. not determined. λ_{max} 205 (ϵ 5500) (MeOH).

Han, B. *et al., J. Nat. Prod.*, 2003, **66**, 1364-1368 (*Semiplenamides E-G*)

Senecrassidiol S-141

[79433-54-8]



$C_{15}H_{26}O_2$ 238.369
Constit. of *Senecio crassissimus*. Cryst. (2-propanol).
Mp 93-96°. $[\alpha]_D^{24}$ -10.9 (c, 0.23 in $CHCl_3$).

6-Deoxy, 5-oxo:
$C_{15}H_{24}O_2$ 236.353
Constit. of *Eurypon* sp. Oil. $[\alpha]_D$ -3.3 (c, 0.9 in $CHCl_3$).

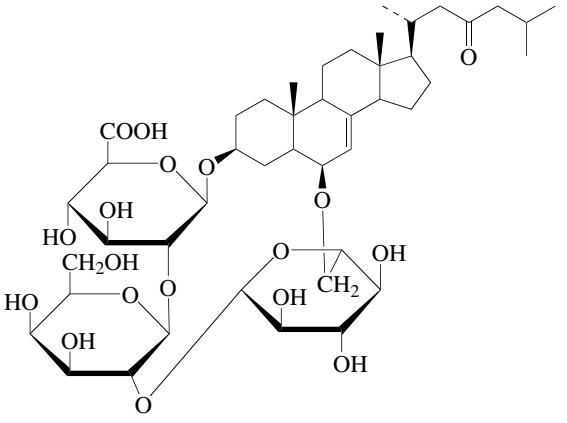
6-Deoxy, 5-oxo, 3-Me ether:
$C_{16}H_{26}O_2$ 250.38
Constit. of a *Eurypon* sp. Oil. $[\alpha]_D$ -5.6 (c, 0.9 in $CHCl_3$).

Dideoxy, 3,4-didehydro, 5α-hydroxy:
$C_{15}H_{24}O$ 220.354
Constit. of a *Eurypon* sp. Oil. $[\alpha]_D$ -12.8 (c, 0.9 in $CHCl_3$).

Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 469 (*isol*)
Barrow, C.J. *et al., Aust. J. Chem.*, 1988, **41**, 1755 (*derivs*)
Iwabachi, H. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1405 (*pmr, cmr*)

Sepositoside A S-142

[79154-52-2]



$C_{45}H_{70}O_{18}$ 899.037

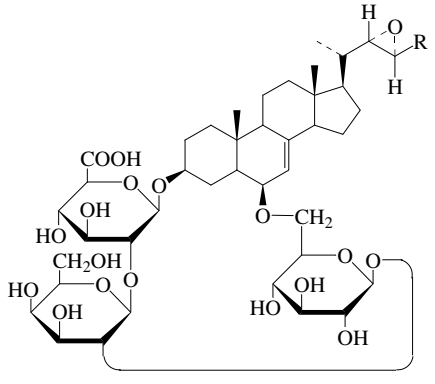
Constit. of *Echinaster sepositus*. Amorph. powder (as Na salt). Sol. H_2O, MeOH; poorly sol. Me_2CO, hexane. $[\alpha]_D$ -68.5 (c, 1 in H_2O) (Na salt).

▶ LD_{50} (mus, ipr) 43 mg/kg.

De Simone, F. *et al., J.C.S. Perkin 1*, 1981, 1855-1862

Sepositoside A analogue 1 S-143

[78747-24-7]



R = -$CH(CH_3)_2$

$C_{44}H_{68}O_{18}$ 885.01

Not named in the paper. Isol. as Na salt. Isol. from the starfish *Echinaster sepositus*.

$[\alpha]_D$ -56.5 (c, 1 in H_2O).

Riccio, R. *et al., Tet. Lett.*, 1981, **22**, 1557-1560; 2242 (*isol, pmr, cmr, struct*)

Sepositoside A analogue 2 S-144

[78731-40-5]

As Sepositoside A analogue 1, S-143 with

R = -$CH_2CH(CH_3)_2$

$C_{45}H_{70}O_{18}$ 899.037

Isol. as Na salt mixed with Sepositoside A analogue 3, S-145. Isol. from the starfish *Echinaster sepositus*.

Riccio, R. *et al., Tet. Lett.*, 1981, **22**, 1557-1560 (*isol, pmr, cmr, struct*)

Sepositoside A analogue 3 S-145

[78731-41-6]

As Sepositoside A analogue 1, S-143 with

R = -$CH(CH_3)CH_2CH_3$

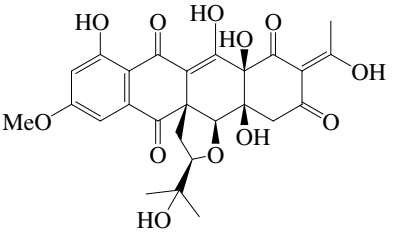
$C_{45}H_{70}O_{18}$ 899.037

Isol. as Na salt in a mixt. with Sepositoside A analogue 2, S-144. Isol. from the starfish *Echinaster sepositus*.

Riccio, R. *et al., Tet. Lett.*, 1981, **22**, 1557-1560 (*isol, pmr, cmr, struct*)

Seragakinone A S-146

[256649-68-0]



Relative Configuration

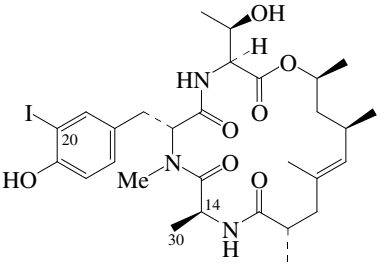
$C_{26}H_{26}O_{12}$ 530.484

Prod. by an unidentified fungus separated from the marine rhodophyte *Ceratodictyon spongiosum*. Amorph. pale yellow solid. $[\alpha]_D^{26}$ +146 (c, 1 in MeOH). λ_{max} 257 (ϵ 25100); 279 (ϵ 20800); 383 (ϵ 12800) (MeOH).

Shigemori, H. *et al., Tetrahedron*, 1999, **55**, 14925-14930

Komatsu, K. *et al., Tetrahedron*, 2000, **56**, 8841-8844 (*biosynth, config*)

Seragamide A S-147



$C_{29}H_{42}IN_3O_7$ 671.571

Depsipeptide antibiotic. Related to Geodiamolide A, G-45. Isol. from the sponge *Suberites japonicus*. Cytotoxic. Amorph. solid. $[\alpha]_D^{27}$ +45.6 (c, 0.21 in $CHCl_3$). λ_{max} 207 (ϵ 34000); 286 (ϵ 2800) (MeOH).

30-Hydroxy: ***Seragamide E***

$C_{29}H_{42}IN_3O_8$ 687.571

Isol. from *Suberites japonicus*. Glass. $[\alpha]_D^{24}$ +33 (c, 0.09 in $CHCl_3$). λ_{max} 218 (ϵ 11000); 285 (ϵ 2500) (MeOH).

20-Chloro analogue: ***Seragamide C***

$C_{29}H_{42}ClN_3O_7$ 580.119

Isol. from *Suberites japonicus*. Glass. $[\alpha]_D^{23}$ +53 (c, 0.1 in $CHCl_3$). λ_{max} 217 (ϵ 12000); 281 (ϵ 2300) (MeOH).

20-Bromo analogue: ***Seragamide B***

$C_{29}H_{42}BrN_3O_7$ 624.571

Isol. from *Suberites japonicus*. Amorph. solid. $[\alpha]_D^{27}$ +39 (c, 0.09 in $CHCl_3$). λ_{max} 205 (ϵ 31000); 283 (ϵ 2300) (MeOH).

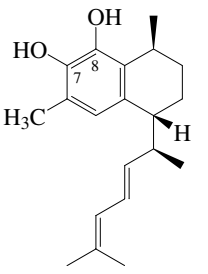
14-Demethyl: ***Seragamide D***

$C_{28}H_{40}IN_3O_7$ 657.544

Isol. from *Suberites japonicus*. Glass. $[\alpha]_D^{23}$ +46 (c, 0.07 in $CHCl_3$). λ_{max} 217 (ϵ 12000); 285 (ϵ 2600) (MeOH).

Tanaka, C. *et al., Tetrahedron*, 2006, **62**, 3536-3542 (*isol, pmr, cmr*)

12,14-Serrulatadiene-7,8-diol S-148



(12*E*)-*form*

$C_{20}H_{28}O_2$ 300.44

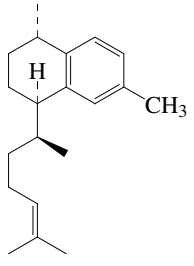
(12*E*)-*form*

7-O-α-D-*Arabinopyranoside:* ***Amphilectosin A***
[862910-66-5]
$C_{25}H_{36}O_6$ 432.556
Constit. of *Pseudopterogorgia elisabethae.* Oil. $[\alpha]_D^{20}$ -85 (c, 0.0038 in CH_2Cl_2).

(12*Z*)-*form*

7-O-α-D-*Arabinopyranoside:* ***Amphilectosin B***
[862910-65-4]
$C_{25}H_{36}O_6$ 432.556
Constit. of *Pseudopterogorgia elisabethae.* Oil. $[\alpha]_D^{20}$ -62 (c, 0.0014 in CH_2Cl_2).
Ferns, T.A. *et al., J.O.C.*, 2005, **70**, 6152-6157 (*Amphilectosins*)

14-Serrulatene S-149

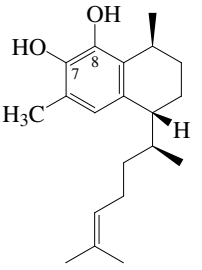


$C_{20}H_{30}$ 270.457

(1α,4α*H*)-*form*
Erogorgiaene
[318513-13-2]
Constit. of *Pseudopterogorgia elisabethae.*
Oil. $[\alpha]_D^{25}$ +24.4 (c, 3.2 in $CHCl_3$). λ_{max} 208 (ϵ 16000); 280 (ϵ 1500) (MeOH).
Rodríguez, A.D. *et al., J. Nat. Prod.*, 2001, **64**, 100-102 (*isol, pmr, cmr*)
Kohl, A.C. *et al., Mar. Drugs*, 2003, **1**, 54-65 (*biosynth*)
Cesati III, R.R. *et al., J.A.C.S.*, 2004, **126**, 96-101 (*synth*)
Davies, H.M.L. *et al., Angew. Chem., Int. Ed.*, 2005, **43**, 1730-1735 (*synth*)
Harmata, M. *et al., Tet. Lett.*, 2005, **46**, 3847-3849 (*synth*)

14-Serrulatene-7,8-diol S-150

7,8-Dihydroxyeriogorgiaene
[199439-75-3]



$C_{20}H_{30}O_2$ 302.456
Constit. of *Pseudopterogorgia elisabethae.*

7-O-α-D-*Arabinopyranoside:* ***Secopseudopterosin J***
[862910-70-1]
$C_{25}H_{38}O_6$ 434.572
Constit. of *Pseudopterogorgia elisabethae.* Oil. $[\alpha]_D^{20}$ -80 (c, 0.0013 in CH_2Cl_2).

7-O-*(2*-O-*Acetyl*-α-D-*arabinopyranoside):* ***Secopseudopterosin I***
[791846-82-7]
$C_{27}H_{40}O_7$ 476.609
Constit. of *Pseudopterogorgia elisabethae.* Powder. $[\alpha]_D^{25}$ -92.4 (c, 2.1 in $CHCl_3$). λ_{max} 208 (ϵ 57500); 228 (ϵ 17300); 278 (ϵ 4200) (MeOH).

7-O-*(4*-O-*Acetyl*-α-D-*arabinopyranoside):* ***Secopseudopterosin H***
[791846-81-6]
$C_{27}H_{40}O_7$ 476.609
Constit. of *Pseudopterogorgia elisabethae.* Powder. $[\alpha]_D^{25}$ -142.3 (c, 0.8 in $CHCl_3$). λ_{max} 208 (ϵ 54600); 228 (ϵ 17000); 280 (ϵ 7900) (MeOH).

8-O-α-L-*Arabinopyranoside:* ***Secopseudopterosin A***
[111466-65-0]
$C_{25}H_{38}O_6$ 434.572
Constit. of sea whip *Pseudopterogorgia* sp. Analgesic and antiinflammatory. Amorph. solid. Fairly sol. MeOH, EtOAc. $[\alpha]_D$ -118 (c, 1.7 in $CHCl_3$). λ_{max} 247; 285; 295 (MeOH/KOH) (Derep). λ_{max} 230 (ϵ 11200); 278 (ϵ 2060); 283 (ϵ 2200) (MeOH) (Derep). λ_{max} 224 (ϵ 10000); 271 (ϵ 1380); 281 (ϵ 1490) (MeOH) (Berdy). λ_{max} 244; 281; 291 (MeOH/NaOH) (Berdy).

8-O-*(2*-O-*Acetyl*-α-L-*arabinopyranoside):* ***Secopseudopterosin B***
[111397-51-4]
$C_{27}H_{40}O_7$ 476.609
Constit. of *Pseudopterogorgia* sp. Antiinflammatory and analgesic agent. Unstable. Sol. MeOH, C_6H_6. λ_{max} 281; 290 (MeOH/KOH) (Derep). λ_{max} 223 (ϵ 7900); 248; 271 (ϵ 2300); 281 (ϵ 2360) (MeOH) (Derep).

8-O-*(3*-O-*Acetyl*-α-L-*arabinopyranoside):* ***Secopseudopterosin C***
[111466-66-1]
$C_{27}H_{40}O_7$ 476.609
Constit. of *Pseudopterogorgia* sp. Antiinflammatory and analgesic agent. Amorph. solid. Sol. MeOH, C_6H_6. $[\alpha]_D$ -89 (c, 0.58 in $CHCl_3$). λ_{max} 223 (ϵ 7900); 248; 271 (ϵ 2300); 281 (ϵ 2360) (MeOH) (Derep). λ_{max} 248; 281; 290 (MeOH/NaOH) (Berdy).

8-O-*(4*-O-*Acetyl*-α-L-*arabinopyranoside):* ***Secopseudopterosin D***
[111466-67-2]
$C_{27}H_{40}O_7$ 476.609
Constit. of *Pseudopterogorgia* sp. Antiinflammatory and analgesic agent. Amorph. solid. Sol. MeOH, C_6H_6. $[\alpha]_D$ -139 (c, 0.6 in $CHCl_3$). λ_{max} 281; 290 (MeOH/KOH) (Derep). λ_{max} 223 (ϵ 7900); 248; 271 (ϵ 2300); 281 (ϵ 2360) (MeOH) (Derep). λ_{max} 248; 283; 292 (MeOH/NaOH) (Berdy).

8-O-*(2*-O-*Acetyl-6-deoxy-β-D-glucopyranoside):* ***Secopseudopterosin E***
[433717-50-1]
$C_{28}H_{42}O_7$ 490.636
Constit. of *Pseudopterogorgia elisabethae.*
$[\alpha]_D^{20}$ -102 (MeOH). λ_{max} 221; 281 (MeOH).

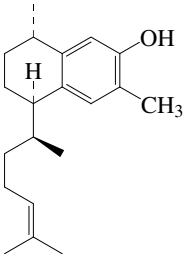
8-O-*(3*-O-*Acetyl-6-deoxy-β-D-glucopyranoside):* ***Secopseudopterosin F***
[433717-53-4]
$C_{28}H_{42}O_7$ 490.636
Constit. of *Pseudopterogorgia elisabethae.*
$[\alpha]_D^{20}$ -55 (MeOH). λ_{max} 223; 283 (MeOH).

8-O-*(4*-O-*Acetyl-6-deoxy-β-D-glucopyranoside):* ***Secopseudopterosin G***
[433717-55-6]
$C_{28}H_{42}O_7$ 490.636
Constit. of *Pseudopterogorgia elisabethae.*
$[\alpha]_D^{20}$ -124 (MeOH). λ_{max} 224; 280 (MeOH).

7-O-*α-L-Fucopyranoside:* ***Secopseudopterosin K***
[890153-95-4]
$C_{26}H_{40}O_6$ 448.598
Constit. of *Pseudopterogorgia elisabethae.* Amorph. solid. $[\alpha]_D^{25}$ -121.3 (c, 0.43 in MeOH). λ_{max} 208 (ε 42000); 230 (sh); 280 (ε 1500) (MeOH).

Look, S.A. *et al., Tetrahedron*, 1987, **43**, 3363-3370 (*Secopseudopterosins A-D*)
Ata, A. *et al., Tetrahedron*, 2003, **59**, 4215-4222 (*Secopseudopterosins E-G*)
Rodriguez, I.I. *et al., J. Nat. Prod.*, 2004, **67**, 1672-1680 (*Secopseudopterosins H and I*)
Ferns, T.A. *et al., J.O.C.*, 2005, **70**, 6152-6157 (*Secopseudopterosin J*)
Ferns, T. *et al., Tetrahedron*, 2005, **61**, 12358-12365 (*isol, biosynth*)
Duque, C. *et al., Tetrahedron*, 2006, **62**, 4205-4213 (*Secopseudopterosin K*)

14-Serrulaten-7-ol S-151

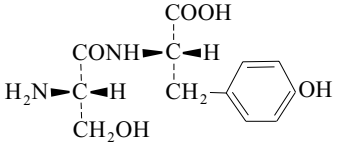


$C_{20}H_{30}O$ 286.456

(1α,4α*H*)-*form*
7-Hydroxyerogorgiaene
[318513-14-3]
Constit. of *Pseudopterogorgia elisabethae.*
Oil. $[\alpha]_D^{25}$ +25.8 (c, 3.8 in $CHCl_3$). λ_{max} 208 (ε 22000); 284 (ε 1800) (MeOH).

Rodríguez, A.D. *et al., J. Nat. Prod.*, 2001, **64**, 100-102 (*isol, pmr, cmr*)
Ferns, T. *et al., Tetrahedron*, 2005, **61**, 12358-12365 (*isol, pmr, cmr*)

N-Seryltyrosine S-152



$C_{12}H_{16}N_2O_5$ 268.269

L-L-*form*
Cryst. (EtOH aq.). Mp 256-260°. $[\alpha]_D^{25}$ +43.1 (c, 0.84 in H_2O).

N-tert-*Butyloxycarbonyl, Me ester:* [10285-64-0]
$C_{18}H_{26}N_2O_7$ 382.413
Cryst. (Et_2O). Mp 117-119°. $[\alpha]_D^{25}$ -5 (c, 1.036 in MeOH).

N-tert-*Butyloxycarbonyl, hydrazide:*
$C_{17}H_{26}N_4O_6$ 382.416
Cryst. + ½ H_2O (H_2O). Mp 193-195° dec., 199-200° dec.
$[\alpha]_D^{24}$ -19.8 (c, 2.035 in 50% AcOH).

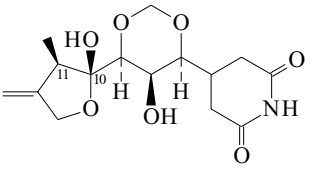
D-D-*form*
N-*(6-Methyloctanoyl):* N-*(6-Methyloctanoyl)seryltyrosine.* ***Tupuseleiamide B***
$C_{21}H_{32}N_2O_6$ 408.494
Prod. by a marine *Bacillus laterosporus.* Solid. $[\alpha]_D$ -78 (MeOH). λ_{max} 262 (ε 41000) (MeOH).

N-*(7-Methyloctanoyl):* N-*(7-Methyloctanoyl)seryltyrosine.* ***Tupuseleiamide A***
$C_{21}H_{32}N_2O_6$ 408.494
Prod. by a marine *Bacillus laterosporus.* Solid. $[\alpha]_D$ -78 (MeOH). λ_{max} 262 (ε 41000) (MeOH).

Fischer, R.F. *et al., J.A.C.S.*, 1954, **76**, 5076 (*synth*)
Hofmann, K. *et al., J.A.C.S.*, 1957, **79**, 1636; 1960, **82**, 3715 (*synth*)
Otsuka, H. *et al., Bull. Chem. Soc. Jpn.*, 1966, **39**, 1171 (*derivs*)
Barsby, T. *et al., J. Nat. Prod.*, 2002, **65**, 1447-1451 (*Tupuseleiamides*)

Sesbanimide A S-153

Sesbanimide



$C_{15}H_{21}NO_7$ 327.333

(+)-*form* [85719-78-4]
Alkaloid from the seeds of *Sesbania drummondii* and *Sesbania punicea* (Leguminosae). Prod. by a marine *Agrobacterium* strain PH-103. Shows notable cytotoxicity against KB cells *in vitro* and potent inhibitory activity against P338 murine leukaemia *in vivo.*
Cryst. (Et_2O/CH_2Cl_2 or MeOH/CH_2Cl_2). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 158-159° (155-156°). $[\alpha]_D^{20}$ +54.7 (c, 0.17 in $CHCl_3$). $[\alpha]_D^{20}$ -3.8 (c, 0.28 in MeOH) (-5.6).

(-)-*form*
Synthetic.
Solid (CH_2Cl_2/Et_2O). Mp 154.5-155.5°. $[\alpha]_D$ +6 (c, 0.27 in MeOH). $[\alpha]_D$ -56.9 (c, 0.21 in $CHCl_3$).

11-Epimer: ***Sesbanimide B***
$C_{15}H_{21}NO_7$ 327.333
Alkaloid from seeds of *Sesbania drummondii* (Leguminosae). Glass. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{20}$ -22.4 (c, 0.17 in $CHCl_3$) (synthetic). Isol. as a mixt. of 2 components, B1 and B2, which are C-10 epimers (assignments of configs. not yet made).

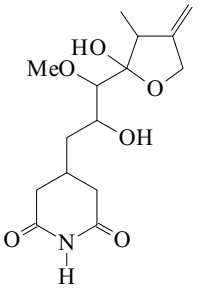
[92282-10-5, 95839-03-5]

Powell, R.G. *et al., J.A.C.S.*, 1983, **105**, 3739-3741 (*isol, uv, ir, pmr, ms, cryst struct*)
Gorst-Allman, C.P. *et al., J.C.S. Perkin 1*, 1984, 1311-1314 (*isol, ir, pmr, cmr*)
Powell, R.G. *et al., Phytochemistry*, 1984, **23**, 2789-2796 (*Sesbanimide B, isol, uv, ir, pmr, cmr, ms, struct*)
U.S. Pat., 1985, 4 532 327; *CA*, **103**, 166147 (*activity*)
Schlessinger, R.H. *et al., J.O.C.*, 1986, **51**, 2621-2623 (*synth*)
Wanner, M.J. *et al., Tetrahedron*, 1987, **43**, 2549-2556 (*synth, ir, pmr*)
Matsuda, F. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 2123 (*synth, props*)
Tomioka, K. *et al., Tet. Lett.*, 1988, **29**, 3095-3096 (*synth*)
Matsuda, F. *et al., Tetrahedron*, 1988, **44**, 4721-4736 (*synth, ir, pmr, abs config*)

Vloon, W.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1991, **110**, 414-419 (*synth*)
Grieco, P.A. *et al., Chem. Comm.*, 1992, 368-370 (*synth*)
Cirillo, P.F. *et al., J.O.C.*, 1994, **59**, 3055-3063 (*synth*)
Honda, T. *et al., Tetrahedron: Asymmetry*, 1994, **5**, 247-254 (*synth*)
Acebal, C. *et al., J. Antibiot.*, 1998, **51**, 64-67 (*marine isol, pmr, cmr*)

Sesbanimide C S-154

[95599-43-2]



$C_{15}H_{23}NO_6$ 313.35
Alkaloid from seeds of *Sesbania drummondii* (Leguminosae). Prod. by a marine *Agrobacterium* strain PH-A034C. Powder. Sol. MeOH. $[\alpha]_D^{25}$ +9.52 (c, 0.21 in $CHCl_3$).

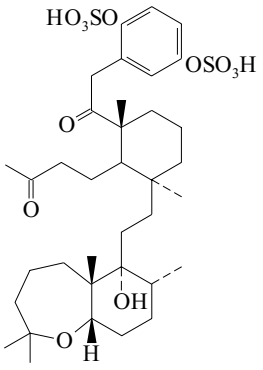
Powell, R.G. *et al., Phytochemistry*, 1984, **23**, 2789-2796 (*isol, pmr, ms, struct*)
Acebal, C. *et al., J. Antibiot.*, 1998, **51**, 64-67 (*isol, pmr, cmr*)

SGFYANRY amide S-155

[638174-62-6]
Ser-Gly-Phe-Tyr-Ala-Asn-Arg-Tyr-NH_2
$C_{45}H_{61}N_{13}O_{12}$ 976.057
Isol. from the pericardial organs of the crab *Cancer borealis*.

Li, L. *et al., J. Neurochem.*, 2003, **87**, 642-656 (*isol*)

Shaagrockol B S-156

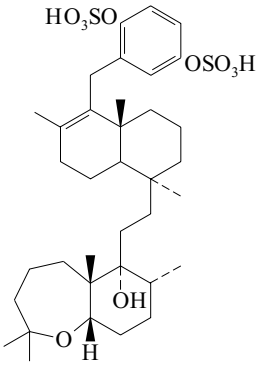


$C_{36}H_{56}O_{12}S_2$ 744.963
Constit. of *Toxiclona toxius*.
$[\alpha]_D$ +4 (c, 0.5 in MeOH) (as di-Na salt).

Isaacs, S. *et al., Tet. Lett.*, 1992, **33**, 2227 (*isol, pmr, cmr*)
Loya, S. *et al., J. Nat. Prod.*, 1993, **56**, 2120 (*isol*)

Shaagrockol C S-157

[141968-27-6]

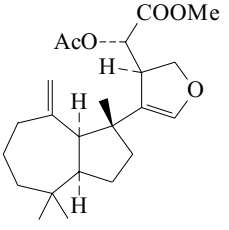


$C_{36}H_{56}O_{10}S_2$ 712.964
Constit. of *Toxiclona toxius*.
$[\alpha]_D$ +8 (c, 0.7 in MeOH) (as di-Na salt).

Isaacs, S. *et al., Tet. Lett.*, 1992, **33**, 2227 (*isol, pmr, cmr*)
Loya, S. *et al., J. Nat. Prod.*, 1993, **56**, 2120 (*isol*)

Shahamin A S-158

[116079-51-7]

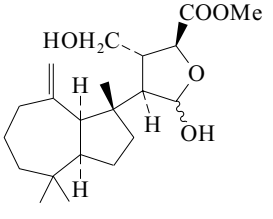


$C_{23}H_{34}O_5$ 390.519
Constit. of *Dysidea* spp. Oil. $[\alpha]_D$ +25 (c, 0.006 in $CHCl_3$).

Carmely, S. *et al., J.O.C.*, 1988, **53**, 4801 (*isol, pmr, cmr*)

Shahamin B S-159

[116079-52-8]

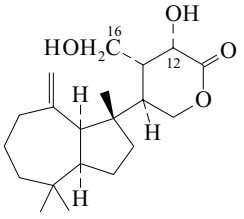


$C_{21}H_{34}O_5$ 366.497
Constit. of *Dysidea* spp. Oil.

Carmely, S. *et al., J.O.C.*, 1988, **53**, 4801 (*isol, pmr, cmr*)

Shahamin E S-160

[116079-55-1]



$C_{20}H_{32}O_4$ 336.47
Constit. of *Dysidea* spp. Oil. $[\alpha]_D$ +72 (c, 0.02 in $CHCl_3$).

16-Ac: ***Shahamin D***
[116079-54-0]
$C_{22}H_{34}O_5$ 378.508
Constit. of *Dysidea* spp. Oil.

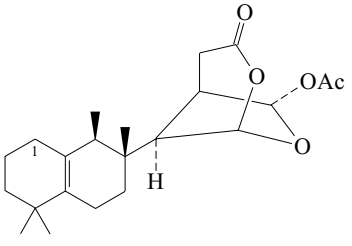
Di-Ac: ***Shahamin C***
[116079-53-9]
$C_{24}H_{36}O_6$ 420.545
Constit. of *Dysidea* spp. Oil. $[\alpha]_D$ +81 (c, 0.01 in $CHCl_3$).

12-Deoxy, 16-Ac: ***12-Desacetoxyshahamin C***
[123332-89-8]
$C_{22}H_{34}O_4$ 362.508
Metab. of *Dendrilla* spp. and *Chromodoris gleniei*. Oil. $[\alpha]_D$ +54 (c, 0.44 in $CHCl_3$).

Carmely, S. *et al., J.O.C.*, 1988, **53**, 4801 (*isol, pmr, cmr*)
Bobzin, S.C. *et al., J.O.C.*, 1989, **54**, 5727 (*isol, pmr, cmr*)
De Silva, E.D. *et al., J. Nat. Prod.*, 1991, **54**, 993 (*12-Desacetoxyshahamin C, isol*)

Shahamin F S-161

[116079-56-2]



$C_{22}H_{32}O_5$ 376.492
Constit. of *Dysidea* spp. and *Chromodoris annulata*. Oil. $[\alpha]_D$ -49.6 (c, 0.001 in $CHCl_3$).

$\Delta^{1(10)}$-Isomer: ***Macfarlandin D***
[105064-36-6]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Chromodoris macfarlandi*. Antimicrobial agent against *Bacillus subtilis*. Needles (Et_2O/hexane). Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. H_2O.
Mp 190-191°. $[\alpha]_D$ -169 (c, 1.2 in $CHCl_3$).

1α-Hydroxy: ***Shahamin G***
[116079-57-3]
$C_{22}H_{32}O_6$ 392.491
Constit of *Dysidea* spp. Oil.

1β-Hydroxy: ***Shahamin H***
[116179-73-8]
$C_{22}H_{32}O_6$ 392.491
Constit. of *Dysidea* spp. Oil.

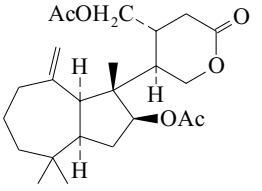
12α-Acetoxy: ***Shahamin I***
[116079-58-4]
$C_{24}H_{34}O_7$ 434.528
Constit. of *Dysidea* spp. Oil. $[\alpha]_D$ -48.3 (c, 0.005 in $CHCl_3$).

12α-Acetoxy, 1β-hydroxy: ***Shahamin J***
[116102-40-0]
$C_{24}H_{34}O_8$ 450.528
Constit. of *Dysidea* spp. Oil.

Molinski, T.F. *et al., J.O.C.*, 1986, **51**, 4564 (*Macfarlandin D*)
Carmely, S. *et al., J.O.C.*, 1988, **53**, 4801 (*Shahamins, isol, pmr, cmr*)
De Silva, E.D. *et al., J. Nat. Prod.*, 1991, **54**, 993 (*isol*)

Shahamin K S-162

[137836-64-7]

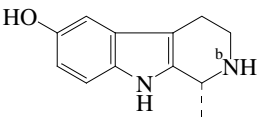


$C_{24}H_{36}O_6$ 420.545
Constit. of *Chromodoris gleniei*. Oil. $[\alpha]_D$ +84 (c, 0.1 in CH_2Cl_2).

De Silva, E.D. *et al., J. Nat. Prod.*, 1991, **54**, 993-997 (*isol, pmr, cmr*)
Lebsack, A.D. *et al., J.A.C.S.*, 2001, **123**, 4851-4852 (*synth*)

Shepherdine S-163

*2,3,4,9-Tetrahydro-1-methyl-1*H*-pyrido[3,4-*b*]indol-6-ol, 9CI. 1,2,3,4-Tetrahydro-6-hydroxy-1-methyl-β-carboline*
[3000-36-0]
[28090-87-1]



(*R*)-*form*

$C_{12}H_{14}N_2O$ 202.255

(R)-form [104485-07-6]
Occurs in urine of man and other mammals.
No phys. props. reported.

(S)-form [104885-06-5]
Occurs in urine of man and other mammals.
No phys. props. reported.

(±)-form
Cryst. (MeOH). Mp 225-230° Mp 257-258°. λ_{max} 276; 298 (sh); 308 (sh) (EtOH) (HCl salt, pH7). λ_{max} 222 (log ε 4.3); 274 (log ε 3.9); 297 (sh) (log ε 3.72) (no solvent reported) (phosphate buffer, pH7).

Me ether: Mp 224-226° (156°, 196-196.5°).

Me ether, picrate: Mp 223-226° dec.

Me ether, N^b-Me: ***1,2,3,4-Tetrahydro-6-methoxy-1,2-dimethyl-β-carboline***
$C_{14}H_{18}N_2O$ 230.309
Constit. of *Piptadenia peregrina*. Cryst. ($CHCl_3$/hexane). Mp 155-157°.

(ξ)-form
Alkaloid from the roots of *Shepherdia canadensis* and from the sponge *Hyrtios* sp. Under certain conditions, a metab. of Serotonin in animals.
Mp 266° dec. (as hydrochloride). $[\alpha]_D$ 0.

N,O-Di-Ac:
Cryst. (MeOH). Mp 192-194°.

N^b-Me: ***1,2,3,4-Tetrahydro-6-hydroxy-1,2-dimethyl-β-carboline.*** *1,2,3,4-Tetrahydro-6-hydroxy-2-methylharman*
$C_{13}H_{16}N_2O$ 216.282
Alkaloid from *Croton moritibensis*.

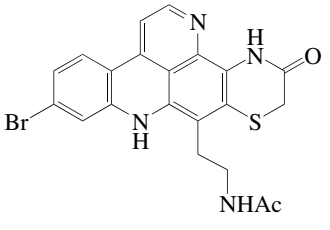
Me ether: 1,2,3,4-Tetrahydro-6-methoxy-1-methyl-β-carboline. ***Adrenoglomerulotropin****. 6-Methoxytetrahydroharman*
[1210-56-6]
[58911-03-8]
$C_{13}H_{16}N_2O$ 216.282
Alkaloid from *Desmodium pulchellum* and *Virola cuspidata* (Leguminosae, Myristicaceae). Also isol. from bovine pineal gland and human urine. Shows some psychotomimetic activity.
▶ UV0740000

Me ether, N^b*-Me:* [21890-60-8]
Alkaloid from *Anadenanthera peregrina* (Leguminosae). No opt. rotn. reported.

Akabori, S. *et al., Ber.*, 1930, **63**, 2245-2248 (*Me ether, synth*)
Farrell, G.L. *et al., Arch. Biochem. Biophys.*, 1961, **94**, 543-544 (*Me ether, isol, struct*)
Taboisky, R.G. *et al., J. Med. Chem.*, 1964, **7**, 135-141 (*synth, uv*)
Agurell, S. *et al., Acta Chem. Scand.*, 1969, **23**, 903-916 (*Me ether* N^b*-Me, occur, synth*)
Ayer, W.A. *et al., Can. J. Chem.*, 1970, **48**, 1980-1984 (*isol, uv, ir, pmr, synth*)
Cassady, J.M. *et al., CA*, 1972, **77**, 98688 (*Me ether, isol*)
Gynther, J. *et al., Acta Chem. Scand., Ser. B*, 1985, **39**, 849-859 (*Me ether, synth, ms*)
Matsubara, K. *et al., Alcohol Alcohol.*, 1986, **21**, 339-345 (*Me ether, hplc, ms, occur*)
Beck, O. *et al., Biochem. Pharmacol.*, 1986, **35**, 2636-2639 (*R-form, S-form, hplc, occur, bibl*)
Zhang, F. *et al., J. Med. Chem.*, 1992, **35**, 82-93 (*synth, hplc, pmr, cmr*)
Callaway, J.C. *et al., J. Het. Chem.*, 1994, **31**, 431-435 (*synth, bibl*)
Herraiz, T. *et al., J. Agric. Food Chem.*, 2000, **48**, 4900-4904 (*hplc, occur*)
Somei, M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1159-1165 (*(±)-form, synth, Me ether, Me ether* N^b*-Me*)
Salmoun, M. *et al., J. Nat. Prod.*, 2002, **65**, 1173-1176 (*isol, pmr, cmr*)
De Araújo-Júnior, V.T. *et al., Pharm. Biol.*, 2004, **42**, 62-67 (N^b*-Me*)

Shermilamine A S-164

[116302-28-4]



$C_{21}H_{17}BrN_4O_2S$ 469.361
Alkaloid from a tunicate *Trididemnum* sp. collected from Guam and from *Chelynotus semperi*. Cytotoxic agent. Orange prisms ($CHCl_3$/MeOH).
Mp 300°. Erroneous spectroscopic data quoted in the original paper. λ_{max} 242 (ϵ 25100); 286 (ϵ 22900); 312 (ϵ 35500); 320 (ϵ 34700); 364 (ϵ 5500); 382 (ϵ 5620); 536 (ϵ 5890) (MeOH/HCl) (Derep). λ_{max} 238 (ϵ 33100); 282 (ϵ 28200); 298 (ϵ 24500); 350 (ϵ 7940); 392 (ϵ 5130); 470 (ϵ 5750) (MeOH) (Derep).

Debromo: ***Shermilamine B****. Debromoshermilamine A*
[122271-41-4]
$C_{21}H_{18}N_4O_2S$ 390.465
Alkaloid from a tunicate *Trididemnum* sp., from the Red Sea tunicate *Eudistoma* sp. and from *Chelynotus semperi*. Fine orange prisms (MeOH).
Mp 254° dec. λ_{max} 232 (ϵ 27500); 282 (ϵ 25100); 302 (ϵ 33900); 318 (ϵ 49000); 364 (ϵ 6030); 382 (ϵ 6170); 536 (ϵ 6760) (MeOH/HCl) (Derep). λ_{max} 234 (ϵ 34700); 282 (ϵ 28200); 298 (ϵ 24500); 348 (ϵ 9330); 390 (ϵ 5750); 468 (ϵ 6460) (MeOH) (Derep).

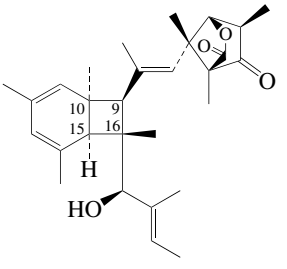
Debromo, N*-de-Ac,* N^{ω},N^{ω}*-di-Me:* ***Shermilamine D***
[211311-08-9]
$C_{21}H_{20}N_4OS$ 376.481
Alkaloid from the tunicate *Cystodytes violatinctus*. Amorph. orange powder. λ_{max} 232 (log ϵ 4.35); 281 (log ϵ 4.25); 297 (log ϵ 4.18); 348 (log ϵ 3.74); 392 (log ϵ 3.51); 468 (log ϵ 3.58) (MeOH). λ_{max} 230; 281; 302; 316; 363; 382; 530 (MeOH/HCl) (Berdy).

Debromo, N*-de-Ac,* N^{ω},N^{ω}*-di-Me,* N*-oxide:* ***Shermilamine E***
[211311-09-0]
$C_{21}H_{20}N_4O_2S$ 392.481
Alkaloid from the tunicate *Cystodytes violatinctus*. Amorph. brown powder. λ_{max} 232 (log ϵ 4.29); 296 (log ϵ 4.1); 349 (log ϵ 3.7); 391 (log ϵ 3.51); 464 (log ϵ 3.49) (MeOH). λ_{max} 230; 281; 300; 315; 361; 382; 526 (MeOH/HCl) (Berdy).

Debromo, N*-de-Ac,* N^{ω}*-(3-methyl-2-butenoyl):* ***Shermilamine C***
[158758-41-9]
$C_{24}H_{22}N_4O_2S$ 430.529
Isol. from *Cystodytes* sp. Antitumour agent. Topoisomerase II inhibitor. DNA intercalator. Orange solid. λ_{max} 231 (ϵ 9185); 279 (ϵ 6670); 296 (ϵ 5690); 350 (ϵ 2680); 390 (ϵ 1896); 463 (ϵ 1664) (MeOH).

Cooray, N.M. *et al., J.O.C.*, 1988, **53**, 4619-4620 (*isol, cryst struct*)
Carroll, A.R. *et al., J.O.C.*, 1989, **54**, 4231-4232 (*isol, uv, ir, pmr, cmr, ms, struct, Shermilamine B*)
Rudi, A. *et al., J.O.C.*, 1989, **54**, 5331 (*isol, uv, ir, pmr, cmr, Shermilamine B*)
Steffan, B. *et al., Tetrahedron*, 1993, **49**, 6223 (*biosynth, Shermilamine B*)
Eldredge, G.S. *et al., J. Med. Chem.*, 1994, **37**, 3819-3827 (*Shermilamine C*)
Ciufolini, M.A. *et al., J.A.C.S.*, 1995, **117**, 12460-12469 (*synth*)
Koren-Goldshlager, G. *et al., J.O.C.*, 1998, **63**, 4601-4603 (*Shermilamines D,E, isol, uv, ir, pmr, cmr*)

Shimalactone A S-165



Absolute Configuration

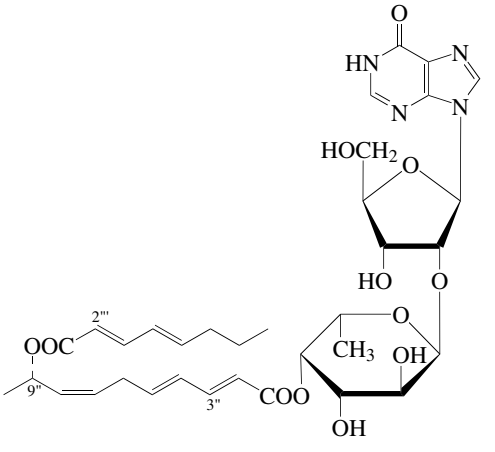
$C_{29}H_{40}O_4$ 452.633
Prod. by the marine fungus *Emericella variecolor* GF10. Neuritogenic agent. Cytotoxic. Oil. $[\alpha]_D^{23}$ +12 (c, 0.57 in MeOH). λ_{max} 280 (ϵ 3700) (MeOH).

9,10,15,16-Tetraepimer: ***Shimalactone B***
$C_{29}H_{40}O_4$ 452.633
Prod. by *Emericella variecolor* GF10. Oil. $[\alpha]_D^{23}$ -48 (c, 1.5 in MeOH). λ_{max} 202 (log ϵ 4.15); 281 (log ϵ 3.57) (MeOH).

Wei, H. *et al., Tetrahedron*, 2005, **61**, 8054-8058 (*Shimalactone A*)
Wei, H. *et al., Heterocycles*, 2006, **68**, 111-123 (*Shimalactone B*)

Shimofuridin A S-166

[152273-80-8]



$C_{34}H_{44}N_4O_{12}$ 700.741

Nucleoside antibiotic. Isol. from the marine tunicate *Aplidium multiplicatum*. Cytotoxic. Also shows activity against fungi and gram-positive bacteria. Protein kinase inhibitor. Solid (MeOH). Sol. MeOH.
Mp 210°. $[\alpha]_D^{19}$ -186 (c, 1,4 in Py). λ_{max} 261 (ϵ 44000); 310 (ϵ 5000) (MeOH).

*(7″*E*)-Isomer:* ***Shimofuridin B***
[157379-40-3]
$C_{34}H_{44}N_4O_{12}$ 700.741
From *Aplidium multiplicatum*. Amorph. solid. Sol. MeOH. $[\alpha]_D^{20}$ -167 (c, 0.1 in MeOH). λ_{max} 261 (ϵ 48000) (MeOH). λ_{max} 261 (ϵ 48000); 370 (ϵ 340) (MeOH) (Berdy).

*(2″*Z*)-Isomer:* ***Shimofuridin C***
[157379-41-4]
$C_{34}H_{44}N_4O_{12}$ 700.741
From *Aplidium multiplicatum*. Amorph. solid. Sol. MeOH. $[\alpha]_D^{20}$ -110 (c, 0.2 in MeOH). λ_{max} 263 (ϵ 32000) (MeOH).

*(4‴*Z*)-Isomer:* ***Shimofuridin D***
[157379-42-5]
$C_{34}H_{44}N_4O_{12}$ 700.741
From *Aplidium multiplicatum*. Amorph. solid. Sol. MeOH. $[\alpha]_D^{20}$ -91 (c, 0.1 in MeOH). λ_{max} 263 (ϵ 30000) (MeOH). λ_{max} 262 (ϵ 42000); 358 (ϵ 240) (MeOH) (Berdy).

*(2‴*Z*)-Isomer:* ***Shimofuridin E***
[157379-43-6]
$C_{34}H_{44}N_4O_{12}$ 700.741
From *Aplidium multiplicatum*. Amorph. solid. Sol. MeOH. $[\alpha]_D^{20}$ -109 (c, 0.1 in MeOH). λ_{max} 262 (ϵ 42000) (MeOH). λ_{max} 262 (ϵ 42000); 353 (ϵ 630) (MeOH) (Berdy).

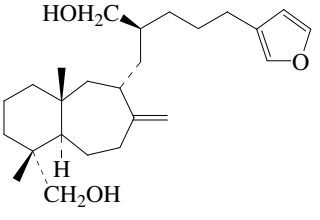
*9″-*O*-Deacyl, 9″-(2,4,7-decatrienoyl)(2*E*,4*E*,7*Z*-):* ***Shimofuridin F***
[157291-78-6]
$C_{36}H_{46}N_4O_{12}$ 726.779
From *Aplidium multiplicatum*. Amorph. solid. Sol. MeOH. $[\alpha]_D^{20}$ -59 (c, 0.07 in MeoH). λ_{max} 263 (ϵ 18000) (MeOH).

*9″-*O*-Deacyl, 9″-(2,4-decadienoyl)(*E,E*-):* ***Shimofuridin G***
[157291-79-7]
$C_{36}H_{48}N_4O_{12}$ 728.795
From *Aplidium multiplicatum*. Amorph. solid. Sol. MeOH. $[\alpha]_D^{20}$ -74 (c, 0.05 in MeOH). λ_{max} 262 (ϵ 16000) (MeOH). λ_{max} 262 (ϵ 16000); 327 (ϵ 780) (MeOH) (Berdy).

Kobayashi, J. *et al., J.O.C.*, 1994, **59**, 255-257 (*isol, uv, ir, pmr, cmr*)
Doi, Y. *et al., Tetrahedron*, 1994, **50**, 8651-8656 (*isol, uv, ir, pmr, cmr, ms*)
Ning, J. *et al., Carbohydr. Res.*, 2003, **338**, 55-60 (*synth, analogues*)

Shinsonefuran S-167

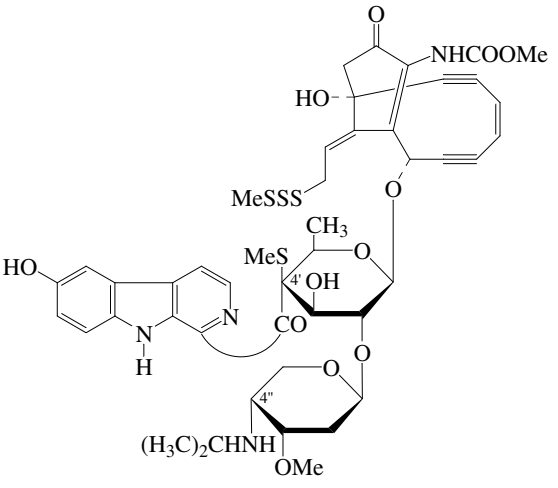
[681127-47-9]



$C_{25}H_{40}O_3$ 388.589
Constit. of *Stoeba extensa*. Oil. $[\alpha]_D^{21}$ +39 (c, 0.2 in MeOH). λ_{max} 211 (log ϵ 3.77) (MeOH).

Phuwapraisirisan, P. *et al., Tet. Lett.*, 2004, **45**, 2125-2128 (*isol, pmr, cmr*)

Shishijimicin A S-168



$C_{46}H_{52}N_4O_{12}S_4$ 981.2
Isol. from the ascidian *Didemnum proliferum*. Cytotoxic.

*4″-*N*-Deisopropyl, 4″-*N*-Et:* ***Shishijimicin C***
$C_{45}H_{50}N_4O_{12}S_4$ 967.174
Isol. from *Didemnum proliferum*. Cytotoxic.

4′-De(methylthio): ***Shishijimicin B***
$C_{45}H_{50}N_4O_{12}S_3$ 935.108
Isol. from *Didemnum proliferum*. Cytotoxic.

Oku, N. *et al., J.A.C.S.*, 2003, **125**, 2044-2045 (*isol*)

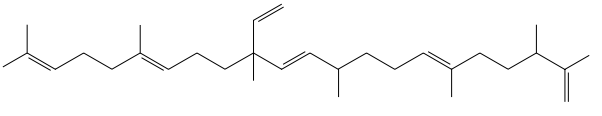
ShK toxin S-169

Peptide containing 35 amino acid residues and 3 intramol. disulfide bonds. Isol. from the sea anemone *Stichodactyla helianthus*. Toxin.

Pennington, M.W. *et al., Int. J. Pept. Protein Res.*, 1995, **46**, 354-358 (*synth*)
Casteneda, O. *et al., Toxicon*, 1995, **33**, 603-613 (*isol*)
Tudor, J.E. *et al., Eur. J. Biochem.*, 1998, **251**, 133-141 (*pmr, cmr, soln struct*)

Showacene S-170

[99461-71-9]



$C_{31}H_{52}$ 424.752
Constit. of *Botryococcus braunii* var. *shawa*.

Wolf, F.R. *et al., J. Phycol.*, 1985, **21**, 388 (*isol*)
Wolf, F.R. *et al., Phytochemistry*, 1985, **24**, 733 (*isol*)
Metzger, P. *et al., Phytochemistry*, 1985, **24**, 2995 (*isol, cmr*)
Huang, Z. *et al., Phytochemistry*, 1989, **28**, 3043 (*isol, ms, pmr, cmr*)

ShPI I S-171

Peptide containing 55 amino acid residues with 3 intramol. disulfide bonds. Isol. from the sea anemone *Stichodactyla helianthus*. Proteinase inhibitor.

Antuch, W. *et al., Eur. J. Biochem.*, 1993, **212**, 675-684 (*isol, pmr, struct*)

Sialic acids S-172

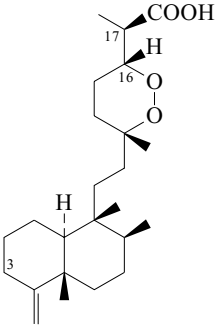
Nonulosaminic acid. Neuraminic acids
A family of acylated amino nonulosonic acids of which Neuraminic acid is the parent. Widely distributed throughout all organisms incl. bacteria and viruses, inn mucopolysaccharides, mucoproteins and lipolysaccharides (mucolipids), mostly in association with 2-Amino-2-deoxyglucose and 2-Amino-2-deoxygalactose. Isol. from bivalves *Crassostrea gigas* and

Modiolus modiolus. Involved in receptor recognition, cell adhesion, aggregation, antigenicity masking, metastatic potential, nerve-signal transmission, viral replication and some genetic disorders.

Zilliken, F. *et al., Adv. Carbohydr. Chem.*, 1958, **13**, 237-263 (*rev*)
Gottschalk, A. *et al., The Chemistry and Biology of Sialic Acids and Related Substances*, Cambridge Univ. Press., 1960, (*book*)
Blix, G. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 246-250 (*isol*)
Sharon, N. *et al., Complex Carbohydrates*, Addison-Welsey Publishing Co., 1975, 142
Codington, J.F. *et al., Methods Carbohydr. Chem.*, 1976, **7**, 226-232 (*isol, detn*)
Downs, F. *et al., Methods Carbohydr. Chem.*, 1976, **7**, 233-240 (*detn*)
Schauer, R. *et al., Adv. Carbohydr. Chem. Biochem.*, 1982, **40**, 131-234 (***rev***)
Sialic Acids: Chem. Metab. and Function, Ed. Schauer, R., Springer-Verlag, 1982, (*book*)
Tunkijjanukij, S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **119**, 705-713 (*isol, molluscs*)

Sigmosceptrellin A S-173

[73436-44-9]



$C_{24}H_{40}O_4$ 392.578

Norsesterterpene. Found in *Sigmosceptrella laevis*. Ichthyotoxin. Poorly sol. hexane.

Me ester: [73436-35-8]
$C_{25}H_{42}O_4$ 406.604
From *Sigmosceptrella laevis*. Oil. $[\alpha]_D$ +54.

16-Epimer: ***Sigmosceptrellin B***. *Prianicin B*
[81738-66-1]
$C_{24}H_{40}O_4$ 392.578
Found in *Sigmosceptrella laevis* and *Prianos* sp. Ichthyotoxin. Active against gram-positive bacteria, fungi and yeasts. Yellow oil.

17-Epimer: ***Sigmosceptrellin C***
[83829-04-3]
$C_{24}H_{40}O_4$ 392.578
From *Sigmosceptrella laevis*. Ichthyotoxin.

Δ^3-Isomer: [110025-81-5]
$C_{24}H_{40}O_4$ 392.578
Constit. of *Mycale ancorina*.

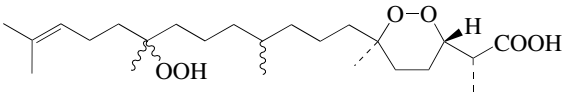
ent-form
ent-*Sigmosceptrellin A*
[120443-84-7]
[110115-10-1 (Me ester)]
Isol. from a sponge Z4967.
Oil (as Me ester). $[\alpha]_D^{25}$ -57.1 (c, 0.7 in $CHCl_3$) (Me ester).

[102917-92-0]

Sokoloff, S. *et al., Experientia*, 1982, **38**, 337-338 (*Prianicin B*)
Piccinni-Leopardi, C. *et al., J.C.S. Perkin 2*, 1982, 1523-1526 (*cryst struct*)
Albericci, M. *et al., Tetrahedron*, 1982, **38**, 1881-1890 (*Sigmosceptrellins A-C*)
Capon, R.J. *et al., Tetrahedron*, 1985, **41**, 3391-3404 (*ent-Sigmosceptrellin A*)
Capon, R.J. *et al., J. Nat. Prod.*, 1987, **50**, 225-229 (*Δ^3-isomer*)
Capon, R.J. *et al., Tetrahedron*, 1988, **44**, 1637-1650 (*abs config*)

Sigmosceptrellin D S-174

[220029-41-4]

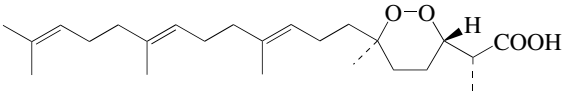


$C_{24}H_{44}O_6$ 428.608
Constit. of a *Sigmosceptrella* sponge.

Me ester: [220029-84-5]
Oil. $[\alpha]_D$ -57.8 (c, 5.9 in $CHCl_3$).

Ovenden, S.P.B. *et al., J. Nat. Prod.*, 1999, **62**, 214-218 (*isol, pmr, cmr*)

Sigmosceptrellin E S-175

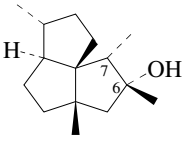


$C_{24}H_{40}O_4$ 392.578
Constit. of a *Sigmosceptrella* sponge.

Me ester: [220029-47-0]
Oil. $[\alpha]_D$ -16.7 (c, 0.23 in $CHCl_3$).

Ovenden, S.P.B. *et al., J. Nat. Prod.*, 1999, **62**, 214-218 (*isol, pmr, cmr*)

6-Silphiperfolanol S-176



(6α,7α)-*form*

$C_{15}H_{26}O$ 222.37

(6α,7α)-*form* [203714-21-0]
Constit. of *Echinops giganteus* var. *lelyi*.
Oil. $[\alpha]_D$ -33.3 (c, 0.9 in $CHCl_3$).

(6α,7β)-*form* [203714-22-1]
Constit. of *Echinops giganteus* var. *lelyi*.
Oil.

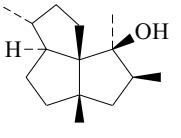
(6β,7α)-*form* [203714-23-2]
Constit. of *Echinops giganteus* var. *lelyi*.
Oil.

(6β,7β)-*form* [203714-24-3]
Struct. revised in 1998. Constit. of *Laurencia majuscula*. Oil. $[\alpha]_D$ -19.4 (c, 0.3 in $CHCl_3$).

Wright, A.D. *et al., J. Nat. Prod.*, 1990, **53**, 845 (*isol, pmr, cmr*)
Weyerstahl, P. *et al., Eur. J. Org. Chem.*, 1998, 1205-1212 (*isol, pmr, cmr, struct*)

7-Silphiperfolanol S-177

[124649-23-6]



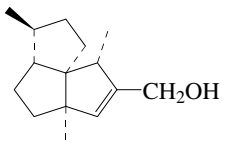
$C_{15}H_{26}O$ 222.37

Numbering systems vary. Metab. of *Laurencia majuscula* and isol. from *Echinops giganteus* var. *lelyi*. Oil. $[\alpha]_D$ -57 (c, 0.01 in $CHCl_3$) (-7.8).

[124596-90-3]

Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1591 (*isol, pmr, cmr*)
Weyerstahl, P. *et al., Eur. J. Org. Chem.*, 1998, 1205-1212 (*isol, pmr, cmr*)

5-Silphiperfolen-13-ol S-178



$C_{15}H_{24}O$ 220.354

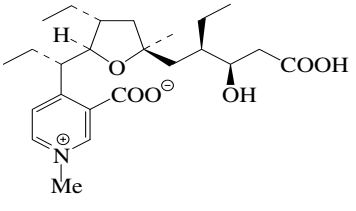
(*ent*-1β)-*form*
Subergorgiol
[444103-23-5]
Constit. of *Subergorgia suberosa*.
Oil. $[\alpha]_D^{31}$ 0 (c, 0.12 in $CHCl_3$).

Ac: [619282-92-7]
$C_{17}H_{26}O_2$ 262.391
Constit. of *Leontopodium alpinum*. Oil. $[\alpha]_D^{20}$ -80 (c, 0.002 in CH_2Cl_2).

13-Carboxylic acid: ***5-Silphiperfolen-13-oic acid***
[173450-48-1 (7*S-form*), 173653-81-1 (7*R-form*)]
$C_{15}H_{22}O_2$ 234.338
Constit. of *Artemisia chamaemelifolia*. Isol. as a mixt. of epimers at C-7. Rel. config. only known.

Marco, J.A. *et al., Phytochemistry*, 1996, **41**, 837-844 (*carboxylic acid*)
Wang, G.-H. *et al., J. Nat. Prod.*, 2002, **65**, 1033-1036 (*isol, pmr, cmr*)
Dobner, M.J. *et al., Helv. Chim. Acta*, 2003, **86**, 733-738 (*Ac*)

Simplakidine A S-179



Absolute Configuration

$C_{24}H_{37}NO_6$ 435.559
Alkaloid from the sponge *Plakortis simplex*. Weakly cytotoxic. Amorph. solid. $[\alpha]_D^{25}$ -21.7 (c, 1.2 in MeOH). λ_{max} 272 (log ϵ 3.55) (MeOH).

Campagnuolo, C. *et al., Org. Lett.*, 2003, **5**, 673-676 (*isol, pmr, cmr, ms*)

Simplexides S-180

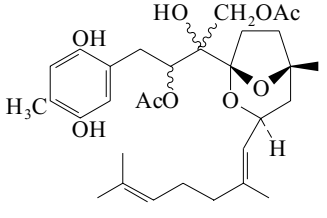
α-D-Glc-(1→4)-β-D-Gal-OCHR$_2$

Glycolipid complex. Consists of a mixt. of long-chain alkyl glycosides derived from symmetrical alcohols such as 18-pentatricontanol (R = *n*-$C_{17}H_{35}$). Isol. from the sponge *Plakortis simplex*. Immunosuppressant. $[\alpha]_D^{25}$ -13 (c, 0.4 in MeOH/$CHCl_3$).

Costantino, V. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 271-276

Sindurol S-181

[172998-30-0]



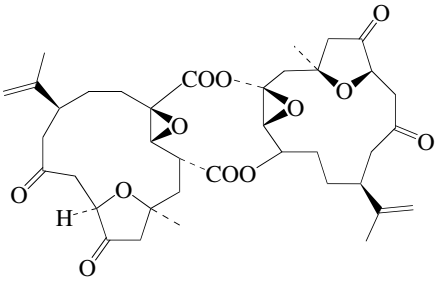
$C_{31}H_{44}O_9$ 560.683

Constit. of *Sinularia dura*. Glass. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D$ -45 (c, 0.01 in $CHCl_3$). λ_{max} 280 (ϵ 3580) (MeOH) (Berdy).

Koren-Goldshlager, G. *et al., J. Nat. Prod.*, 1996, **59**, 262 (*isol, pmr, cmr*)

Singardin S-182

[178062-99-2]

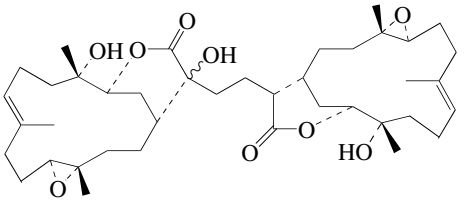


$C_{38}H_{48}O_{12}$ 696.79
Constit. of *Sinularia gardineri*. Needles.
Mp 185-186°. Related to 5,8-Epoxy-18-nor-3,6-dioxo-11,15-cembradien-20,10-olide, E-469.

El Sayed, K.A. *et al., J. Nat. Prod.*, 1996, **59**, 687-689 (*isol, pmr, cmr*)

Sinuflexlin S-183

[214767-82-5]

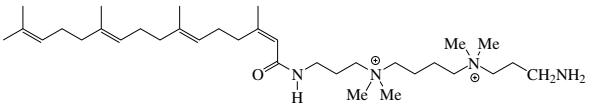


$C_{40}H_{62}O_9$ 686.924
Constit. of *Sinularia flexibilis*. Cryst.
Mp 248-249°. $[\alpha]_D$ -25 (c, 0.11 in $CHCl_3$).

Duh, C.-Y. *et al., Tet. Lett.*, 1998, **39**, 7121-7122 (*isol, pmr, cmr*)

Sinulamide S-184

[122027-56-9]
[122027-57-0, 221278-53-1]

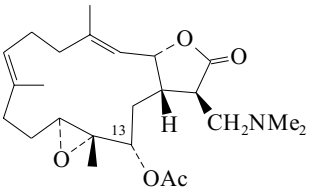


$C_{34}H_{67}N_4O^{2\oplus}$ 547.93
Alkaloid from a soft coral *Sinularia* sp. ATP-ase inhibitor. Cytotoxic agent. Powder (as dichloride, hydrochloride).

Japan. Pat., 1988, 88 307 849; *CA*, **111**, 102689j
Sata, N.U. *et al., Tet. Lett.*, 1999, **40**, 719-722 (*isol, synth, pmr, cmr*)

Sinulamine II S-185

[139579-28-5]



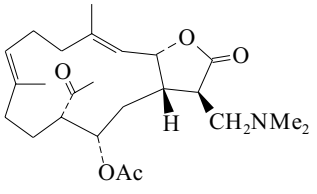
$C_{24}H_{37}NO_5$ 419.56
Constit. of a *Sinularia* coral. Needles.
Mp 147-148°. $[\alpha]_D$ +40 (c, 0.1 in $CHCl_3$).

O^{13}*-De-Ac, 13-ketone:* ***Sinulamine I***
[139579-27-4]
$C_{22}H_{33}NO_4$ 375.507
Constit. of a *Sinularia* coral. Needles.
Mp 139-140°. $[\alpha]_D$ +34 (c, 0.4 in $CHCl_3$).

Iguchi, K. *et al., Chem. Lett.*, 1992, 127 (*isol, pmr, cmr*)
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1992, 340 (*struct*)

Sinulamine III S-186

[139579-29-6]

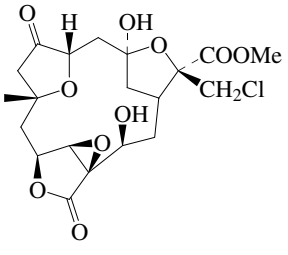


$C_{24}H_{37}NO_5$ 419.56
Constit. of a *Sinularia* coral. Pale yellow viscous oil. $[\alpha]_D$ -57.7 (c, 1.02 in $CHCl_3$).

Iguchi, K. *et al., Chem. Lett.*, 1992, 127 (*isol, pmr, cmr*)
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1992, 340 (*struct*)

Sinularectin S-187

[886984-61-8]

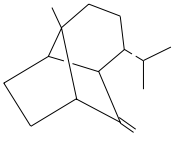


$C_{20}H_{25}ClO_{10}$ 460.864
Constit. of *Sinularia erecta*. Oil.

Rudi, A. *et al., Tet. Lett.*, 2006, **47**, 2937-2939

7(15)-Sinularene S-188

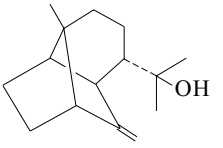
Sinularene
[64845-75-6]



$C_{15}H_{24}$ 204.355
Constit. of *Sinularia mayi*. Oil. $[\alpha]_D^{20}$ -142 (c, 0.55 in CCl_4).

Beechan, C.M. *et al., Tet. Lett.*, 1977, 2395 (*isol*)
Collins, P.A. *et al., Aust. J. Chem.*, 1979, **32**, 1819 (*synth*)
Oppolzer, W. *et al., Tet. Lett.*, 1982, **23**, 4673 (*synth*)
Piers, E. *et al., Can. J. Chem.*, 1985, **58**, 996 (*synth*)
Antczak, K. *et al., Can. J. Chem.*, 1987, **65**, 114 (*synth*)

7(15)-Sinularen-12-ol S-189



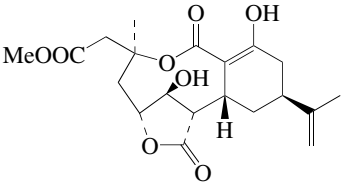
$C_{15}H_{24}O$ 220.354

Ac: ***12-Acetoxysinularene***
$C_{17}H_{26}O_2$ 262.391
Constit. of *Clavularia inflata*. Oil. $[\alpha]_D$ -92.2 (c, 0.346 in $CHCl_3$).

Braekman, J.C. *et al., Tetrahedron*, 1981, **37**, 179
Oppolzer, W. *et al., Tet. Lett.*, 1984, **25**, 825 (*synth*)

Sinulariadiolide S-190

[179669-33-1]

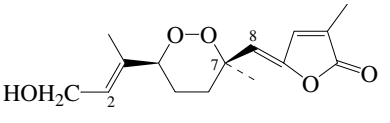


$C_{20}H_{26}O_8$ 394.421
Constit. of a *Sinularia* sp. Powder. $[\alpha]_D$ +91.1 (c, 0.3 in $CHCl_3$).

Iguchi, K. *et al., J.O.C.*, 1996, **61**, 5998-6000 (*isol, pmr, cmr*)

Sinularioperoxide A S-191

[883886-71-3]



$C_{15}H_{20}O_5$ 280.32
Constit. of a *Sinularia* sp. Oil. $[\alpha]_D^{25}$ -2 (c, 1.64 in $CHCl_3$).

2Z-Isomer: ***Sinularioperoxide B***
[883886-72-4]
$C_{15}H_{20}O_5$ 280.32
Constit. of a *Sinularia* sp. Oil. $[\alpha]_D^{25}$ -40 (c, 0.8 in $CHCl_3$).

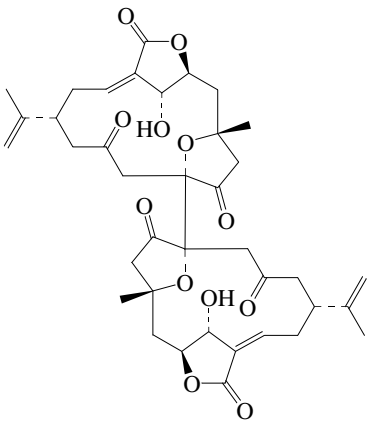
7-Epimer: ***Sinularioperoxide C***
[883886-73-5]
$C_{15}H_{20}O_5$ 280.32
Constit. of a *Sinularia* sp. Oil. $[\alpha]_D^{25}$ -2 (c, 1.68 in $CHCl_3$).

*7-Epimer, 8*E*-isomer:* ***Sinularioperoxide D***
[883886-74-6]
$C_{15}H_{20}O_5$ 280.32
Constit. of a *Sinularia* sp. Oil. $[\alpha]_D^{25}$ -2 (c, 1.68 in $CHCl_3$).

Chao, C.-H. *et al., Tet. Lett.*, 2006, **47**, 2175-2178

Sinulochmodin A S-192

[864685-94-9]

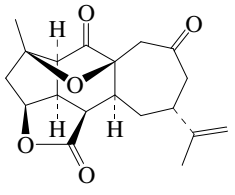


$C_{38}H_{46}O_{12}$ 694.774
Constit. of *Sinularia lochmodes*. Powder. $[\alpha]_D^{25}$ -129 (c, 1.2 in $CHCl_3$).

Tseng, Y.-J. *et al., Org. Lett.*, 2005, **7**, 3813-3816 (*Sinulochmodin A*)

Sinulochmodin C S-193

[864685-96-1]



$C_{19}H_{22}O_5$ 330.38
Constit. of *Sinularia lochmodes*. Powder. $[\alpha]_D^{25}$ -12.5 (c, 0.4 in $CHCl_3$).

Tseng, Y.-J. *et al., Org. Lett.*, 2005, **7**, 3813-3816 (*Sinulochmodin C*)

Sipalosterol B S-194

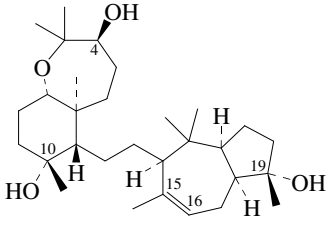
[82196-45-0]

Struct. apparently not determined. Isol. from a Chinese soft coral *Sinularia sipalosa*. A C_{28} compd. Lit. inaccessible.

Long, K. *et al., CA*, 1981, **97**, 21005

Sipholenol A S-195

[78518-73-7]



Absolute Configuration

$C_{30}H_{52}O_4$ 476.738
Constit. of *Siphonochalina siphonella*. Cryst. (Me_2CO/petrol). Mp 169-171°. $[\alpha]_D^{24}$ -60 (c, 7.2 in $CHCl_3$).

19-O-α-L-Rhamnopyranoside: ***Sipholenoside B***
[329050-23-9]
$C_{36}H_{62}O_8$ 622.881
Constit. of *Siphonochalina siphonella*. Powder ($CHCl_3$/Me_2CO). Mp 237°. $[\alpha]_D$ -22 (c, 0.5 in $CHCl_3$).

4-Ketone: ***Sipholenone A***
[78518-74-8]
$C_{30}H_{50}O_4$ 474.723
Cryst. (Me_2CO/petrol). $[\alpha]_D^{24}$ -29 (c, 9 in $CHCl_3$).

15α,16α-Epoxide: ***Sipholenol G***
[329050-19-3]
$C_{30}H_{52}O_5$ 492.738
Constit. of *Siphonochalina siphonella*. Amorph. powder. Mp 173-175°. $[\alpha]_D$ -30 (c, 0.05 in $CHCl_3$).

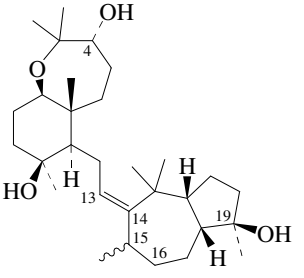
15α,16α-Epoxide, 4-ketone: ***Sipholenone B***
[86748-27-8]
$C_{30}H_{52}O_5$ 492.738
From *Siphonochalina siphonella*. Oil. $[\alpha]_D^{24}$ +5 (c, 4.4 in $CHCl_3$).

10-Epimer: ***Sipholenol B***
[86783-84-8]
$C_{30}H_{52}O_4$ 476.738
From *Siphonochalina siphonella*. Oil. $[\alpha]_D^{24}$ -37 (c, 5.2 in $CHCl_3$).

Shmueli, U. *et al., Tet. Lett.*, 1981, 709-712 (*cryst struct*)
Carmely, S. *et al., J.O.C.*, 1983, **48**, 3517-3525 (*isol*)
Carmely, S. *et al., Magn. Reson. Chem.*, 1986, **24**, 332-336 (*pmr, cmr*)
Inouye, Y. *et al., Chem. Lett.*, 1990, 2073 (*abs config, cryst struct*)
Ohtani, I. *et al., J.O.C.*, 1991, **56**, 1296-1298 (*abs config*)
Kashman, Y. *et al., J. Nat. Prod.*, 2001, **64**, 175-180 (*Sipholenol G, Sipholenoside B*)

Sipholenol C S-196

[86748-29-0]



$C_{30}H_{52}O_4$ 476.738
Constit. of *Siphonochalina siphonella*. Oil. $[\alpha]_D^{24}$ -28 (c, 1.7 in $CHCl_3$).

Δ[14]-Isomer, 16-oxo: ***Sipholenol D***
[86748-30-3]
$C_{30}H_{50}O_5$ 490.722
From *Siphonochalina siphonella*. Oil. $[\alpha]_D^{24}$ -31 (c, 0.2 in $CHCl_3$).

Δ[14]-Isomer, 16α-hydroxy: ***Sipholenol H***
[329197-87-7]
$C_{30}H_{52}O_5$ 492.738
Constit. of *Siphonochalina siphonella*. Oil. $[\alpha]_D$ -42 (c, 0.1 in $CHCl_3$).

Δ[14]-Isomer, 16β-hydroxy: ***Sipholenol E***
[86748-31-4]
$C_{30}H_{52}O_5$ 492.738
Constit. of *Siphonochalina siphonella*.

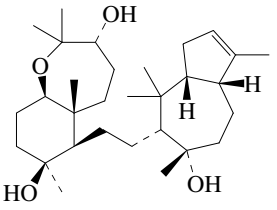
4-Ketone: ***Sipholenone D***
[329050-20-6]
$C_{30}H_{50}O_4$ 474.723
Constit. of *Siphonochalina siphonella*. Oil. $[\alpha]_D$ -35 (c, 0.05 in $CHCl_3$).

4-Ketone, 19-O-α-L-rhamnopyranoside: ***Sipholenoside A***
[329050-22-8]
$C_{36}H_{60}O_8$ 620.865
Constit. of *Siphonochalina siphonella*. Amorph. solid. $[\alpha]_D$ -18 (c, 0.1 in $CHCl_3$).

Carmely, S. *et al., J.O.C.*, 1983, **48**, 3517-3525 (*Sipholenols C-E*)
Kashman, Y. *et al., J. Nat. Prod.*, 2001, **64**, 175-180 (*Sipholenol H, Sipholenone D, Sipholenoside A*)

Sipholenol F S-197

[329050-21-7]

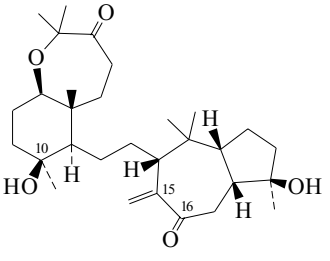


$C_{30}H_{52}O_4$ 476.738
Constit. of *Siphonochalina siphonella*. Oil. $[\alpha]_D$ -24 (c, 0.5 in $CHCl_3$).

Kashman, Y. *et al., J. Nat. Prod.*, 2001, **64**, 175-180 (*isol, pmr, cmr*)

Sipholenone C S-198

[86766-01-0]

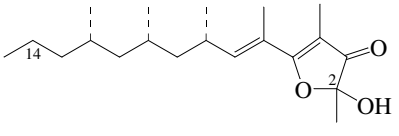


$C_{30}H_{48}O_5$ 488.706
Constit. of *Siphonochalina siphonella*. Oil. $[\alpha]_D^{24}$ +1 (c, 0.9 in $CHCl_3$).

Carmely, S. *et al., J.O.C.*, 1983, **48**, 3517

Siphonarienfuranone S-199

[128008-16-2]



$C_{20}H_{34}O_3$ 322.487
Metab. of *Siphonaria grisea*. Antimicrobial and antifungal. Oil. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D$ +101.5 (c, 0.14 in $CHCl_3$). Occurs as mixt. of epimers at C-2. λ_{max} 240 (ϵ 5201); 305 (ϵ 10717) (EtOH) (Berdy).

2-Deoxy: ***2-Deoxysiphonarienfuranone***
$C_{20}H_{34}O_2$ 306.487
Metab. of *Siphonaria pectinata*. Oil. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{25}$ +40 (c, 0.1 in $CHCl_3$). λ_{max} 235 (ϵ 2344); 300 (ϵ 3252) ($CHCl_3$). λ_{max} 235 (ϵ 2345); 300 (ϵ 3282) ($CHCl_3$) (Berdy).

(Z)-Isomer: ***Isosiphonarienfuranone***
[188296-66-4]
$C_{20}H_{34}O_3$ 322.487
Metab. of *Siphonaria grisea* and *Siphonaria pectinata*. Antimicrobial and antifungal. Occurs as a mixt. of C-2 epimers.

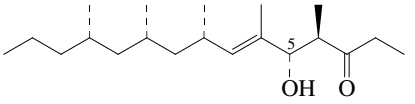
14-Nor: ***14-Norsiphonarienfuranone***
$C_{19}H_{32}O_3$ 308.46
Metab. of *Siphonaria lessoni*. Not mentioned in the CAS abstract. Information on its nat. occurrence comes from a review.

14-Nor, 10-epimer: ***10-Epi-14-norsiphonarienfuranone***
[90220-13-6]
$C_{19}H_{32}O_3$ 308.46
Metab. of *Siphonaria lessoni*. Oil. $[\alpha]_D^{20}$ +90.5 (c, 2.2 in $CHCl_3$).
Obt. as a mixt. of *E*/*Z*-isomers for which the data is given.

Capon, R.J. *et al., J.O.C.*, 1984, **49**, 2506-2508 (*10-Epi-14-norsiphonarienfuranone*)
Norte, M. *et al., Tetrahedron*, 1990, **46**, 1669-1678 (*isol, struct, abs config*)
Rovirosa, J. *et al., Bol. Soc. Chil. Quim.*, 1991, **36**, 233-238 (*14-Norsiphonarienfuranone*)
Paul, M.C. *et al., Tetrahedron*, 1997, **53**, 2303 (*Deoxysiphonarienfuranone*)

Siphonarienolone S-200

5-Hydroxy-4,6,8,10,12-pentamethyl-6-pentadecen-3-one, 9CI
[115883-19-7]



Absolute Configuration

$C_{20}H_{38}O_2$ 310.519
Stereochem. revised in 2002. Metab. of marine mollusc *Siphonaria grisea* and *Siphonaria pectinata*. Antimicrobial and antifungal. Oil. Sol. MeOH, $CHCl_3$, EtOAc; poorly sol. H_2O, hexane. $[\alpha]_D$ +19.6 (c, 0.11 in $CHCl_3$). λ_{max} 335 (ϵ 12800) (EtOH) (Derep). λ_{max} 203 (ϵ 7218) (EtOH) (Berdy).

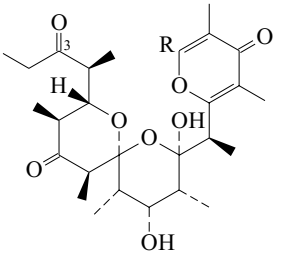
5-Ketone: 4,6,8,10,12-Pentamethyl-6-pentadecene-3,5-dione. ***Siphonarienedione***
[115883-20-0]
$C_{20}H_{36}O_2$ 308.503
Metab. of *Siphonaria grisea*. Antimicrobial, andtifungal. Oil. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D$ +32.5 (c, 0.52 in $CHCl_3$). λ_{max} 335 (ϵ 12800) (EtOH) (Derep). λ_{max} 234 (ϵ 12781); 335 (ϵ 12781) (EtOH) (Berdy).

5-Ketone, 3α-alcohol: 3-Hydroxy-4,6,8,10,12-pentamethyl-6-pentadecen-5-one. ***Isosiphonarienolone***
[188296-63-1]
$C_{20}H_{38}O_2$ 310.519
Metab. of *Siphonaria pectinata*. Oil. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{25}$ +17.6 (c, 0.2 in $CHCl_3$). λ_{max} 242 (ϵ 4615) ($CHCl_3$).

Norte, M. *et al., Tetrahedron*, 1990, **46**, 1669-1678 (*isol, struct*)
Paul, M.C. *et al., Tetrahedron*, 1997, **53**, 2303-2308 (*Isosiphonarienolone*)
Calter, M.A. *et al., J.A.C.S.*, 2002, **124**, 13127-13129 (*synth, abs config*)
Magnin-Lachaux, M. *et al., Org. Lett.*, 2004, **6**, 1425-1427 (*synth*)

Siphonarin A S-201

[92125-67-2]



R = CH_3

$C_{28}H_{42}O_8$ 506.635
Constit. of marine pulminates *Siphonaria zelandica* and *Siphonaria denticulata*. Cryst.
Mp 164-166°. $[\alpha]_D$ +21.7 (c, 0.014 in $CHCl_3$).

*3*R*-Alcohol:* ***Dihydrosiphonarin A***
[92125-69-4]
$C_{28}H_{44}O_8$ 508.651
Isol. from *Siphonaria laciniosa* and *Siphonaria normalis*.
$[\alpha]_D$ -24.9 (c, 1 in CH_2Cl_2).

Hochlowski, J. *et al., J.A.C.S.*, 1984, **106**, 6748-6750 (*isol, uv, cmr, pmr, ms, cryst struct*)
Garson, M.J. *et al., Tet. Lett.*, 1994, **35**, 6921-6924 (*biosynth, struct*)
Paterson, I. *et al., Tet. Lett.*, 1994, **35**, 6925-6928; 6929-6932 (*abs config*)

Siphonarin B S-202

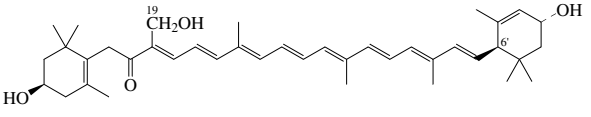
[92125-68-3]
As Siphonarin A, S-201 with
R = CH_2CH_3
$C_{29}H_{44}O_8$ 520.662
Constit. of marine pulmonates *Siphonaria zelandica*, *Siphonaria atra* and *Siphonaria denticulata*. Oil. $[\alpha]_D$ +13.2 (c, 0.0136 in $CHCl_3$).

*3*R-*Alcohol:* ***Dihydrosiphonarin B***
[92125-70-7]
$C_{29}H_{46}O_8$ 522.678
Isol. from *Siphonaria laciniosa* and *Siphonaria normalis*.
$[\alpha]_D$ -32.6 (c, 0.33 in CH_2Cl_2).

Hochlowski, J. *et al., J.A.C.S.*, 1984, **106**, 6748-6750 (*isol, pmr, cmr*)
Garson, M.J. *et al., Tet. Lett.*, 1994, **35**, 6921-6924 (*biosynth, struct*)
Paterson, I. *et al., Tet. Lett.*, 1994, **35**, 6925-6928; 6929-6932 (*abs config*)
Paterson, I. *et al., Org. Lett.*, 2002, **4**, 391-394 (*synth*)

Siphonaxanthin S-203

7,8-Dihydro-3,3′,19-trihydroxy-β,ϵ-caroten-8-one. Xanthophyll K_1S
[28526-44-5]



$C_{40}H_{56}O_4$ 600.88
Pigment from *Caulerpa prolifera* and other algae belonging to the Prasinophyceae.

19-O-*(2*E-*Decenoyl):* [189016-94-2]
$C_{50}H_{72}O_5$ 753.116
Constit. of *Pyramimonas amylifera*. λ_{max} 448 (Me_2CO).

19-O-*(2*E-*Dodecenoyl):* ***Siphonein***. *Xanthophyll K_1*
[39704-43-3]
$C_{52}H_{76}O_5$ 781.169
Isol. from *Eutreptiella gymnastica*.

19-O-*(2*E-*Tetradecenoyl):* [448298-70-2]
$C_{54}H_{80}O_5$ 809.223
Isol. from *Pterosperma cristatum*.

6′-Hydroxy: 7,8-Dihydro-3,3′,6′,19-tetrahydroxy-β,ϵ-caroten-8-one. ***6′-Hydroxysiphonaxanthin***
$C_{40}H_{56}O_5$ 616.879
Isol. from *Pyramimonas amylifera*. λ_{max} 442 (Me_2CO). λ_{max} 461 ($CHCl_3$).

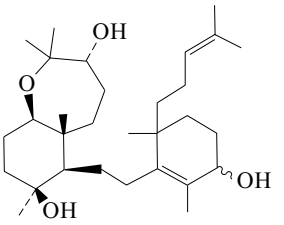
6′-Hydroxy, 19-O-*(2*E-*dodecenoyl):* ***6′-Hydroxysiphonein***
[189073-54-9]
$C_{52}H_{76}O_6$ 797.169
Constit. of *Pyramimonas amylifera*. λ_{max} 449 (Me_2CO). λ_{max} 452 (MeOH). λ_{max} 452 (heptane). λ_{max} 463 ($CHCl_3$).

6′-Hydroxy, 19-O-*(2*E-*tetradecenoyl):* [448298-71-3]
$C_{54}H_{80}O_6$ 825.222
Isol. from *Pterosperma cristatum*.

Walton, T.J. *et al., Phytochemistry*, 1970, **9**, 2545 (*Siphonaxanthin*)
Fiksdahl, A. *et al., Phytochemistry*, 1984, **23**, 649 (*Siphonein*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 350; 351 (*bibl*)
Yokohama, Y. *et al., Jpn. J. Phycol.*, 1992, **40**, 25 (*occur*)
Egeland, E.S. *et al., Phytochemistry*, 1997, **44**, 1087-1097 (*isol, pmr*)
Yoshii, Y. *et al., J. Phycol.*, 2002, **38**, 297-303 (*Pterosperma cristatum esters*)

Siphonellinol S-204

[87978-31-2]

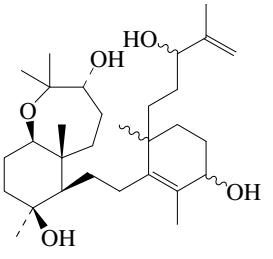


$C_{30}H_{52}O_4$ 476.738
Constit. of the sponge *Siphonochalina siphonella*. Amorph. Mp 109-111°. $[\alpha]_D$ -52 (c, 3.8 in $CHCl_3$).

Carmely, S. *et al., Tet. Lett.*, 1983, **24**, 3673

Siphonellinol B S-205

[329050-24-0]

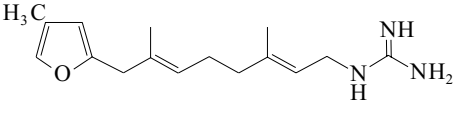


$C_{30}H_{52}O_5$ 492.738
Constit. of *Siphonochalina siphonella*. Oil.

Kashman, Y. *et al., J. Nat. Prod.*, 2001, **64**, 175-180 (*isol, pmr, cmr*)

Siphonodictidine S-206

[88316-91-0]

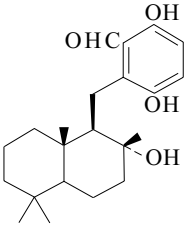


$C_{16}H_{25}N_3O$ 275.393
Constit. of the sponge *Siphonodictyon* sp. Sol. MeOH, EtOAc.

Sullivan, B. *et al., Science (Washington, D.C.)*, 1983, **221**, 1175-1176 (*isol, pmr, cmr, ms*)
Jefford, C.W. *et al., Synlett*, 1990, 745-746 (*synth*)
Jefford, C.W. *et al., Gazz. Chim. Ital.*, 1993, **123**, 317-320 (*synth*)
Jefford, C.W. *et al., J. Nat. Prod.*, 2004, **67**, 1383-1386 (*synth*)

Siphonodictyal A S-207

[78853-02-8]



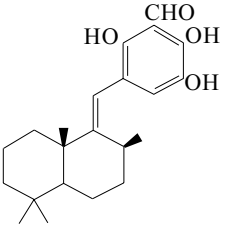
$C_{22}H_{32}O_4$ 360.492
Constit. of *Siphonodictyon coralliphagum*. Cryst. (MeOH). Sol. MeOH.

Mp 192-193°. $[\alpha]_D$ +3.2 (c, 0.5 in MeOH). λ_{max} 280 (ϵ 12000); 390 (ϵ 5000) (MeOH) (Derep).

Sullivan, B. *et al., Tetrahedron*, 1981, **37**, 979-982 (*isol*)

Siphonodictyal B S-208

[78835-08-2]

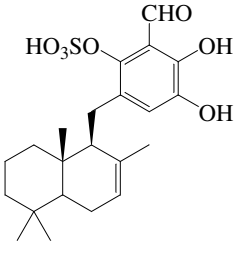


$C_{22}H_{30}O_4$ 358.477
Constit. of *Siphonodictyon coralliphagum*. Cryst. (MeOH aq.). Poorly sol. MeOH, hexane.
Mp 145-147°. λ_{max} 304 (ϵ 7300); 403 (ϵ 1800) (MeOH/NaOH) (Derep). λ_{max} 280 (ϵ 6400); 380 (ϵ 1540) (MeOH) (Derep).

Sullivan, B. *et al., Tetrahedron*, 1981, **37**, 979-982 (*isol*)
Sullivan, B. *et al., J.O.C.*, 1986, **51**, 4568-4573 (*struct*)
Bernet, A. *et al., Helv. Chim. Acta*, 2006, **89**, 784-796 (*synth*)

Siphonodictyal C S-209

[105064-29-7]

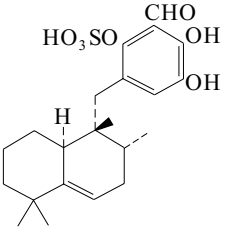


$C_{22}H_{30}O_7S$ 438.541
Struct. revised in 2003. Constit. of *Siphonodictyon coralliphagum* and an *Aka* sp. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -23.6 (c, 0.47 in MeOH). λ_{max} 209 (ϵ 11800); 228 (sh) (ϵ 7900); 276 (ϵ 5800); 368 (ϵ 1600) (MeOH) (Derep). λ_{max} 212 (ϵ 16300); 244 (ϵ 7840); 291 (ϵ 4470); 406 (ϵ 1800) (MeOH/NaOH) (Berdy).

Sullivan, B. *et al., J.O.C.*, 1986, **51**, 4568-4573
Mukku, V.J.R.V. *et al., J. Nat. Prod.*, 2003, **66**, 686-689 (*isol, pmr, cmr, struct*)

Siphonodictyal D S-210

[105064-30-0]



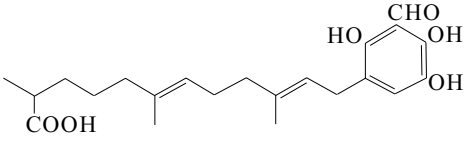
$C_{22}H_{30}O_7S$ 438.541
Constit. of *Siphonodictyon coralliphagum*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Na salt:
Cryst. Mp 131-132°. $[\alpha]_D$ -56.54 (c, 1.12 in MeOH). λ_{max} 212 (ϵ 18000); 244 (ϵ 13000); 288 (ϵ 6600); 401 (ϵ 3000) (MeOH/NaOH) (Derep). λ_{max} 214 (ϵ 14110); 228 (sh) (ϵ 12360); 276 (ϵ 9350); 367 (ϵ 2700) (MeOH) (Derep).

Sullivan, B.W. *et al., J.O.C.*, 1986, **25**, 4568-4573 (*isol*)

Siphonodictyal E S-211

[105064-31-1]

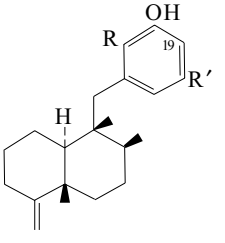


$C_{22}H_{30}O_6$ 390.475
Constit. of *Siphonodictyon coralliphagum*. Oil. λ_{max} (MeOH/NaOH) (Derep). λ_{max} 276 (ϵ 5500); 366 (ϵ 1600) (MeOH) (Derep).

Sullivan, B.W. *et al., J.O.C.*, 1986, **51**, 4568

Siphonodictyoic acid S-212

[105064-34-4]



R = OH, R′ = COOH

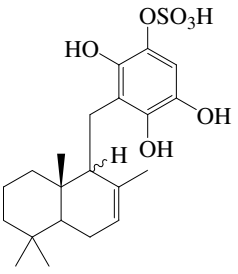
$C_{22}H_{30}O_4$ 358.477
Constit. of *Siphonodictyon coralliphagum*. Oil. $[\alpha]_D$ -5.69 (c, 0.25 in MeOH). λ_{max} 216; 244 (sh); 295 (MeOH/NaOH) (Derep). λ_{max} 216 (ϵ 8400); 245 (ϵ 3340); 294 (ϵ 1650) (MeOH) (Derep).

Me ester: ***Smenospondiol***. *Dictyoceratin A*
[104900-68-7]
$C_{23}H_{32}O_4$ 372.503
Constit. of *Smenospongia* sp. and *Hippospongia* sp. Antimicrobial and cytotoxic. Needles.
Mp 180-182°. $[\alpha]_D$ +12.8 (c, 0.9 in $CHCl_3$). λ_{max} 218 (ϵ 24900); 268 (ϵ 10000); 300 (ϵ 4350) (EtOH) (Derep). λ_{max} 226 (ϵ 10000) (MeOH) (Derep). λ_{max} 219 (ϵ 27300); 269 (ϵ 15600) (EtOH) (Derep).

19-Hydroxy, Me ester: ***Dictyoceratin B***
[104900-67-6]
$C_{23}H_{32}O_5$ 388.503
Constit. *Hippospongia* sp. Antimicrobial. Amorph. solid.
Mp 154.5-155.5°. $[\alpha]_D^{25}$ -1.22 (c, 1.12 in $CHCl_3$). λ_{max} 221 (ϵ 33800); 275 (ϵ 12600) (EtOH) (Derep).

Sullivan, B.W. *et al., J.O.C.*, 1986, **51**, 4568 (*Siphonodictyoic acid*)
Nakamuta, H. *et al., Tetrahedron*, 1986, **42**, 4197 (*deriv*)
Kondracki, M.L. *et al., Tetrahedron*, 1989, **45**, 1995 (*Smenospondiol*)
Shen, Y.C. *et al., J. Nat. Prod.*, 1997, **60**, 93 (*cmr*)

Siphonodictyol I S-213



$C_{21}H_{30}O_7S$ 426.53

Tentative struct. Isol. from the sponge *Aka* sp.

Mukku, V.J.R.V. *et al., J. Nat. Prod.*, 2003, **66**, 686-689 (*isol, pmr, cmr*)

Siphonodictyol G S-214

[105064-32-2]

As Siphonodictyoic acid, S-212 with

R = OSO_3H, R′ = CH_2OH

$C_{22}H_{32}O_6S$ 424.557

Constit. of *Siphonodictyon coralliphagum*. Sol. MeOH, $CHCl_3$. λ_{max} 212 (ϵ 8340); 276 (ϵ 1390); 282 (ϵ 1440) (MeOH) (Berdy). λ_{max} 218 (ϵ 10275); 244 (ϵ 2950); 284 (ϵ 1550); 299 (ϵ 1700) (MeOH-NaOH) (Berdy).

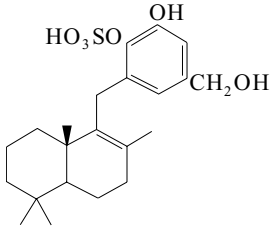
Na salt:

Oil. $[\alpha]_D$ -24.92 (c, 0.65 in MeOH).

Sullivan, B.W. *et al., J.O.C.*, 1986, **51**, 4568

Siphonodictyol H S-215

[105064-33-3]



$C_{22}H_{32}O_6S$ 424.557

Constit. of *Siphonodictyon coralliphagum*. Sol. MeOH, $CHCl_3$. λ_{max} 218 (ϵ 11000); 244 (ϵ 3000); 283 (ϵ 2000); 295 (ϵ 2000) (MeOH/NaOH) (Derep). λ_{max} 213 (ϵ 9100); 220 (sh); 275 (ϵ 1500); 281 (ϵ 1550) (MeOH) (Derep). λ_{max} 213 (ϵ 9100); 274 (ϵ 1500); 280 (ϵ 1550) (MeOH) (Berdy). λ_{max} 218 (ϵ 10900); 244 (ϵ 3100); 282 (ϵ 1650); 292 (ϵ 1575) (MeOH-NaOH) (Berdy).

Na salt:

Oil. λ_{max} 218 (ϵ 11000); 244 (ϵ 3000); 283 (ϵ 2000); 295 (ϵ 2000) (MeOH/NaOH) (Derep). λ_{max} 213 (ϵ 9100); 220 (sh) (ϵ); 275 (ϵ 1500); 281 (ϵ 1550) (MeOH) (Derep).

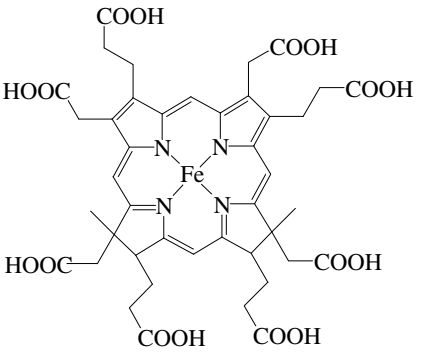
Sullivan, B.W. *et al., J.O.C.*, 1986, **51**, 4568

Siroheme S-216

Octahydrogen [3,8,13,17-tetrakis(carboxymethyl)-2,3,17,18-tetrahydro-3,17-dimethyl-21H,23H-porphine-2,7,12,18-tetrapropanoato(2-)-N^{21},N^{22},N^{23},N^{24}]iron(8-), 10CI. Sirohaem

[52553-42-1]

[42720-57-0]

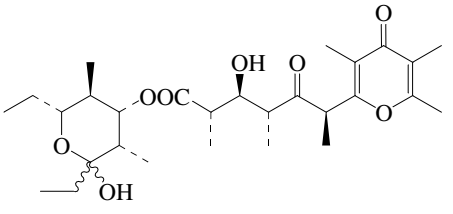


$C_{42}H_{44}FeN_4O_{16}$ 916.674

Isol. from numerous bacterial sulfite reducing strains, incl. *Escherichia* coli, *Desulfovibrio* sp. and *Porphyra* sp. Prosthetic group of a number of microbial and plant sulfite and nitrite reductases.

Vega, J.M. *et al., J. Biol. Chem.*, 1975, **250**, 7980-7989 (*isol*)
Siegel, L.M. *et al., Biochem. J.*, 1977, **167**, 669-674 (*isol*)
Siegel, L.M. *et al., Dev. Biochem.*, 1978, **1**, 201-214 (*rev*)
Siegel, L.M. *et al., Methods Enzymol.*, 1978, **52**, 436-447 (*rev*)
Chang, C.K. *et al., NATO ASI Ser., Ser. C*, 1982, **89**, 313-334 (*rev*)

Siserrone A S-217

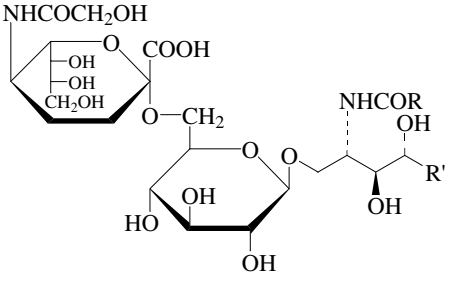


$C_{28}H_{44}O_8$ 508.651

Isol. from the mollusc *Siphonaria serrata*. Unstable pale yellow oil.

Brecknell, D.J. *et al., Tetrahedron*, 2000, **56**, 2497-2502

SJG 1 S-218



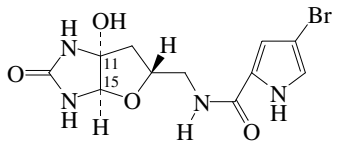
R,R' = various
(R' = mostly C_{13})

Glycosphingolipid complex. Isol. from lipid fraction of the sea cucumber *Stichopus japonicus*. Shows neuritogenic activity. Amorph. powder.
Mp 159-160°.

Kaneko, M. *et al., Eur. J. Org. Chem.*, 1999, 3171-3174 (*isol, pmr, cmr, ms, struct*)

Slagenine A S-219

[246136-98-1]



Absolute Configuration

$C_{11}H_{13}BrN_4O_4$ 345.152
Alkaloid from the sponge *Agelas nakamurai*. Cytotoxic. Amorph. solid. $[\alpha]_D^{27}$ +11 (c, 1.2 in MeOH). λ_{max} 270 (ϵ 10500) (MeOH).

11-Me ether: ***Slagenine B***
[246137-00-8]
$C_{12}H_{15}BrN_4O_4$ 359.179
Alkaloid from *Agelas nakamurai*. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{26}$ +33 (c, 0.2 in MeOH). λ_{max} 269 (ϵ 9000) (MeOH).

11,15-Diepimer, 11-Me ether: ***Slagenine C***
[246137-03-1]
$C_{12}H_{15}BrN_4O_4$ 359.179
Alkaloid from *Agelas nakamurai*. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{25}$ -35 (c, 0.2 in MeOH). λ_{max} 269 (ϵ 9000) (MeOH).

Tsuda, M. *et al., Tet. Lett.*, 1999, **40**, 5709-5712 (*isol, ir, uv, pmr, cmr*)
Gurjar, M.K. *et al., Org. Lett.*, 2002, **4**, 3569-3570 (*synth*)
Jiang, B. *et al., J.O.C.*, 2003, **68**, 2376-2384 (*synth, abs config*)

Mytilus Small cardioactive peptide S-220

Mytilus SCP
[150213-97-1]
H-Ala-Pro-Asn-Phe-Leu-Ala-Tyr-Pro-Arg-Leu-NH_2
$C_{56}H_{85}N_{15}O_{12}$ 1160.381
Constit. of the anterior byssus retractor muscles of *Mytilus edulis* (blue mussel). Muscle relaxant in host.

Fujisawa, Y. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1993, **104**, 469-475; **105**, 471-477 (*isol, struct, pharmacol*)

Aplysia Small cardioactive peptides S-221

SCP
H-Ala-Arg-Pro-Gly-Tyr-Leu-Ala-Phe-Pro-Arg-Met-NH_2
Struct. shown is SCP_A.

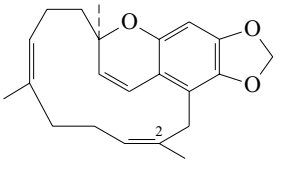
SCP_A
Small cardioactive peptide A
[98035-79-1]
$C_{59}H_{92}N_{18}O_{12}S$ 1277.555
Isol. from *Aplysia californica*. Cardioactive agent.

SCP_B
Small cardioactive peptide B
[84746-43-0]
$C_{52}H_{80}N_{14}O_{11}S_2$ 1141.423
Isol. from *Aplysia californica*, *Aplysia brasiliana* and *Helix aspersa*. Cardioactive agent.

Morris, H.R. *et al., Nature (London)*, 1982, **300**, 643 (*isol, ms, struct*)
Mahon, A.C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1985, **82**, 3925 (*isol*)
Lloyd, P.E. *et al., Trends Neurosci.*, 1986, **9**, 428 (*rev*)
Lloyd, P.E. *et al., Peptides (N.Y.)*, 1987, **8**, 179 (*synth, struct*)
Price, D.A. *et al., J. Exp. Biol.*, 1990, **154**, 421-437 (*isol*)

Smenochromene A S-222

[135823-94-8]

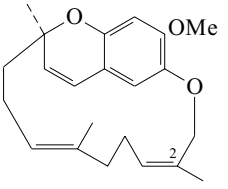


$C_{22}H_{26}O_3$ 338.446
Constit. of a *Smenospongia* sp. Cryst.
Mp 98°. λ_{max} 242 (ϵ 11000); 334 (ϵ 5320) ($CHCl_3$) (Derep). λ_{max} 242 (ϵ 11020); 334 (ϵ 5320) (MeOH) (Berdy).

*2*E-*Isomer:* ***Smenochromene B***
[135823-95-9]
$C_{22}H_{26}O_3$ 338.446
Constit. of a *Smenospongia* sp. Cryst.
Mp 80-82°. $[\alpha]_D$ +6.4 (c, 0.35 in CH_2Cl_2). λ_{max} 242 (ϵ 11000); 334 (ϵ 5320) ($CHCl_3$) (Derep).
Venkateswarlu, Y. *et al., J.O.C.*, 1991, **56**, 6271 (*isol, pmr, cmr, cryst struct*)

Smenochromene C S-223

[135823-96-0]

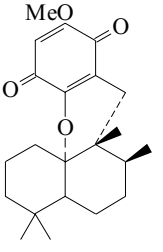


$C_{22}H_{28}O_3$ 340.461
Constit. of a *Smenospongia* sp. Cryst.
Mp 52°. $[\alpha]_D$ -217 (c, 0.3 in CH_2Cl_2). λ_{max} 242 (ϵ 11300); 321 (ϵ 6400) ($CHCl_3$) (Derep).

*2*E-*Isomer:* ***Smenochromene D***
[135823-97-1]
$C_{22}H_{28}O_3$ 340.461
Constit. of a *Smenospongia* sp. Glass. $[\alpha]_D$ -68.5 (c, 0.35 in CH_2Cl_2). λ_{max} 242 (ϵ 11300); 321 (ϵ 6400) ($CHCl_3$) (Derep).
Venkateswarlu, Y. *et al., J.O.C.*, 1991, **56**, 6271 (*isol, pmr, cmr*)

Smenoqualone S-224

[146387-56-6]

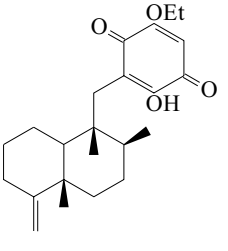


$C_{22}H_{30}O_4$ 358.477
Constit. of a *Smenospongia* sp. Pale yellow oil. $[\alpha]_D$ +70 (c, 0.00125 in $CHCl_3$). λ_{max} 204 (ϵ 5550); 291 (ϵ 5900) (MeOH no shifts reported) (Derep).

Bourguet-Kondracki, M.-L. *et al., Tet. Lett.*, 1992, **33**, 8079 (*isol, pmr, cmr*)

Smenorthoquinone S-225

[121994-49-8]

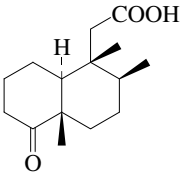


$C_{23}H_{32}O_4$ 372.503
Struct. revised in 1992. Constit. of *Smenospongia* sp. Antimicrobial and cytotoxic. Yellow needles (MeOH). Sol. MeOH,

$CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 209 (ϵ 24000); 283 (ϵ 18400) (EtOH) (Derep).

Kondracki, M.-L. *et al., Tetrahedron*, 1989, **45**, 1995
Urban, S. *et al., J. Nat. Prod.*, 1992, **55**, 1638 (*struct*)

Smenospongic acid S-226

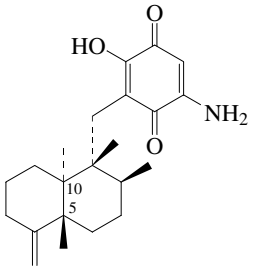


$C_{15}H_{24}O_3$ 252.353
Constit. of *Dactylospongia elegans.*
$[\alpha]_D$ -53.8 (c, 0.3 in $CHCl_3$).

Rodríguez, J. *et al., Tetrahedron*, 1992, **48**, 6667-6680 (*isol, pmr*)

Smenospongine S-227

[113021-53-7]



Absolute Configuration

$C_{21}H_{29}NO_3$ 343.465

Quinoterpenoid antibiotic. Prod. by the sponges *Smenospongia* sp., *Dactylospongia elegans* and *Petrosaspongia metachromia*. Cytotoxic and antimicrobial agent. Red cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 153-155°. λ_{max} 209 (ϵ 16200); 317 (ϵ 15600) (EtOH) (Derep).

N-*(2-Methylpropyl):* ***Smenospongorine***
[121994-53-4]
$C_{25}H_{37}NO_3$ 399.572
Constit. of *Smenospongia* sp. and *Dactylospongia elegans.* Antimicrobial and cytotoxic agent. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 210 (ϵ 14000); 329 (ϵ 20200) (EtOH) (Derep).

N-*Pentyl:* ***Pentylsmenospongine****. Sesquiterpenylamylaminohydroxyquinone*
[127524-59-8]
$C_{26}H_{39}NO_3$ 413.599
Isol. from a *Smenospongia* sp. Red needles (EtOH aq.).
Mp 131-134°. No stereochem. indicated. Presumed here to be a Smenospongine deriv. Named by the authors as Sesquiterpenylamylaminohydroxyquinone.

N-*(3-Methylbutyl):* ***Smenospongiarine***
[121994-52-3]
$C_{26}H_{39}NO_3$ 413.599
Constit. of *Smenospongia* sp. and *Dactylospongia elegans.* Antimicrobial and cytotoxic agent. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 170-172°. λ_{max} 210 (ϵ 14000); 329 (ϵ 20200) (EtOH) (Derep). λ_{max} 210; 325 (MeOH) (Berdy). λ_{max} 204 (ϵ 27230); 324 (ϵ 14700) (EtOH) (Berdy).

N-*(2-Phenylethyl):* ***Smenospongidine***
[121994-51-2]
$C_{29}H_{37}NO_3$ 447.616
Constit. of *Smenospongia* sp. and *Dactylospongia elegans.* Antimicrobial and cytotoxic agent. Cryst. (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 168-170°. λ_{max} 207 (ϵ 25000); 327 (ϵ 17000) (EtOH) (Derep). λ_{max} 210; 330 (MeOH) (Berdy).

N-*(Carboxymethyl):* ***Glycinylilimaquinone***
[159240-55-8]
$C_{23}H_{31}NO_5$ 401.502
Constit. of a *Fasciospongia* sp. Amorph. red powder. λ_{max} 203 (ϵ 23000); 320 (ϵ 11000); 454 (ϵ 1900); 492 (ϵ 2000) (MeOH) (Berdy).

5-Epimer: ***5-Epismenospongine***
[287967-28-6]
$C_{21}H_{29}NO_3$ 343.465
Constit. of *Petrosaspongia metachromia*. Purple powder. $[\alpha]_D^{23}$ +73.1 (c, 0.03 in $CHCl_3$).

5-Epimer, N-*(3-methylbutyl):* ***5-Epismenospongiarine***
$C_{26}H_{39}NO_3$ 413.599
Constit. of *Dactylospongia elegans.* Oil. $[\alpha]_D$ +96.7 (c, 0.12 in $CHCl_3$). CAS no. not found 9-14CI.

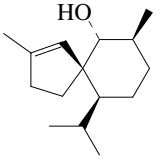
5-Epimer, N-*(2-phenylethyl):* ***5-Epismenospongidine***
[144335-13-7]
$C_{29}H_{37}NO_3$ 447.616
Constit. of *Dactylospongia elegans.* Oil. $[\alpha]_D$ +37.5 (c, 0.16 in $CHCl_3$).

5-Epimer, N-*(2-methylpropyl):* ***5-Epismenospongorine***
[764648-37-5]
$C_{25}H_{37}NO_3$ 399.572
Constit. of *Dactylospongia elegans.*
$[\alpha]_D$ +23 (c, 0.06 in $CHCl_3$). λ_{max} 205 (ϵ 20500); 320 (ϵ 9800) (no solvent reported).

Kondracki, M.-L. *et al., Tetrahedron*, 1989, **45**, 1995-2004 (*isol, ir, uv, pmr, cmr*)
Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1990, **26**, 47-51; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 37-40 (*Pentylsmenospongine*)
Rodriquez, J. *et al., Tetrahedron*, 1992, **48**, 6667-6680 (*isol, pmr, cmr, abs config, bibl*)
Evans, T.P. *et al., Nat. Prod. Lett.*, 1994, **4**, 287-291 (*Glycinylilimaquinone, isol, pmr, cmr, uv, ir, activity*)
Kwak, J.H. *et al., J. Nat. Prod.*, 2000, **63**, 1153-1156 (*5-Epismenospongine*)
Ling, T. *et al., J.A.C.S.*, 2002, **124**, 12261-12267 (*synth*)
Aoki, S. *et al., Chem. Pharm. Bull.*, 2004, **52**, 935-937 (*Dactylospongia elegans constits, bibl*)

Snapirol S-228

2,7-Dimethyl-10-(1-methylethyl)spiro[4.5]dec-1-en-6-ol

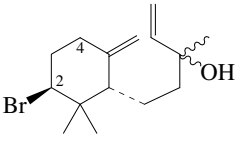


$C_{15}H_{26}O$ 222.37
Isol. from an unidentified Red Sea sponge.

Kashman, Y. *et al., New J. Chem.*, 1990, **14**, 729-740 (*isol, pmr*)

β-Snyderol S-229

[59403-81-5]



$C_{15}H_{25}BrO$ 301.266

Numbering systems vary. Constit. of *Laurencia snyderae.* Oil. $[\alpha]_D$ +14.6 (c, 3.9 in $CHCl_3$).

Ac: ***β-Snyderyl acetate***
$C_{17}H_{27}BrO_2$ 343.303
Metab. of *Laurencia obtusa*. Oil. $[\alpha]_D^{24}$ -9 (c, 1 in $CHCl_3$).

Δ^4-Isomer: ***α-Snyderol***
[59403-83-7]
$C_{15}H_{25}BrO$ 301.266
Constit. of *Laurencia obtusa*. Oil. $[\alpha]_D$ +10.4 (c, 4.65 in $CHCl_3$).

Δ^4-Isomer, Ac: ***α-Snyderyl acetate***
[68690-91-5]
$C_{17}H_{27}BrO_2$ 343.303
Metab. of *Laurencia obtusa*.

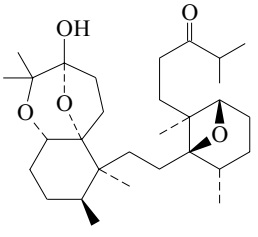
4α-Bromo: ***4-Bromo-β-snyderol***
[636599-34-3]
$C_{15}H_{24}Br_2O$ 380.162
Constit. of *Laurencia obtusa*.
$[\alpha]_D^{25}$ +115.3 (c, 0.2 in $CHCl_3$).

2-Epimer, 4α-bromo: ***4-Bromo-2-epi-β-snyderol***
[636599-33-2]
$C_{15}H_{24}Br_2O$ 380.162
Constit. of *Laurencia obtusa*.
$[\alpha]_D^{25}$ +137.5 (c, 0.4 in $CHCl_3$).

Kato, T. *et al., Chem. Comm.*, 1976, 518 (*synth*)
Howard, B.M. *et al., Tet. Lett.*, 1976, 41 (*isol, struct*)
González, A.G. *et al., Tet. Lett.*, 1976, 137 (*synth*)
Murai, A. *et al., Chem. Lett.*, 1981, 1125 (*synth*)
Imre, S. *et al., Phytochemistry*, 1981, **20**, 833 (*α-Snyderyl acetate*)
Ayyad, S.-E.N. *et al., Phytochemistry*, 1990, **29**, 3193 (*acetate*)
Topcu, G. *et al., J. Nat. Prod.*, 2003, **66**, 1505-1508 (*bromo derivs*)
Carter-Franklin, J.N. *et al., J.A.C.S.*, 2004, **126**, 15060-15066 (*biosynth*)

Sodwanone I S-230

[172923-51-2]

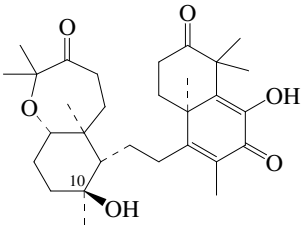


$C_{30}H_{50}O_5$ 490.722
Constit. of *Axinella weltneri* and *Ptilocaulis spiculifer*. Oil. $[\alpha]_D$ +2 (c, 0.2 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 1995, **58**, 1702-1712 (*isol, pmr, cmr*)

Sodwanone A S-231

[150050-12-7]



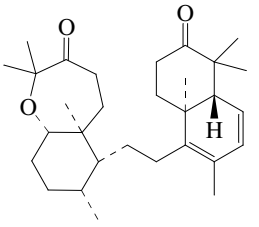
$C_{30}H_{44}O_6$ 500.674
Constit. of *Axinella weltneri* collected in Sodwana Bay, South Africa. Also from *Ptilocaulis spiculifer*. Shows cytotoxic activity. Cryst.
Mp 253°. $[\alpha]_D$ -9 (c, 0.1 in $CHCl_3$).

10-Deoxy: ***Sodwanone B***
[150050-13-8]
$C_{30}H_{44}O_5$ 484.675
Constit. of *Axinella weltneri* and *Ptilocaulis spiculifer*. Glass. $[\alpha]_D$ -6 (c, 0.1 in $CHCl_3$).

Rudi, A. *et al., Tet. Lett.*, 1993, **34**, 3943-3944 (*isol, pmr, cmr, cryst struct*)
Rudi, A. *et al., J. Nat. Prod.*, 1994, **57**, 1416-1423 (*isol, pmr, cmr, cryst struct, activity*)

Sodwanone C S-232

[150079-95-1]

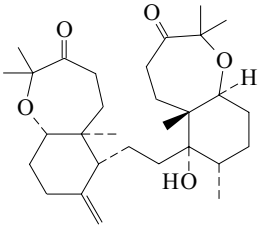


$C_{30}H_{46}O_3$ 454.692
Constit. of *Axinella weltneri* and *Ptilocaulis spiculifer*. Amorph. powder. $[\alpha]_D$ -35 (c, 0.15 in $CHCl_3$).

Rudi, A. *et al., Tet. Lett.*, 1993, **34**, 3943-3944 (*isol, pmr, cmr*)
Rudi, A. *et al., J. Nat. Prod.*, 1994, **57**, 1416-1423 (*isol, pmr, cmr*)

Sodwanone D S-233

[163136-04-7]

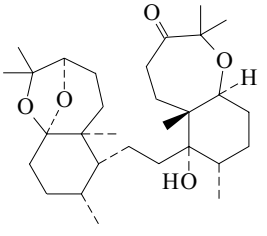


$C_{30}H_{48}O_5$ 488.706
Constit. of *Axinella weltneri* and *Ptilocaulis spiculifer*. Oil. $[\alpha]_D$ +19 (c, 0.3 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 1994, **57**, 1416 (*isol, pmr, cmr*)

Sodwanone E S-234

[163136-05-8]

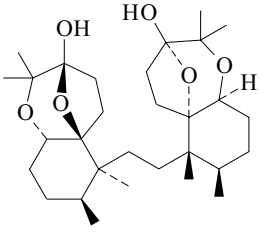


$C_{30}H_{50}O_5$ 490.722
Constit. of *Axinella weltneri*. Oil. $[\alpha]_D$ +3 (c, 0.1 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 1994, **57**, 1416; 1995, **58**, 1702 (*isol, pmr, cmr, cryst struct*)

Sodwanone F S-235

[163136-06-9]



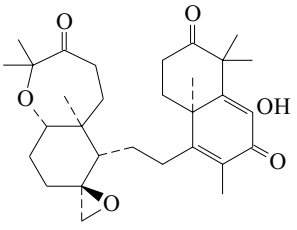
$C_{30}H_{50}O_6$ 506.721

Constit. of *Axinella weltneri* and *Ptilocaulis spiculifer*. Oil. $[\alpha]_D$ -4 (c, 0.1 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 1994, **57**, 1416; 1995, **58**, 1702 (*isol, pmr, cmr, cryst struct*)

Sodwanone G **S-236**

[172854-77-2]

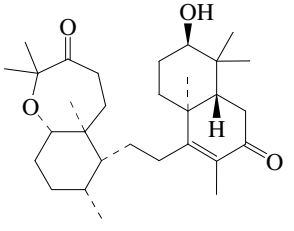


$C_{30}H_{42}O_6$ 498.658
Constit. of *Axinella weltneri*. Cryst. (MeOH).
Mp 245°. $[\alpha]_D$ -14.5 (c, 0.9 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 1995, **58**, 1702 (*isol, pmr, cmr, cryst struct*)

Sodwanone H **S-237**

[172854-78-3]

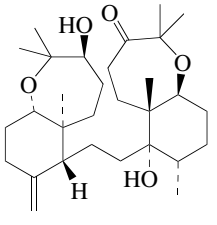


$C_{30}H_{48}O_4$ 472.707
Constit. of *Axinella weltneri*. Shows strong cytotoxic activity.
Amorph. powder. $[\alpha]_D$ -8 (c, 0.1 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 1995, **58**, 1702-1712 (*isol, pmr, activity*)

Sodwanone K **S-238**

[191212-37-0]

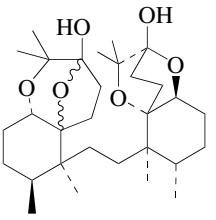


$C_{30}H_{50}O_5$ 490.722
Constit. of *Axinella weltneri*. Oil. $[\alpha]_D$ +6.5 (c, 0.15 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 1997, **60**, 700-703 (*isol, pmr, cmr*)

Sodwanone L **S-239**

[191212-38-1]

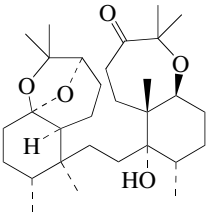


$C_{30}H_{50}O_6$ 506.721
Constit. of *Axinella weltneri*. Oil. $[\alpha]_D$ +19.1 (c, 0.15 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 1997, **60**, 700-703 (*isol, pmr, cmr*)

Sodwanone M **S-240**

[191212-36-9]

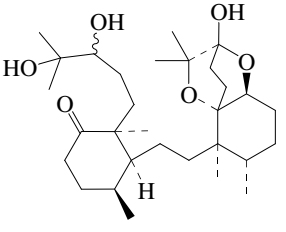


$C_{30}H_{50}O_5$ 490.722
Constit. of *Axinella weltneri*. Oil. $[\alpha]_D$ +18 (c, 0.1 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 1997, **60**, 700-703 (*isol, pmr, cmr*)

Sodwanone N **S-241**

[233607-68-6]

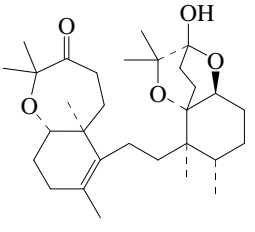


$C_{30}H_{52}O_6$ 508.737
Constit. of *Axinella weltneri*. Oil.

Rudi, A. *et al., Tetrahedron*, 1999, **55**, 5555-5566 (*isol, pmr, cmr*)

Sodwanone O **S-242**

[233607-69-7]

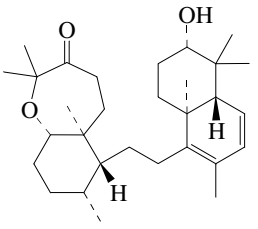


$C_{30}H_{48}O_5$ 488.706
Constit. of *Axinella weltneri*. Oil. $[\alpha]_D$ +18 (c, 0.15 in MeOH).

Rudi, A. *et al., Tetrahedron*, 1999, **55**, 5555-5566 (*isol, pmr, cmr*)

Sodwanone Q S-243

[233607-71-1]

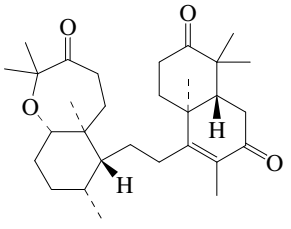


$C_{30}H_{48}O_3$ 456.707
Constit. of *Axinella weltneri*. Oil. $[\alpha]_D$ -22 (c, 0.15 in MeOH).

Rudi, A. *et al., Tetrahedron*, 1999, **55**, 5555-5566 (*isol, pmr, cmr*)

Sodwanone R S-244

[233607-72-2]

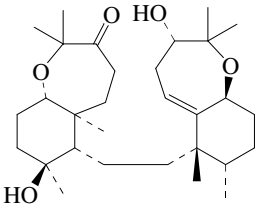


$C_{30}H_{46}O_4$ 470.691
Constit. of *Axinella weltneri*. Oil. $[\alpha]_D$ -18 (c, 0.25 in MeOH).

Rudi, A. *et al., Tetrahedron*, 1999, **55**, 5555-5566 (*isol, pmr, cmr*)

Sodwanone S S-245

[865308-60-7]

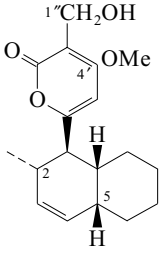


$C_{30}H_{50}O_5$ 490.722
Constit. of *Axinella weltneri*. Powder. $[\alpha]_D^{25}$ +187 (c, 0.033 in CH_2Cl_2).

Bon, C.F.-L. *et al., J. Nat. Prod.*, 2005, **68**, 1284-1287 (*Sodwanone S*)

Solanapyrone B S-246

[88899-60-9]



$C_{18}H_{24}O_4$ 304.385
Isol. from the fungi *Alternaria solanii* and *Ascochyta rabiei*. Phytotoxin. Oil. Sol. MeOH, C_6H_6, EtOAc. $[\alpha]_D$ -59 (c, 0.4 in $CHCl_3$). λ_{max} 302 (ϵ 9010); 303 (ϵ 8500) (EtOH) (Derep).

1″-Aldehyde: ***Solanapyrone A***
[88899-61-0]
$C_{18}H_{22}O_4$ 302.369
Isol. from *Alternaria solanii* and *Ascochyta rabiei*. Phytotoxin. Oil. Sol. MeOH, C_6H_6, EtOAc. $[\alpha]_D$ -67.3 (c, 2.26 in $CHCl_3$). λ_{max} 232 (ϵ 9200); 325 (ϵ 11700); 327 (ϵ 9400) (EtOH) (Derep). λ_{max} 325 (ϵ 11700) (MeOH) (Berdy).

4′-Demethoxy, 4′-amino, 1″-aldehyde: ***Solanapyrone G***
[220924-51-6]
$C_{17}H_{21}NO_3$ 287.358
Isol. from an unidentified fungus from the surface of the marine alga *Halimeda monile*. Antialgal agent. Solid. λ_{max} 236 (log ϵ 3.94); 266 (log ϵ 3.69); 312 (log ϵ 3.83) (MeOH).

4′-Demethoxy, 4′-[(2-hydroxyethyl)amino], 1″-aldehyde: ***Solanapyrone C***
[88899-59-6]
$C_{19}H_{25}NO_4$ 331.411
Constit. of *Alternaria solanii* and *Ascochyta rabiei*. Phytotoxin, algicide. Oil. Sol. MeOH, C_6H_6, EtOAc. $[\alpha]_D$ -5 (c, 0.88 in $CHCl_3$). λ_{max} 238 (ϵ 19900); 282 (ϵ 6900); 320 (ϵ 7300) (EtOH) (Derep).

7α-Hydroxy, 4′-demethoxy, 4′-amino, 1″-aldehyde: ***Solanapyrone F***
[220924-50-5]
$C_{17}H_{21}NO_4$ 303.357
Isol. from an unidentified fungus from the surface of the marine alga *Halimeda monile*. Antialgal agent. Solid. $[\alpha]_D^{25}$ -53.2 (c, 0.3 in MeOH). λ_{max} 228 (log ϵ 4.01); 266 (log ϵ 3.62); 304 (log ϵ 3.71) (MeOH).

7β-Hydroxy, 4′-demethoxy, 4′-amino, 1″-aldehyde: [220924-49-2]
$C_{17}H_{21}NO_4$ 303.357
Isol. from an unidentified fungus from the surface of the marine alga *Halimeda monile*. Antialgal agent. Solid. $[\alpha]_D^{25}$ -16.4 (c, 0.28 in MeOH). λ_{max} 228 (log ϵ 4.01); 267 (log ϵ 3.56); 304 (log ϵ 3.72) (MeOH).

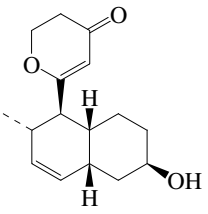
7β-Hydroxy, 4′-demethoxy, 4′-[(2-hydroxyethyl)amino], 1″-aldehyde: ***Solanapyrone I***
$C_{19}H_{25}NO_5$ 347.41
Prod. by the marine-derived *Microsphaeropsis* sp. Stamm 6288. Amorph. solid.
Mp 121°. λ_{max} 237 (log ϵ 4.03); 247 (sh) (log ϵ 3.49); 281 (log ϵ 3.56); 317 (log ϵ 3.6) (MeOH).

2,5-Diepimer: ***Solanapyrone E***
[218773-71-8]
$C_{18}H_{24}O_4$ 304.385
Isol. from *Alternaria solanii* and from an unidentified marine fungus. Phytotoxin. Oil. $[\alpha]_D^{22}$ -76.4 (c, 1 in $CHCl_3$). λ_{max} 302 (ϵ 8180); 308 (ϵ 8180) (EtOH).

2,5-Diepimer, 1″-aldehyde: ***Solanapyrone D***
[106973-16-4]
$C_{18}H_{22}O_4$ 302.369
Constit. of *Alternaria solanii*. Phytotoxic. Oil. $[\alpha]_D^{24}$ -125.2 (c, 0.8 in $CHCl_3$). λ_{max} 232 (ϵ 9200); 327 (ϵ 9400); 328 (ϵ 11800) (EtOH) (Derep).

Ichihara, A. *et al., Tet. Lett.*, 1983, **24**, 5373; 1985, **26**, 2453; 1987, **28**, 1175 (*isol, synth, abs config*)
Oikawa, H. *et al., Chem. Comm.*, 1989, 1282; 1284 (*biosynth, isol*)
Alam, S.S. *et al., Phytochemistry*, 1989, **28**, 2627-2630 (*isol, uv, pmr, cmr, cryst struct*)
Hoehl, B. *et al., Phytopathol. Z.*, 1991, **132**, 193 (*isol*)
Benning, G. *et al., Z. Naturforsch., C*, 1995, **50**, 181 (*cmr, biosynth*)
Ichihara, A. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 12-18 (*rev, biosynth*)
Oikawa, H. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 2016-2022 (*isol, uv, cd, ir, pmr, cmr, conformn, Solanapyrone E*)
Oikawa, H. *et al., J.O.C.*, 1998, **63**, 8748-8756 (*Solanapyrone A, synth*)
Jenkins, K.M. *et al., Phytochemistry*, 1998, **49**, 2299-2304 (*Solanapyrones E-G*)
Hagiwara, H. *et al., J.O.C.*, 2002, **67**, 5969-5976 (*Solanapyrones D,E, synth*)
Lygo, B. *et al., Tet. Lett.*, 2003, **44**, 2529-2532 (*synth*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*Solanapyrone I*)

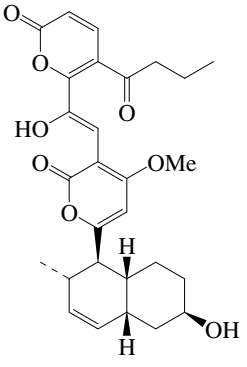
Solanapyrone H S-247



$C_{16}H_{22}O_3$ 262.348
Prod. by the marine-derived *Microsphaeropsis* sp. Stamm 6288.
Oil. $[\alpha]_D^{20}$ +43 (c, 0.1 in MeOH). λ_{max} 266 (log ϵ 4.1) (MeOH).

Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*isol, pmr, cmr, ms*)

Solanapyrone J S-248

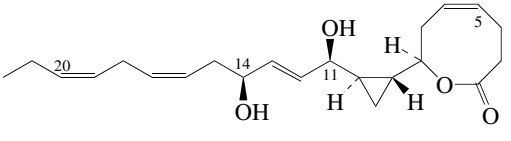


$C_{28}H_{32}O_8$ 496.556
Prod. by the marine-derived *Microsphaeropsis* sp. Stamm 6288.
Yellow solid.
Mp 102°. λ_{max} 274 (log ϵ 3.78); 387 (sh) (log ϵ 3.38) (MeOH).

Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*isol, pmr, cmr, ms*)

Solandelactone G S-249

[180251-01-8]



Absolute Configuration

$C_{22}H_{32}O_4$ 360.492
Isol. from the hydroid *Solanderia secunda*. Oil. $[\alpha]_D^{25}$ +3.7 (c, 0.8 in MeOH).

11-Epimer: ***Solandelactone H***
[180468-72-8]
$C_{22}H_{32}O_4$ 360.492
Isol. from *Solanderia secunda*. Oil. $[\alpha]_D^{25}$ +2.4 (c, 0.5 in MeOH).

5,6-Dihydro: ***Solandelactone C***
[180250-99-1]
$C_{22}H_{34}O_4$ 362.508
Isol. from *Solanderia secunda*. Oil. $[\alpha]_D^{25}$ +2.9 (c, 0.2 in MeOH).

11-Epimer, 5,6-dihydro: ***Solandelactone D***
[180468-70-6]
$C_{22}H_{34}O_4$ 362.508
Isol. from *Solanderia secunda*. Oil. $[\alpha]_D^{25}$ +5.7 (c, 0.2 in MeOH).

19,20-Dihydro: ***Solandelactone E***
[180251-00-7]
$C_{22}H_{34}O_4$ 362.508
Isol. from *Solanderia secunda*. Oil. $[\alpha]_D^{25}$ +2 (c, 0.7 in MeOH).

11-Epimer, 19,20-dihydro: ***Solandelactone F***
[180468-71-7]
$C_{22}H_{34}O_4$ 362.508
Isol. from *Solanderia secunda*. Oil. $[\alpha]_D^{25}$ +3 (c, 1 in MeOH).

5,6,19,20-Tetrahydro: ***Solandelactone A***
[180250-98-0]
$C_{22}H_{36}O_4$ 364.524
Isol. from *Solanderia secunda*. Oil. $[\alpha]_D^{25}$ +0.5 (c, 0.8 in MeOH).

11-Epimer, 5,6,19,20-tetrahydro: ***Solandelactone B***
[180468-69-3]
$C_{22}H_{36}O_4$ 364.524
Isol. from *Solanderia secunda*. Oil. $[\alpha]_D^{25}$ +6.5 (c, 0.8 in MeOH).

11-Deoxy, $\Delta^{11,12}$-isomer, 5,6,19,20-tetrahydro, 13-hydroxy: ***Solandelactone I***
[180251-02-9]
$C_{22}H_{36}O_4$ 364.524
Isol. from *Solanderia secunda*. Oil. $[\alpha]_D^{25}$ -37.7 (c, 0.3 in MeOH).
Stereochem. at C-13 and C-14 not determined.

Seo, Y. *et al., Tetrahedron*, 1996, **52**, 10583 (*isol, pmr, cmr, ms*)

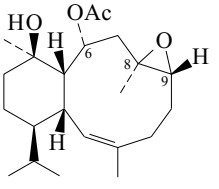
Solenin S-250

Protein. Isol. from the fish *Solenognathus hardwickii*. Shows translation-inhibiting activity.

Ng, T.B. *et al., Int. J. Biochem. Cell Biol.*, 2002, **34**, 625-631 (*isol*)

Solenopodin A S-251

[138629-93-3]



$C_{22}H_{36}O_4$ 364.524
Constit. of *Solenopodium stechei*. Oil. $[\alpha]_D$ -75.3 (c, 0.19 in $CHCl_3$).

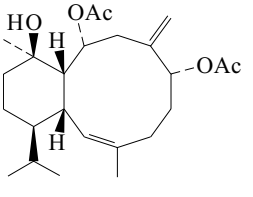
8,9-Diepimer: ***Solenopodin B***
[138749-85-6]
$C_{22}H_{36}O_4$ 364.524
Constit. of *Solenopodium stechei*. Oil.

6-Deacetoxy: ***Solenopodin C***
[138629-94-4]
$C_{20}H_{34}O_2$ 306.487
Constit. of *Solenopodium stechei*. Oil. $[\alpha]_D$ +105.6 (c, 0.36 in $CHCl_3$).

Bloor, S.J. *et al., J.O.C.*, 1992, **57**, 1205 (*isol, pmr, cmr*)

Solenopodin D S-252

[138629-95-5]



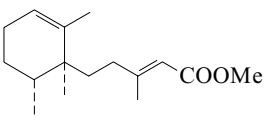
$C_{24}H_{38}O_5$ 406.561
Constit. of *Solenopodium stechei*. Cryst. (C_6H_6/hexane). $[\alpha]_D$ +29.3 (c, 0.15 in $CHCl_3$).

Bloor, S.J. *et al., J.O.C.*, 1992, **57**, 1205 (*isol, pmr, cmr, cryst struct*)

Sollasin A S-253

Fulvanin 1

[149297-97-2]



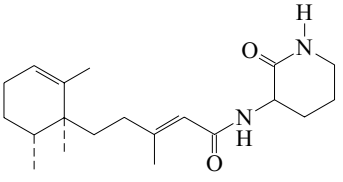
$C_{16}H_{26}O_2$ 250.38

Constit. of *Poecillastra sollasi* and *Reniera fulva*. Oil. $[\alpha]_D^{24}$ +12.2 (c, 1 in $CHCl_3$). Sollasin A and Fulvanin 1 not compared.

Killday, K.B. *et al., J. Nat. Prod.*, 1993, **56**, 500 (*isol, pmr, cmr*)
Casapullo, A. *et al., J. Nat. Prod.*, 1993, **56**, 527 (*isol, pmr, cmr*)
Angers, P. *et al., Tet. Lett.*, 1995, **36**, 2397 (*synth*)
Dagneau, P. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 2817 (*synth*)
Hatsui, T. *et al., Chem. Lett.*, 1998, 113-114 (*synth*)

Sollasin B S-254

[149297-98-3]



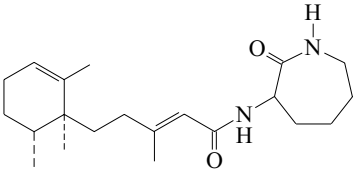
$C_{20}H_{32}N_2O_2$ 332.485

Constit. of *Poecillastra sollasi*. Solid. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{24}$ +29.8 (c, 2.14 in $CHCl_3$). λ_{max} 215 (ϵ 18900) (heptane).

Killday, K.B. *et al., J. Nat. Prod.*, 1993, **56**, 500-507 (*isol, pmr, cmr*)

Sollasin C S-255

[149297-99-4]



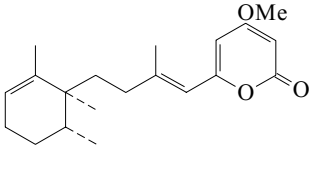
$C_{21}H_{34}N_2O_2$ 346.512

Constit. of *Poecillastra sollasi*. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{24}$ +10 (c, 1.26 in $CHCl_3$). λ_{max} 222 (ϵ 21772) (heptane) (Berdy).

Killday, K.B. *et al., J. Nat. Prod.*, 1993, **56**, 500 (*isol, pmr, cmr*)

Sollasin D S-256

[149298-00-0]



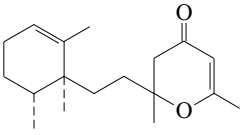
$C_{20}H_{28}O_3$ 316.439

Constit. of *Poecillastra sollasi*. Yellow oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{24}$ -22.1 (c, 2.13 in $CHCl_3$). λ_{max} 226 (ϵ 23510); 308 (ϵ 11579) (heptane).

Killday, K.B. *et al., J. Nat. Prod.*, 1993, **56**, 500-507 (*isol, pmr, cmr*)
Hatsui, T. *et al., Chem. Lett.*, 1998, 113-114 (*synth*)

Sollasin E S-257

[149298-01-1]



$C_{18}H_{28}O_2$ 276.418

Constit. of *Poecillastra sollasi*. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{24}$ +57.6 (c, 0.75 in $CHCl_3$). λ_{max} 266 (ϵ 14723) (heptane) (Berdy).

Killday, K.B. *et al., J. Nat. Prod.*, 1993, **56**, 500-507 (*isol, pmr, cmr*)

Solnin S-258

Isol. from the marine red alga *Soliera robusta*. Isoagglutinins; show mitogenic and antitumour activities.

Solnin A

Monomeric glycoprotein.

Solnin B

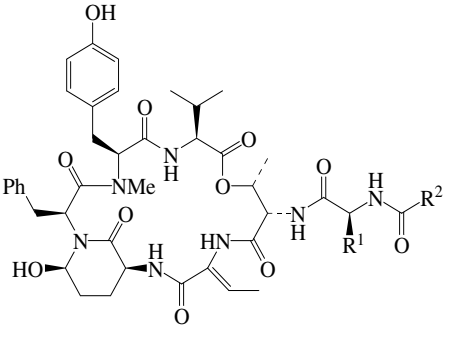
Monomeric glycoprotein.

Solnin C

Monomeric glycoprotein.

Hori, K. *et al., Phytochemistry*, 1988, **27**, 2063-2067 (*isol*)

Somamide A S-259



R^1 = -CH_2CH_2SOMe, R^2 = -$(CH_2)_4CH_3$

Absolute Configuration

$C_{48}H_{67}N_7O_{12}S$ 966.163

Depsipeptide antibiotic. Related to Dolastatin 13, D-1207. Isol. from an assemblage of *Lyngbya majuscula* and *Schizothrix* sp. Oil. $[\alpha]_D^{22}$ -2.5 (c, 0.08 in MeOH).

Nogle, L.M. *et al., J. Nat. Prod.*, 2001, **64**, 716-719 (*isol*)
Yokokawa, F. *et al., Tet. Lett.*, 2002, **43**, 8673-8677 (*synth*)

Somamide B S-260

As Somamide A, S-259 with
R^1 = -$CH_2CH_2CONH_2$, R^2 = -$CH_2CH_2CH_3$

$C_{46}H_{62}N_8O_{12}$ 919.042

Depsipeptide antibiotic. Only gross struct. confirmed. Isol. from an assemblage of *Lyngbya majuscula* and *Schizothrix* sp. Oil. $[\alpha]_D^{22}$ -10.2 (c, 0.05 in MeOH).

Nogle, L.M. *et al., J. Nat. Prod.*, 2001, **64**, 716-719

Somatolactin S-261

[131322-00-4]

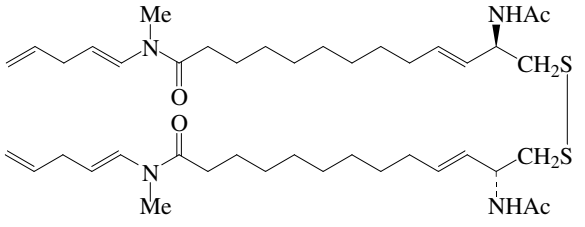
Protein containing 209 amino acid residues and 3 disulfide bonds; member of the growth hormone/prolactin family. First isol.

from the pituitary of the Atlantic cod *Gadus morhua*; present in other fish.

Rand-Weaver, M. *et al., Biochemistry*, 1991, **30**, 1509-1515 (*isol*)
Takayama, Y. *et al., Gen. Comp. Endocrinol.*, 1991, **83**, 366-374 (*struct*)
Takeno, T. *et al., Int. Rev. Cytol.*, 1996, **169**, 1-24 (*rev*)

Somocystinamide A S-262

[422312-35-4]



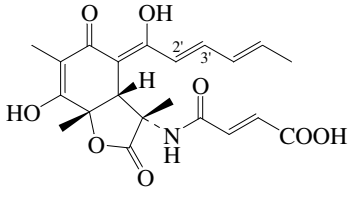
Absolute Configuration

$C_{42}H_{70}N_4O_4S_2$ 759.171
Isol. from a cyanobacterial assemblage of *Lyngbya majuscula* and *Schizothrix* sp. Cytotoxic. Amorph. solid. $[\alpha]_D^{22}$ +13.5 (c, 0.75 in $CHCl_3$). λ_{max} 210 (ϵ 17700); 241 (ϵ 9900) (MeOH).

Nogle, L.M. *et al., Org. Lett.*, 2002, **4**, 1095-1098 (*isol, pmr, cmr*)

Sorbicillactone A S-263

[664987-12-6]



Absolute Configuration

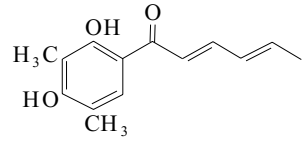
$C_{21}H_{23}NO_8$ 417.415
Prod. by *Penicillium chrysogenum* isol. from the sponge *Ircinia fasciculata*. Cytotoxic. Anti-HIV agent. Yellow needles (MeOH aq.).
Mp 205° dec. $[\alpha]_D^{20}$ -939 (c, 0.2 in MeOH).

2′,3′-Dihydro: ***Sorbicillactone B***
[861434-14-2]
$C_{21}H_{25}NO_8$ 419.43
Prod. by *Penicillium chrysogenum* isol. from *Ircinia fasciculata*. Light brown solid (MeOH aq.).
Mp 109-115°. $[\alpha]_D^{20}$ -327 (c, 0.2 in MeOH).

Bringmann, G. *et al., Tetrahedron*, 2005, **61**, 7252-7265 (*isol, cd, pmr, cmr*)

Sorbicillin S-264

1-(2,4-Dihydroxy-3,5-dimethylphenyl)-2,4-hexadien-1-one, 9CI
[79950-85-9]



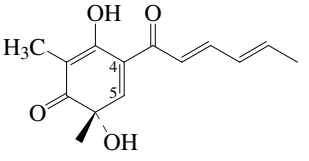
$C_{14}H_{16}O_3$ 232.279
Prod. by *Penicillium notatum*, *Penicillium chrysogenum*, *Trichoderma* spp. incl. *Trichoderma* sp. USF-2690 and *Verticillium intertextum*. Antibiotic. Shows DPPH-radical scavenging activity. Mycotoxin. Orange plates.
Mp 122-125°. λ_{max} 230; 324; 410 (MeOH) (Berdy).

2′,3′-Dihydro: ***Dihydrosorbicillin***
[79950-82-6]
$C_{14}H_{18}O_3$ 234.294
Prod. by *Penicillium notatum* and *Verticillium intertextum*. Mycotoxin. Needles (Et_2O/pentane).
Mp 67-70°. λ_{max} 214; 234; 283; 328 (MeOH) (Berdy).

Cram, D.J. *et al., J.A.C.S.*, 1948, **70**, 4238; 4240 (*struct, isol, uv*)
McOmie, J.F.W. *et al., J.C.S.*, 1958, 3226 (*synth*)
Trifonov, L.S. *et al., Tetrahedron*, 1983, **39**, 4243-4256 (*isol, bibl*)
Bigi, F. *et al., Tetrahedron*, 1984, **40**, 4081 (*synth*)
Andrade, R. *et al., Can. J. Chem.*, 1992, **70**, 2526-2535 (*isol, pmr, cmr*)
Abe, N. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 2120-2126 (*isol, cmr, activity*)
Abe, N. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 2090-2099 (*biosynth*)
Maskey, R.P. *et al., J. Nat. Prod.*, 2005, **68**, 865-870 (*2′,3′-Dihydrosorbicillin*)
Bringmann, G. *et al., Tetrahedron*, 2005, **61**, 7252-7265 (*marine isol*)

Sorbicillinol S-265

3,6-Dihydroxy-2,6-dimethyl-4-(1-oxo-2,4-hexadienyl)-2,4-cyclohexadien-1-one

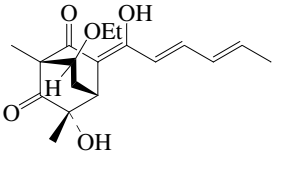


$C_{14}H_{16}O_4$ 248.278
Prod. by *Trichoderma* sp. USF-2690. Biosynth. intermed. of biosorbicillinoids. Yellow amorph. powder (as 6-Ac). $[\alpha]_D^{20}$ -80 (c, 0.05 in MeOH) (6-Ac). λ_{max} 218 (ϵ 8000); 293 (ϵ 12000) (H_2O) (uv refers to parent compd.).

4α,5α-Epoxide: ***Epoxysorbicillinol***
$C_{14}H_{16}O_5$ 264.277
Prod. by *Trichoderma longibrachiatum* from a *Haliclona* sp. sponge. Amorph. yellow powder. $[\alpha]_D$ +75 (c, 0.15 in MeOH). λ_{max} 287 (ϵ 16900) (MeOH).

Sperry, S. *et al., J.O.C.*, 1998, **63**, 10011-10014 (*Epoxysorbicillinol*)
Abe, N. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 2271-2279 (*isol, uv, pmr*)
Wood, J.L. *et al., J.A.C.S.*, 2001, **123**, 2097-2098 (*Epoxysorbicillinol, synth*)
Abe, N. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 2090-2099 (*biosynth*)

Sorbivinetone S-266

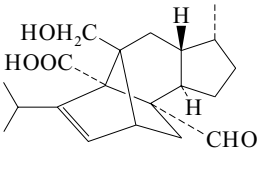


$C_{18}H_{24}O_5$ 320.385
Enolised β-diketone. Prod. by *Penicillium chrysogenum* isol. from the sponge *Ircinia fasciculata*. Light brown solid (MeOH aq.). Mp 100-118°. $[\alpha]_D^{20}$ +219 (c, 0.1 in MeOH). Possible artifact.

Bringmann, G. *et al., Tetrahedron*, 2005, **61**, 7252-7265 (*isol, cd, pmr, cmr, ms*)

Sordaricin S-267

[51493-69-7]



$C_{20}H_{28}O_4$ 332.439

Cryst. (MeOH/pentane). Mp 188-190° dec. $[\alpha]_D^{20}$ -62 (c, 0.33 in MeOH).

O-*(4-O-Methyl-β-D-altropyranoside)*: ***Hydroxysordarin***
$C_{27}H_{40}O_9$ 508.608
Prod. by *Sordaria araneosa*. Powder.
Mp 135-137°. $[\alpha]_D^{22}$ -59 (c, 0.2 in $CHCl_3$).

O-*(6-Deoxy-4-O-methyl-β-D-altropyranoside)*: ***Sordarin***. *SL 2266*. *Antibiotic SL 2266*
[11076-17-8]
$C_{27}H_{40}O_8$ 492.608
Metab. of *Sordaria araneosa*. Shows antifungal and *in vitro* antitumour props. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 253-255° (as K salt). $[\alpha]_D^{20}$ -45.2 (c, 0.57 in MeOH).
▶ LD_{50} (mus, ivn) 250 mg/kg.

O-*(3-O-Acetyl-6-deoxy-4-O-methyl-β-D-altropyranoside)*:
[219744-95-3]
$C_{29}H_{42}O_9$ 534.645
Prod. by *Graphium putredinis*.

O-*[2Z,4E-Hexadienoyl-(→3)-6-deoxy-4-O-methyl-β-D-altropyranoside]*: ***Zofimarin***
[108687-47-4]
$C_{33}H_{46}O_9$ 586.721
Prod. by *Graphium putredinis* and *Zopfiella marina*. Antifungal agent. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D$ -13.2 (MeOH). λ_{max} 210; 262 (ε 21700) (MeOH) (Berdy).

O-*[2-Methyl-2Z,4E-hexadienoyl-(→3)-4-O-methyl-β-D-altropyranoside]*: [219744-96-4]
$C_{34}H_{48}O_{10}$ 616.747
Prod. by *Graphium putredinis*.

O-*[2-Methyl-2E,4E-hexadienoyl-(→3)-6-deoxy-4-O-methyl-β-D-altropyranoside]*: [219744-93-1]
$C_{34}H_{48}O_9$ 600.748
Prod. by *Graphium putredinis*.

O-*[2-Methyl-2E,4Z-hexadienoyl-(→3)-6-deoxy-4-O-methyl-β-D-altropyranoside]*: [219744-94-2]
$C_{34}H_{48}O_9$ 600.748
Prod. by *Graphium putredinis*.

O-*[2-Methyl-2Z,4E-hexadienoyl-(→3)-6-deoxy-4-O-methyl-β-D-altropyranoside]*: ***Antibiotic GR 135402***. *GR 135402*
[204199-15-5]
$C_{34}H_{48}O_9$ 600.748
Prod. by *Graphium putredinis*. Antifungal agent. Cryst. (MeCN aq.). Sol. MeOH, EtOAc. λ_{max} 265 (ε 19860) (MeCN).

O-*[2-Methyl-2Z,4Z-hexadienoyl-(→3)-6-deoxy-4-O-methyl-β-D-altropyranoside]*: [219744-92-0]
$C_{34}H_{48}O_9$ 600.748
Prod. by *Graphium putredinis*.

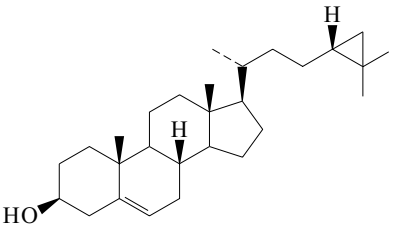
O-*[4S,5R:6S,7S-Diepoxy-2-methyl-2Z-octenoyl-(→3)-6-deoxy-4-O-methyl-β-D-altropyranoside]*: ***Hypoxysordarin***
[251298-72-3]
$C_{36}H_{50}O_{11}$ 658.784
Metab. of *Hypoxylon croceum*. Antifungal agent. Oil. $[\alpha]_D$ +17 (c, 0.35 in $CHCl_3$). λ_{max} 222 (ε 11700) (MeOH).

O-*[7ξ-Hydroxy-2-methyl-4-oxo-2Z,5E-octadienoyl-(→3)-6-deoxy-4-O-methyl-β-D-altropyranoside]*: ***Neosordarin***
$C_{36}H_{50}O_{11}$ 658.784
Prod. by *Sordaria araneosa*. Brownish solid.
Mp 53-57°. $[\alpha]_D^{22}$ -44 (c, 0.8 in $CHCl_3$). λ_{max} 243 (log ε 3.61) (MeOH).

Fr. Pat., 1967, 1 503 235; *CA*, **69**, 95102 (*isol*)
Hauser, D. *et al., Helv. Chim. Acta*, 1971, **54**, 1178 (*isol, ir, uv, ms, nmr*)
Sharpless, K.B. *et al., J.A.C.S.*, 1973, **95**, 7917 (*struct*)
Japan. Pat., 1987, 62 040 292; *CA*, **107**, 5745j (*Zofimarin*)
Kato, N. *et al., Chem. Comm.*, 1993, 1002-1004 (*synth*)
Kinsman, O.S. *et al., J. Antibiot.*, 1998, **51**, 41-49; 1012-1018 (*isol, pmr, cmr, activity*)
Daferner, M. *et al., Z. Naturforsch., C*, 1999, **54**, 474-480 (*Hypoxysordarin*)
Davoli, P. *et al., J. Antibiot.*, 2002, **55**, 377-382 (*Hydroxysordarin, Neosordarin*)
Kitamura, M. *et al., Chem. Lett.*, 2004, **33**, 942-943 (*synth*)
Mander, L.N. *et al., J.O.C.*, 2005, **70**, 1654-1670 (*synth*)
Chiba, S. *et al., J.A.C.S.*, 2006, **128**, 6931-6937 (*Sordarin, synth*)

Sormosterol S-268

25,28-Cycloergost-5-en-3-ol. 24,25-Methylenecholest-5-en-3-ol
[131487-01-9]

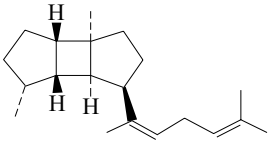


$C_{28}H_{46}O$ 398.671
Constit. of *Lissodendoryx topsenti*.

Silva, C.J. *et al., Coll. Czech. Chem. Comm.*, 1991, **56**, 1093-1105 (*isol, struct*)
Giner, J.-L. *et al., Acta Chem. Scand.*, 1992, **46**, 678-679 (*biosynth*)

13(15),17-Spatadiene S-269

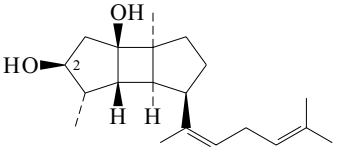
[81575-09-9]



$C_{20}H_{32}$ 272.473

(13(15)*Z*)-*form*
Obt. from *Dilophus marginatus*.
Oil. $[\alpha]_D^{20}$ +128.5 (c, 1.1 in CCl_4).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 129 (*isol*)
Dauben, W.G. *et al., Tet. Lett.*, 1990, **31**, 635 (*synth*)

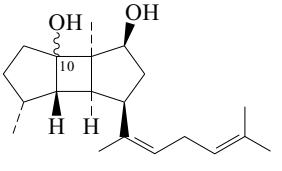
13(15),17-Spatadiene-2,10-diol S-270



$C_{20}H_{32}O_2$ 304.472

(2β,10β,13(15)*Z*)-*form*
Cryst. (Et_2O). Mp 143-145°. $[\alpha]_D$ +180 (c, 1.2 in $CHCl_3$).
2-Ac: [140671-30-3]
$C_{22}H_{34}O_3$ 346.509
Constit. of *Dictyota fenestrata*. Oil. $[\alpha]_D$ +147 (c, 1.3 in $CHCl_3$).
Van Altena, I.A. *et al., Aust. J. Chem.*, 1991, **45**, 541 (*isol, pmr, cmr*)

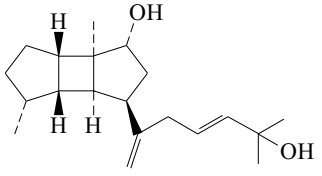
13(15),17-Spatadiene-5,10-diol S-271



$C_{20}H_{32}O_2$ 304.472

(5*S*,10ξ)-*form* [81575-17-9]
10-Ac: ***10-Acetoxy-3(15),17-spatadien-5-ol***
[81575-13-5]
$C_{22}H_{34}O_3$ 346.509
Isol. from *Dilophus marginatus*. Oil. $[\alpha]_D^{20}$ +85 (c, 0.3 in CCl_4).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 129

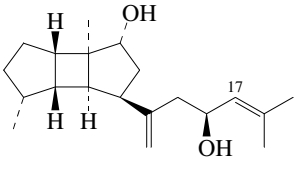
13,16-Spatadiene-5,18-diol S-272



$C_{20}H_{32}O_2$ 304.472

(5*R*,16*E*)-*form* [77136-65-3]
Constit. of *Stoechospermum marginatum*.
Oil. $[\alpha]_D$ +1.9 (c, 1.4 in $CHCl_3$).
Wicklow, W.H. *et al., J.O.C.*, 1981, **46**, 2239

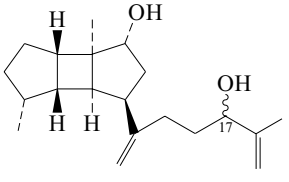
13,17-Spatadiene-5,16-diol S-273



$C_{20}H_{32}O_2$ 304.472
Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

(5*R*,16*S*)-*form* [77136-83-5]
Constit. of *Stoechospermum marginatum*.
Oil. $[\alpha]_D$ +6.3 (c, 1.9 in $CHCl_3$).
Di-Ac: [246547-32-0]
$C_{24}H_{36}O_4$ 388.546
Constit. of *Stoechospermum marginatum*.
$[\alpha]_D$ +10.5 (c, 2 in $CHCl_3$).
17ξ,18-Epoxide: ***17,18-Epoxy-13-spatene-5,16-diol***
$C_{20}H_{32}O_3$ 320.471
Isol. from *Stoechospermum marginatum*.
Gerwick, W.H. *et al., J.O.C.*, 1981, **46**, 2233
Venkateswarlu, Y. *et al., Phytochemistry*, 1995, **40**, 331 (*epoxide*)
De Rosa, S. *et al., Phytochemistry*, 1999, **51**, 1009-1012 (*di-Ac, abs config*)

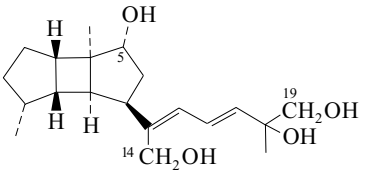
13,18-Spatadiene-5,17-diol S-274



$C_{20}H_{32}O_2$ 304.472

(5*R*,17ξ)-*form* [77136-64-2]
Constit. of *Stoechospermum marginatum*.
Oil. $[\alpha]_D$ +35.2 (c, 0.83 in $CHCl_3$).
17-Epimer: [77209-25-7]
Constit. of *Stoechospermum marginatum*.
Oil. $[\alpha]_D$ +18.4 (c, 0.7 in $CHCl_3$).
Gerwick, W.H. *et al., J.O.C.*, 1981, **46**, 2233

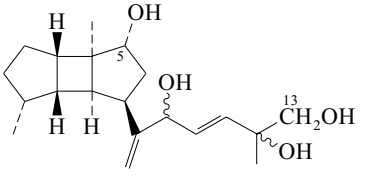
13(15),16-Spatadiene-5,14,18,19-tetrol S-275



$C_{20}H_{32}O_4$ 336.47

(5*R*,13(15)*E*,16*Z*)-*form* [86887-34-5]
5,14,19-Tri-Ac: 18-Hydroxy-5,14,19-triacetoxy-13(15),16-spatadiene
[86900-72-3]
$C_{26}H_{38}O_7$ 462.582
Constit. of *Spatoglossum howlii*. Oil. $[\alpha]_D$ +42.7 (c, 0.98 in $CHCl_3$).
Gerwick, W.H. *et al., J.O.C.*, 1983, **48**, 3325

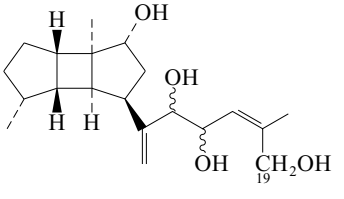
13,16-Spatadiene-5,15,18,19-tetrol S-276



$C_{20}H_{32}O_4$ 336.47

(5*R*,15ξ,16*E*,18ξ)-*form* [77136-60-8]
Constit. of *Stoechospermum marginatum*.
Oil. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D$ -10.7 (c, 1.8 in $CHCl_3$).
19-Ac: [77136-61-9]
$C_{22}H_{34}O_5$ 378.508
Constit. of *Stoechospermum marginatum*. Oil. Sol. MeOH; poorly sol. H_2O, hexane. $[\alpha]_D$ -16.1 (c, 1.5 in $CHCl_3$).
5-Ketone: ***15,18,19-Trihydroxy-13,16E-spatadien-5-one***
[77136-62-0]
$C_{20}H_{30}O_4$ 334.455
Constit. of *Stoechospermum marginatum*. Oil. $[\alpha]_D$ -136.5 (c, 1.2 in $CHCl_3$).
19-Deoxy: ***13,16-Spatadiene-5,15,18-triol***
$C_{20}H_{32}O_3$ 320.471
Isol. from *Spatoglossum schmittii* and *Spatoglossum howleii*.
Cryst.
Mp 55-57°. $[\alpha]_D$ -33.4 (c, 0.73 in $CHCl_3$).
Gerwick, W.H. *et al., J.O.C.*, 1981, **46**, 2233-2241 (*Stoechospermum marginatum constits*)
Gerwick, W.H. *et al., J.O.C.*, 1983, **48**, 3325-3329 (*Spatoglossum constit*)
Salomon, R.G. *et al., J.A.C.S.*, 1991, **113**, 3096-3106 (*synth*)

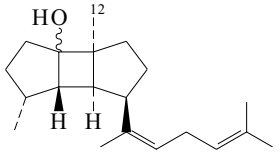
13,17-Spatadiene-5,15,16,19-tetrol S-277



$C_{20}H_{32}O_4$ 336.47

(5*R*,15ξ,16ξ,17*Z*)-*form*
19-Ac: [77136-63-1]
$C_{22}H_{34}O_5$ 378.508
Constit. of *Stoechospermum marginatum*. Oil. $[\alpha]_D$ -8.8 (c, 1.2 in $CHCl_3$).
Gerwick, W.H. *et al., J.O.C.*, 1981, **46**, 2233

13(15),17-Spatadien-10-ol S-278

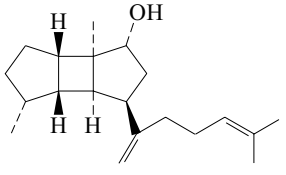


$C_{20}H_{32}O$ 288.472

(10ξ,13(15)*Z*)-*form* [81575-10-2]
Constit. of *Dilophus marginatus*.
Viscous oil. $[\alpha]_D^{20}$ +115 (c, 1.8 in $CHCl_3$).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 129

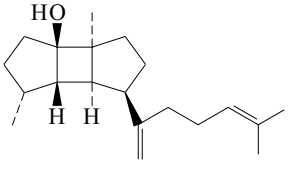
13,17-Spatadien-5-ol S-279

Stoechospermol
[77129-32-9]



$C_{20}H_{32}O$ 288.472
Struct. revised in 1981. Constit. of *Stoechospermum marginatum*.
Oil or cryst. (hexane).
Mp 64-65°. $[\alpha]_D$ +29.4 (c, 1 in $CHCl_3$). $[\alpha]_D^{27}$ +21.8 (EtOH).
Ac:
$C_{22}H_{34}O_2$ 330.509
Constit. of *Stoechospermum marginatum*. Cryst.
Mp 65-66°.
Solimabi, L. *et al., Tet. Lett.*, 1980, **21**, 2249 (*isol*)
Gerwick, W.H. *et al., J.O.C.*, 1981, **46**, 2233 (*isol*)
Salomon, R.G. *et al., J.A.C.S.*, 1984, **106**, 2211; 1991, **113**, 3096 (*synth*)
Tanaka, M. *et al., Tet. Lett.*, 1985, **26**, 3035 (*synth*)
Wahidullah, S. *et al., Planta Med.*, 1988, **54**, 270 (*isol, pmr*)
Miesch, M. *et al., Tet. Lett.*, 1994, **35**, 7031 (*synth*)
Tanaka, M. *et al., Tetrahedron*, 1994, **50**, 12829 (*synth*)

13,17-Spatadien-10-ol S-280



$C_{20}H_{32}O$ 288.472

10β-*form* [81575-11-3]
Constit. of *Dilophus marginatus* and *Dilophus okamurai*. Feeding deterrent. Foam. $[\alpha]_D^{20}$ +96 (c, 0.8 in CCl_4). The spectroscopic properties of the compds. from the two spp. are not in complete agreement.
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 129-144 (*isol*)
Kurata, K. *et al., Phytochemistry*, 1988, **27**, 1321 (*isol*)

Glyptocidaris crenularis Sperm activating peptides S-281

H-X-Leu-Cys-Pro-Gly-Gly-Y-Cys-Val-OH
Reduced form shown. Isol. from the sea urchin *Glyptocidaris crenularis*. Sperm activating factor in host organism.

Sperm activating peptide A
Alloresact
[117627-63-1]
$C_{36}H_{61}N_{11}O_{11}S_2$ 888.077
X = Lys, Y = Asn.

Sperm activating peptide B [117788-28-0]
$C_{42}H_{71}N_{13}O_{14}S_2$ 1046.234
X = Ser-Ala-Lys, Y = Asn.

Sperm activating peptide C [117788-29-1]
$C_{37}H_{63}N_{11}O_{11}S_2$ 902.104
X = Lys, Y = Gln.

Sperm activating peptide D [117788-30-4]
$C_{49}H_{77}N_{13}O_{14}S_2$ 1136.358
X = Ser-Phe-Lys, Y = Gln.

Sperm activating peptide E
LCPGGNCV
[117788-31-5]
$C_{30}H_{49}N_9O_{10}S_2$ 759.903
X = no residue, Y = Asn.

Sperm activating peptide F [117788-32-6]
$C_{31}H_{51}N_9O_{10}S_2$ 773.93
X = no residue, Y = Gln.

Suzuki, N. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1988, **90**, 305-311 (*isol, props*)
Yoshino, K. *et al., FEBS Lett.*, 1991, **294**, 179-182 (*struct*)

Arbacia punctulata Sperm-activating peptide S-282

Resact
[140668-76-4]
H-Cys-Val-Thr-Gly-Ala-Pro-Gly-Cys-Val-Gly-Gly-Gly-Arg-Leu-NH_2
$C_{50}H_{86}N_{18}O_{15}S_2$ 1243.473
Reduced form shown. Isol. from the egg jelly coat of the sea urchin *Arbacia punctulata*. Activates sperm regulation.
[91316-25-5]
Yoshino, K. *et al., FEBS Lett.*, 1991, **294**, 179-182 (*struct*)

Brissus agassizi Sperm-activating peptide S-283

Sperm activating peptide V. SAP V
[144313-67-7]
[144313-51-9]
H-Gly-Cys-Glu-Gly-Leu-Phe-His-Gly-Met-Gly-Asn-Cys-OH
$C_{49}H_{73}N_{15}O_{16}S_3$ 1224.405
Isol. from the egg jelly coat of sea urchin (*Brissus agassizi*). Activates sperm regulation.
Yoshino, K. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1992, **102**, 691-700 (*isol, struct*)

Clypeaster japonicus Sperm-activating peptide S-284

Mosact
[112714-09-7]
H-Asp-Ser-Asp-Ser-Ala-Gln-Asn-Leu-Ile-Gly-OH
$C_{40}H_{66}N_{12}O_{19}$ 1019.03
Isol. from the egg jelly coat of the sea urchin *Clypeaster japonicus*. Activates sperm regulation. Two analogues were also isol.
6-Phenylalanine analogue: [112766-92-4]
$C_{40}H_{61}N_9O_{16}$ 923.973
Isol. from the egg jelly coat of the sea urchin *Clypeaster japonicus*.
6-(5-Bromohistidine) analogue: [112756-80-6]
$C_{37}H_{58}BrN_{11}O_{16}$ 992.833

Isol. from the egg jelly coat of the sea urchin *Clypeaster japonicus*.
Suzuki, N. *et al., Zool. Sci.*, 1987, **4**, 649-656 (*isol, struct*)

Diadema setosum Sperm-activating peptide S-285

[127027-49-0]

Gly-Cys-Pro-Trp-Gly-Gly-Ala-Val-Cys

$C_{36}H_{50}N_{10}O_{10}S_2$ 846.984

Reduced form shown. Isol. from egg jelly of the sea urchin *Diadema setosum*. Activates sperm regulation.

Yoshino, K. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1990, **95**, 423-429 (*isol*)

Stomopneustes variolaris Sperm-activating peptide S-286

KFCPEGKCV

[140653-26-5]

Lys-Phe-Cys-Pro-Glu-GLy-Lys-Cys-Val

$C_{44}H_{69}N_{11}O_{12}S_2$ 1008.228

Reduced form shown. Isol. from egg jelly of the sea urchin *Stomopneustes variolaris*. Activates sperm regulation.

Yoshino, K. *et al., FEBS Lett.*, 1991, **294**, 179-182 (*isol*)

Hemicentrotus pulcherrimus Sperm-activating peptide H1 S-287

[78020-12-9]

H-Gly-Phe-Asp-Leu-Thr-Gly-Gly-Gly-Val-Gly-OH

$C_{38}H_{58}N_{10}O_{14}$ 878.935

Isol. from the egg jelly coat of the sea urchins *Hemicentrotus pulcherrimus* and *Anthocidaris crassispina*. Activates sperm regulation. Many related peptides have been isol. from other sea urchin species incl. a series of 2-bromo-L-phenylalanine-containing peptides from *Tripneustes gratilla*.

5-L-Asparagine analogue: Sperm-activating peptide H_2. Speract
[76901-59-2]
$C_{38}H_{57}N_{11}O_{14}$ 891.934
Isol. from the egg jelly coat of *Hemicentrotus pulcherrimus*.

5-L-Serine analogue: Sperm-activating peptide A_2
[86030-82-2]
$C_{37}H_{56}N_{10}O_{14}$ 864.908
Isol. from the egg jelly coat of *Anthocidaris crassispina*.

Nomura, K. *et al., Biochem. Biophys. Res. Commun.*, 1983, **117**, 147-153 (*isol, struct*)
Suzuki, N. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1988, **89**, 687-693 (*isol*)
Yoshino, K. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **94**, 739 (*isol*)

Sepia officinalis Sperm-attracting peptide S-288

[476342-05-9]

Pro-Ile-Asp-Pro-Gly-Val-NH_2

$C_{27}H_{45}N_7O_8$ 595.695

Isol. from the egg mass of *Sepia officinalis*. Shows sperm-attracting activity.

Zatylny, C. *et al., Biochem. Biophys. Res. Commun.*, 2002, **296**, 1186-1193 (*isol*)

Spermidine S-289

N-*(3-Aminopropyl)-1,4-butanediamine, 9CI*

[124-20-9]

$H_2NCH_2CH_2CH_2N'HCH_2CH_2CH_2CH_2N''H_2$

$C_7H_{19}N_3$ 145.247

Prod. by many microorganisms. Isol. from the edible shaggy ink cap mushroom (*Coprinus comatus*). Bp_{14} 128-130°.

▶ LD_{50} (mus, ivn) 78 mg/kg. EJ7000000

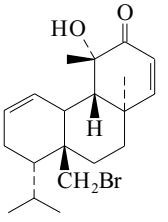
N''-*(3,5-Dibromo-4-methoxy*-E-*cinnamoyl): N^{10}-(3,5-Dibromo-4-methoxycinnamoyl)spermidine.* ***Tokaradine C***
[368422-40-6]
$C_{17}H_{25}Br_2N_3O_2$ 463.211
Isol. from the sponge *Pseudoceratina purpurea*. Amorph. yellow solid. λ_{max} 229 (ε 12200); 279 (ε 9900) (MeOH).

[49721-50-8]

Fusetani, N. *et al., Tetrahedron*, 2001, **57**, 7507-7511 (*Tokaradine C*)

Sphaerococcenol A S-290

[60244-34-0]



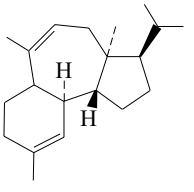
Absolute configuration

$C_{20}H_{29}BrO_2$ 381.352
Constit. of *Sphaerococcus coronopifolius*. Cryst. (CCl_4).
Mp 184-185°. $[\alpha]_D^{25}$ -93 (c, 2 in $CHCl_3$).

Fenical, W. *et al., Tet. Lett.*, 1976, 731

6,11-Sphaerodiene S-291

[80981-65-3]



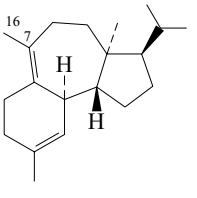
$C_{20}H_{32}$ 272.473
Constit. of *Sphaerococcus coronopifolius*. Oil. $[\alpha]_D$ +44.93 (c, 1.0 in $CHCl_3$).

Cafieri, F. *et al., Tet. Lett.*, 1981, **22**, 4123

7,11-Sphaerodiene S-292

Isosphaerodiene 1

[80981-70-0]

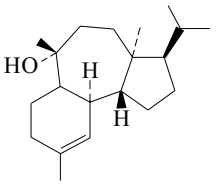


$C_{20}H_{32}$ 272.473
Constit. of *Sphaerococcus coronopifolius*. Cryst.
Mp 58-59°. $[\alpha]_D$ +28 ($CHCl_3$).

$\Delta^{7(16)}$-Isomer: 7(16),11-Sphaerodiene. ***Isosphaerodiene 2***
[108907-24-0]
$C_{20}H_{32}$ 272.473
Constit. of *Sphaerococcus coronopifolius*. Oil. $[\alpha]_D$ +18 ($CHCl_3$).

Cafieri, F. *et al., Tet. Lett.*, 1981, **22**, 4123 (*synth*)
Cafieri, F. *et al., Phytochemistry*, 1987, **26**, 471 (*isol*)
Lee, J. *et al., J.O.C.*, 2004, **69**, 6433-6440 (*abs config*)

11-Sphaeroen-7-ol S-293



$C_{20}H_{34}O$ 290.488

7α-*form*

Presphaerol

[71386-39-5]

Constit. of *Sphaerococcus coronopifolius.*

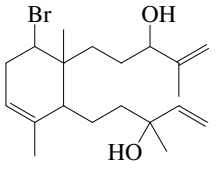
Oil. $[\alpha]_D$ +26 (c, 1.0 in $CHCl_3$).

Cafieri, F. *et al., Tet. Lett.*, 1979, **20**, 963; 1981, **22**, 4123

Lee, J. *et al., J.O.C.*, 2004, **69**, 6433-6440 (*abs config*)

Sphaerolabdadiene-3,14-diol S-294

[361344-21-0]



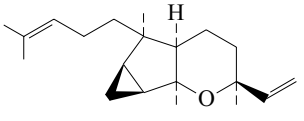
$C_{20}H_{33}BrO_2$ 385.384

Constit. of *Sphaerococcus coronopifolius.* Amorph. powder. $[\alpha]_D$ +9.6 (c, 0.6 in CH_2Cl_2).

Etahiri, S. *et al., J. Nat. Prod.*, 2001, **64**, 1024-1027 (*isol, pmr, cmr*)

Sphaeropyrane S-295

[115610-51-0]

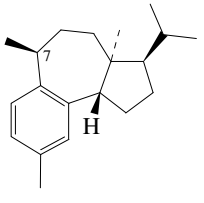


$C_{20}H_{32}O$ 288.472

Constit. of *Sphaerococcus coronopifolius.* Cryst. Mp 136-138°. $[\alpha]_D$ -43.9 (c, 0.8 in $CHCl_3$).

Cafieri, F. *et al., Phytochemistry*, 1988, **27**, 621

8,11,13-Sphaerotriene S-296



$C_{20}H_{30}$ 270.457

7β-*form*

Presphaerene

[88142-52-3]

Constit. of *Sphaerococcus coronopifolius.*

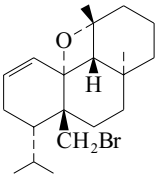
Oil. $[\alpha]_D^{20}$ -46.

Cafieri, F. *et al., Phytochemistry*, 1983, **22**, 1824 (*isol, struct*)

Lee, J. *et al., J.O.C.*, 2004, **69**, 6433-6440 (*synth, abs config*)

Sphaeroxetane S-297

[116310-65-7]



$C_{20}H_{31}BrO$ 367.368

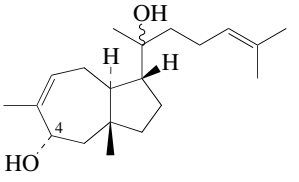
Constit. of *Sphaerococcus coronopifolius.* Oil. $[\alpha]_D$ -9 (c, 0.57 in $CHCl_3$).

De Rosa, S. *et al., Phytochemistry*, 1988, **27**, 1875

2,17-Sphenolobadiene-4,13-diol S-298

Polasol B

[210969-52-1]



$C_{20}H_{34}O_2$ 306.487

Constit. of an *Epipolasis* sp. Oil. $[\alpha]_D^{25}$ +11.4 (c, 0.56 in $CHCl_3$).

4-Ketone: 13-Hydroxy-2,17-sphenolobadien-4-one. ***Polasol A***

[210969-51-0]

$C_{20}H_{32}O_2$ 304.472

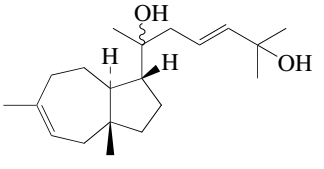
Constit. of an *Epipolasis* sp. Oil. $[\alpha]_D^{25}$ +60.1 (c, 0.44 in $CHCl_3$). λ_{max} 240 (log ϵ 2.9) (MeOH).

Umeyama, A. *et al., J. Nat. Prod.*, 1998, **61**, 945-947 (*isol, pmr, cmr*)

3,16-Sphenolobadiene-13,18-diol S-299

Polasol C

[210969-53-2]



$C_{20}H_{34}O_2$ 306.487

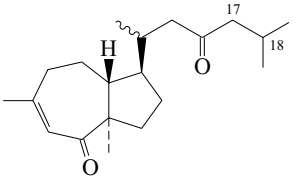
Constit. of *Epipolasis* sp. Oil. $[\alpha]_D^{25}$ -5.37 (c, 0.62 in $CHCl_3$).

Umeyama, A. *et al., J. Nat. Prod.*, 1998, **61**, 945-947 (*isol, pmr, cmr*)

3-Sphenolobene-5,16-dione S-300

Reiswigin A

[116428-62-7]



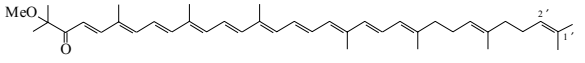
$C_{20}H_{32}O_2$ 304.472

Constit. of sponge *Epipolasis reiswigi.* Antiviral agent. Tan oil. $[\alpha]_D^{20}$ -10 (c, 0.1 in $CHCl_3$). λ_{max} 239 (ϵ 11000) (EtOH) (Derep).

17,18-Didehydro: 3,17-Sphenolobadiene-5,16-dione. ***Reiswigin B***
[116428-63-8]
$C_{20}H_{30}O_2$ 302.456
Constit. of *Epipolasis reiswigi*. Antiviral agent. Tan oil. $[\alpha]_D^{20}$ -20 (c, 0.1 in $CHCl_3$). λ_{max} 239 (ϵ 18000) (EtOH) (Derep).
Kashman, Y. *et al., Tet. Lett.*, 1987, **28**, 5461
Snider, B.B. *et al., J.O.C.*, 1990, **55**, 4392-4399 (*synth, abs config*)
Kun, D. *et al., Tet. Lett.*, 1994, **35**, 7957 (*synth*)
MaGee, D.I. *et al., Can. J. Chem.*, 2004, **82**, 333-343 (*synth*)

Spheroidenone S-301

3,4-Didehydro-1,2,7′,8′-tetrahydro-1-methoxy-ψ,ψ-caroten-2-one. Pigment R
[13836-70-9]



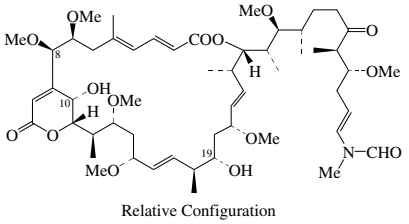
$C_{41}H_{58}O_2$ 582.908
Prod. by *Rhodopseudomonas spheroides*, *Erythrobacter* spp. and a marine-derived *Roseobacter* sp. Red platelets (petrol).
Mp 166-167° (157.5-159°). λ_{max} 461; 482; 513 (petrol).

O-*De-Me: 1-Hydroxy-3,4-didehydro-1,2,7′,8′-tetrahydro-ψ,ψ-caroten-2-one.* ***Desmethylspheroidenone***
$C_{40}H_{56}O_2$ 568.881
Isol. from aerobic cultures of *Rhodopseudomonas capsulata*.
λ_{max} 487 (approx) (EtOH).

1′,2′-Dihydro, 1′-hydroxy: **OH-*Spheroidenone***
[1119-39-7]
$C_{41}H_{60}O_3$ 600.923
Isol. from cultures of *Rhodopseudomonas* sp. and *Erythrobacter* sp.
Mp 158.5-159.5°. λ_{max} 501; 530 (C_6H_6).
Davis, J.B. *et al., Proc. Chem. Soc., London*, 1961, 261 (*struct*)
Jensen, S.L. *et al., Acta Chem. Scand.*, 1963, **17**, 489 (*isol, deriv*)
Jackman, L.M. *et al., Acta Chem. Scand.*, 1964, **18**, 1403 (*struct*)
Barber, M.S. *et al., J.C.S.(C)*, 1966, 2166 (*synth*)
Manchand, P.S. *et al., Tet. Lett.*, 1966, 989 (*synth*)
Harashima, K. *et al., Agric. Biol. Chem.*, 1983, **47**, 1057 (*isol, deriv*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)

Sphinxolide A S-302

[120614-97-3]



Relative Configuration

$C_{54}H_{87}NO_{15}$ 990.279
Macrolide antibiotic. Constit. of an unidentified marine nudibranch and the sponge *Neosiphonia superstes*. Antitumour agent, apoptosis inducer. Microcryst. powder (EtOAc). Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 90-92°. $[\alpha]_D^{25}$ -10.5 (c, 0.15 in MeOH). λ_{max} 273 (ϵ 32000) (MeOH).

19-Me ether: ***Sphinxolide C***
[152340-45-9]
$C_{55}H_{89}NO_{15}$ 1004.306
Isol. from *Neosiphonia superstes*. Antitumour agent. Apoptosis inducer. $[\alpha]_D$ -11.8 (MeOH).

4,5-Epoxide, 19-Me ether: ***Sphinxolide E***
[256381-68-7]
$C_{55}H_{89}NO_{16}$ 1020.305
Isol. from *Neosiphonia superstes*. Antitumour agent. Amorph. powder. $[\alpha]_D^{20}$ +2.9 (c, 0.004 in $CHCl_3$). λ_{max} 226 (log ϵ 4.1) (MeOH).

8-Demethoxy: ***Sphinxolide B***
[152340-44-8]
$C_{53}H_{85}NO_{14}$ 960.253
Isol. from *Neosiphonia superstes*. Antitumour agent. $[\alpha]_D$ +2.8 (MeOH).

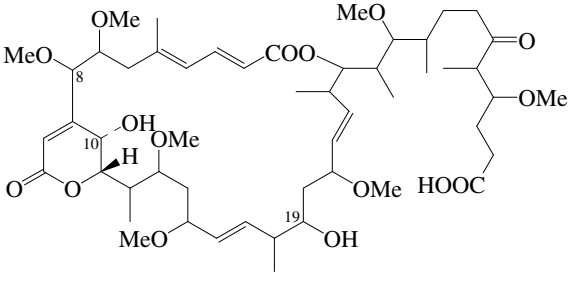
8-Demethoxy, 19-Me ether: ***Sphinxolide D***
[152340-46-0]
$C_{54}H_{87}NO_{14}$ 974.28
Isol. from *Neosiphonia superstes* and *Reidispongia coerulea*. Antitumour agent, apoptosis inducer. $[\alpha]_D$ -3.2 (MeOH).

8-Demethoxy, 10-deoxy: ***Reidispongiolide B***
[156343-57-6]
$C_{53}H_{85}NO_{13}$ 944.253
Isol. from the sponge *Reidispongia coerulea*. Cytotoxic agent. $[\alpha]_D$ +3.5.

8-Demethoxy, 10-deoxy, 19-Me ether: ***Reidispongiolide A***
[156343-56-5]
$C_{54}H_{87}NO_{13}$ 958.28
Isol. from the sponge *Reidispongia coerulea*. Cytotoxic agent. $[\alpha]_D$ -4.8.
Guella, G. *et al., Helv. Chim. Acta*, 1989, **72**, 237-246 (*isol*)
D'Auria, M.V. *et al., Tetrahedron*, 1993, **49**, 8657-8664; 10439 (*Sphinxolides A-C*)
D'Auria, M.V. *et al., Tetrahedron*, 1994, **50**, 4829-4834 (*Reidispongiolides*)
Carbonelli, S. *et al., Tetrahedron*, 1999, **55**, 14665-14674 (*Sphinxolide E*)
Bassarello, C. *et al., Eur. J. Org. Chem.*, 2001, 39-44 (*pmr, cmr, abs config*)

Sphinxolide F S-303

[256381-69-8]



$C_{52}H_{84}O_{16}$ 965.226
Isol. from the sponge *Neosiphonia superstes*. Cytotoxic agent. Amorph. powder. $[\alpha]_D^{20}$ +24.3 (c, 0.001 in $CHCl_3$). λ_{max} 208 (log ϵ 3.9); 280 (log ϵ 4) (MeOH).

8-Demethoxy, 19-Me ether: ***Sphinxolide G***
[256381-70-1]
$C_{52}H_{84}O_{15}$ 949.227
Isol. from the sponge *Reidispongia coerulea*. Cytotoxic agent. Amorph. powder. $[\alpha]_D^{20}$ +8 (c, 0.004 in $CHCl_3$). λ_{max} 212 (log ϵ 3.9); 280 (log ϵ 4) (MeOH).

8-Demethoxy, 10-deoxy, 19-Me ether: ***Reidispongiolide C***
[256381-71-2]
$C_{52}H_{84}O_{14}$ 933.227
Isol. from *Reidispongia coerulea*. Cytotoxic agent. Amorph. powder. $[\alpha]_D^{20}$ +9 (c, 0.004 in $CHCl_3$). λ_{max} 212 (log ϵ 3.9); 276 (log ϵ 4.1) (MeOH).
Carbonelli, S. *et al., Tetrahedron*, 1999, **55**, 14665-14674

Sphyrnastatin S-304

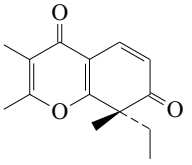
Isol. from the hammerhead shark *Sphyrna lewini*. Shows antitumour activity. Sol. H_2O.

Sphyrnastatin 1
Glycoprotein containing 22% carbohydrate.

Sphyrnastatin 2
Glycoprotein containing 26% carbohydrate.
Pettit, G.R. *et al., J. Pharm. Sci.*, 1977, **66**, 757-758 (*isol*)

Spiciferone A S-305

[123421-05-6]



$C_{14}H_{16}O_3$ 232.279

(R)-form

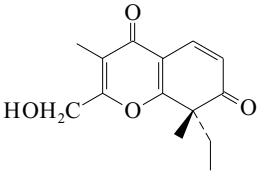
Prod. by *Cochliobolus spicifer* and *Drechslera hawaiiensis*. Plant growth regulator. Phytotoxin. Cryst. (EtOH aq.).
Mp 100-102°. $[\alpha]_D^{20}$ -44.2 (c, 1 in $CHCl_3$). λ_{max} 202 (ϵ 10600); 244 (ϵ 10800); 318 (ϵ 5200) (EtOH) (Berdy).

8S-Alcohol: ***Spiciferol A***
$C_{14}H_{18}O_3$ 234.294
Prod. by *Drechslera hawaiiensis* isol. from the sponge *Callyspongia aerizusa*. Powder. $[\alpha]_D$ +18.1 (c, 0.27 in EtOH). λ_{max} 202 (ϵ 12200); 239 (ϵ 9200); 260 (sh) (ϵ 6600); 325 (ϵ 1200) (EtOH).

Nakajima, H. *et al., Agric. Biol. Chem.*, 1989, **53**, 2297 (*isol*)
Nakajima, H. *et al., J.C.S. Perkin 1*, 1994, 1865 (*abs config, biosynth*)
Edrada, R.A. *et al., Z. Naturforsch., C*, 2000, **55**, 218-221 (*Spiciferol A*)

Spiciferone B S-306

[137181-62-5]



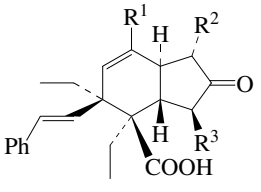
$C_{14}H_{16}O_4$ 248.278

(R)-form

Constit. of *Cochliobolus spicifer* and the marine-derived *Drechslera hawaiiensis*. Phytotoxin. Oil. $[\alpha]_D^{20}$ -34 (c, 0.695 in EtOH). λ_{max} 204 (ϵ 9550); 243 (ϵ 7762); 320 (ϵ 4265) (EtOH) (Berdy).

Nakajima, H. *et al., Phytochemistry*, 1991, **30**, 2563 (*isol, pmr, cmr*)
Nakajima, H. *et al., J.C.S. Perkin 1*, 1994, 1865 (*abs config, biosynth*)
Edrada, R.A. *et al., Z. Naturforsch., C*, 2000, **55**, 218-221 (*marine, isol*)

Spiculoic acid A S-307



Absolute Configuration

$R^1 = R^3 = CH_2CH_3$, $R^2 = CH_3$

$C_{27}H_{36}O_3$ 408.58
Isol. from the marine sponge *Plakortis angulospiculatus*. Cytotoxic. Oil. $[\alpha]_D$ +110 (c, 0.1 in CH_2Cl_2).

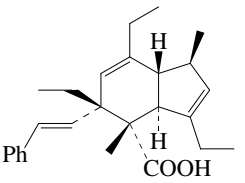
Lower homologue ($R^1 = CH_2CH_3$, $R^2 = R^3 = CH_3$): ***Norspiculoic acid***
$C_{26}H_{34}O_3$ 394.553
Isol. from *Plakortis zyggompha*. Oil. $[\alpha]_D^{24}$ +147.8 (c, 0.11 in CH_2Cl_2).

Lower homologue ($R^1 = R^2 = R^3 = CH_3$): ***Dinorspiculoic acid***
$C_{25}H_{32}O_3$ 380.526
Isol. from *Plakortis zyggompha*. Oil. $[\alpha]_D^{24}$ +65.4 (c, 0.09 in CH_2Cl_2).

Analogue ($R^1 = R^2 = CH_2CH_3$, $R^3 = CH_3$): ***Isospiculoic acid A***
$C_{27}H_{36}O_3$ 408.58
Isol. from *Plakortis zyggompha*. Oil. $[\alpha]_D^{24}$ +134.4 (c, 0.16 in CH_2Cl_2).

Huang, X.-H. *et al., Org. Lett.*, 2004, **6**, 75-78 (*isol, pmr, cmr*)
Berrué, F. *et al., J. Nat. Prod.*, 2005, **68**, 547-549 (*analogues*)
Kirkham, J.E.D. *et al., Chem. Comm.*, 2006, 2863-2865 (*synth, abs config*)

Spiculoic acid B S-308

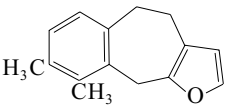


$C_{26}H_{34}O_2$ 378.553
Isol. from the marine sponge *Plakortis angulospiculatus*. Oil. $[\alpha]_D$ -22 (c, 0.1 in CH_2Cl_2).

Huang, X.-H. *et al., Org. Lett.*, 2004, **6**, 75-78 (*isol, pmr, cmr*)

Spiniferin 2 S-309

[59806-74-5]



$C_{15}H_{16}O$ 212.291
Constit. of *Pleraplysilla spinifera* and mollusc *Hypselodoris daniellae*. Unstable oil. λ_{max} 223 (ϵ 9200); 229 (ϵ 10500); 265 (ϵ 550) (hexane) (Berdy).

Cimino, G. *et al., Tet. Lett.*, 1975, 3727 (*isol*)
Cimino, G. *et al., Experientia*, 1978, **34**, 1425 (*struct*)
Schulte, G.R. *et al., Tetrahedron*, 1982, **38**, 1857 (*isol*)

Spinochrome G S-310

Pigment from spines of *Paracentrotus lividus*.
Deep-violet cryst. (EtOAc/petrol).
Mp 340°.

Goodwin, T.W. *et al., Experientia*, 1951, **7**, 375 (*isol*)
Lederer, E. *et al., Biochim. Biophys. Acta*, 1952, **9**, 92 (*isol*)

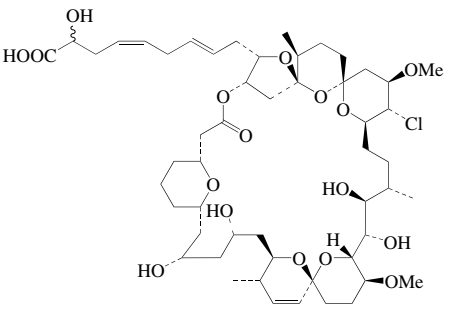
Spinochrome P S-311

$C_{12}H_{10}O_7$ 266.207
Struct. unknown. Pigment of sea urchin, Mediterranean *Paracentrotus lividus*. Deep garnet-red cryst. (dioxan aq.).

Tri-Me ether:
$C_{15}H_{16}O_7$ 308.287
Cryst. Mp 165-166°.

Musajo, L. *et al., Gazz. Chim. Ital.*, 1940, **70**, 287 (*isol*)
Goodwin, T.W. *et al., Experientia*, 1951, **7**, 375 (*isol*)

Spirastrellolide A S-312



Relative Configuration

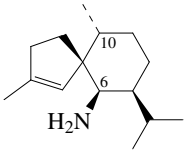
$C_{52}H_{81}ClO_{17}$ 1013.654

Struct. revised in 2004. Isol. from the sponge *Spirastrella coccinea*. Antimitotic agent. Oil (as Me ester). $[\alpha]_D^{25}$ +27 (c, 0.16 in CH_2Cl_2) (Me ester).

Williams, D.E. *et al., J.A.C.S.*, 2003, **125**, 5296-5297 (*isol*)
Williams, D.E. *et al., Org. Lett.*, 2004, **6**, 2607-2610 (*struct*)

1-Spiroaxen-6-amine S-313

6-Amino-1-spiroaxene



$C_{15}H_{27}N$ 221.385

(6β,10α)-*form*

N-*Formyl:* ***Axamide 3***
[59633-82-8]
$C_{16}H_{27}NO$ 249.395
Constit. of sponges *Axinella cannabina* and *Axinella cavernosa*. Oil. $[\alpha]_D$ -6.86 (c, 1 in $CHCl_3$).

Isocyanide: ***Axisonitrile 3***
[59633-83-9]
$C_{16}H_{25}N$ 231.38
Isol. from *Axinella cannabina*, *Topsentia*sp., *Ciocalypta* sp., *Acanthella* sp., *Axinyssa aplysinoides* and *Phyllidia pustulosa*. Shows strong antimycobacterial activity. Anthelmintic, antifouling agent, larval settlement inhibitor, spongicide. Cryst. (petrol). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 101-103°. $[\alpha]_D$ +68.44 (c, 1 in $CHCl_3$). Has -NCS replacing -NH_2.

Isothiocyanate: ***Axisothiocyanate 3***
[59633-81-7]
$C_{16}H_{25}NS$ 263.446
From *Axinella cannabina*. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +165.2 (c, 1 in $CHCl_3$). Has -NCS replacing -NHCHO.

(6β,10β)-*form* [509078-99-3]

N-*Formyl:* ***Exiguamide***
[481054-36-8]
$C_{16}H_{27}NO$ 249.395
Constit. of *Geodia exigua*. Cryst. (MeOH aq.).
Mp 139-140°. $[\alpha]_D^{25}$ +31.7 (c, 0.08 in $CHCl_3$).

N-*Methoxycarbonyl:* ***Exicarbamate***
[509095-16-3]
$C_{17}H_{29}NO_2$ 279.422
Constit. of *Geodia exigua*. Oil. $[\alpha]_D^{25}$ +28 (c, 0.02 in $CHCl_3$).

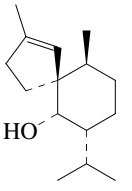
N-*[[(*N-*Methoxycarbonylmethyl)*-N-*methylamino]acetyl]:* ***Exigurin***
[509095-20-9]
$C_{21}H_{36}N_2O_3$ 364.527
Constit. of *Geodia exigua*. Oil. $[\alpha]_D^{25}$ -32 (c, 0.03 in $CHCl_3$).

Isocyanide: ***10-Epiaxisonitrile 3***
[178963-62-7]
$C_{16}H_{25}N$ 231.38
Constit. of *Phyllidia pustulosa* and *Phyllidia acelata*. Antifouling agent; larval settlement inhibitor. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{23}$ -5.6 (c, 0.025 in $CHCl_3$).

Blasio, B.Di. *et al., Tetrahedron*, 1976, **32**, 473-478 (*Axisonitrile 3, Axisothiocyanate 3, Axamide 3*)
Fusetani, N. *et al., Tet. Lett.*, 1992, **33**, 6823-6826 (*Axisonitrile 3*)
Hirota, H. *et al., Tetrahedron*, 1996, **52**, 2359-2368 (*Axisothiocyanate 3, Axamide 3*)
Okino, T. *et al., Tetrahedron*, 1996, **52**, 9447-9454 (*10-Epiaxisonitrile 3*)
Koenig, G.M. *et al., Planta Med.*, 2000, **66**, 337-342 (*Axisonitrile 3, activity*)
Uy, M.M. *et al., Bioorg. Med. Chem. Lett.*, 2002, **12**, 3037-3038 (*Exiguamide, cryst struct*)
Uy, M.M. *et al., Tetrahedron*, 2003, **59**, 731-736 (*Exiguamide, Exicarbamate, Exigurin, cryst struct*)

1-Spiroaxen-6-ol S-314

2,10-Dimethyl-7-(1-methylethyl)spiro[4.5]dec-1-en-6-ol, 8CI. 7-Isopropyl-2,10-dimethylspiro[4.5]dec-1-en-6-ol



6α-*form*

$C_{15}H_{26}O$ 222.37

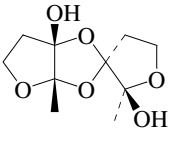
6α-form [119432-99-4]
Constit. of a *Eurypon* sp.
Oil. $[\alpha]_D$ +1.3 (c, 0.6 in $CHCl_3$).

(*ent*-6α)-*form*
Gleenol. *Glehnol*
[72203-99-7]
Constit. of *Picea glehnii* and *Juniperus oxycedrus*.
Oil. $[\alpha]_D^{20}$ -15 (c, 5 in $CHCl_3$).

Kurvyakov, P.I. *et al., Khim. Prir. Soedin.*, 1979, **15**, 164-167; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 138-140 (*Gleenol*)
Barrow, C.J. *et al., Aust. J. Chem.*, 1988, **41**, 1755-1761 (*6α-form*)
Barrero, A.F. *et al., Phytochemistry*, 1991, **30**, 1551-1554 (*Gleenol*)
Ohira, S. *et al., Chem. Lett.*, 1998, 739-740 (*Gleenol, synth abs config*)

Spirobispinnaketal S-315

[96817-38-8]



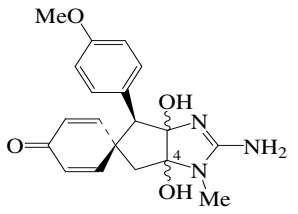
Relative Configuration

$C_{10}H_{16}O_6$ 232.233

Dimer of 5-Hydroxy-2,3-pentanedione, H-891. Constit. of *Laurencia pinnatifida*.

Wiedenfeld, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1985, **318**, 289-293 (*isol, cryst struct*)
Bernart, M.W. *et al., Phytochemistry*, 1992, **31**, 1273-1276 (*synth*)

Spirocalcaridine A S-316



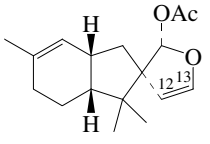
$C_{19}H_{21}N_3O_4$ 355.393
Isol. from the calcareous sponge *Leucetta* sp.
Yellow oil. $[\alpha]_D$ -59.3 (c, 0.11 in MeOH).

4-Me ether: ***Spirocalcaridine B***
$C_{20}H_{23}N_3O_4$ 369.419
Isol. from *Leucetta* sp. Yellow oil. $[\alpha]_D$ -50.8 (c. 0.13 in MeOH).

Edrada, R.A. *et al., J. Nat. Prod.*, 2003, **66**, 939-942 (*isol, pmr, cmr*)

Spirodysin S-317

[70546-66-6]



$C_{17}H_{24}O_3$ 276.375
Constit. of *Dysidea herbacea*. Unstable oil. $[\alpha]_D^{20}$ +24 (c, 1 in $CHCl_3$).

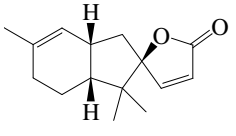
O-*De-Ac, Me ether:* [258874-64-5]
$C_{16}H_{24}O_2$ 248.364
Constit. of *Dysidea fragilis.* Oil. $[\alpha]_D^{25}$ -47 (c, 1 in $CHCl_3$).

12,13-Dihydro, O-*de-Ac, Me ether:* [258874-65-6]
$C_{16}H_{26}O_2$ 250.38
Constit. of *Dysidea fragilis.* Oil. $[\alpha]_D^{25}$ +195 (c, 1 in $CHCl_3$).

Kazlauskas, R. *et al., Tet. Lett.*, 1978, 4949
Reddy, N.S. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 1002-1004 (*Dysidea fragilis constits*)
Cameron, G.M. *et al., Tetrahedron*, 2000, **56**, 5247-5252 (*struct*)

Spirofragilide S-318

[313510-14-4]

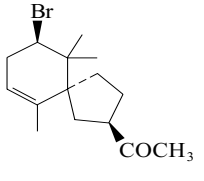


$C_{15}H_{20}O_2$ 232.322
Constit. of *Dysidea fragilis.* Oil. $[\alpha]_D^{25}$ -96 (c, 1 in $CHCl_3$). λ_{max} 224 (ϵ 8400) (EtOH).

Reddy, N.S. *et al., Indian J. Chem., Sect. B*, 2000, **39**, 393-395 (*isol, pmr, cmr*)

Spirolaurenone S-319

[30925-25-8]

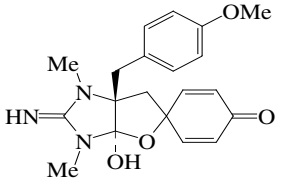


$C_{15}H_{23}BrO$ 299.25
Constit. of the essential oil of *Laurencia glandulifera*. Oil. $[\alpha]_D$ -70.6 (c, 1.26 in $CHCl_3$).

Semicarbazone:
Cryst. Mp 165-170°.

Suzuki, M. *et al., Tet. Lett.*, 1970, 4995 (*isol, struct*)
Suzuki, M. *et al., Tetrahedron*, 1980, **36**, 1551 (*abs config*)
Murai, A. *et al., Tet. Lett.*, 1982, **23**, 2887 (*synth*)

Spiroleucettadine S-320



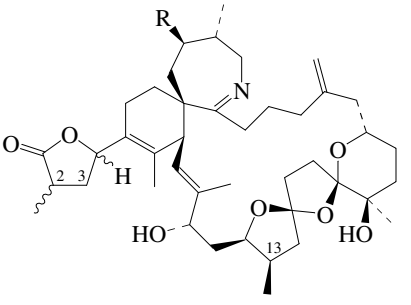
Absolute Configuration

$C_{20}H_{23}N_3O_4$ 369.419
Alkaloid from a *Leucetta* sp. Yellow powder. $[\alpha]_D$ -27.1 (c, 0.38 in MeOH). λ_{max} 227 (ϵ 2410) (MeOH).

Ralifo, P. *et al., J.O.C.*, 2004, **69**, 9025-9029 (*isol, pmr, cmr*)

Spirolide B S-321

[170713-72-1]



Relative Configuration

R = H

$C_{42}H_{63}NO_7$ 693.962
Isol. from *Alexandrium ostenfeldii* found in various contaminated shellfish such as *Mytilus edulis*, *Placopecten magellanicus.* Calcium channel activating agent, phycotoxin.

2,3-Didehydro: ***Spirolide A***
$C_{42}H_{61}NO_7$ 691.946
Isol. from *Alexandrium ostenfeldii* in contaminated shellfish.

Hu, T. *et al., Chem. Comm.*, 1995, 2159-2161 (*isol, pmr, cmr, ms*)
Hu, T. *et al., J. Nat. Prod.*, 2001, **64**, 308-312 (*Spirolide A*)
Falk, M. *et al., Tetrahedron*, 2001, **57**, 8659-8665 (*config*)
Sleno, L. *et al., Anal. Bioanal. Chem.*, 2004, **378**, 969-976; 977-986 (*isol, ms*)

Spirolide D S-322

[170713-73-2]
As Spirolide B, S-321 with
R = CH_3
$C_{43}H_{65}NO_7$ 707.989
Isol. from *Alexandrium ostenfeldii* found in contaminated shellfish. Ca channel activator; phycotoxin.

2,3-Didehydro: ***Spirolide C***
[318996-49-5]
$C_{43}H_{63}NO_7$ 705.973
Isol. from *Alexandrium ostenfeldii* in contaminated shellfish.

13-Demethyl: ***13-Demethylspirolide D***
$C_{42}H_{63}NO_7$ 693.962
Isol. from *Alexandrium ostenfeldii*.

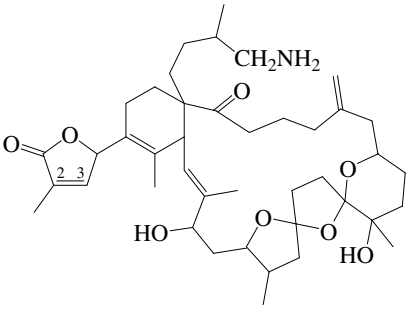
13-Demethyl, 2,3-didehydro: ***13-Demethylspirolide C****. 13-Desmethylspirolide C*
[334974-07-1]
$C_{42}H_{61}NO_7$ 691.946
Isol. from *Alexandrium ostenfeldii* in contaminated shellfish.

13,19-Didemethyl, 2,3-didehydro: ***13,19-Didemethylspirolide C***
$C_{41}H_{59}NO_7$ 677.92
Isol. from *Alexandrium ostenfeldii*.

Hu, T. *et al., Chem. Comm.*, 1995, 2159-2161 (*isol, pmr, cmr, ms*)
Hu, T. *et al., J. Nat. Prod.*, 2001, **64**, 308-312 (*Spirolide C, 13-Demethylspirolide C*)
Falk, M. *et al., Tetrahedron*, 2001, **57**, 8659-8665 (*config*)
Sleno, L. *et al., Anal. Bioanal. Chem.*, 2004, **378**, 969-976; 977-986 (*isol, ms*)
MacKinnon, S.L. *et al., J. Nat. Prod.*, 2006, **69**, 983-987 (*13,19-Didemethylspirolide C*)
MacKinnon, S.L. *et al., J.O.C.*, 2006, **71**, 8724-8731 (*13-Demethylspirolide C, biosynth*)

Spirolide E S-323

[183159-71-9]



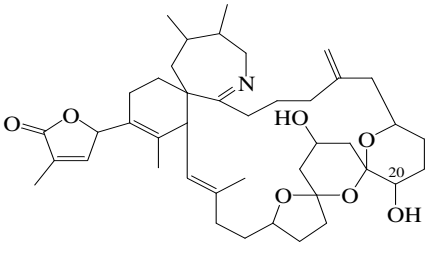
$C_{42}H_{63}NO_8$ 709.962
Isol. from *Alexandrium ostenfeldii* found in contaminated shellfish.

2,3-Dihydro: ***Spirolide F***
[183159-73-1]
$C_{42}H_{65}NO_8$ 711.977
Isol. from *Alexandrium ostenfeldii* in contaminated shellfish.

Hu, T. *et al., Tet. Lett.*, 1996, **37**, 7671-7674 (*isol, pmr, cmr, ms*)
Sleno, L. *et al., Anal. Bioanal. Chem.*, 2004, **378**, 969-976; 977-986 (*isol, ms*)

Spirolide G S-324

[849215-96-9]



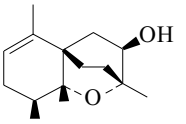
$C_{42}H_{61}NO_7$ 691.946
Isol. from *Alexandrium ostenfeldii* in contaminated shellfish.

20-Methyl: ***20-Methylspirolide G***
[849215-95-8]
$C_{43}H_{63}NO_7$ 705.973
Isol. from *Alexandrium ostenfeldii* in contaminated shellfish.

Aasen, J. *et al., Chem. Res. Toxicol.*, 2005, **18**, 509-515 (*isol, pmr, cmr, ms*)
MacKinnon, S.L. *et al., J. Nat. Prod.*, 2006, **69**, 983-987 (*isol, pmr, cmr, ms*)
Aasen, J. *et al., Rapid Commun. Mass Spectrom.*, 2006, **20**, 1531-1537 (*20-Methylspirolide G esters*)

Spironippol S-325

[80981-64-2]



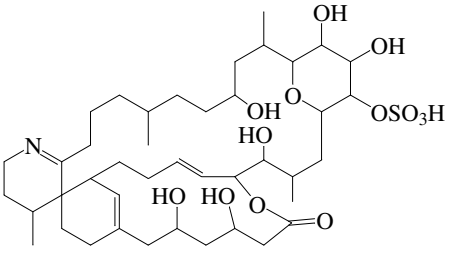
Relative configuration

$C_{15}H_{24}O_2$ 236.353
Constit. of *Laurencia nipponica*. Cryst.
Mp 135-136°. $[\alpha]_D$ +59.1.

Fukuzawa, A. *et al., Tet. Lett.*, 1981, **22**, 4087 (*cryst struct*)

Spiroprorocentrimine S-326

[339176-79-3]

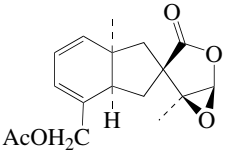


$C_{42}H_{69}NO_{13}S$ 828.072
Isol. from the marine dinoflagellate *Prorocentrum* sp. Cryst. (MeOH). $[\alpha]_D$ -51.4 (c, 0.28 in MeOH). Dec. at 230°. λ_{max} 214 (ϵ 5200) (MeOH).

Lu, C.-K. *et al., Tet. Lett.*, 2001, **42**, 1713-1716 (*isol, pmr, cmr, cryst struct*)

Spirotubipolide S-327

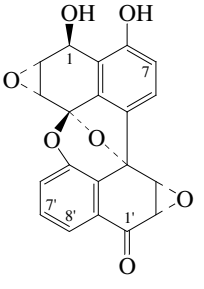
[111233-41-1]



$C_{17}H_{20}O_5$ 304.342
Isol. from the marine stolonifer *Tubipora musica*. Cryst. $[\alpha]_D$ -194 (c, 0.3 in $CHCl_3$). λ_{max} 262 (ϵ 4520) (No solvent reported).

Iguchi, K. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3531-3533 (*isol, uv, pmr, cmr*)

Spiroxin D S-328



Relative Configuration

$C_{20}H_{12}O_7$ 364.311
Prod. by a marine-derived fungus sp.Ll374248. Antitumour agent.

1-Ketone: ***Spiroxin C***
$C_{20}H_{10}O_7$ 362.295
Prod. by a marine-derived fungus sp. Ll374248. Antitumour agent. $[\alpha]_D^{25}$ -706 (c, 0.26 in MeOH). λ_{max} 256 (ϵ 13180); 329 (ϵ 4690) (MeOH). λ_{max} 265 (ϵ 13184); 329 (ϵ 4688) (MeOH) (Berdy).

1-Ketone, 7-chloro, 8′-hydroxy: ***Spiroxin A***
[225233-83-0]
$C_{20}H_9ClO_8$ 412.739
Prod. by a marine-derived fungus sp. Ll374248. Antitumour agent. $[\alpha]_D^{25}$ -644 (c, 0.18 in MeOH). λ_{max} 265 (ϵ 14090); 382 (ϵ 5600) (MeOH).

1-Ketone, 7,7′-dichloro, 8′-hydroxy: ***Spiroxin B****. Antibiotic F 12517. F 12517*
[208466-53-9]
$C_{20}H_8Cl_2O_8$ 447.184
Prod. by a marine-derived fungus sp. Ll374248 and by *Vibrissea filisporia* sp. SANK18796. Antitumour and antibacterial agent. $[\alpha]_D^{25}$ -475 (c, 0.21 in MeOH). λ_{max} 265 (sh) (ϵ 11630); 385 (ϵ 6220) (MeOH).

1-Ketone, 1′β-alcohol, 7,7′-dichloro, 8′-hydroxy: ***Spiroxin E***
$C_{20}H_{10}Cl_2O_8$ 449.2
Prod. by a marine-derived fungus sp.Ll374248. Antitumour agent.

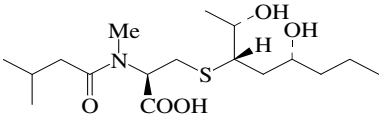
Japan. Pat., 1998, 98 114 778; *CA*, **129**, 40198j
McDonald, L.A. *et al., Tet. Lett.*, 1999, **40**, 2489-2492 (*isol, uv, pmr, cmr, ms*)
Wang, T. *et al., Can. J. Chem.*, 2001, **79**, 1786-1791 (*Spiroxin A, abs config*)
Miyashita, K. *et al., Org. Lett.*, 2003, **5**, 2683-2686 (*synth*)
Krohn, K. *et al., Prog. Chem. Org. Nat. Prod.*, 2003, **85**, 1-49 (*rev*)

Spirulan S-329

[172929-12-3]
Sulfated polysaccharide antibiotic of unknown struct. Composed of two types of repeating disaccharide units; *O*-rhamnosylacofriose and *O*-hexuronosylrhamnose (aldobiuronic acid). Characterised as the Ca deriv. Calcium spirulan, to which CAS no. refers. Isol. from the blue-green alga *Spirulina platensis*. Antiviral agent. Amorph. powder. (as Ca deriv.). $[\alpha]_D$ +14.7 (c, 0.6 in H_2O) (Ca deriv.).

Hayashi, T. *et al., J. Nat. Prod.*, 1996, **59**, 83-87; 1998, **61**, 1101-1104 (*isol, purifn, hplc, activity, ms*)
Lee, J.-B. *et al., J. Nat. Prod.*, 2000, **63**, 136-138 (*ms, struct*)

Spongiacysteine S-330



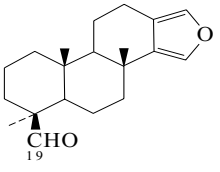
Absolute Configuration

$C_{17}H_{33}NO_5S$ 363.517
Isol. from the Japanese sponge *Spongia* sp. Oil. $[\alpha]_D^{20}$ -238 (c, 0.02 in MeOH) (natural). $[\alpha]_D^{24}$ -115 (c, 0.02 in MeOH) (synthetic).

Kobayashi, K. *et al., Chem. Lett.*, 2004, **33**, 1262-1263 (*isol, synth, pmr, cmr*)

13(16),14-Spongiadien-19-al S-331

[74804-01-6]



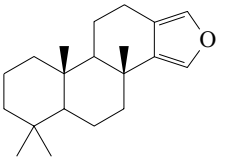
$C_{20}H_{28}O_2$ 300.44
Constit. of *Spongia officinalis*. Amorph. $[\alpha]_D$ -26.5 (c, 1 in $CHCl_3$). λ_{max} 220 (ϵ 3000) (EtOH) (Berdy).

19-Carboxylic acid: ***13(16),14-Spongiadien-19-oic acid***
[74813-86-8]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Spongia officinalis*. Cryst.
Mp 175-176°. $[\alpha]_D$ +15 (c, 1 in $CHCl_3$). λ_{max} 220 (ϵ 3600) (EtOH) (Berdy).

Capelle, N. *et al., Bull. Soc. Chim. Belg.*, 1980, **89**, 399
Vlad, P.F. *et al., Khim. Prir. Soedin.*, 1984, **20**, 725; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 685 (*synth*)

13(16),14-Spongiadiene S-332

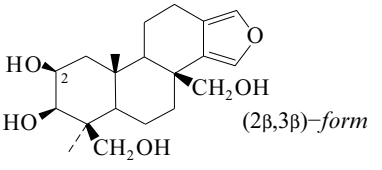
[74804-03-8]



$C_{20}H_{30}O$ 286.456
Constit. of *Spongia officinalis*. Cryst.
Mp 115-116°. $[\alpha]_D$ -32.7 (c, 0.26 in $CHCl_3$). λ_{max} 220 (ϵ 2900) (EtOH) (Berdy).

Capelle, N. *et al., Bull. Soc. Chim. Belg.*, 1980, **89**, 399
Nakano, T. *et al., J. Chem. Res., Synop.*, 1989, 54 (*synth*)
Sakamoto, T. *et al., Tetrahedron*, 1995, **51**, 5771 (*synth*)
Abad, A. *et al., J.C.S. Perkin 1*, 1996, 2193 (*synth*)
Arnó, M. *et al., Tetrahedron*, 1999, **55**, 12419-12428 (*synth*)

13(16),14-Spongiadiene-2,3,17,19-tetrol S-333



(2β,3β)–*form*

$C_{20}H_{30}O_5$ 350.454

(2β,3β)-*form*
Constit. of a *Spongia* sp.
Gum.

Tetra-Ac:
$C_{28}H_{38}O_9$ 518.603
Constit. of *Glossodoris atromarginata*. Oil. $[\alpha]_D$ -1.5 (c, 0.1 in $CHCl_3$).

2-Ketone: 3,17,19-Trihydroxy-13(16),14-spongiadien-2-one. ***Epispongiatriol***
[71302-29-9]
$C_{20}H_{28}O_5$ 348.438
Constit. of *Spongia* spp. Cryst. (EtOAc).
Mp 194.5-197°. $[\alpha]_D^{21}$ +26.3 (c, 0.5 in $CHCl_3$).

2-Ketone, 3-Ac:
$C_{22}H_{30}O_6$ 390.475
Constit. of *Glossodoris atromarginata*. Oil. $[\alpha]_D$ +8.3 (c, 0.1 in $CHCl_3$).

2-Ketone, 3,19-di-Ac:
$C_{24}H_{32}O_7$ 432.513
Constit. of *Glossodoris atromarginata*. Oil.

2-Ketone, 17,19-di-Ac:
$C_{24}H_{32}O_7$ 432.513
Constit. of *Glossodoris atromarginata*. Oil. $[\alpha]_D$ +2.1 (c, 0.14 in $CHCl_3$).

2-Ketone, tri-Ac: [71302-31-3]
Constit. of *Spongia* spp.
Cryst. (MeOH).
Mp 185-186.5°. $[\alpha]_D^{21}$ +31.5 (c, 1 in $CHCl_3$).

3α-form

2-Ketone: ***Spongiatriol***
[71302-27-7]
Constit. of *Spongia* spp. Hypotensive agent. Cryst. (EtOAc).
Mp 157.5-160.5°. $[\alpha]_D^{21}$ +142.5 (c, 0.5 in $CHCl_3$).

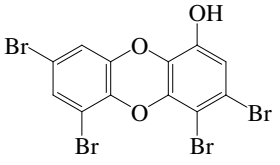
2-Ketone, 3,19-di-Ac:
$C_{24}H_{32}O_7$ 432.513
Constit. of *Glossodoris atromarginata*. Oil.

2-Ketone, tri-Ac: [71302-25-5]
$C_{26}H_{34}O_8$ 474.55
Constit. of *Spongia* spp. Cryst. (MeOH).
Mp 157.5-158.5°. $[\alpha]_D^{25}$ +11.8 (c, 1 in $CHCl_3$).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1979, **32**, 867 (*Spongiatriol, Epispongiatriol*)
Gunasekera, S.P. *et al., J.O.C.*, 1991, **56**, 1250 (*isol, pmr, cmr*)
Fontana, A. *et al., J. Nat. Prod.*, 1997, **60**, 444-448 (*isol, pmr, cmr*)

Spongiadioxin A S-334

*3,4,6,8-Tetrabromodibenzo[*b,e*][1,4]dioxin-1-ol. 3,4,6,8-Tetrabromo-1-hydroxydibenzo[*b,e*]dioxin*
[329040-77-9]



$C_{12}H_4Br_4O_3$ 515.778
Isol. from the sponge *Dysidea dendyi*. Cytotoxic. Needles ($CHCl_3$).
Mp 241-242°. λ_{max} 242 (log ϵ 3.97); 295 (log ϵ 3.06) (EtOH).

*Me ether: 1,2,7,9-Tetrabromo-4-methoxydibenzo[*b,e*][1,4]dioxin.* **O-*Methylspongiadioxin A***
[329025-15-2]
$C_{13}H_6Br_4O_3$ 529.805
Isol. from *Dysidea dendyi*. Needles ($CHCl_3$) (semisynthetic).
Mp 208-209° (semisynthetic).

*4-Debromo: 3,6,8-Tribromodibenzo[*b,e*][1,4]dioxin-1-ol. 3,6,8-Tribromo-1-hydroxydibenzo[*b,e*]dioxin.* ***Spongiadioxin C***
[460092-06-2]
$C_{12}H_5Br_3O_3$ 436.882
Isol. from *Dysidea dendyi*. Needles ($CHCl_3$).
Mp 203-205°. λ_{max} 241 (log ϵ 3.97); 295 (log ϵ 2.88) (EtOH).

*4-Debromo, Me ether: 1,3,8-Tribromo-6-methoxydibenzo[*b,e*][1,4]dioxin.* **O-*Methylspongiadioxin C***
[459433-06-8]
$C_{13}H_7Br_3O_3$ 450.909
Isol. from *Dysidea dendyi*. Needles ($CHCl_3$).
Mp 205-207°. λ_{max} 239 (log ϵ 3.97); 294 (log ϵ 2.86) (EtOH).

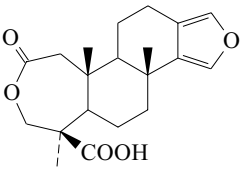
*4-Debromo, 2-bromo: 2,3,6,8-Tetrabromodibenzo[*b,e*][1,4]dioxin-1-ol. 2,3,6,8-Tetrabromo-1-hydroxydibenzo[*b,e*]dioxin.* ***Spongiadioxin B***
[329040-81-5]
$C_{12}H_4Br_4O_3$ 515.778
Isol. from *Dysidea dendyi*. Cytotoxic. Needles ($CHCl_3$).
Mp 245-247°. λ_{max} 242 (log ϵ 3.97); 295 (log ϵ 3.06) (EtOH).

*4-Debromo, 2-bromo, Me ether: 2,3,6,8-Tetrabromo-1-methoxydibenzo[*b,e*][1,4]dioxin.* **O-*Methylspongiadioxin B***
[329025-16-3]
$C_{13}H_6Br_4O_3$ 529.805
Isol. from *Dysidea dendyi*. Needles ($CHCl_3$) (semisynthetic).
Mp 204-206° (semisynthetic).

Utkina, N.K. *et al., J. Nat. Prod.*, 2001, **64**, 151-153; 2002, **65**, 1213-1215 (*isol, synth, uv, ir, pmr, cmr, cryst struct*)

Spongialactone A S-335

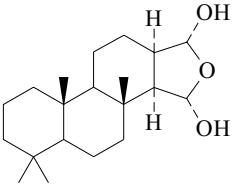
2,3-Seco-2,3-spongianolid-19-oic acid
[120030-04-8]



$C_{20}H_{26}O_5$ 346.422
Constit. of *Spongia arabica*. Amorph. powder.

Hirsch, S. *et al., J. Nat. Prod.*, 1988, **51**, 1243 (*isol, pmr, cmr*)

15,16-Spongianediol S-336



$C_{20}H_{34}O_3$ 322.487

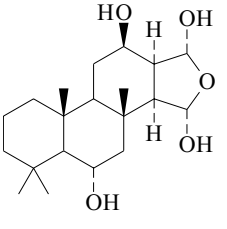
(15α,16α)-form

Di-Ac: ***15α,16α-Diacetoxyspongian***
[84809-50-7]
$C_{24}H_{38}O_5$ 406.561
Constit. of *Spongia officinalis*. Cryst.
Mp 151-153°. $[\alpha]_D$ -23 (c, 1.1 in $CHCl_3$).

Diketone: ***15,16-Spongianedione***
$C_{20}H_{30}O_3$ 318.455
Isol. from *Dictyodendrilla cavernosa*. Cryst.
Mp 154°. $[\alpha]_D$ +21.4 (c, 0.0014 in $CHCl_3$).

Cimino, G. *et al., Tet. Lett.*, 1982, **23**, 4139
Kernan, M.R. *et al., J. Nat. Prod.*, 1990, **53**, 724

6,12,15,16-Spongianetetrol S-337



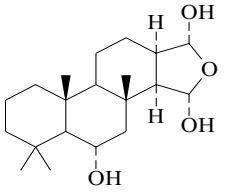
$C_{20}H_{34}O_5$ 354.486

(6α,12β,15α,16α)-form

Tetra-Ac: 6,12,15,16-Tetraacetoxyspongiane
[137836-66-9]
$C_{28}H_{42}O_9$ 522.634
Constit. of *Chromodoris geminus*. Glass. $[\alpha]_D$ +40 (c, 0.7 in $CHCl_3$).

De Silva, E.D. *et al., J. Nat. Prod.*, 1991, **54**, 993 (*isol, pmr, cmr*)

6,15,16-Spongianetriol S-338

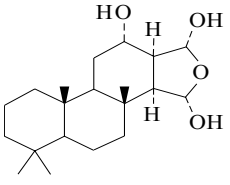


$C_{20}H_{34}O_4$ 338.486

(6α,15α,16α)-*form*

Tri-Ac: 6,15,16-Triacetoxyspongiane
[137836-65-8]
$C_{26}H_{40}O_7$ 464.598
Constit. of *Chromodoris geminus*. Glass. $[\alpha]_D$ +3 (c, 0.3 in $CHCl_3$).
De Silva, E.D. *et al., J. Nat. Prod.*, 1991, **54**, 993 (*isol, pmr, cmr*)

12,15,16-Spongianetriol S-339



$C_{20}H_{34}O_4$ 338.486

(12α,15α,16α)-*form*

15,16-Di-Ac: ***12-Deacetylaplysillin***
$C_{24}H_{38}O_6$ 422.561
Constit. of *Spongia zimocca*.
$[\alpha]_D^{25}$ +7.5 (c, 1.33 in $CHCl_3$).

Tri-Ac: ***Aplysillin***
[71393-11-8]
$C_{26}H_{40}O_7$ 464.598
Constit. of *Aplysilla rosea*. Cryst.
Mp 169-171°. $[\alpha]_D^{20}$ +13 (c, 0.5 in $CHCl_3$).

(12β,15α,16α)-*form*

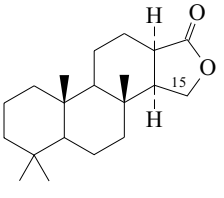
15,16-Di-Ac: ***12-Deacetyl-12-epiaplysillin***
[128269-69-2]
$C_{24}H_{38}O_6$ 422.561
Constit. of *Chromodoris luteorosea*. Ichtyotoxic. Cryst.
Mp 192-197°. $[\alpha]_D^{25}$ +2.5 (c, 0.4 in $CHCl_3$).

Tri-Ac: ***12-Epiaplysillin***
[128201-23-0]
$C_{26}H_{40}O_7$ 464.598
Constit. of *Chromodoris luteorosea* and *Chromodoris geminus*.
Ichthyotoxic. $[\alpha]_D^{25}$ +8.2 (c, 0.4 in $CHCl_3$).

Kazlauskas, R. *et al., Tet. Lett.*, 1979, 903 (*cryst struct*)
Cimino, G. *et al., J. Nat. Prod.*, 1990, **53**, 102 (*isol, pmr, cmr*)
De Silva, E.D. *et al., J. Nat. Prod.*, 1991, **54**, 993 (*12-Epiaplysillin, isol*)
Zubia, E. *et al., J. Nat. Prod.*, 1994, **57**, 725 (*12-Deacetylaplysillin*)

16-Spongianone S-340

[129704-83-2]



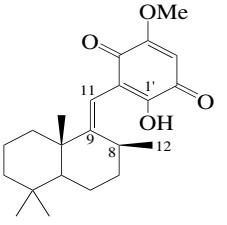
$C_{20}H_{32}O_2$ 304.472

Isol. from *Chelonaplysilla violacea*, *Chromodoris inopinata* and *Dictyodendrilla cavernosa*. Platelets (pentane/Et_2O).
Mp 200° (155-159°). $[\alpha]_D$ +53 (c, 0.001 in $CHCl_3$). $[\alpha]_{Hg}$ -2.3 (c, 1 in $CHCl_3$).

Hambley, T.W. *et al., Aust. J. Chem.*, 1990, **43**, 1861-1870 (*isol, pmr, cmr, ms*)
Kernan, M.R. *et al., J. Nat. Prod.*, 1990, **53**, 724-727 (*isol, pmr, cmr*)
Dilip de Silva, E. *et al., J. Nat. Prod.*, 1991, **54**, 993-997 (*isol*)
Pattenden, G. *et al., J.C.S. Perkin 1*, 1998, 863-868 (*synth*)

Spongiaquinone S-341

[69672-67-9]



$C_{22}H_{30}O_4$ 358.477
Constit. of *Stelospongia conulata*. Red cryst. (hexane).
Mp 159-160°. λ_{max} 286 (ϵ 19500); 530 (ϵ 1740) (EtOH/KOH) (Derep). λ_{max} 282 (ϵ 18200); 450 (ϵ 891) (EtOH) (Derep). λ_{max} 282 (ϵ 18200); 450 (ϵ 990) (EtOH) (Berdy). λ_{max} 286 (ϵ 19500); 530 (ϵ 1740) (EtOH-NaOH) (Berdy).

9α,11-Dihydro, 8,12-didehydro: See Hyatellaquinone, H-423

1′-Deoxy: ***Deoxyspongiaquinone***
[179900-96-0]
$C_{22}H_{30}O_3$ 342.477
Constit. of a sponge *Euryspongia* sp. Yellow oil. $[\alpha]_D$ +164 (c, 7.48 in $CHCl_3$). λ_{max} 203 (ϵ 15000); 222 (sh) (ϵ 13000); 255 (sh) (ϵ 8700); 320 (ϵ 4000); 404 (ϵ 1250) (EtOH). λ_{max} 203 (ϵ 15000); 320 (ϵ 4000); 404 (ϵ 1250) (MeOH) (Berdy).

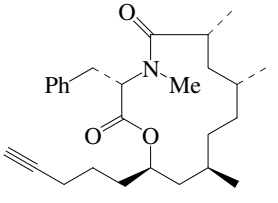
1′-Deoxy, 2′,5′-quinol: ***Deoxyspongiaquinol***
[179900-98-2]
$C_{22}H_{32}O_3$ 344.493
Constit. of *Euryspongia* sp. Yellow oil. $[\alpha]_D$ +67 (c, 10.8 in $CHCl_3$). λ_{max} 207 (ϵ 23000); 218 (sh) (ϵ 20000); 246 (sh) (ϵ 7000); 252 (sh) (ϵ 5700); 300 (ϵ 3600) (EtOH).

*1′-Deoxy, 11-chloro, 9(11)*E*-isomer:* ***Chlorodeoxyspongiaquinone***
[179900-97-1]
$C_{22}H_{29}ClO_3$ 376.922
Constit. of *Euryspongia* sp. Pale pink oil. $[\alpha]_D$ +40 (c, 0.1 in $CHCl_3$). Error in CAS struct. λ_{max} 202 (ϵ 38000); 218 (ϵ 25000); 260 (sh) (ϵ 8500); 293 (ϵ 5000) (EtOH).

*1′-Deoxy, 2′,5′-quinol, 11-chloro, 9(11)*E*-isomer:* ***Chlorodeoxyspongiaquinol***
[179900-99-3]
$C_{22}H_{31}ClO_3$ 378.938
Constit. of *Euryspongia* sp. Pale pink oil. $[\alpha]_D$ +37 (c, 0.27 in $CHCl_3$). Error in CAS struct. λ_{max} 203 (ϵ 47000); 218 (ϵ 44000); 256 (ϵ 15000); 294 (ϵ 5000) (EtOH).

Kazlauskas, R. *et al., Aust. J. Chem.*, 1978, **31**, 2685
Urban, S. *et al., Aust. J. Chem.*, 1996, **49**, 611-615 (*deoxy derivs*)
Bernet, A. *et al., Helv. Chim. Acta*, 2003, **86**, 2009-2020 (*synth*)

Spongidepsin S-342



Absolute Configuration

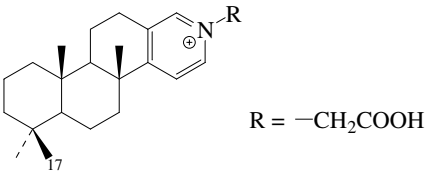
$C_{27}H_{39}NO_3$ 425.61

Isol. from a Vanuatu sponge *Spongia* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D$ -61.8 (c, 0.01 in MeOH). λ_{max} 210 (ϵ 2310); 258 (ϵ 750) (MeOH).

Grassia, A. *et al., Tetrahedron*, 2001, **57**, 6257-6260 (*isol, pmr, cmr*)
Chen, J. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 2148-2152 (*synth, abs config*)
Ferrié, L. *et al., Org. Lett.*, 2006, **8**, 3441-3443 (*synth*)

Spongidine A S-343

[263143-53-9]



$C_{23}H_{34}NO_2^{\oplus}$ 356.527
Alkaloid from a *Spongia* sp. Inhibitor of human phospholipase A_2. $[\alpha]_D$ -16.2 (c, 0.01 in MeOH). Counterion not specified.

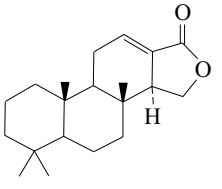
17-Acetoxy: ***Spongidine B***
[263143-54-0]
$C_{25}H_{36}NO_4^{\oplus}$ 414.564
Alkaloid from a *Spongia* sp. Inhibitor of human phospholipase A_2. $[\alpha]_D$ +7.8 (c, 0.01 in MeOH). Counterion not specified.
De Marino, S. *et al., J. Nat. Prod.*, 2000, **63**, 323-326

Spongidine D S-344

[263143-56-2]
As Spongidine A, S-343 with
R=-$CH_2CH_2SO_3H$
$C_{23}H_{36}NO_3S^{\oplus}$ 406.608
Alkaloid from a *Spongia* sp. Inhibitor of human phospholipase A_2. $[\alpha]_D$ -6 (c, 0.02 in MeOH). Counterion not specified.
De Marino, S. *et al., J. Nat. Prod.*, 2000, **63**, 323-326

12-Spongien-16-one S-345

Isoagatholactone
[53823-04-4]

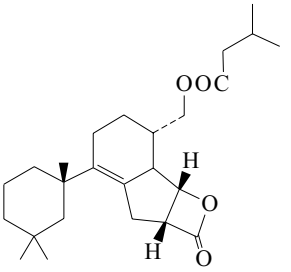


$C_{20}H_{30}O_2$ 302.456
Constit. of *Spongia officinalis*. Cryst. (MeOH). Poorly sol. hexane. Mp 153-155°. $[\alpha]_D$ +6.3 (c, 3 in $CHCl_3$). λ_{max} 222 (ϵ 6000) (cyclohexane) (Berdy).

Cimino, G. *et al., Tetrahedron*, 1974, **30**, 645 (*isol*)
Imamura, P.M. *et al., Chem. Comm.*, 1981, 734 (*synth*)
Nakano, T. *et al., Tet. Lett.*, 1982, **23**, 1423 (*synth*)
Vlad, P.F. *et al., Khim. Prir. Soedin.*, 1984, **20**, 725; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 685 (*synth*)
Abad, A. *et al., J.C.S. Perkin 1*, 1996, 2193 (*synth*)

Spongiolactone S-346

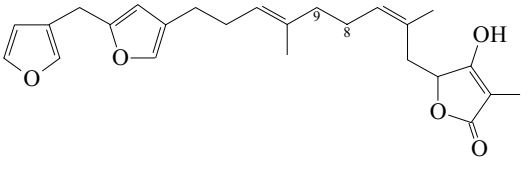
[113597-03-8]



$C_{25}H_{38}O_4$ 402.573
Constit. of *Spongionella gracilis*. Oil. $[\alpha]_D$ +67.6 (c, 1.7 in $CHCl_3$).
Mayol, L. *et al., Tet. Lett.*, 1987, **28**, 3601

Spongionellin† S-347

[99957-22-9]

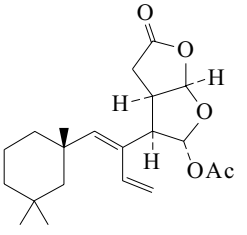


$C_{25}H_{30}O_5$ 410.509
Constit. of *Spongionella* spp. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ +16 (c, 0.1 in CH_2Cl_2).

*8,9-Didehydro(*E-*):* ***Dehydrospongionellin***
[99957-23-0]
$C_{25}H_{28}O_5$ 408.493
Constit. of *Spongionella* spp. Oil. $[\alpha]_D$ +21 (c, 0.1 in CH_2Cl_2). λ_{max} 221 (ϵ 5200); 270 (ϵ 9100); 279 (ϵ 11000); 290 (ϵ 8200) (EtOH) (Berdy).
Kato, Y. *et al., Chem. Lett.*, 1985, **10**, 1521 (*isol, pmr, cmr*)

Spongionellin† S-348

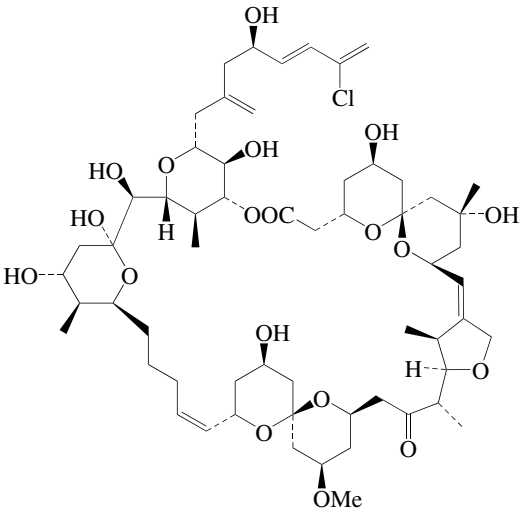
[106199-82-0]



$C_{21}H_{30}O_5$ 362.465
Constit. of sponge *Spongionella gracilis*. Amorph. solid. $[\alpha]_D$ +1.2 (c, 1.0 in $CHCl_3$). λ_{max} 234 (ϵ 11370) (MeOH) (Derep).
Mayol, L. *et al., Tetrahedron*, 1986, **42**, 5369

Spongistatin 5 S-349

[153698-80-7]



$C_{59}H_{89}ClO_{19}$ 1137.793

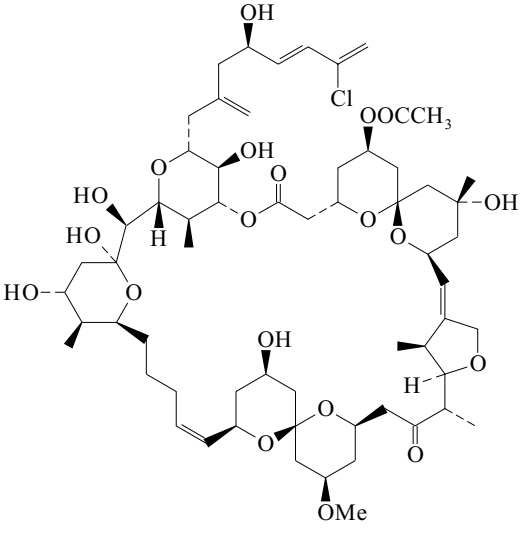
Macrocyclic lactone antibiotic. Isol. from the sponge *Spirastrella spinispirulifera*. Cytotoxic.
Mp 186-187°. $[\alpha]_D^{22}$ -11.1 (c, 0.2 in MeOH). λ_{max} 228 (ϵ 14840) (MeOH).

Dechloro: ***Spongistatin 7***
[158681-42-6]
$C_{59}H_{90}O_{19}$ 1103.349
Isol. from *Spirastrella spinispirulifera*. λ_{max} 223 (ϵ 17780) (MeOH).

Pettit, G.R. *et al., Chem. Comm.*, 1993, 1805-1807 (*isol, uv, ir, pmr, cmr, ms*)
Pettit, G.R. *et al., Nat. Prod. Lett.*, 1993, **3**, 239-244 (*Spongistatin 7*)

Spongistatin 9 S-350

[158734-19-1]



$C_{61}H_{91}ClO_{20}$ 1179.831

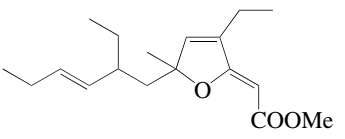
Polyether antibiotic. Isol. from the sponge *Spirastrella spinispirulifera*. Cytotoxic agent. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 164-165°. $[\alpha]_D^{22}$ -33.3 (c, 0.1 in MeOH). λ_{max} 227 (ϵ 13800); 268 (ϵ 1740) (MeOH) (Derep).

Dechloro: ***Spongistatin 8***
[158734-18-0]
$C_{61}H_{92}O_{20}$ 1145.386
Isol. from *Spirastrella spinispirulifera*. Cytotoxic agent. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane.
Mp 158-159°. $[\alpha]_D^{22}$ -32 (c, 0.2 in MeOH). λ_{max} 220 (ϵ 16000) (MeOH) (Derep).

Pettit, G.R. *et al., Chem. Comm.*, 1994, 1605 (*isol, pmr, cmr*)

Spongosoritin A S-351

[767314-30-7]

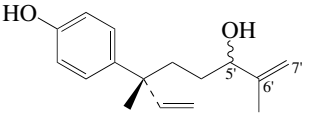


$C_{18}H_{28}O_3$ 292.417
Constit. of a Fijian marine sponge *Spongosorites* sp. and a Jamaican sponge *Plakortis* sp. Cytotoxic agent. Oil. $[\alpha]_D$ -148.1 (c, 1.54 in MeOH). λ_{max} 272 (ϵ 55700) (MeOH).

Hoye, T.R. *et al., CA*, 2004, **14**, 310907a
Capon, R.J. *et al., Aust. J. Chem.*, 2005, **58**, 18-20 (*isol, pmr, cmr*)

Sporochnol C S-352

[147821-61-2]



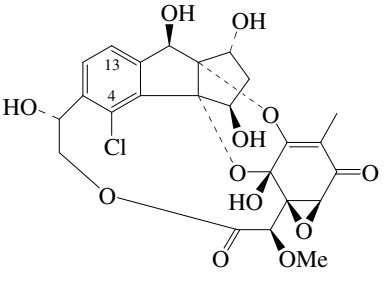
$C_{16}H_{22}O_2$ 246.349
Constit. of *Sporochnus bolleanus*. Feeding deterrent. Pale yellow gum. λ_{max} 224 (ϵ 6800); 277 (ϵ 1740) (MeOH) (Berdy).

6′,7′-Epoxide: ***Sporochnol B***
[147821-60-1]
$C_{16}H_{22}O_3$ 262.348
Constit. of *Sporochnus bolleanus*. Feeding deterrent. Pale yellow gum. λ_{max} 224 (ϵ 7400); 276 (ϵ 1470) (MeOH) (Berdy).

5′-Deoxy, Δ5′-Isomer: ***Sporochnol A***
[147821-59-8]
$C_{16}H_{22}O$ 230.349
Isol. from *Sporochnus bolleanus*. Feeding deterrent. Amorph. solid. $[\alpha]_D$ +10 (c, 1 in $CHCl_3$). λ_{max} 224 (ϵ 11000); 277 (ϵ 2180) (MeOH) (Berdy).

Shen, Y.-C. *et al., Phytochemistry*, 1993, **32**, 71-75 (*isol, pmr, cmr*)
Takahashi, M. *et al., Tetrahedron: Asymmetry*, 1997, **8**, 1235 (*Sporochnol A, synth, abs config*)
Bassindale, M.J. *et al., Tet. Lett.*, 2001, **42**, 9055-9057 (*Sporochnol A, synth*)
Ohira, S. *et al., Tet. Lett.*, 2002, **43**, 4641-4644 (*synth*)
Shan, S. *et al., Synth. Commun.*, 2004, **34**, 4005-4008 (*Sporochnol A, synth*)

Sporolide A S-353



Absolute Configuration

$C_{24}H_{23}ClO_{12}$ 538.891
Prod. by *Salinospora tropica* CNB-392. Amorph. solid.

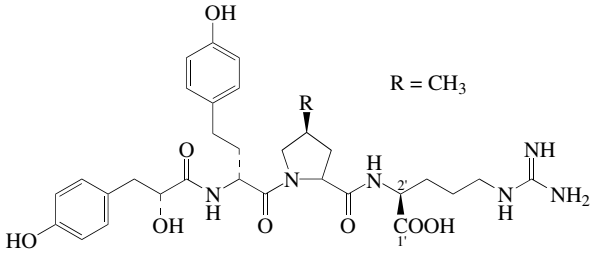
Mp 230-233° dec. $[\alpha]_D$ +80.7 (c, 0.22 in MeOH). λ_{max} 206 (log ϵ 4.5); 268 (log ϵ 3.9) (MeOH).

4-Dechloro, 13-chloro: ***Sporolide B***
$C_{24}H_{23}ClO_{12}$ 538.891
Prod. by *Salinospora tropica* CNB-392. Gum. $[\alpha]_D$ +8.6 (c, 0.17 in MeOH). λ_{max} 206 (log ϵ 4.5); 269 (log ϵ 3.9) (MeOH).

Buchanan, G.O. *et al., Org. Lett.*, 2005, **7**, 2731-2734 (*isol, pmr, cmr, cryst struct*)

Spumigin B1 S-354

[184682-39-1]



$C_{31}H_{42}N_6O_8$ 626.708
Isol. from the marine cyanobacterium *Nodularia spumigena* AV1. Phycotoxin, hepatotoxin. Sol. MeOH. $[\alpha]_D$ -9.9 (c, 0.04 in MeOH).

2′-Epimer: ***Spumigin B2***
[184682-40-4]
$C_{31}H_{42}N_6O_8$ 626.708
Isol. from the marine cyanobacterium *Nodularia spumigena* AV1. Phycotoxin, hepatotoxin. Sol. MeOH. $[\alpha]_D^{26}$ +2.8 (c, 0.04 in MeOH).

1′-Alcohol: ***Spumigin A***
[184682-38-0]
$C_{31}H_{44}N_6O_7$ 612.725
Isol. from the marine cyanobacterium *Nodularia spumigena* AV1. Phycotoxin, hepatotoxin. $[\alpha]_D^{26}$ -5.4 (c, 0.02 in MeOH). C-2′ config. not certain.

Fujii, K. *et al., Tet. Lett.*, 1997, **38**, 5525-5528 (*isol, pmr, ms*)

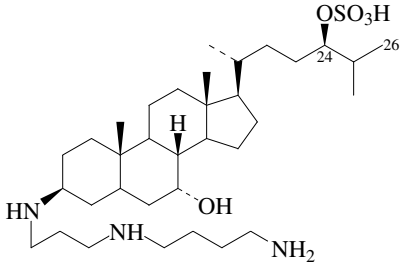
Spumigin C S-355

[184682-41-5]
As Spumigin B1, S-354 with
R = H
$C_{30}H_{40}N_6O_8$ 612.681
Isol. from the marine cyanobacterium *Nodularia spumigena* AV1. Phycotoxin, hepatotoxin. Sol. MeOH. $[\alpha]_D^{26}$ -2.5 (c, 0.05 in MeOH). C-2′ epimeric mixture.

Fujii, K. *et al., Tet. Lett.*, 1997, **38**, 5525-5528 (*isol, pmr, ms*)

Squalamine S-356

[148717-90-2]



$C_{34}H_{65}N_3O_5S$ 627.971
Constit. of the shark *Squalus acanthias*. Active against gram-positive and -negative bacteria. Broad-spectrum steroidal antibiotic. Inhibits angiogenesis and solid tumour growth. Antineoplastic agent, haemolytic, laxative, gastric secretion inhibitor, diuretic. ATP-ase inhibitor. Currently (2000) in Phase II clinical trials. Granted fast track designation by FDA (2004) for the treatment of "wet" age-related macular degeneration. Sol. H_2O, MeOH.

Lactate: ***Squalamine lactate, USAN***. *Evizon. MSI 1256F*
[320725-47-1] Angiogenesis inhibitor. Antineoplastic used in the treatment of advanced malignancies.

N^{ω}*-(3-Aminopropyl):* ***Trodusquemine, INN, USAN***. *7′*-N-*(3-Aminopropyl)squalamine. MSI 1436*
[186139-09-3]
$C_{37}H_{72}N_4O_5S$ 685.066
Constit. of liver of *Squalus acanthias*. Used for treatment of medically significant obesity. Appetite suppressant. Powder.

24-O-*Desulfo, 26-sulfooxy:* [259173-54-1]
$C_{34}H_{65}N_3O_6S$ 643.97
Constit. of liver of *Squalus acanthias*. Powder.

24-Desulfo, 24-ketone, 26-sulfooxy: [232613-79-5]
$C_{34}H_{63}N_3O_6S$ 641.954
Constit. of liver of *Squalus acanthias*. Powder.

24-Desulfo, 24-ketone, 26-[(2-amino-2-carboxyethy)lthio]:
[259173-51-8]
$C_{37}H_{68}N_4O_4S$ 665.035
Constit. of the liver of the dogfish shark *Squalus acanthias*. Powder.

25,26-Didehydro, 24-desulfo, 24-ketone: 3-[[3-[(4-Aminobutyl)amino]propyl]amino]-7-hydroxycholest-25-en-24-one
[186139-08-2]
$C_{34}H_{61}N_3O_2$ 543.875
Constit. of liver of *Squalus acanthias*. Powder.

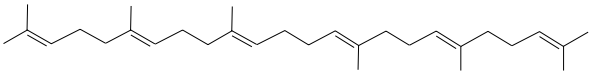
12α-Hydroxy: ***12-Hydroxysqualamine***
[268733-21-7]
$C_{34}H_{65}N_3O_6S$ 643.97
Constit. of liver of *Squalus acanthias*. Powder.

24-Hydroxymethyl: [268733-22-8]
$C_{35}H_{67}N_3O_6S$ 657.997
Constit. of liver of *Squalus acanthias*. Powder.

Moore, K.S. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1993, **90**, 1354-1358 (*isol*)
Wehrli, S.L. *et al., Steroids*, 1993, **58**, 370-378 (*pmr, cmr*)
Moriarty, R.M. *et al., Tet. Lett.*, 1994, **35**, 8103; 1995, **36**, 5139-5142 (*synth*)
Sills, A.K. *et al., Cancer Res.*, 1998, **58**, 2784-2792 (*pharmacol*)
Jones, S.R. *et al., J.O.C.*, 1998, **63**, 3786-3789 (*synth*)
Zhang, X. *et al., J.O.C.*, 1998, **63**, 8599-8603 (*synth*)
Selinsky, B.S. *et al., Biochim. Biophys. Acta*, 2000, **1464**, 135-141 (*pharmacol*)
Rao, M.N. *et al., J. Nat. Prod.*, 2000, **63**, 631-635 (*isol, pmr, cmr, config, derivs*)
Zhang, X. *et al., Org. Lett.*, 2000, **2**, 2921-2922 (*synth*)
Bhargava, P. *et al., Clin. Cancer Res.*, 2001, **7**, 3912-3919 (*Squalamine lactate, pharmacol*)
Ahima, R.S. *et al., Diabetes*, 2002, **51**, 2099-2104 (*MSI 1436, pharmacol*)
Okamura, K. *et al., Chem. Pharm. Bull.*, 2003, **51**, 117-1182 (*synth*)
Hao, D. *et al., Clin. Cancer Res.*, 2003, **9**, 2465-2471 (*clin trial*)
Zhang, D.-H. *et al., Org. Lett.*, 2003, **5**, 3257-3259 (*synth*)
Ciulla, T.A. *et al., Retina*, 2003, **23**, 808-814 (*pharmacol*)
Zhang, D.-H. *et al., Chin. J. Chem.*, 2005, **23**, 176-181 (*synth*)
Zhang, D.-H. *et al., Chin. J. Chem.*, 2005, **23**, 176-181 (*synth*)

Squalene S-357

2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaene, 9CI. Spinacene
[7683-64-9]



$C_{30}H_{50}$ 410.725
▶ XB6010000

(All-E)-form [111-02-4]
Found in fish liver oils, yeast lipids and many vegetable oils, e.g. palm oil, cottonseed oil, rapeseed oil. Obt. comly. from oils

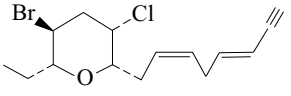
of various sharks *Centrophorus*, *Dalatias* and *Centroscymnus* spp. Volatile component of scent material from *Saguinus oedipus* (cotton-top tamarin monkey) and *Saguinus fuscicollis* (saddle-back tamarin monkey). Component of adult human sebum principally responsible for the fixing of fingerprints. Used in cosmetics. Cause of buoyancy in shark tissues. Oil. Insol. H_2O; sl. sol. EtOH.

Mp -4.8°. Bp_{25} 284-285°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 46A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 33B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 48A (*ir*)
Johnson, W.S. *et al., J.A.C.S.*, 1970, **92**, 741 (*synth*)
Bhalerao, U.T. *et al., J.A.C.S.*, 1971, **93**, 531 (*synth*)
Biellmann, J.F. *et al., Tetrahedron*, 1971, **27**, 5861 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 34 (*occur*)
Grieco, P.A. *et al., J.O.C.*, 1974, **39**, 2135 (*synth*)
Suga, T. *et al., Phytochemistry*, 1975, **14**, 2411 (*biosynth*)
v. Dommelen, M.E. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1975, **94**, 182 (*cmr*)
Johnson, W.S. *et al., Angew. Chem., Int. Ed.*, 1976, **15**, 9 (*rev*)
Ernst, J. *et al., Angew. Chem., Int. Ed.*, 1976, **15**, 778 (*cryst struct*)
Ernst, J. *et al., Annalen*, 1979, 1635 (*cryst struct*)
Belcher, A. *et al., J. Chem. Ecol.*, 1988, **14**, 1367
Nes, W.D. *et al., Phytochemistry*, 1988, **27**, 628 (*biosynth*)
Nordstrom, K.M. *et al., J. Chem. Ecol.*, 1989, **15**, 629

Srilankenyne S-358

[84119-17-5]



Relative configuration

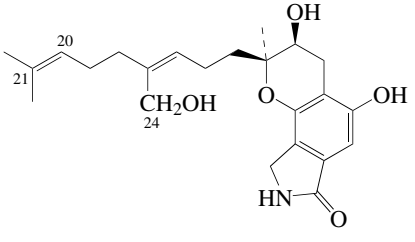
$C_{15}H_{20}BrClO$ 331.679

Metab. of *Aplysia oculifera*. Liq. $[\alpha]_D$ +7.14 (c, 0.98 in CH_2Cl_2).

De Silva, E.D. *et al., J.O.C.*, 1983, **48**, 395-396 (*isol*)

Stachybotrin A S-359

[144373-26-2]



$C_{23}H_{31}NO_5$ 401.502

Alkaloid from an aquatic isolate of the fungus *Stachybotrys* sp. Exhibits antibacterial and antifungal activity. Sol. EtOAc, $CHCl_3$, MeOH; poorly sol. H_2O. $[\alpha]_D$ +8.8 (c, 0.61 in MeOH). λ_{max} 220 (ϵ 17000); 254 (ϵ 6400); 302 (ϵ 2900) (MeOH) (Derep).

24-Deoxy: ***Stachybotrin B***
[144385-02-4]
$C_{23}H_{31}NO_4$ 385.502
From *Stachybotrys* sp. Exhibits antibacterial and antifungal activity. Sol. EtOAc, $CHCl_3$, MeOH; poorly sol. H_2O.
Mp 178-180° dec. $[\alpha]_D$ +39.1 (c, 0.11 in MeOH). λ_{max} 220 (ϵ 17000); 254 (ϵ 6400); 302 (ϵ 2900) (MeOH) (Derep). λ_{max} 254; 270; 302 (MeOH) (Berdy).

24-Deoxy, N-*(2-hydroxyethyl):* ***Antibiotic SMTP 1***. *SMTP 1. NG 243. Antibiotic NG 243*
[189819-17-8]
[161128-86-5]
$C_{25}H_{35}NO_5$ 429.555
Prod. by *Stachybotrys microspora* and *Stachybotrys parvispora*. Light brown oil. $[\alpha]_D^{20}$ -7.1 (c, 2 in Me_2CO). Config. not determined. λ_{max} 214 (ϵ 39700); 254 (ϵ 7200); 299 (ϵ 2800) (MeOH).

24-Deoxy, N-*(2-oxopropyl):* ***Antibiotic NG 129***. *Antibiotic F 4708. NG 129. F 4708*
[157758-74-2]
$C_{26}H_{35}NO_5$ 441.566
Prod. by *Stachybotrys parvispora*. Nerve growth factor-like substance. Powder. Stereochem. not determined. λ_{max} 243 (ϵ 12000) (MeOH) (Berdy).

24-Deoxy, N-*(4-hydroxy-2-oxobutyl):* ***Antibiotic NG 242***. *NG 242*
[160632-28-0]
$C_{27}H_{37}NO_6$ 471.592
Prod. by *Stachybotrys parvispora*. Nerve growth factor-like substance. Powder. Stereochem. not detd.

24-Deoxy, N-*(4-carboxybutyl):* ***Staplabin***
[183006-79-3]
$C_{28}H_{39}NO_6$ 485.619
Prod. by *Stachybotrys microspora*. Plasminogen activator. Fibrin binding enhancer. Light brown oil. Sol. MeOH, butanol; poorly sol. EtOAc, hexane. $[\alpha]_D^{20}$ -11 (c, 0.1 in $CHCl_3$). No stereochem. determined. λ_{max} 216 (ϵ 33500); 258 (ϵ 7300); 300 (ϵ 2500) (MeOH).

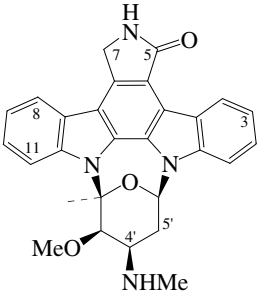
24-Deoxy, N-*[2-(4-hydroxyphenyl)ethyl]:* ***Stachybotrin C***. *NG 245. Antibiotic NG 245*
[150351-23-8]
$C_{31}H_{39}NO_5$ 505.653
Isol. from *Stachybotrys parvispora*. Neuritogenic agent. Yellowish powder.
Mp 89-92°. $[\alpha]_D^{28}$ -28.2 (c, 0.1 in MeOH). λ_{max} 216 (ϵ 52800); 258 (ϵ 12600); 301 (ϵ 4000) (MeOH).

24-Deoxy, 20,21-dihydro, 20,21-dihydroxy, N-*(2-hydroxyethyl):* ***Antibiotic SMTP 2***. *SMTP 2*
[189819-19-0]
$C_{25}H_{37}NO_7$ 463.57
Prod. by *Stachybotrys microspora*. Light brown oil. Sol. $CHCl_3$, MeOH, Me_2CO, DMSO; poorly sol. H_2O. $[\alpha]_D^{20}$ -2.7 (c, 0.2 in Me_2CO). Config. not determined. λ_{max} 212 (ϵ 34000); 252 (ϵ 8000); 294 (ϵ 3000) (MeOH).

Xu, X. *et al., J.O.C.*, 1992, **57**, 6700-6703 (*isol, uv, ir, pmr, cmr, ms, struct*)
Japan. Pat., 1994, 94 128 264; 94 239 869; 94 256 350; *CA*, **121**, 177851w; **122**, 29880k; 142492y (*NG 129,242,243,245*)
Shinohara, C. *et al., J. Antibiot.*, 1996, **49**, 961 (*Staplabin*)
Takayasu, R. *et al., FEBS Lett.*, 1997, **418**, 58-62 (*activity*)
Kohyama, T. *et al., J. Antibiot.*, 1997, **50**, 172 (*SMTP1, SMTP2*)
Nozawa, Y. *et al., J. Antibiot.*, 1997, **50**, 635-640; **59**, 641-645 (*Stachybotrin C*)
Hasumi, K. *et al., J. Antibiot.*, 1998, **51**, 1059-1068 (*activity*)

Staurosporine S-360

AM 2282. CGP 39360. M 193. Antibiotic 230. Antibiotic AM 2282. Antibiotic CGP 39360. Antibiotic M 193
[62996-74-1]



Absolute Configuration

$C_{28}H_{26}N_4O_3$ 466.538

Alkaloid from *Streptomyces staurosporeus*, *Streptomyces* sp. M 193 and the marine actinomycete strain N96C-47. Isol. from *Eudistoma toealensis* and its predator *Pseudoceros* sp. Active against fungi and yeasts. Possesses high hypotensive activity and is a potent platelet aggregation inhibitor. Antiparasitic, nematocide, vasorelaxant, antiamnesic, smooth muscle relaxant, neurotropic, antihyperplastic, endothelin agonist, cell cycle progression inhibitor. Pale yellow plates. Sol. Py; fairly sol. $CHCl_3$, MeOH; poorly sol. butanol, C_6H_6, Me_2CO-EtOAc, hexane.

Mp 270° dec. $[\alpha]_D^{25}$ +35 (c, 1 in MeOH). λ_{max} 207 (ϵ 25000); 243 (ϵ 25000); 267 (sh) (ϵ 31800); 292 (ϵ 57200); 322 (sh) (ϵ 14200); 335 (ϵ 14600); 356 (ϵ 10300); 372 (ϵ 11400) (MeOH) (Derep).

▶ LD_{50} (mus, ipr) 6.6 mg/kg (as hydrochloride). KD5084000

4′-N-*Formyl:* **N-*Formylstaurosporine***
[161973-03-1]
$C_{29}H_{26}N_4O_4$ 494.549
From *Streptomyces longisporoflavus* and the marine *Streptomyces* sp. QD518. Cryst. (EtOAc/CH_2Cl_2).
Mp 221-226°.

4′-N-*Ac:* [120685-33-8]
$C_{30}H_{28}N_4O_4$ 508.576
Prod. by *Saccharothrix aerocolonigenes copiosa* ATCC53856. Protein kinase C inhibitor; antihypertensive; diuretic. Yellow powder. λ_{max} 206 (ϵ 34000); 243 (ϵ 22000); 292 (ϵ 49000); 320 (ϵ 9000); 334 (ϵ 12000); 355 (ϵ 8000); 372 (ϵ 9000) (MeOH).

4′-N-*Benzoyl:* ***Midostaurin, INN, USAN***. N-*Benzoylstaurosporine. CGP 41251. PKC 412*
[120685-11-2]
$C_{35}H_{30}N_4O_4$ 570.646
Selective protein kinase C inhibitor. Antineoplastic agent.

4′-N-*Me:* **N-*Methylstaurosporine***
[129623-30-9]
$C_{29}H_{28}N_4O_3$ 480.565
Prod. by *Streptomyces longisporoflavus*. Isol. from *Eudistoma toealensis* and *Pseudoceros* sp. Cryst. (CH_2Cl_2/2-propanol).
Mp 133-137°.

4′-N-*De-Me:* ***4′*-N-*Demethylstaurosporine***
[126221-77-0]
$C_{27}H_{24}N_4O_3$ 452.512
Isol. from *Eudistoma toealensis* and *Pseudoceros* sp.

O-*De-Me:* ***De*-O-*methylstaurosporine***. *CGP 58546*. *Antibiotic CGP 58546*
[161743-35-7]
$C_{27}H_{24}N_4O_3$ 452.512
Prod. by a blocked mutant of *Streptomyces longisporoflavus* and the marine actinomycete strain N96C-47. Isol. from *Eudistoma toealensis* and *Pseudoceros* sp. Inhibitor of protein kinase C. Pale yellow cryst. (EtOAc). Sol. MeOH, $CHCl_3$.
Mp 220° dec. $[\alpha]_D^{20}$ +82 (c, 1 in DMSO). λ_{max} 207 (ϵ 25000); 243 (ϵ 25000); 267 (sh) (ϵ 31800); 292 (ϵ 57200); 322 (sh) (ϵ 14200); 335 (ϵ 14600); 356 (ϵ 10300); 372 (ϵ 11400) (MeOH) (Derep).

O-*De-Me, 4′*-N-*de-Me:* ***4′*-N,O-*Didemethylstaurosporine***
[406703-32-0]
$C_{26}H_{22}N_4O_3$ 438.485
Isol. from the flatworm *Pseudoceros* sp. Yellowish amorph. powder. λ_{max} 206 (ϵ 2190); 291 (ϵ 3440); 322 (ϵ 690); 334 (ϵ 760); 355 (ϵ 510); 372 (ϵ 550) (MeOH).

4′-N-*Hydroxy:* [161973-04-2]
[137888-67-6]
$C_{28}H_{26}N_4O_4$ 482.538
Prod. by *Saccharothrix aerocolonigenes copiosa* ATCC53856.

4′-N-*Hydroxy, 4′*-N-*de-Me, 4′*-N-*formyl:* [161927-20-4]
$C_{28}H_{24}N_4O_5$ 496.521
From *Streptomyces longisporoflavus*. Cryst. (MeCN aq.).
Mp 220° dec.

4′-N-*Hydroxy,* O-*de-Me:* [137888-68-7]
$C_{27}H_{24}N_4O_4$ 468.511
Prod. by *Saccharothrix aerocolonigenes copiosa* ATCC53856.

4′-N-*(Acetoxymethoxy):* ***4′*-N-*(Acetoxymethoxy)staurosporine***
[161927-21-5]
$C_{31}H_{30}N_4O_6$ 554.601
From *Streptomyces longisporoflavus*. Cryst. (CH_2Cl_2/propanol).
Mp 140-143°.

4′-De(methylamino), 4′α-nitro: ***4′-Demethylamino-4′-nitrostaurosporine***
[161927-19-1]
$C_{27}H_{22}N_4O_5$ 482.495
From *Streptomyces longisporoflavus*. Enzyme inhibitor. Powder (CH_2Cl_2/2-propanol).
Mp 237-242°. λ_{max} 233 (ϵ 29400); 244 (sh) (ϵ 28000); 263 (sh) (ϵ 31300); 275 (sh) (ϵ 42000); 289 (ϵ 71000); 319 (sh) (ϵ 13400); 333 (ϵ 17700); 352 (ϵ 12100); 369 (ϵ 13400) (MeOH) (Derep). λ_{max} 209 (ϵ 23000); 230 (ϵ 7800); 263; 295 (ϵ 16000); 336; 364 (EtOH) (Berdy).

4′-De(methylamino), 4′-hydroxy: 4′-Demethylamino-4-hydroxystaurosporine. ***Antibiotic RK 286C***. *RK 286C*
[126572-73-4]
$C_{27}H_{23}N_3O_4$ 453.496
Prod. by *Streptomyces* sp. RK 286C. Protein kinase C inhibitor; platelet aggregation inhibitor; antiinflammatory; cell cycle progression inhibitor; bleb formn. inhibitor. Pale yellow powder. Sol. EtOAc, DMSO; fairly sol. MeOH; poorly sol. H_2O.
Mp 265° dec. $[\alpha]_D^{20}$ +45.3 (c, 0.22 in EtOAc). λ_{max} 207 (ϵ 25000); 243 (ϵ 25000); 267 (sh) (ϵ 31800); 292 (ϵ 57200); 322 (sh) (ϵ 14200); 335 (ϵ 14600); 356 (ϵ 10300); 372 (ϵ 11400) (MeOH) (Derep). λ_{max} 237 (ϵ 30450); 245 (ϵ 30120); 292 (ϵ 69500); 335 (ϵ 16550); 356 (ϵ 13240); 372 (ϵ 14890) (MeOH) (Berdy). λ_{max} 237; 245; 292; 335; 356; 372 (MeOH/HCl) (Berdy). λ_{max} 237; 245; 292; 335; 356; 372 (MeOH/NaOH) (Berdy).

4′-De(methylamino), 4′α,5′α-dihydroxy: 4′-Demethylamino-4′,5′-dihydroxystaurosporine. ***Antibiotic MLR 52***. *MLR 52*
[155416-34-5]
$C_{27}H_{23}N_3O_5$ 469.496
Prod. by a *Streptomyces* sp. Inhibitor of protein kinase C. Sol. MeOH.
Mp 263-268°. $[\alpha]_D$ +68 (c, 0.09 in MeOH). λ_{max} 206 (ϵ 48500); 234 (ϵ 48500); 286 (ϵ 72100); 317 (ϵ 25000); 332 (ϵ 30000); 351 (ϵ 21500); 368 (ϵ 22600) (MeOH) (Derep).

4′-De(methylamino), 4′,7-dihydroxy: [137888-70-1]
$C_{27}H_{23}N_3O_5$ 469.496
Prod. by *Saccharothrix aerocolonigenes copiosa* ATCC53856. Enzyme inhibitor. λ_{max} 207; 239; 292; 300; 358; 375 (MeOH) (Berdy).

4′-De(methylamino), 4′,7-dihydroxy, O-*de-Me:* [137888-71-2]
$C_{26}H_{21}N_3O_5$ 455.469
Prod. by *Saccharothrix aerocolonigenes copiosa* ATCC53856. Enzyme inhibitor. λ_{max} 208 (ϵ 24000); 239 (ϵ 15000); 301 (ϵ 27000); 358 (ϵ 4000); 376 (ϵ 4000) (MeOH) (Berdy).

3-Hydroxy: ***3-Hydroxystaurosporine***
[320384-51-8]
$C_{28}H_{26}N_4O_4$ 482.538
Isol. from *Eudistoma toealensis* and *Pseudoceros* sp.

3-Hydroxy, 4′-N-*Me:* ***3-Hydroxy-4′*-N-*methylstaurosporine***
[399031-46-0]
$C_{29}H_{28}N_4O_4$ 496.565
Isol. from *Eudistoma toealensis* and *Pseudoceros* sp.

3-Hydroxy, 4′-N-*de-Me:* ***3-Hydroxy-4′*-N-*demethylstaurosporine***
[406703-29-5]
$C_{27}H_{24}N_4O_4$ 468.511
Isol. from *Eudistoma toealensis* and *Pseudoceros* sp. Yellowish amorph. powder. λ_{max} 204 (ϵ 2710); 287 (ϵ 3100); 297 (ϵ 4080); 342 (ϵ 1150); 366 (ϵ 700); 384 (ϵ 700) (MeOH).

3-Hydroxy, O-*de-Me:* ***3-Hydroxy*-O-*demethylstaurosporine***
[399031-45-9]
$C_{27}H_{24}N_4O_4$ 468.511
Isol. from *Eudistoma toealensis* and *Pseudoceros* sp. Amorph. yellow powder. λ_{max} 237 (ϵ 8350); 251 (ϵ 6600); 270 (ϵ 7120); 297 (ϵ 13380); 342 (ϵ 3790); 366 (ϵ 2400); 384 (ϵ 2420) (MeOH).

5′α-Hydroxy: ***5′-Hydroxystaurosporine***
[308847-74-7]
$C_{28}H_{26}N_4O_4$ 482.538
Prod. by a marine *Micromonospora* sp. Pale yellow powder. Mp > 220° dec. $[\alpha]_D^{25}$ +53 (c, 0.1 in MeOH). λ_{max} 206; 242; 291; 320; 334; 354; 370 (MeOH).

5′α-Hydroxy, N-*Me:* ***5′-Hydroxy-4′*-N-*methylstaurosporine***
[308847-73-6]
$C_{29}H_{28}N_4O_4$ 496.565
Prod. by a marine *Micromonospora* sp. Pale yellow powder. Mp > 220° dec. $[\alpha]_D^{25}$ +30 (c, 0.11 in $CHCl_3$). λ_{max} 206; 242; 291; 320; 334; 354; 370 (MeOH).

7ξ-Hydroxy: ***7-Hydroxystaurosporine****. UCN 01. Antibiotic UCN 01. NSC 638850*
[112953-11-4]
$C_{28}H_{26}N_4O_4$ 482.538
From *Streptomyces* sp. N-126 and *Streptomyces longisporoflavus* R19. Selective inhibitor of protein kinase C. Cytotoxic. Pale yellow needles. Sol. MeOH, $CHCl_3$, DMSO; poorly sol. H_2O, hexane. Mp 245-250° dec. $[\alpha]_D^{22}$ +132 (c, 0.3 in MeOH). λ_{max} 240 (ϵ 29000); 264 (sh) (ϵ 20000); 274 (sh) (ϵ 21000); 300 (ϵ 55000); 326 (sh) (ϵ 9600); 338 (sh) (ϵ 8300); 358 (ϵ 7500); 374 (ϵ 8500) (MeOH) (Derep). λ_{max} 241; 266; 280; 298; 325; 356; 375 (EtOH) (Berdy).
▶ LD_{50} (mus, ipr) 30 mg/kg. KC6600010

11-Hydroxy: ***11-Hydroxystaurosporine***
[143682-17-1]
$C_{28}H_{26}N_4O_4$ 482.538
Isol. from the marine tunicate *Eudistoma* sp. Cytotoxic. Inhibitor of protein kinase C. Amorph. $[\alpha]_D$ +10.3 (c, 0.3 in MeOH).

*11-Hydroxy, 4′-*N*-de-Me:* ***11-Hydroxy-4′-N-demethylstaurosporine***
[272766-45-7]
$C_{27}H_{24}N_4O_4$ 468.511
Isol. from *Eudistoma toealensis*, *Pseudoceros* sp., and from the mollusc *Coriocella nigra*. Amorph. yellow powder. λ_{max} 290 (ϵ 1040); 356 (ϵ 180); 373 (ϵ 180) (MeOH).

3,11-Dihydroxy: ***3,11-Dihydroxystaurosporine***
[143682-18-2]
$C_{28}H_{26}N_4O_5$ 498.537
Isol. from *Eudistoma* sp. and the mollusc *Coriocella nigra*. Cytotoxic. Amorph.

7-Oxo: ***7-Oxostaurosporine****. BMY 41950. RK 1409. Antibiotic BMY 41950. Antibiotic RK 1409*
[125035-83-8]
$C_{28}H_{24}N_4O_4$ 480.522
Prod. by *Streptomyces platensis* ssp. *malvinus* and *Streptomyces staurosporeus* ATCC55006. Inhibitor of protein kinase C. Yellow powder.
Mp 235° dec. $[\alpha]_D^{20}$ +38.3 (c, 0.06 in $CHCl_3$). λ_{max} 208 (ϵ 19600); 238 (ϵ 26400); 260 (ϵ 13600); 287 (ϵ 16800); 305 (sh) (ϵ 20800); 317 (ϵ 33600); 340 (sh) (ϵ 8800); 410 (ϵ 2400) (MeOH) (Derep).

*7ξ-Methoxy, 4′-*N*-hydroxy:* [137888-69-8]
$C_{29}H_{28}N_4O_5$ 512.564
Prod. by *Saccharothrix aerocolonigenes copiosa* ATCC53856.

10-Methoxy: ***10-Methoxystaurosporine****. Antibiotic TAN 999. TAN 999*
[124843-68-1]
$C_{29}H_{28}N_4O_4$ 496.565
From *Nocardiopsis dassonvillei*. Possesses macrophage-activating props. Pale yellow cryst. + $\frac{1}{2}H_2O$. Sol. MeOH; poorly sol. H_2O. Mp 221° dec. $[\alpha]_D^{24}$ +42 (c, 0.5 in DMF). λ_{max} 245 (ϵ 31200); 296 (ϵ 60300); 341 (ϵ 19500); 352 (sh) (ϵ 16200); 368 (ϵ 11000) (MeOH) (Derep).

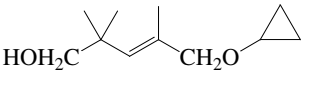
3′-Epimer, 4′-de(methylamino), 4′-hydroxy: 4′-Demethylamino-4′-hydroxy-3′-epistaurosporine. ***Antibiotic RK 1409B****. RK 1409B*
[145212-39-1]
$C_{27}H_{23}N_3O_4$ 453.496
Prod. by *Streptomyces platensis* ssp. *malvinus*. Inhibitor of protein kinase C; antiinflammatory; cell cycle progression inhibitor. Pale yellow powder. Sol. DMSO; fairly sol. MeOH, EtOAc, $CHCl_3$, Me_2CO; poorly sol. H_2O, hexane.
Mp 260° dec. $[\alpha]_D^{22}$ +147 (c, 0.2 in DMSO). λ_{max} 203 (ϵ 37870); 245 (ϵ 25370); 293 (ϵ 58710); 336 (ϵ 13140); 357 (ϵ 9970); 374 (ϵ 10870) (MeOH) (Berdy).

7-Epimer, 7-hydroxy: ***Antibiotic UCN 02****. UCN 02*
[121569-61-7]
$C_{28}H_{26}N_4O_4$ 482.538
From *Streptomyces* sp. N-126. Cytotoxic, protein kinase C inhibitor. Pale yellow needles. Sol. $CHCl_3$, DMSO, MeOH; poorly sol. H_2O. Mp 245-250° dec. $[\alpha]_D^{22}$ -38.6 (c, 0.35 in MeOH). λ_{max} 240 (ϵ 29000); 264 (sh) (ϵ 20000); 274 (sh) (ϵ 21000); 300 (ϵ 55000); 326 (sh) (ϵ 9600); 338 (sh) (ϵ 8300); 358 (ϵ 7500); 374 (ϵ 8500) (MeOH) (Derep).

Omura, S. *et al., J. Antibiot.*, 1977, **30**, 275-282 (*isol, ms, uv, ir, pmr*)
Cordell, G.A. *et al., Alkaloids (N.Y.)*, 1981, **20**, 4-5 (*rev, tox*)
Furusaki, A. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 3681-3685 (*cryst struct*)
Weinreb, S.M. *et al., Heterocycles*, 1984, **21**, 309-324 (*synth*)
Oka, S. *et al., Agric. Biol. Chem.*, 1986, **50**, 2723-2727 (*isol, props*)
Eur. Pat., 1988, (*Ciba-Geigy*)296 110; *CA*, **111**, 96977h (*synth, pharmacol*)
Meyer, T. *et al., Int. J. Cancer*, 1989, **43**, 851-856 (*Midostaurin, pharmacol*)
Takahashi, I. *et al., J. Antibiot.*, 1989, **42**, 564-570; 571-576 (*UCN01, 02*)
Tanida, S. *et al., J. Antibiot.*, 1989, **42**, 1619-1630 (*TAN 999*)
Osada, H. *et al., J. Antibiot.*, 1990, **43**, 168-173 (*RK 286C*)
Pat. Coop. Treaty (WIPO), 1991, 9 034; *CA*, **116**, 39768v (*Saccharothrix aerocolonigenes copsia constits*)
Tsuboi, S. *et al., Tetrahedron*, 1991, **47**, 3565-3574 (*TAN 999, cmr*)
Krause, K.H. *et al., Eur. J. Pharmacol., Mol. Pharmacol.*, 1992, **227**, 221-224 (*Midostaurin, pharmacol*)
Osada, H. *et al., J. Antibiot.*, 1992, **45**, 189-194; 195-198 (*7-Oxostaurosporine*)
Koshino, H. *et al., J. Antibiot.*, 1992, **45**, 1428-1432 (*RK 1409B*)
Kinnel, R.B. *et al., J.O.C.*, 1992, **57**, 6327-6329 (*11-Hydroxystaurosporine, 3,11-Dihydroxystaurosporine*)
Caravatti, G. *et al., Bioorg. Med. Chem. Lett.*, 1994, **4**, 399-404 (*Midostaurin, synth, pharmacol*)
McAlpine, J.B. *et al., J. Antibiot.*, 1994, **47**, 281-288 (*MLR 52*)
Funato, N. *et al., Tet. Lett.*, 1994, **35**, 1251-1254 (*cryst struct, abs config*)
Sedlak, J. *et al., Anti-Cancer Drugs*, 1995, **6**, 70-76 (*Midostaurin, pharmacol*)
Cai, Y. *et al., J. Antibiot.*, 1995, **48**, 143-148 (*Demethylaminonitrostaurosporine, Acetoxymethoxystaurosporine, N-Formylstaurosporine*
Hoehn, P. *et al., J. Antibiot.*, 1995, **48**, 300-305 (*De-O-methylstaurosporine*)
Omura, S. *et al., J. Antibiot.*, 1995, **48**, 535-548 (*rev*)
Link, J.T. *et al., J.A.C.S.*, 1995, **117**, 552-553 (*synth*)
Begemann, M. *et al., Clin. Cancer Res.*, 1996, **2**, 1017-1030 (*Midostaurin, pharmacol*)
Cai, Y. *et al., J. Antibiot.*, 1996, **49**, 1060-1062 (*N-Methylstaurosporine*)
Yang, S.W. *et al., J. Nat. Prod.*, 1996, **59**, 828-833; 1997, **60**, 236-241 (*biosynth, ms*)
Wood, J.L. *et al., J.A.C.S.*, 1996, **118**, 10656-10657; 1997, **119**, 9652-9661 (*synth*)
Wood, J.L. *et al., Tet. Lett.*, 1996, **37**, 7335-7338 (*synth, RK 286C*)
Beltran, P.J. *et al., Biochem. Pharmacol.*, 1997, **53**, 245-247 (*Midostaurin, pharmacol*)
Weidner, S. *et al., J. Antibiot.*, 1998, **51**, 679-682 (*biosynth*)
Schupp, P. *et al., J. Nat. Prod.*, 1999, **62**, 959-962 (*isol, pmr, cmr*)
Contrell, C.L. *et al., Nat. Prod. Lett.*, 1999, **14**, 39-46 (*Coriocella nigra constits*)
Williams, D.E. *et al., Tet. Lett.*, 1999, **40**, 7171-7174 (*marine strain N96C-47, isol*)
Hernandez, L.M.C. *et al., J. Antibiot.*, 2000, **53**, 895-902 (*5′-Hydroxystaurosporine, 5′-Hydroxy-N-methylstaurosporine*)
Cantrell, C.L. *et al., Nat. Prod. Lett.*, 2000, **14**, 39-46 (*11-Hydroxy-4′-N-demethylstaurosporine*)
Schupp, P. *et al., Cancer Lett. (Shannon, Irel.)*, 2001, **174**, 165-172; 2003, **190**, 119 (*Eudistoma, Pseudoceros, isol*)
Zaugg, K. *et al., Cancer Res.*, 2001, **61**, 732-738 (*Midostaurin, pharmacol*)
Schupp, P. *et al., J. Nat. Prod.*, 2002, **65**, 295-298 (*N,O-Didemethylstaurosporine, 3-Hydroxy-N-demethylstaurosporine, 3-Hydroxy-N-methylstaurosporine*)
Wu, S.J. *et al., J. Antibiot.*, 2006, **59**, 331-337 (*marine strain QD518, isol*)

Stellatol S-361

5-(Cyclopropyloxy)-2,2,4-trimethyl-3-penten-1-ol, 9CI
[240421-19-6]

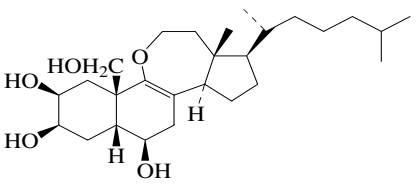


$C_{11}H_{20}O_2$ 184.278
Isol. from the brown alga *Iyengaria stellata*. Mobile oil.

Ali, M.S. *et al., Turk. J. Chem.*, 1999, **23**, 181-183 (*isol, pmr, cmr, ms*)

Stellattasterenol S-362

9,11-Epoxy-9,11-secocholest-8-ene-2,3,6,19-tetrol
[250653-49-7]



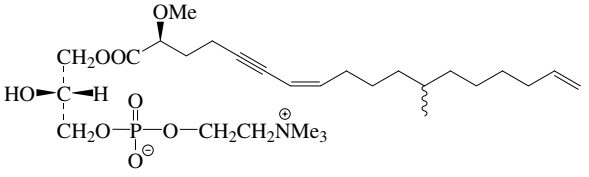
$C_{27}H_{46}O_5$ 450.657

Constit. of *Euryspongia arenaria*. Solid. $[\alpha]_D^{25}$ +70 (c, 0.025 in $CHCl_3$/MeOH).

Van Altena, I.A. *et al., J. Nat. Prod.*, 1999, **62**, 1154-1157 (*isol, pmr, cmr*)

Stellettacholine A S-363

1-(2-Methoxy-12-methyl-7,17-octadecadien-5-ynoyl)glycero-3-phosphocholine
[540466-93-1]

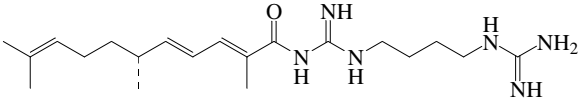


$C_{28}H_{50}NO_8P$ 559.679

Isol. from the sponge *Stelletta* sp. Pale yellow oil. $[\alpha]_D^{21}$ -0.1 (c, 0.25 in MeOH).

Zhao, Q. *et al., J. Nat. Prod.*, 2003, **66**, 725-728 (*isol, pmr, cmr, ms*)

Stellettadine A S-364



Absolute Configuration

$C_{20}H_{36}N_6O$ 376.544

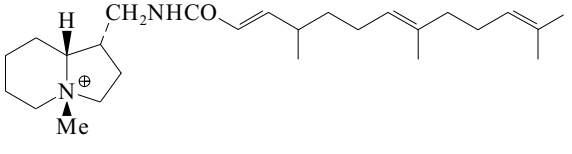
(R)-form [179732-83-3]

Alkaloid from the marine sponge *Stelletta* sp. Induces larval metamorphosis in ascidians, RNA cleaving agent. $[\alpha]_D^{24}$ -42.7 (c, 0.09 in MeOH). $[\alpha]_D^{24}$ -32.8 (c, 1.00 in MeOH). λ_{max} 285 (ϵ 11100) (MeOH).

Tsukamoto, S. *et al., Tet. Lett.*, 1996, **37**, 5555-5556 (*isol, uv, ir, pmr, cmr, struct*)
Nozawa, D. *et al., Bioorg. Med. Chem. Lett.*, 2001, **11**, 1481-1483 (*synth, abs config*)
Takikawa, H. *et al., J.C.S. Perkin 1*, 2001, 657-661 (*synth, abs config*)

Stellettamide A S-365

Octahydro-4-methyl-1-[[(4,8,12-trimethyl-1-oxo-2,7,11-tridecatrienyl)amino]methyl]indolizinium(1+), 9CI
[129744-24-7]
[129744-25-8]



$C_{26}H_{45}N_2O^{\oplus}$ 401.654

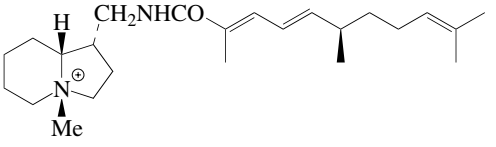
Alkaloid from the marine sponge *Stelletta* sp. Antifungal agent. Cytotoxic. Semisolid (as phosphate). $[\alpha]_D$ +23.1 (c, 0.3 in EtOH) (phosphate).

$\Delta^{3'}$-Isomer: ***Stellettamide C***
$C_{26}H_{45}N_2O^{\oplus}$ 401.654
Alkaloid from *Stelletta* sp. Antibacterial agent. Amorph. solid. Counterion not specified.

Hirota, H. *et al., Tet. Lett.*, 1990, **31**, 4163 (*isol, ir, pmr, cmr, struct*)
Whitlock, G.A. *et al., J.O.C.*, 1997, **62**, 7916-7917 (*synth, enantiomer*)
Matsunaga, S. *et al., J. Nat. Prod.*, 1999, **62**, 1202-1204 (*Stellettamide C*)
Whitlock, G.A. *et al., Helv. Chim. Acta*, 2000, **83**, 2007-2022 (*synth*)

Stellettamide B S-366

[189580-08-3]



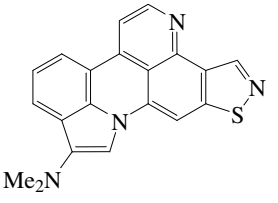
$C_{24}H_{41}N_2O^{\oplus}$ 373.601

Alkaloid from the sponge *Stelletta* sp. Antifungal agent. Yellow gum (as chloride). $[\alpha]_D^{25}$ -24.2 (c, 0.5 in $CHCl_3$) (chloride). CAS no. refers to chloride.

Shin, J. *et al., J. Nat. Prod.*, 1997, **60**, 611-613 (*isol, uv, ir, pmr, cmr*)
Yamazaki, N. *et al., Org. Lett.*, 2001, **3**, 193-196 (*synth*)

Stellettamine S-367

[139427-07-9]



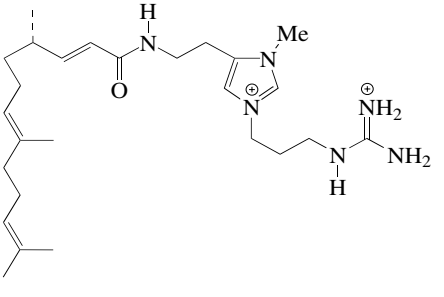
$C_{20}H_{14}N_4S$ 342.423

Alkaloid from the marine sponge *Stelletta* sp. Dark brown cryst. ($CHCl_3$).

Mp 280-282°. λ_{max} 205 (ϵ 15700); 260 (ϵ 9400); 309 (ϵ 10800); 364 (ϵ 3760); 391 (ϵ 3420); 460 (ϵ 1370) (MeOH) (Derep).

Gunawardana, G.P. *et al., J.O.C.*, 1992, **57**, 1523 (*isol, ir, uv, pmr, cmr, cryst struct*)

Stellettazole A S-368



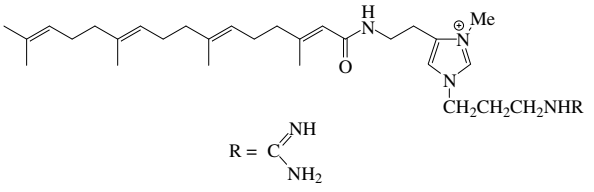
$C_{26}H_{46}N_6O^{2\oplus}$ 458.689

Alkaloid from a marine sponge, *Stelletta* sp. Antibacterial agent. Also inhibits Ca/calmodulin-dependent phosphodiesterase. $[\alpha]_D^{24}$ -35 (c, 0.08 in MeOH). Counterion not specified.

Tsukamoto, S. *et al., Tet. Lett.*, 1999, **40**, 737-738 (*isol, pmr, cmr*)

Stellettazole B S-369

[247086-88-0]



$C_{30}H_{51}N_6O^{\oplus}$ 511.773

The +ve charge is delocalised over the imidazole N's. Alkaloid from the sponge *Stelletta* sp. Antibacterial agent. Amorph. solid. Counterion not specified.

Matsunaga, S. *et al., J. Nat. Prod.*, 1999, **62**, 1202-1204 (*isol, pmr, cmr*)

Stellettazole C S-370

[247086-89-1]

As Stellettazole B, S-369 with

R = H

$C_{29}H_{49}N_4O^{\oplus}$ 469.732

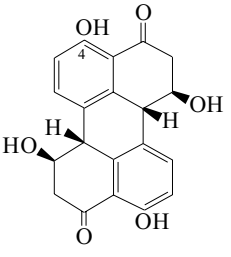
Alkaloid from the sponge *Stelletta* sp. Antibacterial agent. Amorph. solid. Counterion not specified.

Matsunaga, S. *et al., J. Nat. Prod.*, 1999, **62**, 1202-1204 (*isol, pmr, cmr*)

Stemphyperylenol S-371

1,2,6b,7,8,12b-Hexahydro-1,4,7,10-tetrahydroxy-3,9-perylenedione, 9CI

[102694-33-7]



$C_{20}H_{16}O_6$ 352.343

Prod. by *Stemphylium botryosum* and *Alternaria cassiae* and a marine *Alternaria* sp. Phytotoxin. Active against gram-positive bacteria. Buff cryst. (CH_2Cl_2/Et_2O). Sol. MeOH, C_6H_6; poorly sol. H_2O. Dec. at 250° without melting. λ_{max} 206 (log ϵ 4.08); 260 (log ϵ 3.91); 340 (log ϵ 3.51) (MeOH).

Tetra-Ac:

Yellow solid. Mp 148-150°.

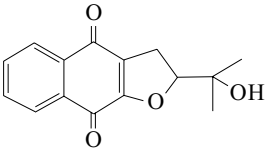
4-Me ether: Mp 176-178°.

Arnone, A. *et al., J.C.S. Perkin 1*, 1986, 525-530 (*isol, pmr, struct*)
Hradil, C.M. *et al., Phytochemistry*, 1988, **28**, 73-75 (*isol, pmr*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

Stenocarpoquinone B S-372

2,3-Dihydro-2-(1-hydroxy-1-methylethyl)naphtho[2,3-b]furan-4,9-dione, 9CI. 4′-Hydroxyiso-α-lapachone. Stenocarpone B

[41192-67-0]



$C_{15}H_{14}O_4$ 258.273

(+)-*form*

Isol. from *Stenocarpus salignus.*

Yellow cryst.

Mp 160-161°. $[\alpha]_D^{20}$ +40 ($CHCl_3$).

2,3-Didehydro: 2-(1-Hydroxy-1-methylethyl)naphtho[2,3-b]furan-4,9-dione. ***Avicequinone C***

$C_{15}H_{12}O_4$ 256.257

Constit. of the stem bark of *Avicennia alba*. Phytoalexin. Yellow powder. Formerly given incorrect struct. λ_{max} 249; 292; 335; 374 (MeOH).

(±)-*form* [66512-82-1]

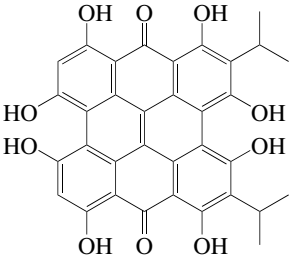
Yellow cryst. (C_6H_6 or Et_2O). Mp 128-129°.

Mock, J. *et al., Aust. J. Chem.*, 1973, **26**, 1121-1130 (*isol*)
Adams, J.H. *et al., J. Chem. Res., Synop.*, 1978, 3 (*synth*)
Ito, C. *et al., Chem. Pharm. Bull.*, 2000, **48**, 339-343 (*Avicequinone C*)

Stentorin S-373

1,3,4,6,8,10,11,13-Octahydroxy-2,5-bis(1-methylethyl)phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 9CI

[157480-38-1]



$C_{34}H_{24}O_{10}$ 592.558

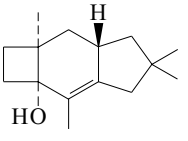
Isol. from the unicellular ciliate *Stentor coeruleus.* Photoreceptor molecule. Dark solid. Mp > 350°. Similar to Hypericin. λ_{max} 595 (MeOH). λ_{max} 595 (MeOH) (Berdy). λ_{max} 587 (MeOH-HCl) (Berdy).

[147395-58-2, 147395-59-3]

Lankester, E.R. *et al., Q. J. Microsc. Sci.*, 1873, **26**, 71 (*isol*)
Tao, N. *et al., J.A.C.S.*, 1993, **115**, 2526 (*isol, uv, ir, ms, pmr*)
Etzelstorfer, C. *et al., Monatsh. Chem.*, 1994, **125**, 955 (*tautom, stereochem*)
Iio, H. *et al., Tet. Lett.*, 1995, **36**, 5921 (*synth*)
Cameron, D.W. *et al., Aust. J. Chem.*, 1997, **50**, 409 (*synth, uv, pmr, struct*)
Falk, H. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 3117-3136 (*rev*)

2-Sterpuren-6-ol S-374

3-Sterpurenol



$C_{15}H_{24}O$ 220.354

Ac: ***3-Acetoxysterpurene***

[126201-36-3]

$C_{17}H_{26}O_2$ 262.391

Metab. of *Alcyonium acaule.* Oil. $[\alpha]_D$ +128.6 (c, 2.2 in $CHCl_3$).

Cimino, G. *et al., Tetrahedron*, 1989, **45**, 6479

Sticholysins S-375

Two polypeptides, Sticholysin I (MW 19401) and Sticholysin II (MW 19290) with 93% sequence identity. Isol. from the venom of the sea anemone *Stichodactyla helianthus.* Cytolysins.

[183449-91-4, 324523-16-2, 324530-31-6]

Lanio, M.E. *et al., Toxicon*, 2001, **39**, 187-194 (*isol, struct*)
Huerta, H. *et al., Toxicon*, 2001, **39**, 1253-1256 (*struct*)

Mancheño, J.M. *et al., Acta Cryst. D*, 2002, **58**, 1229-1231 (*Sticholysin II, cryst struct*)
Anderluh, G. *et al., Toxicon*, 2002, **40**, 111-124 (*rev*)

Stichopin S-376

[213022-72-1]

Asp-Arg-Gln-Gly-Trp-Pro-Ala-Cys-Tyr-Asp-Ser-Lys-Gln-Asn-Tyr-Lys-Cys

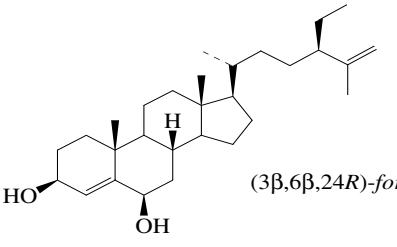
$C_{85}H_{121}N_{25}O_{27}S_2$ 1989.174

Struct. of reduced form shown. Isol. from the body wall of the sea cucumber *Stichopus japonicus*. Neuropeptide.

Birenheide, R. *et al., Biol. Bull. (Woods Hole, Mass.)*, 1998, **194**, 253-259 (*isol*)

Stigmasta-4,25-diene-3,6-diol S-377

24-Ethylcholesta-4,25-diene-3,6-diol



(3β,6β,24*R*)-*form*

$C_{29}H_{48}O_2$ 428.697

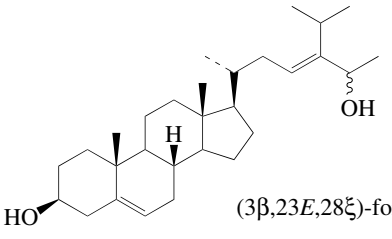
(3β,6β,24*R*)-*form* [429681-36-7]
Constit. of *Laurencia majuscula*.

(3β,6β,24*S*)-*form* [189248-42-8]
Constit. of the alga *Laurencia majuscula*. Cytotoxic agent.
Needles.
Mp 242-243°.

3-Ketone: ***6-Hydroxystigmasta-4,25-dien-3-one***
[173681-52-2]
$C_{29}H_{46}O_2$ 426.681
Constit. of *Codium arabicum*. Amorph. powder.
Mp 194°.

Sheu, J.-H. *et al., J. Nat. Prod.*, 1995, **58**, 1521 (*isol, pmr, cmr, ketone*)
Xu, X.H. *et al., Chin. Chem. Lett.*, 1997, **8**, 235-236 (*isol, pmr, cmr, ms*)
Xu, X.H. *et al., Tianran Chanwu Yanjiu Yu Kaifa*, 2001, **13**, 5-8; *CA*, **136**, 398242k (*isol, pmr, cmr*)

Stigmasta-5,23-diene-3,28-diol S-378



(3β,23*E*,28ξ)-form

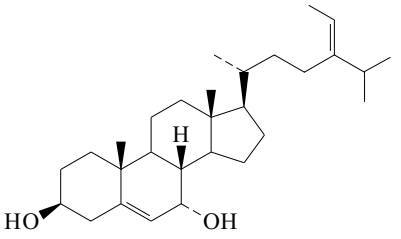
$C_{29}H_{48}O_2$ 428.697

(3β,23*E*,28ξ)-*form* [489459-62-3]
Constit. of the marine brown alga *Ishige okamurae*.

(3β,23*Z*,28ξ)-*form* [477935-96-9]
Constit. of *Sargassum carpophyllum*.
Solid.
Mp 139-141°.

Tang, H.-F. *et al., J. Asian Nat. Prod. Res.*, 2002, **4**, 95-101 (*Sargassum carpophyllum constit*)
Tang, H. *et al., Zhongguo Haiyang Yaowu*, 2003, **22**, 8-12; *CA*, **142**, 276545q (*Ishige okamurae constit*)

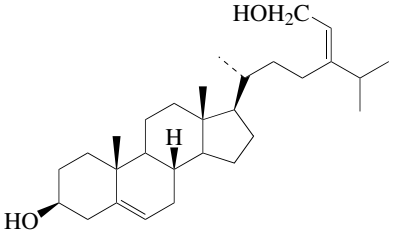
Stigmasta-5,24(28)-diene-3,7-diol S-379



$C_{29}H_{48}O_2$ 428.697

(3β,7α,24*E*)-*form* [37976-89-9]
Constit. of *Fucus evanescens*.
Cryst. (EtOH).
Mp 180°. $[\alpha]_D$ -25.6.
Ikekawa, N. *et al., Phytochemistry*, 1972, **11**, 2317

Stigmasta-5,24(28)-diene-3,29-diol S-380



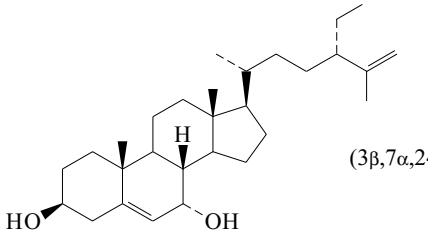
$C_{29}H_{48}O_2$ 428.697

(3β,24(28)*E*)-*form* [81256-58-8]
Cryst. Mp 159-161°. $[\alpha]_D^{25}$ -22 (c, 0.2 in $CHCl_3$).

29-Hydroperoxide: ***29-Hydroperoxystigmasta-5,24(28)-dien-3-ol***
[88147-19-7]
$C_{29}H_{48}O_3$ 444.696
Constit. of *Turbinaria ornata*. Cryst.
Mp 135-136°. $[\alpha]_D^{25}$ -35.9 (c, 0.1 in $CHCl_3$).
Sheu, J.-H. *et al., Planta Med.*, 1997, **63**, 571-572 (*isol, pmr, cmr*)

Stigmasta-5,25-diene-3,7-diol S-381

24-Ethylcholesta-5,25-diene-3,7-diol



(3β,7α,24*S*)–*form*

$C_{29}H_{48}O_2$ 428.697

(3β,7α,24*S*)-*form*
Decortinol
[151345-06-1]
Constit. of *Codium decorticatum* and *Codium arabicum*.
Gum.

3-O-*(6*-O-*Heptadecanoyl-β-*D*-glucopyranoside):* ***Colebrin D***
[329315-71-1]
$C_{52}H_{90}O_8$ 843.278
Constit. of *Clerodendrum colebrookianum*. Wax. $[\alpha]_D^{24}$ -21.3 (c, 0.2 in $CHCl_3$).

7-Formyl: ***Colebrin A***
[263744-73-6]
$C_{30}H_{48}O_3$ 456.707
Constit. of *Clerodendrum colebrookianum*. Wax. $[\alpha]_D^{20.5}$ -117 (c, 0.0112 in MeOH).

3-Ketone: ***7-Hydroxystigmasta-5,25-dien-3-one****. 24-Ethyl-7-hydroxycholesta-5,25-dien-3-one*
[474417-54-4]
$C_{29}H_{46}O_2$ 426.681
Constit. of *Ajuga relicta*.

7-Ketone: 3-Hydroxystigmasta-5,25-dien-7-one. 24-Ethyl-3-hydroxycholesta-5,25-dien-7-one. ***Decortinone***
[151345-08-3]
$C_{29}H_{46}O_2$ 426.681
Constit. of *Codium decorticatum* and *Teucrium chamaedrys* ssp. *chamaedrys*. Gum.

3,7-Diketone: Stigmasta-5,25-diene-3,7-dione. ***Iyengadione***
[494862-71-4]
$C_{29}H_{44}O_2$ 424.665
Constit. of *Codium iyengarii*. Oil. $[\alpha]_D$ -50 (c, 0.04 in $CHCl_3$). λ_{max} 240 (log ε 3.2) ($CHCl_3$).

7-Hydroperoxide: ***7-Hydroperoxystigmasta-5,25-dien-3-ol***
$C_{29}H_{48}O_3$ 444.696
Constit. of *Codium arabicum*. Amorph. powder.
Mp 127-128°. $[\alpha]_D$ -87.6 (c, 0.4 in $CHCl_3$).

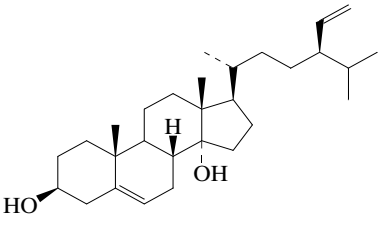
(3β,7β,24*S*)-*form*
Isodecortinol
[151345-07-2]
Constit. of *Codium decorticatum*.
Gum.

3-O-(6-O-Heptadecanoyl-β-D-glucopyranoside): ***Colebrin E***
[329315-72-2]
$C_{52}H_{90}O_8$ 843.278
Constit. of *Clerodendrum colebrookianum*. Wax. $[\alpha]_D^{24}$ -42.2 (c, 0.450 in $CHCl_3$).

Ahmad, V.U. *et al., Phytochemistry*, 1993, **33**, 1189-1192 (*Codium decorticatum constit*)
Ulubelen, A. *et al., Phytochemistry*, 1994, **36**, 171 (*isol, pmr, cmr*)
Sheu, J.-H. *et al., J. Nat. Prod.*, 1995, **58**, 1521 (*isol, pmr, cmr*)
Yang, H. *et al., Fitoterapia*, 2000, **71**, 641-648 (*Colebrins*)
Ali, M.S. *et al., Nat. Prod. Lett.*, 2002, **16**, 407-413 (*Iyengadione*)
Kökdil, G. *et al., Z. Naturforsch., B*, 2002, **57**, 957-960 (*3-ketone*)

Stigmasta-5,28-diene-3,14-diol S-382

24-Ethenylcholest-5-ene-3,14-diol. 24-Vinylcholest-5-ene-3,14-diol



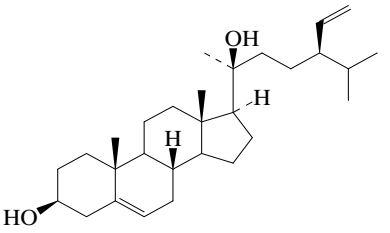
$C_{29}H_{48}O_2$ 428.697

(3β,14α,24*R*)-*form*
Spatosterol
[253340-29-3]
Constit. of *Spatoglossum variabile*.
$[\alpha]_D^{25}$ -38.1 (c, 1 in $CHCl_3$). λ_{max} 198 (log ε 3.89) (no solvent reported).

Atta-ur-Rahman, *et al., Nat. Prod. Lett.*, 1999, **13**, 255-261 (*isol, pmr, cmr*)

Stigmasta-5,28-diene-3,20-diol S-383

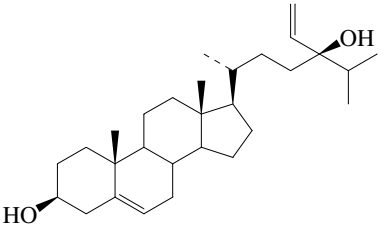
24-Ethenylcholest-5-ene-3,20-diol. 24-Vinylcholest-5-ene-3,20-diol



$C_{29}H_{48}O_2$ 428.697

(3β,20*S*,24*R*)-*form*
Varninasterol
[250147-19-4]
Constit. of *Spatoglossum variabile*.
Cryst.
Mp 225°. $[\alpha]_D^{25}$ -39 (c, 0.1 in $CHCl_3$).
Atta-ur-Rahman, *et al., Phytochemistry*, 1999, **52**, 495-499 (*isol, pmr, cmr*)

Stigmasta-5,28-diene-3,24-diol, 9CI S-384



(3β,24*R*)-*form*

$C_{29}H_{48}O_2$ 428.697

(3β,24*R*)-*form* [87859-99-2]
Constit. of *Hizikia fusiformis* and *Petrosia hebes*.
Cryst. (hexane).
Mp 167-167.5°. $[\alpha]_D$ -27 (c, 0.005 in $CHCl_3$).

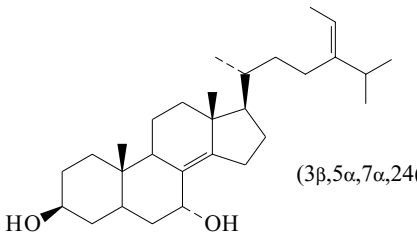
(3β,24*S*)-*form* [87859-98-1]
Cryst. (hexane). Mp 168.5-169°. $[\alpha]_D$ -55 (c, 0.006 in $CHCl_3$).

(3β,24ξ)-*form*
24-Hydroxy-24-vinylcholesterol. ***Saringosterol***
[6901-60-6]
Constit. of *Sargassum ringgoldianum* and *Xestospongia muta*. Also from green algae *Ulva rigida* and *Ulva fasciata*.
Cryst. (C_6H_6/hexane).
Mp 160-161°. $[\alpha]_D$ -31 ($CHCl_3$). Isol. as a 85:15 mixt. of 24*S*-/24*R*-isomers. Artifact of air oxidn. of Stigmasta-5,24(28)-dien-3-ol, S-401.

3-O-β-D-Glucopyranoside:
$C_{35}H_{58}O_7$ 590.839
Constit. of immature French bean seeds (*Phaseolus vulgaris*).

Ikekawa, N. *et al., Chem. Ind. (London)*, 1966, 1179
Catalan, C.A.N. *et al., J.O.C.*, 1983, **48**, 5207-5214 (*synth, pmr*)
Popov, S.S. *et al., Phytochemistry*, 1985, **24**, 1987-1990 (*isol, green algae*)
Cho, J.H. *et al., J.C.S. Perkin 1*, 1987, 1307-1318 (*3β,24R-form*)
Duque, C. *et al., Rev. Colomb. Quim.*, 1987, **14**, 81-88 (*isol, sponge*)
Kim, S.-K. *et al., J. Plant Biol.*, 1994, **37**, 441; *CA*, **123**, 79492b (*glucoside*)
Milkova, T. *et al., Phytochemistry*, 1997, **45**, 93-95
Ayyad, S.-E.N. *et al., Z. Naturforsch., C*, 2003, **58**, 333-336 (*Saringosterol, pmr, cmr*)

Stigmasta-8(14),24(28)-diene-3,7-diol **S-385**
24-Ethylidenecholest-8(14)-ene-3,7-diol



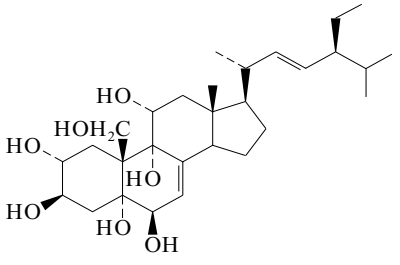
(3β,5α,7α,24(28)*E*)–*form*

$C_{29}H_{48}O_2$ 428.697

(3β,5α,7α,24(28)*E*)-*form* [141860-01-7]
Constit. of *Pellina semitubulosa*.

(3β,5α,7α,24(28)*Z*)-*form* [141860-00-6]
Constit. of *Pellina semitubulosa*.
Notaro, G. *et al., J. Nat. Prod.*, 1992, **55**, 773 (*isol, pmr*)

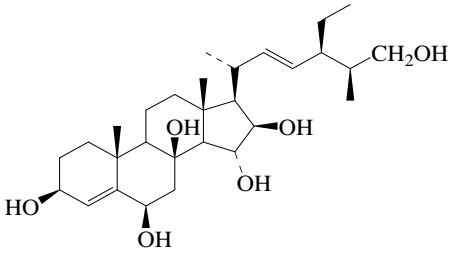
Stigmasta-7,22-diene-2,3,5,6,9,11,19-heptol **S-386**
24-Ethylcholesta-7,22-diene-2,3,5,6,9,11,19-heptol



$C_{29}H_{48}O_7$ 508.694

(2α,3β,5α,6β,11α,24*S*)-*form*
11,19-Di-Ac: [114422-36-5]
$C_{33}H_{52}O_9$ 592.768
Isol. from *Dysidea etheria*. Cryst.
Mp 147°. $[\alpha]_D^{25}$ -47.5 (c, 1.6 in EtOH).
West, R.R. *et al., J.O.C.*, 1988, **53**, 2782

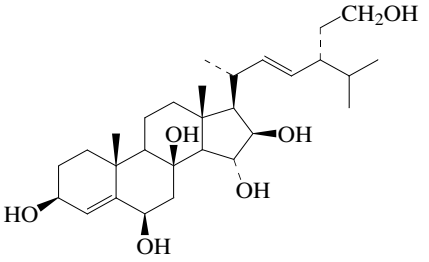
Stigmasta-4,22-diene-3,6,8,15,16,26-hexol **S-387**



$C_{29}H_{48}O_6$ 492.695

(3β,6β,15α,16β,22*E*,24*R*,25*S*)-*form*
3-O-*(2*-O-*Methyl-β-D-xylopyranoside), 15*-sulfate: ***Echinasteroside D***
[156398-64-0]
$C_{35}H_{58}O_{13}S$ 718.901
Isol. from *Echinaster brasiliensis*.
$[\alpha]_D$ -7.5. Isol. as Na salt to which CAS no. refers.
Iorizzi, M. *et al., J. Nat. Prod.*, 1993, **56**, 2149-2162 (*Echinasteroside D*)

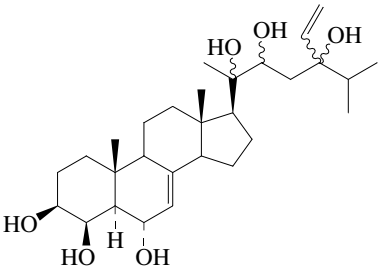
Stigmasta-4,22-diene-3,6,8,15,16,29-hexol **S-388**



$C_{29}H_{48}O_6$ 492.695

(3β,6β,15α,16β,22*E*,24*R*)-*form*
3-O-*(2*-O-*Methyl-β-D-xylopyranoside),15*-O-*sulfate:* ***Echinasteroside E***
[156398-65-1]
$C_{35}H_{58}O_{13}S$ 718.901
Isol. from *Echinaster brasiliensis*. Isol. as the Na salt to which the CAS no. refers.
Iorizzi, M. *et al., J. Nat. Prod.*, 1993, **56**, 2149-2162

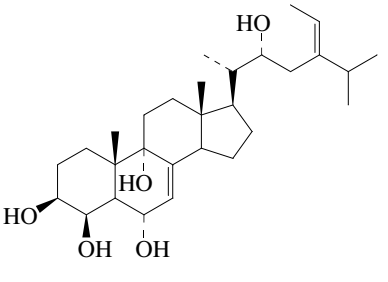
Stigmasta-7,28-diene-3,4,6,20,22,24-hexol **S-389**



$C_{29}H_{48}O_6$ 492.695

(3β,4β,5α,6α,20ξ,22ξ,24ξ)-*form*
4,6-Di-Ac: ***Agosterol C6***
[255832-09-8]
$C_{33}H_{52}O_8$ 576.769
Constit. of a *Spongia* sp.
$[\alpha]_D$ +37.7 (c, 0.2 in $CHCl_3$).
Aoki, S. *et al., Tetrahedron*, 1999, **55**, 13965-13972 (*isol, pmr, cmr*)

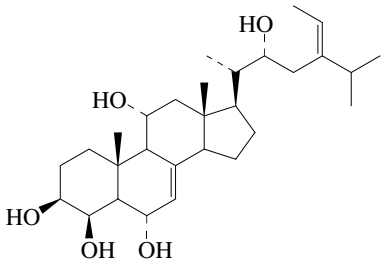
Stigmasta-7,24(28)-diene-3,4,6,9,22-pentol **S-390**



$C_{29}H_{48}O_5$ 476.695

(3β,4β,5α,6α,22*R*,24*E*)-*form*
3,4,6-Tri-Ac: ***Agosterol E3***
[603113-60-6]
$C_{35}H_{54}O_8$ 602.807
Constit. of *Acanthodendrilla* sp.
$[\alpha]_D^{26}$ +12.6 (c, 0.132 in $CHCl_3$).
Tsukamoto, S. *et al., J. Nat. Prod.*, 2003, **66**, 1181-1185 (*isol, pmr, cmr*)

Stigmasta-7,24(28)-diene-3,4,6,11,22-pentol S-391

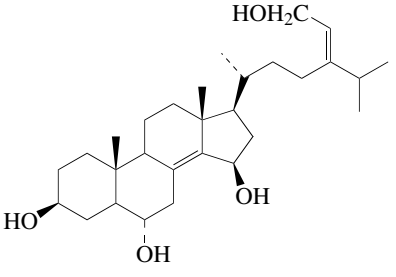


$C_{29}H_{48}O_5$ 476.695

(3β,4β,5α,6α,11α,22*R*,24*E*)-*form*

3,4,6-Tri-Ac: ***Agosterol A₃***
[603113-64-0]
$C_{35}H_{54}O_8$ 602.807
Constit. of *Acanthodendrilla* sp.
$[\alpha]_D^{26}$ +32 (c, 0.428 in $CHCl_3$).
Tsukamoto, S. *et al., J. Nat. Prod.*, 2003, **66**, 1181-1185 (*isol, pmr, cmr*)

Stigmasta-8(14),24(28)-diene-3,6,15,29-tetrol S-392



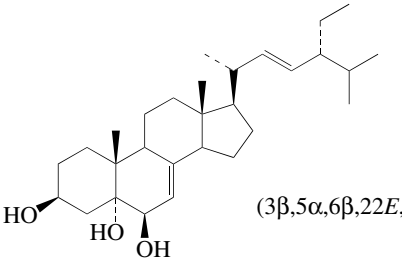
$C_{29}H_{48}O_4$ 460.696

(3β,6α,15β,24(28)*E*)-*form*

29-O-β-D-Xylopyranoside: ***Acodontasteroside I***
[195063-96-8]
$C_{34}H_{56}O_8$ 592.812
Constit. of *Acodontaster conspicuus.*
$[\alpha]_D$ -20.8 (c, 1 in MeOH).
De Marino, S. *et al., J. Nat. Prod.*, 1997, **60**, 959-966 (*isol, pmr, cmr*)

Stigmasta-7,22-diene-3,5,6-triol, 9CI S-393

24-Ethylcholesta-7,22-diene-3,5,6-triol



(3β,5α,6β,22*E*,24*R*)-*form*

$C_{29}H_{48}O_3$ 444.696

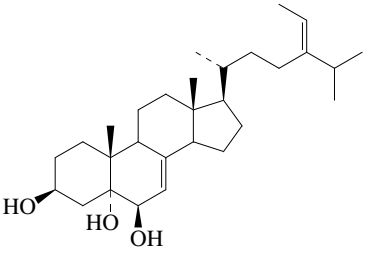
(3β,5α,6β,22*E*,24*R*)-*form* [124596-61-8]
Isol. from *Heliometra gracialis maxima.*

6-Butyl ether: ***Homaxisterol A₄***
[849906-47-4]
$C_{33}H_{56}O_3$ 500.804
Constit. of a *Homaxinella* sp. Oil.

(3β,5α,6β,22*E*,24*S*)-*form* [124649-15-6]
[100667-75-2]
Constit. of *Patinopecten yessoensis*, *Myriapora truncata* and *Heliometra gracialis maxima*.
Mp 227-232°. $[\alpha]_D$ -4.6 (MeOH).
Cafieri, F. *et al., J. Nat. Prod.*, 1985, **48**, 944-947 (*isol*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1988, **51**, 1098-1103 (*isol, pmr*)
Madaio, A. *et al., J. Nat. Prod.*, 1989, **52**, 952-961 (*isol, pmr*)
Kovganko, N.V. *et al., Khim. Prir. Soedin.*, 1989, 664-669; *Chem. Nat. Compd. (Engl. Transl.)*, 1989, **25**, 564-568 (*synth, pmr, config*)
Shubina, L.K. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **119**, 505-511 (*Heliometra gracialis constits*)
Mansoor, T.A. *et al., J. Nat. Prod.*, 2005, **68**, 331-336 (*Homaxisterol A₄*)

Stigmasta-7,24(28)-diene-3,5,6-triol S-394

24-Ethylcholesta-7,24(28)-diene-3,5,6-triol. 24-Ethylidenecholest-7-ene-3,5,6-triol



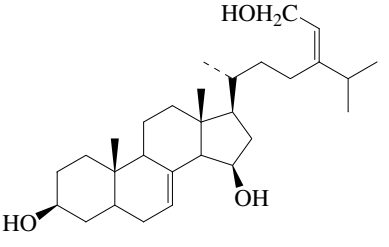
(3β,5α,6β,24*E*)-*form*

$C_{29}H_{48}O_3$ 444.696

(3β,5α,6β,24*E*)-*form* [124596-63-0]
Constit. of *Hippospongia communis, Spongia officinalis*, and *Ircinia variabilis.*

(3β,5α,6β,24*Z*)-*form* [124596-62-9]
Constit. of *Hippospongia communis* and *Spongia officinalis.*
Madaio, A. *et al., J. Nat. Prod.*, 1989, **52**, 952-961 (*isol, pmr, ms*)

Stigmasta-7,24(28)-diene-3,15,29-triol S-395



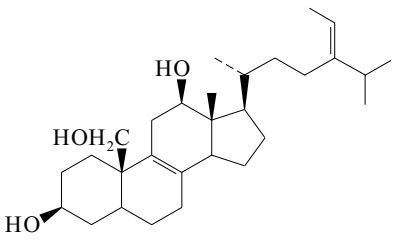
$C_{29}H_{48}O_3$ 444.696

(3β,15β,24(28)*E*)-*form*

3-O-[β-D-Galactopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→4)]-β-D-glucopyranoside]: ***Mycaloside I***
[593280-58-1]
$C_{52}H_{86}O_{22}$ 1063.238
Constit. of *Mycale laxissima*. Solid.
Mp 222-225°. $[\alpha]_D^{25}$ -6.5 (c, 0.7 in MeOH).
Antonov, A.S. *et al., J. Nat. Prod.*, 2003, **66**, 1082-1088 (*isol, pmr, cmr*)

Stigmasta-8,24(28)-diene-3,12,19-triol S-396

24-Ethylidenecholest-8-ene-3,12,19-triol. 24-Ethylcholesta-8,24(28)-diene-3,12,19-triol

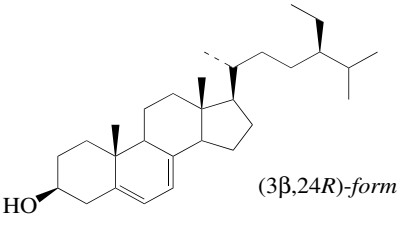


$C_{29}H_{48}O_3$ 444.696

(3β,5α,12β,24(28)*E*)-*form* [160581-13-5]
Constit. of *Litophyton arboreum*.
Flakes (Me_2CO).
Mp 187-189°.
Li, R. *et al., Steroids*, 1994, **59**, 503-505 (*isol, pmr, cmr*)

Stigmasta-5,7-dien-3-ol S-397

24-Ethylcholesta-5,7-dien-3-ol
[21632-41-7]



(3β,24*R*)-*form*

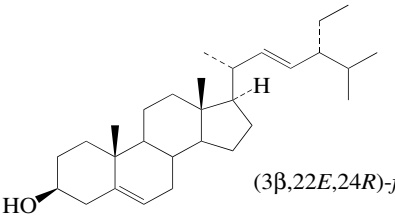
$C_{29}H_{48}O$ 412.698

(3β,24*R*)-*form*
***7*-Dehydrositosterol**. *Provitamin D_5*
[521-04-0]
Minor sterol present in sponges *Tethya amamensis* and *Spongionella gracilis*; also in *Aplysilla tango*, *Axinella cannabina*, *Cacospongia mollior* and molluscs. Isol. from the roots of *Rauwolfia serpentina*.
Cryst.
Mp 138° Mp 144-145°. $[\alpha]_D^{21}$ -116. $[\alpha]_D$ -107 ($CHCl_3$). λ_{max} 261 (log ϵ 3.83); 270 (log ϵ 3.92); 281 (log ϵ 3.94); 292 (log ϵ 3.76) (EtOH).

(3β,24*S*)-*form*
***7*-Dehydroclionasterol**. *Moonisterol*
[24057-73-6]
Constit. of *Capparis moonii* fruits; also from *Axinella cannabina*, *Chlorella vulgaris* and *Eutreptia viridis*.
Cryst. ($CHCl_3$/MeOH).
Mp 85-87°.
Kircher, H.W. *et al., Lipids*, 1974, **9**, 623-624 (*synth*)
Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*synth, pmr*)
Cafieri, F. *et al., Gazz. Chim. Ital.*, 1976, **106**, 761-763 (*isol*)
Weete, J.D. *et al., Lipids*, 1977, **12**, 398-404 (*isol*)
Zielinski, J. *et al., Steroids*, 1982, **40**, 403-411 (*isol, Eutreptia*)
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol*)
Teshima, S. *et al., Lipids*, 1983, **18**, 193-197 (*occur*)
Karmakar, T. *et al., Phytochemistry*, 1983, **22**, 608-609 (*isol, Rauwolfia*)
Sica, D. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **81**, 115-118 (*Spongionella gracilis constit*)
Poiner, A. *et al., Aust. J. Chem.*, 1990, **43**, 1713-1727 (*isol, ms*)
Akihisa, T. *et al., Phytochemistry*, 1992, **31**, 1769-1772 (*isol, Chlorella*)
Ramachandram, R. *et al., Indian J. Nat. Prod.*, 2004, **20**, 40-42 (*Moonisterol*)

Stigmasta-5,22-dien-3-ol S-398

24-Ethylcholesta-5,22-dien-3-ol



(3β,22*E*,24*R*)-*form*

$C_{29}H_{48}O$ 412.698

(3β,22*E*,24*R*)-*form*
***Poriferasterol**. Poriferasta-5,22-dien-3-ol. Strumasterol*
[481-16-3]
[32345-19-0]
Constit. of sponges, e.g. *Cliona celata*, *Spheciospongia vesparia*, *Haliclona variabilis*, green algae *Chlorella* spp., *Ochromonas malhamensis* and clam *Patinopecten yessoensis*.
Cryst. (EtOH).
Mp 156°. $[\alpha]_D$ -46 ($CHCl_3$).
Ac: [1900-51-2]
Mp 146.5-147°. $[\alpha]_D$ -53 ($CHCl_3$).

(3β,22*E*,24*S*)-*form*
***Stigmasterol**. Serposterol*
[83-48-7]
[32345-19-0]
Widely occurring sterol. Present in potato (*Solanum tuberosum*), chick pea (*Cicer arietinum*), artichoke (*Cynara scolymus*), sunflower oil, olive oil, beans (*Phaseolus vulgaris*), oats and strawberry fruit. Also widely distributed in marine organisms such as *Phakellia aruensis*, *Spirastrella inconstans*, *Sargassum filipendula*, *Dictyota dichotoma*, *Dysidea fragilis*, *Chaetoceros simplex* and *Botryocladia leptopoda*. Antimutagenic agent. Cryst. (EtOH).
Mp 170°. $[\alpha]_D^{22}$ -57 ($CHCl_3$).
3-O-*β*-D-*Galactopyranoside:* [145164-14-3]
$C_{35}H_{58}O_6$ 574.84
Constit. of *Rhynchosia minima*. Cryst.
Mp 245-247°. $[\alpha]_D$ -5 (c, 0.2 in $CHCl_3$).
3-O-*β*-D-*Glucopyranoside:* [19716-26-8]
$C_{35}H_{58}O_6$ 574.84
Isol. from soya bean oil (*Glycine max*), and tobacco (*Nicotiana tabacum*), roots of *Angelica japonica* and in *Corydalis bulbosa*.
Cryst. (EtOH/Py).
Mp 299°.
3-O-*[6*-O-*(9Z,12Z,15Z*-octadecatrienoyl)-*β*-D-glucopyranoside]:*
[79380-27-1]
$C_{53}H_{86}O_7$ 835.258
Constit. of *Caryopteris terniflora*.
Hexadecanoyl: ***Palmitoylstigmasterol***
[2308-84-1]
$C_{45}H_{78}O_2$ 651.11
Isol. from fennel (*Foeniculum vulgare*) roots and seeds, *Plantago asiatica* and *Plagiochasma intermedium* .
Mp 94-96°.
Octadecanoyl: Stearoylstigmasterol
[23838-16-6]
$C_{47}H_{82}O_2$ 679.164
Isol. from *Drypetes gossweileri*.
3-O-*(4-Hydroxycinnamoyl): 4-Hydroxycinnamoylstigmasterol*
[208927-15-5]
$C_{38}H_{54}O_3$ 558.843
Constit. of *Argyreia speciosa*. Cryst.
Mp 92°. $[\alpha]_D$ -27 ($CHCl_3$). λ_{max} 225; 326 (MeOH).

3-Ketone: Stigmasta-5,22-dien-3-one. ***Stigmasterone***
[51529-12-5]
$C_{29}H_{46}O$ 410.682
Constit. of *Eupatorium adenoforum*, *Eupatorium fidjiana*, *Eurycoma apiculatta* and *Piptocarpha opaca*. Needles (EtOH).
Mp 124.5-125°. $[\alpha]_D^{25}$ +63 ($CHCl_3$).

3-Ketone, oxime: Mp 187-188°.

3-Ketone, 2,4-dinitrophenylhydrazone:
Red cryst. Mp 244-245° dec.

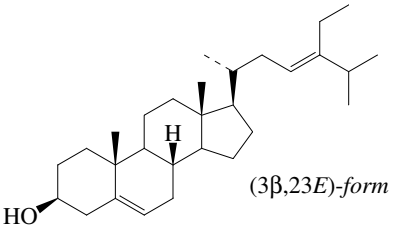
3-O-*Sulfate:* [140460-04-4]
[151890-99-2 (Na salt)]
$C_{29}H_{48}O_4S$ 492.762
Constit. of *Eupentacta fraudatrix* and *Gymnocrinus richeri*.

(3β,17ξ,20ξ,22*E*,24ξ)-*form*
Euphorbosterol
[80735-61-1]
Constit. of the latex of *Euphorbia tirucalli*.

(3β,22*E*,24ξ)-*form* [32345-19-0]
Constit. of *Pseudostichopus trachus*, *Synapta maculata*, *Paracentrotus lividus*, *Cladophora vagabunda*, *Polyneura hilliae*, *Lubomirskia baicalensis*, *Hydrodictyon reticulatum*, *Artemesia feddei*, pollen of *Pachycereus pringlei* and many other terrestrial and marine organisms.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 569B (*nmr*)
Fernholz, E. *et al., J.A.C.S.*, 1939, **61**, 2956-2957 (*synth*)
Jones, E.R.H. *et al., J.C.S.*, 1942, 391-392 (*synth*)
Heyl, F.W. *et al., J.A.C.S.*, 1953, **75**, 1918-1920 (*synth*)
Schwartz, J.J. *et al., J.A.C.S.*, 1955, **77**, 5442-5443 (*Stigmasterol, isol*)
Kishada, Y. *et al., Chem. Ind. (London)*, 1960, 465-466 (*abs config*)
Atherinos, A.E. *et al., J.C.S.*, 1962, 1700-1704 (*Stigmasterol, isol*)
Wright, H.E. *et al., J.O.C.*, 1962, **27**, 918-920 (*glucopyranoside*)
Von Ardenne, M. *et al., Experientia*, 1963, **19**, 178-180 (*ms*)
Kozin, N.I. *et al., CA*, 1964, **61**, 12213 (*Stigmasterol, occur*)
Kartnig, T. *et al., Fette, Seifen, Anstrichm.*, 1965, **67**, 10-13 (*Palmitoylstigmasterol*)
Knights, B.A. *et al., Phytochemistry*, 1965, **4**, 857-862 (*Stigmasterol, occur*)
Tomita, Y. *et al., Phytochemistry*, 1971, **10**, 573-575 (*biosynth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 2077 (*Stigmasterol, occur*)
Sucrow, W. *et al., Chem. Ber.*, 1975, **108**, 3721-3729 (*Poriferasterol, Stigmasterol, synth*)
Lenton, J.R. *et al., Phytochemistry*, 1975, **14**, 1523-1528 (*biosynth*)
Kobayashi, M. *et al., Steroids*, 1975, **26**, 605-624 (*Poriferasterol, isol*)
Wright, J.L.C. *et al., Can. J. Chem.*, 1978, **56**, 1898-1903 (*cmr*)
Holland, H.L. *et al., Can. J. Chem.*, 1978, **56**, 3121-3127 (*cmr*)
Mancuso, A.J. *et al., J.O.C.*, 1978, **43**, 2480-2482 (*synth*)
Malik, A. *et al., Pak. J. Sci. Ind. Res.*, 1981, **24**, 1-3; *CA*, **96**, 82679x (*Euphorbosterol*)
Goodfellow, R.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **76**, 575-578 (*3β,22E,24S-form, occur*)
Nicotra, F. *et al., J.C.S. Perkin 1*, 1985, 521-524 (*Poriferasterol*)
Bano, S. *et al., Planta Med.*, 1987, **53**, 117-118 (*Stigmasterol, occur*)Ronchetti, F. *et al., Chem. Comm.*, 1988, 1375-1376 (*Poriferasterol*)
Rao, R. *et al., Indian J. Chem., Sect. B*, 1988, **27**, 160-162 (*Stigmasterol, occur*)
Couture, R. *et al., Phytochemistry*, 1989, **28**, 1276-1277 (*Stigmasterol, occur*)
Malik, S. *et al., Steroids*, 1989, **53**, 271-284 (*Stigmasterol, occur*)
De Riccardis, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **100**, 647-651 (*Gymnocrinus richeri sulfate*)
Colombo, D. *et al., J.C.S. Perkin 1*, 1991, 962-964 (*Poriferasterol*)
Cambie, R.C. *et al., Phytochemistry*, 1991, **30**, 287-292 (*ketone, isol*)
Kolesnikova, I.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1992, **103**, 501-503 (*3β,22E,24ξ-form, occur*)
Tan, R.X. *et al., Phytochemistry*, 1992, **31**, 3135-3138 (*3β,22E,24ξ-form, occur*)
Ahmed, W. *et al., Phytochemistry*, 1992, **31**, 4038-4039 (*galactopyranoside*)
Lusby, W.R. *et al., Lipids*, 1993, **28**, 468-470 (*3β,22E,24ξ-form, occur*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constit*)
Bert, M. *et al., Phytochemistry*, 1995, **38**, 797-798 (*3β,22E,24ξ-form, occur*)
Marsan, M.-P. *et al., J.O.C.*, 1996, **61**, 4252-4257 (*Stigmasterol, synth*)
Alam, M.S. *et al., Phytochemistry*, 1996, **41**, 1197-1200 (*glucoside, pmr, cmr*)
Gaspar, H. *et al., Phytochemistry*, 1996, **43**, 613-615 (*isol, pmr, cmr*)
Dupont, M.P. *et al., Planta Med.*, 1997, **63**, 282-284 (*Stearoylstigmasterol*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **128**, 337-347 (*3β,22E,24ξ-form*)
Srivastava, A. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 192-194 (*Hydroxycinnamoylstigmasterol*)
Wang, F.-Q. *et al., Yaoxue Xuebao*, 2000, **35**, 587-591 (*Palmitoylstigmasterol*)
Jiang, R.W. *et al., J. Nat. Prod.*, 2001, **64**, 1266-1272 (*cryst struct*)
Benavides, G.A. *et al., Acta Cryst. C*, 2002, **58**, o131-o132 (*Stigmasterol, cryst struct*)
Itoh, D. *et al., J. Nat. Prod.*, 2003, **66**, 332-336 (*biosynth*)
De-Eknamkul, W. *et al., Phytochemistry*, 2003, **62**, 389-398 (*biosynth*)
Zhang, Y.H. *et al., Chin. Chem. Lett.*, 2004, **15**, 1445-1447 (*Caryopteris terniflora constit*)

Stigmasta-5,23-dien-3-ol S-399



(3β,23*E*)-*form*

$C_{29}H_{48}O$ 412.698

(3β,23*E*)-*form*
Sitosta-5,23-dien-3β-ol
[77715-86-7]
Constit. of *Holarrhena antidysenterica* and *Calyx nicaeensis*.
Cryst. (Me_2CO).
Mp 130°. $[\alpha]_D$ -16.3 ($CHCl_3$).

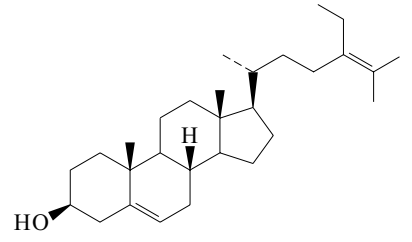
(3β,23*Z*)-*form* [84621-35-2]
Constit. of *Calyx nicaeensis*.

5β,6-Dihydro: 5β-Stigmast-23-en-3-ol
[123158-95-2]
$C_{29}H_{50}O$ 414.713
Minor sterol of *Calyx nicaeensis*, prob. as endobacterial metab.

Steiner, E. *et al., Helv. Chim. Acta*, 1977, **60**, 475-481 (*isol, synth*)
Narayanan, C.R. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 62
Itoh, T. *et al., J.O.C.*, 1983, **48**, 890-892 (*isol*)
Ha, T.B.T. *et al., Steroids*, 1989, **53**, 487-499 (*dihydro*)

Stigmasta-5,24-dien-3-ol S-400

24-Ethylcholesta-5,24-dien-3-ol



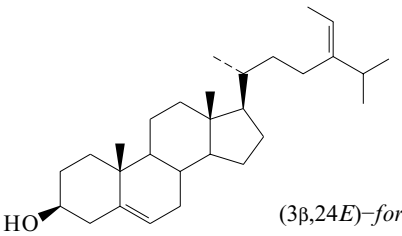
$C_{29}H_{48}O$ 412.698

3β-*form* [28949-66-8]
Constit. of a sponge *Stelletta* sp. and *Withania somnifera*.
Cryst. (MeOH).
Mp 135-137°. $[\alpha]_D$ -40.4 (c, 0.8 in $CHCl_3$).

Ac: [20224-70-8]
Mp 134-136°. $[\alpha]_D$ -45.6 (c, 0.48 in $CHCl_3$).

Lockley, W.J.S. *et al., Tet. Lett.*, 1974, 3773-3776 (*isol*)
Sucrow, W. *et al., Chem. Ber.*, 1975, **108**, 754-758 (*synth, pmr*)
Largeau, C. *et al., Phytochemistry*, 1977, **16**, 1925 (*synth*)
Guerriero, A. *et al., Helv. Chim. Acta*, 1991, **74**, 487-494 (*isol, pmr, cmr*)
Okuzumi, T. *et al., Tet. Lett.*, 1999, **40**, 8863-8866 (*biosynth*)

Stigmasta-5,24(28)-dien-3-ol, 9CI S-401



(3β,24*E*)–*form*

$C_{29}H_{48}O$ 412.698

(3β,24(28)*E*)-*form*

Fucosterol

[17605-67-3]

Characteristic sterol of brown algae; isol. from bladderwrack *Fucus vesiculosus*. Also present in *Sargassum tortile*, *Cystoseira* sp., *Bifurcaria* sp., *Turbinaria conoides*, scallop *Patinopecten yessoensis* and a marine unicellular alga. Also in sponges *Stelletta clarella*, *Tethya aurantia*, *Lissodendoryx noxiosa*, *Haliclona permollis* and other *Haliclona* spp.

Needles (MeOH).

Mp 124°. $[\alpha]_D^{20}$ -38.4 ($CHCl_3$).

3-O-*Sulfate:* [152005-13-5]

$C_{29}H_{48}O_4S$ 492.762

Constit. of *Eupentacta fraudatrix*.

3-O-*β-D-Xylopyranoside:* [151890-84-5]

$C_{34}H_{56}O_5$ 544.813

Constit. of *Eupentacta fraudatrix*.

(3β,24(28)*Z*)-*form*

Isofucosterol. *28-Isofucosterol*

[481-14-1]

Present in oats (*Avena sativa*). Major sterol of *Callyspongia diffusa* and other sponges and some green algae. Also found in scallop *Patinopecten yessoensis* and in lipids of a marine unicellular alga.

Plates (MeOH).

Mp 137° (130-131°). $[\alpha]_D^{26}$ -37.6 (MeOH).

(3β,24(28)ξ)-*form*

Δ⁵-Avenasterol

[18472-36-1]

Isol. from yeast, algal and fern lipids.

Platelets (MeOH).

Mp 137°. $[\alpha]_D^{26}$ -37.6 ($CHCl_3$). Originally considered to have the 5,11-diene struct.

(3β,20*S*,24(28)*E*)-*form*

Sargasterol. *20S-Fucosterol*

[481-15-2]

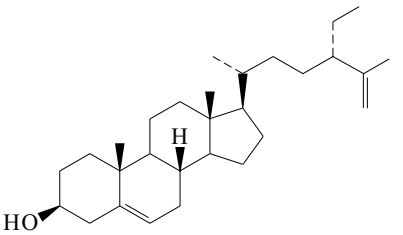
Isol. from the alga *Sargassum ringgoldianum*.

Cryst. (EtOH). $[\alpha]_D$ -47.5 ($CHCl_3$).

[6793-19-7, 20584-62-7, 55870-01-4, 83997-22-2]

Heilbron, I. *et al., J.C.S.*, 1934, 1572 (*isol*)
Idler, D.R. *et al., J.A.C.S.*, 1953, **75**, 1712 (*Isofucosterol, isol*)
Hayazu, R. *et al., Pharm. Bull.*, 1957, **5**, 452 (*synth*)
Tsuda, K. *et al., J.A.C.S.*, 1958, **80**, 921 (*Sargasterol*)
Dusza, J.P. *et al., J.O.C.*, 1960, **25**, 93 (*synth, Isofucosterol*)
Goad, L.J. *et al., Nature (London)*, 1966, **210**, 1322 (*biosynth*)
Nes, W.R. *et al., Steroids*, 1966, **8**, 655 (*pmr*)
Bates, R.B. *et al., Tet. Lett.*, 1968, 6163 (*struct*)
Brooks, C.J.W. *et al., Steroids*, 1972, **20**, 487 (*ms, struct*)
Yu, P.L.C. *et al., J. Nat. Prod.*, 1974, **37**, 593 (*Sargasterol*)
Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*isol, sponges*)
Erdman, T.R. *et al., Lloydia*, 1975, **38**, 359-360 (*Isofucosterol, isol, sponge*)
Kobayashi, M. *et al., Steroids*, 1975, **26**, 605 (*isol, Patinopecten yessoensis constits*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195 (*pmr*)
Bu'Lock, J.D. *et al., Phytochemistry*, 1976, **15**, 1249 (*biosynth*)
Massey, I.J. *et al., J.O.C.*, 1979, **44**, 2448 (*ms, synth*)
Nicotra, F. *et al., Gazz. Chim. Ital.*, 1980, **110**, 579
McInnes, A.G. *et al., Org. Magn. Reson.*, 1980, **13**, 302 (*cmr*)
Srivastava, S.K. *et al., Phytochemistry*, 1980, **19**, 2510 (*isol*)
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*Fucosterol, Isofucosterol, occur, alga*)
Seo, S. *et al., J.C.S. Perkin 1*, 1990, 105-108 (*biosynth*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
De Rosa, S. *et al., Phytochemistry*, 1997, **44**, 861-864; 1998, **48**, 103-105 (*Isofucosterol glucoside, acylglucosylisofucosterols*)
Okuzumi, T. *et al., Tet. Lett.*, 2000, **41**, 3623-3626 (*biosynth*)

Stigmasta-5,25-dien-3-ol S-402



$C_{29}H_{48}O$ 412.698

(3β,24*S*)-*form*

Clerosterol. *Poriferasta-5,25-dien-3-ol*

[2364-23-0]

Constit. of *Clerodendrum infortunatum*. Also from *Momordica charantia* (bitter melon) *Codium arabicum* , *Codium fragile* and *Codium iyengarii*. Component of lipids of a marine unicelluar alga.

Cryst. (petrol).

Mp 147° (120-121°). $[\alpha]_D^{23}$ -50.5 (c, 1.2 in $CHCl_3$).

3-O-*β-D-Glucopyranoside:* [123621-00-1]

$C_{35}H_{58}O_6$ 574.84

Isol. from fruits of bitter melon (*Momordica charantia*) and leaves of *Clerodendrum colebrookianum*. Cryst.

Mp 258-262° dec. Obt. as mixt. with β-sitosterol glucoside.

3-O-*(6*-O-*Heptadecanoyl-β-D-glucopyranoside):* ***Colebrin C***

[329315-70-0]

$C_{52}H_{90}O_7$ 827.279

Constit. of *Clerodendrum colebrookianum*. Wax. $[\alpha]_D^{25}$ -48.1 (c, 0.243 in $CHCl_3$).

3-O-*[6*-O-*(8Z-Octadecanoyl)-β-D-glucopyranoside]:*

[618458-18-7]

$C_{53}H_{90}O_7$ 839.29

Constit. of *Quisqualis fructus*.

3-O-*(6*-O-*Acyl-β-D-glucopyranoside):* Constit. of *Teucrium fruticans*.

$[\alpha]_D^{18}$ -51.5 (c, 0.163 in $CHCl_3$). Mixt. of fatty acid esters (palmitic, stearic, oleic, linoleic, linolenic, tetradecanoic, pentadecanoic, heptadecanoic, eicosanoic, docosanoic).

3-O-*β-D-Galactopyranoside:* ***Clerosterol galactoside***

[142435-67-4]

$C_{35}H_{58}O_6$ 574.84

Constit. of *Codium iyengarii* and *Codium dwarkense*. Powder.

O-*[3-Methylbutanoyl-(→6)-α-L-idopyranoside]:* ***Iyengaroside B***

[494862-73-6]

$C_{40}H_{66}O_7$ 658.957

Constit. of *Codium iyengarii*. Gum. $[\alpha]_D$ +11.8 (c, 1 in $CHCl_3$). Sugar may be misdrawn in ref.

3-Butanoyl: ***Mighavide***

[256512-61-5]

$C_{33}H_{54}O_2$ 482.788

Constit. of *Ajuga pseudoiva*.

3-O-*Hexadecanoyl: Clerosterol palmitate*

[883222-10-4]

$C_{45}H_{78}O_2$ 651.11

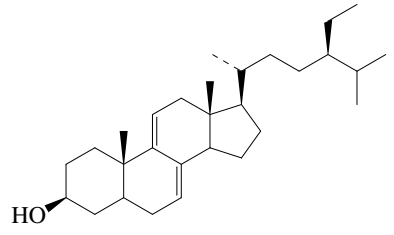
Constit. of *Codium fragile*.

Sucrow, W. *et al., Chem. Ber.*, 1966, **99**, 2765 (*glucoside*)
Manzoor-i-Khuda, M. *et al., Tetrahedron*, 1966, **22**, 2377
Wilkomirski, B. *et al., Phytochemistry*, 1983, **22**, 929 (*biosynth*)
Kokke, W.C.M.C. *et al., J.O.C.*, 1984, **49**, 3742-3752 (*occur, alga*)

Stoilov, I.L. *et al., Tetrahedron*, 1987, **43**, 2213 (*biosynth*)
Ahmad, V.U. *et al., Phytochemistry*, 1993, **33**, 1189 (*cmr*)
Goswami, P. *et al., Phytochemistry*, 1996, **41**, 279 (*isol, pmr, cmr, glucoside*)
Yagi, T. *et al., Phytochemistry*, 1996, **41**, 1057 (*biosynth*)
Gaspar, H. *et al., Phytochemistry*, 1996, **43**, 613 (*isol, pmr, cmr*)
Chaari, A. *et al., J. Soc. Chim. Tunis.*, 1998, **4**, 257-265; *CA*, **132**, 134733u (*3-butanoyl*)
Fontana, G. *et al., Phytochemistry*, 1999, **50**, 283-285 (*6′-Acylglucopyranoside*)
Yang, H. *et al., Fitoterapia*, 2000, **71**, 641-648 (*Colebrin C*)
Jannet, H.B. *et al., Industrial Crops and Products*, 2001, **14**, 213-222 (*Mighavide*)
Siddhanta, A.K. *et al., J. Indian Chem. Soc.*, 2002, **79**, 294-297 (*galactopyranoside*)
Ali, M.S. *et al., Nat. Prod. Lett.*, 2002, **16**, 407-413 (*Iyengaroside B, Clerosterol galactoside*)
Koami, T. *et al., Tet. Lett.*, 2002, **43**, 5479-5781 (*biosynth*)
Kwon, H.C. *et al., Arch. Pharmacal Res.*, 2003, **26**, 275-278; *CA*, **139**, 348070u (*Quisqualis fructus constit*)
Yin, S.-W. *et al., Biochem. Syst. Ecol.*, 2005, **33**, 1288-1292 (*Clerosterol palmitate*)

Stigmasta-7,9(11)-dien-3-ol S-403

24-Ethylcholesta-7,9(11)-dien-3-ol



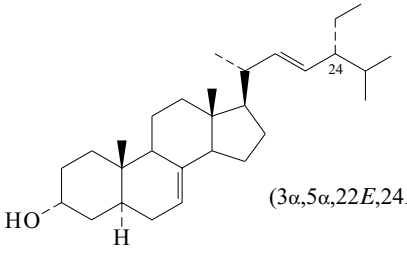
(3β,5α,24*R*)-*form*

$C_{29}H_{48}O$ 412.698

(3β,5α,24*R*)-*form* [59957-40-3]
Constit. of *Bryonia dioica*.
Ac:
Cryst. Mp 159-162°. λ_{max} 233; 240; 250 (no solvent reported).

(3β,5α,24ξ)-*form*
Me ether: 3-Methoxystigmasta-7,9(11)-diene
[139765-32-5]
$C_{30}H_{50}O$ 426.724
Constit. of the sponge *Jereicopsis graphidiophora*.
D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*3-Methoxystigmastadiene*)
Akihisa, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1202-1207 (*isol, pmr, ms*)

Stigmasta-7,22-dien-3-ol S-404



(3α,5α,22*E*,24*R*)–*form*

$C_{29}H_{48}O$ 412.698

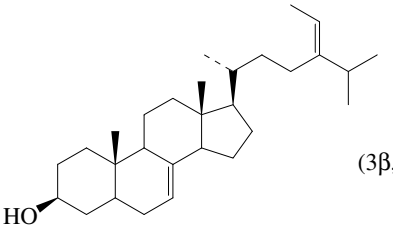
(3β,5α,22*E*,24*R*)-*form*
Chondrillasterol. *Poriferasta-7,22-dien-3-ol*
[481-17-4]
Constit. of *Axinella cannabina*, *Chondrilla nucula* and the green alga *Scenedesmus obliquus*.
Cryst. (Me_2CO/MeOH).
Mp 174.5-175.5°. $[\alpha]_D^{20}$ -2 ($CHCl_3$).

(3β,5α,22*E*,24*S*)-*form*
α-Spinasterol. *Bessisterol*
[481-18-5]
Constit. of spinach (*Spinacia oleracea*) leaves, cucumber (*Cucumis sativus*), alfalfa meal, bark of *Acacia concinu*, *Acacia caesia*, pumpkin seeds and senega root. Isol. from various marine sponges incl. *Axinella cannabina*. Shows antifungal activity. Cryst. ($EtOH/C_6H_6$).
Mp 171-173°. $[\alpha]_D^{22}$ -2.5 ($CHCl_3$).
▶ WJ2480000

Thompson, M.J. *et al., Phytochemistry*, 1972, **11**, 1781-1790 (*pmr*)
Kircher, H.W. *et al., J.O.C.*, 1973, **38**, 2259-2260 (*α-Spinasterol, synth*)
Armarego, W.L.F. *et al., Phytochemistry*, 1973, **12**, 2181-2187 (*biosynth*)
Sucrow, W. *et al., Phytochemistry*, 1976, **15**, 1533-1535 (*pmr, config*)
Banerji, N. *et al., J. Indian Chem. Soc.*, 1980, **57**, 417-419; 1043-1044 (*α-Spinasterol, α-Spinasterone*)
Anastasia, M. *et al., J.C.S. Perkin 1*, 1981, 2561-2562 (*α-Spinasterol, Chondrillasterol, synth, pmr*)
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*Axinella, isol*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Hearth, H.M.T.B. *et al., ACGC Chem. Res. Commun.*, 1999, **9**, 3-8; *CA*, **133**, 147489q (*α-Spinasterol, activity*)

Stigmasta-7,24(28)-dien-3-ol S-405

24-Ethylidenecholest-7-en-3-ol



(3β,5α,24(28)*E*)-*form*

$C_{29}H_{48}O$ 412.698

(3β,5α,24*E*)-*form* [22850-11-9]
Constit. of *Bryonia dioica*, *Pseudostichopus trachus*, *Bathyplotes natans*, *Echinaster sepositus*, *Liolophura japonica*, *Dictyuchus monosporus*, *Olea madagascariensis*, *Stichopus japonicus* and many other terrestrial and marine organisms.
3-O-*Sulfate:* [152005-21-5]
$C_{29}H_{48}O_4S$ 492.762
Constit. of *Eupentacta fraudatrix* and *Stichopus japonicus*.
3-O-*β*-D-*Xylopyranoside:* [151890-88-9]
$C_{34}H_{56}O_5$ 544.813
Constit. of *Eupentacta fraudatrix*.
*24*R,*28*R-*Epoxide: 24,28-Epoxystigmast-7-en-3-ol*. ***24,28-Epoxyisoavenasterol***
[260390-78-1]
$C_{29}H_{48}O_2$ 428.697
Constit. of *Bryonia dioica*.
*24*S,*28*S-*Epoxide:* [260390-79-2]
Constit. of *Bryonia dioica*.

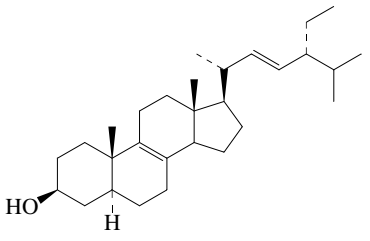
(3β,5α,24*Z*)-*form*
Δ⁷-Avenasterol
[23290-26-8]
Constit. of oats, pumpkin seeds, *Uromyces phaseoli*, *Vernonia anthelmintica* seeds and *Axinella cannabina*.
Cryst. (MeOH).
Mp 148-151°. $[\alpha]_D^{22}$ +12.7 (c, 1.28 in $CHCl_3$). Originally considered to be the 7,11-diene.
3-O-*Sulfate:* [152005-22-6]
Constit. of *Eupentacta fraudatrix*.
3-O-*β*-D-*Xylopyranoside:* [151890-89-0]
Constit. of *Eupentacta fraudatrix*.

Idler, D.R. *et al., J.A.C.S.*, 1953, **75**, 1712-1715 (*isol*)
Frost, D.J. *et al., Tet. Lett.*, 1968, 3779-3782 (*struct*)
Sucrow, W. *et al., Chem. Ber.*, 1970, **103**, 2711-2717 (*synth*)
Lin, H.-K. *et al., Phytochemistry*, 1972, **11**, 2319-2322 (*Uromyces constit*)

De Simone, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **66**, 351-357 (*Echinaster sepositus constit*)
Itoh, T. *et al., J. Chem. Res.*, 1982, **234**, 65-76 (*glc*)
Kalinovskaya, N.I. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **76**, 167-171 (*Stichopus japonicus constits*)
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*Axinella constit*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Akihisa, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1202-1207 (*isol, pmr, ms*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*occur*)
Akihisa, T. *et al., Phytochemistry*, 1999, **52**, 1601-1605 (*epoxides*)

Stigmasta-8,22-dien-3-ol S-406

24-Ethylcholesta-8,22-dien-3-ol



(3β,5α,22*E*,24*R*)-*form*

$C_{29}H_{48}O$ 412.698

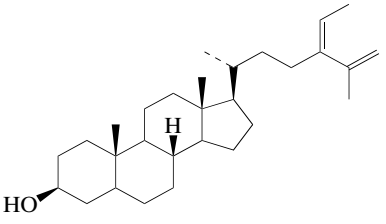
(3β,5α,22*E*,24*R*)-*form* [85798-14-7]
Constit. of the sponge *Axinella cannabina*.

(3β,5α,22*E*,24*S*)-*form* [85733-80-8]
Constit. of the sponge *Axinella cannabina*.

(3β,5β,22*Z*,24*R*)-*form* [173328-30-8]
Constit. of the aerial parts of *Koelpinia linearis*.
Cryst. (petrol/MeOH).
Mp 153.5°. $[\alpha]_D^{25}$ +23.8 (c, 1 in MeOH).
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol, pmr, ms*)
Shah, W.A. *et al., Phytochemistry*, 1996, **41**, 595-597 (*isol, pmr, cmr*)

Stigmasta-24(28),25-dien-3-ol S-407

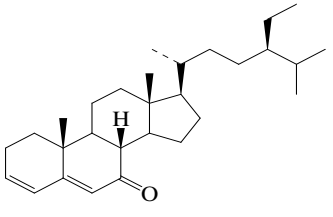
24-Ethylidenecholest-25-en-3-ol



$C_{29}H_{48}O$ 412.698

(3β,5α,24(28)*Z*)-*form* [214483-15-5]
Constit. of *Bathyplotes natans*.
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*isol, ms*)

Stigmasta-3,5-dien-7-one S-408



(24*R*)-*form*

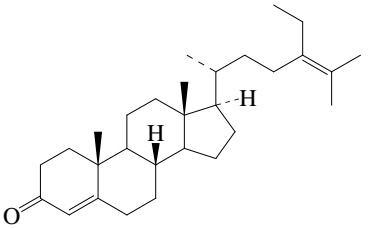
$C_{29}H_{46}O$ 410.682

(24*R*)-*form*
Tremulone
[2034-72-2]
Constit. of the heartwood of *Populus tremuloides*. Also in traces from *Pinus* spp. Pale-yellow cryst. (Me_2CO or MeOH). Mp 111°. $[\alpha]_D^{22}$ -288 ($CHCl_3$).

(24*S*)-*form*
Poriferasta-3,5-dien-7-one
Constit. of *Gracilaria edulis*. Cryst. Mp 117-118°. $[\alpha]_D$ -293.5 (c, 0.22 in $CHCl_3$).
Abramovitch, R.A. *et al., Can. J. Chem.*, 1962, **40**, 2017
Rowe, J.W. *et al., Phytochemistry*, 1965, **4**, 1 (*isol*)
Das, B. *et al., Phytochemistry*, 1992, **31**, 2427 (*isol, pmr*)

Stigmasta-4,24-dien-3-one, 9CI S-409

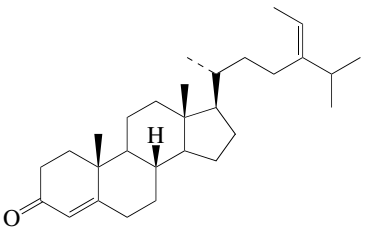
24-Ethylcholesta-4,24-dien-3-one
[103005-20-5]



$C_{29}H_{46}O$ 410.682
Constit. of a *Stelletta* sp. Oil. $[\alpha]_D^{20}$ +54 (c, 0.66 in EtOH).
Guerriero, A. *et al., Helv. Chim. Acta*, 1991, **74**, 487 (*isol, pmr, cmr*)

Stigmasta-4,24(28)-dien-3-one S-410

24-Ethylidenecholest-4-en-3-one

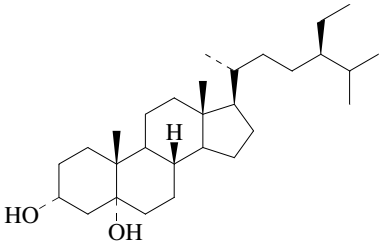


$C_{29}H_{46}O$ 410.682

24*E*-*form* [53755-09-2]
Constit. of *Stelletta clarella* and *Turbinaria conoides*.
Powder. Mp 94-95° (83-84°). $[\alpha]_D^{20}$ +80 ($CHCl_3$). λ_{max} 242 (log ϵ 4.06) (EtOH).
Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*isol, pmr, ms*)
Sheu, J.-H. *et al., J. Nat. Prod.*, 1999, **62**, 224-227 (*isol, pmr, cmr*)

Stigmastane-3,5-diol S-411

24-Ethylcholestane-3,5-diol



(3α,5α,24*R*)-*form*

$C_{29}H_{52}O_2$ 432.729

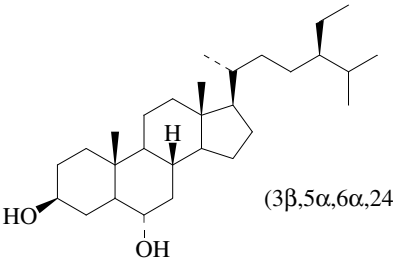
(3α,5α,24*R*)-*form*

3-O-*β*-D-*Glucopyranoside:* [135531-80-5]
$C_{35}H_{62}O_7$ 594.871
Constit. of *Rosa laevigata*.

(3β,5α,24*S*)-*form* [156178-11-9] Constit. of *Gracilaria edulis*. Cryst. (MeOH). Mp 238-240°. $[\alpha]_D$ +35.7 (c, 0.2 in MeOH).
Fang, J.M. *et al., J. Chin. Chem. Soc. (Taipei)*, 1991, **38**, 297 (*3-glucoside*)
Das, B. *et al., Planta Med.*, 1993, **59**, 572 (*isol, pmr, cmr*)

Stigmastane-3,6-diol S-412

24-Ethylcholestane-3,6-diol



(3β,5α,6α,24*R*)-*form*

$C_{29}H_{52}O_2$ 432.729

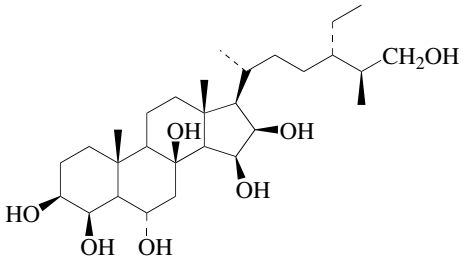
(3β,5α,6α,24*R*)-*form* [112244-29-8]
Constit. of *Spatholobus suberetus*, *Trichosanthes kirilowii* and *Urtica dioica*.
Prisms.
Mp 207-209°. $[\alpha]_D^{20}$ +41.8 (C, 0.74 in EtOH).

(3β,5α,6α,24*S*)-*form* [145985-30-4]
Constit. of *Gracilaria edulis* and seeds of *Trichosanthes kirilowii*.
Cryst. (MeOH).
Mp 214-215°. $[\alpha]_D^{25}$ +46.2 (c, 0.25 in $CHCl_3$).

(3β,5α,6β,24*R*)-*form*
Mp 208-210°.
Diketone: ***Stigmastane-3,6-dione****. 24-Ethylcholestane-3,6-dione*
[22149-69-5]
$C_{29}H_{48}O_2$ 428.697
Isol. from *Aristolochia indica*, *Lycium chinense* and *Typha angustata*. Constit. of mature wheat straw (*Triticum aestivum*).
Cryst.
Mp 195-198°.

(3β,5α,6β,24*S*)-*form*
Poriferastane-3,6-diol
[34427-63-9]
Constit. of *Gracilaria edulis*.
Cryst.
Mp 211-212°. $[\alpha]_D$ +29.5 (c, 0.2 in MeOH).
Chaurasia, N. *et al., J. Nat. Prod.*, 1987, **50**, 881-885 (*isol, Urtica*)
Fukuyama, Y. *et al., Planta Med.*, 1988, **54**, 34-36 (*isol, Spatholobes*)
Das, B. *et al., Phytochemistry*, 1992, **31**, 4371-4373 (*isol, Gracilaria, pmr*)
Gaspar, E.M.M. *et al., Phytochemistry*, 1993, **34**, 523 (*diketone*)
Das, B. *et al., Planta Med.*, 1993, **59**, 572-573 (*isol, Gracilaria, pmr, cmr*)
Kimura, Y. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1813-1817 (*isol, Trichosanthes, pmr, cmr*)
Wei, K. *et al., Magn. Reson. Chem.*, 2004, **42**, 355-359 (*diketone, pmr, cmr*)

Stigmastane-3,4,6,8,15,16,26-heptol S-413

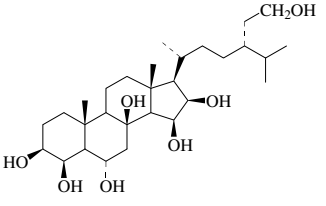


$C_{29}H_{52}O_7$ 512.726

(3β,4β,6α,8β,15β,16β,24*S*,25*S*)-*form* [194935-36-9]
Constit. of *Acodontaster conspicuus*.
$[\alpha]_D$ +6.6 (c, 1 in MeOH).
De Marino, S. *et al., J. Nat. Prod.*, 1997, **60**, 959-966 (*isol, pmr, cmr*)

Stigmastane-3,4,6,8,15,16,29-heptol S-414

24-(2-Hydroxyethyl)cholestane-3,4,6,8,15,16-hexol



(3β,4β,5α,6α,8β,15β,16β,24*R*)-*form*

$C_{29}H_{52}O_7$ 512.726

(3β,4β,5α,6α,8β,15β,16β,24*R*)-*form*
Certonardosterol P₁
[681240-58-4]
Constit. of *Certonardoa semiregularis*.
Cryst. $[\alpha]_D^{21}$ +36.4 (c, 0.11 in MeOH).
3-O-*(4*-O-*Methyl-β*-D-*xylopyranoside):* ***Certonardoside I₂***
[681225-99-0]
$C_{35}H_{62}O_{11}$ 658.868
Constit. of *Certonardoa semiregularis*. Cryst.
29-O-*(4*-O-*Methyl-β*-D-*xylopyranoside), 6*-O-*sulfate:* ***Certonardoside I***
[476437-88-4]
$C_{35}H_{62}O_{14}S$ 738.932
Constit. of *Certonardoa semiregularis*. Cryst.
29-O-*[α*-L-*Arabinopyranosyl-(1→4)-3*-O-*methyl-β*-D-*xylopyranoside]:* ***Moniloside E***
[147362-18-3]
$C_{40}H_{70}O_{15}$ 790.984
Constit. of echinoderm *Fromia monilis*.
29-O-*[2,4-Di*-O-*methyl-β*-D-*xylopyranosyl-(1→2)-α*-L-*arabinofuranoside]:* ***Halityloside H***
[102040-09-5]
$C_{41}H_{72}O_{15}$ 805.011
Constit. of *Halityle regularis*.
$[\alpha]_D$ -5 (MeOH).
29-O-*[2,4-Di*-O-*methyl-β*-D-*xylopyranosyl-(1→2)-α*-L-*arabinofuranoside], 6*-O-*sulfate:*
$C_{41}H_{72}O_{18}S$ 885.075
Constit. of *Halityle regularis*.
29-O-*[2*-O-*Methyl-β*-D-*xylopyranosyl-(1→2)-β*-D-*xylopyranoside]:* ***Halityloside A***
[102046-48-0]
$C_{40}H_{70}O_{15}$ 790.984
Constit. of echinoderm *Halityle regularis*. Sol. MeOH. $[\alpha]_D$ -3.1 (MeOH).

29-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-β-D-xylopyranoside], 6*-O-*sulfate: Halityloside A 6-sulfate*
$C_{40}H_{70}O_{18}S$ 871.048
Isol. from starfish *Nardoa tuberculata*.
$[\alpha]_D$ +3.7.

29-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-4*-O-*methyl-β-D-xylopyranoside], 6*-O-*sulfate:* ***Certonardoside I₃***
[856452-90-9]
$C_{41}H_{72}O_{18}S$ 885.075
Constit. of *Certonardoa semiregularis*.

29-O-*[3*-O-*Methyl-β-D-xylopyranosyl-(1→4)-3*-O-*methyl-β-D-xylopyranoside]:* ***Milleporoside A***
[887141-45-9]
$C_{41}H_{72}O_{15}$ 805.011
Constit. of *Fromia milleporella*. Cryst. (MeOH).
Mp 153-155.5°. $[\alpha]_D^{20}$ -12.6 (c, 0.53 in MeOH).

29-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→2)-β-D-xylopyranoside], 6*-O-*sulfate: 4″*-O-*Methylhalityloside A 6-sulfate*
$C_{41}H_{72}O_{18}S$ 885.075
Isol. from *Nardoa tuberculata*.

29-O-*[3*-O-*Methyl-β-D-xylopyranosyl-(1→4)-β-D-xylopyranosyl-(1→4)-β-D-xylopyranoside]:* ***Moniloside I***
[147362-21-8]
$C_{45}H_{78}O_{19}$ 923.1
Constit. of *Fromia monilis*.
$[\alpha]_D$ -3.5 (MeOH).

29-O-*[3*-O-*Methyl-β-D-xylopyranosyl-(1→4)-3*-O-*methyl-β-D-xylopyranosyl-(1→4)-β-D-xylopyranoside]:* ***Moniloside G***
[147362-20-7]
$C_{46}H_{80}O_{19}$ 937.127
Constit. of *Fromia monilis*.
$[\alpha]_D$ -17.5 (MeOH).

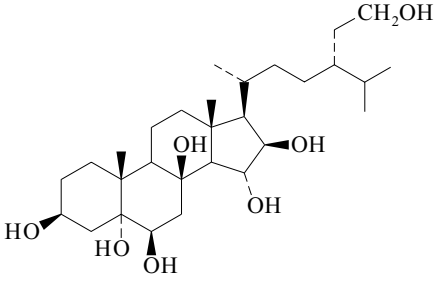
(3β,4β,5α,6β,8β,15α,16β,24*R*)-*form*

29-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-β-D-galactofuranoside]:* ***Crossasteroside P₂***
[125338-05-8]
$C_{41}H_{72}O_{16}$ 821.01
Constit. of *Crossaster pappopus*.
$[\alpha]_D$ -14 (MeOH).

Iorizzi, M. *et al., J. Nat. Prod.*, 1986, **49**, 67-78 (*Halitylosides*)
Kicha, A.A. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1989, **25**, 569-572 (*Crossasteroside P₂*)
Casapullo, A. *et al., J. Nat. Prod.*, 1993, **56**, 105-115 (*Monilosides*)
Bruno, I. *et al., J. Nat. Prod.*, 1993, **56**, 1057-1064 (*Halityloside A 6-sulfate, 4″*-O-*Methylhalityloside A 6-sulfate*)
Wang, W. *et al., J. Nat. Prod.*, 2002, **65**, 1649-1656; 2004, **67**, 584-591 (*Certonardoside I, Certonardosterol P₁, Certonardoside I₂*)
Wang, W. *et al., Arch. Pharmacal Res.*, 2005, **28**, 285-289 (*Certonardoside I₃*)
Levina, E.V. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2006, **32**, 84-88 (*Milleporoside A*)

Stigmastane-3,5,6,8,15,16,29-heptol S-415

24-(2-Hydroxyethyl)cholestane-3,5,6,8,15,16-hexol



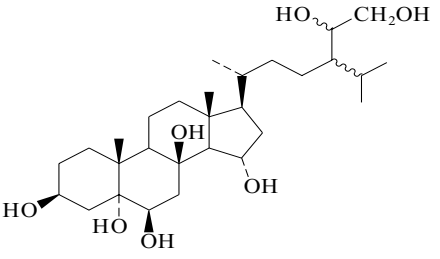
$C_{29}H_{52}O_7$ 512.726

(3β,5α,6β,8β,15α,16β,24*R*)-*form*

29-Sulfate: [160538-72-7]
$C_{29}H_{52}O_{10}S$ 592.79
Constit. of *Styracaster caroli* and *Tremaster novaecaledoniae*.
$[\alpha]_D$ +25 (MeOH).
Iorizzi, M. *et al., J. Nat. Prod.*, 1994, **57**, 1361-1373 (*isol*)

Stigmastane-3,5,6,8,15,28,29-heptol S-416

24-(1,2-Dihydroxyethyl)cholestane-3,5,6,8,15-pentol



$C_{29}H_{52}O_7$ 512.726

(3β,5α,6β,8β,15α,24ξ,28ξ)-*form*

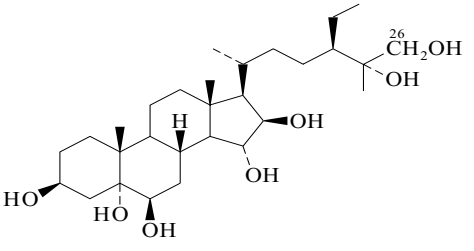
Amorph. $[\alpha]_D$ +29.3 (c, 0.5 in MeOH).

29-Sulfate:
$C_{29}H_{52}O_{10}S$ 592.79
Constit. of *Ctenodiscus crispatus*. Amorph. $[\alpha]_D$ +25.9 (c, 0.8 in MeOH).

Kicha, A.A. *et al., Izv. Akad. Nauk, Ser. Khim.*, 1994, **43**, 1821; *Russ. Chem. Bull. (Engl. Transl.)*, 1994, **43**, 1726 (*isol, pmr, cmr*)

Stigmastane-3,5,6,15,16,25,26-heptol S-417

24-Ethylcholestane-3,5,6,15,16,25,26-heptol

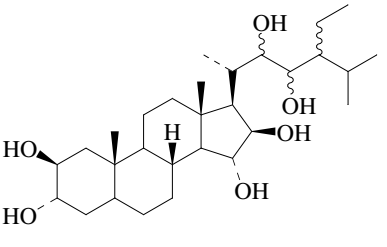


$C_{29}H_{52}O_7$ 512.726

(3β,5α,6β,15α,16β,24*R*,25*R*)-*form*

26-Sulfate: [174587-04-3]
$C_{29}H_{52}O_{10}S$ 592.79
Constit. of *Styracaster caroli*.
$[\alpha]_D$ +15.4 (MeOH).
De Riccardis, F. *et al., J. Nat. Prod.*, 1996, **59**, 386 (*isol, pmr, cmr*)

Stigmastane-2,3,15,16,22,23-hexol S-418

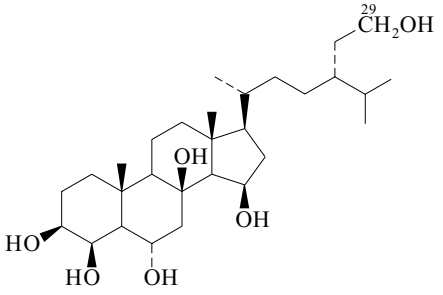


$C_{29}H_{52}O_6$ 496.726

(2β,3α,15α,16β,22ξ,23ξ,24ξ)-*form*

22,23-Dibutanoyl, 15-Ac, 2,3-bis(hydrogen sulfate): ***Clathsterol***
[377080-84-7]
$C_{39}H_{66}O_{15}S_2$ 839.073
Constit. of a *Clathria* sp. Powder. $[\alpha]_D$ +28 (c, 0.35 in MeOH).
Rudi, A. *et al., J. Nat. Prod.*, 2001, **64**, 1451-1453 (*isol, pmr, cmr*)

Stigmastane-3,4,6,8,15,29-hexol S-419



$C_{29}H_{52}O_6$ 496.726

(3β,4β,5α,6α,8β,15β,24*R*)-*form*

29-O-*[2,4-Di*-O-*methyl-β-D-xylopyranosyl-(1→2)-α-L-arabinofuranoside]:* ***Gomophioside B***
[99481-52-4]
$C_{41}H_{72}O_{14}$ 789.011
Constit. of *Gomophia watsoni*.

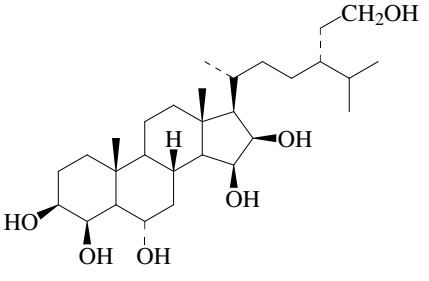
29-O-*[β-D-Xylopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Acodontasteroside D***
[195061-85-9]
$C_{39}H_{68}O_{14}$ 760.958
Constit. of *Acodontaster conspicuus*.
$[\alpha]_D$ +8 (c, 1 in MeOH).

29-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Acodontasteroside F***
[195062-02-3]
$C_{40}H_{70}O_{14}$ 774.985
Constit. of *Acodontaster conspicuus*.
$[\alpha]_D$ -14.4 (c, 1 in MeOH).

29-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-β-D-xylopyranoside], 6*-O-*sulfate:* ***Acodontasteroside B***
[195061-76-8]
$C_{40}H_{70}O_{17}S$ 855.049
Constit. of *Acodontaster conspicuus*.

Riccio, R. *et al., Gazz. Chim. Ital.*, 1985, **115**, 405-409 (*Gomophioside B*)
De Marino, S. *et al., J. Nat. Prod.*, 1997, **60**, 959-966 (*Acodontasterosides*)

Stigmastane-3,4,6,15,16,29-hexol S-420



$C_{29}H_{52}O_6$ 496.726

(3β,4β,5α,6α,15β,16β,24*R*)-*form*

29-O-*(4*-O-*Methyl-β-D-xylopyranoside):* ***Certonardoside J₂***
[681225-97-8]
$C_{35}H_{62}O_{10}$ 642.869
Constit. of *Certonardoa semiregularis*. Cryst. $[\alpha]_D^{21}$ -6.5 (c, 0.16 in MeOH).

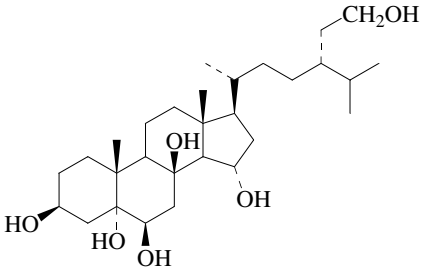
29-O-*(4*-O-*methyl-β-D-xylopyranoside), 6*-O-*sulfate:* ***Certonardoside J***
[476437-89-5]
$C_{35}H_{62}O_{13}S$ 722.933
Constit. of *Certonardoa semiregularis*. Cryst.

*22,23-Didehydro(*E-*): Stigmast-22-ene-3,4,6,15,16,29-hexol*
$C_{29}H_{50}O_6$ 494.71

*22,23-Didehydro(*E-*), 29*-O-*(4*-O-*methyl-β-D-xylopyranoside):* ***Certonardoside J₃***
[681225-98-9]
$C_{35}H_{60}O_{10}$ 640.853
Constit. of *Certonardoa semiregularis*. Cryst.

Wang, W. *et al., J. Nat. Prod.*, 2002, **65**, 1649-1656; 2004, **67**, 584-591 (*isol, pmr, cmr*)

Stigmastane-3,5,6,8,15,29-hexol S-421



$C_{29}H_{52}O_6$ 496.726

(3β,5α,6β,8β,15α,24*R*)-*form*

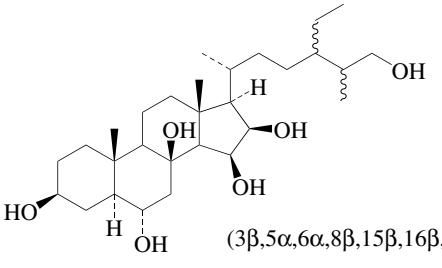
29-O-*β-D-Glucopyranoside:* ***Leptasteroside L***
[169063-30-3]
$C_{35}H_{62}O_{11}$ 658.868
Isol. from the starfish *Leptasterias polaris acervata*. Amorph. $[\alpha]_D$ -3.3 (c, 0.15 in MeOH).

29-(2-O-*Sulfo-β-D-glucopyranoside):* ***Aphelasteroside D***
[369384-73-6]
$C_{35}H_{62}O_{14}S$ 738.932
Constit. of the starfish *Aphelasterias japonica*.

Kicha, A.A. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1995, **44**, 1125-1126; 2001, **50**, 724-727 (*isol, pmr, cmr*)

Stigmastane-3,6,8,15,16,26-hexol S-422

24-Ethylcholestane-3,6,8,15,16,26-hexol



(3β,5α,6α,8β,15β,16β,24ξ,25ξ)-*form*

$C_{29}H_{52}O_6$ 496.726

(3β,5α,6α,8β,15β,16β,24ξ,25ξ)-*form*

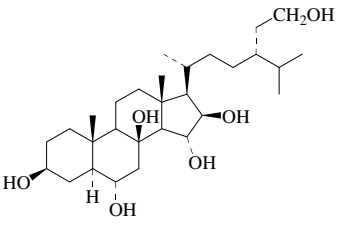
26-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-3*-O-*sulfo-β-D-xylopyranoside]:* ***Certonardoside P₂***
[856452-87-4]
$C_{40}H_{70}O_{17}S$ 855.049
Constit. of *Certonardoa semiregularis*.

(3β,5α,6β,8β,15α,16β,24ξ,25ξ)-*form*

26-O-*β-D-Xylopyranoside, 3-sulfate:* ***Attenuatoside SIII***
[92593-73-2]
$C_{34}H_{60}O_{13}S$ 708.906
Constit. of *Hacelia attenuata*.
$[\alpha]_D$ +3.

Minale, L. *et al., Gazz. Chim. Ital.*, 1984, **114**, 151-158 (*Attenuatoside SIII*)
Wang, W. *et al., Arch. Pharmacal Res.*, 2005, **28**, 285-289 (*Certonardoside P₂*)

Stigmastane-3,6,8,15,16,29-hexol S-423



(3β,5α,6α,15α,16β,24*R*)-*form*

$C_{29}H_{52}O_6$ 496.726

(3β,5α,6α,15α,16β,24*R*)-*form*

*29-(2-*O*-Sulfo-α-L-arabinofuranoside):* ***Asterosaponin P₂***
[329320-38-9]
$C_{34}H_{60}O_{13}S$ 708.906
Constit. of *Patiria pectinifera* (*Asterina pectinifera*) and an *Echinaster* sp.

(3β,5α,6α,15β,16β,24*R*)-*form*

Certonardosterol O₁
[681240-57-3]
Constit. of *Certonardoa semiregularis.*
Cryst.

*3-(4-*O*-Methyl-β-D-xylopyranoside):* ***Certonardoside P₁***
[681225-96-7]
$C_{35}H_{62}O_{10}$ 642.869
Constit. of *Certonardoa semiregularis.* Cryst.

*29-*O*-(6-*O*-Sulfo-β-D-glucopyranoside):* ***Pisasteroside F***
[131985-14-3]
$C_{35}H_{62}O_{14}S$ 738.932
Isol. from the starfish *Pisaster giganteus* (as Na salt).
$[\alpha]_D$ +10 (c, 1 in MeOH).

*29-(5-*O*-Methyl-β-D-galactofuranoside):* ***Oreasteroside F***
[162023-52-1]
$C_{36}H_{64}O_{11}$ 672.895
Constit. of *Oreaster reticulatus.*
$[\alpha]_D$ +10.

*29-(5-*O*-Methyl-β-D-galactofuranoside), 6-sulfate:* ***Oreasteroside G***
[161996-28-7]
$C_{36}H_{64}O_{14}S$ 752.959
Constit. of *Oreaster reticulatus.*
$[\alpha]_D$ +13.8.

*29-[2-*O*-Methyl-β-D-xylopyranosyl-(1→2)-β-D-xylopyranoside]:* ***Halityloside B***
[102072-01-5]
$C_{40}H_{70}O_{14}$ 774.985
Constit. of *Halityle regularisNardoa tuberculata*, *Culcita novaguineae* and *Sphaerodiscus piacenta*. Sol. MeOH. $[\alpha]_D$ -5 (MeOH).

*29-*O*-[β-D-Galactofuranosyl-(1→6)-β-D-galactofuranoside]:* ***Solasteroside S₂***
$C_{41}H_{72}O_{16}$ 821.01
Constit. of *Solaster dawsoni*. Amorph. solid. $[\alpha]_D$ -25.7 (c, 0.6 in MeOH).

(3β,5α,6β,15α,16β,24*R*)-*form*

*3-*O*-(2-*O*-Methyl-β-D-xylopyranoside), 15-sulfate:* ***Laeviuscoloside E***
[129393-25-5]
$C_{35}H_{62}O_{13}S$ 722.933
Constit. of *Henricia laeviuscola*.
$[\alpha]_D$ +2.6.

*29-*O*-[2-*O*-Methyl-β-D-xylopyranosyl-(1→2)-β-D-galactofuranoside]:* ***Crossasteroside P₁***
[125338-06-9]
$C_{41}H_{72}O_{15}$ 805.011
Constit. of *Crossaster papposus.*
$[\alpha]_D$ -12.9 (MeOH).

*29-*O*-α-L-Arabinofuranoside:*
$C_{34}H_{60}O_{10}$ 628.842
Constit. of *Patiria pectinifera.* Cryst.
Mp 248-249°. $[\alpha]_D$ +3.8 (MeOH).

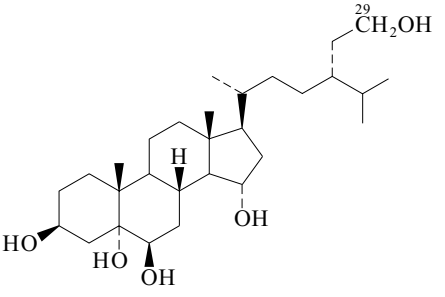
*29-*O*-(5-*O*-Methyl-2-sulfo-α-L-arabinofuranoside):* ***Miniatoside A***
[128269-48-7]
$C_{35}H_{62}O_{13}S$ 722.933
Constit. of *Patiria miniata*.
$[\alpha]_D$ +19 (MeOH).

(3β,5α,6β,15α,16β,24ξ)-*form*

29-β-D-Xylopyranoside, 15-sulfate: ***Attenuatoside SI***
[92593-75-4]
$C_{34}H_{60}O_{13}S$ 708.906
Constit. of *Hacelia attenuata*.
$[\alpha]_D$ +10.

Minale, L. *et al., Gazz. Chim. Ital.*, 1984, **114**, 151-158 (*Attenuatoside SI*)
Kicha, A.A. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 332-337 (*Patiria pectinifera saponin*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1986, **49**, 67-78 (*Halityloside B*)
Kicha, A.A. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1989, **25**, 569-572 (*Crossasteroside P1*)
D'Auria, M.V. *et al., Gazz. Chim. Ital.*, 1990, **120**, 155-163 (*Laeviuscoloside E*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1990, **53**, 94-101 (*Miniatoside A*)
Zollo, F. *et al., J. Nat. Prod.*, 1990, **53**, 1000-1005 (*Pisasteroside F*)
Kicha, A.A. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1993, **42**, 943-949 (*Solasteroside S2*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1995, **58**, 10-26 (*Oreasterosides*)
Kicha, A.A. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2000, **49**, 1794-1795 (*Asterosaponin P2*)
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 584-591 (*Certonardosterol O₁, Certonardoside P₁*)

Stigmastane-3,5,6,15,29-pentol S-424



$C_{29}H_{52}O_5$ 480.727

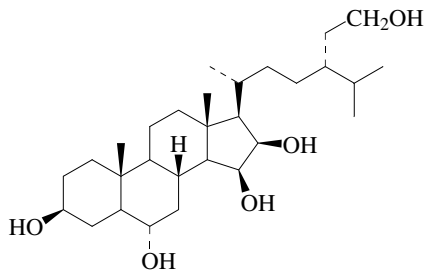
(3β,5α,6β,15α,24*R*)-*form*

29-Sulfate:
$C_{29}H_{52}O_8S$ 560.791
Constit. of *Luidia clathrata*.
$[\alpha]_D$ +15.

29-Carboxylic acid: ***3,5,6,15-Tetrahydroxystigmastan-29-oic acid***
[130799-38-1]
$C_{29}H_{50}O_6$ 494.71
Constit. of *Myxoderma platyacanthum*.
$[\alpha]_D$ +6.7 (MeOH).

Finamore, E. *et al., J.O.C.*, 1991, **56**, 1146-1153 (*isol, pmr, cmr*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1995, **58**, 653-671 (*isol, pmr, cmr*)

Stigmastane-3,6,15,16,29-pentol S-425

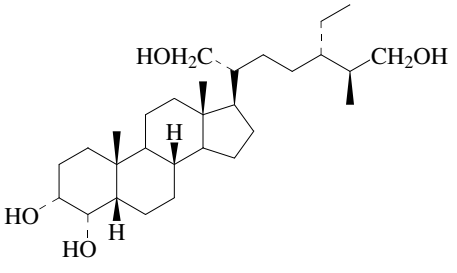


$C_{29}H_{52}O_5$ 480.727

(3β,6α,15β,16β,24*R*)-*form*
Certonardosterol N₁
[681240-56-2]
Constit. of *Certonardoa semiregularis.*
Cryst.
29-O-*(4*-O-*Methyl-β-D-xylopyranoside):* ***Certonardoside O₁***
[681225-95-6]
$C_{35}H_{62}O_9$ 626.869
Constit. of *Certonardoa semiregularis.* Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 584-591 (*isol, pmr, cmr*)

Stigmastane-3,4,21,26-tetrol S-426

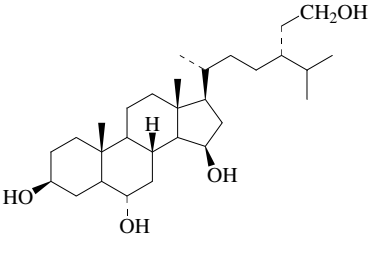
24-Ethylcholestane-3,4,21,26-tetrol



$C_{29}H_{52}O_4$ 464.727

(3α,4α,5β,24*S*,25*S*)-*form*
3,21-Disulfate: [116407-19-3]
$C_{29}H_{52}O_{10}S_2$ 624.856
Isol. from the Pacific ophiuroid *Ophiolepis superba*.
$[\alpha]_D$ +18.8 (MeOH) (as di-Na salt).
D'Auria, M.V. *et al., J.O.C.*, 1989, **54**, 234-239 (*isol, pmr, cmr, struct*)
D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1990, 2895 (*stereochem*)

Stigmastane-3,6,15,29-tetrol S-427



(3β,6α,15β,24*R*)-*form*

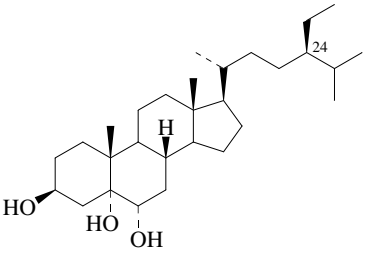
$C_{29}H_{52}O_4$ 464.727

(3β,6α,15β,24*R*)-*form*
Certonardosterol D₃
[681240-55-1]
Constit. of *Certonardoa semiregularis.*
Cryst.

(3β,6β,15α,24*R*)-*form*
Certonardosterol E₂
[681240-59-5]
Constit. of *Certonardoa semiregularis.*
Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 584-591 (*isol, pmr, cmr*)

Stigmastane-3,5,6-triol S-428

24-Ethylcholestane-3,5,6-triol



(3β,5α,6α,24*R*)-*form*

$C_{29}H_{52}O_3$ 448.728

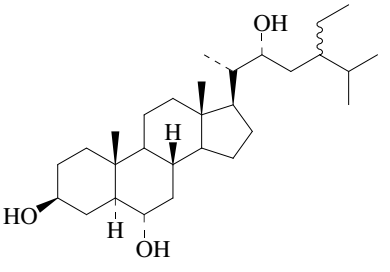
(3β,5α,6α,24*R*)-*form* [332875-49-7]
Constit. of *Euonymus mupinensis.*

(3β,5α,6β,24*R*)-*form* [20835-91-0]
Constit. of cane sugar (*Saccharum officinarum*). Also from ferns *Plenasium banksiifolium* (preferred genus name *Osmunda*) and *Osmundastrum cinnamomeum* (preferred genus name *Osmunda*) and from *Cliona copiosa*.
Cryst. (EtOH).
Mp 250-252°. $[\alpha]_D$ 0 ($CHCl_3$). $[\alpha]_D$ -2.9 (Py).

(3β,5α,6β,24*S*)-*form*
Constit. of *Spirastrella inconstans.*
Cryst. (MeOH).
Mp 242-243°. $[\alpha]_D^{25}$ +35.63 (c, 0.25 in MeOH).
Deshmane, S.S. *et al., Tetrahedron*, 1971, **27**, 1109 (*isol, struct*)
Atabekyan, V.G. *et al., Zh. Org. Khim.*, 1976, **12**, 1231 (*synth*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 1980, **28**, 3137 (*isol*)
Dawidar, A.M. *et al., Z. Naturforsch., B*, 1980, **35**, 102 (*synth*)
Notaro, G. *et al., J. Nat. Prod.*, 1991, **54**, 1570 (*isol, pmr*)
Das, B. *et al., J. Nat. Prod.*, 1993, **56**, 2210 (*isol, pmr, cmr*)
Mao, S. *et al., Tianran Chanwu Yanjiu Yu Kaifa*, 2000, **12**, 14-16; *CA*, **134**, 277901z (*Euonymus mupinensis constit*)

Stigmastane-3,6,22-triol S-429

24-Ethylcholestane-3,6,22-triol

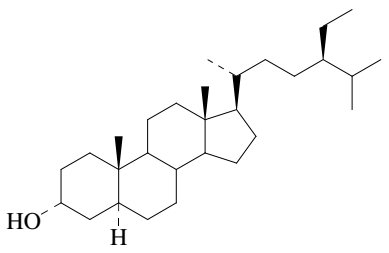


$C_{29}H_{52}O_3$ 448.728

(3β,5α,6α,22*R*,24ξ)-*form*
6-O-*Phosphate, 3*-O-*sulfate:* ***Tremasterol D***
[149298-24-8]
$C_{29}H_{53}O_9PS$ 608.772
Isol. from the starfish *Tremaster novaecaledoniae.*
$[\alpha]_D$ +28.2 (MeOH) (as di-Na salt). CAS no. refers to di-Na salt.
De Riccardis, F. *et al., Gazz. Chim. Ital.*, 1993, **123**, 79-86 (*isol, cmr, struct*)

Stigmastan-3-ol S-430

24-Ethylcholestan-3-ol
[78419-36-0]



(3α,5α,24*R*)-*form*

$C_{29}H_{52}O$ 416.729

(3α,5α,24*R*)-*form* [19043-95-9]
Constit. of *Neolitsea sericea*.

O-*(6*-O-*Hexadecanoyl-β-*D*-glucopyranoside):* [403724-75-4]
$C_{51}H_{92}O_7$ 817.284
Constit. of *Codonopsis convolvulacea*.

(3α,5β,24*S*)-*form* [84472-32-2]
Minor sterol from *Petrosia ficiformis*, prob. as endobacterial metab.

(3β,5α,24*R*)-*form*
Fucostanol. *β-Sitostanol. Stigmastanol. Spinastanol. Dihydro-β-sitosterol*
[83-45-4]
[19466-47-8]
Isol. from *Ascidia nigra* and various crustaceans and molluscs. Constit. of pot marigold (*Calendula officinalis*). Also in other higher plants, e.g. sweet corn (*Zea mays*), Carolina allspice (*Calycanthus floridus*) and from *Sphagnum* moss.
Cryst. (EtOH).
Mp 136-137°. $[\alpha]_D^{20}$ +24.8 ($CHCl_3$).

3-O-*Sulfate:* [151891-03-1]
$C_{29}H_{52}O_4S$ 496.793
Constit. of *Eupentacta fraudatrix*.
Mp 188-190° (as Py salt).

3-O-*β-*D*-Xylopyranoside:* [74185-02-7]
$C_{34}H_{60}O_5$ 548.845
Constit. of *Eupentacta fraudatrix*.

O-*β-*D*-Glucopyranoside:* [69343-51-7]
$C_{35}H_{62}O_6$ 578.871
Constit. of *Gliricidia sepium*. Cryst. ($MeOH/CH_2Cl_2$).
Mp 208°.

O-*Formyl:* ***Sitostanyl formate***
[648428-32-4]
Constit. of *Cyathea podophylla*.
Cryst.
Mp 105-107°. $[\alpha]_D$ -9.9 (c, 0.3 in $CHCl_3$).

O-*(4-Hydroxy-3-methoxy-*E*-cinnamoyl):* ***Feruloyldihydro-β-sitosterol***
[117857-70-2]
$C_{39}H_{60}O_4$ 592.901
Isol. from maize bran oil, rice bran and *Coix lacryma-jobi*. Cryst. ($CHCl_3$/MeOH).
Mp 156-157°. $[\alpha]_D^{20}$ +22.3 (c, 1.33 in $CHCl_3$).

O-*(4-Hydroxy-3-methoxy-*Z*-cinnamoyl):* ***Z-Feruloyldihydro-β-sitosterol***
[117857-72-4]
$C_{39}H_{60}O_4$ 592.901
Constit. of *Coix lacryma-jobi* and rice bran.
Mp 120-121°.

(3β,5α,24*S*)-*form*
Clionastanol. *Poriferastanol*
[55529-51-6]
Isol. from the sponge *Stelletta clarella*; also from *Haliclona flavescens* and *Zooxanthella microadriatica*. Constit. of Zooxanthellae from *Briareum asbestinum*, *Codium dichotomum*, *Codium elongatum*, *Physarum polycephalum*, *Physarum flavicomum*, *Phakellia aruensis*, *Petrosia ficiformis*, *Ascidia nigra* and human faeces.
Cryst. (MeOH).
Mp 144-146° Mp 155-157°. $[\alpha]_D$ +21.4 (c, 0.75 in $CHCl_3$). $[\alpha]_D^{20}$ +43 (c, 6.7 in MeOH).

(3β,5α,24ξ)-*form* [19044-02-1]
Constit. of *Bathyplotes natans*, *Holothuria nobilis*, *Holothuria scabra*, *Pseudostichopus trachus*, *Synapta maculata*, *Trochostoma orientale*, *Patinigera megallanica*, *Homaxinella balfourensis*, *Haliclona chilensis*, *Curcurbita maxima* and many other terrestrial and marine spp.

3-O-*Sulfate:* [80677-69-6]
[80735-06-4]
Constit. of *Parathyona* sp., *Cucumaria japonica*, *Psolus fabricii* and *Eupentacta fraudatrix*.

3-Me ether: ***3-Methoxystigmastane***
[139894-64-7]
$C_{30}H_{54}O$ 430.756
Constit. of *Jereicopsis graphidiophora*.

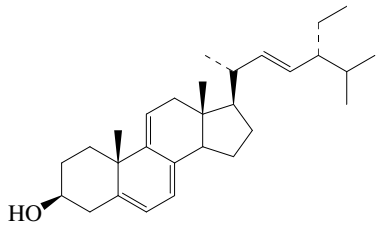
(3β,5β,24*S*)-*form* [387-80-4]
Minor sterol from sponge *Petrosia ficiformis*, prob. as endobacterial metab. Also from human and rat faeces.
Cryst. (MeOH).
Mp 127°.

(3β,5β,24ξ)-*form* [4736-91-8]
Constit. of *Ascidia nigra*.

Marker, R.E. *et al., J.A.C.S.*, 1937, **59**, 2704-2708 (*3β,5β,24*S*-form, synth*)
Larsen, C.D. *et al., J.A.C.S.*, 1938, **60**, 2431-2434 (*Fucostanol*)
Coleman, D.L. *et al., Arch. Biochem. Biophys.*, 1957, **72**, 219-225 (*synth*)
Tamura, T. *et al., Nippon Kagaku Zasshi*, 1958, **79**, 1011; *CA*, **54**, 24857 (*Feruloyldihydro-β-sitosterol*)
Khaletskii, A.M. *et al., Zh. Obshch. Khim.*, 1961, **31**, 2996-3000; *J. Gen. Chem. USSR (Engl. Transl.)*, 1961, **31**, 2794-2797 (*sulfate*)
Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095-4103 (*3β,5α,24S-form*)
Sucrow, W. *et al., Chem. Ber.*, 1975, **108**, 1101-1110 (*3β,5α,24R-form, 3β,5α,24S-form, synth, bibl*)
Bullock, E. *et al., J. Lipid Res.*, 1976, **17**, 565-571 (*Poriferastanol*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195-200 (*pmr*)
McNamara, D.J. *et al., J. Lipid Res.*, 1981, **22**, 474-484 (*3β,5β,24S-form, glc, tlc*)
Smetanina, O.F. *et al., Khim. Prir. Soedin.*, 1981, 585-586; *Chem. Nat. Compd. (Engl. Transl.)*, 1981, **17**, 422-424 (*sulfate*)
Bohlin, L. *et al., Phytochemistry*, 1981, **20**, 2397-2401 (*3β,5α,24S-form, occur*)
Aknin, M. *et al., Phytochemistry*, 1981, **20**, 4167-4169 (*3β,5α,24S-form, occur*)
Li, L.N. *et al., J.A.C.S.*, 1982, **104**, 6726-6732 (*3β,5α,24R-form, 3β,5α,24S-form, synth*)
Zielinski, J. *et al., Steroids*, 1982, **39**, 675-680 (*Clionastanol*)
Ha, T.B.T. *et al., Steroids*, 1982, **40**, 433-453 (*3β,5β,24ξ-form, occur*)
Caputo, O. *et al., Planta Med.*, 1983, **49**, 176-180 (*3β,5α,24ξ-form, occur*)
Jackson, E.M. *et al., J. Lipid Res.*, 1985, **26**, 893-897 (*3β,5α,24S-form, hplc*)
Seldes, A.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **83**, 841-842 (*3β,5α,24ξ-form, occur*)
Romero, M.S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **84**, 125-129 (*3β,5α,24ξ-form, occur*)
Goad, L.J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **84**, 189-196 (*3β,5α,24ξ-form, sulfate, occur*)
Seidel, S.B. *et al., Steroids*, 1986, **47**, 49-62 (*3β,5α,24S-form, 3β,5β,24S-form, occur*)
Kondo, Y. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3147-3152 (*ferulate*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*3-Methoxystigmastane*)
Yano, K. *et al., Phytochemistry*, 1992, **31**, 1741-1746 (*Neolitsea sericea constit*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*3β,5α,24ξ-form, occur*)
Herath, H.M.T.B. *et al., Fitoterapia*, 2000, **71**, 722-724 (*glucoside*)
Akihisa, T. *et al., J. Agric. Food Chem.*, 2000, **48**, 2313-2319 (*ferulates*)
Chen, Q. *et al., Huaxi Yaoxue Zazhi*, 2001, **16**, 245-247; *CA*, **136**, 229371w (*hexadecanoyl glucoside*)
Condo, A.M. *et al., J. Agric. Food Chem.*, 2001, **49**, 4961-4964 (*ferulate*)
Arai, Y. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1311-1313 (*Sitostanyl formate*)

Stigmasta-5,7,9(11),22-tetraen-3-ol S-431

24-Ethylcholesta-5,7,9(11),22-tetraen-3-ol
[71977-14-5]



(3β,22*E*,24*R*)-*form*

$C_{29}H_{44}O$ 408.666

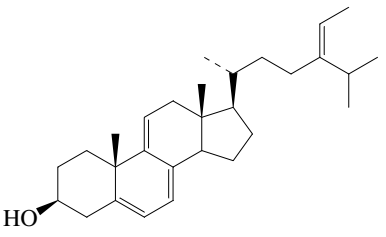
(3β,22*E*,24*R*)-*form* [85733-72-8]
Constit. of the sponge *Axinella cannabina*.

22,23-Dihydro: Stigmasta-5,7,9(11)-trien-3-ol. 24-Ethylcholesta-5,7,9(11)-trien-3-ol
[85733-74-0]
$C_{29}H_{46}O$ 410.682
Constit. of *Axinella cannabina*. Possesses 24*S*-config.

(3β,22*E*,24*S*)-*form* [85761-59-7]
Constit. of *Axinella cannabina* and the green alga *Chlorella vulgaris*.
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-151 (*Axinella constits*)
Akihisa, T. *et al., Phytochemistry*, 1992, **31**, 1769-1772 (*Chlorella constit*)

Stigmasta-5,7,9(11),24(28)-tetraen-3-ol S-432

24-Ethylidenecholesta-5,7,9(11)-trien-3-ol

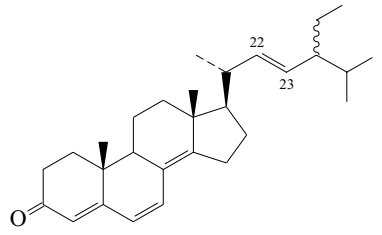


$C_{29}H_{44}O$ 408.666

(3β,24(28)*Z*)-*form* [85733-73-9]
Constit. of the sponge *Axinella cannabina*.
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol, pmr, ms*)

Stigmasta-4,6,8(14),22-tetraen-3-one S-433

24-Ethylcholesta-4,6,8(14),22-tetraen-3-one



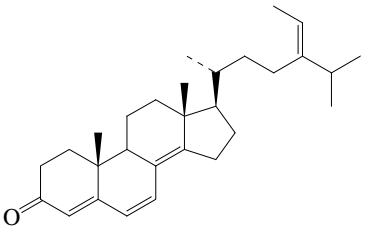
$C_{29}H_{42}O$ 406.65

(22*E*,24ξ)-*form* [142796-31-4]
Constit. of the sponge *Dysidea herbacea*. Oil.

22,23-Dihydro: Stigmasta-4,6,8(14)-trien-3-one. 24-Ethylcholesta-4,6,8(14)-trien-3-one
[142755-15-5]
$C_{29}H_{44}O$ 408.666
Constit. of *Dysidea herbacea*. Oil.
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 72-74 (*isol, pmr*)

Stigmasta-4,6,8(14),24(28)-tetraen-3-one S-434

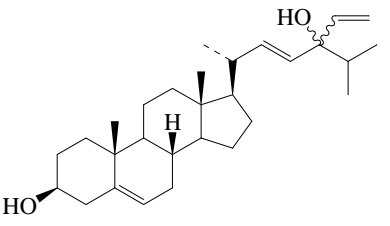
24-Ethylidenecholesta-4,6,8(14)-trien-3-one



$C_{29}H_{42}O$ 406.65

(24*E*)-*form* [142755-14-4]
Constit. of *Dysidea herbacea*. Oil. λ_{max} 348 (EtOH).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 72-74 (*isol*)

Stigmasta-5,22,28-triene-3,24-diol S-435

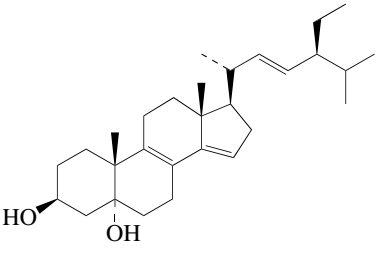


$C_{29}H_{46}O_2$ 426.681

(3β,22*E*,24ξ)-*form*
Cystosphaerol
[754983-91-0]
Constit. of *Cystosphaera jacquinotii*.
Powder. $[\alpha]_D^{25}$ -32 (c, 0.1 in $CHCl_3$). λ_{max} 199 (log ϵ 1.21) (hexane).
Ankisetty, S. *et al., J. Nat. Prod.*, 2004, **67**, 1295-1302 (*isol, pmr, cmr*)

Stigmasta-8,14,22-triene-3,5-diol S-436

24-Ethylcholesta-8,14,22-triene-3,5-diol

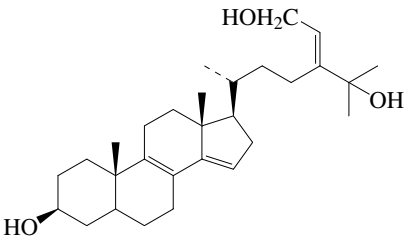


$C_{29}H_{46}O_2$ 426.681

(3β,5α,22*E*,24*S*)-*form* [211358-71-3]
Cryst. Mp 140-142°. $[\alpha]_D^{25}$ -29.

3-O-β-D-Xylopyranoside: [211358-66-6]
$C_{34}H_{54}O_6$ 558.797
Constit. of *Synapta maculata*. Cryst.
Mp 245-247°. $[\alpha]_D^{25}$ +16.8 (c, 0.2 in MeOH). λ_{max} 248 (ϵ 18000) (EtOH).
Kumar, S.V.A.S.P. *et al., J. Chem. Res., Synop.*, 1998, 404-405 (*isol, pmr, cmr*)

Stigmasta-8,14,24(28)-triene-3,25,29-triol S-437

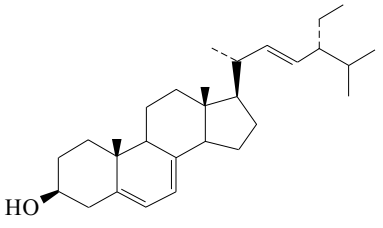


$C_{29}H_{46}O_3$ 442.681

(3β,5α,24(28)*E*)-*form* [678183-93-2]
Constit. of *Vernonia colorata*.
Cryst. (MeOH). $[\alpha]_D^{25}$ +48 (c, 0.1 in MeOH). λ_{max} 236; 242; 250 (MeOH).
Cioffi, G. *et al., J. Nat. Prod.*, 2004, **67**, 389-394 (*isol, pmr, cmr*)

Stigmasta-5,7,22-trien-3-ol S-438

24-Ethylcholesta-5,7,22-trien-3-ol

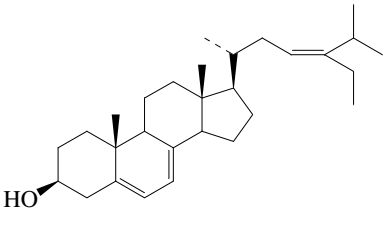


$C_{29}H_{46}O$ 410.682

(3β,24*R*)-*form*
Corbisterol. *7-Dehydroporiferasterol*. *Δ^7-Stigmasterol*
[481-19-6]
Constit. of *Corbicula leana* and green algae. Also isol. from the amoeba *Phellodendron* sp.
Mp 151-152°. $[\alpha]_D$ -105.5 (EtOH).
Ac: [39533-73-8]
Minor sterol in sponge *Tethya amamensis* (stereochem. not explicit) and present in other marine invertebrates.
Mp 152-153° (172-173°). $[\alpha]_D$ -72.8.
[19432-13-4, 21674-20-4]
Toyama, Y. *et al., Bull. Chem. Soc. Jpn.*, 1952, **25**, 355 (*isol*)
Hori, T. *et al., Nippon Kagaku Zasshi*, 1954, **75**, 1144; *CA*, **52**, 10443 (*isol*)
Matsumoto, T. *et al., Nippon Kagaku Zasshi*, 1956, **77**, 1596; *CA*, **53**, 22071 (*isol*)
Nishioki, I. *et al., Yakugaku Zasshi*, 1958, **78**, 1432
Smith, F.R. *et al., J. Lipid Res.*, 1968, **9**, 405
Itoh, T. *et al., Lipids*, 1974, **9**, 173 (*isol*)
Knights, B.A. *et al., Biochim. Biophys. Acta*, 1976, **44**, 341 (*metab*)
Eichenberger, W. *et al., Chimia*, 1976, **30**, 75 (*isol*)
Teshima, S. *et al., Lipids*, 1983, **18**, 193-197 (*Ac, occur*)

Stigmasta-5,7,23-trien-3-ol S-439

24-Ethylcholesta-5,7,23-trien-3-ol

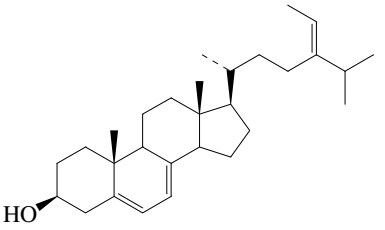


$C_{29}H_{46}O$ 410.682

(3β,23*Z*)-*form* [84873-14-3]
Constit. of *Eutreptia viridis*.
Zielinski, J. *et al., Steroids*, 1982, **40**, 403-410 (*isol, ms*)

Stigmasta-5,7,24(28)-trien-3-ol S-440

24-Ethylidenecholesta-5,7,24(28)-trien-3-ol



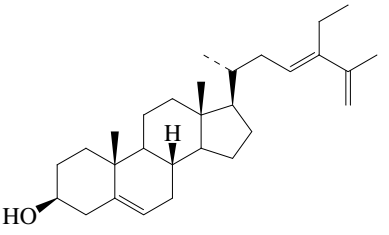
(3β,24(28)*E*)-*form*

$C_{29}H_{46}O$ 410.682

(3β,24*E*)-*form* [29560-26-7]
Isol. from *Axinella cannabina*, *Ircinia foetida*, *Ircinia variabilis* and *Tethya amamensis*.

(3β,24*Z*)-*form* [29560-28-9]
Constit. of *Axinella cannabina*, *Dysidea herbacea*, *Ircinia pipetta* and *Tethya amamensis*.
Cryst. (MeOH).
Mp 119-121°.
Delseth, C. *et al., Helv. Chim. Acta*, 1979, **62**, 101-109 (*Dysidea, isol*)
Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*Axinella, isol*)
Teshima, S. *et al., Lipids*, 1983, **18**, 193-197 (*Tethya, isol*)
Dini, A. *et al., Comp. Biochem. Physiol.*, 1984, **78**, 741-744 (*isol, pmr, ms*)
Sica, D. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1987, **88**, 293-296 (*isol*)

Stigmasta-5,23,25-trien-3-ol S-441

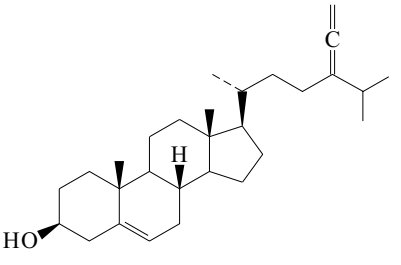


$C_{29}H_{46}O$ 410.682

(3β,23*E*)-*form* [405095-94-5]
Constit. of *Sargassum polycystum*.
Cryst.
Mp 141-142°.
Xu, S.-H. *et al., Youji Huaxue*, 2002, **22**, 138-140 (*isol, pmr, cmr*)

Stigmasta-5,24(28),28-trien-3-ol S-442

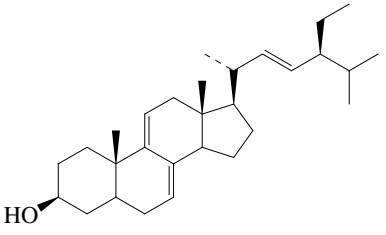
24-Ethylcholesta-5,24(28),28-trien-3-ol. *24-Vinylidenecholest-5-en-3β-ol*



$C_{29}H_{46}O$ 410.682

3β-*form* [56525-73-6]
Constit. of *Callyspongia diffusa*.
Cryst.
Mp 113-114°.
Fujimoto, T. *et al., J.C.S. Perkin 1*, 1975, 2302 (*synth*)
Theobald, N. *et al., J.A.C.S.*, 1978, **100**, 5574 (*isol*)

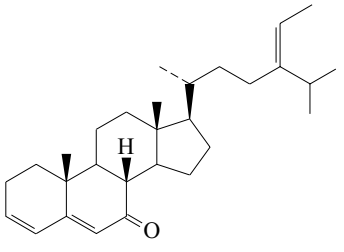
Stigmasta-7,9(11),22-trien-3-ol S-443



$C_{29}H_{46}O$ 410.682

(3β,22*E*,24*S*)-*form* [874221-89-3]
Constit. of *Haloxylon recurvum* and marine algae.
Neal, A.C. *et al., J. Mar. Biol. Assoc. U.K.*, 1986, **66**, 1-13 (*algal constit*)
Ahmed, E. *et al., Bioorg. Med. Chem. Lett.*, 2006, **16**, 573-580 (*isol, Haloxylon*)

Stigmasta-3,5,24(28)-trien-7-one S-444

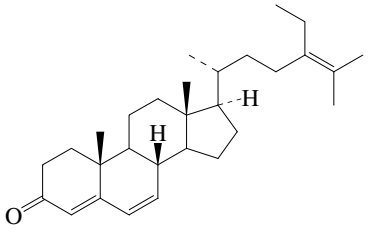


$C_{29}H_{44}O$ 408.666

(24*E*)-*form* [37976-88-8]
Constit. of *Fucus evanescens*.
Cryst. (petrol).
Mp 85°. $[\alpha]_D$ -180.
Irekawa, N. *et al., Phytochemistry*, 1972, **11**, 2317 (*isol*)

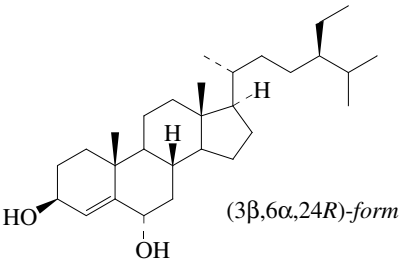
Stigmasta-4,6,24-trien-3-one, 9CI S-445

24-Ethylcholesta-4,6,24-trien-3-one
[134887-25-5]



$C_{29}H_{44}O$ 408.666
Constit. of a *Stelletta* sp. Oil. $[\alpha]_D^{20}$ -6 (c, 0.05 in EtOH).
Guerriero, A. *et al., Helv. Chim. Acta*, 1991, **74**, 487 (*isol, pmr, cmr*)

Stigmast-4-ene-3,6-diol S-446



(3β,6α,24*R*)-*form*

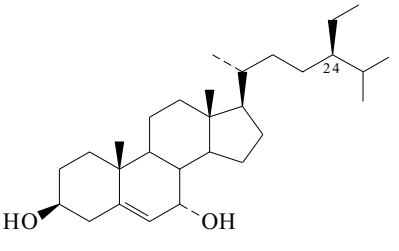
$C_{29}H_{50}O_2$ 430.713

(3β,6α,24*R*)-*form*
Constit. of *Lagerstroemia lancasteri*.
Cryst. (MeOH).
Mp 220°. $[\alpha]_D$ +21.5 (c, 0.5 in $CHCl_3$).
3,6-Diketone: ***Stigmast-4-ene-3,6-dione***. *24-Ethylcholest-4-ene-3,6-dione*
[57458-57-8]
[23670-94-2]
$C_{29}H_{46}O_2$ 426.681
Constit. of *Cinachyra tarentina*, *Sambucus ebulis* roots, *Echium vulgare* roots and mature wheat straw (*Triticum aestivum*). Shows phytotoxic and cytotoxic activities. Cryst.
Mp 170-172°. $[\alpha]_D$ -60.5 (c, 0.99 in $CHCl_3$).
3,6-Diketone, 6-oxime: ***6-Hydroxyiminostigmast-4-en-3-one***
$C_{29}H_{47}NO_2$ 441.696
Constit. of a *Cinachyrella* sponge. Amorph. solid. $[\alpha]_D$ +99.
λ_{max} 271 (no solvent reported).

(3β,6β,24*R*)-*form* [113626-76-9]
Constit. of *Halimeda xishaensis*.

(24ξ)-*form*
3,6-Diketone: ***Pulvinatadione***
[845882-30-6]
$C_{29}H_{46}O_2$ 426.681
Constit. of *Selaginella pulvinata*. Cryst. (MeOH).
Mp 168-170°. May be identical with the diketone descr. above.
Tumann, P. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1974, **307**, 891 (*diketone*)
Chaudhuri, P.K. *et al., Phytochemistry*, 1987, **26**, 3361
Aiello, A. *et al., J. Nat. Prod.*, 1991, **54**, 281 (*diketone*)
Gaspar, E.M.M. *et al., Phytochemistry*, 1993, **34**, 523-527 (*isol, pmr, cmr*)
Rodriguez, J. *et al., Tet. Lett.*, 1997, **38**, 1833 (*oxime, isol*)
Wu, J. *et al., Yaoxue Xuebao*, 1999, **34**, 682 (*diketone, isol, activity*)
Pardo, F. *et al., Biochem. Syst. Ecol.*, 2000, **28**, 911-913 (*diketone, activity*)
Shen, C.-C. *et al., J. Nat. Prod.*, 2002, **65**, 1857-1862 (*diketone, pmr, cmr*)
Yang, K. *et al., Jiegou Huaxue*, 2004, **23**, 531-534 (*Halimeda xishaensis constit, cryst struct*)
Wei, K. *et al., Magn. Reson. Chem.*, 2004, **42**, 355-359 (*diketone, pmr, cmr*)
Tan, G.-S. *et al., Youji Huaxue*, 2004, **24**, 1082-1085; *CA*, **142**, 257722d (*Pulvinatadione*)

Stigmast-5-ene-3,7-diol S-447



(3β,7α,24*R*)–*form*

$C_{29}H_{50}O_2$ 430.713

(3β,7α,24*R*)-*form*
Ikshusterol. *7α-Hydroxysitosterol*
[34427-61-7]
Constit. of cane sugar (*Saccharum officinarum*) wax, pineapple leaves (*Ananas comosus*), *Spatholobus suberetus* and the sponge *Corallistes undulatus*. Fibrinolytic agent. Cryst. (MeOH).
Mp 129-133° (202-204°). $[\alpha]_D$ -27 ($CHCl_3$).

(3β,7α,24*S*)-*form*
Poriferast-5-ene-3β,7α-diol
[145985-29-1]
Constit. of *Gracilaria edulis*.
Cryst. (C_6H_6).
Mp 225-226°. $[\alpha]_D^{25}$ -32.6 (c, 0.23 in $CHCl_3$).

(3β,7β,24*R*)-*form*
7-Epiikshusterol. *7β-Hydroxysitosterol*
[15140-59-7]
Constit. of *Iris missouriensis*, cane sugar wax and the sponges *Corallistes undulatus* and *Cliona copiosa*. Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 211-214°. $[\alpha]_D$ -22.5 ($CHCl_3$).

7-Ketone: 3-Hydroxystigmast-5-en-7-one. ***7-Oxo-β-sitosterol***
[2034-74-4]
$C_{29}H_{48}O_2$ 428.697
Constit. of *Pinus* spp. and *Cryptocarya foveolata* and the sponges *Cliona copiosa* and *Corallistes undulatus*. Isol. after saponification from *Brassica napus* (rapeseed) and *Glycine max* (soyabean) oils. Shows antihypertensive activity. Prisms (MeOH) or needles (hexane).
Mp 165-167° Mp 129° (synthetic).

(3β,7β,24*S*)-*form*
Poriferast-5-ene-3β,7β-diol
[145163-98-0]
Isol. from *Gracilaria edulis* and *Cliona copiosa*.
Mp 157-158°. $[\alpha]_D^{25}$ -29.5 (c, 0.217 in $CHCl_3$).

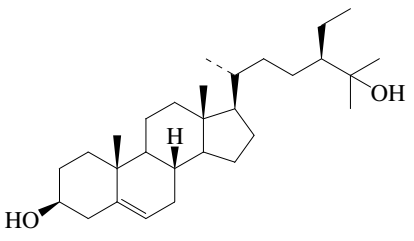
7-Ketone: 3-Hydroxyporiferast-5-en-7-one
[145163-97-9]
$C_{29}H_{48}O_2$ 428.697
Constit. of *Cliona copiosa* and *Gracilaria edulis*. Cryst.
Mp 140-141°. $[\alpha]_D^{25}$ -105.6 (c, 0.23 in $CHCl_3$).

[80666-94-0]

Rowe, J.W. *et al., Phytochemistry*, 1965, **4**, 1 (*isol*)
Bishara, R.H. *et al., J. Nat. Prod.*, 1970, **33**, 477 (*isol, props*)
Deshmane, S.S. *et al., Tetrahedron*, 1971, **27**, 1109 (*isol, struct*)
Mondon, A. *et al., Chem. Ber.*, 1975, **108**, 1989 (*pmr*)
Pakrashi, S.C. *et al., Indian J. Chem.*, 1975, **13**, 755 (*isol*)
Notaro, G. *et al., J. Nat. Prod.*, 1992, **55**, 1588 (*7-ketone, isol, pmr, ms*)
Das, B. *et al., Phytochemistry*, 1992, **31**, 2427; 4371 (*Poriferast-5-ene-3,7-diol*)
Achenbach, H. *et al., Phytochemistry*, 1992, **31**, 4263
Guerriero, A. *et al., J. Nat. Prod.*, 1993, **56**, 1962 (*7-Hydroxysitosterols, 7-ketone, pmr, cmr*)
Kovganko, N.V. *et al., Khim. Prir. Soedin.*, 1999, **35**, 484-487; *Chem. Nat. Compd. (Engl. Transl.)*, 1999, **35**, 433-436 (*synth*)
Ulubelen, A. *et al., Planta Med.*, 2000, **66**, 627-629 (*activity*)

Stigmast-5-ene-3,25-diol S-448

24-Ethylcholest-5-ene-3,25-diol



$C_{29}H_{50}O_2$ 430.713

(3β,24*R*)-*form*
25-Hydroxysitosterol
[10583-04-7]
Isol. from sponge *Damiriana hawaiiana* and leaves of *Bryophyllum pinnatum*.

Delseth, C. *et al., Helv. Chim. Acta*, 1978, **61**, 1470-1476 (*Damiriana hawaiiana constit*)
Siddiqui, S. *et al., Phytochemistry*, 1989, **28**, 2433-2438 (*Bryophyllum pinnatum constit*)

Stigmast-7-ene-3,6-diol S-449

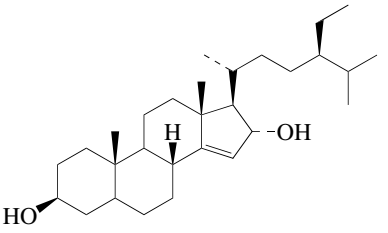
24-Ethylcholest-7-ene-3,6-diol
$C_{29}H_{50}O_2$ 430.713

(3β,5α,6α,24ξ)-*form*
Constit. of *Spongionella gracilis*.

Madaio, A. *et al., J. Nat. Prod.*, 1989, **52**, 952 (*isol, pmr*)

Stigmast-14-ene-3,16-diol S-450

24-Ethylcholest-14-ene-3,16-diol



$C_{29}H_{50}O_2$ 430.713

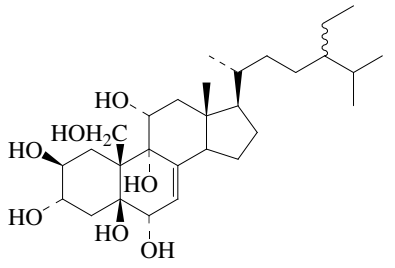
(3β,5α,15α,24*R*)-*form* [139953-33-6]
Constit. of *Topsentia aurantiaca*.

(3β,5α,16α,24*S*)-*form* [140147-34-8]
Constit. of *Topsentia aurantiaca*.

Ciminiello, P. *et al., Steroids*, 1992, **57**, 62-666 (*isol, pmr, cmr*)

Stigmast-7-ene-2,3,5,6,9,11,19-heptol S-451

24-Ethylcholest-7-ene-2,3,5,6,9,11,19-heptol



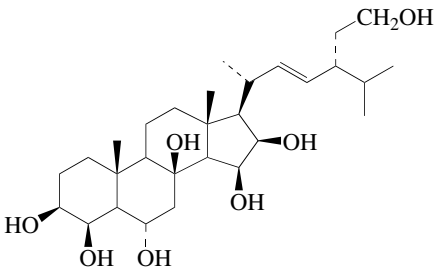
$C_{29}H_{50}O_7$ 510.71

(2β,3α,5β,6α,11α,24ξ)-*form* [120711-50-4]
Isol. from sponge *Dysidea etheria*.
Mp 235-245° dec. $[\alpha]_D^{25}$ +17.7 (c, 1.3 in EtOH).

West, R.R. *et al., J.O.C.*, 1989, **54**, 3234-3236

Stigmast-22-ene-3,4,6,8,15,16,29-heptol **S-452**

24-(2-Hydroxyethyl)cholest-22-ene-3,4,6,8,15,16-hexol



$C_{29}H_{50}O_7$ 510.71

(3β,4β,5α,6α,8β,15β,16β,22*E*,24*R*)-*form*

29-O-[α-L-Arabinopyranosyl-(1→4)-3-O-methyl-β-D-xylopyranoside]: ***Moniloside F***

[147362-19-4]

$C_{40}H_{68}O_{15}$ 788.968

Constit. of *Fromia monilis.*

29-O-[3-O-Methyl-β-D-xylopyranosyl-(1→4)-3-O-methyl-β-D-xylopyranosyl-(1→4)-β-D-xylopyranoside]: ***Moniloside H***

[147385-58-8]

$C_{46}H_{78}O_{19}$ 935.111

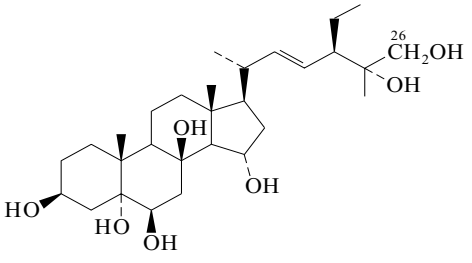
Constit. of *Fromia monilis.*

$[\alpha]_D$ +23.5 (MeOH).

Casapullo, A. *et al., J. Nat. Prod.*, 1993, **56**, 105-115 (*isol, pmr, cmr*)

Stigmast-22-ene-3,5,6,8,15,25,26-heptol **S-453**

24-Ethylcholest-22-ene-3,5,6,8,15,25,26-heptol



$C_{29}H_{50}O_7$ 510.71

(3β,5α,6β,8β,15α,24*R*,25*R*)-*form*

26-Sulfate: [174587-03-2]

$C_{29}H_{50}O_{10}S$ 590.774

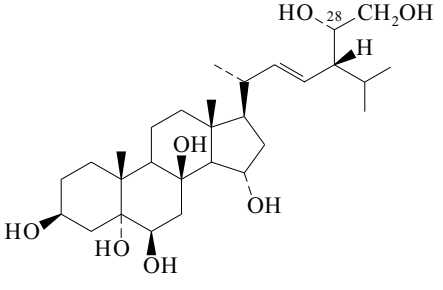
Constit. of *Styracaster caroli.*

$[\alpha]_D$ +4.6 (MeOH).

De Riccardis, F. *et al., J. Nat. Prod.*, 1996, **59**, 386 (*isol, pmr, cmr*)

Stigmast-22-ene-3,5,6,8,15,28,29-heptol **S-454**

24-(1,2-Dihydroxyethyl)cholest-22-ene-3,5,6,8,15-pentol



$C_{29}H_{50}O_7$ 510.71

(3β,5α,6β,8β,15α,22*E*,24*R*,28*S*)-*form*

28-Sulfate: [160538-75-0]

$C_{29}H_{50}O_{10}S$ 590.774

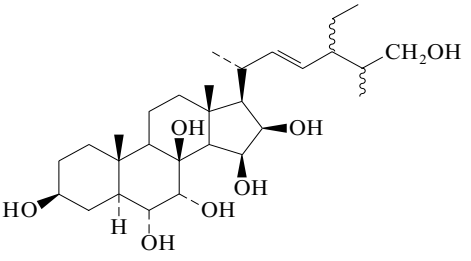
Constit. of *Styracaster caroli.*

$[\alpha]_D$ -0.7 (MeOH).

Iorizzi, M. *et al., J. Nat. Prod.*, 1994, **57**, 1361 (*isol, pmr, cmr*)

Stigmast-22-ene-3,6,7,8,15,16,26-heptol **S-455**

24-Ethylcholest-22-ene-3,6,7,8,15,16,26-heptol



$C_{29}H_{50}O_7$ 510.71

(3β,5α,6α,7α,8β,15β,16β,22*E*,24ξ,25ξ)-*form*

26-O-[3-O-Methyl-2-sulfate-β-D-xylopyranoside]: ***Oreasteroside J***

[161996-31-2]

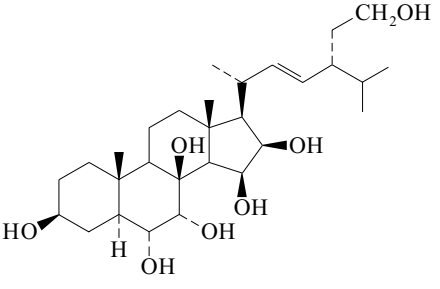
$C_{35}H_{60}O_{14}S$ 736.917

Constit. of *Oreaster reticulatus.*

Iorizzi, M. *et al., J. Nat. Prod.*, 1995, **58**, 10-26 (*isol, pmr, cmr*)

Stigmast-22-ene-3,6,7,8,15,16,29-heptol **S-456**

24-(2-Hydroxyethyl)cholest-22-ene-3,6,7,8,15,16-hexol



$C_{29}H_{50}O_7$ 510.71

(3β,5α,6α,7α,8β,15β,16β,22*E*,24*R*)-*form*

29-O-[3-O-Methyl-2-sulfo-β-D-xylopyranoside]: ***Oreasteroside K***

[161996-32-3]

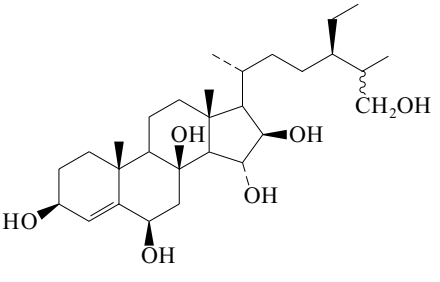
$C_{35}H_{60}O_{14}S$ 736.917

Constit. of *Oreaster reticulatus.*

Iorizzi, M. *et al., J. Nat. Prod.*, 1995, **58**, 10-26 (*isol, pmr, cmr*)

Stigmast-4-ene-3,6,8,15,16,26-hexol **S-457**

24-Ethylcholest-4-ene-3,6,8,15,16,26-hexol



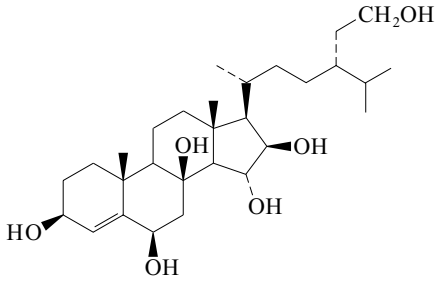
$C_{29}H_{50}O_6$ 494.71

(3β,6β,15α,16β,25ξ)-*form*

3-O-*(2*-O-*Methyl-β-D-xylopyranoside)*: ***Forbeside L***
[134985-05-0]
$C_{35}H_{60}O_{10}$ 640.853
Isol. from the starfish *Asterias forbesi*. Powder.
Mp 210° dec. $[\alpha]_D$ -7.8 (c, 0.4 in H_2O).
Findlay, J.A. *et al., J. Nat. Prod.*, 1991, **54**, 428

Stigmast-4-ene-3,6,8,15,16,29-hexol S-458

24-(2-Hydroxyethyl)cholest-4-ene-3,6,8,15,16-pentol



$C_{29}H_{50}O_6$ 494.71

(3β,6β,8β,15α,16β,24*R*)-*form*

3-O-*(2*-O-*Methyl-β-D-xylopyranoside), 15*-sulfate: ***Echinasteroside B***
[98166-58-6]
$C_{35}H_{60}O_{13}S$ 720.917
Constit. of *Echinaster sepositus*, *Echinaster brasiliensis* and *Henricia laeviuscola*. Isol. as Na salt to which CAS registry number refers.

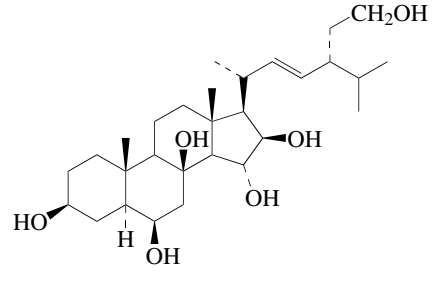
3-O-*(2*-O-*Methyl-β-D-xylopyranoside), 29*-O-*α-L-arabinofuranoside*: ***Linckoside A***
[460357-08-8]
$C_{40}H_{68}O_{14}$ 772.969
Constit. of *Linckia laevigata*. Powder. $[\alpha]_D^{25}$ -35 (c, 0.37 in MeOH).

3-O-*(2*-O-*Methyl-β-D-xylopyranoside), 29*-O-*β-D-xylopyranoside*: ***Linckoside B***
[460357-09-9]
$C_{40}H_{68}O_{14}$ 772.969
Constit. of *Linckia laevigata*. Powder. $[\alpha]_D^{25}$ -27 (c, 0.17 in MeOH).

3-O-*(2*-O-*Methyl-β-D-xylopyranoside), 29*-O-*β-D-xylopyranoside, 15-sulfate*: ***Echinasteroside F***
[156398-66-2]
$C_{40}H_{68}O_{17}S$ 853.033
Isol. from *Echinaster brasiliensis*.
$[\alpha]_D$ -1.2. Isol. as Na salt to which CAS registry number refers.
Zollo, F. *et al., Gazz. Chim. Ital.*, 1985, **115**, 303-306 (*isol, struct*)
D'Auria, M.V. *et al., Gazz. Chim. Ital.*, 1990, **120**, 155-163 (*isol, pmr, cmr*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1993, **56**, 2149-2162 (*Echinasteroside F*)
Qi, J. *et al., Bioorg. Med. Chem.*, 2002, **10**, 1961-1966 (*Linckosides*)

Stigmast-22-ene-3,6,8,15,16,29-hexol S-459

24-(2-Hydroxyethyl)cholest-22-ene-3,6,8,15,16-pentol

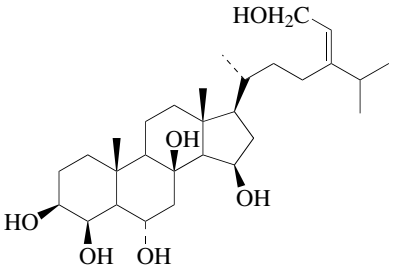


$C_{29}H_{50}O_6$ 494.71

(3β,5α,6β,8β,15α,16β,22*E*,24*R*)-*form*

29-O-*β-D-Xylopyranoside, 15*-sulfate: ***Attenuatoside SII***
[92593-74-3]
$C_{34}H_{58}O_{13}S$ 706.89
Constit. of *Hacelia attenuata*. $[\alpha]_D$ +7.4 (MeOH).
Minale, L. *et al., Gazz. Chim. Ital.*, 1984, **114**, 151-158 (*isol, pmr, cmr*)

Stigmast-24(28)-ene-3,4,6,8,15,29-hexol S-460

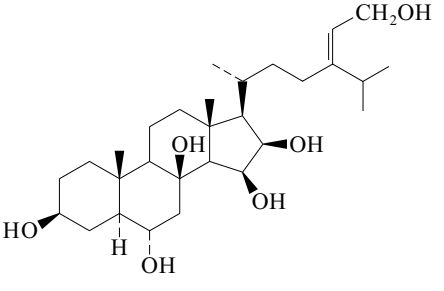


$C_{29}H_{50}O_6$ 494.71

(3β,4β,6α,8β,15β,24(28)*E*)-*form*

29-O-*[2*-O-*Methyl-β-D-xylopyranosyl-(1→2)-β-D-xylopyranoside], 6*-sulfate: ***Acodontasteroside C***
[195061-78-0]
$C_{40}H_{68}O_{17}S$ 853.033
Constit. of *Acodontaster conspicuus*. $[\alpha]_D$ -11.1 (c, 1 in MeOH).
De Marino, S. *et al., J. Nat. Prod.*, 1997, **60**, 959-966 (*isol, pmr, cmr*)

Stigmast-24(28)-ene-3,6,8,15,16,29-hexol S-461



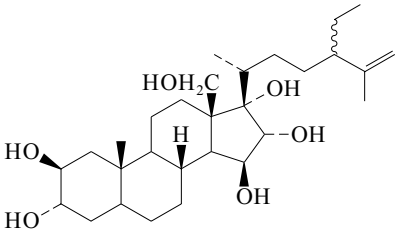
$C_{29}H_{50}O_6$ 494.71

(3β,5α,6α,15β,16β,24(28)*Z*)-*form*

29-O-*(4*-O-*Sulfo-β-D-xylopyranoside)*: ***Pisasteroside C***
[123154-35-8]
$C_{34}H_{58}O_{13}S$ 706.89
Isol. from the starfish *Pisaster giganteus* (as Na salt).
$[\alpha]_D$ +12 (c, 1 in MeOH).
Zollo, F. *et al., J. Nat. Prod.*, 1989, **52**, 693-700 (*isol*)

Stigmast-25-ene-2,3,15,16,17,18-hexol S-462

24-Ethylcholest-25-ene-2,3,15,16,17,18-hexol

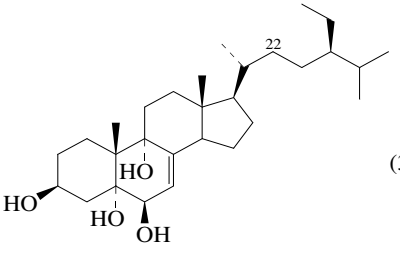


$C_{29}H_{50}O_6$ 494.71

(2β,3α,15β,16α,17α,24ξ)-*form*
Echinoclasterol
2-O-*Sulfate:* [152369-47-6]
$C_{29}H_{50}O_9S$ 574.775
Constit. of the marine sponge *Echinoclathria subhispida*. Solid (as phenethylammonium salt). $[\alpha]_D$ +0.3 (c, 0.15 in MeOH). λ_{max} 205 (ϵ 8900); 260 (ϵ 340) (MeOH) (Berdy).
Li, H. *et al., Tet. Lett.*, 1993, **34**, 5733 (*isol, pmr, cmr*)

Stigmast-7-ene-3,5,6,9-tetrol S-463

24-Ethylcholest-7-ene-3,5,6,9-tetrol



(3β,5α,6β,24*R*)-*form*

$C_{29}H_{50}O_4$ 462.712

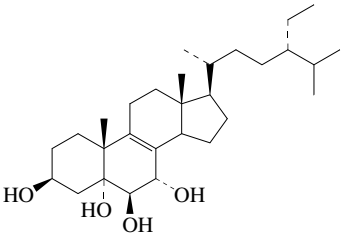
(3β,5α,6β,24*R*)-*form* [133161-21-4]
Constit. of *Spongia officinalis*.

(3β,5α,6β,24*S*)-*form* [133056-67-4]
Constit. of *Spongia officinalis*.

(3β,5α,6β,9α,24ξ)-*form*
*22,23*E-*Didehydro:* ***Stigmasta-7,22-diene-3,5,6,9-tetrol***
[119325-39-2]
$C_{29}H_{48}O_4$ 460.696
Isol. from *Patinopecten yessoensis*.
$[\alpha]_D$ -66.5 (MeOH).
Iorizzi, M. *et al., J. Nat. Prod.*, 1988, **51**, 1098-1103 (*Patinopecten yessoensis constit*)
Migliuolo, A. *et al., J. Nat. Prod.*, 1990, **53**, 1414-1424 (*Spongia officinalis constits*)

Stigmast-8-ene-3,5,6,7-tetrol S-464

24-Ethylcholest-8-ene-3,5,6,7-tetrol

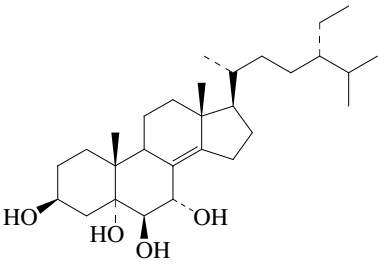


$C_{29}H_{50}O_4$ 462.712
Erroneously named as triol in the lit.

(3β,5α,6β,7α,24*S*)-*form* [169565-87-1]
Isol. from the Caribbean sponge *Neofibularia nolitangere*.
Costantino, V. *et al., Steroids*, 1995, **60**, 768-772 (*isol, pmr, cmr*)

Stigmast-8(14)-ene-3,5,6,7-tetrol S-465

24-Ethylcholest-8(14)-ene-3,5,6,7-tetrol

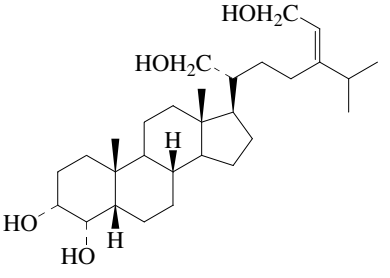


$C_{29}H_{50}O_4$ 462.712
Erroneously named as triol in the lit.

(3β,5α,6β,7α,24*S*)-*form* [169565-88-2]
Isol. from the Caribbean sponge *Neofibularia nolitangere*.
Costantino, V. *et al., Steroids*, 1995, **60**, 768-772 (*isol, pmr, cmr*)

Stigmast-24(28)-ene-3,4,21,29-tetrol S-466

24-Ethylcholest-24(28)-ene-3,4,21,29-tetrol



$C_{29}H_{50}O_4$ 462.712

(3α,4α,5β,24(28)*E*)-*form*
3,21-Disulfate: [116407-23-9]
$C_{29}H_{50}O_{10}S_2$ 622.84
Isol. from the Pacific ophiuroid *Ophiolepis superba*.
$[\alpha]_D$ +21.9 (MeOH) (as di-Na salt).
D'Auria, M.V. *et al., J.O.C.*, 1989, **54**, 234-239 (*isol, pmr, cmr, struct*)

Stigmast-7-ene-3,5,6-triol S-467

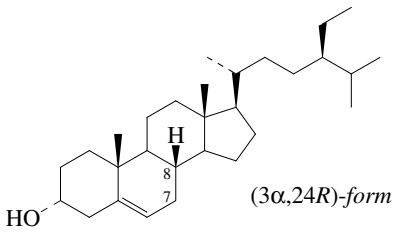
24-Ethylcholest-7-ene-3,5,6-triol
$C_{29}H_{50}O_3$ 446.712

(3β,5α,6β,24*R*)-*form*
Constit. of the sponge *Spongionella gracilis* and *Patinopecten yessoensis*.
Cryst. (MeOH).
Mp 254-256°. $[\alpha]_D$ -12.7 (MeOH).

(3β,5α,24ξ)-*form*
6-Ketone: 3,5-Dihydroxystigmast-7-en-6-one
$C_{29}H_{48}O_3$ 444.696
Constit. of *Oscarella lobularis*.
[112058-05-6]
Piccialli, V. *et al., J. Nat. Prod.*, 1987, **50**, 915
Aiello, A. *et al., Steroids*, 1991, **56**, 337 (*isol, pmr, ketone*)

Stigmast-5-en-3-ol S-468

24-Ethylcholest-5-en-3-ol



(3α,24*R*)-*form*

$C_{29}H_{50}O$ 414.713
Log P 10.45 (uncertain value) (calc).

(3β,24*R*)-*form*

***β*-Sitosterol**. *Nimbosterol. Cupreol. Quebrachol. Rhamnol. Cinchol. Verosterol. Slanutosterol. Raphanisterol. Papaveristerol. Sitosterol. Angelicin†. 22,23-Dihydrostigmasterol*
[83-46-5]
Widely distributed in plants; the commonest sterol of higher plants. Also occurs in marine organisms, incl. the scallop *Placopecten magellanicus*, the sponge *Reniera* sp. and the alga *Cladophora densa*. Antihypercholesterolaemic, estrogenic and hypolipidaemic agent. Shows antibacterial and antifungal props. Cryst. (MeOH).
Mp 136-137°. $[\alpha]_D^{22}$ -35 ($CHCl_3$). Log P 10.45 (uncertain value) (calc). Early isolates usually contd. *ca*. 5-30%.
▶ Exp. reprod. effects. WJ2600000

O-*Sulfate:* ***Phytocohesine***
[107013-12-7]
$C_{29}H_{50}O_4S$ 494.778
Constit. of *Eupentacta fraudatrix*.
Mp 151-152° (as Na salt).

O-*β-D-Galactopyranoside:* [55057-29-9]
[51704-25-7]
$C_{35}H_{60}O_6$ 576.855
Constit. of *Hibiscus sabdariffa* (roselle) leaves and *Cladophora densa*. Cryst. ($CHCl_3$).
Mp 275-277°. $[\alpha]_D$ -63 (c, 0.52 in Py).

(3β,24*S*)-*form*

***γ*-Sitosterol**. *Clionasterol. Poriferast-5-en-3β-ol. β-Dihydroeucosterol*
[83-47-6]
Constit. of *Spheciospongia vesparia*, *Cliona celata*, *Tethya aurantia*, liverworts, green algae *Chaetomorpha aurea*, *Caulerpa prolifera*, *Bryopsis plumosa*, *Udotea petiolata*, green-lipped mussel *Perna canaliculus* and many other marine organisms.
Cryst. (EtOH).
Mp 147-148°. $[\alpha]_D$ -47.7 ($CHCl_3$). Earlier isolates of γ-Sitosterol were shown to be mixts. and the proposal was made to discontinue the name (Linde *et al*, 1966 and other workers).

(3β,24ξ)-*form*

Lobophytol A
[257939-67-6]
Constit. of *Bugula neritina*, *Lobophytum* sp., *Eupentacta fraudatrix*, *Bathyplotes natans*, *Holothuria nobilis*, *Holothuria scabra*, *Pseudostichopus trachus*, *Synapta maculata* and *Trochostoma orientale*. Occurs in dinoflagellate *Prorocentrum micans*. The isolates may not necessarily have the same 24-configs.

3-O-*Sulfate:* [80735-04-2]
$C_{29}H_{50}O_4S$ 494.778
Constit. of *Euretaster insignis*, *Parathyona* sp., *Psolus fabricii*, *Echinus esculentus*, *Echinocardium cordatum*, *Antedon bifida*, *Ophiocomina nigra* and other marine organisms.

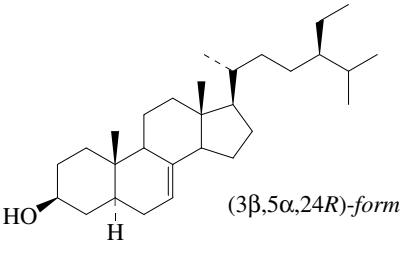
Tetracosanoyl:
$C_{53}H_{96}O_2$ 765.34
Isol. from the sponge *Tedania annhelans*. Need not have the same 24-config. as Lobophytol A.

Me ether: 3-Methoxystigmast-5-ene
[139894-63-6]
$C_{30}H_{52}O$ 428.74
Constit. of *Jereicopsis graphidiophora*.

[19044-06-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1048C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 569A (*nmr*)
Slomp, G. *et al., J.A.C.S.*, 1962, **84**, 204-206 (*pmr*)
Khaletskii, A.M. *et al., Zh. Obshch. Khim.*, 1963, **33**, 1104-1107; *J. Gen. Chem. USSR (Engl. Transl.)*, 1963, **33**, 1089-1091 (*sulfate*)
Idler, D.R. *et al., Comp. Biochem. Physiol., A: Comp. Physiol.*, 1971, **38**, 581 (*β-Sitosterol, isol, Placopecten*)
Ikan, R. *et al., J.O.C.*, 1971, **36**, 3944-3945 (*synth*)
Naqui, S.H. *et al., Steroids*, 1973, **22**, 285-292 (*ms*)
Aizawa, K. *et al., Org. Mass Spectrom.*, 1974, **9**, 470-479 (*ms*)
Sucrow, W. *et al., Chem. Ber.*, 1975, **108**, 3721-3729 (*synth*)
Lenton, J.R. *et al., Phytochemistry*, 1975, **14**, 1523-1528 (*biosynth*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195-200 (*pmr*)
Sliwowski, J.K. *et al., J.A.C.S.*, 1977, **99**, 4479-4485 (*biosynth*)
Fujimoto, Y. *et al., J.O.C.*, 1979, **44**, 1011-1012 (*synth*)
Smetanina, O.F. *et al., Khim. Prir. Soedin.*, 1981, 585-588; *Chem. Nat. Compd. (Engl. Transl.)*, 1981, **17**, 422-424 (*3β,24ξ-form, sulfate*)
Okano, M. *et al., Nippon Suisan Gakkaishi*, 1982, **48**, 1485-1490 (*β-Sitosterol, Cladophora densa constit, galactoside*)
De Napoli, L. *et al., Phytochemistry*, 1982, **21**, 1993-1994 (*Clionasterol, occur*)
Goodfellow, R.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **76**, 575-578 (*3β,24ξ-form, sulfate, occur*)
Weston, R.J. *et al., N.Z. J. Sci.*, 1983, **26**, 15-20 (*Clionasterol, occur*)
Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3779-3782 (*hplc*)
D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1984, 2277-2282 (*3β,24ξ-form, sulfate*)
Seo, S. *et al., Chem. Comm.*, 1986, 1139-1141 (*biosynth*)
Goad, L.J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **84**, 189-196 (*3β,24ξ-form, sulfate, occur*)
Yamaguchi, T. *et al., Tohoku J. Agric. Res.*, 1986, **37**, 5 (*occur, dinoflagellates*)
Lawson, M.P. *et al., Lipids*, 1988, **23**, 750-754 (*β-Sitosterol, Reniera constit, isol*)
Zimmerman, M.P. *et al., Lipids*, 1990, **25**, 383-390 (*Clionasterol, occur*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*3-Methoxystigmastene*)
Nes, W.D. *et al., Phytochemistry*, 1992, **31**, 805-811 (*biosynth*)
Seo, S. *et al., Phytochemistry*, 1992, **31**, 3029-3031 (*biosynth*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*sulfate, isol*)
Reynolds, W.F. *et al., Magn. Reson. Chem.*, 1997, **35**, 455-462 (*Clionasterol, pmr, cmr*)
Yamada, J. *et al., Tetrahedron*, 1997, **53**, 877-884 (*biosynth*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*3β,24ξ-form, occur*)
Chen, C.S. *et al., CA*, 1999, **132**, 149197w (*Lobophytol A*)
Okuzumi, T. *et al., Tet. Lett.*, 1999, **40**, 8863-8866 (*biosynth*)
Nasu, K. *et al., Phytochemistry*, 2000, **54**, 381-385 (*biosynth*)
De-Eknamkul, W. *et al., Phytochemistry*, 2003, **62**, 389-398 (*biosynth*)

Stigmast-7-en-3-ol S-469



(3β,5α,24*R*)-*form*

$C_{29}H_{50}O$ 414.713

(3β,5α,24*R*)-*form*

Schottenol. *22-Dihydrochondrillasterol. 22,23-Dihydro-α-spinasterol. Poriferast-7-en-3-ol*
[521-03-9]
Isol. from *Arenaria kansuensis*, *Asterias rubens*, *Bupleurum falcatum*, *Bryonia dioica*, *Lophocereus schottii*, *Trichosanthes kirilowii*, *Cucumis sativus*, *Helianthus annuus*, wheat and rye germ, avocado oil and the uredospores of *Uromyces phaseoli*. Also in *Acheta domesticus* (house cricket).

Cryst. (MeOH or EtOAc/hexane).
Mp 153-154° (137-140°). $[\alpha]_D^{30}$ +9.1 (c, 0.95 in $CHCl_3$). $[\alpha]_D^{26}$ +4.5 (c, 0.2 in $CHCl_3$). Prob. identical with β-Spinasterol.

3-O-*Sulfate:* [152139-43-0]
$C_{29}H_{50}O_4S$ 494.778
Constit. of *Eupentacta fraudatrix*.

3-O-*β-D-Xylopyranoside:* [74185-06-1]
$C_{34}H_{58}O_5$ 546.829
Constit. of *Eupentacta fraudatrix*.

3-O-*β-D-Glucopyranoside:* [61376-86-1]
$C_{35}H_{60}O_6$ 576.855
Constit. of *Baccharis cordifolia*, *Citrullus lanatus* var. *citroides*, *Cucumis trigonus*, *Cucurbita foetidissima*, *Ipomopsis aggregata*, *Phytolacca esculenta*, *Styrax officinalis*. Also from the cultured cells of *Camellia sinensis*, *Codonopsis pilosula*, leaves of *Cucumis sativus*, dried seeds of *Trichosanthes uniflora* and dried roots of *Trichosanthes* spp. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

O-*(6-O-Hexadecanoyl-β-D-glucopyranoside):* [83177-33-7]
$C_{51}H_{90}O_7$ 815.268
Constit. of *Codonopsis convolvulacea*.

O-*(Eicosenoyl-β-D-glucopyranoside):* [403699-20-7]
$C_{55}H_{96}O_7$ 869.359
Constit. of *Codonopsis convolvulacea*. Posn. of double bond in eicosenoyl residue not specified in the abstract.

Ac: [14473-77-9]
Cryst. (EtOH aq.). Mp 154-156°. $[\alpha]_D^{30}$ +12.5 (c, 0.96 in $CHCl_3$).

Hexadecanoyl: [76201-82-6]
$C_{45}H_{80}O_2$ 653.126
Isol. from *Arenaria kansuensis*. Amorph. powder. $[\alpha]_D^{26}$ +4.4 (c, 0.3 in $CHCl_3$).

(3β,5α,24*S*)-*form*
Chondrillast-7-enol. *Dihydrochondrillasterol*
[18525-35-4]
Constit. of *Oocystis polymorpha*, *Spirulina* spp., *Calothrix* sp., *Nostoc commune*, *Scenedesmus quadricauda*, *Chlorella* sp., *Uronema* spp., *Selenastrum gracile*, the sponge *Petrosia hebes*, *Perna canaliculus* (green lipped mussel), *Mytilus edulis* (blue mussel) and *Crassostrea virginica*.
Mp 173-174°.

Me ether: 3-Methoxystigmast-7-ene
[156472-89-8]
$C_{30}H_{52}O$ 428.74
Constit. of *Microscleroderma spirophora*.

(3β,5α,24ξ)-*form* [18725-34-3]
Isol. from the starfish *Protoreaster nodosus*, *Protoreaster lincki*, *Culcita schmideliana*, *Asterias rubens*, *Cucumaria* sp., *Bathyplotes natans*, *Holothuria nobilis*, *Holothuria scabra*, *Pseudostichopus trachus*, *Trochostoma orientale* and the sponge *Axinella cannabina*.

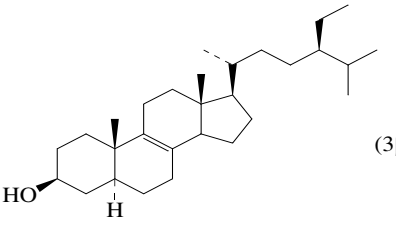
Me ether: [139894-65-8]
Constit. of the sponge *Jereicopsis graphidiophora*.

[6869-99-4]

Takeda, K. *et al., Chem. Pharm. Bull.*, 1958, **6**, 437-440 (*isol*)
Terauchi, H. *et al., Chem. Pharm. Bull.*, 1970, **18**, 213-216 (*isol, struct*)
Orcutt, D.M. *et al., Steroids*, 1970, **16**, 429-446 (*Poriferast-7-en-3β-ol*)
Lin, H.-K. *et al., Phytochemistry*, 1972, **11**, 2319-2322 (*isol*)
Smith, A.G. *et al., Biochem. J.*, 1973, **135**, 443-455 (*occur*)
Kircher, H.W. *et al., J.O.C.*, 1973, **38**, 2259-2260 (*synth*)
Sheikh, Y.M. *et al., Steroids*, 1973, **22**, 835-850 (*3β,5α,24ξ-form, occur, glc*)
Itoh, T. *et al., Lipids*, 1974, **9**, 173-184 (*3β,5α,24R-form, isol*)
Jeong, J.M. *et al., Lipids*, 1974, **9**, 921-927 (*3β,5α,24R-form, glc-ms, occur*)
Paoletti, C. *et al., Lipids*, 1976, **11**, 266-271 (*3β,5α,24S-form, occur, glc*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195-200 (*pmr*)
Ulubelen, A. *et al., Planta Med.*, 1976, **30**, 144-145 (*glucoside, isol*)
Siefert, K. *et al., Pharmazie*, 1977, **32**, 125 (*isol*)
Weston, R.J. *et al., N.Z. J. Sci.*, 1983, **26**, 15-20 (*3β,5α,24S-form, occur*)
Seo, S. *et al., Chem. Comm.*, 1987, 1876-1878 (*biosynth*)
Wu, F.-E. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2281-2282 (*3β,5α,24R-form, hexadecanoyl*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*3-Methoxystigmastene*)
Uomori, A. *et al., Phytochemistry*, 1992, **31**, 3861-3864 (*biosynth*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Costantino, V. *et al., Steroids*, 1994, **59**, 181-184 (*3-Methoxystigmastene*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*3β,5α,24ξ-form, occur*)
Chen, Q. *et al., Huaxi Yaoxue Zazhi*, 2001, **16**, 245-247; *CA*, **136**, 229371w (*acyl glucosides*)

Stigmast-8-en-3-ol S-470

24-Ethylcholest-8-en-3-ol
[56710-74-8, 108942-93-4]



(3β,5α,24*R*)-*form*

$C_{29}H_{50}O$ 414.713

(3β,5α,24*R*)-*form* [34350-84-0]
Isol. from the sponges *Axinella cannabina* and *Haliclona* sp.

(3β,5α,24*S*)-*form* [37936-73-5]
Isol. from *Axinella cannabina*.

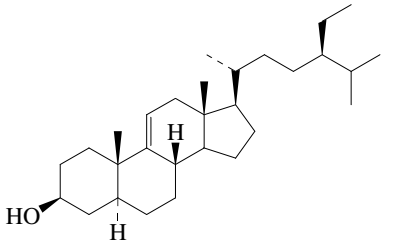
Me ether: 3-Methoxystigmast-8-ene
[156472-88-7]
$C_{30}H_{52}O$ 428.74
Constit. of *Microscleroderma spirophora*.

(3β,5α,24ξ)-*form*
Me ether: [139765-31-4]
Constit. of *Jereicopsis graphidiophora*.

Itoh, T. *et al., J.C.S. Perkin 1*, 1983, 147-153 (*isol*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1992, **55**, 311-320 (*isol, pmr, ms*)
Costantino, V. *et al., Steroids*, 1994, **59**, 181-184 (*Me ether*)

Stigmast-9(11)-en-3-ol S-471

[152697-23-9]



(3β,5α,24*R*)-*form*

$C_{29}H_{50}O$ 414.713

(3β,5α,24*R*)-*form*
Lindesterol
[77794-81-1]
Constit. of *Costus speciosus*, *Lindenbergia urticaefolia* and *Malva parviflora*.
Cryst. (Me_2CO).
Mp 132-133°. $[\alpha]_D^{24}$ +50 ($CHCl_3$). λ_{max} 214 (log ε 5.6) (MeOH).

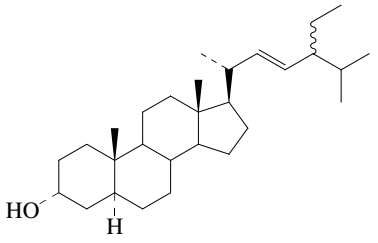
Ac: [64548-16-9]
Needles (MeOH). Mp 108-110°. $[\alpha]_D^{22}$ +23.7 (c, 1.2 in $CHCl_3$).

Ketone: Stigmast-9(11)-en-3-one. ***Malvasterone***
[81474-61-5]
$C_{29}H_{48}O$ 412.698
Constit. of *Malva parviflora*. Cryst. ($CHCl_3$/MeOH).
Mp 102-103°. $[\alpha]_D^{18}$ +4.4 (c, 0.07 in $CHCl_3$). λ_{max} 215 (log ε 4.5) (MeOH).

(3β,5α,24*S*)-*form*
Poriferast-9(11)-en-3β-ol
[140631-28-3]
Constit. of *Gracilaria edulis.*
Cryst. (C_6H_6).
Mp 133-134°. $[\alpha]_D^{25}$ +46 (c, 0.27 in $CHCl_3$).
Gupta, M.M. *et al., Phytochemistry*, 1981, **20**, 2557-2559 (*isol, pmr, ms*)
Das, B. *et al., Phytochemistry*, 1992, **31**, 1054-1055 (*Poriferast-9(11)-en-3β-ol*)
Mori, K. *et al., Annalen*, 1993, 657-663 (*synth, pmr*)
Sharma, S.K. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 746-748 (*Malvasterone*)

Stigmast-22-en-3-ol S-472

24-Ethylcholest-22-en-3-ol



(3α,5α,22*E*,24ξ)-*form*

$C_{29}H_{50}O$ 414.713

(3α,5α,22*E*,24ξ)-*form* [115305-07-2]
Isol. from the sponge *Esperiopsis edwardii* and from the roots of *Holoptelea integrifolia*.
Cryst. ($CHCl_3$/MeOH).
Mp 193-195°.
Ac:
Cryst. (Ac_2O/Py). Mp 125-127°.

(3β,5α,22*E*,24*S*)-*form*
3-O-*Sulfate:* [152005-15-7]
$C_{29}H_{50}O_4S$ 494.778
Constit. of *Eupentacta fraudatrix*.
3-O-*β-D-Xylopyranoside:* [74185-05-0]
$C_{34}H_{58}O_5$ 546.829
Constit. of *Eupentacta fraudatrix*.

(3β,5α,22*E*,24ξ)-*form* [65494-30-6]
Constit. of *Bathyplotes natans*, *Holothuria nobilis*, *Holothuria scabra* and *Trochostoma orientale.*

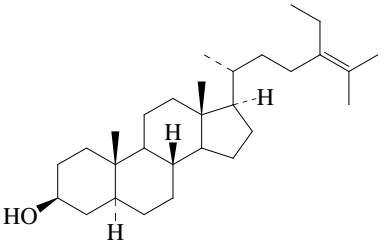
(3β,5α,22*Z*,24*R*)-*form*
5α-Poriferast-22-en-3β-ol
Mp 154-156°. $[\alpha]_D^{21}$ +46 (c, 0.67 in $CHCl_3$).
Ac: Mp 151-153°. $[\alpha]_D^{21}$ -44 (c, 1.17 in $CHCl_3$).

(3β,5α,22*Z*,24*S*)-*form* [4736-56-5]
Present in the slime mould *Dictyostelium discoideum*. Chemotactic agent. Cryst. (EtOH).
Mp 158-159°. $[\alpha]_D$ +3.3 (c, 1.5 in $CHCl_3$).
Ac: Mp 144-146°. $[\alpha]_D^{20}$ -7.2 ($CHCl_3$).

(3β,5α,22ξ,24ξ)-*form* [886993-54-0]
Constit. of *Geodia* and *Tedania* spp.
Takeda, K. *et al., Chem. Pharm. Bull.*, 1958, **6**, 536 (*isol, struct*)
Johnson, D.F. *et al., Arch. Biochem. Biophys.*, 1962, **97**, 232 (*biosynth*)
Sucrow, W. *et al., Chem. Ber.*, 1975, **108**, 1101 (*synth*)
Seldes, A.M. *et al., Tetrahedron*, 1988, **44**, 1359-1362 (*isol*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta fraudatrix constits*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*3β,5α,22E,24ξ-form, occur*)
Jain, R. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 190-191 (*isol*)
De Rosa, S. *et al., Z. Naturforsch., C*, 2006, **61**, 129-134 (*sponge constit*)

Stigmast-24-en-3-ol S-473

24-Ethylcholest-24-en-3-ol

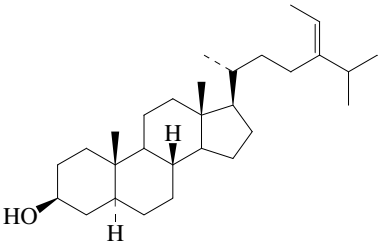


$C_{29}H_{50}O$ 414.713

(3β,5α)-*form* [134887-29-9]
Constit. of a sponge *Stelletta* sp. Genus name incorr. given as Stelleta.
Guerriero, A. *et al., Helv. Chim. Acta*, 1991, **74**, 487-494 (*isol, pmr, cmr*)

Stigmast-24(28)-en-3-ol S-474

24-Ethylidenecholestan-3-ol



(3β,5α,24*E*)-*form*

$C_{29}H_{50}O$ 414.713

(3β,5α,24*E*)-*form* [65941-69-7]
Constit. of the marine fungus *Haliphthoros milfordensis*, *Echinaster sepotisus* and various sponges.
O-*Sulfate:* [152005-16-8]
$C_{29}H_{50}O_4S$ 494.778
Constit. of the sea cucumber *Eupentacta fraudatrix*.
3-O-*β-D-Xylopyranoside:* [151890-85-6]
$C_{34}H_{58}O_5$ 546.829
Constit. of *Eupentacta fraudatrix*.

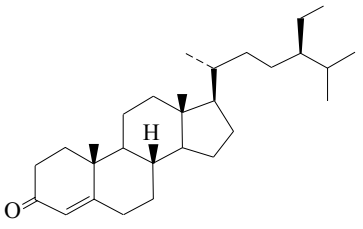
(3β,5α,24*Z*)-*form*
Isofucostanol
[55309-68-7]
Constit. of *Artemisina appollinis*, *Echinaster sepotisus*, *Jaspis stellifera*, *Holothuria nobilis*, *Pseudostichopus trachus* and *Periphylla periphylla*.
O-*Sulfate:* [152005-17-9]
Constit. of *Eupentacta fraudatrix*.
3-O-*β-D-Xylopyranoside:* [151890-86-7]
$C_{34}H_{58}O_5$ 546.829
Constit. of *Eupentacta fraudatrix*.
9Z,12Z-Octadecadienoyl: [120584-18-1]
$C_{47}H_{80}O_2$ 677.148
Isol. from corn oil.

(3β,5α,24ξ)-*form* [60208-82-4]
Constit. of the leaves of *Cassia tomentosa*. Isol. from *Gigartina skottsbergii* and *Rhizosolenia* sp.
Ballantine, J.A. *et al., Tet. Lett.*, 1975, **16**, 105-108 (*Periphylla constit*)
Theobald, N. *et al., J.A.C.S.*, 1978, **100**, 7677-7684 (*Jaspis constit*)
De Simone, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **66**, 351-357 (*Echinaster constits*)
Morris, R.J. *et al., J. Mar. Biol. Assoc. U.K.*, 1984, **64**, 721-722 (*Rhizosolenium constit*)
Palermo, J.A. *et al., Phytochemistry*, 1984, **23**, 2688-2689 (*Gigartina constit*)

Trost, V.W. *et al., J. Am. Oil Chem. Soc.*, 1989, **66**, 325-333 (*octadecadienoate*)
Seldes, A.M. *et al., Z. Naturforsch., B*, 1990, **45**, 83-86 (*Artemisia constit*)
Makarieva, T.N. *et al., Steroids*, 1993, **58**, 508-517 (*Eupentacta constits*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **128**, 337-347 (*3β,5α,24Z-form*)

Stigmast-4-en-3-one S-475

Sitost-4-en-3-one. ***β-Sitostenone***
[1058-61-3]



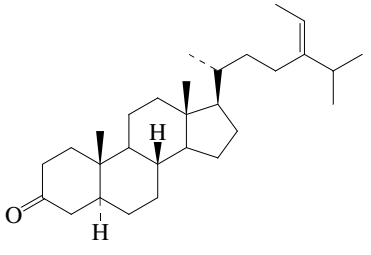
$C_{29}H_{48}O$ 412.698
Constit. of the wood of *Quassia amara* (Surinam quassia), *Cabralea* spp. and *Pinus taeda*. Also from lichens. Isol. from marine sponge *Geodia cydonium*, as an inseparable mixt. of C-24 epimers. Needles (Et_2O/MeOH).
Mp 95-96.5°. $[\alpha]_D$ +81.3.

Oxime:
Cryst. (EtOAc). Mp 175-176°.

Jones, E.R.H. *et al., J.C.S.*, 1942, 391 (*synth*)
Barton, D.H.R. *et al., J.C.S.*, 1943, 599 (*synth*)
Lavie, D. *et al., J.C.S.*, 1963, 5001 (*isol*)
Joshi, K.C. *et al., Indian J. Chem.*, 1974, **12**, 903 (*ms, pmr*)
Smith, A.G. *et al., Biomed. Mass Spectrom.*, 1976, **3**, 64 (*ms, synth*)
Migliuolo, A. *et al., J. Nat. Prod.*, 1990, **53**, 1262-1266 (*isol, sponge*)
Gaspar, E.M.M. *et al., Phytochemistry*, 1993, **34**, 523 (*isol, pmr, cmr*)

Stigmast-24(28)-en-3-one S-476

24-Ethylidenecholestan-3-one
[84711-17-1]



(5α,24(28)*E*)-*form*

$C_{29}H_{48}O$ 412.698

(5α,24(28)*E*)-*form* [53755-10-5]
Constit. of the seeds of *Setaria italica* (foxtail millet).
Mp 137-138.5°.

(5α,24(28)*Z*)-*form* [126576-88-3]
Constit. of *Setaria italica* (foxtail millet). Also isol. from the sponge *Artemisina apollinis*.

Sheikh, Y.M. *et al., J.C.S. Perkin 1*, 1974, 909-914 (*synth*)
Seldes, A.M. *et al., Z. Naturforsch., B*, 1990, **45**, 83-86 (*isol, pmr*)
Narumi, Y. *et al., Nihon Yukagakkaishi*, 1999, **48**, 1307-1313; *CA*, **132**, 194547w (*isol, pmr, cmr, synth*)

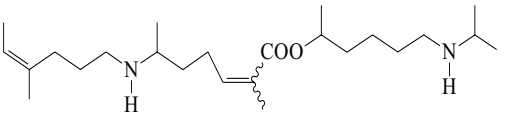
Stiparin S-477

Glycoprotein. Isol. from the dermis of the sea cucumber *Cucumaria frondosa*. Aggregates collagen fibrils.

Trotter, J.A. *et al., Matrix Biol.*, 1996, **15**, 99-110; *CA*, **125**, 138185 (*isol*)

Stockerine S-478

[136771-39-6]

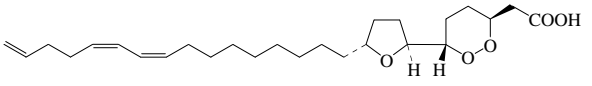


$C_{24}H_{46}N_2O_2$ 394.64
Metab. from the alga *Stockeyia indica*. Amorph.

Atta-ur-Rahman, *et al., Fitoterapia*, 1991, **62**, 77 (*isol, ir, pmr, cmr, ms, struct*)

Stolonic acid A S-479

3,6-Epidioxy-9,10-epoxy-19,21,25-hexacosatrienoic acid
[294203-16-0]



Relative Configuration

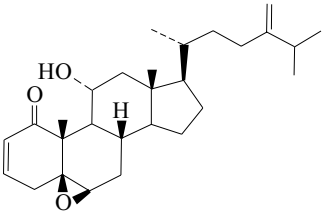
$C_{26}H_{42}O_5$ 434.615
Isol. from the ascidian *Stolonica* sp. Cytotoxic agent. Pale yellow oil. $[\alpha]_D$ -30.5 (c, 0.43 in $CHCl_3$). λ_{max} 239 (ϵ 4855) (MeOH/$CHCl_3$).

25,26-Dihydro: 3,6-Epidioxy-7,10-epoxy-19,21-hexacosadienoic acid. ***Stolonic acid B***
[294203-17-1]
$C_{26}H_{44}O_5$ 436.631
Isol. from *Stolonica* sp. Cytotoxic agent. Pale yellow oil. $[\alpha]_D$ -18.4 (c, 0.42 in $CHCl_3$). λ_{max} 239 (ϵ 8200) (MeOH/$CHCl_3$).

Davies-Coleman, M.T. *et al., J. Nat. Prod.*, 2000, **63**, 1411-1413

Stoloniferone A S-480

5,6-Epoxy-11-hydroxyergosta-2,24(28)-dien-1-one, 9CI
[94806-02-7]

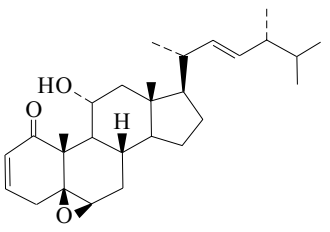


$C_{28}H_{42}O_3$ 426.638
Constit. of the soft coral *Clavularia viridis*. Cytotoxin. Cryst. (MeCN). Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 148°. $[\alpha]_D$ +38.5 ($CHCl_3$). λ_{max} 225 (ϵ 7800) (solvent not reported) (Derep). λ_{max} 225 (ϵ 8000) (MeOH) (Berdy).

Kobayashi, M. *et al., Tet. Lett.*, 1984, **25**, 5925

Stoloniferone B S-481

5,6-Epoxy-11-hydroxyergosta-2,22-dien-1-one, 9CI
[94806-03-8]



$C_{28}H_{42}O_3$ 426.638
Constit. of the soft coral *Clavularia viridis*. Cytotoxic. Cryst. (MeCN). Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 150°. $[\alpha]_D$ +33 ($CHCl_3$). λ_{max} 225 (ϵ 7800) (solvent not reported) (Derep). λ_{max} 225 (ϵ 8000) (MeOH) (Berdy).

Ac:
$C_{30}H_{44}O_4$ 468.675
Constit. of *Clavularia viridis*. Cryst. (MeCN).
Mp 143.5-144°. $[\alpha]_D$ -75.6 (c, 0.14 in $CHCl_3$). λ_{max} 224 (ϵ 5600) (EtOH).

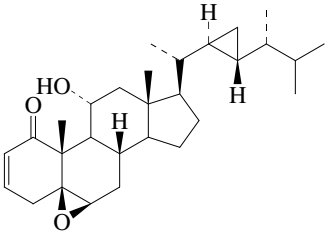
22,23-Dihydro: 5,6-Epoxy-11-hydroxyergost-2-en-1-one, 9CI. ***Stoloniferone C***
[94806-05-0]
$C_{28}H_{44}O_3$ 428.654
Constit. of *Clavularia viridis*. Cytotoxin. Cryst. (MeCN). Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 148°. $[\alpha]_D$ +40 ($CHCl_3$). λ_{max} 225 (ϵ 7800) (solvent not reported) (Derep). λ_{max} 225 (ϵ 7800) (MeOH) (Berdy).

22,23-Dihydro, Ac:
$C_{30}H_{46}O_4$ 470.691
Constit. of *Clavularia viridis*. Plates (MeCN).
Mp 140.5-141°. $[\alpha]_D$ -72.9 (c, 0.28 in $CHCl_3$). λ_{max} 224 (ϵ 5360) (EtOH).

Kobayashi, M. *et al., Tet. Lett.*, 1984, **25**, 5925
Watanabe, K. *et al., Steroids*, 1996, **61**, 439 (*isol, pmr, cmr*)

Stoloniferone D S-482

5,6-Epoxy-11-hydroxy-23-norgorgost-2-en-1-one, 9CI
[94806-04-9]

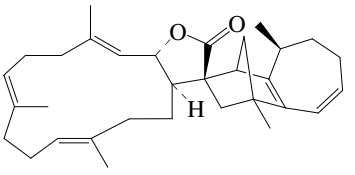


$C_{29}H_{44}O_3$ 440.665
Constit. of the soft coral *Clavularia viridis*. Cytotoxin. Cryst. (MeCN). Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 142°. $[\alpha]_D$ +31 ($CHCl_3$). λ_{max} 225 (ϵ 7800) (solvent not reported) (Derep). λ_{max} 225 (ϵ 8000) (MeOH) (Berdy).

Kobayashi, M. *et al., Tet. Lett.*, 1984, **25**, 5925 (*cryst struct*)

Stolonilactone S-483

[720681-08-3]

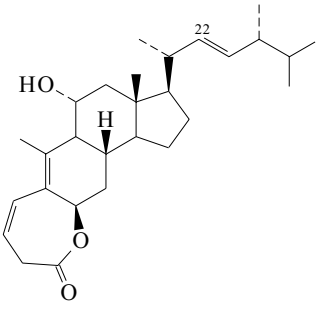


$C_{32}H_{44}O_2$ 460.698
Constit. of *Clavularia koellikeri*. Oil. $[\alpha]_D^{25}$ +100 (c, 0.21 in $CHCl_3$). λ_{max} 269 (ϵ 4200) (EtOH).

Iguchi, K. *et al., J.O.C.*, 2004, **69**, 4351-4355 (*isol, pmr, cmr*)

Stoloniolide I S-484

[171784-09-1]



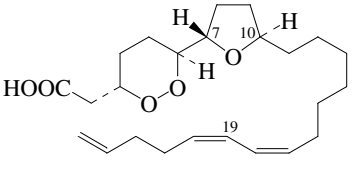
$C_{28}H_{42}O_3$ 426.638
Constit. of *Clavularia viridis*.

22,23-Dihydro: ***Stoloniolide II***
[171784-10-4]
$C_{28}H_{44}O_3$ 428.654
Constit. of *Clavularia viridis*.

Iguchi, K. *et al., Chem. Lett.*, 1995, 1109 (*isol, pmr, cmr*)

Stolonoxide A S-485

3,6-Epidioxy-7,10-epoxy-17,19,23-tetracosatrienoic acid
[259728-97-7]



Absolute Configuration

$C_{24}H_{38}O_5$ 406.561
Isol. from the marine tunicate *Stolonica socialis*. Cytotoxic agent. Oil (as Me ester). $[\alpha]_D$ -50.8 (c, 039 in $CHCl_3$) (Me ester). λ_{max} 235 (ϵ 22000) (EtOH) (Me ester).

*19*E-*Isomer:* ***Stolonoxide B***
[300811-92-1]
$C_{24}H_{38}O_5$ 406.561
Isol. from *Stolonica socialis*. Oil (as Me ester). $[\alpha]_D^{25}$ -37.7 (c, 0.26 in $CHCl_3$) (Me ester). λ_{max} 233 (ϵ 19900) (MeOH) (Me ester).

7,10-Diepimer: ***Stolonoxide C***
[300811-96-5]
$C_{24}H_{38}O_5$ 406.561
Isol. from *Stolonica socialis*.

*7,10-Diepimer, 19*E-*isomer:* ***Stolonoxide D***
[300811-97-6]
$C_{24}H_{38}O_5$ 406.561
Isol. from *Stolonica socialis*.

Fontana, A. *et al., Tet. Lett.*, 2000, **41**, 429-432 (*Stolonoxide A*)
Duran, R. *et al., Tetrahedron*, 2000, **56**, 6031-6037 (*Stolonoxides B-D*)

Stonustoxin S-486

SNTX

[137803-80-6]

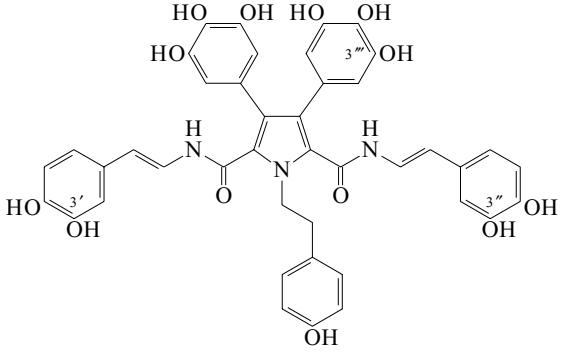
Protein consisting of 2 subunits (α and β) with MW 71000 and 79000. Isol. from the venom of the stonefish *Synanceia horrida*. Lethal factor.

[182373-44-0, 182577-50-0, 193026-01-6]

Poh, C.H. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **99**, 793-798 (*isol*)
Ghadessy, F.J. *et al., J. Biol. Chem.*, 1996, **271**, 25575-25578 (*struct*)
Yew, W.S. *et al., J. Struct. Biol.*, 1999, **128**, 216-218 (*cryst struct*)
Khoo, H.E. *et al., Clin. Exp. Pharmacol. Physiol.*, 2002, **29**, 802-806 (*rev*)

Storniamide D S-487

[174285-74-6]



$C_{42}H_{35}N_3O_{13}$ 789.751

Alkaloid from a Patagonian sponge *Cliona* sp. Shows antibiotic activity against gram-positive bacteria. Yellow oil. λ_{max} 212 (ϵ 29500); 284 (ϵ 11500); 338 (ϵ 12400) (MeOH) (Berdy).

3′-Deoxy: ***Storniamide B***
[174232-39-4]
$C_{42}H_{35}N_3O_{12}$ 773.751
From *Cliona* sp. Active against gram-positive bacteria. Yellow oil. λ_{max} 210 (ϵ 24500); 282 (ϵ 10200); 334 (ϵ 10800) (MeOH) (Berdy).

3‴-Deoxy: ***Storniamide C***
[174232-40-7]
$C_{42}H_{35}N_3O_{12}$ 773.751
From *Cliona* sp. Active against gram-positive bacteria. Yellow oil. λ_{max} 214 (ϵ 27000); 284 (ϵ 11100); 342 (ϵ 14300) (MeOH) (Berdy).

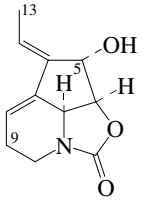
3′,3″-Dideoxy: ***Storniamide A***
[174232-38-3]
$C_{42}H_{35}N_3O_{11}$ 757.752
From *Cliona* sp. Active against gram-positive bacteria. Yellow oil. λ_{max} 208 (ϵ 22500); 286 (ϵ 11300); 334 (ϵ 11500) (MeOH) (Berdy).

Palermo, J.A. *et al., Tetrahedron*, 1996, **52**, 2727 (*isol, uv, ir, pmr, cmr, struct*)
Ebel, H. *et al., Tet. Lett.*, 1998, **39**, 9165-9166 (*synth*)
Boger, D.L. *et al., J.A.C.S.*, 1999, **121**, 54-62 (*Storniamide A, synth*)
Iwao, M. *et al., Tet. Lett.*, 2003, **44**, 4443-4446 (*Storniamide A, synth*)

Streptazoline S-488

*4-Ethylidene-2*a,*3,4,6,7,7*b-*hexahydro-3-hydroxy-1*H-*2-oxa-7*a-*azacyclopent[*cd*]inden-1-one, 9CI*

[80152-07-4]



Absolute Configuration

$C_{11}H_{13}NO_3$ 207.229

Authors' numbering shown (Puder *et al*). Isol. from *Streptomyces viridochromogenes* and the marine-derived *Streptomyces* sp. B5525.
$[\alpha]_D^{25}$ +22 (c, 2.8 in $CHCl_3$). Readily polymerises. λ_{max} 256 (ϵ 8510) (EtOH) (Derep). λ_{max} 256 (ϵ 9000) (EtOH) (Berdy).

*5-*O*-β-D-Xylopyranoside:* ***5-O-β-D-Xylopyranosylstreptazolin***
$C_{16}H_{21}NO_7$ 339.344
Prod. by *Streptomyces* sp. strain A1. Solid.
Mp 118°. $[\alpha]_D^{22}$ +1.3 (c, 0.8 in MeOH). λ_{max} 252 (log ϵ 4.23) (MeOH).

*9*R*-Hydroxy:* ***9-Hydroxystreptazolin***
$C_{11}H_{13}NO_4$ 223.228
Prod. by *Streptomyces* sp. strain A1. Oil. $[\alpha]_D^{22}$ +38 (c, 1.1 in MeOH). λ_{max} 256 (log ϵ 3.84) (MeOH).

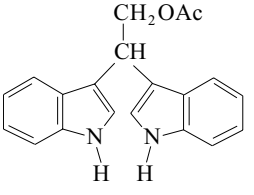
13-Hydroxy: ***13-Hydroxystreptazolin***
$C_{11}H_{13}NO_4$ 223.228
Prod. by *Streptomyces* sp. strain A1. Oil. $[\alpha]_D^{22}$ +39 (c, 1.1 in MeOH). λ_{max} 256 (log ϵ 4.04); 315 (log ϵ 2.7) (MeOH).

Drautz, H. *et al., Helv. Chim. Acta*, 1981, **64**, 1752-1765 (*isol*)
Karrer, A. *et al., Helv. Chim. Acta*, 1982, **65**, 1432 (*cryst struct*)
Flann, C.J. *et al., J.A.C.S.*, 1987, **109**, 6115 (*synth*)
Kozikowski, A.P. *et al., J.O.C.*, 1990, **55**, 4668 (*synth*)
Mayer, M. *et al., J.O.C.*, 1993, **58**, 3486 (*biosynth, bibl*)
Huang, S. *et al., Chem. Comm.*, 2000, 569-570 (*synth*)
Cossy, J. *et al., Eur. J. Org. Chem.*, 2001, 2841-2850 (*Dihydrostreptazolin, synth*)
Puder, C. *et al., J. Nat. Prod.*, 2001, **64**, 42-45 (*9-hydroxy, 13-hydroxy, 5-xylosyl*)
Maskey, R.P. *et al., Z. Naturforsch., B*, 2002, **57**, 823-829 (*marine, isol*)
Trost, B.M. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 4327-4329 (*synth*)
Li, F. *et al., J.O.C.*, 2006, **71**, 5221-5227 (*synth*)

Streptindole S-489

*β-1*H*-Indol-3-yl-1*H*-indole-3-ethyl acetate, 9CI. 2,2-Di(3-indolyl)ethyl acetate*

[88321-08-8]



$C_{20}H_{18}N_2O_2$ 318.374

Metab. from intestinal bacteria (*Streptococcus faecium* IB 37). Sol. MeOH, EtOAc; poorly sol. H_2O. Uncertain low mp. λ_{max} 273 (ϵ 6100); 283 (ϵ 6500); 290 (ϵ 5800) (EtOH) (Derep).

▶ Genotoxic agent.

Deacetoxy: ***Vibrindole A***. *1,1-Di(3-indolyl)ethane*
[5030-91-1]
$C_{18}H_{16}N_2$ 260.338
Metab. from the marine bacterium *Vibrio parahaemolyticus*, isol. from the toxic mucus of the boxfish *Ostracion cubicus*. Exhibits antimicrobial activity. Oil. λ_{max} 241 (ϵ 12200); 275 (ϵ 8100); 282 (ϵ 8160) ($CHCl_3$) (Berdy).

Thesing, J. *et al., Chem. Ber.*, 1954, **87**, 692-699 (*synth, deacetoxy*)
Osawa, T. *et al., Tet. Lett.*, 1983, **24**, 4719-4722 (*isol, uv, ir, pmr, ms, struct*)
Hogan, I.T. *et al., Synthesis*, 1984, 872 (*synth, uv, ir, pmr*)
Jackson, A.H. *et al., J.C.S. Perkin 1*, 1987, 2543-2551 (*Vibrindole A, synth*)
Singh, H. *et al., Tetrahedron*, 1988, **44**, 5897-5904 (*synth, ir, pmr*)
Bell, R. *et al., J. Nat. Prod.*, 1994, **57**, 1587-1590 (*Vibrindole A*)
Chakrabarty, M. *et al., Tet. Lett.*, 2002, **43**, 4075-4078 (*Vibrindole A, synth*)
Bartoli, G. *et al., Synthesis*, 2004, 895-900 (*synth*)

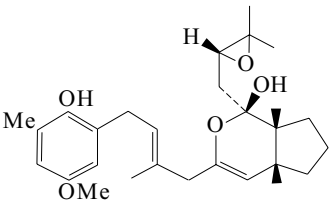
Striatoxin S-490

[82030-90-8]

Glycoprotein. Isol. from the venom of the marine snail *Conus striatus*. Cardiotonic.

Kobayashi, J. *et al., Biochem. Biophys. Res. Commun.*, 1982, **105**, 1389-1395

Strictaepoxide S-491

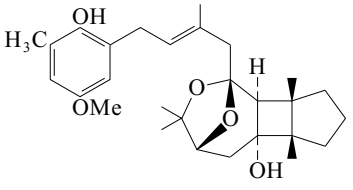


$C_{28}H_{40}O_5$ 456.621
Constit. of brown alga *Cystoseira stricta*. Oil. $[\alpha]_D$ -5.1 (c, 5.6 in EtOH).

Amico, V. *et al., Tetrahedron*, 1986, **42**, 6015

Strictaketal S-492

[110612-28-7]



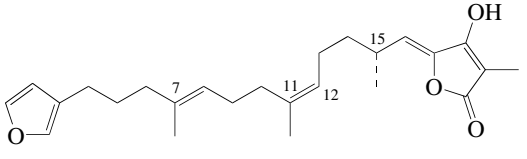
$C_{28}H_{40}O_5$ 456.621
Constit. of *Cystoseira stricta*. Oil. $[\alpha]_D$ +21.7 (c, 0.9 in EtOH). λ_{max} 215 (ϵ 10700); 290 (ϵ 3690) (EtOH) (Derep).

Z-Isomer: ***Isostrictaketal***
[110322-47-9]
$C_{28}H_{40}O_5$ 456.621
Constit. of *Cystoseira stricta*. Cryst.
Mp 94-95°. $[\alpha]_D^{20}$ +1.3 (c, 0.94 in EtOH).

Amico, V. *et al., J. Nat. Prod.*, 1987, **50**, 449
Amico, V. *et al., Phytochemistry*, 1987, **26**, 1719 (*deriv*)
Amico, V. *et al., Acta Cryst. C*, 1988, **44**, 686-689 (*Isostrictaketal, cryst struct*)

Strobilinin S-493

[56394-06-0]



(7*E*,11*Z*,15*R*)-*form*

$C_{25}H_{34}O_4$ 398.541

(7*E*,11*Z*,15*R*)-*form* [158252-27-8]
Constit. of *Ircinia strobilina*, *Ircinia felix* and *Ircinia campana*. Oil. λ_{max} 273 (MeOH) (Berdy).

(7*Z*,11*E*,15*R*)-*form* [158252-28-9]
Constit. of *Ircinia strobilina*.
Oil.

(7*Z*,11*Z*,15*R*)-*form*
Constit. of *Ircinia strobilina*, *Ircinia felix* and *Ircinia campana*. λ_{max} 273 (MeOH) (Berdy).

(7*Z*,11*Z*,15*S*)-*form* [193001-60-4]
Constit. of *Ircinia oros.*

Me ether: 18-O-*Methylstrobilinin*
$C_{26}H_{36}O_4$ 412.568
Oil. $[\alpha]_D^{20}$ -43.7 (c, 0.4 in $CHCl_3$). λ_{max} 263 (ϵ 19900) (EtOH).

(7ξ,15ξ)-*form*

11,12-Dihydro, 11-hydroxy: ***Strobilinol***
$C_{25}H_{36}O_5$ 416.556
Constit. of *Ircinia strobilina*.

Rothberg, I. *et al., Tet. Lett.*, 1975, **16**, 769-772 (*Strobilinin, 7Z,11E,15R-form*)
Shubiak, P. *et al., Diss. Abstr. Int., B*, 1978, **38**, 4775; *CA*, **89**, 20649 (*Strobilinol*)
Crews, P. *et al., Prog. Chem. Org. Nat. Prod.*, 1985, **48**, 203-269 (*Strobilinol*)
Davis, R. *et al., Aust. J. Chem.*, 1994, **47**, 933-936 (*struct*)
Martinez, A. *et al., Chem. Pharm. Bull.*, 1997, **45**, 181-184 (*Strobilinins*)
Höller, U. *et al., J. Nat. Prod.*, 1997, **60**, 832-835 (*Ircinia oros constit*)

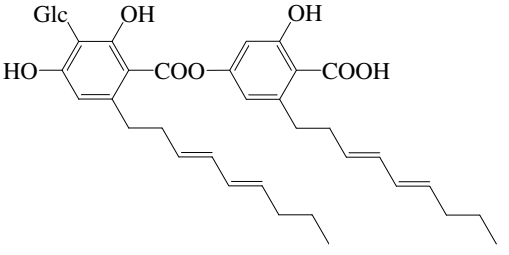
Strombine dehydrogenase S-494

E.C. 1.5.1.22. N-*(Carboxymethyl)-D-alanine:NAD*$^{\oplus}$ *oxidoreductase (glycine-forming)*
[79393-84-3]
Oxidoreductase enzyme. Isol. from *Mytilus edulis.* Catalyses the reaction of *N*-(Carboxymethyl)alanine, C-106 with $NAD^{\oplus}$ and H_2O to give Glycine, pyruvate and NADH.

Dando, P.R. *et al., Biochem. Soc. Trans.*, 1981, **9**, 297-298

Stromemycin S-495

[345295-46-7]

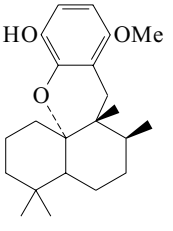


$C_{38}H_{48}O_{12}$ 696.79
Isol. from the fungus *Emericella variecolor* derived from the sponge *Haliclona valliculata*. Metalloproteinase inhibitor.
Amorph. red powder.
Mp 139°. $[\alpha]_D^{20}$ +29 (c, 0.1 in EtOH). λ_{max} 229; 273; 307 (EtOH).

Pat. Coop. Treaty (WIPO), 2001, 01 44 264; *CA*, **135**, 60263d (*isol*)
Bringmann, G. *et al., Phytochemistry*, 2003, **63**, 437-443 (*isol, cd*)

Strongylin A S-496

Sch 50678
[136978-48-8]

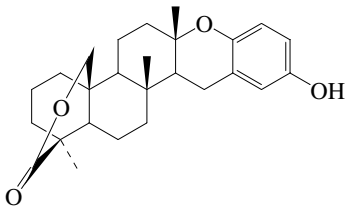


$C_{22}H_{32}O_3$ 344.493
Constit. of *Strongylophora hartmani* and *Xestospongia wiedenmayeri*. Oil. $[\alpha]_D^{20}$ +72 (c, 0.023 in CH_2Cl_2). λ_{max} 215 (ϵ 1370); 276 (ϵ 1030) (MeOH) (Derep). λ_{max} 201 (ϵ 52200); 225 (sh) (ϵ 9470); 284 (ϵ 3440) (heptane).

Wright, A.E. *et al., J. Nat. Prod.*, 1991, **54**, 1108 (*isol, pmr, cmr*)
Coval, S.J. *et al., Bioorg. Med. Chem. Lett.*, 1995, **5**, 605-610 (*isol, uv, pmr, cmr*)

Strongylophorine 2 S-497

[70214-92-5]



Absolute Configuration

$C_{26}H_{34}O_4$ 410.552
Constit. of sponge *Strongylophora durissima*. Ichthyotoxic. Oil.

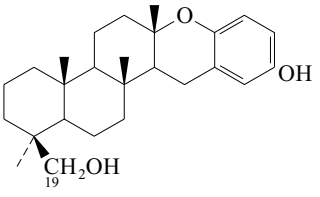
Ac: ***Strongylophorine 11***
[70214-98-1]
$C_{28}H_{36}O_5$ 452.589
Constit. of *Strongylophora durissima*. Fine needles. $[\alpha]_D^{25}$ -71 (c, 0.05 in $CHCl_3$). λ_{max} 228 (log ϵ 3.9); 283 (log ϵ 3.51); 290 (log ϵ 3.45) (MeOH).

Me ether: ***Strongylophorine 9***
[70214-99-2]
$C_{27}H_{36}O_4$ 424.579
Constit. of *Strongylophora durissima*. Fine needles. $[\alpha]_D^{25}$ -43.7 (c, 0.1 in MeOH). λ_{max} 229 (log ϵ 3.5); 294 (log ϵ 3.23) (MeOH).

Braekman, J.C. *et al., Bull. Soc. Chim. Belg.*, 1978, **87**, 917
Shen, Y.-C. *et al., J. Chin. Chem. Soc. (Taipei)*, 2000, **47**, 567-570 (*isol, pmr, cmr, ms*)

Strongylophorine 5 S-498

[125282-12-4]



$C_{26}H_{38}O_3$ 398.584
Metab. of *Strongylophora durissima*. Oil. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 303 (MeOH/NaOH) (Derep). λ_{max} 295 (ϵ 1300) (MeOH) (Derep). λ_{max} 296 (ϵ 2440) (MeOH) (Berdy). λ_{max} 305 (MeOH/NaOH) (Berdy).

19-Aldehyde: ***Strongylophorine 4***
[125282-11-3]
$C_{26}H_{36}O_3$ 396.569
Metab. of *Strongylophora durissima*. Ichthyotoxin. Cryst. (EtOAc/hexane). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 196-198°. $[\alpha]_D$ -55 (c, 0.5 in $CHCl_3$). λ_{max} 303 (MeOH/NaOH) (Derep). λ_{max} 295 (ϵ 1300) (MeOH) (Derep).

19-Carboxylic acid: ***Strongylophorine 3***
[70214-93-6]
$C_{26}H_{36}O_4$ 412.568
Constit. of *Strongylophora durissima*. Ichthyotoxin, insecticide. Cryst.
Mp 183-186°. $[\alpha]_D$ -35 (c, 0.32 in CH_2Cl_2).

19-Carboxylic acid, Ac: ***Strongylophorine 12***
[315209-08-6]
$C_{28}H_{38}O_5$ 454.605
Constit. of *Strongylophora durissima*. Amorph. powder. $[\alpha]_D^{25}$ -9.4 (c, 0.1 in $CHCl_3$). λ_{max} 229 (log ϵ 3.41); 283 (log ϵ 4.13); 290 (log ϵ 3.53) (MeOH).

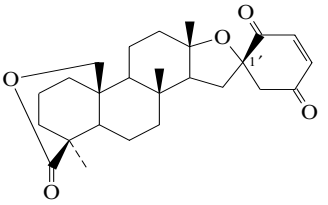
19-Carboxylic acid, Me ether: ***Strongylophorine 1***
[70214-91-4]
$C_{27}H_{38}O_4$ 426.595
Constit. of *Strongylophora durissima*. Ichthyotoxin. Cryst.
Mp 160°. $[\alpha]_D$ -27 (c, 0.5 in $CHCl_3$).

19-Deoxy: ***Strongylophorine 22***
[648883-30-1]
$C_{26}H_{38}O_2$ 382.585
Constit. of *Petrosia* (*Strongylophora*) *corticata*. Cryst. (MeOH). Mp 190-191°. $[\alpha]_D^{25}$ -75.2 (c, 1.1 in $CHCl_3$). λ_{max} 221 (ϵ 6684); 229 (ϵ 5932); 298 (ϵ 4432) (EtOH).

Braekman, J.C. *et al., Bull. Soc. Chim. Belg.*, 1978, **87**, 917
Salvá, J. *et al., J.O.C.*, 1990, **55**, 1941 (*isol, pmr, cmr*)
Shen, Y.-C. *et al., J. Nat. Prod.*, 2000, 1686-1688 (*Strongylophorine 12*)
Hoshino, A. *et al., J. Nat. Prod.*, 2003, **66**, 1600-1605 (*Strongylophorine 22*)

Strongylophorine 6 S-499

[125282-13-5]



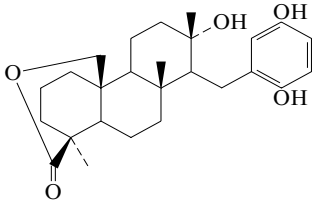
$C_{26}H_{34}O_5$ 426.552
Metab. of *Strongylophora durissima*. Cryst. (Et_2O). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 243-244° dec. $[\alpha]_D$ -47.1 (c, 0.42 in $CHCl_3$). λ_{max} 223 (ϵ 11800) (MeOH) (Derep).

1′-Epimer: ***Strongylophorine 7***
[125302-26-3]
$C_{26}H_{34}O_5$ 426.552
Metab. of *Strongylophora durissima*. Cryst. (Et_2O). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 237-238° dec. $[\alpha]_D$ -18.3 (c, 3.3 in $CHCl_3$). λ_{max} 223 (ϵ 11800) (MeOH) (Derep).

Salvá, J. *et al., J.O.C.*, 1990, **55**, 1941 (*isol, pmr, cmr*)

Strongylophorine 8 S-500

[125329-09-1]

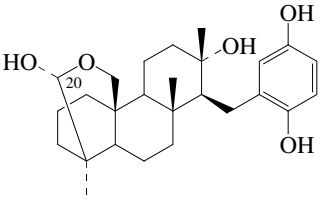


$C_{26}H_{36}O_5$ 428.567
Metab. of *Strongylophora durissima*. Cryst. (MeOH). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 246-247°. $[\alpha]_D$ -9.1 (c, 0.55 in Me_2CO). λ_{max} 312 (MeOH/NaOH) (Derep). λ_{max} 295 (ϵ 9340) (MeOH) (Derep). λ_{max} 295 (ϵ 9840) (MeOH) (Berdy).

Salvá, J. *et al., J.O.C.*, 1990, **55**, 1941 (*isol, pmr, cmr*)

Strongylophorine 13 S-501

[866403-71-6]



$C_{26}H_{38}O_5$ 430.583

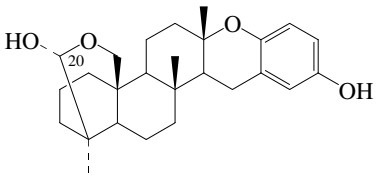
Constit. of *Strongylophora strongylata*. λ_{max} 204 (ϵ 13000); 230 (sh) (ϵ 3100); 296 (ϵ 2100) (MeOH).

20-Epimer: ***Strongylophorine 14***
[866403-72-7]
$C_{26}H_{38}O_5$ 430.583
Constit. of *Strongylophora strongylata*.

Liu, H. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 661-670

Strongylophorine 15 S-502

[866403-73-8]



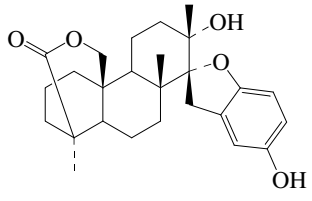
$C_{26}H_{36}O_4$ 412.568
Constit. of *Strongylophora strongylata*. λ_{max} 204 (ϵ 13000); 230 (sh) (ϵ 3100); 296 (ϵ 2100) (MeOH).

20-Epimer: ***Strongylophorine 16***
[866403-74-9]
$C_{26}H_{36}O_4$ 412.568
Constit. of *Strongylophora strongylata*.

Liu, H. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 661-670

Strongylophorine 19 S-503

[866403-75-0]

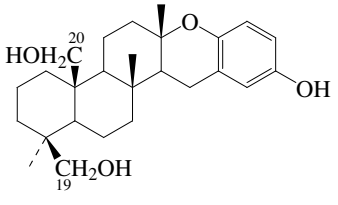


$C_{26}H_{34}O_5$ 426.552
Constit. of *Strongylophora strongylata*. Powder. $[\alpha]_D$ -3.6 (c, 0.15 in Py). λ_{max} 207 (ϵ 22000); 229 (sh) (ϵ 5400); 257 (ϵ 2500); 297 (ϵ 1600) (MeOH).

Liu, H. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 661-670

Strongylophorine 25 S-504

Strongylophorine 17
[648883-33-4]



$C_{26}H_{38}O_4$ 414.584
Constit. of *Petrosia corticata* (*Strongylophora corticata*) and *Strongylophora strongylata*. Cryst. (MeOH).
Mp 262-263°. $[\alpha]_D^{22}$ -60 (c, 0.1 in $CHCl_3$). λ_{max} 221 (ϵ 6299); 228 (ϵ 5405); 298 (ϵ 3993) (EtOH).

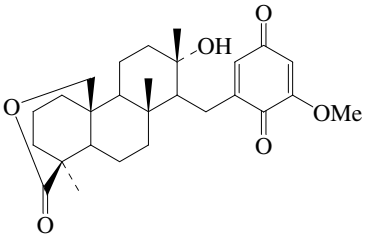
19-Deoxy: ***Strongylophorine 23***. *Strongylophorine 18*
[648883-31-2]
$C_{26}H_{38}O_3$ 398.584
Constit. of *Petrosia corticata* (*Strongylophora corticata*) and *Strongylophora strongylata*. Amorph. solid. $[\alpha]_D^{23}$ -52.2 (c, 1.2 in $CHCl_3$). λ_{max} 220 (ϵ 5950); 229 (ϵ 5066); 298 (ϵ 3822) (MeOH).

19-Deoxy, 20-aldehyde: ***Strongylophorine 24***
[648883-32-3]
$C_{26}H_{36}O_3$ 396.569
Constit. of *Petrosia* (*Strongylophora*) *corticata*. Cryst. (MeOH aq.). Mp 214-216°. $[\alpha]_D^{26}$ -25.5 (c, 1 in $CHCl_3$). λ_{max} 220 (ϵ 6273); 228 (ϵ 5290); 297 (ϵ 3803) (EtOH).

Hoshino, A. *et al., J. Nat. Prod.*, 2003, **66**, 1600-1605 (*Strongylophorines 23-25*)
Liu, H. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 661-670 (*Strongylophorines 17 and 18*)

Strongylophorine 26 S-505

[664992-27-2]



$C_{27}H_{36}O_6$ 456.578
Metab. of *Petrosia corticata* (*Strongylophora corticata*). Amorph. solid. $[\alpha]_D^{28}$ +11 (c, 0.35 in MeCN). λ_{max} 202 (ϵ 10000); 241 (ϵ 6200); 276 (ϵ 6900); 347 (sh) (MeCN).

Warabi, K. *et al., J. Nat. Prod.*, 2004, **67**, 1387-1389 (*isol, pmr, cmr*)

Strongylostatin S-506

Isol. from the sea urchin *Strongylocentrotus droebachiensis*. Shows antitumour activity.

Strongylostatin 1 [71950-63-5]
Glycoprotein.
▶ LD_{50} (mus, ipr) 10 mg/kg.

Strongylostatin 2 [80893-49-8]
Glycoprotein. Fairly sol. H_2O; poorly sol. MeOH, hexane.

Pettit, G.R. *et al., J. Nat. Prod.*, 1979, **42**, 407-409; 1981, **44**, 701-704 (*isol*)

Styelins S-507

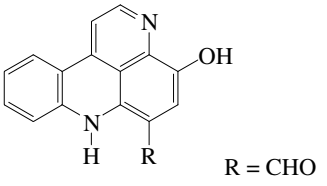
A family of peptides containing 31-32 amino acid residues. Isol. from haemocytes of the solitary tunicate *Styela clava*. Show antimicrobial activity.

[202421-35-0, 202421-36-1]

Lee, I.H. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1997, **118**, 515-521 (*isol*)
Zhou, C. *et al., FEBS Lett.*, 1997, **412**, 144-148 (*isol*)
Taylor, S.W. *et al., J. Biol. Chem.*, 2000, **275**, 38417-38426 (*isol*)
Lehrer, R.I. *et al., Adv. Exp. Med. Biol.*, 2001, **484**, 71-76 (*rev*)

Styelsamine C S-508

[216446-11-6]



$C_{16}H_{10}N_2O_2$ 262.267
Isol. from the ascidian *Eusynstyela latericius*. Cytotoxic. Orange solid (as TFA salt). λ_{max} 248 (log ϵ 4.9); 284 (log ϵ 4.82); 334 (log ϵ 4.22); 350 (log ϵ 4.27); 418 (log ϵ 4.75); 480 (log ϵ 4.41) ($CHCl_3$).

Copp, B.R. *et al., J.O.C.*, 1998, **63**, 8024-8026 (*isol, pmr, cmr*)
Nakahara, S. *et al., Heterocycles*, 2003, **60**, 2017-2022; 2005, **65**, 1925-1929 (*synth*)

Styelsamine D S-509

[216365-44-5]

As Styelsamine C, S-508 with

R = -$^{13}CH_2^{14}CH_2NH_2$

$C_{17}H_{15}N_3O$ 277.325

Closely related to *N*-Deacylcystodytin, D-34. Isol. from the ascidian *Eusynstyela latericius*. Purple solid (as bistrifluoroacetate salt). λ_{max} 222 (log ϵ 4.3); 238 (log ϵ 4.17); 276 (log ϵ 4.37); 294 (log ϵ 4.38); 320 (log ϵ 3.8); 372 (log ϵ 3.54); 386 (log ϵ 3.6); 560 (log ϵ 3.43) (MeOH/trifluoroacetate). λ_{max} 270 (log ϵ 4.26); 376 (log ϵ 3.95) (MeOH/KOH).

N^{14}-Ac: ***Styelsamine B***

[216387-14-3]

$C_{19}H_{17}N_3O_2$ 319.362

Isol. from *Eusynstyela latericius*. Purple solid (as trifluoroacetate salt). λ_{max} 222 (sh) (log ϵ 4.43); 244 (log ϵ 4.28); 278 (log ϵ 4.55); 294 (log ϵ 4.6); 372 (sh) (log ϵ 3.57); 388 (log ϵ 3.7); 572 (log ϵ 3.72) (MeOH/trifluoroacetate). λ_{max} 262 (log ϵ 4.38); 378 (log ϵ 3.97) (KOH).

13-Hydroxy: ***Styelsamine A***

[216446-06-9]

$C_{17}H_{15}N_3O_2$ 293.324

Isol. from *Eusynstyela latericius*. Purple solid (as bistrifluoroacetate salt). λ_{max} 222 (sh) (log ϵ 3.86); 244 (log ϵ 3.71); 276 (log ϵ 3.93); 294 (log ϵ 3.96); 386 (log ϵ 3.17); 554 (log ϵ 3.02) (MeOH/trifluoroacetate). λ_{max} 272 (log ϵ 3.85); 378 (log ϵ 3.39) (MeOH/KOH).

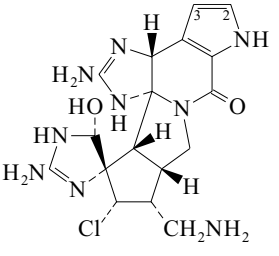
Copp, B.R. *et al., J.O.C.*, 1998, **63**, 8024-8026 (*Styelsamines A,B, isol, ir, pmr, cmr, uv*)

Skyler, D. *et al., Org. Lett.*, 2001, **3**, 4323-4324 (*Styelsamine B, synth*)

Styloguanidine S-510

Isopalauamine

[163089-72-3]



$C_{17}H_{22}ClN_9O_2$ 419.873

Alkaloid from the marine sponge *Stylotella aurantium*. Potent chitinase inhibitor. Antifouling agent. Amorph. solid. $[\alpha]_D$ +20.7 (c, 3.5 in MeOH). λ_{max} 273 (ϵ 4700) (MeOH) (Derep). λ_{max} 224 (ϵ 7800); 272 (ϵ 7900) (MeOH) (Derep).

3-Bromo: ***3-Bromostyloguanidine***

[162339-62-0]

$C_{17}H_{21}BrClN_9O_2$ 498.769

From *Stylotella aurantium*. Potent chitinase inhibitor; antifouling agent. Tan solid. $[\alpha]_D$ +57.5 (c, 0.7 in MeOH). λ_{max} 277 (ϵ 5000) (MeOH) (Derep).

2,3-Dibromo: ***2,3-Dibromostyloguanidine***

[162339-63-1]

$C_{17}H_{20}Br_2ClN_9O_2$ 577.665

From *Stylotella aurantium*. Potent chitinase inhibitor; antifouling agent. Off-white cryst. (2-propanol/MeOH). $[\alpha]_D$ -70.8 (c, 0.6 in MeOH). λ_{max} 283 (ϵ 5800) (MeOH) (Derep).

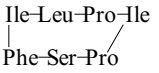
Kato, T. *et al., Tet. Lett.*, 1995, **36**, 2133 (*isol, uv, ir, pmr, cmr, struct*)

Kinnel, R.B. *et al., J.O.C.*, 1998, **63**, 3281-3286 (*isol, pmr, cmr*)

Stylopeptide 1 S-511

Stylostatin 2

[170968-92-0]



$C_{40}H_{61}N_7O_8$ 767.964

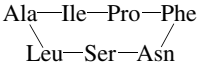
Cyclic peptide. Isol. from the marine sponges *Phakellia costata* and *Stylotella* sp. Cryst. (MeOH aq.).
Mp 228-229°. $[\alpha]_D^{25}$ -128 (c, 0.2 in MeOH).

Pettit, G.R. *et al., J.O.C.*, 1995, **60**, 8257-8261; 1996, **61**, 2322-2325 (*isol, pmr, cmr, cryst struct, synth*)

U.S. Pat., 1996, 5 494 893; *CA*, **124**, 333059p (*isol*)

Stylostatin 1 S-512

[145190-76-7]



$C_{36}H_{54}N_8O_9$ 742.871

Cyclic peptide. Isol. from the sponge *Stylotella* sp. Cytotoxic agent. Cryst. (MeOH aq.).
Mp 210°. $[\alpha]_D^{25}$ -116 (c, 0.3 in MeOH). λ_{max} 212 (ϵ 4059); 231 (ϵ 5072); 282 (ϵ 3087) (EtOH) (Berdy).

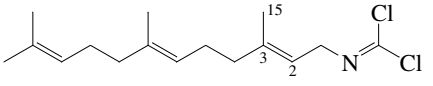
Pettit, G.R. *et al., J.O.C.*, 1992, **57**, 7217-7220; 1993, **58**, 3222 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)

Bourne, G.T. *et al., J.O.C.*, 1999, **64**, 3095-3101 (*synth*)

Rosenbaum, C. *et al., Tet. Lett.*, 2001, **42**, 5677-5680 (*synth*)

Stylotellane A S-513

[199732-52-0]



$C_{16}H_{25}Cl_2N$ 302.286

Constit. of *Stylotella aurantium*.

$\Delta^{3(15)}$-Isomer, 2ξ-chloro: ***Stylotellane B***

[64789-89-5]

$C_{16}H_{24}Cl_3N$ 336.73

Constit. of the sponge *Pseudaxinyssa pitys* and *Stylotella aurantium*.

*$\Delta^{3(15)}$-Isomer, 1,2-didehydro(*E-*):* ***Ulosin A***

[321557-59-9]

$C_{16}H_{23}Cl_2N$ 300.27

Constit. of *Stylotella aurantium* and *Ulosa spongia*. Oil. λ_{max} 284 (log ϵ 4.5) (MeOH).

Wratten, S.J. *et al., J.A.C.S.*, 1977, **99**, 7367-7368 (*isol, pmr, cmr*)

Simpson, J.S. *et al., Tet. Lett.*, 1997, **38**, 7947-7950 (*isol, pmr, cmr, biosynth*)

Musman, M. *et al., J. Nat. Prod.*, 2001, **64**, 111-113 (*Ulosin A*)

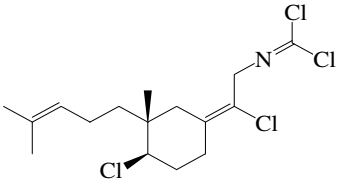
Kehraus, S. *et al., J. Nat. Prod.*, 2001, **64**, 939-941 (*isol, pmr, cmr*)

Brust, A. *et al., Tet. Lett.*, 2003, **44**, 327-330 (*biosynth*)

Simpson, J.S. *et al., Org. Biomol. Chem.*, 2004, **2**, 949-956 (*biosynth*)

Stylotellane D S-514

[693253-52-0]



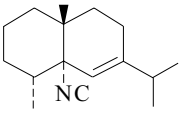
$C_{16}H_{23}Cl_4N$ 371.175

Constit. of *Stylotella aurantium*.

Brust, A. *et al., ACGC Chem. Res. Commun.*, 2004, **17**, 33-37
Simpson, J.S. *et al., Org. Biomol. Chem.*, 2004, **2**, 949-956

Stylotellin S-515

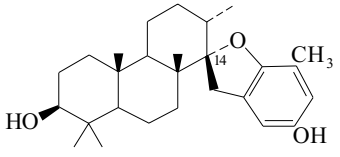
[108648-45-9]



$C_{16}H_{25}N$ 231.38
Constit. of sponge *Stylotella* sp. Oil. $[\alpha]_D$ -47 (c, 1.7 in $CHCl_3$).

Paś, M. *et al., Tet. Lett.*, 1987, **28**, 1409

Stypodiol S-516



(14*S*)–*form*

$C_{27}H_{40}O_3$ 412.611
λ_{max} 230 (ϵ 6350); 304 (ϵ 5650) (MeOH) (Derep).

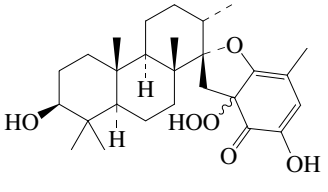
(14*R*)-*form*
Epistypodiol
[75578-65-3]
Constit. of *Stypopodium zonale*.
Oil. $[\alpha]_D$ -4.5 (c, 1.4 in $CHCl_3$). λ_{max} 230 (ϵ 6350); 304 (ϵ 5650) (MeOH) (Derep). λ_{max} 230 (ϵ 6250); 304 (ϵ 5650) (MeOH) (Berdy).

(14*S*)-*form* [75657-53-3]
Constit. of *Stypopodium zonale*.
Unstable, amorph. $[\alpha]_D$ -3.1 (c, 1 in $CHCl_3$). λ_{max} 305 (ϵ 2020) (MeOH) (Berdy).

Gerwick, W.H. *et al., J.O.C.*, 1981, **46**, 22
Abad, A. *et al., J.O.C.*, 1998, **63**, 5100-5106 (*synth*)

Stypohydroperoxide S-517

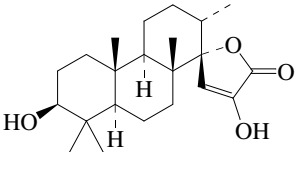
[863548-88-3]



$C_{27}H_{40}O_6$ 460.609
Constit. of the tropical marine alga *Stypopodium flabelliforme*. Oil. $[\alpha]_D^{25}$ -21 (c, 0.12 in $CHCl_3$). λ_{max} 266 (ϵ 658); 290 (ϵ 675) (MeOH).

Sabry, O.M.M. *et al., J. Nat. Prod.*, 2005, **68**, 1022-1030 (*Stypohydroperoxide*)

Stypolactone S-518



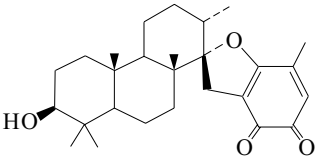
$C_{22}H_{34}O_4$ 362.508

Constit. of the brown alga *Stypopodium zonale*. Amorph. powder. $[\alpha]_D^{25}$ -67 (c, 0.06 in MeOH).

Dorta, E. *et al., Tet. Lett.*, 2002, **43**, 9043-9046 (*isol, pmr, cmr*)

Stypoldione S-519

[71103-05-4]

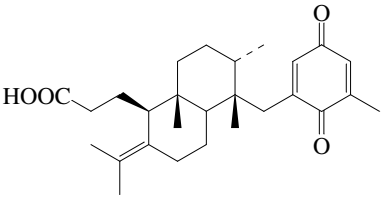


$C_{27}H_{38}O_4$ 426.595
Constit. of algae *Stypopodium zonale*, *Stypopodium flabelliforme* and mollusc *Aplysia dactyomela*. Ichtyotoxin, algicide, toxic to sea urchin eggs. Phospholipase A2 inhibitor, microtubule inhibitor. Red cryst. (Et_2O).
Mp 170° dec. $[\alpha]_D$ -65.1 (c, 0.46 in $CHCl_3$). λ_{max} 270 (ϵ 2470); 475 (ϵ 882) (MeOH) (Derep).

Gerwick, W.H. *et al., J.O.C.*, 1981, **46**, 22-27 (*isol, ir, pmr, cmr, uv*)
Jacobs, R.S. *et al., Tetrahedron*, 1985, **41**, 981-984 (*rev*)
Gerwick, W.H. *et al., J. Chem. Ecol.*, 1989, **15**, 677-683 (*isol*)
Mori, K. *et al., Bioorg. Med. Chem. Lett.*, 1992, **2**, 391-394 (*synth*)
Falck, J.R. *et al., J.A.C.S.*, 1993, **115**, 11606-11607 (*synth*)
Rovirosa, J. *et al., Bol. Soc. Chil. Quim.*, 1994, **39**, 219-221 (*isol, pmr, cmr*)
Mori, K. *et al., Annalen*, 1995, 1755-1763 (*synth*)
Abad, A. *et al., Synlett*, 1996, 913-915 (*synth*)

Stypoquinonic acid S-520

[232585-15-8]

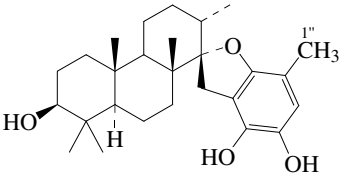


$C_{27}H_{38}O_4$ 426.595
Stereochem. revised in 2003. Constit. of *Stypopodium zonale*. Oil. $[\alpha]_D^{25}$ +68.9 (c, 0.27 in MeOH). λ_{max} 255 (ϵ 1240) (MeOH).

Wessels, M. *et al., J. Nat. Prod.*, 1999, **62**, 927-930 (*isol, pmr, cmr*)
Dorta, E. *et al., Tetrahedron*, 2003, **59**, 2059-2062 (*pmr, cmr, stereochem*)

Stypotriol S-521

[71106-25-7]



$C_{27}H_{40}O_4$ 428.611
Isol. from *Stypopodium zonale*. Ichthyotoxin. Oil. Sol. MeOH, Et_2O, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{25}$ -10 (c, 0.82 in $CHCl_3$). λ_{max} 291 (ϵ 2990) (MeOH) (Derep). λ_{max} 270 (ϵ 2470); 475 (ϵ 882) (MeOH) (Berdy).

Tri-Ac:
Cryst. Mp 248-250°.

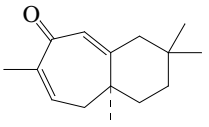
1″-Oxo: ***Stypotriolaldehyde***. *Stypoltrial*
[863548-87-2]
$C_{27}H_{38}O_5$ 442.594
Constit. of the tropical marine alga *Stypopodium flabelliforme*.

Oil. $[\alpha]_D^{25}$ +22 (c, 0.12 in $CHCl_3$). λ_{max} 216 (ϵ 7910); 288 (ϵ 2560); 348 (ϵ 1190) (MeOH).

Gerwick, W.H. *et al., J.O.C.*, 1981, **46**, 22 (*Stypotriol*)
Sabry, O.M.M. *et al., J. Nat. Prod.*, 2005, **68**, 1022-1030 (*Stypotriolaldehyde*)

Styxone A S-522

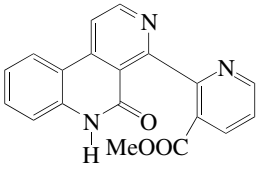
[498552-75-3]



$C_{15}H_{22}O$ 218.338
Constit. of *Myrmekioderma styx*. Oil. $[\alpha]_D$ +164 (c, 0.09 in MeOH). λ_{max} 252 (ϵ 6808) (no solvent reported).

Peng, J. *et al., Tet. Lett.*, 2002, **43**, 9699-9702 (*isol, pmr, cmr*)

Subarine S-523

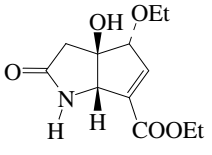


$C_{19}H_{13}N_3O_3$ 331.33
Alkaloid from a Singaporean ascidian. Pale yellow gum. λ_{max} 233 (log ϵ 4.45); 267 (log ϵ 4.14); 335 (log ϵ 3.72) (MeOH).

Nilar, *et al., J. Nat. Prod.*, 2002, **65**, 1198-1200 (*isol, pmr, cmr, ms*)
Bijeire, L. *et al., Eur. J. Org. Chem.*, 2004, 1891-1893 (*synth, pmr, cmr*)

Subereatensin S-524

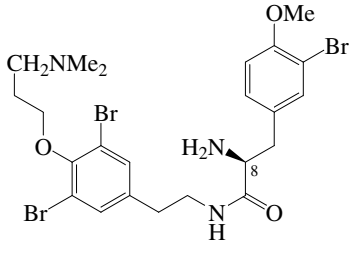
[474670-21-8]



$C_{12}H_{17}NO_5$ 255.27
Isol. from the sponge *Suberea* aff. *praetensa*. Gum.

Kijjoa, A. *et al., Z. Naturforsch., C*, 2002, **57**, 732-738 (*isol, pmr, cmr, ms*)

Suberedamine A S-525



$C_{23}H_{30}Br_3N_3O_3$ 636.22
Related to Purpuramine H, P-725.

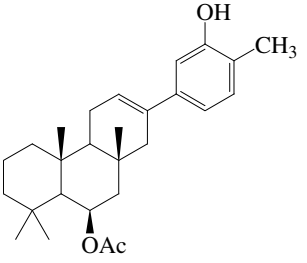
(S)-form
Isol. from a sponge, *Suberea* sp. Cytotoxic. Amorph. solid.
Mp 64-67°. $[\alpha]_D^{25}$ +21 (c, 1 in MeOH). λ_{max} 281 (ϵ 2400) (MeOH).

N^8*-Me:* ***Suberedamine B***
$C_{24}H_{32}Br_3N_3O_3$ 650.247
Isol. from a *Suberea* sp. Cytotoxic. Amorph. solid.
Mp 79-81°. $[\alpha]_D^{25}$ +16 (c, 1 in MeOH). λ_{max} 281 (ϵ 2900) (MeOH).

Tsuda, M. *et al., J. Nat. Prod.*, 2001, **64**, 980-982

Suberiphenol S-526

[676271-83-3]

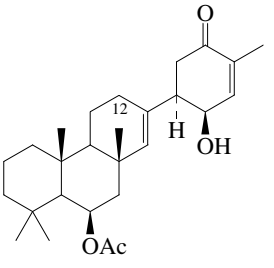


$C_{27}H_{38}O_3$ 410.595
Constit. of a *Suberites* sp. Amorph. solid.
Mp 93-94°. $[\alpha]_D^{25}$ -9.3 (c, 0.02 in MeOH). λ_{max} 214 (log ϵ 4.14); 251 (log ϵ 3.91); 291 (log ϵ 3.32) (MeOH).

Lee, H.S. *et al., J. Nat. Prod.*, 2004, **67**, 672-674 (*isol, pmr, cmr*)

Suberitenone A S-527

[169340-00-5]



Absolute Configuration

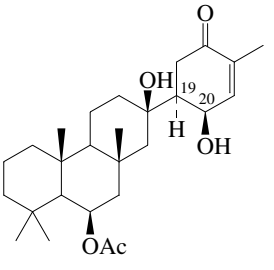
$C_{27}H_{40}O_4$ 428.611
Constit. of a *Suberites* sp. Inhibitor of cholesteryl ester transfer protein activity. Gum. $[\alpha]_D$ -152.8 (c, 0.5 in $CHCl_3$).

Δ^{12}*-Isomer:* ***Suberitenone C***
[676271-85-5]
$C_{27}H_{40}O_4$ 428.611
Constit. of a *Suberites* sp. Amorph. solid.
Mp 89-92°. $[\alpha]_D^{25}$ -18 (c, 0.02 in MeOH). λ_{max} 229 (log ϵ 4.15) (MeOH).

Shin, J. *et al., J.O.C.*, 1995, **60**, 7582-7588 (*Suberitenone A*)
Lee, H.-S. *et al., J. Nat. Prod.*, 2004, **67**, 672-674 (*Suberitenone C*)

Suberitenone B S-528

[169340-01-6]



Absolute Configuration

$C_{27}H_{42}O_5$ 446.626

Constit. of a *Suberites* sp. Inhibitor of cholesteryl ester transfer protein activity. Cryst.
Mp 232-234°. $[\alpha]_D$ -15.9 (c, 0.7 in $CHCl_3$). λ_{max} 226 (ϵ 14000) (MeOH) (Berdy).

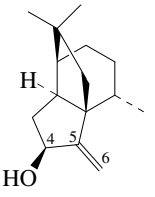
20-Ac: ***Suberitenone D***
[676271-84-4]
$C_{29}H_{44}O_6$ 488.663
Constit. of a *Suberites* sp. Amorph. solid.
Mp 102-104°. $[\alpha]_D^{25}$ -67.5 (c, 0.05 in MeOH). λ_{max} 227 (log ϵ 3.99) (MeOH).

19-Epimer, 20-deoxy: ***19-Episuberitenone***
[720681-63-0]
$C_{27}H_{42}O_4$ 430.626
Constit. of *Suberites caminatus*. Oil. $[\alpha]_D^{25}$ +100 (c, 0.13 in $CHCl_3$).

Shin, J. *et al., J.O.C.*, 1995, **60**, 7582-7588 (*Suberitenone B*)
Lee, H.S. *et al., J. Nat. Prod.*, 2004, **67**, 672-674 (*Suberitenone D*)
Díaz-Marrero, A.R. *et al., Tet. Lett.*, 2004, **45**, 4707-4710 (*19-Episuberitenone*)

Suberosenol A S-529

[313242-60-3]



$C_{15}H_{24}O$ 220.354
Constit. of *Isis hippuris*. Powder.
Mp 106-108°. $[\alpha]_D^{25}$ -232 (c, 0.1 in $CHCl_3$).

Ac: Suberosenol A acetate
[313242-63-6]
$C_{17}H_{26}O_2$ 262.391
Constit. of *Isis hippuris*. Oil. $[\alpha]_D^{25}$ -110 (c, 0.1 in $CHCl_3$).

4-Ketone: ***Suberosenone***
[176714-39-9]
$C_{15}H_{22}O$ 218.338
Constit. of *Subergorgia suberosa*. Oil. $[\alpha]_D$ +55.7 (c, 0.78 in $CHCl_3$). λ_{max} 233 (ϵ 11100) (MeOH). λ_{max} 233 (ϵ 11100) (MeOH) (Berdy).

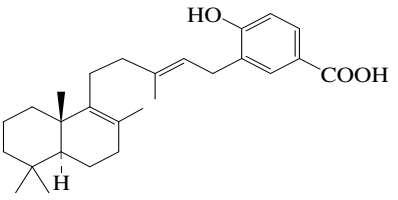
4-Ketone, 5α,6-dihydro: ***Suberosanone***
[313242-62-5]
$C_{15}H_{24}O$ 220.354
Constit. of *Isis hippuris*.

4-Epimer: ***Suberosenol B***
[313242-61-4]
$C_{15}H_{24}O$ 220.354
Constit. of *Isis hippuris*. Powder.
Mp 74-75°. $[\alpha]_D^{25}$ -10 (c, 0.1 in $CHCl_3$).

4-Epimer, Ac: Suberosenol B acetate
[313242-64-7]
$C_{17}H_{26}O_2$ 262.391
Constit. of *Isis hippuris*. Oil. $[\alpha]_D^{25}$ -8 (c, 0.03 in $CHCl_3$).

Bokesch, H.R. *et al., Tet. Lett.*, 1996, **37**, 3259 (*Suberosenone, isol, pmr, cmr*)
Sheu, J.-H. *et al., J. Nat. Prod.*, 2000, **63**, 1603-1607 (*Isis hippuris constits*)
Lee, H.-Y. *et al., Org. Lett.*, 2000, **2**, 1951-1953 (*synth*)
Stephens, P.J. *et al., J. Nat. Prod.*, 2006, **69**, 1055-1064 (*abs config*)

Subersic acid S-530



(+)-*form*

$C_{27}H_{38}O_3$ 410.595

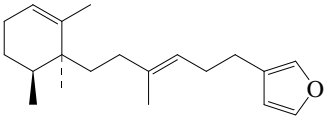
(+)-form [672922-56-4]
Constit. of an *Acanthodendrilla* sp.
Oil. $[\alpha]_D^{25}$ +39.3 (c, 3.26 in MeOH).

(-)-form [374819-08-6]
Constit. of *Jaspis splendens*.
Yellow oil. $[\alpha]_D$ -46 (c, 0.5 in $CHCl_3$).

Carroll, J. *et al., J.O.C.*, 2001, **66**, 6847-6851 (*(-)-form, isol, pmr, cmr*)
Tanada, Y. *et al., Eur. J. Org. Chem.*, 2003, 848-854 (*synth, abs config*)
Basabe, P. *et al., Tetrahedron*, 2003, **59**, 9173-9177 (*synth*)
Williams, D.E. *et al., J. Nat. Prod.*, 2004, **67**, 2127-2129 (*(+)-form*)

Subersin S-531

[375378-29-3]



$C_{20}H_{30}O$ 286.456
Constit. of *Jaspis splendens*. Yellow oil. $[\alpha]_D$ +30 (c, 2.6 in $CHCl_3$).

Carroll, J. *et al., J.O.C.*, 2001, **66**, 6847-6851 (*isol, pmr, cmr*)

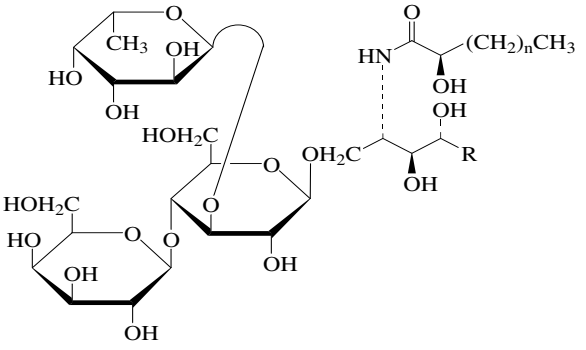
Neoceratodus forsteri Substance P S-532

Lungfish substance P
H-Lys-Pro-Arg-Pro-Asp-Glu-Phe-Tyr-Gly-Leu-Met-NH_2
$C_{62}H_{94}N_{16}O_{16}S$ 1351.588
Isol. from the spiral intestine of the Australian lungfish *Neoceratodus forsteri*.

Liu, L. *et al., Gen. Comp. Endocrinol.*, 2002, **125**, 104-112 (*isol, struct*)

Sulcaceramide S-533

[433228-20-7]



n = 19, 20 or 21
R = $C_{12}H_{25}$, $C_{13}H_{27}$, $C_{14}H_{29}$, $C_{15}H_{31}$

Triglycosylceramide complex. Isol. from the marine ascidian *Microcosmus sulcatus*. Oil. $[\alpha]_D^{25}$ -36 (c, 0.003 in $CHCl_3$). Obt. as a mixt. of homologues.

Aiello, A. *et al., Eur. J. Org. Chem.*, 2002, 1047-1050 (*isol, pmr, cmr, ms*)

Penaeus monodon Sulfakinins S-534

5-OxoPro-Phe-Asp-Glu-Tyr(SO_3H)-Gly-His-Met-Arg-Phe-NH_2
Struct. of Pem-SK-I shown. Isol. from the tiger prawn *Penaeus monodon*. Neuropeptides.

Pem-SK-I [264906-57-2]
$C_{60}H_{78}N_{16}O_{19}S_2$ 1391.504
X = *O*-sulfotyrosine.

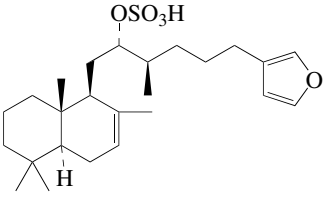
Pem-SK-II [264906-58-3]
$C_{83}H_{117}N_{25}O_{31}S$ 1993.052
X = *O*-sulfotyrosine.

Pem-SK-III [264906-59-4]
$C_{69}H_{95}N_{19}O_{24}S$ 1606.688
X = *O*-sulfotyrosine.

Johnsen, A.H. *et al., Eur. J. Biochem.*, 2000, **267**, 1153-1160 (*isol, struct*)

Sulfircin S-535

[120927-18-6]



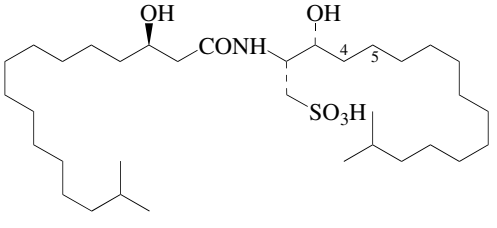
$C_{25}H_{40}O_5S$ 452.654
Isol. from the sponge *Ircinia* sp. CCR7 receptor binding inhibitor. Needles (CH_2Cl_2/MeOH) (as dimethylguanidinium salt).
Mp 199-200°. $[\alpha]_D^{20}$ +5 (c, 0.006 in MeOH). λ_{max} 208 (ϵ 1024) (EtOH).

$\Delta^{8,9}$-Isomer: ***Antibiotic Sch 599473***. *Sch 599473*
$C_{25}H_{40}O_5S$ 452.654
Isol. from an *Ircinia* sp. Stereochem. not fully confirmed.

Wright, A.E. *et al., J.O.C.*, 1989, **54**, 3472-3474 (*isol, uv, ir, pmr, cmr, cryst struct*)
Yang, S.-W. *et al., J. Antibiot.*, 2003, **56**, 783-786 (*Sch 599473*)

Sulfobacin A S-536

Flavocristamide B
[169217-35-0]



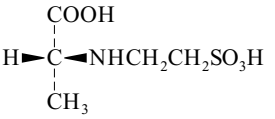
$C_{34}H_{69}NO_6S$ 619.988
Prod. by *Chryseobacterium* sp. NR 2993 and from a *Flavobacterium* sp. in the marine bivalve *Cristaria plicata*. Von Willebrand factor receptor antagonist. Powder. $[\alpha]_D^{24}$ -35 (c, 0.1 in MeOH).

*4,5-Didehydro(*E-*):* ***Flavocristamide A***
[169217-34-9]
$C_{34}H_{67}NO_6S$ 617.972
Prod. by a *Flavobacterium* sp. in the marine bivalve *Cristaria plicata*. DNA polymerase inhibitor. Amorph. solid. $[\alpha]_D^{20}$ -17 (c, 0.3 in MeOH).

Kamiyama, T. *et al., J. Antibiot.*, 1995, **48**, 924-928; 929-936 (*isol, ir, pmr, cmr*)
Kobayashi, J. *et al., Tetrahedron*, 1995, **51**, 10487-10490 (*isol, ir, pmr, cmr, ms*)
Irako, N. *et al., Tet. Lett.*, 1998, **39**, 5793-5796 (*synth*)
Takikawa, H. *et al., J.C.S. Perkin 1*, 1999, 2467-2477 (*synth*)
Shioiri, T. *et al., Tetrahedron*, 2000, **56**, 9129-9142 (*synth*)
Labeeuw, O. *et al., Tet. Lett.*, 2003, **44**, 6383-6386 (*synth*)
Gupta, P. *et al., Tet. Lett.*, 2004, **45**, 9641-9643 (*synth*)

N-(2-Sulfoethyl)alanine S-537

N-*(1-Carboxyethyl)taurine.* ***Rhodoic acid***. *Tauropine*



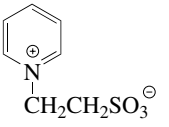
$C_5H_{11}NO_5S$ 197.212

(R)-form
D-form
[33497-79-9]
Isol. from various red algae incl. *Chondrus ocellatus* and *Rhodoglossum japonicum*. Also obt. from the muscles of abalone *Haliotis discus hannai* and *Haliotis lamellosa*.
Cryst.
Mp 258°. $[\alpha]_D^{13}$ -1.15 (c, 5 in 1*M* NaOH).

Kuriyama, M. *et al., Nature (London)*, 1961, **192**, 969 (*isol*)
Sato, M. *et al., Nippon Suisan Gakkaishi*, 1985, **51**, 1681; 1986, **52**, 1025; *CA*, **104**, 17840; **105**, 58213 (*isol, biosynth*)
Sato, M. *et al., Hydrobiologia*, 1987, **151-152**, 457; *CA*, **108**, 3459r (*occur*)

N-(2-Sulfoethyl)pyridinium betaine S-538

2-Pyridinioethanesulfonic acid. ***Pyridinebetaine B***
[24020-66-4]



$C_7H_9NO_3S$ 187.219
Isol. from the sponge *Agelas dispar*. Cryst. (EtOH).
Mp 260°. λ_{max} 222 (ϵ 6500); 260 (ϵ 4500) (MeOH).

Le Berre, A. *et al., Bull. Soc. Chim. Fr.*, 1970, 954 (*synth, pmr*)
King, J.F. *et al., Can. J. Chem.*, 1984, **62**, 1977-1995 (*synth*)
Cafieri, F. *et al., J. Nat. Prod.*, 1998, **61**, 1171-1173 (*isol, uv, ir, pmr, cmr*)

Litopenaeus vannamei Sulfokinins S-539

*Pev-SK*Isol. from the white shrimp *Litopenaeus vannamei*.
Myotropic neuropeptides.

Pev-SK 1
$C_{83}H_{117}N_{25}O_{34}$ 2008.984
Peptide with tyrosine sulfate residues at positions 11 and 14; position 17 is leucine or isoleucine.

Pev-SK 2
Peptide with a tyrosine sulfate residue at position 5.

Torfs, P. *et al., Biochem. Biophys. Res. Commun.*, 2002, **299**, 312-320 (*isol*)

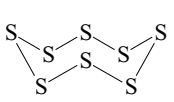
2,2′-Sulfonylbis(ethanol) dicarbamate, 9CI S-540

Bis(2-carbamoyloxyethyl) sulfone
[205448-99-3]
$H_2NCOOCH_2CH_2SO_2CH_2CH_2OOCNH_2$
$C_6H_{12}N_2O_6S$ 240.237
Isol. from the alga *Caloglossa leprieurii*.

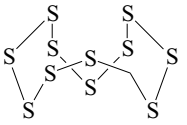
Xu, X.-H. *et al., CA*, 1998, **128**, 254981n (*isol*)

Sulfur, 11CI, ESA, ISO, JMAF S-541

Sulphur. Brimstone. Liquamat. Sastid
[7704-34-9]



Octasulfur
(crown conform)



Dodecasulfur

[S]

Atomic No. 16. Ground state electron config. [Ne]$3s^2 3p^4$. 10 Isotopes are known of which 4 are stable. ^{33}S is used in nmr spectroscopy. Known since Biblical times. Two of many oligomeric forms shown. Has a strong tendency to catenate. Allotropic. Widely distributed in lithosphere (0.048%). Major component of atmosphere of Venus. Occurs as elemental sulfur and vast range of metal sulfides and as atmospheric H_2S and SO_2. Manuf. from H_2S, pyrites and other sulfide minerals. Mined via Frasch Process. Commercially available. Used in manuf. of H_2SO_4, CS_2, sulfites, insecticides, fungicides, plastics; for vulcanisation of rubber, in gunpowder, in bleaches, pharmaceuticals. Component of Crystex. Scabicide and ectoparasiticide. Yellow solid. Insol. H_2O; sol. CS_2; sl. sol. other org. solvs. Various metastable forms of sulfur include e.g. Plastic sulfur, Catena sulfur , Lamina sulfur, Fibrous sulfur. These are mixts. of allotropes that revert to S_8 at r.t. Dissolves in oleum → coloured solns. contg. $S_4^{2\oplus}$, $S_8^{2\oplus}$ and $S_{16}^{2\oplus}$ ions. Pharmaceutical sulfur has ≥99.5% purity.

▶ Eye irritant, poison, fungicide; explosive as dust, combustible. On heating, burns to emit toxic fumes of sulfur oxides. WS4250000

Sulfur (S_8)

Cyclooctasulfur. Orthorhombic sulfur. α-Sulfur. ***Antibiotic MS 146****. MS 146*
[10544-50-0]

S_8 256.528

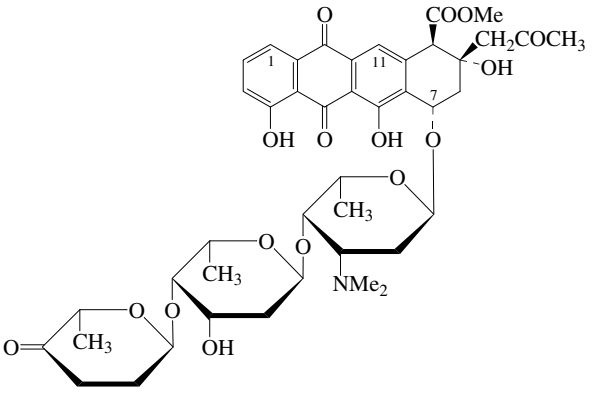
Struct. comprises non-planar rings in crown conformn., S–S 203.7 pm; angle SSS 107° 48′. Prod. by *Streptomyces verticillus-tsukushiensis* and the marine *Streptomyces* sp. strain GWS-BW-HS. Myosin light chain kinase inhibitor. Yellow cryst. solid, stable at r.t., yellow liq. On melting, forms v. mobile liq.; at *ca.* 159° viscosity rapidly increases to a max. at *ca.* 195°, then decreases as liq. becomes more mobile and dark red at the Bp. Sol. polar solvs., CS_2.
Mp 112.8° (α-S) Mp 119° (β-S) Mp 106.8° (γ-S). Bp 444.6°. Exists as α-form (orthorhombic, stable) and β-form (monoclinic, stable above 95.4°). γ-Sulfur (stable at *ca.* 95-115°) formed as pale yellow needles; reverts slowly to α-S.

[9035-99-8, 12185-15-8, 12597-04-5, 14127-58-3, 14127-59-4, 14280-16-1, 14337-03-2, 14700-95-9, 14701-12-3, 14841-24-8, 16734-12-6, 16884-99-4, 16885-00-0, 16885-01-1, 16999-01-2, 18496-25-8, 19709-28-5, 20681-10-1, 22537-26-4, 22541-72-6, 23778-11-2]

Mellor Compr. Treat. Inorg. Theor. Chem., 1930, **10**, 1
Gmelin Handbook Inorg. Chem., Syst. No. 9, 1942, **A1**, ; 1953, **A2, A3**, 1 (*rev, bibl*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 795 (*rev*)
Templeton, L.K. *et al., Inorg. Chem.*, 1976, **15**, 1994-2001 (*S_8, cryst struct*)
Steudel, R. *et al., Stud. Inorg. Chem.*, 1984, **5**, 3 (*rev*)
Sander, U.H.F. *et al., Sulfur, Sulfur Dioxide and Sulfuric Acid*, Verlag Chemie, Weinheim, 1984,
Greenwood, N.N. *et al., Chemistry of the Elements*, Pergamon, Oxford, 1986, 757 (*rev*)
Nakanishi, S. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1333-1335 (*MS 146*)
Emsley, J. *et al., The Elements*, 3rd edn., Clarendon Press, 1998, 198; 250
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 837-865 (*S_8, isol*)

Sulfurmycin A S-542

[78173-90-7]



$C_{43}H_{53}NO_{16}$ 839.889

Anthracycline antibiotic. Numbering systems vary. Isol. from *Streptomyces galilaeus* (OB111; ATCC31533; P4780). Active against gram-positive bacteria, mycobacteria and tumours. Yellow powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 140°. $[\alpha]_D^{20}$ -23.2 (c, 0.1 in $CHCl_3$). Strain also produces Sulfurmycin B, Auramycin A, A-745 and Auramycin B.

▶ LD_{50} (mus, ipr) 100 mg/kg. QI9290600

Aglycone: ***Sulfurmycinone***
[78173-88-3]
$C_{23}H_{20}O_9$ 440.406
From *Streptomyces galilaeus*. Yellow powder.
Mp 159°. $[\alpha]_D^{20}$ +232.2 (c, 0.1 in $CHCl_3$).

1-Hydroxy: ***1-Hydroxysulfurmycin A****. 10-Hydroxysulfurmycin A*
[79234-80-3]
$C_{43}H_{53}NO_{17}$ 855.888
Prod. by *Streptomyces galilaeus* (AC628) and *Streptomyces melanogenes* (AC180). Active against gram-positive bacteria and tumours. Sol. $CHCl_3$, MeOH; poorly sol. H_2O, hexane.
Mp 126°. $[\alpha]_D^{20}$ +57.88 (c, 0.1 in $CHCl_3$). λ_{max} 234 (E1%/1cm 570); 256 (E1%/1cm 345); 292 (E1%/1cm 115); 493 (E1%/1cm 175); 511 (E1%/1cm 165); 526 (ϵ 160); 570 (E1%/1cm 75) (MeOH) (Berdy). λ_{max} 241 (E1%/1cm 530); 292 (E1%/1cm 170); 565 (E1%/1cm 230); 602 (E1%/1cm 180) (MeOH/NaOH) (Berdy).

1-Hydroxy, aglycone: 1-Hydroxysulfurmycinone. 10-Hydroxysulfurmycinone
[79206-71-6]
Mp 169.5°.

11-Hydroxy, aglycone: ***11-Hydroxysulfurmycinone***
[95663-90-4]
$C_{23}H_{20}O_{10}$ 456.405
Prod. by *Streptomyces* sp. (MST-77755). Red solid. $[\alpha]_D^{20}$ +545 (c, 0.008 in $CHCl_3$). λ_{max} 234 (ϵ 37000); 253 (ϵ 22000); 291 (ϵ 7600); 492 (ϵ 11400); 526 (ϵ 7700); 579 (ϵ 1000) (MeOH).

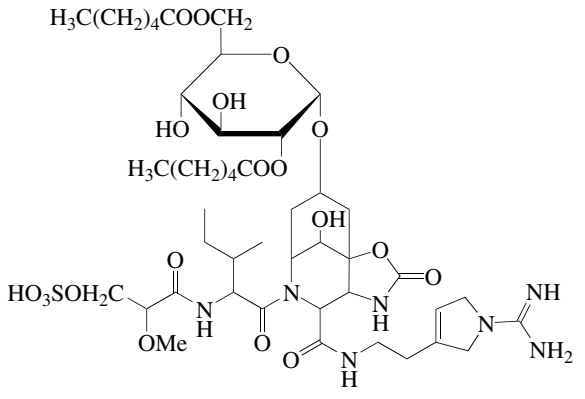
7-Deoxy, aglycone: ***7-Deoxysulfurmycinone****. 4-Deoxysulfurmycinone, 9CI*
[78173-94-1]
$C_{23}H_{20}O_8$ 424.406
Prod. by *Streptomyces galilaeus*.
Mp 219.5°. $[\alpha]_D^{20}$ +73.9 ($CHCl_3$).

9-Epimer, 1-hydroxy, 4′-O-deglycosyl: ***1-Hydroxysulfurmycin T***
$C_{31}H_{35}NO_{12}$ 613.617
Prod. by marine-derived *Streptomyces* sp. (CANU Fox 21-2-6a). Cytotoxic. Deep red solid. λ_{max} 202; 234; 258; 290; 492 (MeOH).

Fujiwara, A. *et al., J. Antibiot.*, 1981, **34**, 912-915; 1982, **35**, 164-175 (*isol, ir, pmr, cmr*)
Hoshino, T. *et al., J. Antibiot.*, 1984, **37**, 1469-1472 (*derivs*)
Phipps, R.K. *et al., ARKIVOC*, 2004, **x**, 94-100 (*1-Hydroxysulfurmycin T*)
Clark, B. *et al., J. Nat. Prod.*, 2004, **67**, 1729-1731 (*11-Hydroxysulfurmycinone*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SON520

Suomilide S-543

[195256-59-8]



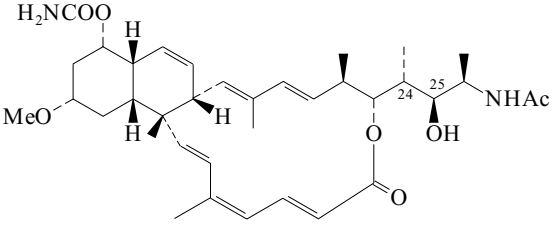
$C_{45}H_{73}N_7O_{19}S$ 1048.173

Isol. from the marine cyanobacterium *Nodularia spumigena* HKUV. Enzyme inhibitor. Amorph. powder. $[\alpha]_D^{26}$ +74.2 (c, 0.1 in MeOH).

Sivonen, K. *et al., Hydrobiologia*, 1989, **185**, 3-8 (*isol*)
Fujii, K. *et al., Tet. Lett.*, 1997, **38**, 5529-5532 (*isol, pmr, cmr, ms*)

Superstolide A S-544

[156368-64-8]



$C_{36}H_{52}N_2O_7$ 624.816

Macrolide antibiotic. Isol. from the marine sponge *Neosiphonia superstes*. Cytotoxic. Amorph. solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ +54.1 (MeOH). λ_{max} 239 (ϵ 16600); 303 (ϵ 4450) (MeOH).

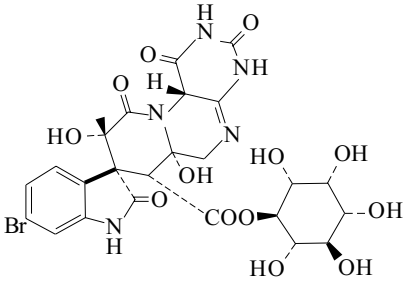
*25-Deoxy, 24,25-didehydro (*E-*):* ***Superstolide B***
[161300-74-9]
$C_{36}H_{50}N_2O_6$ 606.801

Isol. from *Neosiphonia superstes*. Cytotoxic. Amorph. solid. $[\alpha]_D$ +47 (MeOH). λ_{max} 236 (ϵ 15360); 303 (ϵ 5000) (MeOH).

D'Auria, M.V. *et al., J. Nat. Prod.*, 1994, **57**, 1595-1597 (*Superstolide B*)
D'Auria, M.V. *et al., J.A.C.S.*, 1994, **116**, 6658-6663 (*isol, pmr, cmr*)

Surugatoxin S-545

[40957-92-4]



$C_{25}H_{26}BrN_5O_{13}$ 684.41

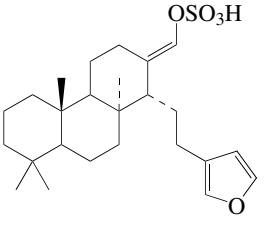
Unique skeleton containing both indole and pteridine subunits. Toxin from the mid-gut gland of the Japanese Ivory shell *Babylonia japonica* (harvested from a particular area only). Prod. from cyanobacteria. Marine toxin, causing shellfish poisoning. Prisms + $7H_2O$.
Mp 300°. Artifact formed during isol. λ_{max} 276 (ϵ 15000) (0.1*N* HCl) (Derep). λ_{max} 279 (ϵ 19000) (0.1*N* NaOH) (Derep). λ_{max} 276 (ϵ 15000) (H_2O) (Derep).

▶ Toxic.

Kosuge, T. *et al., Tet. Lett.*, 1972, 2545-2548 (*isol, uv, ir, cryst struct*)
Inoue, S. *et al., Tet. Lett.*, 1984, **25**, 4407 (*synth*)
Okado, K. *et al., Yakugaku Zasshi*, 1985, **105**, 375; 381 (*synth*)
Inoue, S. *et al., Tetrahedron*, 1994, **50**, 2729 (*synth*)

Suvanine S-546

[94203-53-9]
[202072-67-1]



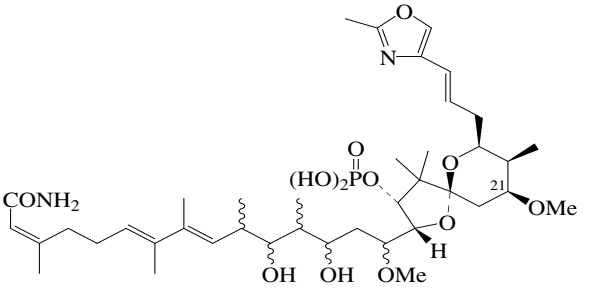
$C_{25}H_{38}O_5S$ 450.638

Constit. of sponges of the genera *Coscinoderma* and *Hippospongia*. Powder (as *N,N*-dimethylguanidine salt).
Mp 224° (dimethylguanidine salt). $[\alpha]_D$ +9.5 (MeOH). Also isol. as the trimethylguanidinium salt. λ_{max} 210 (ϵ 6300) (MeOH) (Derep).

Manes, L.V. *et al., J.O.C.*, 1985, **50**, 284; 1988, **53**, 570 (*struct*)
Kimura, J. *et al., J. Nat. Prod.*, 1998, **61**, 248-250; 862 (*isol*)

Swinhoeiamide A S-547

[209408-31-1]



$C_{40}H_{65}N_2O_{12}P$ 796.934

Related to Calyculin A, C-70 and Clavosine A, C-690. Isol. from the sponge *Theonella swinhoei*. Insecticide and antifungal agent. Cell proliferation inhibitor. Powder. $[\alpha]_D^{20}$ -21.6 (c, 0.35 in EtOH). λ_{max} 223 (MeOH).

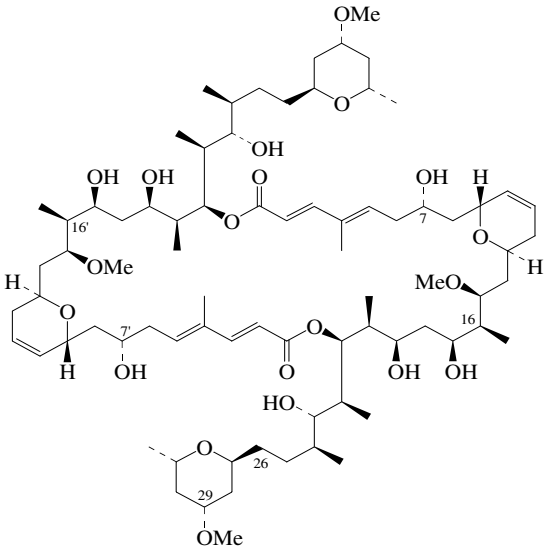
O^{21}*-De-Me:* ***Geometricin A***
[443769-46-8]
$C_{39}H_{63}N_2O_{12}P$ 782.907

Isol. from the sponge *Luffariella geometrica*. Cytotoxic. Amorph. solid. $[\alpha]_D^{23}$ -36.3 (c, 0.29 in MeOH). λ_{max} 206 (ϵ 16280); 221 (ϵ 16370) (MeOH).

Kehraus, S. *et al., J. Nat. Prod.*, 2002, **65**, 1056-1058 (*Geometricin A*)
Edrada, R.A. *et al., J. Nat. Prod.*, 2002, **65**, 1168-1172 (*Swinhoeiamide A*)

Swinholide A S-548

[95927-67-6]



$C_{78}H_{132}O_{20}$ 1389.889
Constit. of sponge *Theonella swinhoei*. Antifungal agent. Cytotoxic. Actin depolymeriser. Microcryst. + H_2O (EtOAc). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 102°. $[\alpha]_D$ +16 ($CHCl_3$). λ_{max} 270 (ϵ 41400) (MeOH).

7,7′-Di-Me ether: ***Swinholide H***
[188292-67-3]
$C_{80}H_{136}O_{20}$ 1417.942
Constit. of the sponge *Lamellomorpha strongylata*. Solid.
Mp 90-91°. $[\alpha]_D^{20}$ -82 (c, 0.16 in EtOH). λ_{max} 270 (ϵ 51000) (EtOH).

*29-*O*-De-Me:* ***Swinholide C***
[132923-51-4]
$C_{77}H_{130}O_{20}$ 1375.862
Constit. of *Theonella* sp. Antitumour agent. Amorph. powder + $2H_2O$. $[\alpha]_D^{24}$ +5.4 (c, 5.4 in $CHCl_3$). λ_{max} 270 (ϵ 41400) (MeOH). λ_{max} 268 (ϵ 42600) (MeOH) (Berdy).

26ξ-Hydroxy: ***Swinholide I***
$C_{78}H_{132}O_{21}$ 1405.888
Constit. of *Theonella swinhoei*. Cytotoxic. Light yellow solid. $[\alpha]_D^{25}$ -42.5 (c, 0.04 in MeOH). λ_{max} 274 (log ϵ 4.58) (MeOH).

16-Demethyl: ***Swinholide B***
[132943-68-1]
$C_{77}H_{130}O_{20}$ 1375.862
Constit. of *Theonella* sp. Antitumour agent. Amorph. powder + $1H_2O$. $[\alpha]_D^{22}$ +2.5 (c, 6.1 in $CHCl_3$). λ_{max} 270 (ϵ 41400) (MeOH).

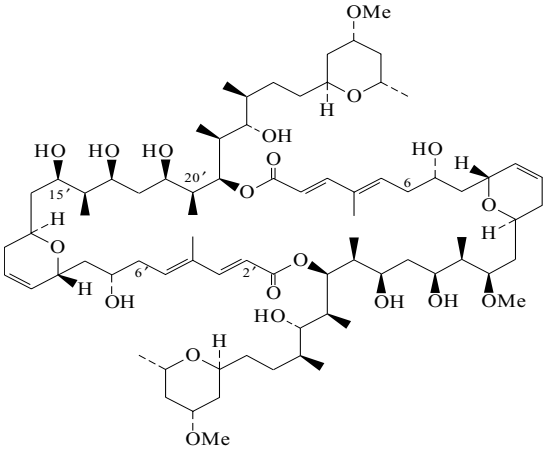
*16-Demethyl, 7,7′-bis-*O*-(2,3-di-*O*-methyl-β-L-lyxopyranoside):* ***Ankaraholide B***
$C_{91}H_{154}O_{28}$ 1696.201
Isol. from *Geitlerinema* sp. Cytotoxic. Yellowish oil. $[\alpha]_D^{25}$ -37 (c, 0.07 in $CHCl_3$). λ_{max} 266 (ϵ 57000) ($CHCl_3$).

*16,16′-Didemethyl, 7,7′-bis-*O*-(2,3-di-*O*-methyl-β-L-lyxopyranoside):* ***Ankaraholide A***
$C_{90}H_{152}O_{28}$ 1682.174
Isol. from the cyanobacterium *Geitlerinema* sp. Cytotoxic. Yellowish oil. $[\alpha]_D^{25}$ -47 (c, 0.12 in $CHCl_3$). λ_{max} 268 (ϵ 57000) ($CHCl_3$).

Carmely, S. *et al., Tet. Lett.*, 1985, **26**, 511 (*isol*)
Carmely, S. *et al., Magn. Reson. Chem.*, 1986, **24**, 343-349 (*pmr, cmr*)
Kobayashi, M. *et al., Tet. Lett.*, 1989, **30**, 2963-2966 (*struct*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2960 (*derivs*)
Kitagawa, I. *et al., J.A.C.S.*, 1990, **112**, 3710 (*stereochem*)
Doi, M. *et al., J.O.C.*, 1991, **56**, 3629 (*abs config, cryst struct*)
Paterson, I. *et al., J.A.C.S.*, 1994, **116**, 9391 (*synth*)
Norcross, R.D. *et al., Chem. Rev.*, 1995, **95**, 2041 (*rev, synth*)
Paterson, I. *et al., Tetrahedron*, 1995, **51**, 9393; 9413; 9437; 9467 (*synth*)
Nicolaou, K.C. *et al., J.A.C.S.*, 1996, **118**, 3059 (*synth*)
Dumdei, E.J. *et al., J.O.C.*, 1997, **62**, 2636 (*Swinholide H*)
Andrianasolo, E.H. *et al., Org. Lett.*, 2005, **7**, 1375-1378 (*Ankaraholides*)
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2006, **69**, 154-157 (*Swinholide I*)

Swinholide D S-549

[139178-92-0]



$C_{77}H_{130}O_{20}$ 1375.862
Constit. of the sponge *Theonella* sp. Amorph. Sol. MeOH, EtOAc. $[\alpha]_D^{19}$ +48 (c, 0.05 in MeOH). λ_{max} 268 (ϵ 50000) (EtOH) (Berdy).

6′-Hydroxy, 15′-Me ether: ***Swinholide E***
[139178-93-1]
$C_{78}H_{132}O_{21}$ 1405.888
Constit. of a *Theonella* sp. Amorph. Sol. MeOH, EtOAc. $[\alpha]_D^{19}$ -43 (c, 0.13 in MeOH). λ_{max} 267 (ϵ 40000) (EtOH) (Berdy).

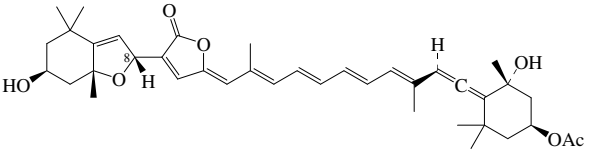
2Z-Isomer, 15′-Me ether: ***Swinholide F***
[139159-67-4]
$C_{78}H_{132}O_{20}$ 1389.889
Constit. of a *Theonella* sp. Amorph. Sol. MeOH, EtOAc. $[\alpha]_D^{19}$ +93 (c, 0.03 in MeOH). λ_{max} 268 (ϵ 50000) (EtOH) (Berdy).

20′-Demethyl, 15′-Me ether: ***Swinholide G***
[139178-94-2]
$C_{77}H_{130}O_{20}$ 1375.862
Constit. of a *Theonella* sp. Amorph. Sol. MeOH, EtOAc. $[\alpha]_D^{19}$ +30 (c, 0.08 in MeOH). λ_{max} 269 (ϵ 50000) (EtOH) (Berdy).

Tsukamoto, S. *et al., J.C.S. Perkin 1*, 1991, 3185-3188 (*isol, pmr, struct*)
Norcross, R.D. *et al., Chem. Rev.*, 1995, **95**, 2041-2114 (*rev, synth*)

Symbiodinium apocarotenoid 1 S-550

[161023-21-8]

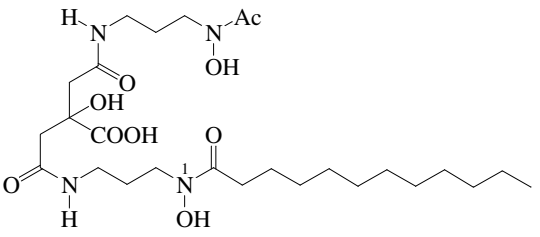


$C_{39}H_{50}O_7$ 630.82
Constit. of the dinoflagellate *Symbiodinium* sp. Red oil. $[\alpha]_D^{25}$ +63.6 (c, 0.07 in $CHCl_3$). Related to, 3-Ac. λ_{max} 449 (ϵ 57800) (MeOH).

8-Epimer: ***Symbiodinium apocarotenoid 2***
[161023-24-1]
$C_{39}H_{50}O_7$ 630.82
Constit. of a *Symbiodinium* sp. Red oil. $[\alpha]_D^{25}$ -69.2 (c, 0.04 in $CHCl_3$). λ_{max} 449 (ϵ 55800) (MeOH).

Suzuki, M. *et al., Chem. Pharm. Bull.*, 2003, **51**, 724-727 (*isol, pmr, cmr*)

Symbioimine S-551



$C_{19}H_{23}NO_5S$ 377.46

Alkaloid from the marine dinoflagellate *Symbiodinium* sp.; also from *Amphiscolops* sp. Inhibitor of cyclooxygenase-2 and osteoclast differentiation. Cryst. $+1H_2O$ (H_2O).

Mp 214-215° dec. $[\alpha]_D^{27}$ +245 (c, 0.1 in DMSO).

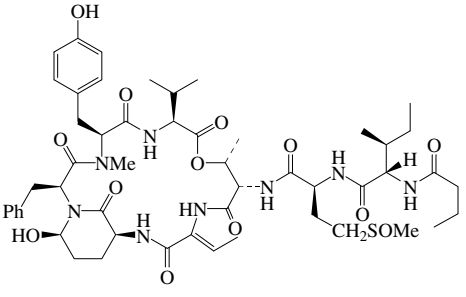
Kita, M. *et al., J.A.C.S.*, 2004, **126**, 4794-4795 (*isol*)

Kita, M. *et al., Bioorg. Med. Chem.*, 2005, **13**, 5253-5258 (*isol, pmr, cmr, activity*)

Varseev, G.N. *et al., Angew. Chem., Int. Ed.*, 2006, **45**, 4767-4771 (*synth*)

Zou, Y. *et al., Org. Lett.*, 2006, **8**, 5605-5608 (*synth*)

Symplostatin 2 S-552



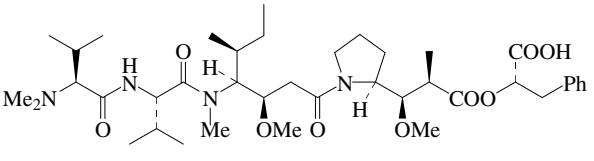
Absolute Configuration

$C_{52}H_{74}N_8O_{13}S$ 1051.268

Depsipeptide antibiotic. Similar to Dolastatin 13, D-1207. Isol. from the marine cyanobacterium *Symploca hydnoides*. Glassy oil. $[\alpha]_D$ -18 (c, 1.2 in MeOH).

Harrigan, G.G. *et al., J. Nat. Prod.*, 1999, **62**, 655-658 (*isol, ir, pmr, cmr*)

Symplostatin 3 S-553



$C_{40}H_{66}N_4O_9$ 746.983

Peptide antibiotic. Similar to Isodolastatin H, I-170. Isol. from the cyanobacteria *Symploca* sp. VP452. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{24}$ -46 (c, 0.35 in MeOH). λ_{max} 203 (log ϵ 4.36) (MeOH).

Luesch, H. *et al., J. Nat. Prod.*, 2002, **65**, 16-20

Synaptoside S2 S-554

Struct. unknown. Isol. from *Synapta maculata*.

Mp 183°. $[\alpha]_D^{20}$ -11.7 (c, 0.28 in Py). Glycoside which gives 3-Hydroxyholost-9(11)-en-23-one, H-684 on hydrol.

Kuznetsova, J.A. *et al., Khim. Prir. Soedin.*, 1985, **21**, 667; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 626

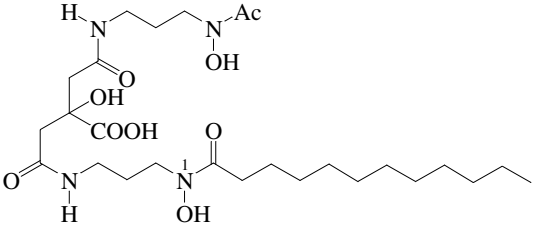
Synaptoside S3 S-555

Struct. unknown. Isol. from *Synapta maculata*.

Mp 201°. $[\alpha]_D^{20}$ -24.4 (c, 0.635 in MeOH aq.). Glycoside which gives 3-Hydroxyholost-9(11)-en-23-one, H-684 on hydrol.

Kuznetsova, J.A. *et al., Khim. Prir. Soedin.*, 1985, **21**, 667; *Chem. Nat. Compd. (Engl. Transl.)*, 626

Synechobactin A S-556



$C_{26}H_{48}N_4O_9$ 560.687

Isol. from the marine cyanobacterium *Synechococcus* sp. PCC 7002. Siderophore. Related to Schizokinen.

N^1-*Deacyl,* N^1-*octanoyl:* ***Synechobactin C***

$C_{22}H_{40}N_4O_9$ 504.579

Isol. from *Synechococcus* sp. PCC 7002.

N^1-*Deacyl,* N^1-*decanoyl:* ***Synechobactin B***

$C_{24}H_{44}N_4O_9$ 532.633

Isol. from *Synechococcus* sp. PCC 7002.

Ito, Y. *et al., Limnol. Oceanogr.*, 2005, **50**, 1918-1923 (*isol, struct*)

Tachycitin T-1

[188793-83-1]
[188737-23-7]

Granular peptide containing 73 amino acid residues and 5 disulfide bonds. Isol. from haemocytes of horseshoe crab *Tachypleus tridentatus*. Shows antimicrobial activity.

Kawabata, S. *et al., J. Biochem. (Tokyo)*, 1996, **120**, 1253-1260 (*isol*)

Petromyzon marinus Tachykinin T-2

[154563-90-3]

H-Arg-Lys-Pro-His-Pro-Lys-Glu-Phe-Val-Gly-Leu-Met-NH_2

$C_{66}H_{108}N_{20}O_{14}S$ 1437.771

Isol. from the brain of the sea lamprey of *Petromyzon marinus* and from the intestine of the river lamprey *Lampetra fluviatilis*. Shows neurokinin A-like immunoreactivity.

Waugh, D. *et al., Peptides (Pergamon)*, 1994, **15**, 155-161; 1995, **16**, 615-621 (*isol*)

Raja rhina Tachykinin 1 T-3

Raja rhina *Substance P*

[154563-88-9]

H-Ala-Lys-His-Asp-Lys-Phe-Tyr-Gly-Leu-Met-NH_2

$C_{56}H_{85}N_{15}O_{13}S$ 1208.446

Isol. from the brain of *Raja rhina*. Shows substance P-like immunoreactivity.

Waugh, D. *et al., Peptides (Pergamon)*, 1994, **15**, 155-161 (*isol*)

Raja rhina Tachykinin 2 T-4

Raja rhina *Neurokinin A*

[154563-89-0]

H-His-Lys-Leu-Gly-Ser-Phe-Val-Gly-Leu-Met-NH_2

$C_{50}H_{82}N_{14}O_{11}S$ 1087.351

Isol. from the brain of *Raja rhina*. Shows neurokinin A-like immunoreactivity.

Waugh, D. *et al., Peptides (Pergamon)*, 1994, **15**, 155-161 (*isol*)

Cancer borealis Tachykinin-related peptides T-5

CabTRP

H-Ala-Pro-Ser-Gly-Phe-Leu-Gly-Met-Arg-NH_2

Struct. of Cab-TRP-1a shown. Isol. from the nervous system of the crab *Cancer borealis*. Myotropic.

Cab-TRP-1a

Pev-tachykinin. Decapod tachykinin-related peptide. Decapod TRP

[197713-54-5]

Also isol. from brain of the white shrimp *Penaeus vannamei*, the crayfish *Procambarus clarkii* and the lobster*Panulirus interruptus*.

Cab-TRP-1b [197713-56-7]

Christie, A.E. *et al., J. Exp. Biol.*, 1997, **200**, 2279-2294 (*isol, Cancer constit*)
Nieto, J. *et al., Biochem. Biophys. Res. Commun.*, 1998, **248**, 406-411 (*isol, Penaeus constit*)
Yasuda-Kamatani, Y. *et al., Eur. J. Biochem.*, 2004, **271**, 1546-1556 (*Decapod TRP*)

Octopus Tachykinins T-6

Lys-Pro-Pro-Ser-Ser-Ser-Glu-Phe-Ile-Gly-Leu-Met-NH_2

Struct. of Oct-Tk-1 shown. Isol. from the posterior salivary glands of the common octopus *Octopus vulgaris*.

Oct-Tk-I [590346-74-0]

$C_{58}H_{94}N_{14}O_{17}S$ 1291.53

Oct-Tk-II [590346-75-1]

$C_{57}H_{92}N_{14}O_{17}S$ 1277.503

Kanda, A. *et al., Peptides (N.Y.)*, 2003, **24**, 35-43 (*isol*)

Tachylectins T-7

Isol. from the haemocytes of haemolymph plasma of the Japanese horseshoe crab *Tachypleus tridentatus*. Lectins.

Tachylectin 1

Protein containing 221 amino acid residues with no *N*-linked sugar and composed of 6 tandem repeats. There are 3 intrachain and 1 interchain disulfide bonds.

Tachylectin 2

Protein containing 236 amino acid residues with no cysteine and no *N*-linked sugar.

Tachylectin 3

Protein containing 123 amino acid residues with no *N*-linked sugar and 3 intramol. disulfide bonds.

Tachylectin 4

Glycoprotein containing 232 amino acid residues.

Tachylectin 5

Two homologous glycoproteins, Tachylectin 5A (269 amino acid residues, incl. 6 cysteines) and Tachylectin 5B (289 amino acid residues incl. 7 cysteines).

Saito, T. *et al., J. Biol. Chem.*, 1995, **270**, 14493-14499 (*Tachylectin 1*)
Okino, N. *et al., J. Biol. Chem.*, 1995, **270**, 31008-31015 (*Tachylectin 2*)
Saito, T. *et al., J. Biol. Chem.*, 1997, **272**, 30703-30708 (*Tachylectin 4*)
Kawabata, S. *et al., Dev. Comp. Immunol.*, 1999, **23**, 391-400 (*rev*)
Beisel, H.G. *et al., EMBO J.*, 1999, **18**, 2313-2322 (*Tachylectin 2, cryst struct*)
Inamori, K. *et al., J. Biol. Chem.*, 1999, **276**, 3272-3278 (*Tachylectin 3*)
Godukan, S. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1999, **96**, 10086-10091 (*Tachylectin 5*)
Kairies, N. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2001, **98**, 13519-13524 (*Tachylectin 5A, cryst struct*)

Tachyplesin T-8

Gigasin

[148045-87-8]

H-Lys-Trp-Cys-Phe-Arg-Val-Cys-Tyr-Arg-Gly-Ile-Cys-Tyr-Arg-Arg-Cys-Arg-NH_2

Peptide complex. Struct. of Tachyplesin I (reduced form) shown. Oxidised form contains ^{3}Cys-^{16}Cys and ^{7}Cys-^{12}Cys disulfide bonds. Isol. from haematocytes of crabs *Tachypleus tridentatus*, *Tachypleus gigas* and *Carcinoscorpius* sp. Shows antimicrobial props. λ_{max} 220 (ϵ 20000); 280 (ϵ 8000); 289 (ϵ 6000) (MeOH) (Derep).

Tachyplesin I [118231-04-2]

[118231-03-1, 121317-18-8]

$C_{99}H_{151}N_{35}O_{19}S_4$ 2263.769

Tachyplesin II

1-L-Arginine-15-L-lysinetachyplesin I

[125139-69-7]
[125139-72-2]

$C_{95}H_{151}N_{35}O_{19}S_4$ 2215.725

Tachyplesin III

15-L-Lysinetachyplesin I

[135200-93-0]

$C_{99}H_{151}N_{33}O_{19}S_4$ 2235.756

Nakamura, T. *et al., J. Biol. Chem.*, 1988, **263**, 16709-16713 (*isol, Tachyplesin I*)
Akaji, K. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2661-2664 (*synth*)
Miyata, T. *et al., J. Biochem. (Tokyo)*, 1989, **106**, 663-668 (*isol, Tachyplesin II*)
Muta, T. *et al., J. Biochem. (Tokyo)*, 1990, **108**, 261-266 (*isol, Tachyplesin III*)
Tamamura, H. *et al., Chem. Pharm. Bull.*, 1993, **41**, 978-980 (*cd, conformn, props*)
Laederach, A. *et al., Biochemistry*, 2002, **41**, 12359-12368 (*soln struct*)

Tachystatins T-9

[189582-26-1]

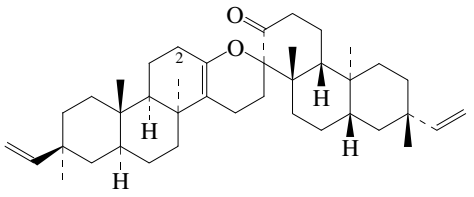
Three peptides, Tachystatins A (44 residues), B (42 residues) and C (41 residues), with 3 disulfide bonds. Isol. from haemocytes of the horseshoe crab *Tachypleus tridentatus*. Show antimicrobial activity.

[249602-53-7, 251312-20-6, 251312-24-0, 251312-27-3, 251312-88-6]

Osaki, T. *et al., J. Biol. Chem.*, 1999, **274**, 26172-26178 (*isol*)
Fujitani, N. *et al., J. Biol. Chem.*, 2002, **277**, 23651-23657 (*soln struct*)

Tagalsin I T-10

[861648-67-1]



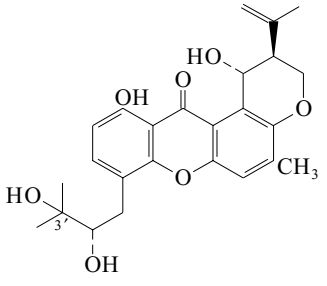
$C_{40}H_{60}O_2$ 572.913
Constit. of the mangrove *Ceriops tagal*. Yellow cryst.
Mp 163-164°. $[\alpha]_D^{25}$ +4.6 (c, 0.12 in $CHCl_3$).

2-Ketone: ***Tagalsin J***
[861648-68-2]
$C_{40}H_{58}O_3$ 586.896
Constit. of *Ceriops tagal*. Amorph. powder. $[\alpha]_D^{25}$ +37.6 (c, 0.59 in $CHCl_3$).

Zhang, Y. *et al., Org. Lett.*, 2005, **7**, 3037-3040 (*Tagalsins I and J, cryst struct*)

Tajixanthone hydrate T-11

8-(2,3-Dihydroxy-3-methylbutyl)-2,3-dihydro-1,11-dihydroxy-5-methyl-2-(1-methylethenyl)pyrano[3,2-a]xanthen-12(1H)-one, 9CI
[54622-51-4]



$C_{25}H_{28}O_7$ 440.492
Prod. by *Aspergillus variecolor*. Yellow needles (Me_2CO).
Mp 195-196°. $[\alpha]_D$ -71.5 (c, 2.3 in $CHCl_3$).

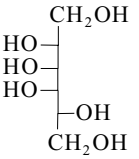
2′-O-Formyl: ***Varixanthone***
$C_{26}H_{28}O_8$ 468.502
Isol. from a marine-derived *Emericella variecolor*. Antibacterial agent. Yellow needles.
Mp 125-127°. $[\alpha]_D^{25}$ +62.1 (c, 1.13 in $CHCl_3$). Not considered to be an artifact. λ_{max} 392 (log ϵ 3.68) (EtOH).

3′-Me ether: ***Tajixanthone methanolate***
[55826-51-2]
$C_{26}H_{30}O_7$ 454.519
Prod. by *Aspergillus variecolor*. Yellow needles (Me_2CO).
Mp 190-191°. $[\alpha]_D$ -65.8 (c, 5.6 in $CHCl_3$).

Holker, J.S.E. *et al., J.C.S. Perkin 1*, 1974, 2135; 1975, 549 (*isol, pmr, cmr, struct*)
Malmstrom, J. *et al., J. Nat. Prod.*, 2002, **65**, 364-367 (*Varixanthone*)

Talitol, 9CI, 8CI T-12

Altritol, 9CI, 8CI. talo-*Hexitol.* altro-*Hexitol*
[5552-13-6]



D–*form*

$C_6H_{14}O_6$ 182.173

D-*form* [643-03-8]
Isol. from various brown algae incl. *Himanthalia elongata* and *Notheia anomala*.
Cryst. (MeOH).
Mp 88°. $[\alpha]_D$ +3.2 (c, 1.8 in H_2O).

*Hexa-Ac: 1,2,3,4,5,6-Hexa-*O*-acetyl-D-talitol*
$C_{18}H_{26}O_{12}$ 434.396
Mp 81-83°. $[\alpha]_D^{25}$ -0.6 (c, 16 in $CHCl_3$).

*2,4-*O*-Methylene: 2,4-*O*-Methylene-D-talitol*
$C_7H_{14}O_6$ 194.184
Mp 144-145°. $[\alpha]_D^{20}$ -4.2 (c, 1.2 in H_2O).

*2,4-*O*-Methylene, tetra-Ac: 1,3,5,6-Tetra-*O*-acetyl-2,4-*O*-methylene-D-talitol*
$C_{15}H_{22}O_{10}$ 362.333
Mp 67-68°. $[\alpha]_D^{20}$ +37.8 (c, 0.94 in $CHCl_3$).

*1,3:4,6-Di-*O*-methylene: 1,3:4,6-Di-*O*-methylene-D-talitol*
$C_8H_{14}O_6$ 206.195
Prisms (EtOH). Mp 182-183°. $[\alpha]_D^{20}$ -41.2 (c, 0.81 in H_2O).

*2,3:4,5-Di-*O*-methylene: 2,3:4,5-Di-*O*-methylene-D-talitol*
$C_8H_{14}O_6$ 206.195
Plates (H_2O). Mp 261-262°. $[\alpha]_D^{60}$ -1 (c, 0.41 in H_2O).

*1,3:2,4:5,6-Tri-*O*-methylene: 1,3:2,4:5,6-Tri-*O*-methylene-D-talitol*
$C_9H_{14}O_6$ 218.206
Mp 118-119°. $[\alpha]_D^{20}$ -32.1 (c, 0.42 in H_2O).

*1,2:5,6-Di-*O*-isopropylidene: 1,2:5,6-Di-*O*-isopropylidene-D-talitol*
$C_{12}H_{22}O_6$ 262.302
Cryst. (petrol). Mp 64.5-65.5°. $[\alpha]_D^{22}$ +5.2 (c, 2.4 in $CHCl_3$).

L-*form*
Needles (EtOH). Mp 87-88°. $[\alpha]_D$ -2.9 (c, 5 in H_2O).

DL-*form*
Prisms (EtOH). Mp 96°.

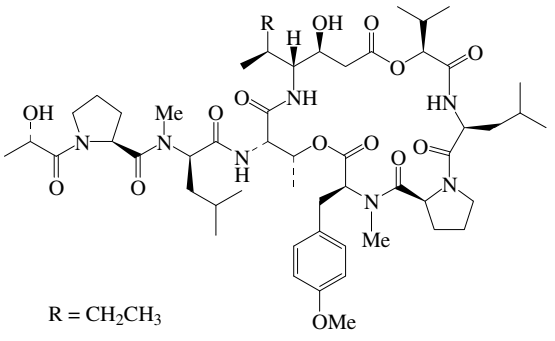
*Hexa-Ac: Hexa-*O*-acetyl-DL-talitol*
$C_{18}H_{26}O_{12}$ 434.396
Mp 85-86°.

[45007-61-2]

Humoller, F.L. *et al., J.A.C.S.*, 1945, **67**, 1226 (*L-form, DL-form*)
Hann, R.M. *et al., J.A.C.S.*, 1947, **69**, 624 (*D-form, synth, D-methylene derivs*)
Barker, S.A. *et al., Adv. Carbohydr. Chem.*, 1952, **7**, 137 (*acetals, rev*)
Sugihara, J.M. *et al., J.A.C.S.*, 1957, **79**, 5780 (*D-form, synth, D-diisopropylidene*)
Wright, L. *et al., J.O.C.*, 1961, **26**, 1588 (*D-hexa-Ac, DL-hexa-Ac*)
Chudek, J.A. *et al., Phytochemistry*, 1984, **23**, 1081-1082 (*isol*)
Kopf, J. *et al., Carbohydr. Res.*, 1991, **217**, 1 (*cryst struct, D-form*)
Kopf, J. *et al., Carbohydr. Res.*, 1992, **229**, 17 (*cryst struct, hexa-Ac*)
Evans, P.A. *et al., J.O.C.*, 1998, **63**, 6768-6769 (*synth*)
Raven, J.A. *et al., Phytochemistry*, 2001, **58**, 389-394 (*occur*)

Tamandarin A T-13

[250211-78-0]



$C_{54}H_{85}N_7O_{14}$ 1056.304

Depsipeptide antibiotic. Isol. from an unidentified Brazilian didemnid ascidian. Cytotoxic agent. Amorph. solid. $[\alpha]_D$ -35 (c, 0.11 in MeOH). λ_{max} 228 (ϵ 24500); 276 (ϵ 4000); 283 (ϵ 3400) (CH_2Cl_2).

Vervoort, H. *et al., J.O.C.*, 2000, **65**, 782-792 (*isol, pmr, cmr*)
Liang, B. *et al., J.A.C.S.*, 2001, **123**, 4469-4474 (*synth*)

Tamandarin B T-14

[258339-38-7]

As Tamandarin A, T-13 with

R = CH_3

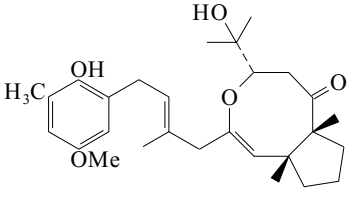
$C_{53}H_{83}N_7O_{14}$ 1042.277

Depsipeptide antibiotic. Isol. from an unidentified didemnid Brazilian ascidian. Cytotoxic agent. Amorph. solid. $[\alpha]_D$ -29 (c, 0.11 in MeOH). λ_{max} 227 (ϵ 14400); 277 (ϵ 1500); 283 (ϵ 1200) (CH_2Cl_2).

Vervoort, H. *et al., J.O.C.*, 2000, **65**, 782-792 (*isol, pmr, cmr*)
Joullie, M.M. *et al., Tet. Lett.*, 2000, **41**, 9373-9376 (*synth*)
Liang, B. *et al., J.A.C.S.*, 2001, **123**, 4469-4474 (*synth*)

Tamariscolone T-15

[124924-81-8]



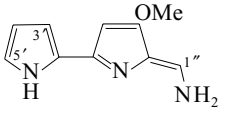
$C_{28}H_{40}O_5$ 456.621

Constit. of *Cystoseira tamariscifolia*. Oil. $[\alpha]_D^{20}$ -50.5 (c, 0.87 in EtOH).

Amico, V. *et al., Gazz. Chim. Ital.*, 1989, **119**, 467 (*isol, pmr, cmr*)

Tambjamine A T-16

[85850-00-6]



$C_{10}H_{11}N_3O$ 189.216

Isol. from the nembrothid nudibranchs *Tambja abdere*, *Tambja eloria*, *Atapozoa* sp., *Nembrotha crista*, *Nembrotha kubaryana* and *Roboastra tigris*, also isol. from the dietary source *Sessibugula translucens*. DNA binding agent. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 255 (ϵ 4600); 397 (ϵ 20000) (MeOH) (Derep).

1″-N-*Et:* ***Tambjamine E***

[126584-10-9]

$C_{12}H_{15}N_3O$ 217.27

Alkaloid from the marine ascidian *Atapozoa* sp. and from *Nembrotha crista* and *Nembrotha kubaryana*. DNA binding agent, feeding deterrent. Yellow cryst. ($CDCl_3$).

Mp 68-70°. λ_{max} 204 (ϵ 26600); 252 (ϵ 6900); 366 (ϵ 17700) (MeOH/NaOH) (Derep). λ_{max} 205 (ϵ 5000); 255 (ϵ 5700); 280 (sh); 405 (ϵ 30500) (MeOH) (Derep).

1″-N-*(2-Methylpropyl):* ***Tambjamine C***

[85850-02-8]

$C_{14}H_{19}N_3O$ 245.324

Isol. from *Tambja abdere*, *Tambja eliora*, *Roboastra tigris*, *Sessibugula* and *Atapozoa* spp. DNA binding agent. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 204 (ϵ 26600); 252 (ϵ 6900); 366 (ϵ 17700) (MeOH/NaOH) (Derep). λ_{max} 205 (ϵ 5000); 255 (ϵ 5700); 280 (sh); 405 (ϵ 30500) (MeOH) (Derep). λ_{max} 204 (ϵ 5300); 251 (ϵ 6600); 258 (ϵ 5700); 405 (ϵ 23000) (MeOH) (Berdy).

1″-N-*(2-Phenylethyl):* ***Tambjamine F***

[126584-09-6]

$C_{18}H_{19}N_3O$ 293.368

Alkaloid from *Atapozoa* sp. and from *Nembrotha crista* and *Nembrotha kubaryana*. DNA binding agent, feeding deterrent. Brown oil. λ_{max} 205 (ϵ 10200); 259 (ϵ 7000); 407 (ϵ 32100) (MeOH) (Berdy). λ_{max} 203 (ϵ 32600); 251 (ϵ 7000); 365 (ϵ 19200) (MeOH/NaOH) (Berdy).

1″-N-*Dodecyl:* ***Antibiotic BE 18591****. BE 18591*

[147138-01-0]

$C_{22}H_{35}N_3O$ 357.538

Prod. by *Streptomyces* sp. BA18591. Antitumour agent. Yellowish-green amorph. solid.

Mp 50-53°. λ_{max} 257 (28400); 325 (100000); 406 (8500) (MeOH).

1″-N-*(3Z-Dodecenyl):* [882419-92-3]

$C_{22}H_{33}N_3O$ 355.522

Prod. by the marine bacterium *Pseudoalteromonas tunicata*. Yellow solid.

3′-Bromo, 1″-N-*(2-methylpropyl):* ***Tambjamine D***

[85850-03-9]

$C_{14}H_{18}BrN_3O$ 324.22

Isol. from *Tambja abdere*, *Tambja eliora*, *Sessibugula* sp. and *Roboastra tigris* spp. DNA binding agent. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 257 (ϵ 6200); 401 (ϵ 23000) (MeOH) (Derep).

5′-Bromo: ***Tambjamine B***

[85850-01-7]

$C_{10}H_{10}BrN_3O$ 268.112

Isol. from *Tambja abdere*, *Tambja eliora*, *Roboastra tigris*, *Sessibugula* and *Roboastra* spp. DNA binding agent. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 255 (ϵ 4600); 397 (ϵ 20000) (MeOH) (Derep).

5′-Bromo, 1″-N-*Et:* ***Tambjamine G***

[157536-53-3]

$C_{12}H_{14}BrN_3O$ 296.166

Alkaloid from the bryozoan *Bugula dentata*.

5′-Bromo, 1″-N-*propyl:* ***Tambjamine H***

[157536-54-4]

$C_{13}H_{16}BrN_3O$ 310.193

Alkaloid from *Bugula dentata*.

5′-Bromo, 1″-N-*(2-methylpropyl):* ***Tambjamine I***

[157536-55-5]

$C_{14}H_{18}BrN_3O$ 324.22

Alkaloid from *Bugula dentata*.

5′-Bromo, 1″-N-*(2-methylbutyl):* ***Tambjamine J***

[157536-56-6]

$C_{15}H_{20}BrN_3O$ 338.246

Alkaloid from *Bugula dentata*.

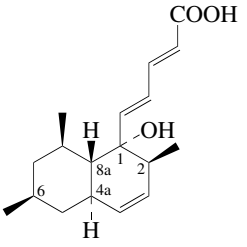
[153231-89-1]

Carté, B. *et al., J.O.C.*, 1983, **48**, 2314-2318 (*isol, uv, ir, pmr, ms, struct, Tambjamines B-D*)
Carté, B. *et al., J. Chem. Ecol.*, 1986, **12**, 795-804
Paul, V.J. *et al., Marine Ecol.: Progr. Ser.*, 1990, **59**, 109 (*occur*)

Lindquist, N. *et al., Experientia*, 1991, **47**, 504-506 (*Tambjamines C,E,F*)
Kojiri, K. *et al., J. Antibiot.*, 1993, **46**, 1799-1803; 1894-1896 (*BE 18591*)
Blackman, A.J. *et al., Aust. J. Chem.*, 1994, **47**, 1625-1629 (*Tambjamines G-J*)
Franks, A. *et al., Molecules*, 2005, **10**, 1286-1291 (*Pseudoalteromonas alkaloid*)

Tanzawaic acid C T-17

[196868-00-5]



$C_{18}H_{26}O_3$ 290.402
Prod. by a marine-derived *Penicillium citrinum*.
$[\alpha]_D$ +2 (c, 0.2 in MeOH).

1-Deoxy: ***Tanzawaic acid B****. GS 1302-1. Antibiotic GS 1302-1*
[169181-33-3]
$C_{18}H_{26}O_2$ 274.402
Prod. by a marine-derived *Penicillium citrinum*. Inhibitor of superoxide anion prodn. $[\alpha]_D$ +16 (c, 0.2 in MeOH).

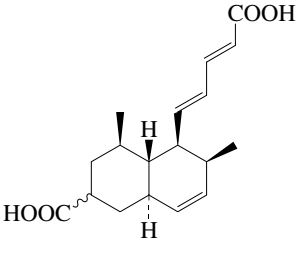
*1-Deoxy, 1,2,4*a,*8*a*-tetradehydro:* ***Tanzawaic acid A****. GS 1302-3. Antibiotic GS 1302-3*
[169181-34-4]
$C_{18}H_{22}O_2$ 270.371
Prod. by a marine-derived *Penicillium citrinum*. Inhibitor of superoxide anion prodn. $[\alpha]_D^{28}$ +147 (c, 0.04 in $CHCl_3$).

1-Deoxy, 6-hydroxy: ***Tanzawaic acid E***
$C_{18}H_{26}O_3$ 290.402
Prod. by a marine-derived *Penicillium steckii*. Yellowish oil. $[\alpha]_D^{20}$ +45.5 (c, 0.11 in MeOH). λ_{max} 265 (log ϵ 3.94) (MeOH).

*1-Deoxy, 6-hydroxy, 1,2,4*a,*8*a*-tetradehydro:* ***Tanzawaic acid D***
[196868-01-6]
$C_{18}H_{22}O_3$ 286.37
Prod. by a marine-derived *Penicillium citrinum*.
$[\alpha]_D$ +118 (c, 0.6 in MeOH).

Kuramoto, M. *et al., Chem. Lett.*, 1997, 885-886 (*isol, pmr, cmr*)
Arimoto, H. *et al., Tet. Lett.*, 1998, **39**, 9513-9516 (*synth, abs config*)
Malmstrom, J. *et al., Phytochemistry*, 2000, **54**, 301-309 (*Tanzawaic acid E*)

Tanzawaic acid F T-18

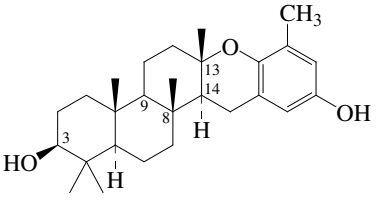


$C_{18}H_{24}O_4$ 304.385
Prod. by the marine-derived *Penicillium steckii*. Yellowish oil. $[\alpha]_D^{20}$ +10 (c, 0.04 in MeOH). λ_{max} 264 (log ϵ 4.07) (MeOH).

Malmstrom, J. *et al., Phytochemistry*, 2000, **54**, 301-309 (*isol, pmr, cmr*)

Taondiol T-19

[34274-99-2]



$C_{27}H_{40}O_3$ 412.611
Constit. of *Taonia atomaria*. Cryst. (C_6H_6).
Mp 283-284°. $[\alpha]_D$ -76 (c, 0.3 in $CHCl_3$).

13-Epimer: Isotaondiol
[52645-59-7]
$C_{27}H_{40}O_3$ 412.611
Cryst. Mp 215-217°. $[\alpha]_D$ +60 (c, 0.47 in $CHCl_3$).

8,9-Diepimer: ***Epitaondiol***
[75598-52-6]
$C_{27}H_{40}O_3$ 412.611
Constit. of *Aplysia dactylomela* and *Stypopodium zonale*. Ichthyotoxic, antimitotic, algicide. Cryst. (Et_2O).
Mp 149-152°. $[\alpha]_D$ +43.1 (c, 1.03 in $CHCl_3$). Stereochem. revised in 1995. λ_{max} 292 (ϵ 3950) (MeOH) (Berdy).

8,9-Diepimer, 3-ketone: ***3-Ketoepitaondiol***
[120963-61-3]
$C_{27}H_{38}O_3$ 410.595
Isol. from *Aplysia dactylomela* feeding on *Stypopodium zonale*.

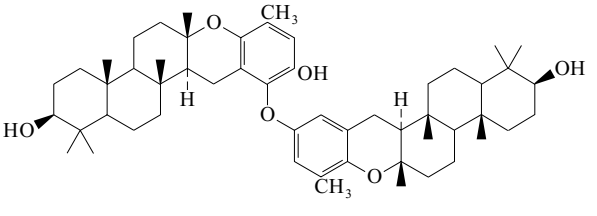
13,14-Diepimer: ***Isoepitaondiol***
[144539-76-4]
$C_{27}H_{40}O_3$ 412.611
Constit. of *Stypopodium flabelliforme*. Oil. λ_{max} 301 (MeOH).

2,3,6,7-Tetraepimer: ***2β,3α-Epitaondiol***
[863548-84-9]
$C_{27}H_{40}O_3$ 412.611
Constit. of the tropical marine alga *Stypopodium flabelliforme*. Cryst. (MeCN). $[\alpha]_D^{25}$ +70 (c, 0.2 in $CHCl_3$). λ_{max} 224 (ϵ 1210); 294 (ϵ 1301) (MeOH).

González, A.G. *et al., J.C.S. Perkin 1*, 1973, 2637-2642 (*synth*)
González, A.G. *et al., Tetrahedron*, 1973, **29**, 1605-1609 (*isol, pmr, ms*)
Gerwick, W.H. *et al., J. Chem. Ecol.*, 1989, **15**, 677-683 (*3-Ketoepitaondiol*)
Rovirosa, J. *et al., Phytochemistry*, 1992, **31**, 2679-2681 (*Isoepitaondiol*)
Sánchez-Ferrando, F. *et al., J.O.C.*, 1995, **60**, 1475-1478 (*Epitaondiol*)
Peters, K. *et al., Z. Kristallogr.*, 1996, **211**, 71-72 (*3-Ac, cryst struct*)
Sabry, O.M.M. *et al., J. Nat. Prod.*, 2005, **68**, 1022-1030 (*2β,3α-Epitaondiol, cryst struct*)

Taondiol dimer T-20

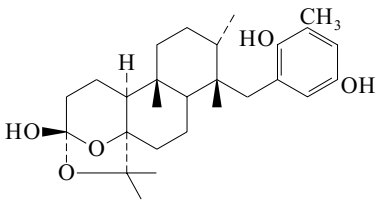
[40663-80-7]



$C_{54}H_{78}O_6$ 823.207
Dimer of Taondiol, T-19. Isol. from *Taonia atomaria*.

Gonzalez, A.G. *et al., An. Quim.*, 1972, **68**, 1187

Taonia hemilactal T-21

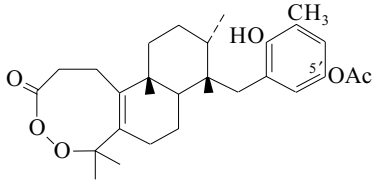


$C_{27}H_{40}O_5$ 444.61

Tri-Ac: [81860-87-9]
$C_{33}H_{46}O_8$ 570.722
Constit. of brown alga *Taonia atomaria*. Cryst.
Mp 180-181°. $[\alpha]_D^{27}$ -11 (c, 0.31 in $CHCl_3$).
Gonzalez, A.G. *et al., Chem. Lett.*, 1984, 1649 (*cryst struct*)

Taonia peroxylactone A T-22

Taonia *Peroxylactone A*
[81855-46-1]

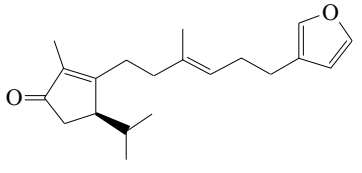


$C_{29}H_{40}O_6$ 484.631
Constit. of brown alga *Taonia atomaria*. Cryst.
Mp 151-152°. $[\alpha]_D^{27}$ -99 (c, 0.14 in $CHCl_3$).

*5′-Deacetyl, 5′-*O*-Me:* ***Taonia peroxylactone B***. Taonia *Peroxylactone B*
[82471-15-6]
$C_{28}H_{40}O_5$ 456.621
Constit. of *Taonia atomaria*. Cryst.
Mp 133-134°. $[\alpha]_D^{27}$ -82 (c, 0.28 in $CHCl_3$).
Gonzalez, A.G. *et al., Chem. Lett.*, 1984, 1649 (*cryst struct*)

Taonianone T-23

[79203-37-5]

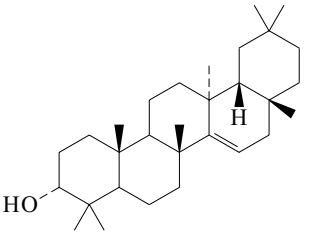


Absolute configuration

$C_{20}H_{28}O_2$ 300.44
Constit. of *Taonia australasica*. Oil. $[\alpha]_D^{21}$ +12.4 (c, 0.5 in $CHCl_3$).
Murphy, P.T. *et al., Tet. Lett.*, 1981, 1555 (*isol*)
Kido, F. *et al., Chem. Comm.*, 1986, 590 (*synth, abs config*)
Huckestein, M. *et al., Helv. Chim. Acta*, 1987, **70**, 445 (*synth, abs config*)

14-Taraxeren-3-ol T-24

D-Friedoolean-14-en-3-ol, 9CI
[81654-73-1]



3α–*form*

$C_{30}H_{50}O$ 426.724

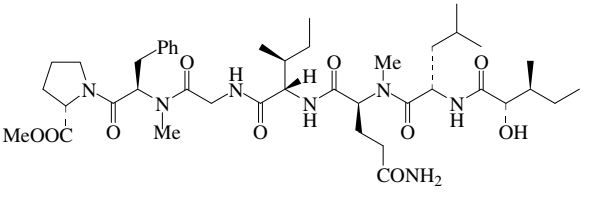
3β-*form*
Taraxerol. *Skinmiol*†. *Alnulin*
[127-22-0]
Constit. of *Taraxacum officinale* (dandelion), *Alnus* spp., *Skimmia japonica, Rhododendron* spp., *Euphorbia* spp. and other plants. Rather widely distributed. Also isol. from the lichen *Pertusaria ophthalmiza* (poss. not a genuine lichen constit.). EBV-EA induction inhibitor. Cancer chemopreventive agent. Possesses antiulcer props. Cryst. (C_6H_6).
Mp 282-283°. $[\alpha]_D^{20}$ +0.72 (c, 0.974 in $CHCl_3$). Log P 10.66 (uncertain value) (calc). Prob. identical with Pertusarin from the lichen *Pertusaria communis* (Hesse, 1898).

O-*(4-Hydroxy-Z-cinnamoyl):* **cis-*Careaborin***
[132046-11-8]
$C_{39}H_{56}O_3$ 572.87
Constit. of *Rhizophora apiculata*. Amorph.
Mp 275° dec.

O-*(3,4-Dihydroxy-*E*-cinnamoyl):* E-*Caffeoyltaraxerol*
[771494-33-8]
$C_{39}H_{56}O_4$ 588.869
Constit. of fruits of *Rhizophora mucronata*. Solid.
Mp 246-248°. $[\alpha]_D^{27}$ +28.84 (c, 0.052 in $CHCl_3$). λ_{max} 237 (log ϵ 3.33); 294 (log ϵ 3.29); 327 (log ϵ 3.33) (MeOH).

O-*(3,4-Dihydroxy-Z-cinnamoyl):* Z-*Caffeoyltaraxerol*
[771494-40-7]
$C_{39}H_{56}O_4$ 588.869
Constit. of fruits of *Rhizophora mucronata*. Solid.
Mp 246° dec. $[\alpha]_D^{27}$ -100 (c, 0.04 in $CHCl_3$). λ_{max} 223 (log ϵ 2.91); 296 (log ϵ 2.65); 316 (log ϵ 2.64) (MeOH).
Kokpol, U. *et al., J. Nat. Prod.*, 1990, **53**, 953-955 (*cis-Careaborin*)
Laphookhieo, S. *et al., Chem. Pharm. Bull.*, 2004, **52**, 883-885 (*caffeoyl esters*)

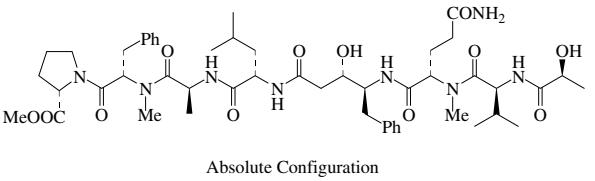
Tasiamide A T-25



Absolute Configuration

$C_{42}H_{67}N_7O_{10}$ 830.032
Isol. from *Symploca* sp. Cytotoxic. Amorph. powder. $[\alpha]_D^{21}$ +15 (c, 0.4 in $CHCl_3$). λ_{max} 201 (log ϵ 4.27); 254 (log ϵ 2.52) (MeOH).
Williams, P.G. *et al., J. Nat. Prod.*, 2002, **65**, 1336-1339 (*Tasiamide A*)

Tasiamide B T-26



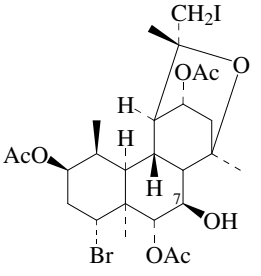
Absolute Configuration

$C_{50}H_{74}N_8O_{12}$Isol. from *Symploca* sp.
Amorph. powder. $[\alpha]_D^{21}$ -28 (c, 0.4 in MeOH). λ_{max} 201 (log ϵ 7.6) (MeOH).

Williams, P.G. *et al., J. Nat. Prod.*, 2003, **66**, 1006-1009 (*Tasiamide B*)

Tasihalide A T-27

[630094-98-3]

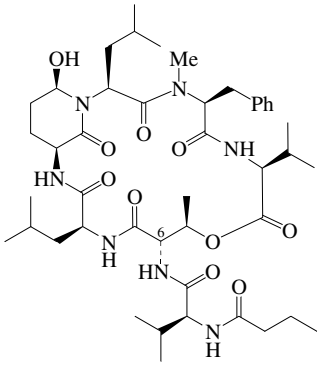


$C_{26}H_{38}BrIO_8$ 685.39
Constit. of an assemblage of a marine cyanobacterium (*Symploca* sp.) and an unidentified red alga. Amorph. powder. $[\alpha]_D^{24}$ -18 (c, 0.6 in MeOH). λ_{max} 207 (log ϵ 4.3); 253 (log ϵ 1.2) (MeOH).

7-Ac: ***Tasihalide B***
[630094-99-4]
$C_{28}H_{40}BrIO_9$ 727.427
Constit. of an assemblage of a marine cyanobacterium (*Symploca* sp.) and an unidentified red alga. Amorph. powder. $[\alpha]_D^{23}$ -13 (c, 0.4 in MeOH).

Williams, P.G. *et al., Org. Lett.*, 2003, **5**, 4167-4170 (*isol, pmr, cmr*)

Tasipeptin A T-28



Absolute Configuration

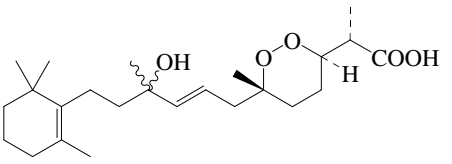
$C_{45}H_{71}N_7O_{10}$ 870.097
Depsipeptide antibiotic. Isol. from a marine *Symploca* sp. NIH304. Cytotoxic. Amorph. powder. $[\alpha]_D^{24}$ -23 (c, 1.5 in MeOH). λ_{max} 202 (log ϵ 4.88) (MeOH).

N^6-*Deacyl,* N^6-*butanoyl:* ***Tasipeptin B***
$C_{40}H_{62}N_6O_9$ 770.965
Isol. from *Symploca* sp. NIH304. Cytotoxic. Amorph. powder. $[\alpha]_D^{21}$ -13 (c, 0.7 in MeOH). λ_{max} 202 (log ϵ 4.88) (MeOH).

Williams, P.G. *et al., J. Nat. Prod.*, 2003, **66**, 620-624 (*isol, pmr, cmr*)

Tasnemoxide A T-29

[655228-40-3]

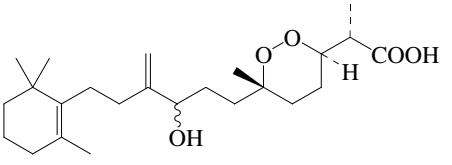


$C_{24}H_{40}O_5$ 408.577
Constit. of *Diacarnus erythraenus.* Oil. $[\alpha]_D^{25}$ +21.8 (c, 0.55 in CH_2Cl_2).

Youssef, D.T.A. *et al., J. Nat. Prod.*, 2004, **67**, 112-114 (*isol, pmr, cmr*)

Tasnemoxide B T-30

[655228-41-4]

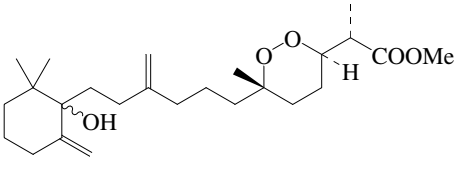


$C_{24}H_{40}O_5$ 408.577
Constit. of *Diacarnus erythraenus.*
$[\alpha]_D^{25}$ +62.5 (c, 0.4 in CH_2Cl_2).

Youssef, D.T.A. *et al., J. Nat. Prod.*, 2004, **67**, 112-114 (*isol, pmr, cmr*)

Tasnemoxide C T-31

[655228-42-5]

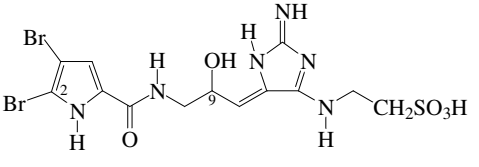


$C_{25}H_{42}O_5$ 422.604
Constit. of *Diacarnus erythraenus.* Oil. $[\alpha]_D^{25}$ +76 (c, 0.3 in CH_2Cl_2).

Youssef, D.T.A. *et al., J. Nat. Prod.*, 2004, **67**, 112-114 (*isol, pmr, cmr*)

Tauroacidin A T-32

[200566-34-3]



$C_{13}H_{16}Br_2N_6O_5S$ 528.181
Isol. as partial racemate. Tautomerism possible in the iminoimidazole ring. Alkaloid from the sponge *Hymeniacidon* sp. Inhibits tyrosine kinase. Amorph. solid. $[\alpha]_D^{28}$ -4.3 (c, 0.1 in MeOH). λ_{max} 273 (ϵ 9700); 312 (ϵ 3800) (MeOH).

2-Debromo: ***Tauroacidin B***
[200566-35-4]
$C_{13}H_{17}BrN_6O_5S$ 449.285
Alkaloid from *Hymeniacidon* sp. Inhibits tyrosine kinase. Amorph. solid. Isol. as a racemate.

9-Deoxy: ***Taurodispacamide A***
[323177-96-4]
$C_{13}H_{16}Br_2N_6O_4S$ 512.181

Alkaloid from the sponge *Agelas oroides*. Antihistaminic agent. Pale yellow solid. λ_{max} 230; 270 (no solvent reported).

2-Debromo, 9-deoxy: ***9-Deoxytauroacidin B****. 2-Debromotaurodispacamide A*
$C_{13}H_{17}BrN_6O_4S$ 433.285
Alkaloid from *Axinella verrucosa*.

Kobayashi, J. *et al., Tetrahedron*, 1997, **53**, 16679-16682 (*isol, uv, ir, pmr, cmr, ms*)
Fattorusso, E. *et al., Tet. Lett.*, 2000, **41**, 9917-9922 (*Taurodispacamide A*)
Aiello, A. *et al., Bioorg. Med. Chem.*, 2006, **14**, 17-24 (*Deoxytauroacidin B*)

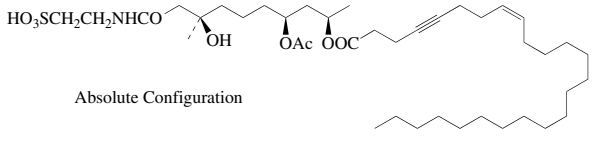
Tauropine dehydrogenase T-33

E.C. 1.5.1.23. N^2*-(D-1-Carboxyethyl)taurine:NAD*$^{\oplus}$ *oxidoreductase (taurine-forming)*
[104645-74-1]
Oxidoreductase enzyme. Isol. from *Haliotis*, *Arabella* and *Asterina* spp. Catalyses the reaction of *N*-(2-Sulfoethyl)alanine, S-537 with $NAD^{\oplus}$ and H_2O to give 2-Aminoethanesulfonic acid, A-289, pyruvate and NADH.

Gäde, G. *et al., Eur. J. Biochem.*, 1986, **160**, 311-318 (*Haliotis lamellosa*)
Kanno, N. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1996, **114**, 409-416 (*Arabella iricolor*)
Kanno, N. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **121**, 323-332 (*Asterina pectinifera*)

Taurospongin A T-34

[185138-92-5]



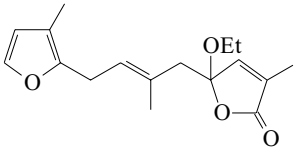
Absolute Configuration

$C_{40}H_{71}NO_9S$ 742.068
Isol. from the sponge *Hippospongia* sp. Inhibitor of DNA polymerase β and HIV reverse transcriptase. Amorph. solid. $[\alpha]_D^{27}$ +2.4 (c, 0.2 in $CHCl_3$).

Ishiyama, H. *et al., J.O.C.*, 1997, **62**, 3831-3836 (*isol, ir, pmr, cmr*)
Lebel, H. *et al., J.O.C.*, 1998, **63**, 9624-9625 (*synth*)
Hollowood, C.J. *et al., Org. Biomol. Chem.*, 2003, 1664-1675 (*synth*)
Moreau, X. *et al., J.A.C.S.*, 2005, **127**, 7288-7289 (*synth*)

Tavacbutenolide 1 T-35

*5-Ethoxy-3-methyl-5-[2-methyl-4-(3-methyl-2-furanyl)-2-butenyl]-2(5*H*)-furanone, 9CI*
[98570-67-3]

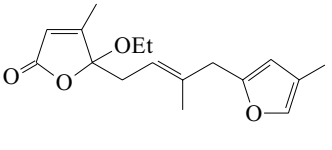


$C_{17}H_{22}O_4$ 290.358
Isol. from a marine sponge. Racemic.

Guella, G. *et al., Helv. Chim. Acta*, 1985, **68**, 1276-1282 (*isol, pmr, cmr*)

Tavacbutenolide 2 T-36

*5-Ethoxy-4-methyl-5-[3-methyl-4-(4-methyl-2-furanyl)-2-butenyl]-2(5*H*)-furanone, 9CI*
[98570-66-2]

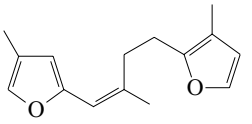


$C_{17}H_{22}O_4$ 290.358
Isol. from a marine sponge. Racemic.

Guella, G. *et al., Helv. Chim. Acta*, 1985, **68**, 1276 (*isol, pmr, cmr, struct*)

Tavacfuran T-37

3-Methyl-2-[3-methyl-4-(4-methyl-2-furanyl)-3-butenyl]furan, 9CI
[98570-64-0]



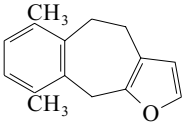
$C_{15}H_{18}O_2$ 230.306
Isol. from a marine sponge. Liq. λ_{max} 220 (ϵ 7300); 274 (ϵ 10800); 285 (ϵ 7100) (MeOH) (Berdy).

*(*E*)-Isomer:* ***Isotavacfuran***
[98570-68-4]
Isol. from the nudibranch *Hypselodoris* sp.
Oil.

Guella, G. *et al., Helv. Chim. Acta*, 1985, **68**, 1276 (*isol, pmr, cmr, struct*)
Avila, C. *et al., J. Chem. Ecol.*, 1991, **17**, 625 (*Isotavacfuran*)

Tavacpallescensin T-38

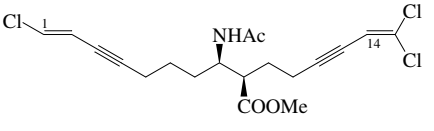
*5,10-Dihydro-6,9-dimethyl-4*H*-benzo[5,6]cyclohepta[1,2-*b*]furan, 9CI*
[98570-65-1]



$C_{15}H_{16}O$ 212.291
Isol. from *Pleraplysilla spinifera*. Oil.

Guella, G. *et al., Helv. Chim. Acta*, 1985, **68**, 1276-1282 (*isol, pmr, cmr, struct*)
Ho, T.-L. *et al., J. Chin. Chem. Soc. (Taipei)*, 1996, **43**, 207-208 (*synth*)
Ho, T.-L. *et al., J.C.S. Perkin 1*, 1999, 1207-1210 (*synth*)

Taveuniamide E T-39



Relative Configuration

$C_{19}H_{22}Cl_3NO_3$ 418.746
Isol. from a mixed assemblage of *Lyngbya majuscula* and *Schizothrix* sp.
$[\alpha]_D^{25}$ +2.1 (c, 0.3 in $CHCl_3$). λ_{max} 242 (ϵ 7200) (EtOH).

12,12,13,13,14,15-Hexahydro: ***Taveuniamide A***
$C_{19}H_{28}Cl_3NO_3$ 424.793
Isol. from a mixt. of *Lyngbya majuscula* and *Schizothrix* sp.
$[\alpha]_D^{25}$ +11.7 (c, 0.4 in $CHCl_3$). Stereochem. not determined.
λ_{max} 236 (ϵ 6700) (EtOH).

1-Chloro, 1,2-dihydro: ***Taveuniamide D***
$C_{19}H_{23}Cl_4NO_3$ 455.206
Isol. from a mixt. of *Lyngbya majuscula* and *Schizothrix* sp.
$[\alpha]_D^{25}$ +5.3 (c, 0.09 in $CHCl_3$). Stereochem. not determined.
λ_{max} 244 (ϵ 16500) (EtOH).

*1-Chloro, 1,2,3*E*,4-tetrahydro:* ***Taveuniamide C***
$C_{19}H_{25}Cl_4NO_3$ 457.222
Isol. from a mixt. of *Lyngbya majuscula* and *Schizothrix* sp.
$[\alpha]_D$ +24 (c, 0.03 in $CHCl_3$). Stereochem. not determined.
λ_{max} 244 (ϵ 15400) (EtOH).

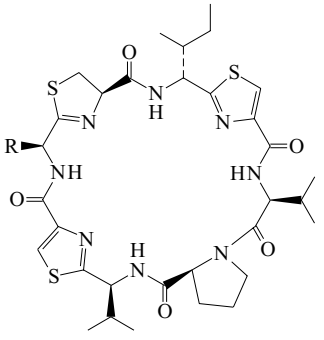
1-Chloro, 12,12,13,13,14,15-hexahydro: ***Taveuniamide B***
$C_{19}H_{27}Cl_4NO_3$ 459.238

Isol. from a mixt. of *Lyngbya majuscula* and *Schizothrix* sp. $[\alpha]_D^{25}$ +10.4 (c, 0.1 in $CHCl_3$). Stereochem. not determined. λ_{max} 244 (ϵ 18300) (EtOH).

Williamson, R.T. *et al., Tetrahedron*, 2004, **60**, 7025-7033 (*isol, pmr, cmr*)

Tawicyclamide A **T-40**

[143007-28-7]



R = CH_2Ph

$C_{39}H_{50}N_8O_5S_3$ 807.073

Cyclic peptide antibiotic. Isol. from the ascidian *Lissoclinum patella*. Weakly cytotoxic. Clear solid. $[\alpha]_D^{25}$ -15 (c, 0.43 in $CHCl_3$). λ_{max} 249 (ϵ 16530) (MeOH) (Berdy).

McDonald, L.A. *et al., J.O.C.*, 1992, **57**, 4616-4624 (*isol, pmr, cmr, cryst struct*)

Tawicyclamide B **T-41**

[143007-29-8]

As Tawicyclamide A, T-40 with

R = $-CH_2CH(CH_3)_2$

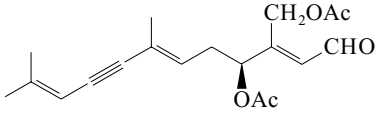
$C_{36}H_{52}N_8O_5S_3$ 773.055

Cyclic peptide antibiotic. Isol. from the ascidian *Lissoclinum patella*. Weakly cytotoxic. Clear solid. $[\alpha]_D^{25}$ +2.1 (c, 0.35 in $CHCl_3$). λ_{max} 249 (ϵ 15029) (MeOH) (Berdy).

McDonald, L.A. *et al., J.O.C.*, 1992, **57**, 4616-4624 (*isol, pmr, cmr, cryst struct*)

Taxifolial A **T-42**

[142474-75-7]



$C_{19}H_{24}O_5$ 332.396

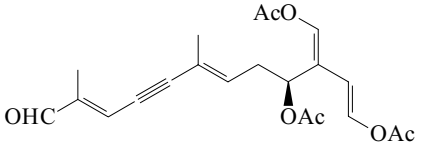
Constit. of *Caulerpa taxifolia*. Oil. $[\alpha]_D^{20}$ -3.9 (c, 0.47 in EtOH). λ_{max} 269 (ϵ 17100) (MeOH) (Berdy).

▶ Toxic.

Guerriero, A. *et al., Helv. Chim. Acta*, 1992, **75**, 689 (*isol, pmr, cmr*)
Santelli, M. *et al., Org. Lett.*, 2001, **3**, 1713-1715 (*synth*)

Taxifolial B **T-43**

[142474-76-8]



$C_{21}H_{24}O_7$ 388.416

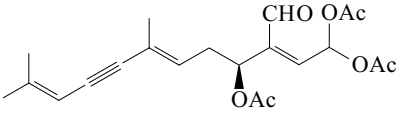
Constit. of *Caulerpa taxifolia*. Oil. $[\alpha]_D^{20}$ 0 (c, 0.17 in EtOH). λ_{max} 251 (ϵ 21300); 306 (ϵ 15400) (MeOH) (Berdy).

▶ Toxic.

Guerriero, A. *et al., Helv. Chim. Acta*, 1992, **75**, 689 (*isol, pmr, cmr*)

Taxifolial C **T-44**

[142474-78-0]



$C_{21}H_{26}O_7$ 390.432

Constit. of *Caulerpa taxifolia*. Oil. $[\alpha]_D^{20}$ 0 (c, 0.04 in EtOH). λ_{max} 260 (ϵ 32000) (MeOH) (Berdy).

▶ Toxic.

Guerriero, A. *et al., Helv. Chim. Acta*, 1992, **75**, 689 (*isol, pmr, cmr*)

Tealiatoxin **T-45**

[106908-69-4]

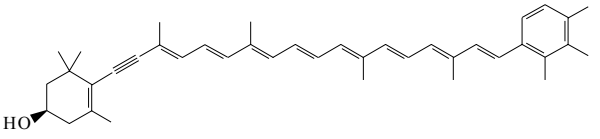
Protein. Isol. from the sea anenome *Tealia felina*. Toxin. Vasoconstrictor. Shows histaminolytic and cardiotoxic props.

Aldeen, S.I. *et al., Br. J. Pharmacol.*, 1981, **72**, 211-220 (*isol*)
Elliott, R.C. *et al., Toxicon*, 1986, **24**, 117-122 (*isol*)

Tedaniaxanthin **T-46**

7,8-Didehydro-β,χ-caroten-3-ol. Allopurpurin

[63893-29-8]



$C_{40}H_{50}O$ 546.834

Constit. of *Tedania digitata* and other sponges. λ_{max} 357; 457 (MeOH).

Me ether: ***7,8-Didehydroaaptopurpurin****. 7,8-Didehydro-3-methoxy-β,χ-carotene*

[115516-52-4]

$C_{41}H_{52}O$ 560.861

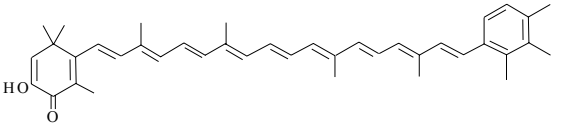
Isol. from *Tedania digitata*.

Tanaka, Y. *et al., Nippon Suisan Gakkaishi*, 1979, **45**, 633; 1988, **54**, 155 (*occur, ir, nmr, ms*)
Litchfield, C. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **66**, 359-365 (*occur, ms, pmr, uv*)
Saxegaard, P. *et al., Biochem. Syst. Ecol.*, 1981, **9**, 325-327 (*struct*)

Tedanin **T-47**

2,3-Didehydro-3-hydroxy-β,χ-caroten-4-one

[55511-20-1]



$C_{40}H_{48}O_2$ 560.818

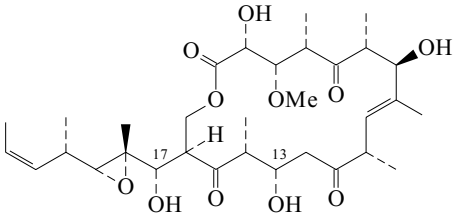
Major pigment from *Tedania digitata*. Purple-black cryst. (CH_2Cl_2/EtOH).

Mp 188-190°.

Okukado, N. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 1061 (*isol, pmr, ir, ms*)
Yashuhara, M. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 1629 (*synth*)
Shimada, A. *et al., Tet. Lett.*, 1981, 773 (*synth*)

Tedanolide T-48

[92471-87-9]



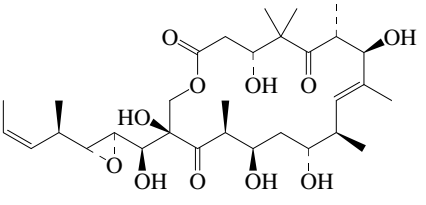
$C_{32}H_{50}O_{11}$ 610.74

Macrolide antibiotic. Isol. from the sponge *Tedania ignis*. Antitumour agent. Cryst. (C_6H_6/$CHCl_3$). Sol. MeOH, $CHCl_3$; poorly sol. hexane, H_2O.
Mp 193-194° dec. $[\alpha]_D$ +18.7 (c, 0.08 in $CHCl_3$). Stereochem. at C-17 incorrectly shown in earliest paper.

13-Deoxy: ***13-Deoxytedanolide***
[134455-11-1]
$C_{32}H_{50}O_{10}$ 594.741
Isol. from the sponge *Mycale adhaerens*. Antitumour agent.
$[\alpha]_D$ +84.4 (c, 0.26 in $CHCl_3$).

Schmitz, F.J. *et al., J.A.C.S.*, 1984, **106**, 7251-7252 (*isol, pmr, cryst struct*)
Fusetani, N. *et al., J.O.C.*, 1991, **56**, 4971-4974 (*13-Deoxytedanolide*)
Smith, A.B. *et al., Org. Lett.*, 1999, **1**, 1249-1252 (*synth*)
Smith, A.B. *et al., J.A.C.S.*, 2003, **125**, 350-351 (*13-Deoxytedanolide, synth*)
Nishimura, S. *et al., Bioorg. Med. Chem.*, 2005, **13**, 449-454; 455-462 (*13-Deoxytedanolide, activity*)
Julian, L.D. *et al., J.A.C.S.*, 2005, **127**, 6186-6187 (*13-Deoxytedanolide, synth*)

Tedanolide C T-49



Relative Configuration

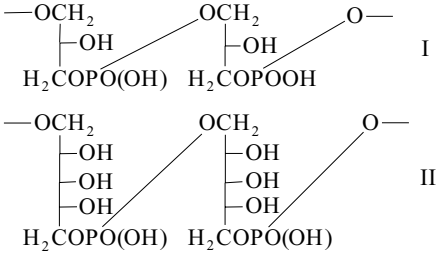
$C_{31}H_{50}O_{11}$ 598.729

Macrolide antibiotic. Constit. of an *Ircinia* sp. Cytotoxic. Amorph. solid. $[\alpha]_D^{24}$ +21.4 (c, 0.21 in MeOH). λ_{max} 208 (ε 8030); 264 (ε 1100) (MeOH).

Chevallier, C. *et al., J.O.C.*, 2006, **71**, 2510-2513 (*isol, pmr, cmr*)

Teichoic acid T-50

[9041-38-7]

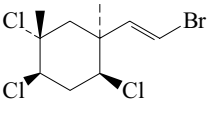


Teichoic acids are polymers of glycerol or ribitol phosphate in which some of the free hydroxyl groups may be glycosylated or esterified with D-alanine. Prominent constits. (along with peptidoglycan and other heteropolysaccharides) of the cell walls or envelopes which surround the cytoplasmic membrane of gram-positive bacteria cells. There are two major classes; those which occur in the wall, covalently linked to the peptidoglycan, and those known as lipoteichoic acids, which are situated on the surface of the cytoplasmic membrane and are covalently linked to the glycolipid located within the membrane. The former class of polymers contain glycerol and ribitol phosphates (I and II) and they comprise a major part of the purified cell walls (30-50%). The lipoteichoic acids are formed exclusively from glycerol phosphate (I); see separate entry Lipoteichoic acids.

Archibald, A.R. *et al., Adv. Carbohydr. Chem.*, 1966, **21**, 323 (*rev*)
Baddiley, J. *et al., Essays Biochem.*, 1972, **8**, 35 (*rev*)
Archibald, A.R. *et al., Methods Carbohydr. Chem.*, 1972, **6**, 162 (*isol*)
Sharon, N. *et al., Complex Carbohydrates*, Addison-Wesley, 1975, 322
Duckworth, M. *et al., Surf. Carbohydr. Prokaryotic Cell*, Academic Press, 1977, 177 (*rev*)
Tarelli, E. *et al., Carbohydr. Res.*, 1979, **75**, 31-37 (*cmr*)
Pooley, H.M. *et al., New Compr. Biochem.*, 1994, **27**, 187 (*rev*)
Komandrova, N.A. *et al., Bioorg. Khim.*, 1998, **24**, 446-448; *Russ. J. Bioorg. Chem. (Engl. Transl.)*, 1998, **24**, 390-392 (*isol, struct*)

Telfairine T-51

1-(2-Bromoethenyl)-2,4,5-trichloro-1,5-dimethylcyclohexane
[120163-22-6]



$C_{10}H_{14}BrCl_3$ 320.483
Constit. of *Plocamium telfairiae*. Amorph. powder (hexane).
Mp 62-63°. $[\alpha]_D^{25}$ -18 (c, 0.1 in MeOH).

Watanabe, K. *et al., Phytochemistry*, 1989, **28**, 77

Temptin T-52

Peptide containing 103 amino acid residues. Present in albumen glands of *Aplysia californica* and *Aplysia brasiliana*. Water-borne pheromone that acts in concert with attractin to stimulate mate attraction.

Cummins, S.F. *et al., J. Biol. Chem.*, 2004, **279**, 25614-25622 (*isol*)

Tenebrosins T-53

Basic proteins with a single polypeptide chain. Isol. from the sea anemone *Actinia tenebrosa*. Cardiac stimulator.

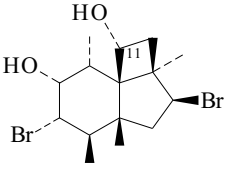
Tenebrosin A [112279-11-5]
Contains 186 amino acid residues.

Tenebrosin B [127652-31-7]
Contains 187 amino acid residues.

Tenebrosin C [127652-32-8]
[129712-22-7, 129712-23-8]
Haemolytic agent. Contains 177 amino acid residues.

Thompson, M. *et al., Biochem. Int.*, 1987, **15**, 1711-1718 (*Tenebrosin A, isol*)
Simpson, R.J. *et al., Eur. J. Biochem.*, 1990, **190**, 319-328 (*Tenebrosin C, struct*)
Norton, R.S. *et al., Toxicon*, 1990, **28**, 29-41 (*Tenebrosins A-C, isol*)

Tenerol T-54



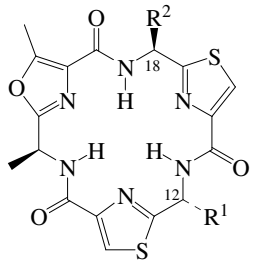
$C_{15}H_{24}Br_2O_2$ 396.161

11-Ac: ***Tenerol acetate***
[148098-28-6]
$C_{17}H_{26}Br_2O_3$ 438.199
Constit. of *Laurencia tenera*. Oil. $[\alpha]_D^{25}$ -4.3 (c, 0.3 in $CHCl_3$).

Wright, A.D. *et al., Phytochem. Anal.*, 1992, **3**, 263 (*isol, pmr, cmr*)

Tenuecyclamide A T-55

[213539-45-8, 213539-46-9]



Absolute Configuration

$R^1 = R^2 = CH_3$

$C_{19}H_{20}N_6O_4S_2$ 460.537
Alkaloidal peptide from *Nostoc spongiaeforme* var. *tenue*. Amorph. solid. $[\alpha]_D^{25}$ -8.8 (c, 2.5 in MeOH). λ_{max} 243 (ϵ 24500) (MeOH).

12-Epimer: ***Tenuecyclamide B***
$C_{19}H_{20}N_6O_4S_2$ 460.537
Alkaloidal peptide from *Nostoc spongiaeforme* var. *tenue*. Glassy solid. $[\alpha]_D^{25}$ -36 (c, 0.5 in MeOH). CAS no. incorrectly assigned by CA. λ_{max} 244 (ϵ 16500) (MeOH).

Banker, R. *et al., J. Nat. Prod.*, 1998, **61**, 1248-1251 (*isol, uv, ir, pmr, cmr, ms*)
You, S.-L. *et al., Org. Lett.*, 2004, **6**, 2627-2630 (*synth, abs config*)

Tenuecyclamide C T-56

[213539-46-9]
As Tenuecyclamide A, T-55 with
$R^1 = -CH_2^{14}CH_2SMe$, $R^2 = H$

$C_{20}H_{22}N_6O_4S_3$ 506.63
Alkaloidal peptide from *Nostoc spongiaeforme* var. *tenue*. Glassy solid. $[\alpha]_D^{25}$ +12 (c, 0.5 in MeOH). λ_{max} 244 (ϵ 17300) (MeOH).

14-S-*Oxide:* ***Tenuecyclamide D***
[213539-47-0]
$C_{20}H_{22}N_6O_5S_3$ 522.629
Alkaloidal peptide from *Nostoc spongiaeforme* var. *tenue*. Glassy solid. $[\alpha]_D^{25}$ +44 (c, 0.5 in MeOH). λ_{max} 247 (ϵ 39170) (MeOH).

Banker, R. *et al., J. Nat. Prod.*, 1998, **61**, 1248-1251 (*isol, uv, ir, pmr, cmr, ms*)
You, S.-L. *et al., Org. Lett.*, 2004, **6**, 2627-2630 (*synth, abs config*)

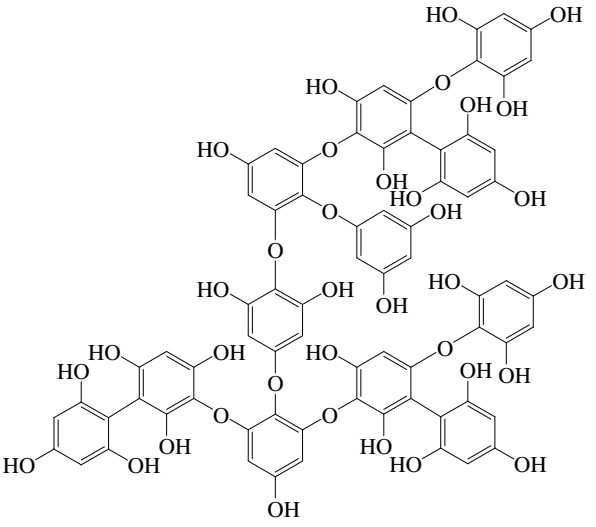
Teprotide, BAN, INN, USAN T-57

Bradykinin potentiator B, 2-L-tryptophan-3-de-L-leucine-4-de-L-proline-8-L-glutamine, 9CI. Bradykinin-potentiating peptide BPP_{9a}. $BPP_{9\alpha}$. SQ 20881. Bothrops jararaca *BPP-9a*
[35115-60-7]
pyroGlu-Trp-Pro-Arg-Pro-Gln-Ile-Pro-Pro

$C_{53}H_{76}N_{14}O_{12}$ 1101.27
Isol. from venom of *Bothrops jararaca*. Used for treatment of hypertension and the diagnosis of renin-dependent hypertension. Inhibitor of angiotensin-converting enzyme.

U.S. Pat., 1976, 3 973 006; *CA*, **86**, 16960z
Fr. Pat., 1977, 2 350 846; *CA*, **89**, 197973m (*synth*)
Ger. Pat., 1977, 2 621 279; *CA*, **88**, 38157m
Netherlands Pat., 1977, 7 605 327; *CA*, **89**, 24824k (*synth*)
Sevast'yanova, N.N. *et al., J. Mol. Struct.*, 1980, **65**, 125 (*conformn*)
Krit, N.A. *et al., Bioorg. Khim.*, 1981, **7**, 965 (*synth*)
Martindale, The Extra Pharmacopoeia, 28thl29th edn., Pharmaceutical Press, 1982, 906
Reissmann, S. *et al., Proc. FEBS Congr., 16th*, 1984, 449 (*biol activity, struct*)
Hofbauer, K.G. *et al., J. Cardiovasc. Pharmacol.*, 1985, **7**, 562 (*activity*)
Murayama, N. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1997, **94**, 1189-1193 (*isol*)

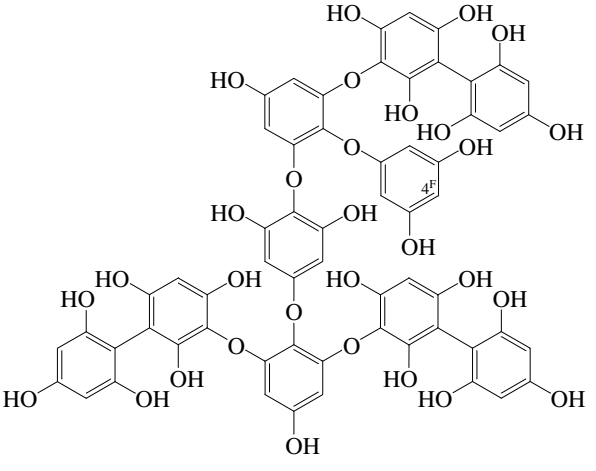
Terfucoheptaphlorethol A T-58



$C_{72}H_{50}O_{36}$ 1491.165
Isol. from brown alga *Cystophora retroflexa*.

Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol, pmr, cmr, ms*)

Terfucohexaphlorethol A T-59

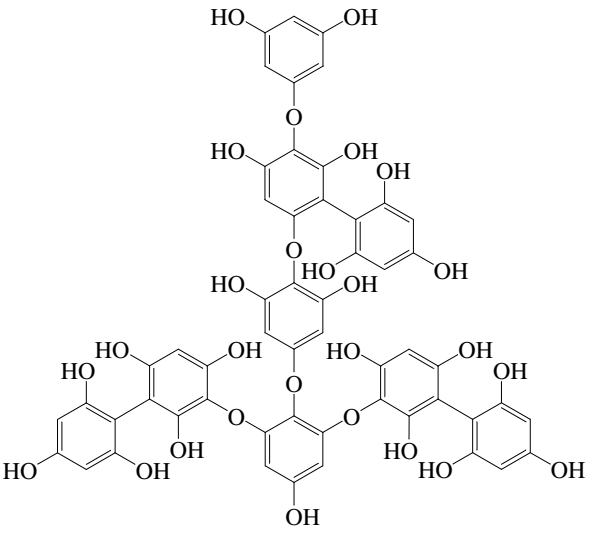


$C_{60}H_{42}O_{30}$ 1242.974
Isol. from brown algae *Cystoseira retroflexa, Carpophyllum maschalocarpum* and *Carpophyllum angustifolium*.

4^F-Hydroxy: ***Hydroxyterfucohexaphlorethol A***
$C_{60}H_{42}O_{31}$ 1258.973
Isol. from *Carpophyllum maschalocarpum*.

Glombitza, K.W. *et al., Phytochemistry*, 1991, **30**, 3423 (*isol, pmr, ms*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)
Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol*)

Terfucopentaphlorethol A T-60

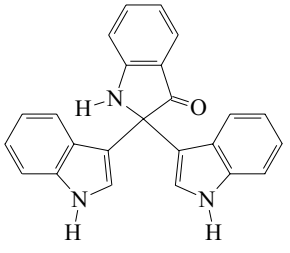


$C_{54}H_{38}O_{27}$ 1118.878
Isol. from brown algae *Cystophora retroflexa* and *Carpophyllum maschalocarpum*.

Glombitza, K.W. *et al., Phytochemistry*, 1991, **30**, 3423 (*isol, pmr, ms*)
Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol, pmr*)

[3,2′:2′(3′*H*),3″-Ter-1*H*-indol]-3′-one, 9CI T-61

2,2-Di-3-indolyl-3-indolone. 2,2-Bis(3-indolyl)indoxyl
[17646-95-6]

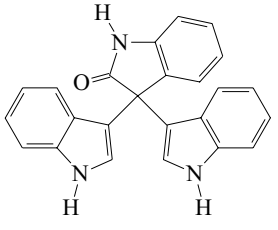


$C_{24}H_{17}N_3O$ 363.418
Metab. from the marine bacterium *Vibrio parahaemolyticus* isol. from the toxic mucus of the boxfish *Ostracion cubicus*. Also isol. as the product of indole oxidation by a strain of *Claviceps purpurea*. Exhibits antibacterial activity. Oil. λ_{max} 242 (ϵ 33600); 268 (ϵ 31800) ($CHCl_3$) (Berdy).

Loo, Y.H. *et al., Chem. Ind. (London)*, 1957, 1123
Bell, R. *et al., J. Nat. Prod.*, 1994, **57**, 1587 (*isol, uv, ir, pmr, cmr*)
Stull, T.L. *et al., J. Biol. Chem.*, 1995, **270**, 5

[3,3′:3′(2′*H*),3″-Ter-1*H*-indol]-2′-one T-62

3,3-Di-3-indolyl-2-indolone. ***Trisindoline***



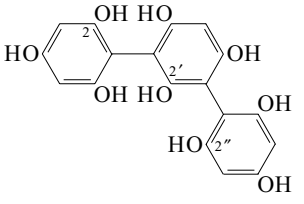
$C_{24}H_{17}N_3O$ 363.418
Prod. by a bacterium of *Vibrio* sp. separated from the Okinawan marine sponge *Hyrtios altum* and *Vibrio parahaemolyticus* Bio249.

Amorph. solid. Incorrectly named in CA; no CAS no. reported. λ_{max} 219 (ϵ 62000); 254 (ϵ 12000); 274 (ϵ 12000); 280 (ϵ 12000); 290 (ϵ 10000) (MeOH).

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 2449-2451 (*isol, synth, uv, ir, pmr, cmr*)
Veluri, R. *et al., J. Nat. Prod.*, 2003, **66**, 1520-1523 (*isol*)

[1,1′:3′,1″-Terphenyl]-2,2′,2″,4,4′,4″,6,6′,6″-nonol, 9CI T-63

Trifucol
[62218-04-6]



$C_{18}H_{14}O_9$ 374.303
Constit. of various brown algae incl. *Analipus japonicus*, *Bifurcaria bifurcata*, *Fucus vesiculosus* and *Himanthalia elongata*. Isol. as nona-Ac.

2-O-Sulfate: [123203-17-8]
$C_{18}H_{14}O_{12}S$ 454.367
Constit. of an alga.

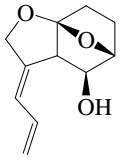
2,2″-Di-O-sulfate: [123203-18-9]
$C_{18}H_{14}O_{15}S_2$ 534.432
Constit. of an alga.

Nona-Ac: [57103-40-9]
$C_{36}H_{32}O_{18}$ 752.638
Mp 217.5-219.5°.

Glombitza, K.W. *et al., Phytochemistry*, 1975, **14**, 1403; 1976, **15**, 1279; 1977, **16**, 1614 (*isol*)

Terpiodiene T-64

[405199-45-3]

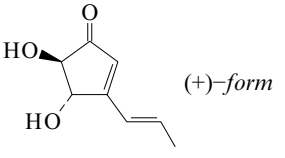


$C_{11}H_{14}O_3$ 194.23
Constit. of *Terpios hoshinota*.

Teruya, T. *et al., Chem. Lett.*, 2002, 38-39 (*isol, pmr, cmr*)

Terrein T-65

4,5-Dihydroxy-3-(1-propenyl)-2-cyclopenten-1-one
[131233-98-2, 154096-62-5, 180682-72-8]



(+)–*form*

$C_8H_{10}O_3$ 154.165

(+)-*form* [582-46-7]
Metab. of *Aspergillus terreus*, *Neosartorya fischeri* and *Penicillium raistrickii*. Phytotoxin. Sol. H_2O, MeOH, EtOAc; poorly sol. C_6H_6, hexane.
Mp 123°. $[\alpha]_{Hg}^{20}$ +185 (c, 1 in H_2O). λ_{max} 271 (ϵ 25700) (MeOH) (Berdy). λ_{max} 276 (ϵ 25000); 282 (ϵ 26500) (EtOH) (Berdy).

Di-Ac, 2,4-dinitrophenylhydrazone: Mp 195-196°. $[\alpha]_D$ -613 (c, 0.53 in $CHCl_3$).

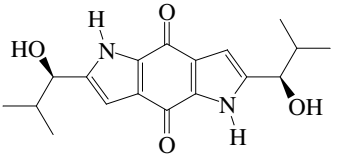
1′,2′-Dihydro: 4,5-Dihydroxy-3-propyl-2-cyclopenten-1-one. ***Dihydroterrein***
$C_8H_{12}O_3$ 156.181
Isol. from a marine-derived *Emericella variecolor*. Oil (as di-Ac). $[\alpha]_D^{25}$ +6.4 (c, 1.15 in $CHCl_3$) (di-Ac). λ_{max} 216 (log ϵ 4.67) (EtOH).

(±)-*form* [54192-03-9]
Prod. by *Penicillium* sp. 20135.
Mp 87-89°.

Raistrick, H. *et al., Biochem. J.*, 1935, **29**, 606-611 (*isol*)
Barton, D.H.R. *et al., J.C.S.*, 1955, 1028 (*struct, abs config*)
Auerbach, J. *et al., Chem. Comm.*, 1974, 298 (*synth*)
Garson, M.J. *et al., Chem. Comm.*, 1977, 624 (*biosynth*)
Barton, D.H.R. *et al., J.C.S. Perkin 1*, 1977, 1103 (*synth, stereoisomers*)
Hill, R.A. *et al., J.C.S. Perkin 1*, 1981, 2570 (*biosynth*)
Klunder, A.J.H. *et al., Tet. Lett.*, 1981, **22**, 4557 (*synth*)
Altenbach, H.-J. *et al., Angew. Chem., Int. Ed.*, 1990, **29**, 67 (*synth*)
Kolb, H.C. *et al., Tetrahedron: Asymmetry*, 1990, **1**, 237 (*synth*)
Kawakubo, J. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1208 (*isol, bibl*)
Mikolajczyk, M. *et al., Angew. Chem., Int. Ed.*, 1996, **35**, 1560 (*synth, isomers*)
Harper, J.K. *et al., Acta Cryst. C*, 2000, **56**, e570-e571 (*cryst struct*)
Malmstrom, J. *et al., J. Nat. Prod.*, 2002, **65**, 364-367 (*Dihydroterrein*)
Lee, S. *et al., Bioorg. Med. Chem. Lett.*, 2005, **15**, 471-473 (*isol, synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 769

Terreusinone T-66

*2,6-Bis(1-hydroxy-2-methylpropyl)-1*H,*5*H*-pyrrolo[2,3*-b*]indole-4,8-dione*
[637334-34-0]



Absolute Configuration

$C_{18}H_{22}N_2O_4$ 330.383
Prod. by the marine fungus *Aspergillus terreus* (MFA-460). Potent Uv-A protectant. Yellowish solid.
Mp 230° dec. $[\alpha]_D$ +47 (c, 0.3 in MeOH). λ_{max} 204 (log ϵ 3.73); 247 (log ϵ 4.08); 277 (log ϵ 3.83); 355 (log ϵ 3.57) (MeOH).

Lee, S.M. *et al., Tet. Lett.*, 2003, **44**, 7707-7710 (*isol, cd, pmr, cmr, ms*)

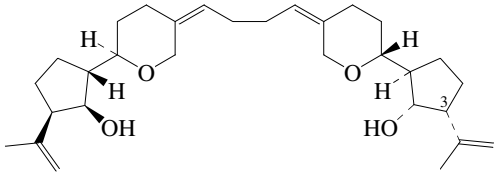
Tessulatoxin T-67

[85497-48-9]
Protein. Isol. from venom of *Conus tessulatus*. Vasoactive and ichthyotoxic agent.

Kobayashi, J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1983, **74**, 381-384 (*isol*)

Testudinariol A T-68

[200567-51-7]



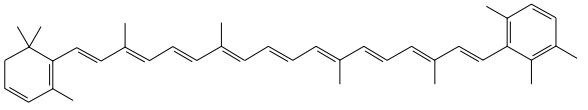
$C_{30}H_{46}O_4$ 470.691
Constit. of *Pleurobranchus testudinarius*. Oil. $[\alpha]_D^{25}$ +15.2 (c, 0.3 in $CHCl_3$).

3-Epimer: ***Testudinariol B***
[200567-52-8]
$C_{30}H_{46}O_4$ 470.691
Constit. of *Pleurobranchus testudinarius*. Oil. $[\alpha]_D^{25}$ +15 (c, 0.05 in $CHCl_3$).

Spinella, A. *et al., Tetrahedron*, 1997, **53**, 16891-16896 (*isol, pmr, cmr*)
Hioki, H. *et al., Chem. Lett.*, 2001, 898-899 (*synth*)
Yoshida, M. *et al., J.C.S. Perkin 1*, 2001, 1007-1017 (*synth*)
Takikawa, H. *et al., Tet. Lett.*, 2001, **42**, 1527-1530 (*synth*)
Amarasinghe, K.K.D. *et al., J.A.C.S.*, 2002, **124**, 9366-9367 (*synth*)

Tethyanin T-69

3,4-Didehydro-β,ϕ-carotene
[94664-02-5]

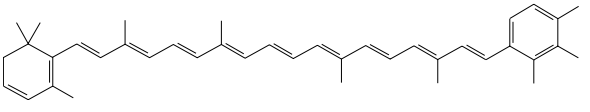


$C_{40}H_{50}$ 530.835
Constit. of *Tethya amamensis*. λ_{max} 456 (petrol).

Tanaka, Y. *et al., Nippon Suisan Gakkaishi*, 1984, **50**, 1787 (*occur, uv, ir, ms, pmr*)

Tethyatene T-70

3,4-Didehydro-β,χ-carotene
[65252-69-9]

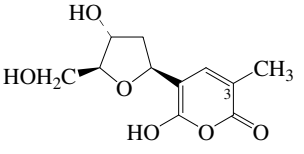


$C_{40}H_{50}$ 530.835
Constit. of *Tethya amamensis* and other sea sponges.
Mp 165°. λ_{max} 468 (petrol).

Tanaka, Y. *et al., Nippon Suisan Gakkaishi*, 1977, **43**, 1229-1232 (*occur, uv, ir, ms*)
Shimada, A. *et al., Tet. Lett.*, 1981, **22**, 773-774 (*synth*)

Tetillapyrone T-71

*5-(Tetrahydro-4-hydroxy-5-hydroxymethyl-2-furanyl)-6-hydroxy-3-methyl-2*H*-pyran-2-one*



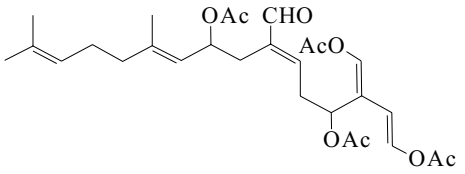
Relative Configuration

$C_{11}H_{14}O_6$ 242.228
Exists as ionic enolate in the solid state, as protonated form (illus.) in soln. Isol. from the sponge *Tetilla japonica*. Needles ($CHCl_3$/MeOH).
Mp 191-192°. $[\alpha]_D^{20}$ +17.6 (Me_2CO). λ_{max} 207 (log ϵ 3.86); 267 (log ϵ 3.85) (MeOH).

Watanadilok, R. *et al., J. Nat. Prod.*, 2001, **64**, 1056-1058 (*isol, pmr, cmr, cryst struct*)

1,4,9,20-Tetraacetoxy-1,3(20),6,10,14-phytapentaen-19-al T-72

4-Acetyloxy-2-[3,6-bis(acetyloxy)-4-(acetyloxymethylene)-5-hexenylidene]-6,10-dimethyl-5,9-undecadienal, 9CI. 4,9-Diacetoxyudoteal. Halimeda tetraacetate
[93888-68-7]



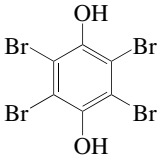
$C_{28}H_{38}O_9$ 518.603
Metab. of many *Halimeda* spp. of green algae. Feeding deterrent to fish. Yellow oil. $[\alpha]_D^{25}$ -1.5 (c, 1.2 in $CHCl_3$). λ_{max} 235 (ϵ 15400) (MeOH) (Derep).

[116560-98-6]

Schmitz, F.J. *et al., Phytochemistry*, 1984, **23**, 1331 (*isol, ir, uv, pmr, cmr, ms*)
Paul, V.J. *et al., Tetrahedron*, 1984, **40**, 3053
Targett, N.M. *et al., Mar. Biol. (Berlin)*, 1986, **92**, 141 (*props*)
Paul, V.J. *et al., J. Exp. Mar. Biol. Ecol.*, 1988, **119**, 15 (*pmr, cmr, metab*)

2,3,5,6-Tetrabromo-1,4-benzenediol, 9CI T-73

Tetrabromohydroquinone, 8CI. Tetrabromoquinol
[2641-89-6]



$C_6H_2Br_4O_2$ 425.697
Isol. from the acorn worm *Ptychodera flava*. Cryst. (EtOH/Et_2O). Mp 244°. Luminescent.

Di-Ac: [7437-72-1]
$C_{10}H_6Br_4O_4$ 509.771
Mp 283-284°.

Bis(4-methylbenzenesulfonyl): [15146-61-9]
Mp 272-273°.

Mono-Me ether: 2,3,5,6-Tetrabromo-4-methoxyphenol
$C_7H_4Br_4O_2$ 439.723
Cryst. (AcOH). Mp 125-126°.

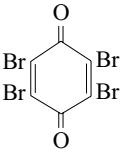
Di-Me ether: 1,2,4,5-Tetrabromo-3,6-dimethoxybenzene, 9CI
[19403-94-2]
$C_8H_6Br_4O_2$ 453.75
Cryst. Mp 194-196°.

Di-Et ether: 1,2,4,5-Tetrabromo-3,6-diethoxybenzene
[120231-44-9]
$C_{10}H_{10}Br_4O_2$ 481.804
Needles (MeOH). Mp 150-151°.

Sarauw, E. *et al., Annalen*, 1881, **209**, 93 (*synth*)
Boehm, J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1967, **41**, 707; 1075 (*synth, uv*)
Wieczorek, M.W. *et al., Acta Cryst. B*, 1980, **36**, 1513 (*cryst struct, deriv*)
Higa, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **65**, 525 (*isol*)
Meador, M.A. *et al., J.O.C.*, 1989, **54**, 2336 (*deriv, synth, pmr, ms*)
Kanakubo, A. *et al., Bioorg. Med. Chem.*, 2005, **13**, 2741-2747 (*isol*)

Tetrabromo-1,4-benzoquinone T-74

2,3,5,6-Tetrabromo-2,5-cyclohexadiene-1,4-dione, 9CI. Bromanil. Tetrabromoquinone
[488-48-2]

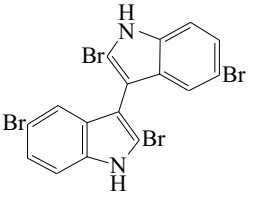


$C_6Br_4O_2$ 423.681
Isol. from the acorn worm *Ptychodera flava*. Golden-yellow cryst. Mp 300° subl. Luminescent.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 715C (*nmr*)
Graebe, C. *et al., Annalen*, 1891, **263**, 31 (*struct, synth*)
Kempf, R. *et al., Ber.*, 1914, **47**, 2615 (*synth*)
Hodgson, H. *et al., J.C.S.*, 1942, 583 (*synth*)
Braude, E.A. *et al., J.C.S.*, 1945, 490 (*uv*)
Iida, Y. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 2955 (*ir*)
Hedayatullah, M. *et al., Bull. Soc. Chim. Fr.*, 1973, 2702 (*synth*)
Yamada, H. *et al., Spectrochim. Acta A*, 1974, **30**, 295 (*ir, Raman*)
Kanakubo, A. *et al., Bioorg. Med. Chem.*, 2005, **13**, 2741-2747 (*isol*)

2,2′,5,5′-Tetrabromo-3,3′-bi-1*H*-indole T-75

3,3′-Bi(2,5-dibromoindole)
[81387-82-8]



$C_{16}H_8Br_4N_2$ 547.869
Isol. from the marine blue-green alga *Rivularia firma*. Anti-inflammatory agent. Rosettes ($CHCl_3$). Mp 239-240°.

Norton, R.S. *et al., J.A.C.S.*, 1982, **104**, 3628-3635 (*isol, uv, ir, pmr, cmr, struct*)

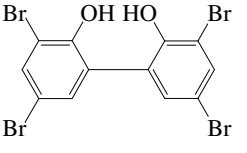
2,2′,6,6′-Tetrabromo-3,3′-bi-1*H*-indole, 9CI T-76

3,3′-Bi(2,6-dibromoindole)
[138779-89-2]
$C_{16}H_8Br_4N_2$ 547.869
Isol. from the cyanobacterium *Rivularia firma*. Viscous oil.

Hodder, A.R. *et al., J. Nat. Prod.*, 1991, **54**, 1661-1663 (*isol, uv, ir, pmr, cmr, ms, struct*)

3,3′,5,5′-Tetrabromo[1,1′-biphenyl]-2,2′-diol, 9CI T-77

3,3′,5,5′-Tetrabromo-2,2′-dihydroxybiphenyl. MC21-A. Antibiotic MC21-A
[21987-62-2]



$C_{12}H_6Br_4O_2$ 501.794
Prod. by the marine-derived *Pseudomonas phenolica* sp. O-BC30T. Antibacterial agent (anti-MRSA). Cryst. ($CHCl_3$). Sol. MeOH, $CHCl_3$; insol. H_2O, hexane. Mp 205-207°. λ_{max} 211; 301 (MeOH).

▶ Exp. fetotoxic and teratogenic effects. DV5185000

Dihydrogen phosphate: ***Bromofenofos, INN****. 3,3′,5,5′-Tetrabromo[1,1′-biphenyl]-2,2′-diol mono(dihydrogen phosphate), 9CI. Bromfenofos. Acedist. Ph 1882*
[21466-07-9]
$C_{12}H_7Br_4O_5P$ 581.774
Fasciolicide. Mp 350° dec.

▶ Exp. reprod. and teratogenic effects. DV5190000

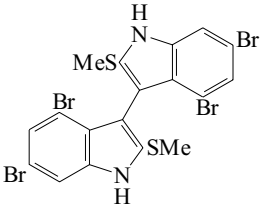
Bis(methoxymethyl) ether: [121169-13-9]
$C_{16}H_{14}Br_4O_4$ 589.9
Cryst. (EtOAc). Mp 110°.

[14957-65-4, 23015-40-9, 63990-95-4]

van der Meer, S. *et al., J. Med. Chem.*, 1969, **12**, 534 (*synth, deriv, pharmacol*)
Perold, G.W. *et al., J. S. Afr. Chem. Inst.*, 1975, **28**, 300 (*synth, pmr*)
Yoshimura, H. *et al., Arch. Toxicol.*, 1987, **60**, 319; 325 (*tox*)
Endoh, Y.S. *et al., J. Chromatogr.*, 1988, **426**, 202 (*hplc*)
Isnansetyo, A. *et al., Antimicrob. Agents Chemother.*, 2003, **47**, 480-488 (*isol, pmr, cmr*)
Alexakis, A. *et al., J.O.C.*, 2004, **69**, 5660-5667 (*synth, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BNV500; DAZ110

4,4′,6,6′-Tetrabromo-2,2′-bis(methylthio)-3,3′-bi-1*H*-indole, 9CI T-78

*3,3′-Bi[4,6-dibromo-2-methylthio-1*H*-indole]*
[128351-82-6]



$C_{18}H_{12}Br_4N_2S_2$ 640.054
Alkaloid from the Okinawan red alga *Laurencia brongniartii*.
Cryst. (hexane/$CHCl_3$).
Mp 186-188°. λ_{max} 236 (ϵ 50000); 306 (ϵ 20000) (EtOH).

*2-*S*-Oxide:* ***4,4′,6,6′-Tetrabromo-2-(methylsulfinyl)-2′-(methylthio)-3,3′-bi-1*H*-indole***
$C_{18}H_{12}Br_4N_2OS_2$ 656.054
Isol. from *Laurencia brongniartii*.
Mp 187-189°. $[\alpha]_D^{25}$ +36 (c, 0.2 in $CHCl_3$). λ_{max} 238 (log ϵ 4.7); 312 (log ϵ 4.1) (MeOH).

*2,2′-Di-*S*-oxide:* ***4,4′,6,6′-Tetrabromo-2,2′-bis(methylsulfinyl)-3,3′-bi-1*H*-indole***
$C_{18}H_{12}Br_4N_2O_2S_2$ 672.053
Isol. from *Laurencia brongniartii*.
Mp 191-193°. λ_{max} 233 (log ϵ 4.5); 309 (log ϵ 3.08) (MeOH).

2-De(methylthio), 2-bromo: ***2,4,4′,6,6′-Pentabromo-2′-(methylthio)-3,3′-bi-1*H*-indole***
[873202-17-6]
$C_{17}H_9Br_5N_2S$ 672.858
Alkaloid from *Laurencia brongniartii*. λ_{max} 212 (sh) (ϵ 28390); 234 (ϵ 40925); 296 (ϵ 11930) (MeOH).

Tanaka, J. *et al., Tetrahedron*, 1989, **45**, 7301-7310 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Kubota, N.K. *et al., Heterocycles*, 2005, **65**, 2675-2682 (*demethylthio-2-bromo*)
El-Gamal, A.A. *et al., J. Nat. Prod.*, 2005, **68**, 815-817 (*oxides*)

1,1,4,4-Tetrabromo-3-buten-2-ol T-79

$Br_2C{=}CHCH(OH)CHBr_2$
$C_4H_4Br_4O$ 387.691

(+)-form [62872-11-1]
Constit. of the red alga *Asparagopsis taxiformis*.
Needles (pentane).
Mp 84.5-85.5°. $[\alpha]_D^{24}$ +7.9 (c, 2.6 in CH_2Cl_2).
Woolard, F.X. *et al., Tetrahedron*, 1976, **32**, 2843 (*isol, ms, synth*)

1,1,4,4-Tetrabromo-3-buten-2-one T-80

[59228-07-8]
$Br_2C{=}CHCOCHBr_2$
$C_4H_2Br_4O$ 385.675
Constit. of the seaweed *Asparagopsis armata* and red alga *Asparagopsis taxiformis*. Originally assigned the 1,1,3,4-tetrabromo struct., revised in 1976.

[55716-05-7, 56020-83-8]

Woolard, F.X. *et al., Tetrahedron*, 1976, **332**, 2843

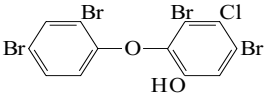
1,3,4,4-Tetrabromo-3-buten-2-one T-81

[69267-74-9]
$Br_2C{=}CBrCOCH_2Br$
$C_4H_2Br_4O$ 385.675
Constit. of the red alga *Ptilonia australasica*.

Kazlauskas, R. *et al., Tet. Lett.*, 1978, 3165-3168 (*isol, struct*)

2,2′,4,4′-Tetrabromo-3-chloro-6-hydroxydiphenyl ether T-82

3,5-Dibromo-4-chloro-2-(2,4-dibromophenoxy)phenol
[79755-45-6]

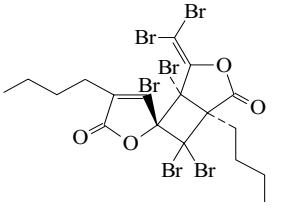


$C_{12}H_5Br_4ClO_2$ 536.239
Isol. from an unidentified Australian sponge. Prisms.
Mp 181-181.5°.

Capon, R. *et al., J.C.S. Perkin 1*, 1981, 2464-2467 (*isol, spectra, cryst struct*)

3,5′,7′,7′-Tetrabromo-1′,4-dibutyl-4′-(dibromomethylene)spiro[furan-2(5*H*),6′-[3]oxabicyclo[3.2.0]heptane]-2′,5-dione, 9CI T-83

[115747-17-6]

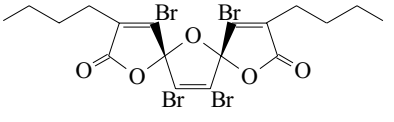


$C_{18}H_{18}Br_6O_4$ 777.762
Constit. of the red alga *Delisea elegans*.
Mp 105.5-106°.

McCombs, J.D. *et al., Tetrahedron*, 1988, **44**, 1489

4,11,12,13-Tetrabromo-3,10-dibutyl-1,6,8-trioxadispiro[4.1.4.2]trideca-3,10,12-triene-2,9-dione, 9CI T-84

[115721-47-6]

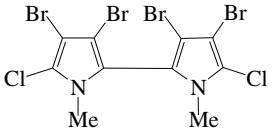


$C_{18}H_{18}Br_4O_5$ 633.953
Constit. of the red alga *Delisea elegans*. Needles (pentane).

McCombs, J.D. *et al., Tetrahedron*, 1988, **44**, 1489

3,3′,4,4′-Tetrabromo-5,5′-dichloro-1,1′-dimethyl-2,2′-bi-1*H*-pyrrole T-85

[253798-64-0]

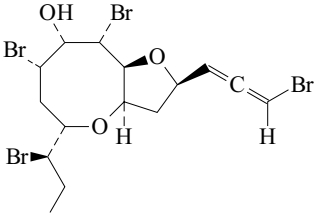


$C_{10}H_6Br_4Cl_2N_2$ 544.692

Isol. from the eggs of various seabirds. Cryst. (Me_2CO). Mp 221° dec.

Gribble, G.W. *et al., Chem. Comm.*, 1999, 2195-2196 (*synth, pmr, ms, cryst struct*)

3,6,8,15-Tetrabromo-4,10:9,12-diepoxy-13,14-pentadecadien-7-ol T-86



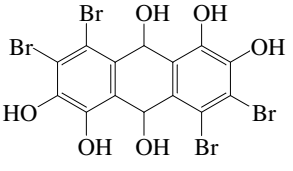
$C_{15}H_{20}Br_4O_3$ 567.937

Not named in reference. Constit. of *Mycale rotalis*. Cryst. ($CHCl_3$). Mp 128-130°. $[\alpha]_D^{20}$ +38.8 (c, 1.3 in $CHCl_3$).

Notaro, G. *et al., J. Nat. Prod.*, 1992, **55**, 626 (*isol, pmr, cmr, cryst struct*)

3,4,7,8-Tetrabromo-9,10-dihydro-1,2,5,6,9,10-anthracenehexol T-87

1,2,5,6-Tetrabromo-9,10-dihydro-3,4,7,8,9,10-hexahydroxyanthracene



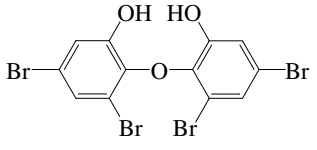
$C_{14}H_8Br_4O_6$ 591.83

9,10-Di-Me ether: 3,4,7,8-Tetrabromo-9,10-dihydro-9,10-dimethoxy-1,2,5,6-anthracenetetrol. 3,4,7,8-Tetrabromo-9,10-dihydro-1,2,5,6-tetrahydroxy-9,10-dimethoxyanthracene
$C_{16}H_{12}Br_4O_6$ 619.883
Constit. of the brown alga *Leathesia nana*. Brown powder (Me_2CO).
Mp 117-119° dec.

Xu, X. *et al., J. Nat. Prod.*, 2004, **67**, 1661-1666 (*isol, pmr, cmr, ms*)

2,2′,4,4′-Tetrabromo-6,6′-dihydroxydiphenyl ether T-88

3,3′,5,5′-Tetrabromo-2,2′-oxybisphenol. 2,2′-Oxybis[3,5-dibromophenol]

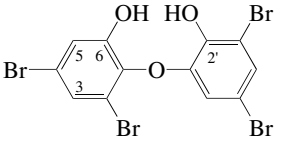


$C_{12}H_6Br_4O_3$ 517.794

Mono-Me ether: 3,5-Dibromo-2-(2,4-dibromo-6-methoxyphenoxy)-phenol. 2,2′,4,4′-Tetrabromo-6-hydroxy-6′-methoxydiphenyl ether
[372478-61-0]
$C_{13}H_8Br_4O_3$ 531.82
Isol. from *Phyllospongia dendyi*.
Hattori, T. *et al., Fish. Sci.*, 2001, **67**, 899-903 (*isol*)

2,3′,4,5′-Tetrabromo-2′,6-dihydroxydiphenyl ether T-89

3,4′,5,6′-Tetrabromo-2,2′-oxybisphenol



$C_{12}H_6Br_4O_3$ 517.794
Mp 143-145°.

2′-Me ether: 2,3′,4,5′-Tetrabromo-6-hydroxy-2′-methoxydiphenyl ether. 3,5-Dibromo-2-(3,5-dibromo-2-methoxyphenoxy)phenol, 9CI. 2,4-Dibromo-6-(2,4-dibromo-6-hydroxyphenoxy)anisole
[80246-35-1]
$C_{13}H_8Br_4O_3$ 531.82
Metab. of the sponge *Dysidea* spp. and from *Vibrio* sp. associated with a *Dysidea* sp. Active against *Staphylococcus aureus* and *Trichophyton meuloprophytes*. Pale green wax.
Mp 32-33°. λ_{max} 284 (sh) (ϵ 3800); 291 (ϵ 4100) (MeOH).

6-Me ether: 2,3′,4,5′-Tetrabromo-2′-hydroxy-6-methoxydiphenyl ether. 2,4-Dibromo-6-(2,4-dibromo-6-methoxyphenoxy)phenol
[170473-60-6]
$C_{13}H_8Br_4O_3$ 531.82
Metab. of *Dysidea* spp.

Di-Me ether: 2,3′,4,5′-Tetrabromo-2′,6-methoxydiphenyl ether
[76652-99-8]
$C_{14}H_{10}Br_4O_3$ 545.847
Metab. of *Phyllospongia foliascens*.
Mp 86-88°. λ_{max} 215 (ϵ 10000) (MeOH).

3-Bromo: 2,3,3′,4,5′-Pentabromo-2′,6-dihydroxydiphenyl ether. 3,4,5-Tribromo-2-(3,5-dibromo-2-hydroxyphenoxy)phenol
[170473-61-7]
$C_{12}H_5Br_5O_3$ 596.69
Metab. of *Dysidea* spp. Inhibitor of inosine monophosphate synthetase and glucosamine monophosphate synthetase. Fine needles (MeOH).
Mp 132-133°.

3-Bromo, 2′-Me ether: 2,3,3′,4,5′-Pentabromo-6-hydroxy-2′-methoxydiphenyl ether. 3,4,5-Tribromo-2-(3,5-dibromo-2-methoxyphenoxy)phenol
[170473-63-9]
$C_{13}H_7Br_5O_3$ 610.717
Metab. of *Dysidea* sp. Inhibitor of inosine monophosphate synthetase and glucosamine monophosphate synthetase. Viscous oil.

3-Bromo, 6-Me ether: 2,3,3′,4,5′-Pentabromo-2′-hydroxy-6-methoxydiphenyl ether. 2,4-Dibromo-6-(2,3,4-tribromo-6-methoxyphenoxy)phenol
[661476-66-0]
$C_{13}H_7Br_5O_3$ 610.717
Isol. from the sponge *Phyllospongia dendyi*. Viscous oil. λ_{max} 232 (ϵ 25000); 294 (ϵ 6100) (EtOH).

3-Bromo, di-Me ether: 2,3,3′,4,5′-Pentabromo-2′,6-dimethoxydiphenyl ether
[170473-62-8]
$C_{14}H_9Br_5O_3$ 624.743
Isol. from *Dysidea herbacea* and *Phyllospongia dendyi*. Cryst. ($CHCl_3$).
Mp 142-144°. λ_{max} 282 (ϵ 3200); 290 (ϵ 4000); 299 (ϵ 3000) (MeOH).

5-Bromo: 2,3′,4,5,5′-Pentabromo-2′,6-dihydroxydiphenyl ether. 2,3,5-Tribromo-6-(3,5-dibromo-2-hydroxyphenoxy)phenol
[80246-26-0]
$C_{12}H_5Br_5O_3$ 596.69
Metab. of *Phyllospongia foliascens* . Cryst. ($CHCl_3$).
Mp 183-184°.

5-Bromo, 6-Me ether: 2,3′,4,5,5′-Pentabromo-2′-hydroxy-6-methoxydiphenyl ether. 2,4-Dibromo-6-(2,4,5-tribromo-6-methoxyphenoxyl)phenol
[80246-34-0]
$C_{13}H_7Br_5O_3$ 610.717
Metab. of *Dysidea* sp. Cryst. ($CHCl_3$).
Mp 202-204°.

3,5-Dibromo: 2,3,3′,4,5,5′-Hexabromo-2′,6-dihydroxydiphenyl ether. 2,3,4,5-Tetrabromo-6-(3,5-dibromo-2-hydroxyphenoxy)phenol
[80246-27-1]
$C_{12}H_4Br_6O_3$ 675.586
Metab. of *Dysidea* sp.

3,5-Dibromo, 6-Me ether: 2,3,3′,4,5,5′-Hexabromo-2′-hydroxy-6-methoxydiphenyl ether. 2,4-Dibromo-6-(2,3,4,5-tetrabromo-6-methoxyphenoxy)phenol
[661476-65-9]
$C_{13}H_6Br_6O_3$ 689.613
Isol. from the sponge *Phyllospongia dendyi*. Viscous oil. λ_{max} 232 (ϵ 22600); 292 (ϵ 5000) (EtOH).

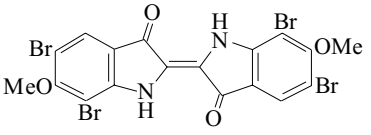
2-Debromo, 2′-Me ether: 3,4′,5-Tribromo-2′-hydroxy-2-methoxydiphenyl ether
[372478-62-1]
$C_{13}H_9Br_3O_3$ 452.924
Isol. from the sponge *Phyllospongia dendyi*.

3′-Debromo, 2′-Me ether: 2,4,5′-Tribromo-6-hydroxy-2′-methoxydiphenyl ether
[372478-63-2]
$C_{13}H_9Br_3O_3$ 452.924
Isol. from the sponge *Phyllospongia dendyi*.

Carté, B *et al., Tetrahedron*, 1981, **37**, 2335-2339 (*di-Me ether, isol, uv, pmr*)
Norton, R.S. *et al., Tetrahedron*, 1981, **37**, 2341-2349 (*2′-Me ether, di-Me ether, isol, ms, pmr*)
Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1987, **23**, 603-605; *Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 508-509 (*2′-Me ether*)
Elyakov, G.B. *et al., Experientia*, 1991, **47**, 632-633 (*2′-Me ether, isol*)
Fu, X. *et al., J. Nat. Prod.*, 1995, **58**, 1384-1391 (*3-bromo di-Me ether, 5-bromo, 5-bromo 6-Me ether, 3,5-dibromo, isol*)
Popov, A.M. *et al., Khim.-Farm. Zh.*, 1999, **33**, 71-73; *CA*, 2000, **132**, 61495 (*2′-Me ether, isol, activity*)
Hattori, T. *et al., Fish. Sci.*, 2001, **67**, 899-903 (*Phyllospongia dendyi ethers*)
Liu, H. *et al., J. Nat. Prod.*, 2004, **67**, 472-474 (*Phyllospongia dendyi ethers*)

5,5′,7,7′-Tetrabromo-6,6′-dimethoxyindigotin T-90

[58933-45-2]



$C_{18}H_{10}Br_4N_2O_4$ 637.904
Pigment from the marine invertebrate *Ptychodera flava laysanica*.
Purple-blue powder.
Mp 300°.

Higa, T. *et al., Heterocycles*, 1976, **4**, 227 (*isol, struct*)

1,1,3,3-Tetrabromo-2-heptanol T-91

[66002-42-4]
$H_3C(CH_2)_3CBr_2CH(OH)CHBr_2$
$C_7H_{12}Br_4O$ 431.787
Constit. of the red algae *Bonnemaisonia* spp.

Ac: [69394-12-3]
$C_9H_{14}Br_4O_2$ 473.824
Constit. of *Bonnemaisonia hamifera*.

Jacobsen, N. *et al., Tet. Lett.*, 1978, **19**, 3065-3068 (*isol*)
McConnell, O.J. *et al., Phytochemistry*, 1980, **19**, 233-247 (*isol*)

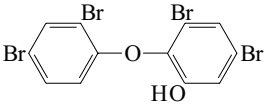
1,1,3,3-Tetrabromo-2-heptanone T-92

[54899-94-4]
$H_3C(CH_2)_3CBr_2COCHBr_2$
$C_7H_{10}Br_4O$ 429.771
Constit. of the red alga *Bonnemaisonia hamifera*.

Siuda, J.F. *et al., J.A.C.S.*, 1975, **97**, 937 (*synth, ms*)

2,2′,4,4′-Tetrabromo-6-hydroxydiphenyl ether T-93

3,5-Dibromo-2-(2,4-dibromophenoxy)phenol
[79755-43-4]



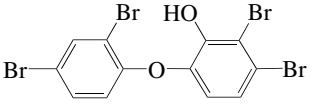
$C_{12}H_6Br_4O_2$ 501.794
Isol. from an unidentified Australian sponge.
Mp 172.5-173°.

Me ether: 2,2′,4,4′-Tetrabromo-6-methoxydiphenyl ether. 3,5-Dibromo-2-(2,4-dibromophenoxy)anisole
[102739-99-1]
$C_{13}H_8Br_4O_2$ 515.821
Constit. of the sponge *Dysidea herbacea*. Needles (EtOAc/petrol or CH_2Cl_2/MeOH).
Mp 116.5-117.5°.

Capon, R. *et al., J.C.S. Perkin 1*, 1981, 2464-2467 (*isol, spectra, cryst struct*)
Francesconi, K.A. *et al., Aust. J. Chem.*, 1985, **38**, 1271-1277 (*synth, pmr*)
Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 89-90 (*Me ether, isol*)
Marsh, G. *et al., Eur. J. Org. Chem.*, 2003, 2566-2576 (*Me ether, synth, pmr, ms*)

2′,3,4,4′-Tetrabromo-2-hydroxydiphenyl ether T-94

2,3-Dibromo-6-(2,4-dibromophenoxy)phenol
[184174-87-6]



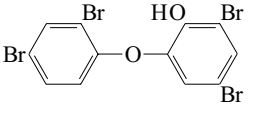
$C_{12}H_6Br_4O_2$ 501.794
Isol. from the sponge *Dysidea* sp.

6-Bromo: 2,3,5-Tribromo-6-(2,4-dibromophenoxy)phenol. 2′,3,4,4′,6-Pentabromo-2-hydroxydiphenyl ether
$C_{12}H_5Br_5O_2$ 580.69
Isol. from *Dysidea herbacea*. Prisms (MeCN).
Mp 113-114°. λ_{max} 218 (sh) (ϵ 22500); 231 (ϵ 24900); 286 (sh) (ϵ 3700); 292 (ϵ 4000) (no solvent reported).

Fu, X. *et al., J. Nat. Prod.*, 1996, **59**, 1102-1103 (*isol, ir, pmr, cmr, ms*)
Bowden, B.F. *et al., Aust. J. Chem.*, 2000, **53**, 299-301 (*6-bromo*)

2′,3,4′,5-Tetrabromo-2-hydroxydiphenyl ether T-95

2,4-Dibromo-6-(2,4-dibromophenoxy)phenol, 9CI
[80246-25-9]



$C_{12}H_6Br_4O_2$ 501.794
Constit. of the marine sponge *Dysidea chlorea* and from a cyanobacterial symbiont of *Dysidea herbacea*. Cryst. (hexane/petrol).
Mp 90-91° (88-90°).

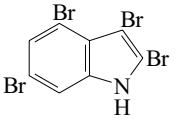
Ac: [80246-32-8]
Mp 118-119°.

Me ether: 2′,3,4′,5-Tetrabromo-2-methoxydiphenyl ether. 4,6-Dibromo-2-(2,4-dibromophenoxy)anisole
[96920-28-4]
$C_{13}H_8Br_4O_2$ 515.821
Isol. from *Aplysia dactylomela*, *Cladophora fascicularis* and *Dysidea* sp. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. λ_{max} 239 (ϵ 11600); 284 (ϵ 1800) (hexane) (Berdy).

Carté, B. *et al., Tetrahedron*, 1981, **37**, 2335 (*isol, pmr*)
Francesconi, K.A. *et al., Aust. J. Chem.*, 1985, **38**, 1271-1277 (*synth*)
Kuniyoshi, M. *et al., Experientia*, 1985, **41**, 523-524 (*Me ether*)
Sakai, R. *et al., Helv. Chim. Acta*, 1986, **69**, 91-105 (*isol, Me ether*)
Unson, M.D. *et al., Mar. Biol. (Berlin)*, 1994, **119**, 1 (*isol*)
Fu, X. *et al., J. Nat. Prod.*, 1995, **58**, 1384 (*isol*)
Cameron, G.M. *et al., Tetrahedron*, 2000, **56**, 5247-5252 (*Me ether, isol, pmr, cmr, ms*)

2,3,4,6-Tetrabromo-1*H*-indole, 9CI T-96

[128351-87-1]



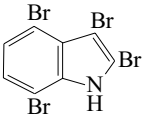
$C_8H_3Br_4N$ 432.734
Alkaloid from the Okinawan red alga *Laurencia brongniartii*.
Cryst. (hexane/CCl_4). Mp 137-141°.

N-*Ac:* [128351-91-7]
$C_{10}H_5Br_4NO$ 474.772
Cryst. (hexane/CCl_4). Mp 176-178°.

Tanaka, J. *et al., Tetrahedron*, 1989, **45**, 7301 (*isol, ir, pmr, ms, struct*)

2,3,4,7-Tetrabromo-1*H*-indole, 9CI T-97

[68234-23-1]



$C_8H_3Br_4N$ 432.734
Alkaloid from the marine red alga *Rhodophyllis membranacea*.
Mp 144.5°.

Brennan, M.R. *et al., Tet. Lett.*, 1978, 1637 (*isol, pmr, struct*)
Ohta, T. *et al., Heterocycles*, 1989, **29**, 1663 (*synth*)

2,3,5,6-Tetrabromo-1*H*-indole, 9CI T-98

[17826-06-1]

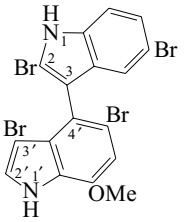
$C_8H_3Br_4N$ 432.734
Alkaloid from the algae *Laurencia brongniartii* and *Laurencia similis*.
Mp 152.5-154° (149-151°). λ_{max} 230 (ϵ 47000); 294 (ϵ 9600); 301 (ϵ 9500) (EtOH) (Derep).

N-*Me:* ***2,3,5,6-Tetrabromo-1-methyl-1*H*-indole***
[25055-55-4]
$C_9H_5Br_4N$ 446.761
Alkaloid from *Laurencia brongniartii*. Cryst. (petrol).
Mp 171.5-172° (168-170°). λ_{max} 233 (ϵ 49000); 296 (ϵ 10000); 303 (ϵ 10000) (EtOH) (Derep).

Settimo, A.D. *et al., Gazz. Chim. Ital.*, 1967, **97**, 1304; 1977, **107**, 367 (*synth*)
Settimo, A.D. *et al., J.O.C.*, 1970, **35**, 2546-2551 (*N-Me, synth*)
Carter, G.T. *et al., Tet. Lett.*, 1978, 4479-4482 (*N-Me, isol, uv, pmr, ms*)
Liu, Y. *et al., J. Nat. Prod.*, 2002, **65**, 748-749 (*N-Me, synth*)

2,3′,5,5′-Tetrabromo-7′-methoxy-3,4′-bi-1*H*-indole T-99

Rivularin D₃



$C_{17}H_{10}Br_4N_2O$ 577.895
λ_{max} 227 (ϵ 66000); 280 (ϵ 16000); 290 (ϵ 17000); 299 (ϵ 14000) (MeCN) (Berdy).

(+)-*form* [81387-83-9]
Isol. from the marine blue-green alga *Rivularia firma*. Shows antiinflammatory, antiallergic, CNS depressant and tremorgenic props. Prisms (CH_2Cl_2/hexane). Sol. MeOH, $CHCl_3$.
Mp 178-179° dec. $[\alpha]_D^{20}$ +71 (c, 1 in $CHCl_3$). Exhibits opt. activity owing to restricted rotn.

1-N-*Ac:*
Prisms (CH_2Cl_2/hexane). Mp 109-111°. $[\alpha]_D^{20}$ +99 (c, 1 in $CHCl_3$).

Di-N-*Ac:*
Prisms (CH_2Cl_2/hexane). Mp 96-98°. $[\alpha]_D^{20}$ +71 (c, 0.75 in $CHCl_3$).

*2-Debromo: 3′,5,5′-Tribromo-7′-methoxy-3,4′-bi-1*H*-indole.* ***Rivularin D₁***
[81387-84-0]
$C_{17}H_{11}Br_3N_2O$ 498.999
Isol. from the marine blue-green alga *Rivularia firma*. Anti-inflammatory agent. Prisms ($CHCl_3$).
Mp 220-223°. $[\alpha]_D^{20}$ +8.5 (c, 1 in $CHCl_3$). Exhibits opt. activity owing to restricted rotn. λ_{max} 283; 288; 297 (MeOH) (Berdy). λ_{max} 291 (ϵ 13100) (MeCN) (Berdy).

*3′-Debromo: 2,5,5′-Tribromo-7′-methoxy-3,4′-bi-1*H*-indole*
[81387-85-1]
$C_{17}H_{11}Br_3N_2O$ 498.999
Isol. from the marine blue-green alga *Rivularia firma*. Foam. $[\alpha]_D^{20}$ +11.3 (c, 1 in $CHCl_3$). Exhibits opt. activity owing to restricted rotn.

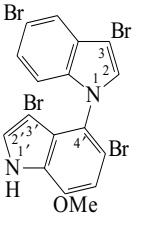
(±)-*form* [95739-89-2]
Synthetic.
Beige prisms (CH_2Cl_2/hexane). Mp 180°.

2-Debromo: [95739-88-1] Synthetic.
Cryst. ($CHCl_3$). Mp 220-223° dec.

Norton, R.S. *et al., J.A.C.S.*, 1982, **104**, 3628-3635 (*isol, uv, ir, pmr, cmr, struct*)
Maehr, H. *et al., J.A.C.S.*, 1985, **107**, 2943-2945 (*synth, uv, ir, pmr, ms*)

3,3′,5,5′-Tetrabromo-7′-methoxy-1,4′-bi-1*H*-indole T-100

[81387-86-2]



$C_{17}H_{10}Br_4N_2O$ 577.895
Isol. from the marine blue-green alga *Rivularia firma*. Poorly cryst. solid ($CHCl_3$/hexane).
Mp 196-200°. $[\alpha]_D^{20}$ -6 (c, 1 in MeCN). Exhibits opt. activity owing to restricted rotn.

Norton, R.S. *et al., J.A.C.S.*, 1982, **104**, 3628-3635 (*isol, uv, ir, pmr, cmr, struct*)

1,1,3,3-Tetrabromo-2-nonanone T-101

[66002-44-6]

$H_3C(CH_2)_5CBr_2COCHBr_2$

$C_9H_{14}Br_4O$ 457.825

Constit. of the red alga *Bonnemaisonia nootkana*.

McConnell, O.J. *et al., Phytochemistry*, 1980, **29**, 233 (*isol*)

1,1,2,4-Tetrabromo-1-octen-3-one T-102

[64822-80-6]

$H_3C(CH_2)_3CHBrCOCBr{=}CBr_2$

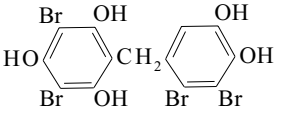
$C_8H_{10}Br_4O$ 441.782

Constit. of the red seaweed *Delisea fimbriata*.

Rose, A.F. *et al., Tet. Lett.*, 1977, 1847

2′,3,3′,5-Tetrabromo-2,4,4′,5′,6-pentahydroxydiphenylmethane T-103

2,4-Dibromo-6-[(2,3-dibromo-4,5-dihydroxyphenyl)methyl]-1,3,5-benzenetriol



$C_{13}H_8Br_4O_5$ 563.819

Penta-Me ether: 2′,3,3′,5-Tetrabromo-2,4,4′,5′,6-pentamethoxydiphenylmethane

Constit. of red alga *Rytiphloea tinctoria*.

Cryst. (MeOH).

Mp 129°. Genus name incorrectly given as Rytiphlea.

Chevolot-Magueur, A.-M. *et al., Phytochemistry*, 1976, **15**, 767 (*isol, struct*)

1,1,1,3-Tetrabromo-2-propanone T-104

1,1,1,3-Tetrabromoacetone

[62874-50-4]

$BrCH_2COCBr_3$

$C_3H_2Br_4O$ 373.664

Metabolite of *Asparagopsis taxiformis*. Needles.

Mp 37-38°. Bp 258° dec. Bp_{14} 139°.

Tetrahydrate:

Prisms. Mp 62°.

Dippy, J.F.J. *et al., J.C.S.*, 1931, 2508 (*synth*)
Weygand, F. *et al., Chem. Ber.*, 1949, **82**, 333 (*synth*)
McConnel, O. *et al., Phytochemistry*, 1977, **16**, 367 (*isol*)

1,1,3,3-Tetrabromo-2-propanone, 9CI T-105

1,1,3,3-Tetrabromoacetone

[22612-89-1]

$Br_2CHCOCHBr_2$

$C_3H_2Br_4O$ 373.664

Found in *Asparagopsis taxiformis, Asparagopsis armata* and *Falkenbergia rufolanosa*. Bp_7 129-130°.

Rappe, C. *et al., Acta Chem. Scand.*, 1962, **16**, 2467 (*synth, pmr*)
Fenical, W. *et al., Tet. Lett.*, 1974, 4463 (*ms*)
McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367-374 (*isol*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **7**, 4717-4719 (*use*)

1,1,3,3-Tetrabromo-1-propene T-106

[56020-79-2]

$Br_2CHCH{=}CBr_2$

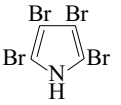
$C_3H_2Br_4$ 357.665

Isol. from the alga *Asparagopsis taxiformis*.

Burreson, B.J. *et al., Tet. Lett.*, 1975, 473 (*isol, ms*)
Lambert, J.B. *et al., Tet. Lett.*, 1978, 4253 (*synth*)
Stavnebrekk, P.J. *et al., J. Mol. Struct.*, 1987, **162**, 101 (*conformn*)

2,3,4,5-Tetrabromo-1*H*-pyrrole, 9CI T-107

[54705-14-5]



C_4HBr_4N 382.675

Metab. of marine *Chromobacterium* sp. Has antibiotic activity.

Spar. sol. H_2O.

Mp 250°. Unstable, v. light-sensitive.

N-*Me:* [56454-29-6]

$C_5H_3Br_4N$ 396.701

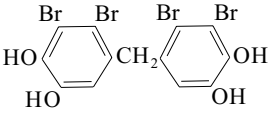
Mp 154-155°. Blue melt.

De Varda, G. *et al., Ber.*, 1888, **21**, 2871 (*synth*)
Andersen, R.J. *et al., Mar. Biol. (Berlin)*, 1974, **27**, 281 (*isol, ms, struct*)
Gilow, H.M. *et al., J.O.C.*, 1981, **46**, 2221 (*synth, glc*)

2,2′,3,3′-Tetrabromo-4,4′,5,5′-tetrahydroxydiphenylmethane T-108

4,4′-Methylenebis[5,6-dibromo-1,2-benzenediol], 9CI. Bis(2,3-dibromo-4,5-dihydroxyphenyl)methane

[65487-76-5]



$C_{13}H_8Br_4O_4$ 547.82

Constit. of the marine algae *Rhodomela larix, Rhodomela confervoides, Polysiphonia nigrescens* and *Polysiphonia brodiaci*.

Cryst. (C_6H_6/MeOH).

Mp 200-201°.

6,6′-Dibromo: 2,2′,3,3′,6,6′-Hexabromo-4,4′,5,5′-tetrahydroxydiphenylmethane. Bis(2,3,6-tribromo-4,5-dihydroxyphenyl)methane

$C_{13}H_6Br_6O_4$ 705.612

Isol. from *Symphyocladia latiuscula*. Pale yellow amorph. solid.

Mp 228-230°.

2-Debromo, 6,6′-dibromo: 2,2′,3,5′,6-Pentabromo-3′,4,4′,5-tetrahydroxydiphenylmethane

$C_{13}H_7Br_5O_4$ 626.716

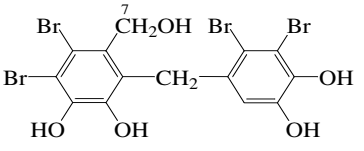
Isol. from *Symphyocladia latiuscula*. Pale yellow amorph. solid.

Mp 168-172°.

Kurata, K. *et al., Chem. Lett.*, 1977, 1435-1438 (*isol, struct*)
Lundgren, L. *et al., Acta Chem. Scand., Ser. B*, 1979, **33**, 105 (*isol, struct, ms*)
Wang, W. *et al., J. Nat. Prod.*, 2005, **68**, 620-622 (*Symphyocladia constits*)

2′,3,3′,4-Tetrabromo-4′,5,5′,6-tetrahydroxy-1-hydroxymethyldiphenyl ether T-109

2,3-Dibromo-6-(2,3-dibromo-4,5-dihydroxybenzyl)-4,5-dihydroxybenzyl alcohol



$C_{14}H_{10}Br_4O_5$ 577.846

7-Me ether: 2′,3,3′,4-Tetrabromo-4′,5,5′,6-tetrahydroxy-1-methoxymethyldiphenyl ether

$C_{15}H_{12}Br_4O_5$ 591.873

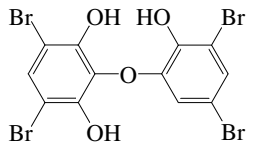
Constit. of the brown alga *Leathesia nana*. Brown powder (Me_2CO).

Mp 171-172° dec.

Xu, X. *et al., J. Nat. Prod.*, 2004, **67**, 1661-1666 (*isol, pmr, cmr, ms*)

3,3′,5,5′-Tetrabromo-2,2′,6-trihydroxydiphenyl ether T-110

4,6-Dibromo-2-(3,5-dibromo-2-hydroxyphenoxy)-1,3-benzenediol



$C_{12}H_6Br_4O_4$ 533.793

2,2′-Di-Me ether: 3,3′,5,5′-Tetrabromo-2-hydroxy-2′,6-dimethoxydiphenyl ether
[372478-64-3]
$C_{14}H_{10}Br_4O_4$ 561.847
Isol. from *Phyllospongia dendyi*.

Hattori, T. *et al., Fish. Sci.*, 2001, **67**, 899-903 (*isol*)

1,1,2,2-Tetrachloroethane, 9CI T-111

sym-*Tetrachloroethane. Acetylene tetrachloride*
[79-34-5]
[25322-20-7]

$Cl_2CHCHCl_2$

$C_2H_2Cl_4$ 167.849
Isol. from the alga *Cytoseira barbata*. Nonflammable solv. for fats, resins, etc. Liq. with chloroform-like odour. d_4^{25} 1.59.
Fp -43.8 Mp -36° (-44°). Bp 146.3° Bp_{45} 62°.

▶ Severe eye and mucous membrane irritant. Prolonged or repeated exposure can cause dermatitis, liver damage and other systemic effects. High vapour conc. cause restlessness, dizziness. LD_{50} (rat, orl) 800 mg/kg. LC_{50} (mus, ihl) 4500 mgm^{-3} (2h exposure). KI8575000

[33685-54-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 86D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 127B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 123B (*ir*)
Timmermans, J. *et al., Bull. Soc. Chim. Belg.*, 1927, **36**, 502
Favorskii, A.E. *et al., CA*, 1935, **29**, 7271 (*synth*)
Field, K. *et al., J.O.C.*, 1971, **36**, 3566 (*synth*)
IARC Monog., 1979, **20**, 477; *Suppl.*, 6; *Suppl.*, 7; 354; 511 (*rev, tox*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1105
Milkova, T. *et al., Phytochemistry*, 1997, **45**, 93 (*isol*)
Hazards in the Chemical Laboratory, 3rd edn., (ed. Bretherick, L.), Royal Society of Chemistry, 1981, 496
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TBQ100

Tetrachloroethylene, 8CI, USAN T-112

Tetrachloroethene, 9CI. Perchloroethylene. Perclene. Perklone. Nema. Ankilostin. Didakene. Kosmovermil. Tetracap. Tetropil. Verminol
[127-18-4]
$Cl_2C{=}CCl_2$

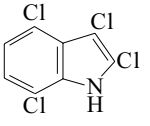
C_2Cl_4 165.833
Manuf. by pyrolysis of CCl_4. Prod. by several spp. of macroalgae and one microalgae (*Porphyridium purpureum*). Widely used non-flammable solv. Used in dry-cleaning, degreasing and textile finishing. Used in manuf. of fluorocarbons. Proposed as a replacement for CCl_4. Anthelmintic, effective against hookworms and intestinal flukes. Liq. with ether-like odour. Insol. H_2O; misc. EtOH, Et_2O, C_6H_6. d_4^{20} 1.62.
Fp -22.35 Mp -19°. Bp 121° Bp_{30} 33.2°. n_D^{20} 1.5053. Log P 3.48 (calc). Vp 18 mmHg (25°). Resistant to radical homopolym. but forms copolymers with some vinyl monomers. Q/e for copolym., Q 0.001, e 1.24.

▶ Probable human carcinogen (IARC 2A). Skin, eye and mucous membrane irritant. Prolonged or repeated exposure can cause dermatitis. High vapour conc. cause dizziness and other CNS effects. LD_{50} (rat, orl) 2629 mg/mg. Exp. carcinogen and teratogen. Exp. reprod. effects. OES: long-term 50 ppm; short-term 150 ppm. KX3850000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 101C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 143A (*ir*)
Weiser, H.B. *et al., J. Phys. Chem.*, 1919, **23**, 415-439 (*synth*)
U.S. Pat., 1934, 1 947 491; *CA*, **28**, 2371 (*synth*)
Frydlender, J.H. *et al., CA*, 1935, **29**, 7935 (*rev*)
Alfrey, T. *et al., J. Polym. Sci.*, 1948, **3**, 297-301 (*copolym*)
Breitenbach, J.W. *et al., Monatsh. Chem.*, 1950, **81**, 21-30 (*copolym*)
Schulman, E.M. *et al., J.A.C.S.*, 1972, **94**, 5972-5979 (*cmr*)
Hawkes, G.E. *et al., J.O.C.*, 1974, **39**, 1276-1290 (*cmr*)
Schmid, W.J. *et al., Chem. Phys. Lett.*, 1977, **45**, 502-503 (*ir, Raman*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427-443 (*Q/e values*)
Reichert, D. *et al., Mutat. Res.*, 1983, **123**, 411-429 (*metab, tox*)
Organo-chlorine Solvents, Royal Society of Chemistry, 1986, 191 (*tox*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 50-59 (*rev*)
Abrahamsson, K. *et al., Limnol. Oceanogr.*, 1995, **40**, 1321-1326 (*occur*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1-423 (*occur*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1380
IARC Monog. (Web), (*tox*)
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 696 (*human tox*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1185
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000 /DATE>PCF275

2,3,4,7-Tetrachloro-1*H*-indole, 9CI T-113

[68234-17-3]



$C_8H_3Cl_4N$ 254.929
Alkaloid from the marine red alga *Rhodophyllis membranacea*.
Mp 119°.

Brennan, M.R. *et al., Tet. Lett.*, 1978, 1637 (*isol, struct*)
Ohta, T. *et al., Heterocycles*, 1989, **29**, 1663 (*synth*)

1,1,3,3-Tetrachloro-2-propanol, 9CI T-114

[18992-39-7]

$Cl_2CHCH(OH)CHCl_2$

$C_3H_4Cl_4O$ 197.875
Isol. from *Asparagopsis taxiformis* and *Caldariomyces fumago*.
Cryst.
Mp 34.5-35.5°. Bp_{12} 94-96°.

4-Nitrobenzoyl:
Cryst. (EtOH). Mp 106.5°.

Neunhoeffer, O. *et al., Annalen*, 1960, **632**, 22-27 (*synth*)
Woolard, F.X. *et al., Tetrahedron*, 1976, **32**, 2843-2846 (*isol*)
Franssen, M.C.R. *et al., Phytochemistry*, 1988, **27**, 1093-1096 (*isol*)

1,1,3,3-Tetrachloro-2-propanone, 9CI T-115

1,1,3,3-Tetrachloroacetone
[632-21-3]
$Cl_2CHCOCHCl_2$

$C_3H_2Cl_4O$ 195.859
Constit. of *Asparagopsis taxiformis*. d_4^{25} 1.59. Bp 182° Bp_{12} 74-77°.

▶ LD_{50} (mus, orl) 176 mg/kg. LD_{50} (rbt, skn) 80 mg/kg. Exp. reprod. and teratogenic effects. UC3815100

Registry of Mass Spectral Data, Wiley-Interscience, 1974, 917-1 (*ms*)
Aldrich Library of Infrared Spectra, 2nd edn., 222H (*ir*)
Aldrich Library of NMR Spectra, **2**, 115B (*pmr*)
Gränacher, C. *et al., Helv. Chim. Acta*, 1949, **32**, 705 (*synth*)
Mountcastle, W.R. *et al., J. Phys. Chem.*, 1960, **64**, 1342 (*uv*)
McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367-374 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TBN300

5,9,23,27-Tetracontatetraenoic acid T-116

$H_3C(CH_2)_5CH{=}CHCH_2CH_2CH{=}CH(CH_2)_{12}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$

$C_{34}H_{60}O_2$ 500.847

(all-Z)-form [187657-50-7]
Isol. from the sponge *Haliclona cinerea*.
Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*isol, ms*)

5,9-Tetracosadienoic acid T-117

[59708-80-4]

$H_3C(CH_2)_{13}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$

$C_{24}H_{44}O_2$ 364.61
Constit. of the marine sponges *Microciona prolifera* and *Spongia tubulifera*.

(Z,Z)-form [118885-07-7]
Constit. of the sponges *Dysidea fragilis* and *Pseudaxinella* cf. *lunaecharta*.
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206
Carballeira, N.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **100**, 489-492 (*isol*)
Christie, W.W. *et al., Lipids*, 1992, **27**, 640-644 (*isol*)

5,15-Tetracosadienoic acid T-118

$H_3C(CH_2)_7CH{=}CH(CH_2)_8CH{=}CH(CH_2)_3COOH$

$C_{24}H_{44}O_2$ 364.61

(Z,Z)-form [160296-62-8]
Constit. of the sponge *Hymeniacidon sanguinea*.
Christie, W.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1994, **109**, 245-252 (*isol*)

13,17-Tetracosadienoic acid T-119

$H_3C(CH_2)_5CH{=}CHCH_2CH_2CH{=}CH(CH_2)_{11}COOH$

$C_{24}H_{44}O_2$ 364.61

(Z,Z)-form [187657-30-3]
Isol. from the sponge *Haliclona cinerea*.
Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*isol, ms*)

6,9,12,15,18,21-Tetracosahexaenoic acid T-120

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_4COOH$

$C_{24}H_{36}O_2$ 356.547

(all-Z)-form [68378-49-4]
Occurs in numerous species of fish. Also found in human sperm and eye retina.
Poulos, A. *et al., Biochem. J.*, 1986, **240**, 891 (*occur*)
Rotstein, N.P. *et al., Biochem. J.*, 1988, **249**, 191 (*occur*)
Vysotskii, M.V. *et al., Bioorg. Khim.*, 1989, **15**, 1133 (*occur*)
Ota, T. *et al., Fish. Sci.*, 1994, **60**, 171 (*occur*)

Tetracosanal, 9CI, 8CI T-121

[57866-08-7]

$H_3C(CH_2)_{22}CHO$

$C_{24}H_{48}O$ 352.643
Isol. from various fruit waxes, oil shales and marine sediments.
Cryst. (Et_2O).
Mp 57.5-62°.

Oxime:
$C_{24}H_{49}NO$ 367.657
Cryst. (C_6H_6/Et_2O or C_6H_6/Me_2CO). Mp 112-113.5°.

Cason, J. *et al., J.O.C.*, 1953, **18**, 850 (*synth, oxime*)
Radler, F. *et al., Aust. J. Chem.*, 1965, **18**, 1059 (*isol, chromatog*)
Stephanoll, E. *et al., Naturwissenschaften*, 1989, **76**, 464 (*isol, ms*)

6,9,12,15,18-Tetracosapentaenoic acid T-122

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_4COOH$

$C_{24}H_{38}O_2$ 358.563

(all-Z)-form [29487-98-7]
Found in bovine retina, mammalian sperm and various marine animals.
Poulos, A. *et al., Biochem. J.*, 1986, **240**, 891 (*isol*)
Rotstein, N.P. *et al., Biochem. J.*, 1988, **249**, 191 (*isol, synth*)
Vysotskii, M.V. *et al., Biochim. Biophys. Acta*, 1991, **1083**, 161 (*isol*)

9,12,15,18,21-Tetracosapentaenoic acid T-123

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_7COOH$

$C_{24}H_{38}O_2$ 358.563

(all-Z)-form [68378-48-3]
Found in bovine retina, mammalian sperm and various marine animals.
[137045-34-2]
Poulos, A. *et al., Biochem. J.*, 1986, **240**, 891 (*isol*)
Rotstein, N.P. *et al., Biochem. J.*, 1988, **249**, 191 (*isol, synth*)

5,9,17-Tetracosatrienoic acid T-124

$H_3C(CH_2)_5CH{=}CH(CH_2)_6CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$

$C_{24}H_{42}O_2$ 362.595

(all-Z)-form [143833-68-5]
Constit. of *Dysidea fragilis*.
Christie, W.W. *et al., Lipids*, 1992, **27**, 640-644 (*isol, ms*)

17-Tetracosenal T-125

$H_3C(CH_2)_5CH{=}CH(CH_2)_{15}CHO$

$C_{24}H_{46}O$ 350.627

(Z)-form [103424-62-0]
Isol. from the sponges *Amphimedon compressa*, *Halichondria panicea* and *Lubomirskia baikalensis*.
Carballeira, N.M. *et al., Chem. Phys. Lipids*, 1986, **39**, 365-368 (*isol*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1992, **55**, 333-339 (*isol*)

11-Tetracosenoic acid T-126

$H_3C(CH_2)_{11}CH{=}CH(CH_2)_9COOH$

$C_{24}H_{46}O_2$ 366.626

(Z)-form [133640-27-4]
Constit. of the sponge *Pseudaxinella* cf. *lunaecharta* and various fish oils.
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol*)

15-Tetracosenoic acid T-127

[26444-06-4]

$H_3C(CH_2)_7CH{=}CH(CH_2)_{13}COOH$

$C_{24}H_{46}O_2$ 366.626

(E)-form [14490-79-0]
Cryst. (EtOH). Mp 66-67° (61°).

Me ester:
$C_{25}H_{48}O_2$ 380.653
Cryst. (Me_2CO). Mp 36.5-37.5°. $Bp_{0.00001}$ 180-190°.

Amide:
$C_{24}H_{47}NO$ 365.641
Mp 97-98°.

(*Z*)-*form*
Nervonic acid. Selacholeic acid
[506-37-6]
[31152-46-2]
Present in cerebrosides and in fish oils. Isol. from the sponge *Pseudaxinella* cf. *lunaecharta*. Also in seed oils of *Lunaria biennis*, rape (*Brassica napus*) and *Carthamus tinctorius*.
Cryst. (EtOH).
Mp 40.5-41° Mp 44-45°.

Me ester: [2733-88-2]
Mp 14-15°. $Bp_{0.02}$ 165° approx.

Amide: [208650-37-7]
Cryst. (EtOH). Mp 86.5-87.5°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 784B (*nmr*)
Hale, J.B. *et al., J.A.C.S.*, 1930, **52**, 4536 (*synth*)
Bounds, D.G. *et al., J.C.S.*, 1954, 448 (*synth*)
Batchelor, J.G. *et al., J.A.C.S.*, 1973, **95**, 6358 (*cmr*)
Lecerf, J. *et al., J. Physiol. (Paris)*, 1975, **70**, 493
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206 (*isol, biosynth*)
Bohannon, M.B. *et al., Lipids*, 1976, **11**, 157-159 (*isol*)
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol, Pseudaxinella*)

17-Tetracosenoic acid T-128

[59708-76-8]
[26444-06-4, 31152-46-2]
$H_3C(CH_2)_5CH{=}CH(CH_2)_{15}COOH$
$C_{24}H_{46}O_2$ 366.626
Isol. from mycelia of *Phycomyces blakesleeanus*. Occurs in *Eurypongia rosea* and other sponges.

[75917-08-7]

Bernhard, K. *et al., Helv. Chim. Acta*, 1948, **31**, 977 (*isol*)
Carballeira, N.M. *et al., Lipids*, 1989, **24**, 665 (*occur*)

19-Tetracosenoic acid T-129

$H_3C(CH_2)_3CH{=}CH(CH_2)_{17}COOH$
$C_{24}H_{46}O_2$ 366.626

(*Z*)-*form* [133530-23-1]
Constit. of various sponges incl. *Amphimedon complanata* and *Lubomirskia baicalensis*.

Carballeira, N.M. *et al., J. Nat. Prod.*, 1991, **54**, 315-317 (*isol*)
Dembitsky, V.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1994, **109**, 415-426 (*isol*)

7,11-Tetradecadiene-5,9-diynoic acid T-130

$H_3CCH_2CH{=}CHC{\equiv}CCH{=}CHC{\equiv}C(CH_2)_3COOH$
$C_{14}H_{16}O_2$ 216.279

(7*E*,11*E*)-*form*
Isol. from the marine sponge *Oceanapia* sp. Antibacterial and antifungal agent. Pale yellow solid. λ_{max} 292 (log ϵ 4.56); 310 (log ϵ 4.53) (1-propanol).

Matsunaga, S. *et al., J. Nat. Prod.*, 2000, **63**, 690-691

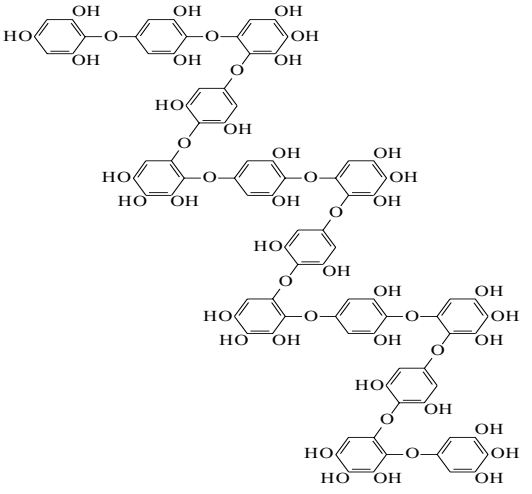
2,4-Tetradecadien-1-ol T-131

[145297-74-1]
$H_3C(CH_2)_8CH{=}CHCH{=}CHCH_2OH$
$C_{14}H_{26}O$ 210.359
Isol. from corals and starfishes. Sperm attractant.

Coll, J.C. *et al., CA*, 1993, **118**, 36147 (*isol*)

Tetradecafuhalol A T-132

[164176-33-4]

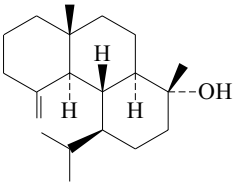


$C_{84}H_{58}O_{49}$ 1851.353
Constit. of the brown alga *Sargassum spinuligerum*.

Glombitza, K.-W. *et al., Phytochemistry*, 1995, **38**, 987-995 (*isol, pmr, cmr, ms*)

Tetradecahydro-1-hydroxy-4-isopropyl-1,8*a*-dimethyl-5-methylenephenanthrene T-133

*Tetradecahydro-1,8*a*-dimethyl-5-methylene-4-(1-methylethyl)-1-phenanthrenol*
[103200-86-8]



$C_{20}H_{34}O$ 290.488
Constit. of a *Briareum* sp. (DD6). Isol. from a reaction of 2,4,7,11-Cembratetraene and formic acid. Solid (CH_2Cl_2/petrol).
Mp 161-164°. $[\alpha]_D$ -12.9 (c, 0.31 in $CHCl_3$).

Raldugin, V. *et al., CA*, 1986, **105**, 43104r (*synth*)
Bagryanskya, I.Yu. *et al., CA*, 1986, **105**, 43105s (*props*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1989, **42**, 1705 (*isol, pmr, cmr*)

Tetradecanoic acid, 9CI T-134

Myristic acid, 8CI. FEMA 2764
[544-63-8]
$H_3C(CH_2)_{12}COOH$
$C_{14}H_{28}O_2$ 228.374
Occurs widely in vegetable glycerides. Major component of the lipids of nutmeg (*Myristica moschata*). Present in lipids of *Physalia physalis* (Portuguese-man-of-war). Defoaming agent, lubricant used in food processing. Cryst. (petrol).
Mp 54°. Bp_{100} 250.5° Bp_{16} 199°.
▶ Skin and eye irritant. LD_{50} (mus, ivn) 43 mg/kg. QH4375000

[822-12-8, 4086-70-8, 13429-27-1, 41669-40-3]

Stillway, L.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 535-537 (*Physalia physalis constit*)

2-Tetradecanone T-135

[2345-27-9]
$H_3C(CH_2)_{11}COCH_3$
$C_{14}H_{28}O$ 212.375

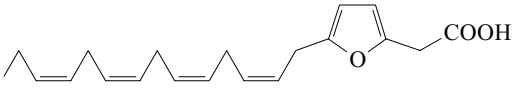
Constit. of hop oil. Prod. by a marine bacterium. Cryst. (EtOH aq.).
Mp 33-34°. Bp_{100} 205-206° Bp_{13} 134°.

Semicarbazone: Mp 125-126°.

Rodd's Chem. Carbon Compd. (2nd edn.), 1965, **1**, 52
Allen, J.E. *et al., Lipids*, 1971, **6**, 448 (*synth*)
Bagnell, L. *et al., Aust. J. Chem.*, 1974, **27**, 1381 (*synth*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*isol*)

5-(2,5,8,11-Tetradecatetraenyl)-2-furanacetic acid T-136

3,6-Epoxy-3,5,8,11,14,17-eicosahexaenoic acid



$C_{20}H_{26}O_3$ 314.424

(*all-Z*)-*form* [136337-72-9]
Isol. from the sponges *Hymeniacidon hauraki* and *Dictyonella incisa*. Cytotoxic agent. Yellow oil.

(8*Z*,11*Z*,14*Z*,17*E*)-*form* [136378-47-7]
Isol. from *Dictyonella incisa*.
No phys. props. reported.

Ciminiello, P. *et al., Experientia*, 1991, **47**, 739 (*isol*)
Prinsep, M.R. *et al., J. Nat. Prod.*, 1994, **57**, 1557 (*isol, pmr, cmr*)

3,5,13-Tetradecatrien-2-amine T-137

2-Amino-3,5,13-tetradecatriene
$H_2C{=}CH(CH_2)_6CH{=}CHCH{=}CHCH(NH_2)CH_3$
$C_{14}H_{25}N$ 207.358

(2*R*,3*E*,5*E*)-*form*

13,14-Dihydro: ***3,5-Tetradecadien-2-amine, 9CI****. 2-Amino-3,5-tetradecadiene*
[356073-87-5]
$C_{14}H_{27}N$ 209.374
Isol. from a *Pseudodistoma* sp. Oil. $[\alpha]_D$ -1.2 (c, 0.25 in MeOH). λ_{max} 229 (log ε 4.24) (MeOH).

(2*S*,3*E*,5*Z*)-*form*
(+)-trans,cis-*form*
[151284-88-7]
Prod. by tunicate *Pseudodistoma novaezelandiae*.
Viscous pale yellow oil. $[\alpha]_D^{25}$ +17.8 (c, 1 in $CHCl_3$) (95% e.e.). λ_{max} 230 (ε 16600) (MeOH) (Berdy).

(2*RS*,3*E*,5*E*)-*form*
(±)-trans,trans-*form*
[134381-24-1]
Constit. of the ascidian *Pseudodistoma novaezelandiae*. λ_{max} 230 (ε 16600) (MeOH) (Berdy).

(2*RS*,3*E*,5*Z*)-*form*
(±)-trans,cis-*form*
[134381-23-0]
Constit. of *Pseudodistoma novaezelandiae*.

13,14-Dihydro: [134381-25-2]
Constit. of *Pseudodistoma novaezelandiae*.

Perry, N.B. *et al., Aust. J. Chem.*, 1991, **44**, 627-633 (*isol, uv, pmr, cmr*)
Enders, D. *et al., Annalen*, 1993, 551-555 (*synth*)
Rashid, M.A. *et al., Tetrahedron*, 2001, **57**, 5751-5755 (*3R,3E,5E-form 13,14-dihydro*)

2,5,8-Tetradecatrien-1-ol T-138

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2OH$
$C_{14}H_{24}O$ 208.343

(*Z,Z,Z*)-*form* [60188-11-6]
Isol. from the sponge *Homaxinella* sp. Key intermed. for icosanoid synth.
Oil.

Tai, H.-H. *et al., Biochemistry*, 1980, **19**, 1989 (*synth*)
Kerdesky, F.A.J. *et al., Tet. Lett.*, 1985, **26**, 2143 (*synth*)
Badone, D. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 629 (*synth, pmr*)
Mansoor, T.A. *et al., J. Nat. Prod.*, 2004, **67**, 721-724 (*isol, pmr, cmr*)

13-Tetradecene-2,4-diyn-1-ol, 9CI T-139

[125906-53-8]
$H_2C{=}CH(CH_2)_7C{\equiv}CC{\equiv}CCH_2OH$
$C_{14}H_{20}O$ 204.311
Isol. from the hard corals *Montipora* spp. and *Pectinia lactuca*. Exhibits ichthyotoxicity and inhibits growth of some bacteria and fungi. Cytotoxic. Sol. MeOH, Me_2CO. λ_{max} 220 (E1%/1cm 340); 230 (E1%/1cm 445); 242 (E1%/1cm 440); 256 (E1%/1cm 250) (MeOH) (Berdy).

2-Hydroxyethyl ether: ***Dihomomontiporyne H***
$C_{16}H_{24}O_2$ 248.364
Isol. from a coral *Montipora* sp. Cytotoxic. Light yellow oil.

Higa, T. *et al., Chem. Lett.*, 1990, 145-148 (*isol, struct*)
Alam, N. *et al., J. Nat. Prod.*, 2001, **64**, 1059-1063 (*isol*)
Alam, N. *et al., Chem. Pharm. Bull.*, 2002, **50**, 661-662 (*Dihomomontiporyne H*)

5-Tetradecenoic acid T-140

Physeteric acid
[544-66-1]
[26444-03-1]
$H_3C(CH_2)_7CH{=}CH(CH_2)_3COOH$
$C_{14}H_{26}O_2$ 226.358

(*Z*)-*form* [5684-70-8]
[28039-98-7]
Occurs in sperm whale oil. Also in lipids of *Euglena gracilis* and *Streptococcus* sp. d_4^{15} 0.91.
Mp 20°. Bp_{15} 192-197°. n_D^{15} 1.4571.

Isopropyl ester: [71597-92-7]
$C_{17}H_{32}O_2$ 268.439
Constit. of the pheromone of the beetle *Dermestes maculatus*.

Tsujimoto, M. *et al., Kogyo Kagaku Zasshi*, 1926, **29**, 102; *CA*, **23**, 1109 (*isol*)
Toyama, Y. *et al., Nippon Kagaku Kaishi*, 1935, **56**, 1050; *CA*, **30**, 315 (*isol*)
Korn, E.D. *et al., J. Lipid Res.*, 1964, **5**, 352 (*isol*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1977, **18**, 115 (*cmr*)
Francke, W. *et al., Angew. Chem., Int. Ed.*, 1979, **18**, 796 (*isopropyl ester*)

7-Tetradecenoic acid T-141

[2197-54-8]
[26444-03-1]
$H_3C(CH_2)_5CH{=}CH(CH_2)_5COOH$
$C_{14}H_{26}O_2$ 226.358
Isol. from various microbial lipids.

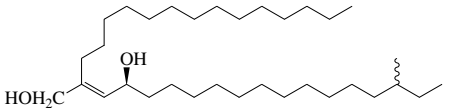
(*Z*)-*form* [2430-95-7]
[28039-98-7]
Constit. of lipids of *Euglena gracilis*.

Isopropyl ester: [71597-93-8]
$C_{17}H_{32}O_2$ 268.439
Constit. of the pheromone of the beetle *Dermestes maculatus*and of *Harrisonia brillians*.

Hofmann, K. *et al., J. Biol. Chem.*, 1959, **234**, 1672 (*synth*)
Scheuerbrandt, G. *et al., J. Biol. Chem.*, 1962, **237**, 2064 (*isol*)
Korn, E.D. *et al., J. Lipid Res.*, 1964, **5**, 352 (*isol*)
Francke, W. *et al., Angew. Chem., Int. Ed.*, 1979, **18**, 796 (*isopropyl ester*)
Myerson, J. *et al., Tet. Lett.*, 1982, **23**, 2757 (*isol, synth*)
Zakharkin, L.I. *et al., Zh. Org. Khim.*, 1982, **18**, 1623 (*synth*)
Nakamura, T. *et al., Bull. Chem. Soc. Jpn.*, 2003, **76**, 1011-1022 (*synth, pmr*)

2-Tetradecyl-16-methyl-2-octadecene-1,4-diol T-142

17-(Hydroxymethyl)-3-methyl-16-hentriaconten-15-ol



(2*E*,4*S*,16ξ)-*form*

$C_{33}H_{66}O_2$ 494.883

(2*E*,4*S*,16ξ)-*form*

1-O-*β*-D-Glucopyranoside: ***Clathroside B***
$C_{39}H_{76}O_7$ 657.025
Isol. from *Agelas clathrodes*.

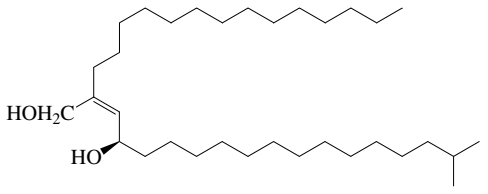
(2*Z*,4*R*,16ξ)-*form*

1-O-*β*-D-Glucopyranoside: ***Isoclathroside B***
$C_{39}H_{76}O_7$ 657.025
Isol. from *Agelas clathrodes*.

Costantino, V. *et al., J. Nat. Prod.*, 2006, **69**, 73-78 (*isol, pmr, cmr*)

2-Tetradecyl-17-methyl-2-octadecene-1,4-diol T-143

17-(Hydroxymethyl)-2-methyl-16-hentriaconten-15-ol



(*R*,*Z*)-*form*

$C_{33}H_{66}O_2$ 494.883

(*R*,*Z*)-*form*

1-O-*β*-D-Glucopyranoside: ***Isoclathroside C***
$C_{39}H_{76}O_7$ 657.025
Isol. from *Agelas clathrodes*.

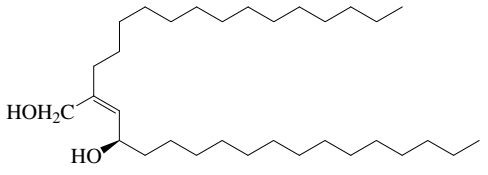
(*S*,*E*)-*form*

1-O-*β*-D-Glucopyranoside: ***Clathroside C***
$C_{39}H_{76}O_7$ 657.025
Isol. from *Agelas clathrodes*.

Costantino, V. *et al., J. Nat. Prod.*, 2006, **69**, 73-78 (*isol, pmr, cmr*)

2-Tetradecyl-2-octadecene-1,4-diol T-144

17-(Hydroxymethyl)-16-hentriaconten-15-ol



(*R*,*Z*)-*form*

$C_{32}H_{64}O_2$ 480.856

(*R*,*Z*)-*form*

1-O-*β*-D-Glucopyranoside: ***Isoclathroside A***
$C_{38}H_{74}O_7$ 642.998
Isol. from *Agelas clathrodes*. Oil. $[\alpha]_D^{25}$ -2 (c, 0.1 in $CHCl_3$).

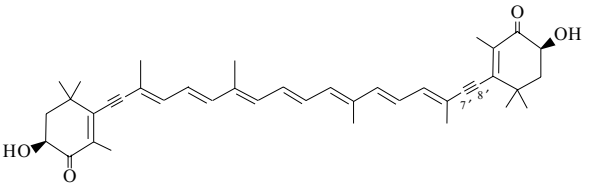
(*S*,*E*)-*form*

1-O-*β*-D-Glucopyranoside: ***Clathroside A***
$C_{38}H_{74}O_7$ 642.998
Isol. from *Agelas clathrodes*. Oil. $[\alpha]_D^{25}$ -6 (c, 0.1 in $CHCl_3$).

Costantino, V. *et al., J. Nat. Prod.*, 2006, **69**, 73-78 (*isol, pmr, cmr*)

7,7′,8,8′-Tetradehydroastaxanthin T-145

7,7′,8,8′-Tetradehydro-3,3′-dihydroxy-β,β-carotene-4,4′-dione. Diketotetrahydrozeaxanthin. 4,4′-Diketocynthiaxanthin
[31687-79-3]

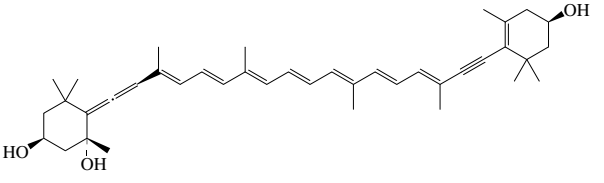


$C_{40}H_{48}O_4$ 592.817
Constit. of *Asterias rubens* and other echinoderms. Bluish cryst. (Et_2O).
Mp 210°.

7′,8′-Dihydro: 7,8-Didehydro-3,3′-dihydroxy-β,β-carotene-4,4′-dione. ***7,8-Dehydroastaxanthianthin***
[19866-02-5]
$C_{40}H_{50}O_4$ 594.833
Isol. from *Asterias rubens* and lobster eggs. Violet plates (CH_2Cl_2/diisopropyl ether).
Mp 211-212°. Asterinic acid was a mixt. of this with 7,7′,8,8′-Tetradehydroastaxanthin above.

Francis, G.W. *et al., Acta Chem. Scand.*, 1970, **24**, 3050 (*isol, struct*)
Thommen, H. *et al., Biochem. Syst. Ecol.*, 1976, **4**, 131 (*isol, deriv*)
Bernhard, K. *et al., Helv. Chim. Acta*, 1980, **63**, 1473 (*synth, ir, uv, pmr, cmr, ms, cd*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 400 (*bibl*)

6,7,7′,8′-Tetradehydro-β,β-carotene-3,3′,5-triol T-146



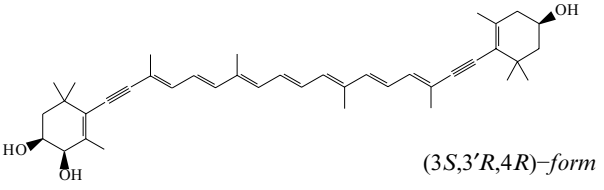
$C_{40}H_{54}O_3$ 582.865

(3*S*,3′*R*,5*R*,6*R*)-*form*
7′,8′-Didehydrodeepoxyneoxanthin
[865866-07-5]
Constit. of the corbicula clam (Shijimi), *Corbicula japonica*, from brackish water. λ_{max} 420; 443; 472 (Et_2O).

Maoka, T. *et al., J. Nat. Prod.*, 2005, **68**, 1341-1344 (*7′,8′-Didehydrodeepoxyneoxanthin*)

7,7′,8,8′-Tetradehydro-β,β-carotene-3,3′,4-triol T-147

4-Hydroxyalloxanthin



(3*S*,3′*R*,4*R*)–*form*

$C_{40}H_{52}O_3$ 580.849

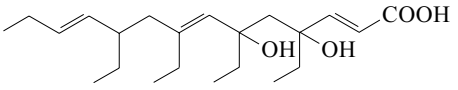
(3*S*,3′*R*,4*R*)-*form*
Constit. of *Mytilus coruscus*.

(3*S*,3′*R*,4*S*)-*form*
Constit. of *Mytilus coruscus*.

Maoka, T. *et al., CA*, 1988, **109**, 226980a (*isol, pmr*)

4,6,8,10-Tetraethyl-4,6-dihydroxy-2,7,11-tetradecatrienoic acid T-148

[152821-47-1]



$C_{22}H_{38}O_4$ 366.54

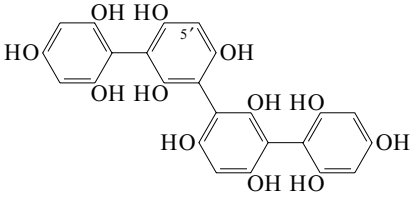
Isol. from the sponge *Plakortis halichondrioides*. Cytotoxic. Oil. $[\alpha]_D$ +1.2 (c, 0.33 in $CHCl_3$).

Rudi, A. *et al., J. Nat. Prod.*, 1993, **56**, 1827 (*isol, pmr*)

Tetrafucol A T-149

[1,1′:3′,1″:3″,1‴]-Quaterphenyl-2,2′,2″,2‴,4,4′,4″,4‴,6,6′,6″,6‴-dodecol, 9CI

[123154-66-5]



$C_{24}H_{18}O_{12}$ 498.399

Constit. of the brown algae *Fucus vesiculosus*, *Analipus japonicus* and *Carpophyllum angustifolium*.

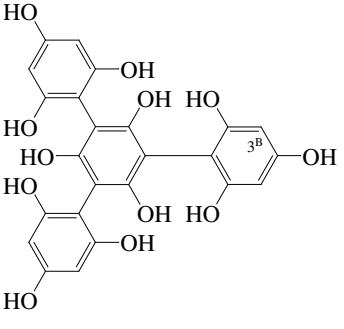
5′-Chloro: ***5′-Chlorotetrafucol A***
[123172-43-0]
$C_{24}H_{17}ClO_{12}$ 532.844
Constit. of *Analipus japonicus*.

5′-Bromo: ***5′-Bromotetrafucol A***
[123154-64-3]
$C_{24}H_{17}BrO_{12}$ 577.295
Constit. of *Analipus japonicus*.

Glombitza, K.W. *et al., Planta Med.*, 1989, **55**, 171-175 (*isol, struct*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

Tetrafucol B T-150

[57103-41-0]



$C_{24}H_{18}O_{12}$ 498.399

Isol. from *Fucus vesiculosus*. Isol. as dodeca-Ac to which CAS no. refers.

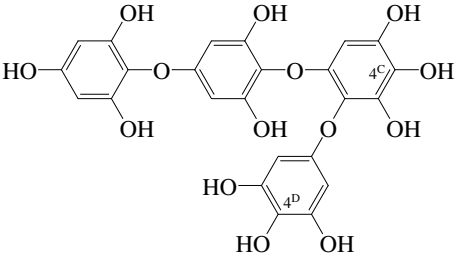
3^B-Hydroxy: ***Hydroxytetrafucol B***
[642487-12-5]
$C_{24}H_{18}O_{13}$ 514.398
Isol. from *Scytothamnus australis*. Isol. as trideca-Ac, to which CAS no. refers.

Glombitza, K.W. *et al., Phytochemistry*, 1975, **14**, 1403-1405 (*Tetrafucol B*)
Glombitza, K.W. *et al., Bot. Mar.*, 2003, **46**, 315-320 (*Hydroxytetrafucol B*)

Tetrafuhalol A T-151

5-[2,6-Dihydroxy-4-(2,4,6-trihydroxyphenoxy)phenoxy]-4-(3,4,5-trihydroxyphenoxy)-1,2,3-benzenetriol

[76689-97-9]



$C_{24}H_{18}O_{14}$ 530.398

Constit. of *Carpophyllum maschalocarpum*.

4^C-Deoxy: ***Deshydroxytetrafuhalol A***
$C_{24}H_{18}O_{13}$ 514.398
Isol. from *Sargassum spinuligerum*. Struct. assumed here to be as shown. Struct. publ. only in a thesis.

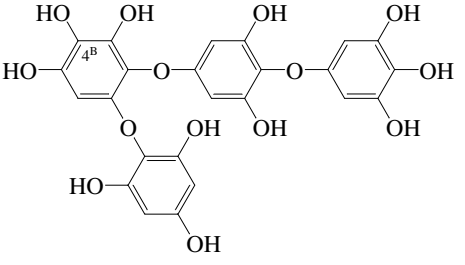
4^D-Deoxy: ***Deshydroxytetrafuhalol C***
$C_{24}H_{18}O_{13}$ 514.398
Isol. from *Sargassum spinuligerum*.

Glombitza, K.-W. *et al., Phytochemistry*, 1976, **15**, 1279; 1981, **30**, 2741; 1995, **38**, 987-995 (*isol, pmr*)
Keusgen, M. *et al., Phytochemistry*, 1997, **46**, 1403-1415 (*cmr*)

Tetrafuhalol B T-152

4-[3,5-Dihydroxy-4-(3,4,5-trihydroxyphenoxy)phenoxy]-5-(2,4,6-trihydroxyphenoxy)-1,2,3-benzenetriol

[76689-96-8]



$C_{24}H_{18}O_{14}$ 530.398

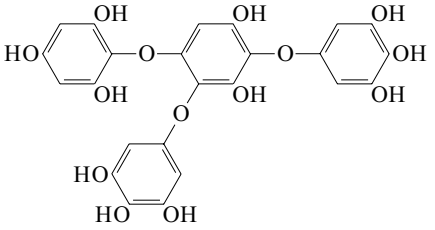
Constit. of *Carpophyllum maschalocarpum*.

4^B-Deoxy: ***Deshydroxytetrafuhalol B***
[164176-22-1]
$C_{24}H_{18}O_{13}$ 514.398
Constit. of the brown alga *Sargassum spinuligerum*.

Koch, M. *et al., Phytochemistry*, 1981, **20**, 1373 (*isol, pmr*)
Glombitza, K.-W. *et al., Phytochemistry*, 1991, **30**, 2741 (*isol*)
Keusgen, M. *et al., Phytochemistry*, 1995, **38**, 975 (*4′-Deoxy, isol, pmr, cmr, ms*)

Tetrafuhalol D T-153

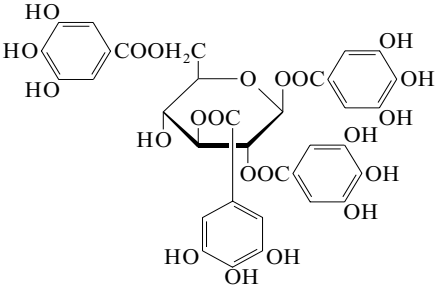
5,5′-[[2,4-Dihydroxy-6-(2,4,6-trihydroxyphenoxy)-1,3-phenylene]bis(oxy)]bis[1,2,3-benzenetriol], 9CI
[137809-89-3]



$C_{24}H_{18}O_{14}$ 530.398
Constit. of *Carpophyllum maschalocarpum*.

Glombitza, K.-W. *et al., Phytochemistry*, 1991, **30**, 2741-2745 (*isol, pmr*)

1,2,3,6-Tetragalloylglucose T-154



$C_{34}H_{28}O_{22}$ 788.582

β-D-Pyranose-*form* [79886-50-3]
Isol. from *Fuchsia* spp. *Quercus infectoria*, *Ceratonia siliqua* (carob), *Epilobium angustifolium* and *Juglans mandshurica*. Inhibits reverse transcriptase. Shows antitumour effects by inhibition of tumour cell adhesion and invasion. Apoptosis inducer. Fine needles (H_2O).
Mp 250°. $[\alpha]_D^{20}$ +41 (c, 0.8 in MeOH). λ_{max} 216; 278 (no solvent reported).

O-*(3,4,5-Trihydroxybenzoyl)(1): 3*-O-*Digalloyl-1,2,6-tri*-O-*galloyl-β-D-glucopyranose*
[99907-48-9]
$C_{41}H_{32}O_{26}$ 940.688
Isol. from green alga (*Spirogyra* sp.). Amorph. powder. Sol. MeOH, EtOAc, H_2O; poorly sol. Et_2O, hexane. $[\alpha]_D^{31}$ +60 (c, 0.53 in Me_2CO). Contains a digalloyl (galloylgalloyl) residue at C-3. λ_{max} 280 (MeOH) (Berdy).

O-*(3,4,5-Trihydroxybenzoyl)(2): 6*-O-*Digalloyl-1,2,3-tri*-O-*galloyl-β-D-glucopyranose*
[86709-52-6]
$C_{41}H_{32}O_{26}$ 940.688
Gallotannin from the twig gall of *Quercus infectoria*. Light brown amorph. powder. $[\alpha]_D^{20}$ +44.1 (c, 0.54 in Me_2CO). Contains a digalloyl (galloylgalloyl) residue at C-6.

O-*Bis(3,4,5-trihydroxybenzoyl): 2,6-Bis*-O-*digalloyl-1,3-di*-O-*galloyl-β-D-glucopyranose*
$C_{48}H_{36}O_{30}$ 1092.794
Gallotannin constit. of the twig gall *Quercus infectoria*. Light brown amorph. powder. $[\alpha]_D^{20}$ +39.4 (c, 0.33 in Me_2CO). Contains galloylgalloyl residues at C-2 and C-6.

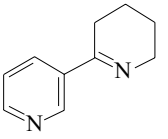
O-*(Galloylgalloyl): 6*-O-*Trigalloyl-1,2,3-tri*-O-*galloyl-β-D-glucopyranose*
$C_{48}H_{36}O_{30}$ 1092.794
Isol. from the twig gall of *Quercus infectoria*. Light brown amorph. powder. $[\alpha]_D^{20}$ +43.4 (c, 0.35 in Me_2CO). Contains a trigalloyl (galloylgalloylgalloyl) residue at C-6.

3^D-Deoxy: 1,2,3-Tri-O-*galloyl-6*-O-*protocatechuoyl-β-D-glucopyranose.* ***Monacanthin B***
$C_{34}H_{28}O_{21}$ 772.583
Constit. of *Cornulaca monacantha*. Off-white powder.

Haddock, E.A. *et al., J.C.S. Perkin 1*, 1982, 2515 (*isol, struct, pmr, cmr*)
Nishizawa, M. *et al., J.C.S. Perkin 1*, 1983, 961 (*derivs*)
Nishioka, I. *et al., Yakugaku Zasshi*, 1983, **103**, 125-142 (*isol*)
Nishizawa, M. *et al., Phytochemistry*, 1985, **24**, 2411 (*deriv*)
Hagenah, S. *et al., Phytochemistry*, 1993, **32**, 637 (*biosynth*)
Saeki, K. *et al., Planta Med.*, 1999, **65**, 124; 227-229 (*isol, activity*)
Min, B.-S. *et al., Chem. Pharm. Bull.*, 2000, **48**, 194-200 (*activity*)
Kandil, F.E. *et al., Phytochemistry*, 2001, **58**, 611-613 (*Monacanthin B*)

3,4,5,6-Tetrahydro-2,3′-bipyridine, 9CI T-155

Anabaseine
[3471-05-4]



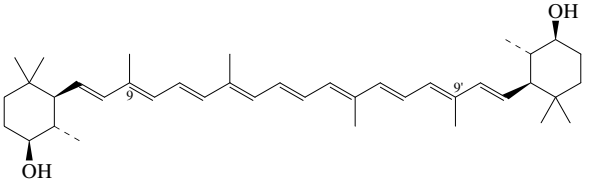
$C_{10}H_{12}N_2$ 160.218
Toxin from the marine hoplonemertean worms *Paranemertes peregrina* and *Amphiporus angulatus*. Also isol. from *Aphaenogaster* ants. Nicotinic receptor agonist with selectivity for α7 subtype. Oil. Bp_1 110-120°.

▶ DW1890000

Dipicrate: Mp 174°.

Späth, E. *et al., Ber.*, 1936, **69**, 1082 (*synth*)
Kem, W.R. *et al., Toxicon*, 1971, **9**, 15-22; 23-32 (*isol, occur*)
Kem, W.R. *et al., Experientia*, 1976, **32**, 684
Wheeler, J.W. *et al., Science (Washington, D.C.)*, 1981, **211**, 1051-1052 (*isol, ants*)
Zoltewicz, J.A. *et al., Heterocycles*, 1993, **35**, 171-179 (*pharmacol, derivs*)
Kem, W.R. *et al., J. Pharmacol. Exp. Ther.*, 1997, **283**, 979-992 (*pharmacol*)
Kem, W.R. *et al., Mar. Drugs*, 2006, **4**, 255-273 (*rev*)

5,5′,6,6′-Tetrahydro-β,β-carotene-4,4′-diol T-156



(4*S*,4′*S*,5*S*,5′*S*,6*S*,6′*S*)-*form*

$C_{40}H_{60}O_2$ 572.913

(4S,4′S,5S,5′S,6S,6′S)-form
4,4′-Dihydroxypirardixanthin
[364062-36-2]
[34781-87-8]
Isol. from the muscle of the spindle shell *Fusinus perplexus*.
λ_{max} 414; 437; 467 (Et_2O).

Monoketone: 5,5′,6,6′-Tetrahydro-4′-hydroxy-β,β-caroten-4-one. ***4′-Hydroxy-4-oxopirardixanthin***
[98502-72-8]
$C_{40}H_{58}O_2$ 570.897
Isol. from the spindle shell *Fusinus perplexus*. Considered to be a metabolite of, Diketone. λ_{max} 414; 437; 467 (Et_2O).

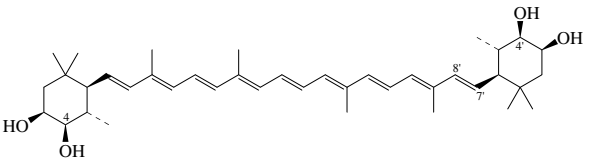
(4S,4′S,5S,5′S,6S,6′S,9Z,9′Z)-form
Cucumariaxanthin C
[167818-25-9]
Constit. of *Cucumaria japonica*. EBV activation inhibitor. Deep orange needles. λ_{max} 407 (ε 89125); 430 (ε 141250); 458 (ε 128820) (Et_2O) (Berdy).

Monoketone: ***Cucumariaxanthin B***
[167818-24-8]
$C_{40}H_{58}O_2$ 570.897
Constit. of *Cucumaria japonica*. EBV activation inhibitor. Deep orange needles. λ_{max} 407; 430; 458 (Et_2O) (Berdy).

Diketone: 5,5′,6,6′-Tetrahydro-β,β-carotene-4,4′-dione. ***Cucumariaxanthin A***
[167613-52-7]
$C_{40}H_{56}O_2$ 568.881
Constit. of *Cucumaria japonica*. EBV activation inhibitor. Deep orange needles. λ_{max} 407; 430; 458 (Et_2O) (Berdy).

Tanaka, Y. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **54B**, 391 (*occur*)
Matsuno, T. *et al., Nippon Suisan Gakkaishi*, 1984, **50**, 1583 (*struct*)
Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **81**, 905-908 (*isol*)
Tsushima, M. *et al., J. Nat. Prod.*, 1996, **59**, 30; 2001, **64**, 1139-1142 (*isol, pmr, cmr, abs config*)

5,5′,6,6′-Tetrahydro-β,β-carotene-3,3′,4,4′-tetrol T-157



$C_{40}H_{60}O_4$ 604.912

(3S,3′S,4R,4′R,5S,5′S,6S,6′S)-form
3,4,3′,4′-Tetrahydroxypirardixanthin. ***Ophioxanthol***
[98502-74-0]
Constit. of *Fusinus perplexus.*
Mp 144-146°. λ_{max} 414; 437; 467 (Et_2O).

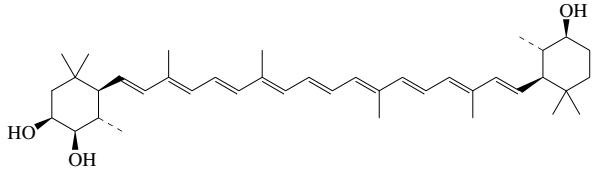
4,4′-Disulfate: ***Ophioxanthin***
[96928-49-3]
$C_{40}H_{60}O_{10}S_2$ 765.04
Constit. of ophiuroid *Ophioderma longicaudum*. Characterised as di-Na salt.

7′,8′-Didehydro, 4,4′-disulfate: ***Dehydroophioxanthin***
$C_{40}H_{58}O_{10}S_2$ 763.024
Isol. from *Ophiocomina nigra*.

Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **81**, 905-908 (*isol, biochem*)
D'Auria, M.V. *et al., Tet. Lett.*, 1985, **26**, 1871-1872 (*Ophioxanthin*)
D'Auria, M.V. *et al., J. Nat. Prod.*, 1991, **54**, 606-608 (*Dehydroophioxanthin*)
Tsushima, M. *et al., J. Nat. Prod.*, 2001, **64**, 1139-1142 (*isol, pmr, abs config*)

5,5′,6,6′-Tetrahydro-β,β-carotene-3,4,4′-triol T-158

3,4,4′-Trihydroxy-5,5′,6,6′-tetrahydro-β,β-carotene

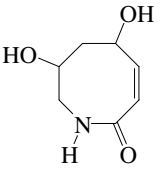


$C_{40}H_{60}O_3$ 588.912

(3S,4R,4′S,5S,5′S,6S,6′S)-form
3,4,4′-Trihydroxypirardixanthin
[98502-73-9]
Isol. from the spindle shell *Fusinus perplexus.* Metab. of Adonirubin, A-118.
Cryst.
Mp 140-142°. λ_{max} 414; 437; 467 (Et_2O).

Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **81**, 905-908 (*isol, pmr*)
Tsushima, M. *et al., J. Nat. Prod.*, 2001, **64**, 1139-1142 (*isol, pmr, abs config*)

5,6,7,8-Tetrahydro-5,7-dihydroxy-1*H*-azocin-2-one T-159

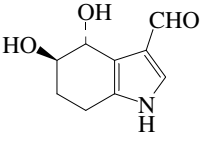


$C_7H_{11}NO_3$ 157.169
Prod. by the marine *Streptomyces* sp. strain QD518.

Fotso, S. *et al., Nat. Prod. Commun.*, 2006, **1**, 9-13 (*isol*)

4,5,6,7-Tetrahydro-4,5-dihydroxy-1*H*-indole-3-carboxaldehyde T-160

*3-Formyl-4,5,6,7-tetrahydro-4,5-dihydroxy-1*H*-indole*



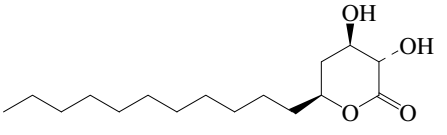
$C_9H_{11}NO_3$ 181.191

(4R*,5R*)-form
5-Ac: [501373-69-9]
$C_{11}H_{13}NO_4$ 223.228
Isol. from a Puerto Rican *Lyngbya majuscula*. Amorph. solid. $[\alpha]_D^{22}$ +104.6 (c, 0.5 in $CHCl_3$). λ_{max} 214 (log ϵ 4.39); 254 (log ϵ 4.04); 287 (log ϵ 3.67) (MeOH).

Nogle, L.M. *et al., J. Nat. Prod.*, 2003, **66**, 217-220 (*isol, pmr, cmr, ms*)

Tetrahydro-3,4-dihydroxy-6-undecyl-2*H*-pyran-2-one T-161

2,3-Dihydroxy-5-hexadecanolide



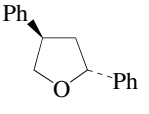
$C_{16}H_{30}O_4$ 286.411

(3S,4R,6S)-form
Prod. by an endophytic fungus No. 2524 isol. from the seeds of the mangrove *Avicennia marina*.
Amorph. powder.
Mp 105-107°. $[\alpha]_D^{20}$ -42 (c, 0.12 in MeOH). λ_{max} 216 (ϵ 120) (MeOH).

Li, H.-J. *et al., J. Asian Nat. Prod. Res.*, 2004, **6**, 185-191 (*isol, pmr, cmr, ms*)

Tetrahydro-2,4-diphenylfuran T-162

2,4-Diphenyloxolane



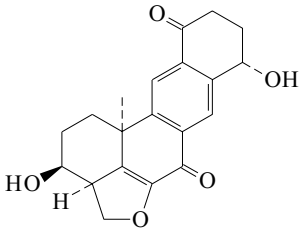
(2*R**,4*R**)-*form*

$C_{16}H_{16}O$ 224.302

(2R*,4R*)-form
(+)-trans-*form.* ***Calyxolane A***
[194999-92-3]
Constit. of the sponge *Calyx podatypa*.
Oil. $[\alpha]_D^{22}$ +34.6 (c, 0.3 in $CHCl_3$). λ_{max} 206 (ϵ 16000) (MeOH).

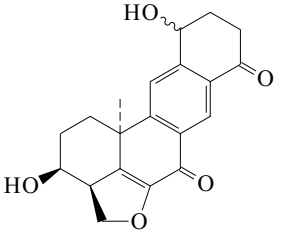
(2*R,4*S**)-*form***
cis-*form*. ***Calyxolane B***
[194999-93-4]
Constit. of *Calyx podatypa*.
Oil. $[\alpha]_D$ 0. Poss. racemic. λ_{max} 206 (ϵ 16000) (MeOH).
Rodriguez, A.D. *et al., J. Nat. Prod.*, 1997, **60**, 915-917 (*isol, uv, ir, pmr, cmr, ms*)

Tetrahydrohalenaquinone A **T-163**
[142508-06-3]



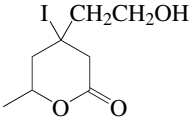
$C_{20}H_{20}O_5$ 340.375
Constit. of *Xestospongia* cf. *carbonaria*. Solid.
Mp 234°. $[\alpha]_D$ +12. λ_{max} 252 (ϵ 16600); 328 (ϵ 9000) (EtOH) (Derep). λ_{max} 216; 258; 334 (MeOH) (Derep).
Alvi, K.A. *et al., J.O.C.*, 1993, **58**, 4871 (*isol, pmr, cmr*)

Tetrahydrohalenaquinone B **T-164**



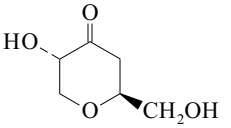
$C_{20}H_{20}O_5$ 340.375
Constit. of *Xestospongia* cf. *carbonaria*. Solid.
Mp 234°. $[\alpha]_D$ +24.
Alvi, K.A. *et al., J.O.C.*, 1993, **58**, 4871 (*isol, pmr, cmr*)

Tetrahydro-4-(2-hydroxyethyl)-4-iodo-6-methyl-2*H*-pyran-2-one, 9CI **T-165**



$C_8H_{13}IO_3$ 284.093
Octadecanoyl: [195971-77-8]
$C_{26}H_{47}IO_4$ 550.559
Isol. from the alga *Laurencia majuscula*. Solid.
Mp 63-64°.
Su, J.-Y *et al., CA*, 1997, **127**, 259825d (*isol*)

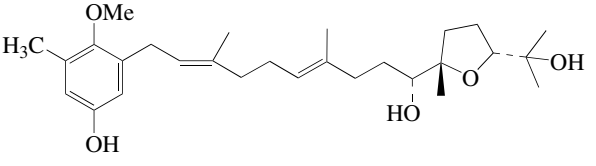
Tetrahydro-5-hydroxy-2-hydroxymethyl-4*H*-pyran-4-one **T-166**
2,3,5,6-Tetrahydrokojic acid



$C_6H_{10}O_4$ 146.143
Bp_{16} 135-140°.

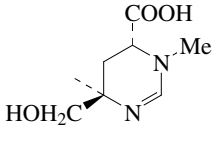
(2*S*,5*S*)-*form*
Haliclonol
[142450-10-0]
Constit. of *Haliclona hogarthi*.
Oil. $[\alpha]_D^{25}$ -21.4 (MeOH).
Ichimoto, I. *et al., Agric. Biol. Chem.*, 1964, **28**, 723 (*synth*)
Ciminiello, P. *et al., Heterocycles*, 1992, **34**, 765 (*isol, pmr, cmr*)

Tetrahydro-α-[9-(5-hydroxy-2-methoxy-3-methylphenyl)-3,7-dimethyl-3,7-nonadienyl]-α′,α′,2-trimethyl-2,5-furandimethanol, 9CI **T-167**
α⁵-[9-(5-Hydroxy-2-methoxy-3-methylphenyl)-3,7-dimethyl-3,7-nonadienyl]-α²,α²,5-trimethyltetrahydrofuran-2,5-dimethanol
[224784-49-0]



$C_{28}H_{44}O_5$ 460.653
Constit. of *Cystophora brownii*. Pale yellow oil. $[\alpha]_D$ +2.8 (c, 5 in $CHCl_3$). λ_{max} 284 (ϵ 2570) (MeOH).
Stereoisomer: [224784-50-3]
$C_{28}H_{44}O_5$ 460.653
Constit. of *Cystophora brownii*. Pale yellow oil. $[\alpha]_D$ +17.6 (c, 0.55 in $CHCl_3$). λ_{max} 285 (ϵ 2580) (MeOH).
Bian, B. *et al., Aust. J. Chem.*, 1998, **51**, 1157-1165 (*isol, pmr, cmr*)

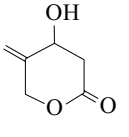
3,4,5,6-Tetrahydro-6-hydroxymethyl-3,6-dimethyl-4-pyrimidinecarboxylic acid, 9CI **T-168**
[246137-84-8]



Relative Configuration

$C_8H_{14}N_2O_3$ 186.21
Isol. from the Palauan sponge *Protophlitaspongia aga*. Antifouling agent against barnacles.
Hattori, T. *et al., Fish. Sci.*, 2001, **67**, 690-693 (*isol*)

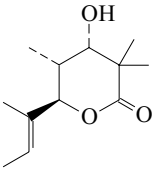
Tetrahydro-4-hydroxy-5-methylene-2*H*-pyran-2-one **T-169**



$C_6H_8O_3$ 128.127

*Ac: 4-(Acetyloxy)tetrahydro-5-methylene-2*H*-pyran-2-one, 9CI.*
3-Acetoxy-4-hydroxymethyl-4-pentenoic acid lactone
[74411-81-7]
$C_8H_{10}O_4$ 170.165
Metab. of the sponge *Plakortis zygompha*.
Faulkner, D.J. *et al., Tet. Lett.*, 1980, 23 (*isol, spectra*)

Tetrahydro-4-hydroxy-5-(1-methyl-2-propenyl)-3,3,5-trimethyl-2*H*-pyran-2-one, 9CI **T-170**



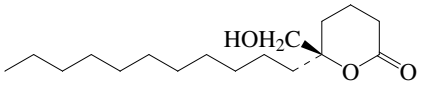
(4*S*,5*S*,6*R*)–*form*

$C_{12}H_{20}O_3$ 212.288

(4*R*,5*S*,6*R*)-*form*
Helicascolide B
[121325-38-0]
Isol. from the mangrove ascomycete *Helicascus kanaloanus* ATCC18591.
Cryst.
Mp 61-62°. $[\alpha]_D^{31}$ -27.6 (c, 0.4 in $CHCl_3$).

(4*S*,5*S*,6*R*)-*form*
Helicascolide A
[121350-98-9]
From *Helicascus kanaloanus* ATCC18591.
Cryst.
Mp 97-98°. $[\alpha]_D^{31}$ -25 (c, 1.4 in $CHCl_3$).
Poch, G.K. *et al., J. Nat. Prod.*, 1989, **52**, 257-260 (*isol, pmr, struct*)

Tetrahydro-6-hydroxymethyl-6-undecyl-2*H*-pyran-2-one **T-171**
Tanikolide

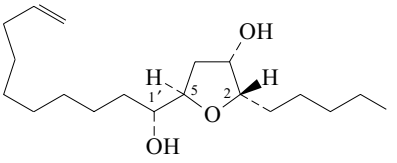


$C_{17}H_{32}O_3$ 284.438

(*R*)-*form* [248278-40-2]
Isol. from *Lyngbya majuscula*. Antifungal and cytotoxic agent.
Oil. $[\alpha]_D^{25}$ +2.3 (c, 0.65 in $CHCl_3$).

(±)-*form* [382136-69-8]
Oil.
Singh, I.P. *et al., J. Nat. Prod.*, 1999, **62**, 1333-1335 (*isol, ir, pmr, cmr, ms*)
Chang, M.-Y. *et al., J. Chin. Chem. Soc. (Taipei)*, 2001, **48**, 787-794 (*synth*)
Krauss, J. *et al., Nat. Prod. Lett.*, 2001, **15**, 393-399 (*synth*)
Zhang, R. *et al., Synth. Commun.*, 2002, **32**, 2187-2194 (*synth, ir, pmr, cmr*)
Mizutani, H. *et al., Tetrahedron*, 2002, **58**, 8929-8936 (*synth*)
Zhai, H. *et al., Tet. Lett.*, 2003, **44**, 2893-2894 (*synth*)
Carda, M. *et al., Tetrahedron*, 2003, **59**, 857-864 (*synth*)
Arasaki, H. *et al., Chem. Pharm. Bull.*, 2004, **52**, 848-852 (*synth*)
Schomaker, J.M. *et al., Org. Biomol. Chem.*, 2004, **2**, 621-624 (*synth*)
Ohgiya, T. *et al., Tet. Lett.*, 2004, **45**, 8273-8275 (*synth*)
Chen, Q. *et al., Tetrahedron*, 2005, **61**, 8390-8393 (*synth*)

Tetrahydro-2-(1-hydroxy-9-nonenyl)-5-pentyl-3-furanol **T-172**
Tetrahydro-4-hydroxy-α-8-nonenyl-5-pentyl-2-furanmethanol, 9CI.
6,9-Epoxy-18-nonadecene-7,10-diol



$C_{19}H_{36}O_3$ 312.492

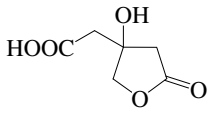
(1′*R*,2*S*,3*S*,5*R*)-*form* [74350-84-8]
Isol. from the brown alga *Notheia anomala*. Nematocidal agent.
Plates (hexane).
Mp 54.5-55°. $[\alpha]_D^{21}$ +15 (c, 1 in $CHCl_3$).
1′-O-*Dodecanoyl:* [129436-96-0]
$C_{31}H_{58}O_4$ 494.797
Isol. from *Notheia anomala*.
3-O-*Dodecanoyl:* [129451-33-8]
$C_{31}H_{58}O_4$ 494.797
Isol. from *Notheia anomala*.
1′-O-*Tetradecanoyl:* [129436-97-1]
$C_{33}H_{62}O_4$ 522.85
Isol. from *Notheia anomala*.
3-O-*Tetradecanoyl:* [129436-99-3]
$C_{33}H_{62}O_4$ 522.85
Isol. from *Notheia anomala*.
1′-O-*Hexadecanoyl:* [129436-86-8]
$C_{35}H_{66}O_4$ 550.904
Isol. from *Notheia anomala*. Visc. oil. $[\alpha]_D$ +172.4 (c, 0.4 in $CHCl_3$).
3-O-*Hexadecanoyl:* [129451-31-6]
$C_{35}H_{66}O_4$ 550.904
Isol. from *Notheia anomala*. Visc. oil. $[\alpha]_D$ +63.6 (c, 0.5 in $CHCl_3$).
1′-O-*Octadecanoyl:* [129436-98-2]
$C_{37}H_{70}O_4$ 578.958
Isol. from *Notheia anomala*.
3-O-*Octadecanoyl:* [129437-00-9]
$C_{37}H_{70}O_4$ 578.958
Isol. from *Notheia anomala*.
3-O-*(5,8,11,14-Eicosatetraenoyl)(*all-Z*): 6,9-Epoxy-18-nonadecene-7,10-diol 7-arachidonate*
[138195-54-7]
$C_{39}H_{66}O_4$ 598.948
Constit. of *Notheia anomala*. Yellow oil. $[\alpha]_D$ +16.6 (c, 0.4 in $CHCl_3$).

(1′*S*,2*S*,3*S*,5*S*)-*form*
Isol. from *Notheia anomala*. Nematocidal agent. Oil. $[\alpha]_D$ +74.5 (c, 0.4 in $CHCl_3$).

[89673-80-3]

Warren, R.G. *et al., Aust. J. Chem.*, 1980, **33**, 891 (*isol, pmr, cmr, ms*)
Hatakeyama, S. *et al., Tet. Lett.*, 1985, **26**, 1333 (*synth*)
Barrow, R.A. *et al., Aust. J. Chem.*, 1990, **43**, 895 (*isol, pmr, cmr*)
Gurjar, M.K. *et al., Heterocycles*, 1990, **31**, 407 (*synth*)
Murray, L.M. *et al., Aust. J. Chem.*, 1991, **44**, 843 (*deriv*)
Chikashita, H. *et al., Chem. Lett.*, 1993, 477 (*synth*)
Capon, R.J. *et al., Tet. Lett.*, 1997, **38**, 7609-7612 (*synth*)
Wang, Z.-M. *et al., J.O.C.*, 1998, **63**, 1414-1418 (*synth*)
Capon, R.J. *et al., Tetrahedron*, 1998, **54**, 2227-2242 (*isol, ir, pmr, cmr, ms*)
Mori, Y. *et al., Tet. Lett.*, 1999, **40**, 731-734 (*synth*)
Garcia, C. *et al., Tet. Lett.*, 2000, **41**, 4127-4130 (*synth*)
Gadikota, R.R. *et al., J.O.C.*, 2002, **66**, 9046-9051 (*synth*)

Tetrahydro-3-hydroxy-5-oxo-3-furanacetic acid T-173

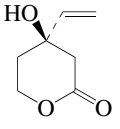


$C_6H_8O_5$ 160.126

Me ester: [164353-60-0]
$C_7H_{10}O_5$ 174.153
Isol. from the cyanobacterium *Lyngbya majuscula*.
$[\alpha]_D^{24}$ -3 (c, 0.23 in $CHCl_3$).
Todd, J. S. *et al., J. Nat. Prod.*, 1995, **58**, 586-589 (*isol, ir, pmr, cmr*)

Tetrahydro-4-hydroxy-4-vinyl-2*H*-pyran-2-one T-174

*4-Ethenyltetrahydro-4-hydroxy-2*H*-pyran-2-one*



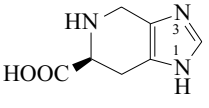
(*R*)-*form*

$C_7H_{10}O_3$ 142.154

(*R*)-*form*
Harzialactone B
[203243-32-7]
Prod. by a *Trichoderma harzianum* isol. from the sponge *Halichondria okadai*.
Oil. $[\alpha]_D$ -23.5 (c, 1.8 in $CHCl_3$). λ_{max} 223 (log ϵ 2.66); 278 (log ϵ 2.89) (EtOH). λ_{max} 223 (ϵ 457); 278 (ϵ 776) (MeOH) (Berdy).
Amagata, T. *et al., J. Antibiot.*, 1998, **51**, 33-40 (*isol, uv, ir, cd, pmr, cmr*)

4,5,6,7-Tetrahydro-1*H*-imidazo[4,5-*c*]pyridine-6-carboxylic acid, 9CI T-175

Spinacine



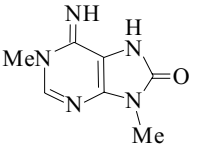
$C_7H_9N_3O_2$ 167.167

(*S*)-*form* [59981-63-4]
Isol. from the crab *Crangon vulgaris*, from the liver of the shark *Acanthias vulgaris* and from spinach. Also isol. from the roots of *Panax ginseng*.
Mp 265°. $[\alpha]_D^{20}$ -174.6 (H_2O). Forms a sesquihydrate.
Hydrochloride: Mp 286-287° (279-280°).
1-Me: [133807-71-3]
$C_8H_{11}N_3O_2$ 181.194
Cryst. (MeOH/Et_2O) (as dihydrochloride). Mp 287-290° dec. (dihydrochloride). $[\alpha]_D^{23}$ -9597 (c, 1.11 in H_2O).
3-Me: [114787-98-3]
$C_8H_{11}N_3O_2$ 181.194
Cryst. (MeOH/Et_2O) (as dihydrochloride). Mp 262-265° dec. (dihydrochloride). $[\alpha]_D^{23}$ -93.5 (c, 1.05 in H_2O).

(±)-*form*
Synthetic. Mp 265°.
Ackermann, D. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1941, **268**, 277-282; 1949, **284**, 129-131; 1962, **328**, 275-276 (*isol, struct, synth*)
Vitali, T. *et al., Gazz. Chim. Ital.*, 1964, **94**, 296-305 (*synth*)
Nardelli, M. *et al., Ric. Sci., Parte 2: Sez. A*, 1964, **7**, 718-719; *CA*, **63**, 12440g (*cryst struct*)
Andreetti, G.D. *et al., Gazz. Chim. Ital.*, 1971, **101**, 625-634 (*cryst struct*)
Eilazyan, O.G. *et al., CA*, 1982, **96**, 85467n (*synth*)
Han, Y.N. *et al., Arch. Pharmacal Res.*, 1987, **10**, 258-259; *CA*, **108**, 201742r (*isol*)
Klutchko, S. *et al., J. Het. Chem.*, 1991, **28**, 97-108 (*synth, pmr, derivs*)

1,6,7,9-Tetrahydro-6-imino-1,9-dimethyl-8*H*-purin-8-one, 9CI T-176

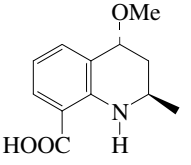
1,9-Dimethyl-6-imino-8-oxopurine
[98601-03-7]



$C_7H_9N_5O$ 179.181
Isol. from the marine sponge *Hymeniacidon sanguinea*.
Mp 300° (synthetic). Isol. and struct. elucidated as the Ac deriv.
Ac: [98601-04-8]
Cryst. ($CHCl_3$). Mp 245-246°.
Cimino, G. *et al., J. Nat. Prod.*, 1985, **48**, 523-528 (*isol, uv, ir, pmr, ms, cryst struct*)
Fujii, T. *et al., Heterocycles*, 1988, **27**, 1145-1148 (*synth, ir, pmr*)

1,2,3,4-Tetrahydro-4-methoxy-2-methyl-8-quinolinecarboxylic acid T-177

Helquinoline

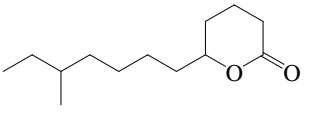


$C_{12}H_{15}NO_3$ 221.255

(2*RS*,4*RS*)-*form*
Prod. by the marine-derived *Janibacter limosus* Hel 1. Antibacterial and antifungal agent. Oil. λ_{max} 221 (log ϵ 4.05); 261 (log ϵ 3.67); 349 (log ϵ 3.49) (MeOH). λ_{max} 201 (log ϵ 3.96); 223 (log ϵ 4.03); 261 (log ϵ 3.59); 358 (log ϵ 3.47) (MeOH/HCl).
Asolkar, R.N. *et al., J. Antibiot.*, 2004, **57**, 17-23 (*isol, uv, pmr, cmr*)

Tetrahydro-6-(5-methylheptyl)-2*H*-pyran-2-one T-178

10-Methyl-5-dodecanolide

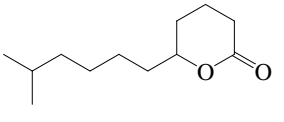


$C_{13}H_{24}O_2$ 212.331

(ξ)-*form*
Prod. by the marine *Streptomyces* sp. strain GWS-BW-H5.
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 837-865 (*isol, synth, pmr, cmr, ms*)

Tetrahydro-6-(5-methylhexyl)-2*H*-pyran-2-one T-179

10-Methyl-5-undecanolide

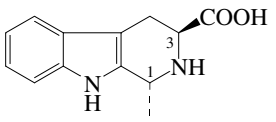


$C_{12}H_{22}O_2$ 198.305

(ξ)-*form*
Prod. by the marine *Streptomyces* sp. strain GWS-BW-H5.
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 837-865 (*isol, synth, pmr, cmr, ms*)

2,3,4,9-Tetrahydro-1-methyl-1*H*-pyrido[3,4-*b*]indole-3-carboxylic acid, 9CI T-180

1,2,3,4-Tetrahydro-1-methyl-β-carboline-3-carboxylic acid
[5470-37-1]
[143396-05-8 (*cis*-form)]



(1*R*,3*S*)-*form*

$C_{13}H_{14}N_2O_2$ 230.266

(1*R*,3*S*)-*form* [42438-72-2]
Constit. of cocoa and maca tubers (*Lepidium meyenii*).
Cryst. (H_2O).
Mp 242-244° (225-228° dec.). $[\alpha]_D$ -69.1 (c, 1 in 1*M* HCl/MeOH 1:1).
N^2-*Me:*
$C_{14}H_{16}N_2O_2$ 244.293
Mp 222-223° (as hydrochloride). $[\alpha]_D^{25}$ -29.6 (c, 1 in 1*M* HCl MeOH/H_2O 1:1).

(1*S*,3*S*)-*form* [40678-46-4]
Alkaloid from the starfish *Lethasterias nanimensis chelifera*.
Constit. of cocoa.
Cryst. (H_2O).
Mp 293° (276-280° dec.). $[\alpha]_D^{25}$ -106.6 (c, 1 in 1*M* HCl/MeOH 1:1).

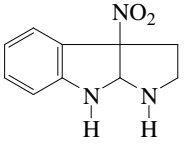
(1ξ,3ξ)-*form*
Formed by Pictet-Spengler condensation between Acetaldehyde and Tryptophan in nature or during food processing. Present in many foods. Alkaloid from the toxic fly agaric mushroom (*Amanita muscaria*). Shows little pharmacol. activity. Needles (H_2O).
Mp 290° dec. $[\alpha]_D$ -142.8 (50 % Py aq.). λ_{max} 219; 271; 277; 280 (sh); 287 (MeOH).

(1*R,3*R**)-*form***
6-Hydroxy: 1,2,3,4-Tetrahydro-6-hydroxy-1-methyl-β-carboline-3-carboxylic acid. ***Hyrtioerectine B***
$C_{13}H_{14}N_2O_3$ 246.265
Isol. from the sponge *Hyrtios erectus*. Amorph. solid. $[\alpha]_D^{25}$ -19.2 (c, 0.18 in MeOH). λ_{max} 231 (log ϵ 3.81); 276 (log ϵ 3.74); 357 (log ϵ 1.82) (MeOH).

[22677-22-1]

Matsumoto, T. *et al., Helv. Chim. Acta*, 1969, **52**, 716-720 (*isol, uv, ir, struct*)
Brossi, A. *et al., J. Med. Chem.*, 1973, **16**, 418-420 (*1R,3S-form, 1S,3S-form, synth, pharmacol, ord*)
Bobbitt, J.M. *et al., J.O.C.*, 1980, **45**, 1978-1984 (*synth*)
Bosin, T.R. *et al., J. Agric. Food Chem.*, 1986, **34**, 843-847 (*isol*)
Herraiz, T. *et al., J. Agric. Food Chem.*, 1996, **44**, 3057-3065; 1998, **46**, 3484-3490; 1999, **47**, 4883-4887; 2000, **48**, 4900-4904; 2004, **52**, 2652-2658 (*hplc, occur, bibl*)
Herraiz, T. *et al., J. Chromatogr., A*, 1997, **765**, 265-277; 2000, **871**, 23-30 (*occur, gc, hplc*)
Piacenta, S. *et al., J. Agric. Food Chem.*, 2002, **50**, 5621-5625 (*1R,3S-form, isol*)
Kicha, A.A. *et al., Tet. Lett.*, 2003, **44**, 1935-1937 (*Lethasterias alkaloid, isol, pmr, cmr*)
Youssef, D.T.A. *et al., J. Nat. Prod.*, 2005, **68**, 1416-1419 (*Hyrtioerectine B*)

2,3,8,8*a*-Tetrahydro-3*a*-nitro-1*H*-pyrrolo[2,3-*b*]indole T-181

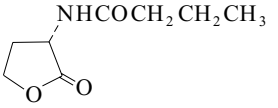


$C_{10}H_{11}N_3O_2$ 205.216
Isol. from the marine-derived *Flavobacterium* sp. T436.

Schuhmann, I. *et al., Dissertation*, Univ. of Göttingen, 2005, (*isol*)

N-(Tetrahydro-2-oxo-3-furanyl)butanamide, 9CI T-182

α-Butyramido-γ-butyrolactone



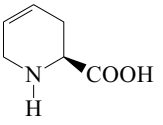
$C_8H_{13}NO_3$ 171.196

(*S*)-*form* [67605-85-0]
Constit. of *Lyngbya majuscula*.
Cryst. (CH_2Cl_2/hexane).
Mp 120-121°. $[\alpha]_D^{25}$ +18.9 (c, 0.74 in $CHCl_3$).

Marner, F.-J. *et al., Phytochemistry*, 1978, **17**, 553 (*isol, struct*)

1,2,3,6-Tetrahydro-2-pyridinecarboxylic acid, 9CI T-183

1,2,3,6-Tetrahydropicolinic acid, 8CI. ***Baikiain***
[498-98-6]



(*S*)–*form*

$C_6H_9NO_2$ 127.143

(*S*)-*form* [31456-71-0]
Amino acid present in *Baikiaea plurijuga, Caesalpinia tinctoria*, red algae and red seaweeds (Leguminosae, Caesalpiniaceae). Also in *Russula subnigricans*. Neurotransmission inhibitor. Prisms (MeOH). V. sol. H_2O, spar. sol. EtOH, insol. Me_2CO, EtOAc, Et_2O, C_6H_6; Sol. H_2O. $[\alpha]_D$ -182.6 (c, 0.3 in H_2O).

Hydrochloride:
Prisms (MeOH or EtOH). Mp 264°. $[\alpha]_D^{20}$ -90.1 (H_2O).

Picrate:
Needles or plates (H_2O). Mp 172-173°.

Me ester:
$C_7H_{11}NO_2$ 141.169
Bp_{15} 110-112°.

Me ester, hydrochloride:
Prisms (MeOH/Me_2CO). Mp 164°.

N-*Benzoyl:*
$C_{13}H_{13}NO_3$ 231.251
Prisms (EtOAc); needles (Et_2O or H_2O). Mp 178-179°. $[\alpha]_D^{20}$ -91.9.

N-*Di-Me, betaine:* ***Baikiain betaine***
[114622-09-2]
$C_8H_{13}NO_2$ 155.196
Isol. from the red alga *Pterocladia capillacea*. Cryst. (2-propanol). Mp 184-186°. $[\alpha]_D^{25}$ -103 (c, 1.6 in H_2O).

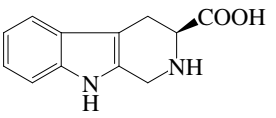
(±)-*form* [7200-16-0]
Small prisms (MeOH/Me_2CO). Mp 251-254° dec Mp 273-274° dec.

Hydrochloride: [111257-58-0]
Cryst. (MeOH/EtOAc). Mp 264° dec.

King, T.J. *et al., J.C.S.*, 1950, 3590 (*isol, struct, abs config*)
Burgstahler, A.W. *et al., J.O.C.*, 1960, **25**, 489 (*synth*)
Watson, R. *et al., Phytochemistry*, 1973, **12**, 617 (*isol*)
Impellizzeri, G. *et al., Phytochemistry*, 1975, **14**, 1549-1557 (*algae, isol*)
Maeda, M. *et al., Agric. Biol. Chem.*, 1980, **44**, 2725 (*isol, pmr, cmr, ir, occur, ms*)
Miyazawa, K. *et al., CA*, 1983, **98**, 194969q (*occur*)
Sciuto, S. *et al., J. Nat. Prod.*, 1988, **51**, 322-325 (*Baikiain betaine*)
Kinderman, S.S. *et al., Adv. Synth. Catal.*, 2002, **344**, 736-748 (*S-form, synth, ir, pmr, cmr*)
Ginesta, X. *et al., Tet. Lett.*, 2002, **43**, 779-782 (*synth*)

2,3,4,9-Tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylic acid, 9CI T-184

1,2,3,4-Tetrahydro-β-carboline-3-carboxylic acid
[6052-68-2]
[41509-88-0 (±-form), 72002-54-1 (*R*-form)]



$C_{12}H_{12}N_2O_2$ 216.239

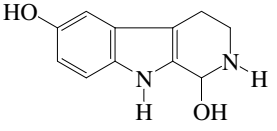
(*S*)-*form*
L-form. ***Lycoperodine 1***
[42438-90-4]
Formed by Pictet-Spengler condensation of Formaldehyde and Tryptophan in nature or during food processing. Alkaloid from *Aleurites fordii* and *Allium tuberosum*. Isol. from starfish *Asterias rollestoni*. Constit. of cocoa and tomatoes.
Cryst. (H_2O).
Mp 282-284° Mp 315°. $[\alpha]_D^{20}$ -124.6 (c, 0.2 in 0.1*M* NaOH) $[\alpha]_D^{25}$ -49.6 (c, 1 in 1*M* HCl MeOH/H_2O 1:1). λ_{max} 274 (3.72); 291 (sh) (3.5) (MeOH).

[129848-94-8]

Harvey, D.G. *et al., J.C.S.*, 1941, **63**, 153-159 (*synth*)
Brossi, A. *et al., J. Med. Chem.*, 1973, **16**, 418-420 (*S-form, synth, pmr, ord, cd, N²-Me*)
Okuda, T. *et al., Phytochemistry*, 1975, **14**, 2304-2305 (*ir, uv, ms, pmr, config*)
Maclaren, J.A. *et al., Aust. J. Chem.*, 1989, **42**, 813-821 (*synth, bibl*)
Tilstra, L. *et al., J.A.C.S.*, 1990, **112**, 9176-9182; 9182-9190 (*synth, pmr, ms, cryst struct*)
Li, G.Q. *et al., J. Chin. Pharm. Sci.*, 2004, **13**, 81-86 (*isol, Asterias*)

2,3,4,9-Tetrahydro-1*H*-pyrido[3,4-*b*]indole-1,6-diol T-185

1,2,3,4-Tetrahydro-1,6-dihydroxy-β-carboline
[452067-34-4]

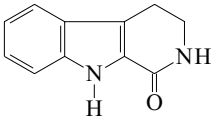


$C_{11}H_{12}N_2O_2$ 204.228
Isol. from the sponge *Hyrtios reticulata*.

Salmoun, M. *et al., J. Nat. Prod.*, 2002, **65**, 1173-1176 (*isol*)

2,3,4,9-Tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-one, 9CI T-186

1,2,3,4-Tetrahydro-1-oxo-β-carboline
[17952-82-8]



$C_{11}H_{10}N_2O$ 186.213
Alkaloid from *Evodia rutaecarpa*. Also isol. from an Indonesian sponge. Needles (EtOH aq.).
Mp 183-185°.

Picrate:
Orange-yellow plates (EtOH). Mp 195-197°.

N^2-*(2-Methylaminobenzoyl)*: ***Rhetsinine***. *Hydroxyevodiamine*
[526-43-2]
$C_{19}H_{17}N_3O_2$ 319.362
Alkaloid from the trunk bark of *Zanthoxylum rhetsa* and the fruits of *Evodia rutaecarpa* (Rutaceae). Also obt. by the mild oxidn. of Evodiamine. Yellow cryst. ($CHCl_3$/EtOH).
Mp 206-207° (192° dec.). λ_{max} 314 (log ε 4.15) (EtOH).

N^2-*(2-Methylaminobenzoyl), hydrochloride:*
Yellow needles. Mp 228-229° dec.

N^2-*(2-Methylaminobenzoyl), picrate:*
Slender orange-yellow needles. Mp 270-272° dec.

N^2-*Me: 2,3,4,9-Tetrahydro-2-methyl-1*H-*pyrido[3,4*-b*]indol-1-one. 1,2,3,4-Tetrahydro-2-methyl-1-oxo-β-carboline.* ***Strychnocarpine***
[59156-98-8]
$C_{12}H_{12}N_2O$ 200.24
Alkaloid from the stem bark of *Strychnos elaeocarpa* and *Strychnos floribunda* (Strychnaceae). Weak muscular relaxant.
Cryst. (EtOAc).
Mp 226° (198-200°). λ_{max} 227 (log ε 4.25); 242 (log ε 4.07); 305 (log ε 4.14) (MeOH).

*6-Hydroxy: 2,3,4,9-Tetrahydro-6-hydroxy-1*H-*pyrido[3,4*-b*]indol-1-one. 1,2,3,4-Tetrahydro-6-hydroxy-1-oxo-β-carboline*
[51085-95-1]
$C_{11}H_{10}N_2O_2$ 202.212
Isol. from the sponge *Hyrtios* sp.

*7-Hydroxy: 2,3,4,9-Tetrahydro-7-hydroxy-1*H-*pyrido[3,4*-b*]indol-1-one, 9CI*
[56409-32-6]
Mp 138°.

*5-Methoxy: 2,3,4,9-Tetrahydro-6-methoxy-1*H-*pyrido[3,4*-b*]indol-1-one.* ***1,2,3,4-Tetrahydro-5-methoxy-1-oxo-β-carboline***
[26579-73-7]
$C_{12}H_{12}N_2O_2$ 216.239
Alkaloid from the root bark of *Alstonia venenata* (Apocynaceae). Prisms (MeOH).
Mp 216-217° (synth.) Mp 182-184° (nat.). The original nat. isolate was impure and the reported spectroscopic data was subsequently revised. λ_{max} 236 (log ε 4.46); 295 (log ε 4.16) (EtOH).

6-Methoxy: 2,3,4,9-Tetrahydro-6-methoxy-1-H-*pyrido[3,4*-b*]indol-1-one, 9CI. 1,2,3,4-Tetrahydro-6-methoxy-1-oxo-β-carboline*
[17952-87-3]
Synthetic. Prisms (EtOH). Mp 275-277° (265°) Mp 275-277°.

*7-Methoxy: 2,3,4,9-Tetrahydro-7-methoxy-1*H-*pyrido[3,4*-b*]indol-1-one. 1,2,3,4-Tetrahydro-7-methoxy-1-oxo-β-carboline.* ***Ketotetrahydronorharmine****. Harmalacidine*
[26579-69-1]
$C_{12}H_{12}N_2O_2$ 216.239
Alkaloid from *Banisteriopsis caapi* (Malphigiaceae) and seeds of *Peganum harmala* (Zygophyllaceae). Needles ($CHCl_3$/MeOH).
Mp 200-201° (197-198° dec.). λ_{max} 220; 250; 325 (MeOH).

8-Methoxy: 2,3,4,9-Tetrahydro-8-methoxy-1-H-*pyrido[3,4*-b*]indol-1-one, 9CI. 1,2,3,4-Tetrahydro-8-methoxy-1-oxo-β-carboline*
[109021-64-9] Synthetic.
Needles (MeOH). Mp 244-246° (241-242°).

Abramovitch, R.A. *et al., J.C.S.*, 1956, 4589-4592 (*6-methoxy, synth*)
Chatterjee, A. *et al., Tetrahedron*, 1959, **7**, 257-261 (*Rhetsinine, isol, uv, ir*)
Pachter, I.J. *et al., J.O.C.*, 1960, **25**, 1680-1682 (*Rhetsinine, uv, struct, synth*)
Hashimoto, Y. *et al., Phytochemistry*, 1976, **15**, 1559-1560 (*Ketotetrahydronorharmine, isol, uv, ir, pmr, ms, struct, synth*)
Rolfsen, W. *et al., Acta Pharm. Suec.*, 1980, **17**, 333-340 (*Strychnocarpine, isol, uv, ir, pmr, cmr, ms, struct*)
Verpoorte, R. *et al., Planta Med.*, 1981, **42**, 32-36 (*Strychnocarpine, isol, uv, pmr, ms*)
Banerji, J. *et al., Phytochemistry*, 1982, **21**, 2765-2767 (*5-methoxy, isol, struct*)
Herdeis, C. *et al., Heterocycles*, 1984, **22**, 2277 (*Strychnocarpine, synth, uv, ir, pmr, cmr*)
Yamada, F. *et al., Heterocycles*, 1986, **24**, 2619-2627 (*5-methoxy, 8-methoxy, synth, uv, ir, pmr, struct*)
Lehmann, J. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1988, **321**, 411-414 (*Strychnocarpine, synth, ir, pmr*)
Siddiqui, S. *et al., Heterocycles*, 1988, **27**, 1401-1410 (*Harmalacidine, isol, uv, ir, pmr, cmr, ms*)
Narayanan, K. *et al., J.O.C.*, 1991, **56**, 359-365 (*pmr, ir, ms*)
Bracher, F. *et al., Annalen*, 1992, 1315-1319 (*synth*)
Abramovitch, R.A. *et al., Synlett*, 1992, 795-796 (*6-methoxy, synth*)
Bracher, F. *et al., Pharmazie*, 1993, **48**, 695 (*Harmalacidine, Strychnocarpine, synth*)
Soti, F. *et al., Synth. Commun.*, 1993, **23**, 1689-1698 (*8-methoxy, synth*)
Salmoun, M. *et al., J. Nat. Prod.*, 2002, **65**, 1173-1176 (*6-hydroxy*)

Rao, K.V. *et al., J. Nat. Prod.*, 2003, **66**, 823-828 (*isol, pmr, cmr*)
Lehmann, I. *et al., Arch. Pharm. (Weinheim, Ger.)*, **1988**, 321-411 (*synth, ir, pmr*)

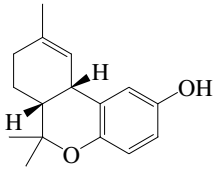
Tetrahydrothiophene 1,1-dioxide, 9CI T-187

Sulfolane. Tetramethylene sulfone. Sulpholane. Cyclotetramethylene sulfone. Bondolane A
[126-33-0]

$C_4H_8O_2S$ 120.172
Constit. of the sponge/tunicate composite, *Batzella* sp./*Lissoclinum* sp. High-boiling polar aprotic solv. Used for extraction of aromatics from hydrocarbon mixts. Used as solv. for measuring polarographic half-wave potentials for alkali metals and Ba. Oil. Mp 27°. Bp 285° Bp_{18} 153-154°. Bitter taste.
▶ Fl. p. 177° (oc). Eye irritant. LD_{50} (rat, orl) 1941 mg/kg.
XN0700000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 882C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1421C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 832B (*ir*)
Arnett, E.M. *et al., J.A.C.S.*, 1964, **86**, 409 (*use*)
Morrow, G.S. *et al., CA*, 1970, **72**, 43508a (*rev*)
Coetzee, J.F. *et al., Anal. Chem.*, 1972, **44**, 1129 (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 651 (*use*)
Riddick, Y.A. *et al., Organic Solvents*, 4th edn., J. Wiley, 1986, 686 (*props*)
Barrow, R.A. *et al., J. Nat. Prod.*, 1992, **55**, 1330 (*isol*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1522
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SNW500

6*a*,7,8,10*a*-Tetrahydro-6,6,9-trimethyl-6*H*-dibenzo[*b*,*d*]pyran-2-ol, 9CI T-188



(6*aR*,10*aS*)-*form*

$C_{16}H_{20}O_2$ 244.333

(6*aR*,10*aS*)-*form*
(+)-cis-*form*. ***Epiconicol***
[149817-72-1]
[868391-33-7]
Isol. from the ascidians *Synoicum castellatum* and *Aplidium* aff. *densum*. Glass. $[\alpha]_D$ +58 (c, 0.09 in $CHCl_3$). λ_{max} 287 (ϵ 28000); 325 (ϵ 7700) (MeOH) (Berdy).

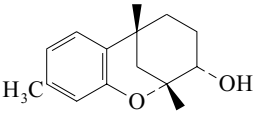
6a,*7,8,10*a-*Tetradehydro:* ***Didehydroconicol***
[868279-76-9]
$C_{16}H_{16}O_2$ 240.301
Constit. of *Aplidium* aff. *densum*. Yellow oil. λ_{max} 230 (log ϵ 3.59); 240 (log ϵ 3.4); 254 (log ϵ 3.29); 272 (log ϵ 3.27); 330 (log ϵ 3) (MeOH).

(6*aS*,10*aS*)-*form*
(+)-trans-*form*. ***Conicol***
[459174-31-3]
Constit. of *Aplidium conicum* and *Aplidium* aff. *densum*.
Oil. $[\alpha]_D^{27}$ +1 (c, 0.4 in $CHCl_3$).

Gosh, R. *et al., J.C.S.*, 1940, 1118-1121; 1393-1396 (*synth*)
Carroll, A.R. *et al., Aust. J. Chem.*, 1993, **46**, 1079-1083 (*isol, struct*)
Garrido, L. *et al., J. Nat. Prod.*, 2002, **65**, 1328-1331 (*Conicol*)
Simon-Levert, A. *et al., J. Nat. Prod.*, 2005, **68**, 1412-1415 (*Conicol, Epiconicol, Didehydroconicol*)

3,4,5,6-Tetrahydro-2,6,9-trimethyl-2,6-methano-2*H*-1-benzoxocin-3-ol, 9CI T-189

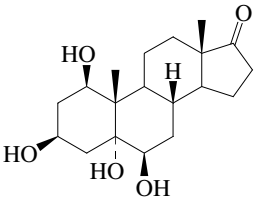
[145382-79-2]



$C_{15}H_{20}O_2$ 232.322
Constit. of *Laurencia majuscula*. Yellow oil. $[\alpha]_D$ 0 (c, 0.1 in $CHCl_3$).

de Nys, R. *et al., Aust. J. Chem.*, 1992, **45**, 1611 (*isol, pmr, cmr*)

1,3,5,6-Tetrahydroxyandrostan-17-one T-190



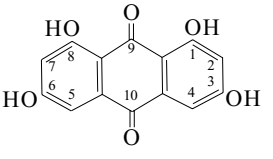
$C_{19}H_{30}O_5$ 338.443

(1β,3β,5α,6β)-*form* [90134-60-4]
Isol. from soft coral *Sarcophyton glaucum*. Cryst. + ¼ H_2O (Me_2CO/hexane). Mp 249-251°. $[\alpha]_D$ +37.2.

Kobayashi, M. *et al., Steroids*, 1982, **40**, 673-677 (*isol, pmr, cmr, struct, synth*)

1,3,6,8-Tetrahydroxyanthraquinone T-191

1,3,6,8-Tetrahydroxy-9,10-anthracenedione, 9CI. ***Rheoemodin***
[52940-12-2]



$C_{14}H_8O_6$ 272.214
Prod. by *Aspergillus versicolor, Rheum hotaoense, Rumex alpinus, Trichoderma viride* and *Verticicladiella* sp. Inhibits growth of pine seedlings. Key intermed. in synth. of Averufin. Orange cryst. (Me_2CO). Mp 340°. λ_{max} 250 (ϵ 20900); 275 (ϵ 25700); 368 (ϵ 4780); 410 (ϵ 3700) (MeOH) (Berdy).

Tetra-Ac:
$C_{22}H_{16}O_{10}$ 440.362
Mp 207°.

3-Me ether: 1,3,8-Trihydroxy-6-methoxyanthraquinone. ***Lunatin***
[314255-80-6]
$C_{15}H_{10}O_6$ 286.24
Isol. from the fungus *Curvularia lunata* obt. from the sponge *Niphates olemda*. Also isol. from the lichen *Xanthoria parietina*. Yellowish amorph. solid. The two different natural isolates showed significant differences in chemical shift data. Identity of the two compds. needs clarification. λ_{max} 266 (ϵ 24000); 292 (ϵ 23100); 435 (ϵ 16300) (MeOH).

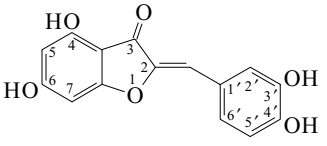
Tetra-Me ether: 1,3,6,8-Tetramethoxyanthraquinone
[2476-76-8]
$C_{18}H_{16}O_6$ 328.321
Cryst. (EtOH). Mp 225-226°.

Castonguay, A. *et al., Can. J. Chem.*, 1977, **55**, 1324-1332 (*synth, bibl*)
Berger, Y. *et al., Org. Magn. Reson.*, 1978, **11**, 375-377 (*cmr, bibl*)
Berger, Y. *et al., Phytochemistry*, 1980, **19**, 2779-2780 (*isol, bibl*)
Ayer, W.A. *et al., Phytochemistry*, 1983, **22**, 2267-2271 (*isol, props*)
O'Malley, G.J. *et al., J.O.C.*, 1985, **50**, 5533-5537 (*synth, bibl*)

Betina, V. *et al., Experientia*, 1986, **42**, 196-197 (*isol*)
Ivanova, V. *et al., Pharmazie*, 2000, **55**, 785-786 (*Lunatin*)
Jadulco, R. *et al., J. Nat. Prod.*, 2002, **65**, 730-733 (*Lunatin*)

3′,4,4′,6-Tetrahydroxyaurone T-192

4,6-Dihydroxy-2-[(3,4-dihydroxyphenyl)methylene]-3(2H)-benzofuranone, 9CI. ***Aureusidin****. Cernuin*
[480-70-6]



$C_{15}H_{10}O_6$ 286.24
Aglycone from *Antirrhinum majus*, also isol. from *Citrus medica* (citron), *Melanorrhoea aptera*, *Cyperus*, *Eleocharis*, *Gahnia*, *Lepironia*, *Ptilanthelium*, *Schoenus*, *Scirpus* and *Remirea* spp. The most widely distributed aurone. Deep-yellow cryst. + $1H_2O$ (MeOH aq.). Mp 270° Mp 295° dec. (double Mp).

Tetra-Ac:
Yellow needles (petrol). Mp 188-189°.

4-O-β-D-Glucopyranoside: ***Cernuoside***
[480-69-3]
$C_{21}H_{20}O_{11}$ 448.382
Pigment from *Oxalis cernua*, also present in *Chirita micromusa, Limonium bonduellii, Petrocosmea kerrii, Mussaenda hirsutissima* and others. Yellow cryst. (EtOH aq.). Mp 250-258°. $[\alpha]_D^{30}$ -13 (Py).

6-O-β-D-Glucopyranoside: ***Aureusin***
[633-15-8]
$C_{21}H_{20}O_{11}$ 448.382
Constit. of *Antirrhinum majus*, also in *Antirrhinum nuttalianum, Linaria maroccana, Oxalis* spp. and others. Needles (EtOAc) (as hepta-Ac). Mp 264.5-265.5° (as hepta-Ac).

6-O-β-D-Glucuronopyranoside: Aureusidin 6-O-glucuronoside
[65604-87-7]
$C_{21}H_{18}O_{12}$ 462.366
Isol. from antheridiophores of the liverworts *Marchantia berteroana, Marchantia polymorpha, Conocephalum supradecompositum* and *Carrpos sphaerocarpus*. No phys. props. reported.

4,6-Di-O-β-D-Glucopyranoside: [89648-26-0]
$C_{27}H_{30}O_{16}$ 610.524
Isol. from *Mussaenda hirsutissima* flowers. No phys. props. reported.

6-O-α-L-Rhamnopyranoside: [124925-02-6]
$C_{21}H_{20}O_{10}$ 432.383
Constit. of *Pterocarpus marsupium*. Mp 264°.

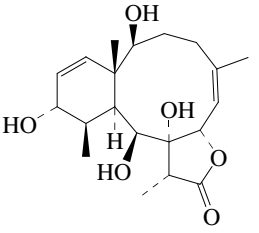
4-Me ether: 3′,4′,6-Trihydroxy-4-methoxyaurone. ***Rengasin***
[54826-89-0]
$C_{16}H_{12}O_6$ 300.267
Constit. of *Melanorrhoea* spp. heartwood. Golden-yellow cryst. Mp 314-316° dec. Originally thought to be the 6-Me ether.

Tetra-Me ether: 3′,4,4′,6-Tetramethoxyaurone
[23053-69-2]
$C_{19}H_{18}O_6$ 342.348
Constit. of *Cyperus capitatus*. Greenish-yellow needles (MeOH aq.). Mp 173° (169-170°).

[38216-54-5]

Geissman, T.A. *et al., J.A.C.S.*, 1950, **72**, 5725; 1955, **77**, 4622 (*isol, struct*)
Farkas, L. *et al., Chem. Ber.*, 1961, **94**, 2221; 1964, **97**, 1044; 1969, **49**, 2221 (*synth, struct*)
Batterham, T.J. *et al., Aust. J. Chem.*, 1964, **17**, 428 (*pmr*)
Harborne, J.B. *et al., Phytochemistry*, 1966, **5**, 111; 589; 1967, **6**, 1643 (*occur, Cernuoside*)
Clifford, H.T. *et al., Phytochemistry*, 1969, **8**, 123 (*occur*)
Hastings, J.S. *et al., J.C.S. Perkin 1*, 1972, 2128 (*pmr, struct*)
Deshmukh, S.W. *et al., Indian J. Chem.*, 1974, **12**, 893 (*synth*)
Ogiyama, K. *et al., Phytochemistry*, 1976, **15**, 2025 (*isol*)
Harborne, J.B. *et al., Phytochemistry*, 1983, **22**, 2741 (*diglycoside*)
Mohan, P. *et al., Phytochemistry*, 1989, **28**, 2529 (*6-rhamnoside*)
Seabra, R.M. *et al., Phytochemistry*, 1997, **45**, 839 (*Tetramethoxyaurone*)

2,8,9,12-Tetrahydroxy-5,13-briaradien-18,7-olide T-193



$C_{20}H_{30}O_6$ 366.453

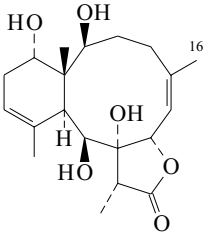
(2β,5Z,7α,8α,9β,12α)-form

2,9-Di-Ac: ***Cavernulin B***
[437651-06-4]
$C_{24}H_{34}O_8$ 450.528
Constit. of a *Cavernularia* sp.
$[\alpha]_D$ -50.3 (c, 0.2 in $CHCl_3$).

12-Butanoyl, 2,9-di-Ac: ***Cavernulin A***
[437651-05-3]
$C_{28}H_{40}O_9$ 520.619
Constit. of a *Cavernularia* sp.
$[\alpha]_D$ -56.4 (c, 0.42 in $CHCl_3$).

Patra, A. *et al., J. Indian Chem. Soc.*, 2001, **78**, 619-626 (*isol, pmr, cmr*)

2,8,9,14-Tetrahydroxy-5,11-briaradien-18,7-olide T-194



$C_{20}H_{30}O_6$ 366.453

(2β,5Z,7α,8α,9β,14α)-form

2,14-Di-Ac: ***9-Deacetylstylatulide lactone***
$C_{24}H_{34}O_8$ 450.528
Constit. of a *Briareum* sp. Cryst.
Mp 229-231°. $[\alpha]_D^{26}$ -3 (c, 0.58 in $CHCl_3$).

2,9,14-Tri-Ac: ***Stylatula lactone A****. Stylatulide lactone*
[74269-51-5]
$C_{26}H_{36}O_9$ 492.565
Constit. of *Stylatula* spp. and a *Briareum* sp. Cryst. (prev. descr. as oil).
Mp 107-109°. $[\alpha]_D^{20}$ -7 (c, 0.1 in $CHCl_3$).

2-Butanoyl, 9,14-di-Ac: ***Renillin C***
[851320-00-8]
$C_{28}H_{40}O_9$ 520.619
Constit. of *Renilla reniformis*. Amorph. powder. $[\alpha]_D^{25}$ -89 (c, 0.015 in $CHCl_3$).

9-Ketone, 2-butanoyl, 14-Ac: ***Briareolide K***
$C_{26}H_{36}O_8$ 476.566
Constit. of *Briareum asbestinum*. Gum. $[\alpha]_D$ +116.1 (c, 0.16 in $CHCl_3$).

11,12-Epoxide: 11,12-Epoxy-2,8,9,14-tetrahydroxy-5-briaren-18,7-olide
$C_{20}H_{30}O_7$ 382.453

11α,12α-Epoxide, 2-butanoyl, 9,14-di-Ac: ***Renillin D***
[851320-01-9]
$C_{28}H_{40}O_{10}$ 536.618
Constit. of *Renilla reniformis*. Amorph. powder. $[\alpha]_D^{25}$ -42 (c, 0.017 in $CHCl_3$).

11β,12β-Epoxide, 2,14-di-Ac: ***Milolide B***
[352335-83-2]
$C_{24}H_{34}O_9$ 466.527
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ +7.1 (c, 0.28 in CH_2Cl_2).

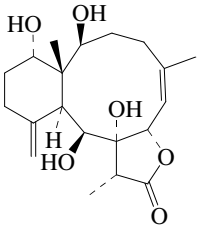
16-Chloro: 16-Chloro-2,8,9,14-tetrahydroxy-5,11-briaradien-18,7-olide
$C_{20}H_{29}ClO_6$ 400.898

16-Chloro, 2,14-di-Ac: ***Milolide L***
[438552-15-9]
$C_{24}H_{33}ClO_8$ 484.973
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ -30.6 (c, 0.46 in CH_2Cl_2).

16-Chloro, 11β,12β-epoxide, 2,14-di-Ac: ***16-Chloromilolide B***
[352273-95-1]
$C_{24}H_{33}ClO_9$ 500.972
Constit. of *Briareum stechei*.
$[\alpha]_D^{23}$ -10 (c, 0.25 in CH_2Cl_2).

Wratten, S.J. *et al., Tetrahedron*, 1979, **35**, 1907
Sheu, J.H. *et al., J. Nat. Prod.*, 1996, **59**, 935 (*isol, pmr, cmr*)
Mootoo, B.S. *et al., Tetrahedron*, 1996, **52**, 9953 (*Briareolide K*)
Kwak, J.H. *et al., J. Nat. Prod.*, 2001, **64**, 754-760 (*Milolide B, 16-Chloromilolide B*)
Kwak, J.H. *et al., J. Nat. Prod.*, 2002, **65**, 704-708 (*Milolide L*)
Barsby, T. *et al., J. Nat. Prod.*, 2005, **68**, 511-516 (*Renillins C,D*)

2,8,9,14-Tetrahydroxy-5,11(20)-briaradien-18,7-olide T-195



$C_{20}H_{30}O_6$ 366.453

(2β,8α,9β,14α)-*form*

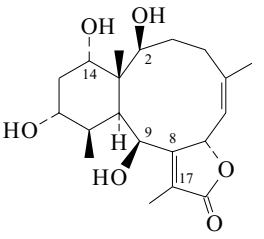
2,14-Di-Ac: ***9-Deacetyllumbraculolide A***
[565430-59-3]
$C_{24}H_{34}O_8$ 450.528
Constit. of *Junceella fragilis.* Powder (EtOAc).
Mp 99-101°. $[\alpha]_D^{25}$ +28 (c, 0.8 in $CHCl_3$).

2,9,14-Tri-Ac: ***Umbraculolide A***
[213269-03-5]
$C_{26}H_{36}O_9$ 492.565
Constit. of *Gorgonella umbraculum.* Cryst. ($CHCl_3$).
Mp 217-219°. $[\alpha]_D^{30}$ -37 (c, 0.51 in $CHCl_3$). Trivial name not used in 1998 paper, assigned in 2000.

2-Propanoyl, 9,14-di-Ac: ***Junceellolide E***
[303963-51-1]
$C_{27}H_{38}O_9$ 506.592
Constit. of *Junceella fragilis.* Cryst.
Mp 195-196°. $[\alpha]_D^{26}$ -111 (c, 0.6 in $CHCl_3$).

Subrahmanyam, C. *et al., J. Nat. Prod.*, 1998, **61**, 1120-1122 (*isol, pmr, cmr*)
Sung, P.-J. *et al., J. Nat. Prod.*, 2000, **63**, 1483-1487 (*Junceellolide E, cryst struct*)
Sung, P.-J. *et al., Heterocycles*, 2003, **60**, 1199-1202, (*9-Deacetylumbraculolide A*)

2,9,12,14-Tetrahydroxy-5,8(17)-briaradien-18,7-olide T-196



$C_{20}H_{30}O_6$ 366.453

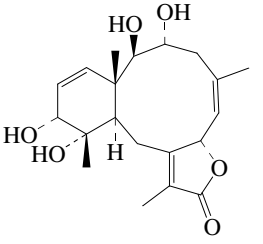
2-Butanoyl, 9,14-di-Ac: ***Briareolide G***
[132750-59-5]
$C_{28}H_{40}O_9$ 520.619
Constit. of a *Briareum* sp. Powder (MeOH aq.). λ_{max} 204 (ε 9020) (MeOH) (Derep).

8α,17α-Epoxide, 2-butanoyl, 9,14-di-Ac: ***Briareolide E***
[132750-57-3]
$C_{28}H_{40}O_{10}$ 536.618
Constit. of a *Briareum* sp. Antiinflammatory agent. Foam.
Mp 182-183° dec.

8α,17α-Epoxide, 2,9,14-tri-Ac: ***Briareolide F***
[132750-58-4]
$C_{26}H_{36}O_{10}$ 508.564
Constit. of a *Briareum* sp. Foam.

Pordesimo, E.O. *et al., J.O.C.*, 1991, **56**, 2344 (*isol, pmr, cmr*)

2,3,11,12-Tetrahydroxy-5,8(17),13-briaratrien-18,7-olide T-197



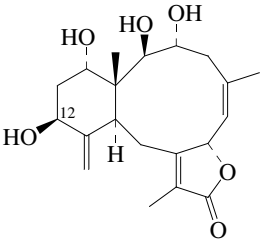
$C_{20}H_{28}O_6$ 364.438

(2β,3α,5*Z*,7α,11α,12α)-*form*

2,3-Di-Ac: ***9-Deacetoxybriviolide D***
[868281-75-8]
$C_{24}H_{32}O_8$ 448.512
Constit. of a *Briareum* sp. Amorph. powder. $[\alpha]_D$ +35 (c, 0.11 in MeOH). λ_{max} 218 (ε 13200) (MeOH).

Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 2083-2093 (*9-Deacetoxybriviolide D*)

2,3,12,14-Tetrahydroxy-5,8(17),11(20)-briaratrien-18,7-olide T-198



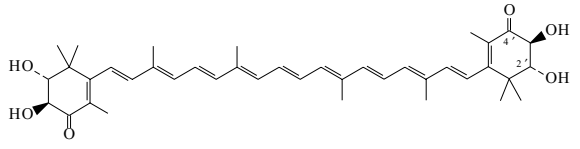
$C_{20}H_{28}O_6$ 364.438

(2β,3α,5*Z*,7α,12β,14α)-*form*

12-Hydroperoxide, 2,3,14-tri-Ac: ***Brianthein B***
[383366-82-3]
$C_{26}H_{34}O_{10}$ 506.549
Constit. of *Briareum excavatum*.
$[\alpha]_D^{20}$ +81.7 (c, 0.4 in EtOH).
Aoki, S. *et al., Tetrahedron*, 2001, **57**, 8951-8957 (*isol, pmr, cmr*)

2,2′,3,3′-Tetrahydroxy-β,β-carotene-4,4′-dione T-199

[72826-80-3]



$C_{40}H_{52}O_6$ 628.847
Isol. from a mutant of *Rhizobium lupini*. λ_{max} 477 (EtOH).

2′-Deoxy: 2,3,3′-Trihydroxy-β,β-carotene-4,4′-dione. ***2-Hydroxyastaxanthin***
[174206-05-4]
$C_{40}H_{52}O_5$ 612.848
Isol. from a marine bacterium strain SD-212.

4′-Deoxo: ***2,2′,3,3′-Tetrahydroxy-β,β-caroten-4-one. 4-Ketonostoxanthin***
[63109-36-4]
$C_{40}H_{54}O_5$ 614.864
Isol. from *Rhizobium lupini*. λ_{max} 457; 475 (no solvent reported).

*4′-Deoxo, 3′-*O*-sulfate: 4-Ketonostoxanthin 3′-sulfate*
$C_{40}H_{54}O_8S$ 694.928
Isol. from a marine *Flavobacterium* sp. Isol. as Na salt. λ_{max} 478 (ϵ 87600) ($CHCl_3$/MeOH).

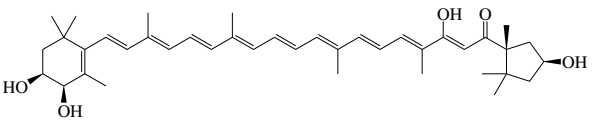
4′-Deoxo, 2-deoxy: 2′,3,3′-Trihydroxy-β,β-caroten-4-one. ***Erythroxanthin***
[174204-81-0]
$C_{40}H_{54}O_4$ 598.864
Isol. from marine bacterium SD-212. λ_{max} 476 (C_6H_6).

*4′-Deoxo, 2-deoxy, 3-*O*-sulfate: Erythroxanthin 3-sulfate*
$C_{40}H_{54}O_7S$ 678.928
Isol. from *Erythrobacter longus*. Red solid. λ_{max} 469 (MeOH/NH_4OH).

4′-Deoxo, 2′-deoxy: 2,3,3′-Trihydroxy-β,β-caroten-4-one. ***2-Hydroxyadonixanthin***
[174206-06-5]
$C_{40}H_{54}O_4$ 598.864
Isol. from marine bacterium strain SD-212.

Kleinig, H. *et al., Helv. Chim. Acta*, 1977, **60**, 254 (*occur, uv, ir, ms*)
Beyer, P. *et al., Helv. Chim. Acta*, 1979, **62**, 2551 (*config*)
Takaichi, S. *et al., Phytochemistry*, 1991, **30**, 3411-3415 (*Erythroxanthin 3-sulfate*)
Yokoyama, A. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 200-203; 1877 (*2-Hydroxyadonixanthin, 2-Hydroxyastaxanthin, Erythroxanthin*)

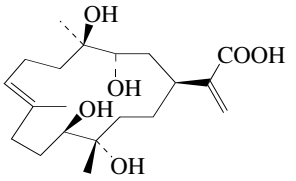
3,3′,4,8′-Tetrahydroxy-β,κ-caroten-6′-one T-200



$C_{40}H_{56}O_5$ 616.879

(3*S*,3′*S*,4*R*,5′*R*,7′*Z*)-*form* [870095-33-3]
Constit. of the oyster *Crassostrea gigas*.
Red solid. λ_{max} 470 (KOH/EtOH).
Maoka, T. *et al., Chem. Pharm. Bull.*, 2005, **53**, 1207-1209 (*Crassostrea gigas constit*)

3,4,11,12-Tetrahydroxy-7,15(17)-cembradien-16-oic acid T-201

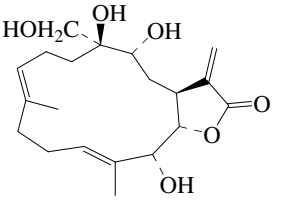


$C_{20}H_{34}O_6$ 370.485

(1*S*,3*S*,4*R*,7*E*,11*R*,12*S*)-*form*

Me ester: ***Sinuflexibilin***
[210706-47-1]
$C_{21}H_{36}O_6$ 384.512
Constit. of *Sinularia flexibilis*. Cryst.
Mp 169-170°. $[\alpha]_D^{25}$ -3.9 (c, 0.14 in MeOH). λ_{max} 206 (log ϵ 4.01) (MeOH).
Duh, C.-Y. *et al., J. Nat. Prod.*, 1998, **61**, 844-847 (*isol, pmr, cmr*)

3,4,13,18-Tetrahydroxy-7,11,15(17)-cembratrien-16,14-olide T-202

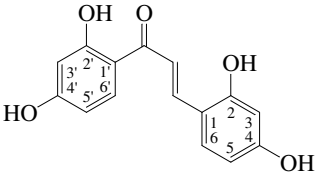


$C_{20}H_{30}O_6$ 366.453

(1*S*,3*R*,4*S*,7*E*,11*E*,13*R*,14*S*)-*form*
Sinularolide A
[852469-24-0]
Constit. of *Sinularia gibberosa*.
Oil. $[\alpha]_D^{25}$ +2.17 (c, 0.05 in $CHCl_3$).
Li, G. *et al., J. Nat. Prod.*, 2005, **68**, 649-652 (*Sinularolide A*)

2,2′,4,4′-Tetrahydroxychalcone, 8CI T-203

1,3-Bis(2,4-dihydroxyphenyl)-2-propen-1-one, 9CI. 2,4-Dihydroxyphenyl 2,4-dihydroxystyryl ketone
[25972-30-9]



$C_{15}H_{12}O_5$ 272.257

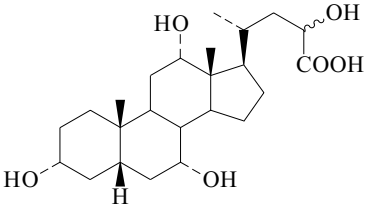
2,4,4′-Tri-Me ether: 2′-Hydroxy-2,4,4′-trimethoxychalcone
[36685-67-3]
$C_{18}H_{18}O_5$ 314.337
Prod. by *Tubastrea micrantha*. Defence chemical. Yellow needles (EtOH).
Mp 157° (145-147°).

2,4,4′-Tri-Me, 2′-Ac:
$C_{20}H_{20}O_6$ 356.374
Pale yellow cryst. (EtOH). Mp 110-112°.

2′,4,4′-Tri-Me ether:
$C_{18}H_{18}O_5$ 314.337
Greenish-yellow needles (Me_2CO). Mp 156°.

Tetra-Me ether: [25110-62-7]
$C_{19}H_{20}O_5$ 328.364
Yellowish needles (EtOH). Mp 128°.
Kostanecki, S. *et al., Ber.*, 1906, **39**, 92 (*synth*)
Kauffmann, H. *et al., Ber.*, 1913, **46**, 3797 (*synth*)
Bhalla, A.L. *et al., J.C.S.*, 1933, 290 (*uv*)
Sanduja, R. *et al., J. Chem. Res., Synop.*, 1986, 450-451 (*isol, struct*)
Delle Monache, G. *et al., Phytochemistry*, 1995, **39**, 575 (*synth, pmr, cmr*)
Khatib, S. *et al., Bioorg. Med. Chem.*, 2005, **13**, 433-443 (*synth, uv, pmr*)

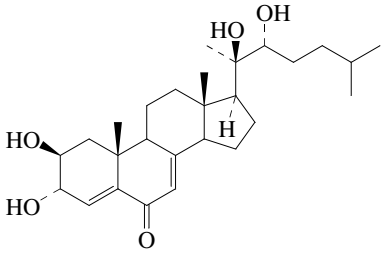
3,7,12,23-Tetrahydroxycholan-24-oic acid T-204



$C_{24}H_{40}O_6$ 424.576

(3α,5β,7α,12α,23ξ)-*form*
α-Phocaecholic acid
Bile acid from the seal.
Cryst. (Me_2CO).
Mp 156-158°. $[\alpha]_D$ +23 ($CHCl_3$).
Hammersten, O. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1909, **61**, 454; 1910, **68**, 109
Bergstrom, S. *et al., Acta Soc. Med. Ups.*, 1959, **64**, 160
Haslewood, G.A.D. *et al., Biochem. J.*, 1961, **78**, 352
Ikawa, S. *et al., Biochem. J.*, 1976, **153**, 343 (*isol*)
Kutner, A. *et al., Steroids*, 1982, **40**, 11 (*synth*)

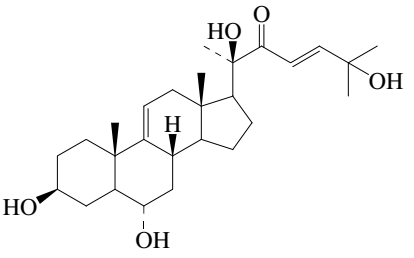
2,3,20,22-Tetrahydroxycholesta-4,7-dien-6-one, 9CI T-205



$C_{27}H_{42}O_5$ 446.626

(2β,3α,20*R*,22*R*)-*form*
Pinnasterol
[80981-63-1]
Constit. of the red alga *Laurencia pinnata*.
Cryst. Sol. MeOH, C_6H_6.
Mp 198-201°. $[\alpha]_D$ +37 (MeOH).
2-Ac: ***2-O-Acetylpinnasterol***
[80981-66-4]
$C_{29}H_{44}O_6$ 488.663
Constit. of *Laurencia pinnata*. Shows moulting hormone activity.
Cryst. Sol. MeOH, C_6H_6.
Mp 105-107°. $[\alpha]_D$ +64 (MeOH).
Fukuzawa, A. *et al., Tet. Lett.*, 1981, **22**, 4085-4086 (*isol, pmr, cmr, cryst struct*)
Fukuzawa, A. *et al., Phytochemistry*, 1986, **25**, 1305-1307 (*isol*)

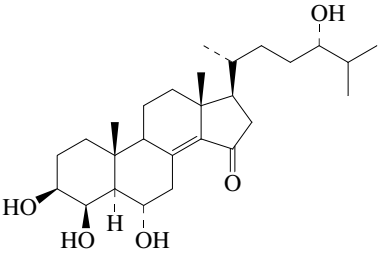
3,6,20,25-Tetrahydroxycholesta-9(11),23-dien-22-one T-206



$C_{27}H_{42}O_5$ 446.626

(3β,5α,6α,22*R*)-*form*
6-O-[β-D-Fucopyranosyl-(1→2)-6-deoxy-β-D-glucopyranosyl-(1→4)-[6-deoxy-3-O-methyl-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-O-sulfate: ***Goniopectenoside A***
[326793-68-4]
$C_{57}H_{94}O_{27}S$ 1243.419
Constit. of *Goniopecten demonstrans*. Amorph. powder. $[\alpha]_D$ +1.9 (c, 0.3 in MeOH).
De Marino, S. *et al., Eur. J. Org. Chem.*, 2000, 4093-4098

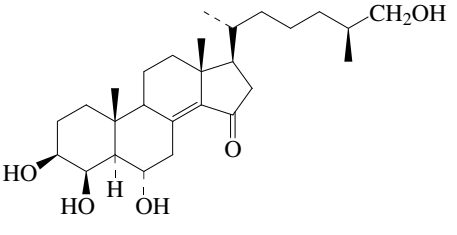
3,4,6,24-Tetrahydroxycholest-8(14)-en-15-one T-207



$C_{27}H_{44}O_5$ 448.642

(3β,4β,5α,6α,25*S*)-*form*
Certonardosterol Q_7
[781646-82-0]
Constit. of *Certonardoa semiregularis*.
Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 1654-1660 (*isol, pmr, cmr*)

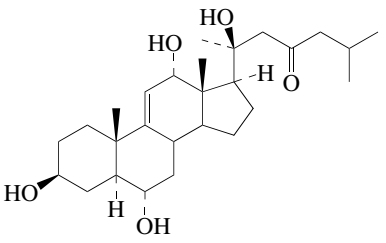
3,4,6,26-Tetrahydroxycholest-8(14)-en-15-one T-208



$C_{27}H_{44}O_5$ 448.642

(3β,4β,5α,6α,25*S*)-*form*
Certonardosterol Q_4
[781646-79-5]
Constit. of *Certonardoa semiregularis*.
Cryst. λ_{max} 258 (log ϵ 3.78) (MeOH).
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 1654-1660 (*isol, pmr, cmr*)

3,6,12,20-Tetrahydroxycholest-9(11)-en-23-one T-209



$C_{27}H_{44}O_5$ 448.642

(3β,5α,6α,12α,20*S*)-*form*

6-O-[β-D-Fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)[β-D-quinovopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-β-D-quinovopyranoside], 3-sulfate: ***Tenuispinoside C***

[105404-83-9 (Na salt)]

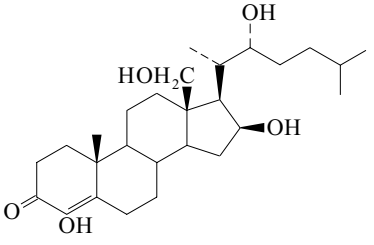
$C_{56}H_{92}O_{29}S$ 1261.391

Constit. of *Coscinasterias tenuispina*.

$[\alpha]_D$ +37.5 (MeOH) (as Na salt).

Riccio, R. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 869-893 (*isol, pmr, cmr, ms*)

4,16,18,22-Tetrahydroxycholest-4-en-3-one T-210



$C_{27}H_{44}O_5$ 448.642

(16β,22*R*)-*form*

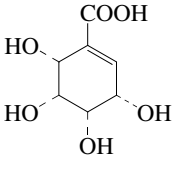
16,18-Di-Ac: [76907-70-5]

$C_{31}H_{48}O_7$ 532.716

Constit. of the hydroids *Eudendrium rameum*, *Eudendrium racemosum* and *Eudendrium ramosum* and their predator nudibranchs, e.g. *Hervia*, *Flabellina* and *Coryphella* spp. Amorph. powder. $[\alpha]_D^{25}$ +55 (c, 0.4 in $CHCl_3$). λ_{max} 277 (MeOH).

Cimino, G. *et al., Tet. Lett.*, 1980, **21**, 3303-3304 (*isol, pmr, struct, synth*)

3,4,5,6-Tetrahydroxy-1-cyclohexene-1-carboxylic acid T-211



$C_7H_{10}O_6$ 190.152

(3α,4α,5α,6α)-*form*

6-Me ether, Me ester: Methyl 3,4,5-trihydroxy-6-methoxy-1-cyclohexene-1-carboxylate. ***Pericosine B***

[200335-69-9]

$C_9H_{14}O_6$ 218.206

Prod. by *Periconia byssoides* isol. from *Aplysia kurodai*. Cytotoxic agent. Oil. $[\alpha]_D$ +22.3 (c, 0.82 in EtOH). λ_{max} 218 (log ε 3.85) (EtOH).

6-Deoxy, 6-chloro, Me ester: Methyl 6-chloro-3,4,5-trihydroxy-1-cyclohexene-1-carboxylate. ***Pericosine A***

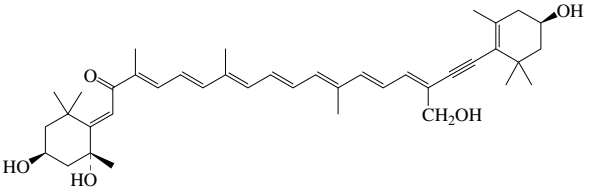
[200335-68-8]

$C_8H_{11}ClO_5$ 222.625

Prod. by *Periconia byssoides* isol. from *Aplysia kurodai*. Cytotoxic agent. Plates (MeOH). Mp 95-97°. $[\alpha]_D$ +57 (c, 3.2 in EtOH). λ_{max} 217 (log ε 3.9) (EtOH).

Numata, A. *et al., Tet. Lett.*, 1997, **38**, 8215-8218 (*isol, uv, ir, pmr, cmr, ms*)
Donohoe, T.J. *et al., Tet. Lett.*, 1998, **39**, 8755-8758 (*Pericosine B, synth*)

3,3′,5,19′-Tetrahydroxy-7′,8′-didehydro-γ,ε-caroten-8-one T-212



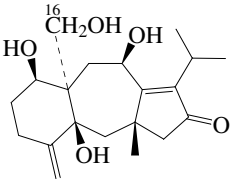
$C_{40}H_{54}O_5$ 614.864

(3*R*,3′*R*,5*S*,6*E*)-*form* [850130-12-0]

Constit. of *Prianos osiros*. Dark red solid. λ_{max} 200 (log ε 4.12); 282 (log ε 3.98); 348 (log ε 3.8) (EtOH).

Rogers, E.W. *et al., J. Nat. Prod.*, 2005, **68**, 450-452 (*isol, pmr, cmr*)

4,7,14,16-Tetrahydroxy-1(15),8-dolastadien-10-one T-213



$C_{20}H_{30}O_5$ 350.454

(4β,7β,14β)-*form*

14-Ac: ***Dichotenone B***

[639476-54-3]

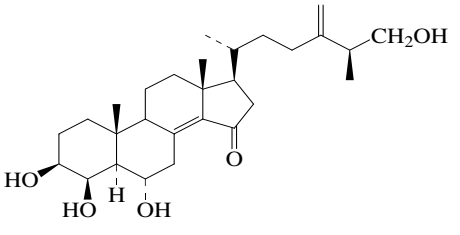
$C_{22}H_{32}O_6$ 392.491

Constit. of *Dictyota dichotoma*. Cryst. Mp 205-208°. $[\alpha]_D^{24}$ -15 (c, 0.04 in Py). λ_{max} 241 (log ε 3.3) (MeOH).

Ali, M.S. *et al., Nat. Prod. Res.*, 2003, **17**, 301-306 (*isol, pmr, cmr*)

3,4,6,26-Tetrahydroxyergosta-8(14),24(28)-dien-15-one T-214

3,4,6,26-Tetrahydroxy-24-methylenecholest-8(14)-en-15-one



$C_{28}H_{44}O_5$ 460.653

(3β,4β,5α,6α,25*S*)-*form*

Certonardosterol Q5

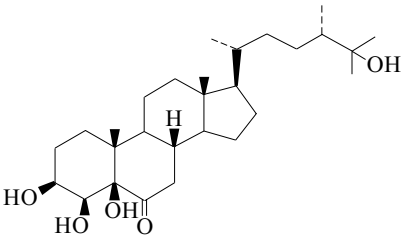
[781646-80-8]

Constit. of *Certonardoa semiregularis*. Cryst.

Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 1654-1660 (*isol, pmr, cmr*)

3,4,5,25-Tetrahydroxyergostan-6-one, 9CI T-215

3,4,5,25-Tetrahydroxy-24-methylcholestan-6-one



$C_{28}H_{48}O_5$ 464.684

(3β,4β,5β,24*S*)-*form*

Constit. of *Sclerophytum* spp. Cryst. Mp 220-225°. $[\alpha]_D^{29}$ -8 (c, 1.7 in $CHCl_3$).

25-Ac: ***Lobosterol***

[59176-66-8]

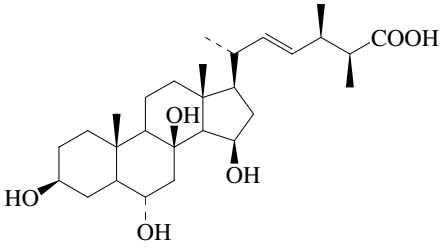
$C_{30}H_{50}O_6$ 506.721

Constit. of *Lobophytum pauciflorum*. Cryst. (MeOH). Mp 210-212°. $[\alpha]_D^{20}$ -16 (c, 0.65 in dioxan).

Losman, D. *et al., Acta Cryst. B*, 1976, **32**, 2513

Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 297 (*isol, pmr, cmr*)

3,6,8,15-Tetrahydroxyergost-22-en-26-oic acid T-216



$C_{28}H_{46}O_6$ 478.668

(3β,5α,6α,8β,15β,22*E*,24*R*,25*S*)-*form*

*26-(2-Sulfoethylamide), 3-*O*-β-D-xylopyranoside:* ***Minutoside B***

[863919-29-3]

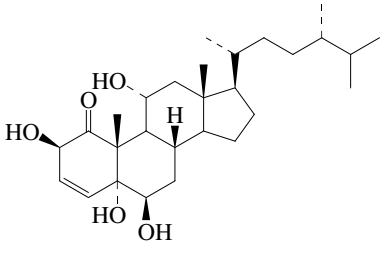
$C_{35}H_{59}NO_{12}S$ 717.917

Constit. of *Anasterias minuta*. Amorph. powder. $[\alpha]_D^{20}$ -22.9 (c, 0.42 in MeOH).

Chludil, H.D. *et al., J. Nat. Prod.*, 2005, **68**, 1279-1283 (*Minutoside B*)

2,5,6,11-Tetrahydroxyergost-3-en-1-one T-217

2,5,6,11-Tetrahydroxy-24-methylcholest-3-en-1-one



$C_{28}H_{46}O_5$ 462.668

(2β,5α,6β,11α,24*S*)-*form*

Stoloniferone F

[475111-79-6]

Constit. of *Clavularia viridis*. Amorph. solid. $[\alpha]_D^{25}$ -30.6 (c, 0.11 in $CHCl_3$). λ_{max} 208 (log ϵ 3.68) (MeOH).

24,28-Didehydro: 2,5,6,11-Tetrahydroxyergosta-3,24(28)-dien-1-one. 2,5,6,11-Tetrahydroxy-24-methylenecholest-3-en-1-one.

Stoloniferone G

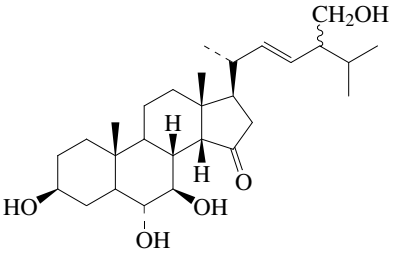
[475111-80-9]

$C_{28}H_{44}O_5$ 460.653

Constit. of *Clavularia viridis*. Amorph. solid. $[\alpha]_D^{25}$ -21.7 (c, 0.12 in $CHCl_3$).

Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1535-1539 (*isol, pmr, cmr*)

3,6,7,28-Tetrahydroxyergost-22-en-15-one T-218



$C_{28}H_{46}O_5$ 462.668

(3β,6α,7β,14β,22*E*,24ξ)-*form*

Clathriol B

[565430-73-1]

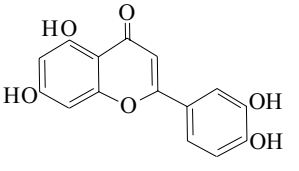
Constit. of *Clathria lissosclera*. $[\alpha]_D$ -29.4 (c, 0.71 in CH_2Cl_2).

Keyzers, R.A. *et al., Aust. J. Chem.*, 2003, **56**, 279-282 (*isol, pmr, cmr*)

3′,4′,5,7-Tetrahydroxyflavone T-219

*2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI.* ***Luteolin****. Digitoflavone. Daphneflavonol. Flavopurpol. Luteolol. C.I. Natural Yellow 2*

[491-70-3]



$C_{15}H_{10}O_6$ 286.24

Various methyl and methylene ethers have separate entries. Occurs in many plants in Leguminosae, Resedaceae, Euphorbiaceae, Umbelliferae, Scrophulariaceae, Fabaceae, Asteraceae, Cistaceae, Passifloraceae, Yerbenaceae and Hepaticae. First isol. in 1832 from *Reseda luteola*. Used in EtOH soln. for colour reactions with Al, Be, Cd, Cu, Zr, B. Antiinflammatory, antispasmodic, antitussive agent. Antitumourigenic activity in mice reported. Shows anti-HIV activity. Potential nutriceutical. Active against *Bacillus subtilis* and *Candida albicans*. Yellow needles. Mp 328-330° (325°). Log P 0.38 (calc). λ_{max} 257 (log ϵ 4.21); 353 (log ϵ 4.3) (EtOH).

▶ LD_{50} (mus, ipr) 180 mg/kg. Exp. reprod. effects. LK9275210

*3′,7-Di-*O*-sulfate: Luteolin 3′,7-disulfate*

[59176-62-4]

$C_{15}H_{10}O_{12}S_2$ 446.369

Isol. from *Zostera marina* and leaves of *Lachenalia unifolia*.

*7-*O*-(2-*O*-Sulfo-β-D-glucopyranoside): 2″-Sulfoglucoluteolin.*

Thalassiolin A

[207683-70-3]

$C_{21}H_{20}O_{14}S$ 528.447

Constit. of *Thalassia testudinum*. Phytoalexin. Inhibitor of HIV integrase.

[18695-03-9, 54985-16-9, 62804-16-4, 98716-92-8, 102506-55-8]

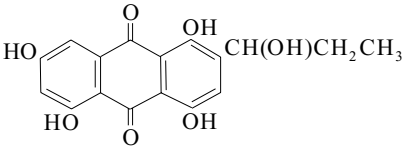
Harborne, J.B. *et al., Biochem. Syst. Ecol.*, 1976, **4**, 37-41 (*3′,7-disulfate*)

Jensen, P.R. *et al., Appl. Environ. Microbiol.*, 1998, **64**, 1490-1496 (*2″-Sulfoglucoluteolin*)

Rowley, D.C. *et al., Bioorg. Med. Chem.*, 2002, **10**, 3619-3625 (*Thalassiolin A*)

1,4,5,7-Tetrahydroxy-2-(1-hydroxypropyl)anthraquinone T-220

[52422-03-4]



$C_{17}H_{14}O_7$ 330.293

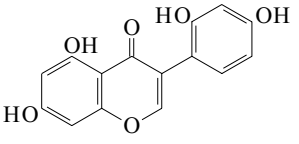
Minor pigment from *Comanthus bennetti*.

Bertolini, G.L. *et al., Tetrahedron*, 1973, **29**, 3699 (*isol*)

2′,4′,5,7-Tetrahydroxyisoflavone T-221

*3-(2,4-Dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI.* ***2′-Hydroxygenistein***

[1156-78-1]



$C_{15}H_{10}O_6$ 286.24

Isol. from *Apios tuberosa*, *Argyrocytisus battandieri*, *Cajanus cajan*, *Crotalaria juncea*, *Dolichos biflorus*, *Hardenbergia violacea*, *Lablab niger*, *Laburnum anagyroides*, *Lupinus albus*, *Moghania macrophylla*, *Neonotonia wightii*, *Phaseolus vulgaris*, *Phaseolus coccineus*, *Spartium junceum*, *Stizolobium deeringianum* and others. Cryst. ($CHCl_3$/MeOH). Mp 270-273°. λ_{max} 209; 262; 288 (MeOH) (Berdy).

2′,4′,7-Tri-Me ether: 5-Hydroxy-2′,4′,7-trimethoxyisoflavone

[54443-60-6]

$C_{18}H_{16}O_6$ 328.321

Constit. of *Virola caducifolia* and marine mollusc *Nerita albicilla*. Cryst. Mp 160-162°.

Tetra-Me ether: 2′,4′,5,7-Tetramethoxyisoflavone

[1100-15-8]

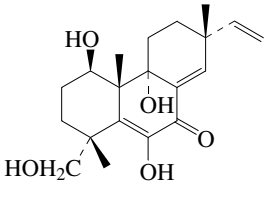
$C_{19}H_{18}O_6$ 342.348

Constit. of *Nerita albicilla*. Cryst. (C_6H_6/petrol or MeOH). Mp 203-204° (197-199°).

Sanduja, R. *et al., J. Chem. Res., Synop.*, 1985, 56 (*2′,4′,7-tri-Me ether, tetra-Me ether, isol, Nerita*)

Parmar, V.S. *et al., Org. Mass Spectrom.*, 1985, **20**, 265-266 (*ms*)

1,6,9,18-Tetrahydroxy-5,8(14),15-isopimaratrien-7-one T-222



$C_{20}H_{28}O_5$ 348.438

Enolised α-diketone.

(1β,9α)-*form*

Libertellenone C

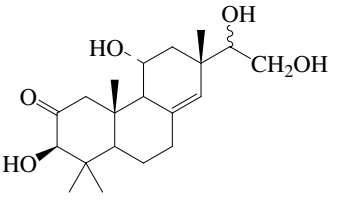
[866413-30-1]

Metab. of a marine-derived *Libertella* sp.

Powder. $[\alpha]_D$ -84.1 (c, 0.387 in MeCN). λ_{max} 216 (log ϵ 3.54); 269 (log ϵ 3.48); 321 (log ϵ 3.7) (MeCN).

Oh, D.-C. *et al., Bioorg. Med. Chem.*, 2005, **13**, 5267-5273 (*Libertellenone C*)

3,11,15,16-Tetrahydroxy-8(14)-isopimaren-2-one T-223



$C_{20}H_{32}O_5$ 352.47

(3β,11α,15ξ)-*form*

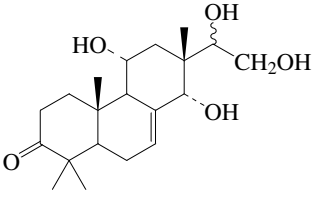
Agallochaol F

[862255-98-9]

Constit. of *Excoecaria agallocha*.

Wang, J.-D. *et al., Helv. Chim. Acta*, 2005, **88**, 979-985 (*Agallochaol F*)

11,14,15,16-Tetrahydroxy-7-isopimaren-3-one T-224



$C_{20}H_{32}O_5$ 352.47

(11α,14α,15ξ)-*form*

Agallochaol E

[862255-97-8]

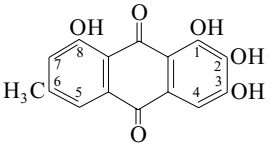
Constit. of *Excoecaria agallocha*.

Wang, J.-D. *et al., Helv. Chim. Acta*, 2005, **88**, 979-985 (*Agallochaol E*)

1,2,3,8-Tetrahydroxy-6-methylanthraquinone T-225

1,2,3,8-Tetrahydroxy-6-methyl-9,10-anthracenedione, 9CI. 7-Hydroxyemodin

[10228-40-7]



$C_{15}H_{10}O_6$ 286.24

Isol. from the insects *Nipaecoccus aurilantus, Pseudococcus albizziae, Eriococcus coriaceus* and *Eriococcus confusus* and cultures of *Aspergillus rugulosus*. Red needles.

Mp 296-298°.

3-Me ether: 1,2,8-Trihydroxy-3-methoxy-6-methylanthraquinone. ***Dermoglaucin***

[7213-59-4]

$C_{16}H_{12}O_6$ 300.267

Isol. from *Dermocybe sanguinea*. Mycotoxin. Possesses mutagenic props. Orange-yellow cryst. (EtOAc).

Mp 236°. λ_{max} 248 (ϵ 8300); 254 (ϵ 9300); 282 (ϵ 19800); 435 (ϵ 7300); 580 (ϵ 1300) (EtOH) (Berdy).

▶ Possibly mutagenic. CB7883000

8-Me ether: 1,2,3-Trihydroxy-8-methoxy-6-methylanthraquinone. ***Evariquinone***

$C_{16}H_{12}O_6$ 300.267

Isol. from *Emericella variecolor* derived from the sponge *Haliclona valliculata*. Orange needles.

Mp 238-242° subl. λ_{max} 213; 248; 285; 424 (EtOH).

1,3-Di-Me ether: 2,8-Dihydroxy-1,3-dimethoxy-6-methylanthraquinone, 8CI
[33982-72-8]
$C_{17}H_{14}O_6$ 314.294
Constit. of *Melanoxylon braunia* and *Cassia greggii*. Orange needles.
Mp 238-240°. The *C. greggii* isolate was originally formulated as the 3,8-di-Me isomer.

1,2,3-Tri-Me ether: 8-Hydroxy-1,2,3-trimethoxy-6-methylanthraquinone
[78308-22-2]
$C_{18}H_{16}O_6$ 328.321
Constit. of *Cassia greggii*. Yellow needles.
Mp 195-196° (189-190°).

Chan, A.W.K. *et al., Aust. J. Chem.*, 1966, **19**, 1701 (*isol, uv, ir, pmr*)
Steglich, W. *et al., Chem. Ber.*, 1969, **102**, 4104; 1972, **105**, 2928 (*isol, struct*)
Gottlieb, O.R. *et al., Phytochemistry*, 1971, **10**, 1379 (*isol, deriv*)
Steglich, W. *et al., Chem. Comm.*, 1972, 102 (*biosynth*)
Banks, H.J. *et al., Aust. J. Chem.*, 1976, **29**, 1509; 2231; 1978, **31**, 2271 (*isol, synth*)
Brown, J.P. *et al., Biochem. Soc. Trans.*, 1977, **5**, 1489
Roberge, G. *et al., J.O.C.*, 1981, **46**, 4161 (*synth*)
Barba, B. *et al., Phytochemistry*, 1994, **37**, 837 (*isol, pmr*)
Schripsema, J. *et al., Phytochemistry*, 1996, **42**, 177 (*pmr, struct*)
Bringmann, G. *et al., Phytochemistry*, 2003, **63**, 437-443 (*Evariquinone*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MEY750

1,4,5,8-Tetrahydroxy-2-methylanthraquinone T-226

1,4,5,8-Tetrahydroxy-2-methyl-9,10-anthracenedione, 9CI. ***Cinodontin****. Cynodontin. 1-Hydroxyhelminthosporin*
[476-43-7]
$C_{15}H_{10}O_6$ 286.24
Isol. from *Phoma* and *Helminthosporium* spp., *Pyrenochaeta terrestris*, *Drechslera* sp., *Bipolaris sorokiniana*, *Curvularia lunata*, *Maesopsis eminii*, *Pyrenochaeta terrestris*, *Aspergillus aculeatus*, *Cercospora cari*, *Asahinea chrysantha* and *Asahinea scholanderi*.
Dyestuff intermediate. Brown leaflets with bronze lustre (Py).
Mp 260-261°. λ_{max} 238 (ϵ 12880); 296; 474; 483; 505; 516; 542; 554 (MeOH) (Berdy). λ_{max} 241; 295; 483; 514; 539; 552 (EtOH) (Berdy). λ_{max} 247; 252 (sh); 297; 462 (sh); 481 (sh); 491; 512; 523; 549; 562 ($CHCl_3$) (Berdy).

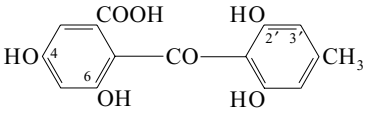
▶ Shows weak mutagenic props. CB8079000

Tetra-Ac:
Yellow cryst. (AcOH). Mp 224-225°.

Raistrick, L. *et al., Biochem. J.*, 1933, **27**, 1170-1175; 1940, **34**, 1546-1548 (*isol, struct*)
Cumming, A.M. *et al., Phytochemistry*, 1970, **9**, 2399-2400 (*isol*)
v. Eijk, G.W. *et al., Experientia*, 1977, **33**, 1283-1284 (*isol*)
Mabadeje, S.A. *et al., Exp. Mycol.*, 1978, **2**, 359-365 (*isol*)
Kurobane, I. *et al., J. Antibiot.*, 1979, **32**, 1256-1266 (*biosynth*)
Laatsch, H. *et al., Annalen*, 1982, 2189-2215 (*synth, spectra*)
Cameron, D.W. *et al., Aust. J. Chem.*, 1982, **35**, 2095-2109 (*synth*)
Krivoshchekova, O.E. *et al., Khim. Prir. Soedin.*, 1983, **19**, 283-289; *Chem. Nat. Compd. (Engl. Transl.)*, 1983, **19**, 270-274 (*isol*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

2′,4,6,6′-Tetrahydroxy-4′-methylbenzophenone-2-carboxylic acid T-227

2-(2,6-Dihydroxy-4-methylbenzoyl)-3,5-dihydroxybenzoic acid



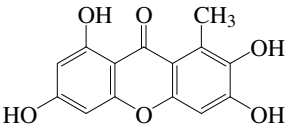
$C_{15}H_{12}O_7$ 304.256

2′,6-Di-Me ether, Me ester: ***Monomethylsulochrin****. Methylsulochrin*
$C_{18}H_{18}O_7$ 346.336
Metab. of *Aspergillus fumigatus* when grown on Raulin-Thom medium and of *Aspergillus terreus-aureus*. Also prod. by the marine-derived *Aspergillus* sp. B-F-2. Elongated plates (EtOAc/petrol).
Mp 198-199°. λ_{max} 260 (log ϵ 2.09); 286 (log ϵ 2.27) ($CHCl_3$).

Turner, W.B. *et al., J.C.S.*, 1965, 6658-6659 (*Monomethlsulochrin*)
Ma, Y.M. *et al., Fitoterapia*, 2004, **75**, 451-456 (*Rhizoctonic acid, Monomethylsulochrin*)
R. *et al., J. Antibiot.*, 2006, **59**, 362-365 (*Monomethylsulochrin, marine isol*)

2,3,6,8-Tetrahydroxy-1-methylxanthone T-228

*2,3,6,8-Tetrahydroxy-1-methyl-9*H*-xanthen-9-one, 9CI.* ***Anomalin A***

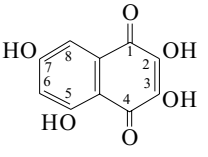


$C_{14}H_{10}O_6$ 274.229
Prod. by the algicolous marine fungi *Apiospora montagnei* and *Wardomyces anomalus*. Antioxidant and tyrosine kinase inhibitor.
Yellow-brown powder. λ_{max} 234 (log ϵ 4.86); 258 (log ϵ 4.86); 311 (log ϵ 4.72); 358 (log ϵ 4.5) (MeOH).

Abdel-Lateff, A. *et al., J. Nat. Prod.*, 2003, **66**, 706-708 (*isol, pmr, cmr*)

2,3,5,7-Tetrahydroxy-1,4-naphthoquinone T-229

2,3,5,7-Tetrahydroxy-1,4-naphthalenedione, 9CI. Spinochrome B. Spinochrome B_1*. Spinochrome* M_2*. Spinochrome N. Spinochrome* P_1
[604-46-6]



$C_{10}H_6O_6$ 222.154
Isol. from many echinoids, including *Paracentrotus lividus*, *Echinothrix calamaris*, *Strongylocentrotus pulcherrimus*, *Anthocidaris crassispina*, *Salmacis sphaeroides* and *Psammechinus microtuberculatus*. Brick-red solvated cryst. (MeOH) or cryst. (dioxan).
Mp 325-330° dec. (MeOH solvate) Mp 350-355°. λ_{max} 272 (ϵ 24000); 323 (ϵ 12550); 385 (ϵ 11000); 480 (ϵ 4900) (EtOH) (Berdy).

Tetra-Ac:
$C_{18}H_{14}O_{10}$ 390.303
Bright yellow cryst. Mp 255° dec.

3-Me ether: 2,5,7-Trihydroxy-3-methoxy-1,4-naphthoquinone. ***2,7-Dihydroxy-3-methoxyjuglone***
[62574-10-1]
$C_{11}H_8O_6$ 236.181
Isol. from cultures of *Cercospora melonis*. Yellow cryst.
Mp 255° dec.

3-Me ether, tri-Ac: [62608-10-0]
$C_{17}H_{14}O_9$ 362.292
Yellow solid (Et_2O). Mp 145-147°.

7-Me ether: 2,3,5-Trihydroxy-7-methoxy-1,4-naphthoquinone. ***2,3-Dihydroxy-7-methoxyjuglone***
[28785-72-0]
$C_{11}H_8O_6$ 236.181
Metab. of *Corynespora cassicola*. Hypotensive agent. Red needles.
Sol. MeOH, C_6H_6; poorly sol. H_2O.
Mp 267°. λ_{max} 272 (ϵ 21380); 322 (ϵ 9770); 383 (ϵ 3630); 483 (ϵ 1660) (EtOH) (Berdy).

▶ QJ5788000

Tetra-Me ether: 2,3,5,7-Tetramethoxy-1,4-naphthoquinone
[65565-44-8]
$C_{14}H_{14}O_6$ 278.261
Cryst. (C_6H_6/petrol). Mp 157-158° (132-132.5°).

Goodwin, T.W. *et al., Biochem. J.*, 1950, **47**, 69-76 (*occur*)
Goodwin, T.W. *et al., Experientia*, 1951, **7**, 375-376 (*isol*)
Lederer, E. *et al., Biochim. Biophys. Acta*, 1952, **9**, 92-100 (*isol*)
Smith, J. *et al., J.C.S.*, 1961, 1008-1012 (*isol*)
Gough, J. *et al., Tet. Lett.*, 1964, 269-275 (*isol, struct, pmr*)
Moore, R.E. *et al., J.O.C.*, 1966, **31**, 3645-3660 (*isol*)
Singh, H. *et al., Experientia*, 1967, **23**, 624-626 (*occur*)

Singh, I. *et al., Tetrahedron*, 1968, **24**, 6053-6073 (*uv*)
Fornasiero, U. *et al., Ann. Chim. (Rome)*, 1973, **63**, 387-390 (*isol*)
Chimura, H. *et al., J. Antibiot.*, 1973, **26**, 618-620 (*7-Me ether*)
Assante, G. *et al., Phytochemistry*, 1977, **16**, 243-247 (*3-Me ether, synth*)
Grandmaison, J.-L. *et al., Tetrahedron*, 1977, **33**, 2047-2053 (*synth*)

2,5,6,8-Tetrahydroxy-1,4-naphthoquinone T-230

2,5,6,8-Tetrahydroxy-1,4-naphthalenedione, 9CI. 2,6-Dihydroxynaphthazarin
[15257-45-1]
$C_{10}H_6O_6$ 222.154
Pigment in calcareous skeleton of sea urchins. Brick-red cryst. ($CHCl_3$).
Mp 270-285° subl.

2,6-Di-Me ether: 4,8-Dihydroxy-1,6-dimethoxy-1,4-naphthoquinone
$C_{12}H_{10}O_6$ 250.207
Dark-red cryst. (Me_2CO). Mp 295-296°.

Tetra-Me ether: 2,5,6,8-Tetramethoxy-1,4-naphthoquinone
$C_{14}H_{14}O_6$ 278.261
Cryst. (EtOH/CCl_4). Mp 192-193°.

Moore, R.E. *et al., Tetrahedron*, 1967, **23**, 3271 (*isol*)
Singh, I. *et al., Tetrahedron*, 1968, **24**, 2969; 6053 (*synth, uv*)
Simoneau, B. *et al., Tetrahedron*, 1986, **42**, 3767 (*deriv, synth, uv, ir, pmr*)

2,5,7,8-Tetrahydroxy-1,4-naphthoquinone T-231

2,5,7,8-Tetrahydroxy-1,4-naphthalenedione, 9CI. Mompain. 2,7-Dihydroxynaphthazarin
[2473-16-7]
$C_{10}H_6O_6$ 222.154
Metab. of *Helicobasidium mompa*; also obt. from the sea urchins *Echinothrix diadema* and *Echinothrix calamaris*. Red needles by subl.
Mp 265-275° subl Mp > 300° dec. λ_{max} 228; 272; 318; 486; 517 (EtOH) (Berdy).

Tetra-Ac:
$C_{18}H_{14}O_{10}$ 390.303
Yellow needles (EtOH). Mp 176-179°.

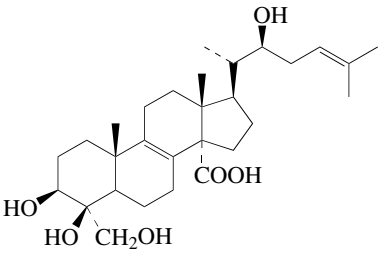
2,7-Di-Me ether: 5,8-Dihydroxy-2,7-dimethoxy-1,4-naphthoquinone
[2808-46-0]
$C_{12}H_{10}O_6$ 250.207
Metab. of *Streptomyces* and *Streptoverticillium* spp. Active against gram-positive bacteria and some fungi. Red needles (2,2,4-trimethylpentane).
Mp 273-275° (275-276°). λ_{max} 285 (ϵ 8625); 308 (ϵ 9450); 480 (ϵ 7125); 512 (ϵ 8500); 550 (ϵ 5500) ($CHCl_3$) (Derep).
▶ QL7975000

5,7,8-Tri-Me ether: 2-Hydroxy-5,7,8-trimethoxy-1,4-naphthoquinone
[13261-43-3]
$C_{13}H_{12}O_6$ 264.234
Bronze needles (MeOH aq.). Mp 174°.

Tetra-Me ether: 2,5,7,8-Tetramethoxy-1,4-naphthoquinone
[2644-68-0]
$C_{14}H_{14}O_6$ 278.261
Cryst. Mp 169-171°.

Nishikawa, H. *et al., Agric. Biol. Chem.*, 1962, **26**, 696-698 (*isol*)
Ballie, A.C. *et al., J.C.S.(C)*, 1966, 2184-2186 (*synth*)
Gerber, N.N. *et al., J.O.C.*, 1966, **31**, 1496-1498 (*2,7-di-Me ether, isol*)
Moore, R.E. *et al., J.O.C.*, 1966, **31**, 3645-3650 (*isol*)
Natori, S. *et al., Chem. Pharm. Bull.*, 1967, **15**, 380-390 (*isol, ms, nmr, uv*)
Baker, P.M. *et al., Chem. Comm.*, 1968, 71-72 (*synth*)
Singh, I. *et al., Tetrahedron*, 1968, **24**, 2969-2978 (*synth*)
Bentley, R. *et al., Biochemistry*, 1975, **14**, 3138-3143 (*biosynth*)
Malinovskaya, G.V. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1998, **48**, 1010-1011 (*synth*)
Ameer, F. *et al., Synth. Commun.*, 2004, **34**, 1247-1258 (*5,7,8-tri-Me ether*)

3,4,22,28-Tetrahydroxy-29-norlanosta-8,24-dien-30-oic acid T-232



$C_{29}H_{46}O_6$ 490.679

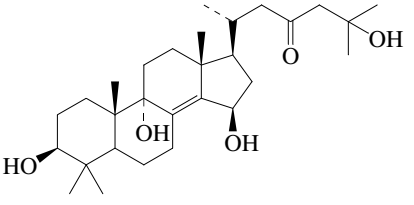
(3β,4β,22*S*)-*form*

3-O-[β-D-Galactopyranosyl-(1→4)-α-L-arabinopyranosyl-(1→2)-β-D-galactopyranoside]: ***Ectyoplaside B***
[220605-12-9]
$C_{46}H_{74}O_{20}$ 947.079
Constit. of *Ectyoplasia ferox*. Amorph. solid. $[\alpha]_D^{25}$ -12 (c, 0.002 in MeOH).

Cafieri, F. *et al., Eur. J. Org. Chem.*, 1999, 231-238 (*isol, pmr, cmr*)

3,9,15,25-Tetrahydroxy-30-norlanost-8(14)-en-23-one T-233

3,9,15,25-Tetrahydroxy-4,4-dimethylcholest-8(14)-en-23-one



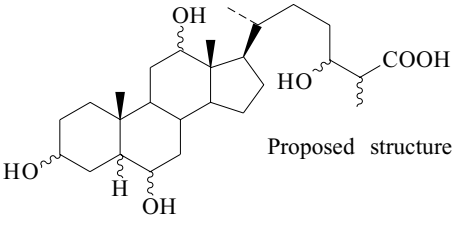
$C_{29}H_{48}O_5$ 476.695

(3β,9α,15β)-*form*

15-Me ether, 3-O-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→4)]-β-D-xylopyranoside]: ***Sarasinoside K***
[865369-06-8]
$C_{63}H_{104}N_2O_{29}$ 1353.511
Constit. of *Melophlus sarassinorum*. Yellow amorph. solid. $[\alpha]_D^{20}$ -6.8 (c, 0.5 in MeOH). λ_{max} 204 (MeOH).

Dai, H.-F. *et al., J. Nat. Prod.*, 2005, **68**, 1231-1237 (*Sarasinoside K*)

Tetrahydroxynorsterocholanic acid T-234



Proposed structure

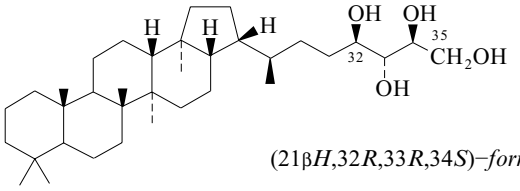
$C_{27}H_{46}O_6$ 466.657
Constit. of the bile of the gigi fish. Cryst. (Me_2CO aq.).
Mp 212-214°. $[\alpha]_D$ +27.2 (EtOH).

Me ester: Mp 204°.

Ohta, M. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1939, **259**, 53

29-(2,3,4,5-Tetrahydroxypentyl)hopane T-235

1,2,3-Trideoxy-2-methyl-2-[A-neo-22,29,30-trinorgammaceran-21-yl]heptitol, 9CI. 7-(A′-Neo-22,29,30-trinorgammaceran-21-yl)-1,2,3,4-octanetetrol. 32,33,34,35-Bacteriohopanetetrol



(21β*H*,32*R*,33*R*,34*S*)–*form*

$C_{35}H_{62}O_4$ 546.872

(21β*H*,32*R*,33*R*,34*S*)-*form*

Bacteriohopanetetrol. *Tetrahydroxybacteriohopane*
[51024-98-7]
Constit. of *Acetobacter aceti* ssp. *xylinum*, *Rhodopseudomonas acidophila* and *Zymomonas mobilis*. Isol. from the sponge *Plakortis simplex*.

*35-*O*-(6-Amino-6-deoxy-β-D-glucopyranoside):* [143113-32-0]
$C_{41}H_{73}NO_8$ 708.03
Constit. of a *Synechocystis* sp.

*35-*O*-β-D-Glucuronopyranoside:* [144599-05-3]
$C_{41}H_{70}O_{10}$ 722.998
Constit. of *Rhodospirillum rubrum*.

*35-*O*-β-D-Galacturonopyranoside:*
$C_{41}H_{70}O_{10}$ 722.998
Constit. of *Prochlorothrix hollandica*.

35-Deoxy, 35-amino: ***35-Amino-32,33,34-bacteriohopanetriol***
[91683-32-8]
$C_{35}H_{63}NO_3$ 545.888
Constit. of *Acetobacter aceti* ssp. *xylinum* and *Rhodopseudomonas* sp.

*35-Deoxy, 35-(*N*-hexadecanoylamino):* **N-*Palmitoylaminobacteriohopanetriol***
[223103-34-2]
$C_{51}H_{93}NO_4$ 784.3
Constit. of *Nitrosomonas europaea*.

*35-Deoxy, 35-(*N*-8Z-hexadecenoylamino):* **N-cis-*Palmitoleylaminobacteriohopanetriol***
[223103-37-5]
$C_{51}H_{91}NO_4$ 782.284
Constit. of *Nitrosomonas europaea*.

35-Deoxy, 35-(ornithylamino): [91683-34-0]
$C_{40}H_{73}N_3O_4$ 660.034
Constit. of *Rhodomicrobium vannielii*.

35-Deoxy, 35-(tryptophanylamino): [91683-33-9]
$C_{46}H_{73}N_3O_4$ 732.1
Constit. of *Rhodomicrobium vannielii*.

35-Carboxylic acid, (35→32)-lactone:
$C_{35}H_{58}O_4$ 542.841
Constit. of *Nitrosomonas europaea*.

(21α*H*,32ξ,33ξ,34ξ)-*form*
Metab. of *Zymomonas mobilis*.

(21β*H*,32*R*,33*R*,34*R*)-*form*
Constit. of *Acetobacter aceti* and *Acetobacter pasteurianus*.
Cryst. (CH_2Cl_2/MeOH) (as tetra-Ac).
Mp 185° (tetra-Ac). $[\alpha]_D$ +54 (c, 0.00092 in $CHCl_3$) (tetra-Ac).

(21β*H*,22*S*,32*R*,33*R*,34*S*)-*form*
Constit. of *Acetobacter aceti* and *Acetobacter pasteurianus*.
Cryst. (CH_2Cl_2/MeOH) (as tetra-Ac).
Mp 120-122° (tetra-Ac). $[\alpha]_D$ +15 (c, 0.00275 in $CHCl_3$) (tetra-Ac).

(21β*H*,22ξ,29ξ,30ξ,33ξ,34ξ)-*form*

*32-Ketone, 35-*O*-(2-amino-2-deoxy-β-D-glucopyranoside):*
[123167-01-1]
$C_{41}H_{71}NO_8$ 706.014
Isol. from *Zymomonas mobilis*.

(21β*H*,22*R*,32ξ,33ξ,34ξ)-*form*

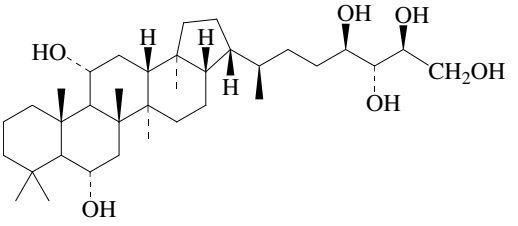
*35-*O*-α-D-Altruronopyranoside:*
$C_{41}H_{70}O_{10}$ 722.998
Constit. of *Prochlorothrix hollandica*.

*35-*O*-(3,6-Anhydro-β-D-galacturonopyranoside):*
$C_{41}H_{68}O_9$ 704.983
Constit. of *Prochlorothrix hollandica*.

Rohmer, M. *et al., Tet. Lett.*, 1976, 3633 (*struct*)
Neunlist, S. *et al., Eur. J. Biochem.*, 1985, **147**, 561 (*isol, pmr, cmr*)
Tahara, Y. *et al., Agric. Biol. Chem.*, 1986, **50**, 1345
Neunlist, S. *et al., Chem. Comm.*, 1988, 830 (*bibl, abs config*)
Flesch, G. *et al., Chem. Comm.*, 1988, 868 (*biosynth, bibl*)
Flesch, G. *et al., Biochem. J.*, 1989, **262**, 673 (*aminoglycoside*)
Rohmer, M. *et al., Chem. Comm.*, 1989, 1471 (*biosynth*)
Bisseret, P. *et al., J.O.C.*, 1989, **54**, 2958 (*abs config, synth*)
Llopiz, P. *et al., Biochem. J.*, 1992, **287**, 159 (*glucuronopyranoside*)
Peisiler, B. *et al., J. Chem. Res., Synop.*, 1992, 298; *J. Chem. Res., Miniprint*, 1992, 2353 (*isol, pmr, cmr*)
Simonin, P. *et al., Tet. Lett.*, 1992, **33**, 3629 (*aminoglycoside*)
Rohmer, M. *et al., Pure Appl. Chem.*, 1993, **65**, 1293 (*biosynth*)
Simonin, P. *et al., Eur. J. Biochem.*, 1996, **241**, 865 (*glycuronopyranosides*)
Seemann, M. *et al., Tet. Lett.*, 1999, **40**, 1681-1684 (*Nitrosomonas europaea constits*)
Costantino, V. *et al., Tetrahedron*, 2001, **57**, 4045-4048 (*isol, Plakortis simplex*)
Vincent, S.P. *et al., Chem. Comm.*, 2003, 782-783 (*biosynth*)
Pan, W. *et al., Chem. Comm.*, 2005, 3445-3447 (*synth*)

29-(2,3,4,5-Tetrahydroxypentyl)-6,11-hopanediol T-236

6,11,32,33,34,35-Bacteriohopanehexol

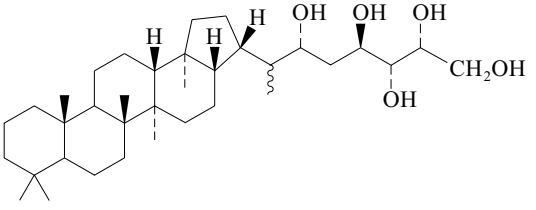


$C_{35}H_{62}O_6$ 578.871

(6α,11α,22*R*,32*R*,33*R*,34*S*)-*form* [303982-48-1]
Constit. of a *Petrosia* sp.
$[\alpha]_D$ +34 (c, 0.02 in $CHCl_3$).
Shatz, M. *et al., J. Nat. Prod.*, 2000, **63**, 1554-1556 (*isol, pmr, cmr, ms*)

29-(2,3,4,5-Tetrahydroxypentyl)-29-hopanol T-237

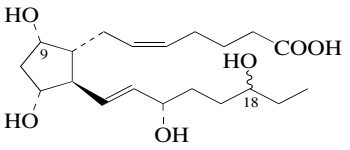
29,32,33,34,35-Bacteriohopanepentol. 30,32,33,34,35-Bacteriohopanepentol



$C_{35}H_{62}O_5$ 562.872

(22ξ,29*R*,32*R*,33*R*,34*R*)-*form* [175669-47-3]
Constit. of *Nostoc* PCC 6720. Cell wall component.
Zhao, N. *et al., Tetrahedron*, 1996, **52**, 2777 (*isol, pmr, cmr*)

9,11,15,18-Tetrahydroxyprosta-5,13-dienoic acid T-238



$C_{20}H_{34}O_6$ 370.485

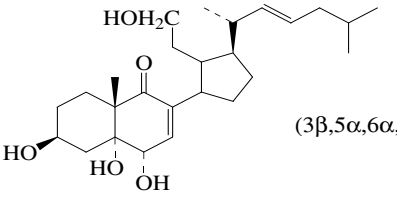
(5*Z*,8*R*,9*S*,11*R*,12*S*,13*E*,15*S*,18ξ)-*form*

11,18-Di-Ac: [74728-09-9]
$C_{24}H_{38}O_8$ 454.559
Constit. of the soft coral *Lobophytum depressum*.

11,18-Di-Ac, Me ester: [74728-07-7]
$C_{25}H_{40}O_8$ 468.586
Constit. of *Lobophytum depressum*. Oil.

Carmely, S. *et al., Tet. Lett.*, 1980, **21**, 875-878 (*isol, ir, pmr, ms*)

3,5,6,11-Tetrahydroxy-9,11-secocholesta-7,22-dien-9-one T-239



(3β,5α,6α,22*E*)-*form*

$C_{27}H_{44}O_5$ 448.642

(3β,5α,6α,22*E*)-*form* [168982-45-4]
Constit. of *Dysidea fragilis* from the lagoon of Venice.

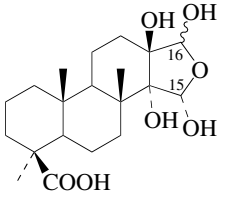
22,23-Dihydro: 3,5,6,11-Tetrahydroxy-9,11-secocholest-7-en-9-one [168982-48-7]
$C_{27}H_{46}O_5$ 450.657
Constit. of *Dysidea fragilis*. λ_{max} 251 (ε 11000) (MeOH) (Berdy).

(3β,5α,6β,22*E*)-*form*

22,23-Dihydro: ***Aplidiasterol B***
[646487-25-4]
$C_{27}H_{46}O_5$ 450.657
Constit. of *Aplidium conicum*.
$[\alpha]_D$ -30 (c, 0.0009 in MeOH).

Aiello, A. *et al., Steroids*, 1995, **60**, 666-673 (*isol, pmr, cmr*)
Aiello, A. *et al., Steroids*, 2003, **68**, 719-723 (*Aplidiasterol B*)

13,14,15,16-Tetrahydroxy-19-spongianoic acid T-240



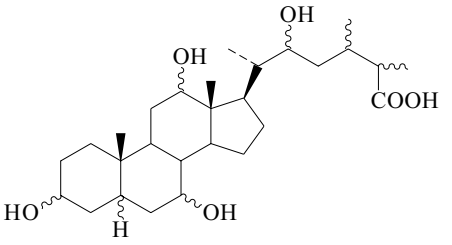
$C_{20}H_{32}O_7$ 384.469

(13β,14α,15α,16ξ)-*form*

15,16-Di-Me ether: 13,14-Dihydroxy-15,16-dimethoxy-19-spongianoic acid
[220304-54-1]
$C_{22}H_{36}O_7$ 412.522
Constit. of *Spongia matamata*. Powder. $[\alpha]_D$ +137 (c, 0.4 in $CHCl_3$/MeOH).

Li, C.-J. *et al., J. Nat. Prod.*, 1999, **62**, 287-290 (*isol, pmr, cmr*)

Tetrahydroxysterocholanic acid T-241

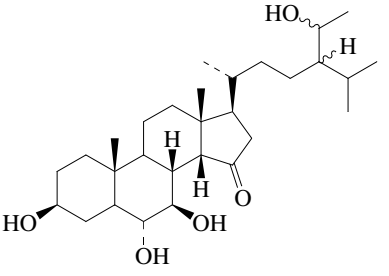


$C_{28}H_{48}O_6$ 480.684
Constit. of the bile of alligator, turtle and tortoise. Cryst. (MeOH).
Mp 149-150°. Readily lactonises.

26→22 lactone:
$C_{28}H_{46}O_5$ 462.668
Mp 208°.

Kanemitu, K. *et al., J. Biochem. (Tokyo)*, 1942, **35**, 155; 173

3,6,7,28-Tetrahydroxystigmastan-15-one T-242



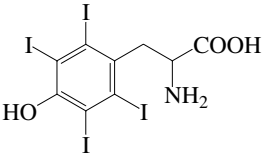
$C_{29}H_{50}O_5$ 478.711

(3β,5α,6α,7β,14β,24ξ,28ξ)-*form*
Clathriol
[424838-85-7]
Constit. of *Clathria lissosclera*.
$[\alpha]_D^{20}$ +22.6 (c, 1.4 in MeOH).

Keyzers, R.A. *et al., J. Nat. Prod.*, 2002, **65**, 598-600 (*isol, pmr, cmr*)

2,3,5,6-Tetraiodotyrosine T-243

[84299-87-6]



$C_9H_7I_4NO_3$ 684.777

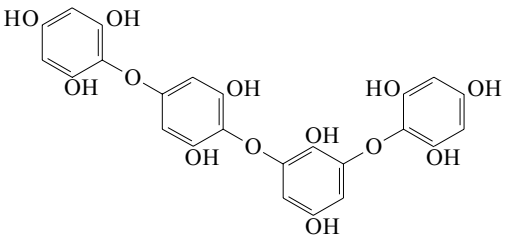
(*S*)-*form*
Hygroscopic cryst. $[\alpha]_D$ -33 (c, 0.6 in H_2O). Synthetic. CAS No. not found 8-14CI.

(±)-*form*
Constit. of *Cladophora densa*.
Hygroscopic cryst. $[\alpha]_D$ 0 (c, 1.7 in H_2O). CAS No. not found 8-14CI.

Okano, M. *et al., Nippon Suisan Gakkaishi*, 1982, **48**, 1485-1490; *CA*, **98**, 50356 (*isol, synth*)

Tetraisofuhalol T-244

[94513-74-3]



$C_{24}H_{18}O_{13}$ 514.398
Constit. of *Chorda filum*.

Grosse-Damhues, J. *et al., Phytochemistry*, 1984, **23**, 2639 (*isol, pmr*)

Tetramethylarsonium(1+) T-245

$Me_4As^{\oplus}$
$C_4H_{12}As^{\oplus}$ 135.06
Isol. from various marine molluscs.

Chloride: [5814-22-2]
$C_4H_{12}AsCl$ 170.513
Phys. props. not reported. Characterised as $Me_4AsCl.2HgCl_2$; Mp 177-178°.

Bromide: Bromotetramethylarsorane, 9CI
[69755-45-9]
$C_4H_{12}AsBr$ 214.964
Deliquescent cryst. (EtOH). Difficult to purify. Mp 350°.

Iodide: [5814-20-0]
$C_4H_{12}AsI$ 261.965
Characterised as I_2 complex below.

▶ CI0525000

Triiodide:
$C_4H_{12}AsI_3$ 515.774
Brown prisms with metallic lustre, or red-violet needle-like cryst. Mp 133°.

Hydroxide: [34618-96-7]
$C_4H_{13}AsO$ 152.068
Synth. from the iodide and moist Ag_2O. Deliquescent colourless plates. Strongly alk. soln. in H_2O.

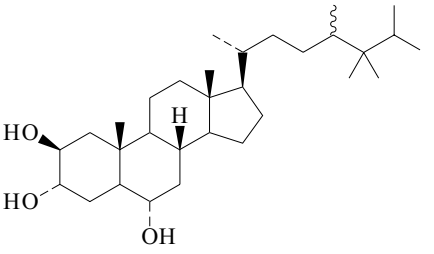
Picrate:
Yellow cryst. (H_2O or EtOH). Mp 290° Mp 308-309°.

Methanesulfonate: [66568-49-8]
Solid. Dec. at *ca.* 130°.

2,4-Dinitrobenzenesulfonate:
Cryst. (EtOH). Mp 186.5-188°.

Steinkopf, W. *et al., Ber., B*, 1921, **65**, 2969 (*synth, iodide*)
Cullen, W. *et al., Can. J. Chem.*, 1960, **38**, 439; 1962, **40**, 426; 1965, **43**, 3193 (*synth, ir, iodide, triiodide*)
Heinekey, D.M. *et al., J.C.S.*, 1963, 725 (*synth*)
Collins, E. *et al., J.C.S.*, 1963, 4051 (*synth, struct*)
Mallion, K.B. *et al., J.C.S.*, 1964, 5716 (*synth*)
Armstrong, R. *et al., Aust. J. Chem.*, 1967, **20**, 2771
Randall, E.W. *et al., Spectrochim. Acta A*, 1967, **23**, 1235 (*pmr*)
Larsen, D.W. *et al., J. Phys. Chem.*, 1971, **75**, 3880 (*nqr*)
Rager, H. *et al., Z. Phys. Chem. (Leipzig)*, 1974, **93**, 299 (*pmr, dta, iodide*)
Balimann, G. *et al., J. Magn. Reson.*, 1977, **26**, 283 (*As-75 nmr*)
Lorenz, I.P. *et al., Z. Naturforsch., B*, 1978, **33**, 47 (*synth, ir*)
Cullen, W.R. *et al., Appl. Organomet. Chem.*, 1989, **3**, 401 (*pmr, ms, iodide*)
Watkins, C.L. *et al., Magn. Reson. Chem.*, 1989, **27**, 616 (*pmr, cmr, iodide*)
Edmonds, J.S. *et al., Nat. Prod. Rep.*, 1993, **10**, 421 (*rev, isol*)
Behrens, U. *et al., Angew. Chem., Int. Ed.*, 1994, **33**, 987 (*triiodide, synth, uv-vis*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TDL250

24,25,26,26-Tetramethylcholestane-2,3,6-triol T-246



$C_{31}H_{56}O_3$ 476.782

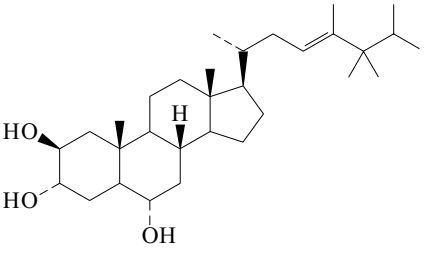
(2β,3α,6α,24ξ)-*form*
Ophirapstanol
Cryst. Mp 258-260°. $[\alpha]_D^{24}$ +23 (c, 0.05 in MeOH).

Trisulfate: ***Ophirapstanol trisulfate***
[162232-39-5]
$C_{31}H_{56}O_{12}S_3$ 716.974
Constit. of *Topsentia ophiraphidites*. Powder. $[\alpha]_D^{24}$ +17.3 (c, 0.12 in MeOH).

Gunasekera, S.P. *et al., J. Nat. Prod.*, 1994, **57**, 1751-1754 (*isol, pmr, cmr*)

24,25,26,26-Tetramethylcholest-23-ene-2,3,6-triol T-247

25-Isopropylergost-23-ene-2,3,6-triol



$C_{31}H_{54}O_3$ 474.766

(2β,3α,5α,6α,23*E*)-*form*
Sokotrasterol
[90352-20-8]
Constit. of a *Halichondria* sp. Inhibits Na^+ and K^+-activated ATPase. Cryst. Mp 223-226°. $[\alpha]_D^{20}$ +45.6 (c, 0.45 in EtOH).

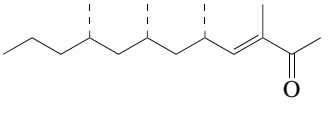
Tri-O-*sulfate:* [102974-62-9]
[85748-14-7]
$C_{31}H_{54}O_{12}S_3$ 714.958
Isol. from a *Halichondria* sp.

[90332-72-2, 102974-62-9]

Makarieva, T.N. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1983, **19**, 115-116 (*isol*)
Makarieva, T.N. *et al., Steroids*, 1983, **42**, 267-281 (*isol*)
Ilyin, S.G. *et al., J. Nat. Prod.*, 1992, **55**, 232-236 (*cryst struct*)

3,5,7,9-Tetramethyl-3-dodecen-2-one T-248

Norsiphonarienone



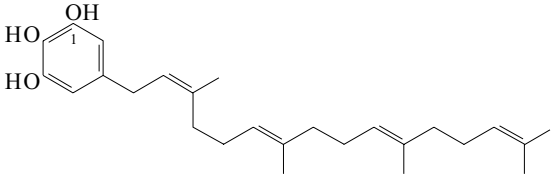
$C_{16}H_{30}O$ 238.412

(3*E*,5*S*,7*S*,9*S*)-*form* [188296-62-0]
Metab. of *Siphonaria pectinata*. Oil. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{25}$ +12 (c, 0.1 in $CHCl_3$). λ_{max} 242 (ϵ 2064) ($CHCl_3$).

Paul, M.C. *et al., Tetrahedron*, 1997, **53**, 2303 (*isol, uv, ir, pmr, cmr, ms*)

5-(3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraenyl)-1,2,3-benzenetriol T-249

5-(2,6,10,14-Phytatetraenyl)-1,2,3-benzenetriol



$C_{26}H_{38}O_3$ 398.584

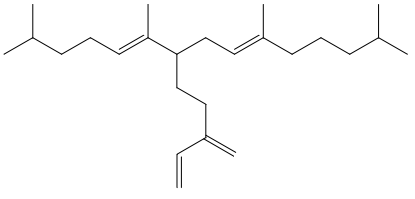
(2′Z,6′E,10′E)-form

1-Me ether: 3-Methoxy-5-(3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)-1,2-benzenediol
[133084-69-2]
$C_{27}H_{40}O_3$ 412.611
Metab. of a *Fasciospongia* sp. Shows weak antimicrobial props. Oil.

Kernan, M.R. *et al., J. Nat. Prod.*, 1991, **54**, 269 (*isol, pmr, cmr*)

2,6,10,14-Tetramethyl-7-(3-methylene-4-pentenyl)-5,9-pentadecadiene T-250

[348614-46-0]

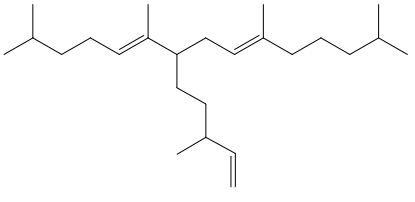


$C_{25}H_{44}$ 344.623
Constit. of *Haslea ostrearia*.

Allard, W.G. *et al., Phytochemistry*, 2001, **56**, 795-800 (*isol, pmr, cmr, ms*)

2,6,10,14-Tetramethyl-7-(3-methyl-4-pentenyl)-5,9-pentadecadiene T-251

[235094-61-8]

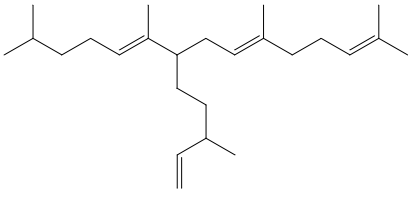


$C_{25}H_{46}$ 346.638
Constit. of *Haslea ostrearia*.

Wraige, E.J. *et al., Phytochemistry*, 1999, **51**, 69-73 (*isol, pmr, cmr*)

2,6,10,14-Tetramethyl-9-(3-methyl-4-pentenyl)-2,6,10-pentadecatriene T-252

[342004-06-2]

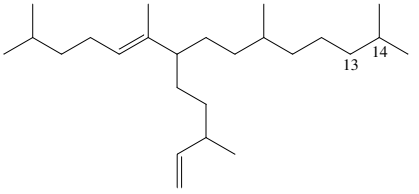


$C_{25}H_{44}$ 344.623
Constit. of *Haslea ostrearia*.

Allard, W.G. *et al., Phytochemistry*, 2001, **56**, 795-800 (*isol, pmr, cmr, ms*)

2,6,10,14-Tetramethyl-7-(3-methyl-4-pentenyl)-5-pentadecene T-253

[160941-81-1]



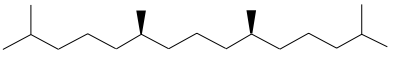
$C_{25}H_{48}$ 348.654
Biomarker isol. from benthic sediments and *Pleurosigma strigosum*.

13,14-Didehydro: ***2,6,10,14-Tetramethyl-9-(3-methyl-4-pentenyl)-2,10-pentadecadiene***
[816458-92-1]
$C_{25}H_{46}$ 346.638
Constit. of marine benthic diatom *Pleurosigma strigosum*.

Belt, S.T. *et al., Chem. Comm.*, 1994, 2077 (*isol, pmr, cmr, ms*)
Grossi, V. *et al., Phytochemistry*, 2004, **65**, 3049-3055 (*isol, pmr, cmr*)

2,6,10,14-Tetramethylpentadecane T-254

Pristane. *Norphytane. Bute hydrocarbon*
[1921-70-6]



$C_{19}H_{40}$ 268.525
▶ Skin irritant. RZ1880000

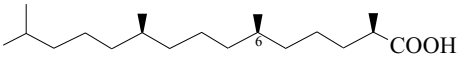
(6RS,10SR)-form

meso-*form*
Obt. from shark liver oil, herring oil, Bute inlet wax, wool wax, zooplankton and other sources.
Oil.
Mp -100°. Bp 296° Bp_{10} 158°. Chiral forms may also occur naturally; in most cases the opt. rotn. of isol. samples has not been measured.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 16C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 12B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 16C (*ir*)
Hallgren, B. *et al., Acta Chem. Scand.*, 1963, **17**, 543
Kates, M. *et al., Biochemistry*, 1967, **6**, 3329 (*abs config, bibl*)
Jain, T.C. *et al., Can. J. Chem.*, 1969, **47**, 4359 (*isol*)
Goodman, R.A. *et al., J.A.C.S.*, 1973, **95**, 7553 (*cmr*)
Carman, C.J. *et al., Macromolecules*, 1973, **6**, 719 (*cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PMD500

2,6,10,14-Tetramethylpentadecanoic acid T-255

Pristanic acid
[1189-37-3]



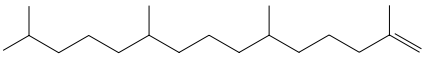
$C_{19}H_{38}O_2$ 298.508
Component of butterfat, fish oil and sheep perinephric fat. Also in petroleum. Metab. of 1-Phytanoic acid, P-379. Oil. A mixture of 6*R*- and 6*S*-forms occurs in nature.

Cason, J. *et al., Tetrahedron*, 1965, **21**, 471 (*isol, struct*)
Eldjarn, L. *et al., Acta Chem. Scand.*, 1966, **20**, 2313 (*synth*)
Nakajima, K. *et al., Agric. Biol. Chem.*, 1974, **38**, 1859 (*biosynth*)

Cox, R.E. *et al., Biochim. Biophys. Acta*, 1974, **360**, 166 (*biosynth, stereochem*)
Ratanayake, W.M.N. *et al., Lipids*, 1989, **24**, 630-637 (*occur, fish oil*)

2,6,10,14-Tetramethyl-1-pentadecene T-256

Zamene. *Norphytene*
[2140-82-1]

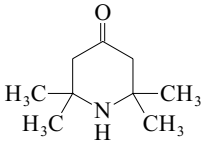


$C_{19}H_{38}$ 266.509
Produced from liver oils of elasmobranch fishes and occurs in shale oil. Oil. Bp_2 128°.

Kikumasa, S. *et al., J.O.C.*, 1967, **32**, 177 (*synth*)
Larcheveque, M. *et al., Tet. Lett.*, 1975, 3851 (*synth*)

2,2,6,6-Tetramethyl-4-piperidinone, 9CI T-257

4-Oxo-2,2,6,6-tetramethylpiperidine. 2,2,6,6-Tetramethyl-γ-piperidone. Triacetonamine. Odoratin†. *Vincubine*
[826-36-8]



$C_9H_{17}NO$ 155.239
Isol. from *Acalypha indica* and *Salsola tetrandra* (Euphorbiaceae, Chenopodiaceae), also from *Viola odorata* (sweet violet). Metab. of the soft coral *Lobophytum strictum* and sponge *Agelas oroides*. Plates + $1H_2O$ (Et_2O); anhyd. needles (dry Et_2O).
Mp 34.9° (anhyd.). Bp 205°. The hydrochloride of the alkaloid from *Salsola tetrandra* was reported to have $[\alpha]_D$ +14.3° (EtOH) which makes the struct. assignment highly dubious. Artifact.

▶ TO0127900

Monohydrate: [10581-38-1]
Mp 61-63° (58°). Bp_{18} 102-105°.

Hydrochloride: [33973-59-0]
Mp 198° dec.

Oxime: [4168-79-0]
$C_9H_{18}N_2O$ 170.254
Prisms (EtOH). Mp 153°.

▶ LD_{50} (mus, ivn) 180 mg/kg. TO0128000

Semicarbazone:
Cryst. (EtOH). Mp 219-220°.

N,N-*Di-Me: 1,1,2,2,6,6-Hexamethyl-4-oxopiperidinium, 9CI. 1,1,2,2,6,6-Hexamethyl-4-piperidinone*
[113308-50-2, 195864-37-0]
$C_{11}H_{22}NO^{\oplus}$ 184.301
Quaternary alkaloid from the alga *Laminaria japonica*.

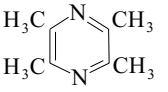
N-*Benzyl:* [52981-86-9]
$C_{16}H_{23}NO$ 245.364
Plates or prisms (EtOH/Et_2O) (as hydrochloride). Mp 137-138° (hydrochloride).

N-*Bromo:*
$C_9H_{16}BrNO$ 234.135
Cryst. (petrol). Mp 44°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 461C; 461D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 720C; 721A (*nmr*)
Frenclowa, I. *et al., Acta Pol. Pharm.*, 1961, **18**, 187; 1964, **21**, 145; *CA*, **57**, 7381; **62**, 10817 (*isol*)
Rees, B. *et al., Acta Cryst. B*, 1971, **27**, 932 (*cryst struct*)
Karawya, M.S. *et al., Phytochemistry*, 1971, **10**, 3303 (*isol*)
Sosnovsky, G. *et al., Synthesis*, 1976, 735 (*synth*)
Ermakov, A.I. *et al., Khim. Geterotsikl. Soedin.*, 1979, 507 (*ms*)
Ozinskas, A.J. *et al., Helv. Chim. Acta*, 1980, **63**, 1407 (*pmr*)
Parameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 1991, **30**, 449 (*isol, pmr, cmr*)
Shimoi, N. *et al., Fish. Sci.*, 1997, **63**, 650-651 (*Hexamethylpiperidone*)
Koenig, G.M. *et al., Planta Med.*, 1998, **64**, 88-89 (*isol, pmr, cmr*)
Bond, A.D. *et al., Acta Cryst. C*, 2002, **58**, o115-o116 (*monohydrate, cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TDU000

Tetramethylpyrazine T-258

Chuanxiongzine. Ligustrazine. Tetrapyrazine. BS Factor. FEMA 3237. NSC 36080. NSC 46451
[1124-11-4]



$C_8H_{12}N_2$ 136.196
Metab. from *Bacillus subtilis* and an arctic marine bacterium; isol. from Galbanum oil. Constit. of *Ligusticum chuanxiong* and *Ligusticum wallichii*. Fragrance and flavouring ingredient. Shows antiinflammatory activity. Bactericidal agent. Trihydrate; cryst. (H_2O).
Mp 74-77° (hyd.) Mp 86° (anhyd.). Bp 190°. pK_{a1} 3.61; pK_{a2} -2.73 (25°, H_2O). pK_{a1} 3.55; pK_{a2} -2.7 (27°, H_2SO_4 aq.). Log P 1.58 (calc). Odour threshold 10^4 ppb in H_2O. λ_{max} 294 (ε 8500) (MeOH) (Berdy).

▶ LD_{50} (rat, orl) 1910 mg/kg. UQ3905000

Hydrochloride: Mp 91° (dihydrate) Mp 156° (anhyd.).

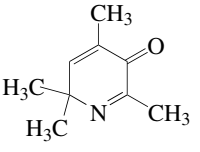
Dipicrate:
Needles. Mp 194-195°.

1,4-Dioxide:
$C_8H_{12}N_2O_2$ 168.195
Mp 224°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 841C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 402A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1559A (*ir*)
Piloty, O. *et al., Ber.*, 1910, **43**, 489
Kipping, F.B. *et al., J.C.S.*, 1929, 2891
Gnitchtel, H. *et al., Chem. Ber.*, 1972, **105**, 1865
Bus, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1973, **92**, 123 (*ir*)
Gumbley, S.J. *et al., J. Het. Chem.*, 1985, **22**, 1143 (*props*)
Eiermann, U. *et al., Chem. Ber.*, 1990, **123**, 523 (*uv*)
Ozaki, Y. *et al., Chem. Pharm. Bull.*, 1992, **40**, 954 (*isol, pharmacol*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*marine isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TDV725

2,4,6,6-Tetramethyl-3(6*H*)-pyridinone T-259

[203524-64-5]

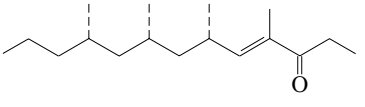


$C_9H_{13}NO$ 151.208
Isol. from the marine sponge *Agelas oroides*. Volatile oil/glass. Possible artifact. λ_{max} 221 (sh) (ε 9310); 245 (ε 7120) (MeOH).

Koenig, G.M. *et al., Planta Med.*, 1998, **64**, 88-89 (*isol, uv, ir, pmr, cmr, ms*)

4,6,8,10-Tetramethyl-4-tridecen-3-one T-260

Siphonarienone
[128008-15-1]



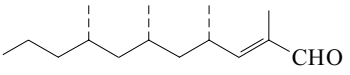
$C_{17}H_{32}O$ 252.439
Metab. of *Siphonaria grisea* and *Siphonaria pectinata*. Oil. Sol.

MeOH, $CHCl_3$, EtOAc; poorly sol. H_2O, hexane. $[\alpha]_D$ +13.3 (c, 0.7 in $CHCl_3$). λ_{max} 229 (ϵ 5288) (EtOH) (Berdy).

Norte, M. *et al., Tetrahedron*, 1990, **46**, 1669 (*isol, struct, abs config*)
Abiko, A. *et al., Tet. Lett.*, 1996, **37**, 1081 (*synth*)

2,4,6,8-Tetramethyl-2-undecenal T-261

Siphonarienal



$C_{15}H_{28}O$ 224.386

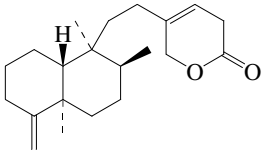
(2*E*,4*S*,6*S*,8*S*)-*form* [156162-12-8]
Isol. from the marine mollusc *Siphonaria grisea*.
Oil. $[\alpha]_D$ +7.5 (c, 0.2 in $CHCl_3$).

Carboxylic acid: ***2,4,6,8-Tetramethyl-2-undecenoic acid***
$C_{15}H_{28}O_2$ 240.385
Isol. from the marine mollusc *Siphonaria capensis*. Oil. $[\alpha]_D^{21}$ +32 (c, 0.19 in $CHCl_3$).

Norte, M. *et al., Tet. Lett.*, 1994, **35**, 3413-3416 (*isol*)
Beukes, D.R. *et al., Tetrahedron*, 1999, **55**, 4051-4056 (*Tetramethylundecenoic acid*)
Calter, M.A. *et al., J.O.C.*, 2001, **66**, 7500-7504 (*synth, pmr, cmr*)

Tetranorcacospongionolide B T-262

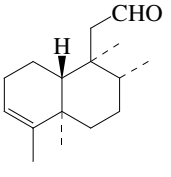
[252643-01-9]



$C_{21}H_{32}O_2$ 316.483
Constit. of *Fasciospongia cavernosa*. Amorph. solid. $[\alpha]_D$ -33.3 (c, 0.03 in $CHCl_3$). Not named in ref.

De dosa, S. *et al., Tetrahedron*, 1999, **55**, 13805-13808 (*isol, pmr, cmr*)

13,14,15,16-Tetranor-3-cleroden-12-al T-263

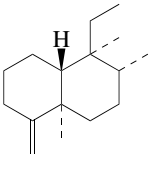


$C_{16}H_{26}O$ 234.381

(*ent*)-*form*
Callicarpenal
[161105-12-0]
Constit. of oil from *Callicarpa americana* and *Callicarpa japonica* (beautyberry). Mosquito bite deterrent. $[\alpha]_D^{25}$ -45.3 (c, 0.0053 in C_6H_6).

Cantrell, C.L. *et al., J. Agric. Food Chem.*, 2005, **53**, 5948-5953 (*Callicarpenal*)

13,14,15,16-Tetranor-4(18)-clerodene T-264



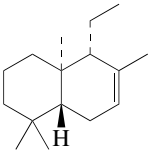
$C_{16}H_{28}$ 220.397

ent-form [199012-88-9]
Constit. of a *Mycale* sp.

Δ^3-Isomer: ***13,14,15,16-Tetranor-3-clerodene***
[199012-89-0]
$C_{16}H_{28}$ 220.397
Constit. of a *Mycale* sp.

Capon, R.J. *et al., J. Nat. Prod.*, 1997, **60**, 1261-1264 (*isol, pmr, cmr*)

13,14,15,16-Tetranor-7-labdene T-265



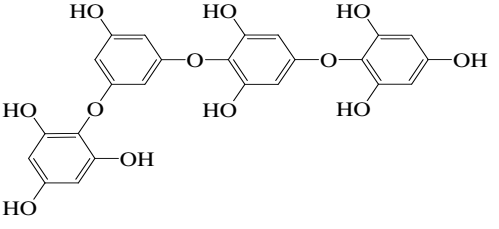
$C_{16}H_{28}$ 220.397

ent-form [199012-90-3]
Constit. of a *Mycale* sp.

Capon, R.J. *et al., J. Nat. Prod.*, 1997, **60**, 1261-1264 (*isol, pmr, cmr*)

Tetraphlorethol A T-266

2-[3,5-Dihydroxy-4-[3-hydroxy-5-(2,4,6-trihydroxyphenoxy) phenoxy]phenoxy]-1,3,5-benzenetriol, 9CI. Tetraphloroethol A
[72380-16-6]
[72380-17-7]

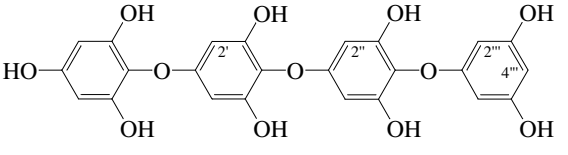


$C_{24}H_{18}O_{12}$ 498.399
Isol. from *Laminaria ochroleuca* and *Himanthalia elongata*.

Glombitza, K.W. *et al., CA*, 1980, **92**, 55043 (*isol*)
Koch, M. *et al., Phytochemistry*, 1980, **19**, 1821-1823 (*isol, struct*)
Glombitza, K.W. *et al., Planta Med.*, 1985, **50**, 42-46 (*isol*)

Tetraphlorethol C T-267

Tetraphloroethol C
[94513-69-6]



$C_{24}H_{18}O_{12}$ 498.399
Constit. of the algae *Laminaria ochroleuca*, *Cystophora congesta*, *Ecklonia maxima*, *Cystophora reflexa*, *Sargassum spinuligerum* and *Carpophyllum angustifolium*. In the naming of the phlorethols, the letters after the name reflect the temporal order of discovery. Some naming confusion in the lit.

4‴-Hydroxy: ***Hydroxytetraphlorethol A***
[137809-87-1]
$C_{24}H_{18}O_{13}$ 514.398
Constit. of *Carpophyllum maschalocarpum* and *Carpophyllum angustifolium*.

2′,4‴-Dihydroxy: ***Dihydroxytetraphlorethol A***
[164176-20-9]
$C_{24}H_{18}O_{14}$ 530.398
Constit. of the brown alga *Sargassum spinuligerum*.

2″,4‴-Dihydroxy: ***Dihydroxytetraphlorethol B***
$C_{24}H_{18}O_{14}$ 530.398
Isol. from *Sargassum spinuligerum*.

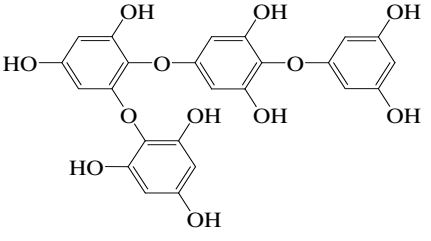
2‴-Bromo: 2^D*-Bromotetraphlorethol C*
[256448-63-2 (per-Ac)]
$C_{24}H_{17}BrO_{12}$ 577.295
Constit. of the alga *Cystophora retroflexa*. Isol. as per-Ac.

[94530-71-9, 163088-07-1]

Koch, M. *et al., Phytochemistry*, 1984, **23**, 2633-2637 (*isol, struct*)
Ragan, M.A. *et al., Prog. Phycol. Res.*, 1986, **4**, 129-241 (*rev*)
Glombitza, K.-W. *et al., Phytochemistry*, 1991, **30**, 2741 (*Hydroxytetraphlorethol A*)
Keusgen, M. *et al., Phytochemistry*, 1995, **38**, 975-985 (*Hydroxytetraphlorethol A, Dihydroxytetraphlorethols*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*Hydroxytetraphlorethol A*)
Sailler, B. *et al., Nat. Toxins*, 1999, **7**, 57-62 (*2‴-bromo*)
Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol*)

Tetraphlorethol E T-268

Tetraphloroethol E
[227085-29-2]

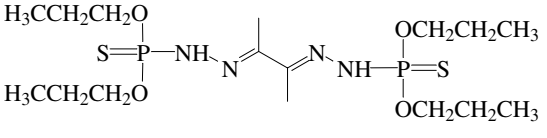


$C_{24}H_{18}O_{12}$ 498.399
Isol. from brown alga *Cystophora retroflexa*. Identified as per-Ac, to which CAS no. refers.

Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol, pmr, cmr, ms*)

O,O,O′,O′-Tetrapropyl 2,2′-(1,2-dimethyl-1,2-ethanediylidene)bis(phosphorohydrazidothioate) T-269

[59895-89-5]

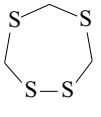


$C_{16}H_{36}N_4O_4P_2S_2$ 474.564
Constit. of *Lignincola laevis*. Cytotoxic agent. Cryst. (EtOH). Mp 124-125°. Poss. a biotransformation prod. of a pesticide, but no coml. prods. with related structs. could be found.

Cates, L.A. *et al., J. Med. Chem.*, 1976, **19**, 1133-1137 (*synth*)
Abraham, S.P. *et al., Pure Appl. Chem.*, 1994, **66**, 2391-2394 (*isol*)

1,2,4,6-Tetrathiepane T-270

1,2,4,6-Tetrathiacycloheptane
[292-45-5]

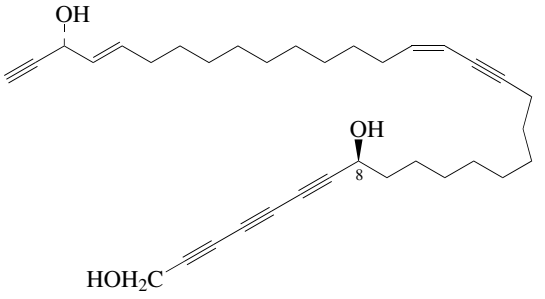


$C_3H_6S_4$ 170.344
Isol. from basidiomycetes shiitake mushroom (*Lentinus edodes*), and *Parkia speciosa*, and from red alga *Chondria californica*. Shows weak activity against gram-positive and -negative bacteria and *Candida albicans*.
Mp 79°.

4,4-Dioxide: [58966-89-5]
$C_3H_6O_2S_4$ 202.343
Constit. of *Chondria californica*. Prisms ($CHCl_3$).
Mp 154-155°.

Morita, K. *et al., Chem. Pharm. Bull.*, 1967, **15**, 998 (*synth, isol*)
Wratten, S.J. *et al., J.O.C.*, 1976, **41**, 2465 (*isol*)
Weissflog, E. *et al., Phosphorus Sulfur Relat. Elem.*, 1980, **8**, 157 (*synth*)
Gmelin, R. *et al., Phytochemistry*, 1981, **20**, 2521
Still, I.W.J. *et al., Tet. Lett.*, 1981, 1939 (*synth*)
Holzmann, G. *et al., Org. Mass Spectrom.*, 1982, **17**, 165 (*ms*)

19,30-Tetratriacontadiene-2,4,6,17,33-pentayne-1,8,32-triol T-271



$C_{34}H_{46}O_3$ 502.736

(8S,19Z,30E,32R)-form
Triangulyne F
[182314-12-1]
Isol. from the sponge *Pellina triangulata*. Cytotoxic agent. Powder. $[\alpha]_D$ -10.6 (c, 1.1 in $CHCl_3$). λ_{max} 202 (log ϵ 3.8); 227 (log ϵ 4.1) (MeOH).

8-Deoxy: 19,30-Tetratriacontadiene-2,4,6,17,33-pentayne-1,32-diol. ***Triangulyne G***
[182314-13-2]
$C_{34}H_{46}O_2$ 486.736
Isol. from *Pellina triangulata*. Cytotoxic agent. Powder. $[\alpha]_D$ -10.5 (c, 0.4 in $CHCl_3$). λ_{max} 203 (log ϵ 4); 227 (log ϵ 4.2); 306 (log ϵ 2.5) (MeOH).

Dai, J.-R. *et al., J. Nat. Prod.*, 1996, **59**, 860-865 (*isol, uv, ir, pmr, cmr, ms*)

18,30-Tetratriacontadiene-2,4,12,33-tetrayne-1,6,32-triol, 9CI T-272

Melyne C
[115276-19-2]
$HC{\equiv}CCH(OH)CH{=}CH(CH_2)_{10}CH{=}CH(CH_2)_4C{\equiv}C(CH_2)_5CH(OH)C{\equiv}CC{\equiv}CCH_2OH$
$C_{34}H_{50}O_3$ 506.767
Isol. from *Xestospongia* sp. Sol. MeOH, $CHCl_3$, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ -6 (c, 2.0 in $CHCl_3$). λ_{max} 230 (ϵ 360); 240 (ϵ 330); 255 (ϵ 200) (MeOH) (Derep). λ_{max} 230 (ϵ 360); 242 (ϵ 330); 256 (ϵ 200) (MeOH) (Berdy).

Quinoa, E. *et al., Tet. Lett.*, 1988, **29**, 2037 (*isol, struct*)

19,22,25,28,31-Tetratriacontapentaenoic acid T-273

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_{17}COOH$
$C_{34}H_{58}O_2$ 498.831

(all-Z)-form [105514-44-1]
Constit. of *Petrosia pellasarca*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1990, **53**, 836-840 (*isol, ms*)

5,9,27-Tetratriacontatrienoic acid T-274

$H_3C(CH_2)_5CH{=}CH(CH_2)_{16}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{34}H_{62}O_2$ 502.863

(*all-Z*)-*form* [187657-48-3]
Isol. from the sponge *Haliclona cinerea*.
Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*isol, ms*)

30-Tetratriacontene-2,4,16,33-tetrayne-1,32-diol T-275

Durissimol B

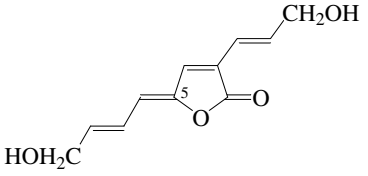
$HC{\equiv}CCH(OH)CH{=}CH(CH_2)_{12}C{\equiv}C(CH_2)_{10}C{\equiv}CC{\equiv}CCH_2OH$

$C_{34}H_{52}O_2$ 492.784

(-)-(*E*)-*form*
Isol. from the sponge *Strongylophora durissima*.
Pale yellow oil. $[\alpha]_D^{25}$ -10.4 (c, 0.1 in $CHCl_3$). λ_{max} 216 (log ϵ 3.23); 254 (log ϵ 3.49); 268 (log ϵ 4.04); 285 (log ϵ 3.17) (MeOH).
Shen, Y.-C. *et al., J. Nat. Prod.*, 2000, **63**, 1686-1688

Tetrenolin T-276

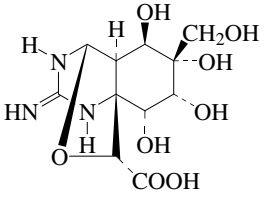
Lissoclinolide
[132074-82-9]
[26047-03-0, 248936-42-7]



$C_{11}H_{12}O_4$ 208.213
Lissoclinolide and Tetrenolin shown to be identical in 1999.
Metab. of *Micropolyspora venezuelensis* and *Lissoclinum patella*. Antibiotic. Yellow cryst. ($CHCl_3$). Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 126-128°. λ_{max} 206 (ϵ 17000); 240 (ϵ 8500); 340 (ϵ 54000) (MeOH) (Derep). λ_{max} 208 (ϵ 12300); 340 (ϵ 42900) (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 150 mg/kg. LU4700000
Octahydro: Mp 60-62°.
Gallo, G.G. *et al., Tetrahedron*, 1969, **25**, 5677-5680 (*isol, pmr, ms*)
Pagani, H. *et al., J. Antibiot.*, 1973, **26**, 1-6 (*isol*)
Davidson, B.S. *et al., J. Nat. Prod.*, 1990, **53**, 1036-1038 (*Lissoclinolide*)
Rossi, R. *et al., Tet. Lett.*, 1998, **39**, 7799-7802 (*synth, Lissoclinolide*)
Gorth, F.C. *et al., Synthesis*, 1999, 1520-1528 (*synth, struct*)

Tetrodonic acid T-277

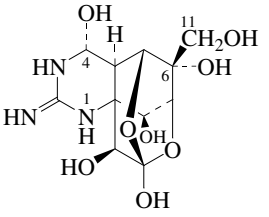
[3270-35-7]



$C_{11}H_{17}N_3O_8$ 319.271
Isol. from the fish *Fugu pardalis*, *Fugu poecilonotus* and *Fugu rubripes*. Amorph.
Tsuda, K. *et al., Chem. Pharm. Bull.*, 1964, **12**, 634-642 (*struct*)
Tamura, C. *et al., Acta Cryst.*, 1966, **21**, 219-225 (*cryst struct*)
Nakamura, M. *et al., Toxicon*, 1985, **23**, 271-276 (*isol*)

Tetrodotoxin T-278

Tarichatoxin. Spheroidine. Tetrodontoxin. Fugu poison. Maculotoxin. Araregai toxin. TTX
[4368-28-9]



$C_{11}H_{17}N_3O_8$ 319.271
Isol. from the ovaries and liver of Japanese puffer fish (*Sphoeroides rubripes*, *Sphoeroides vermicularis*, *Sphoeroides phyreus*), skin of Californian newt (*Taricha torosa*), from the Japanese ivory shell (*Babylonia japonica*), from the dinoflagellate *Alexandrium tarnavense*, xanthid crab *Atergatis floridus* and *Cynops ensicauda*. Believed to be a metab. prod. of a *Pseudomonas* sp. Sodium channel (I, II, III, μ1, h1) blocker. Highly potent toxin. Of practical significance as a cause of accidental poisoning in Japan. Used in neurophysiological research. Anaesthetic synergist. Cryst. Sol. acids; fairly sol. H_2O; poorly sol. EtOAc, hexane. $[\alpha]_D^{25}$ -8.64 (c, 8.55 in AcOH aq.). pK_a 8.76. Darkens at 225° but does not melt.
▶ LD_{50} (mus, orl) 435 μg/kg; LD_{50} (mus, ivn) 9 μg/kg; LD_{50} (mus, ipr) 0.08 mg/kg. Highly toxic to mammals, birds, reptiles, amphibians and fish. IO1450000
Hydrobromide:
Prisms (EtOH aq.). No definite Mp.
Picrate:
Yellow needles + $1H_2O$ (H_2O). Darkens >200° without melting.
Hepta-Ac: Mp 188.5-191.5°. $[\alpha]_D^{30}$ +15.8 (c, 0.39 in $CHCl_3$).
11-Deoxy: ***11-Deoxytetrodotoxin***
[112174-24-0]
$C_{11}H_{17}N_3O_7$ 303.271
Isol. from *Arothron nigropunctatus*, *Cynops ensicauda*, *Fugu* spp. and other marine spp. Paralytic poison, phycotoxin, Na ion blocker. Needles (AcOH aq.).
Mp 202° (dec.). $[\alpha]_D^{25}$ +5.4 (c, 0.3 in AcOH aq.).
▶ LD_{50} (mus, ipr) 0.71 mg/kg.
11-Hydroxy: ***11-Hydroxytetrodotoxin***. *11-Oxotetrodotoxin*
[123665-88-3]
$C_{11}H_{17}N_3O_9$ 335.27
Isol. from the puffer fish *Arothron nigropunctatus*, the frog *Brachycephalus ephippium* and the newt *Notophthalmus viridescens*. Also from the xanthid crab *Atergatis floridus*. Amorph. Exists as covalent hydrate.
*4-Deoxy, 4*R*-[(2*S*-amino-2-carboxyethyl)thio]:* ***4-S-Cysteinyltetrodotoxin***
[853013-71-5]
$C_{14}H_{22}N_4O_9S$ 422.415
Isol. from *Fugu pardalis*.
4-Epimer: ***4-Epitetrodotoxin***
[98242-82-1]
$C_{11}H_{17}N_3O_8$ 319.271
Isol. from *Arothron nigropunctatus, Cynops ensicauda*, *Fugu* spp., *Octopus maculosus* and other marine spp. Phycotoxin, sodium channel blocker, paralytic poison. Amorph.
4-Epimer, 11-deoxy: ***11-Deoxy-4-epitetrodotoxin***
[113564-23-1]
$C_{11}H_{17}N_3O_7$ 303.271
Isol. from the newt *Cynops ensicauda*. Amorph.
6-Epimer: ***6-Epitetrodotoxin***
[112318-40-8]
$C_{11}H_{17}N_3O_8$ 319.271
Isol. from *Arothron nigropunctatus*, *Cynops ensicauda*, *Fugu* spp. and other marine spp. Phycotoxin. Amorph. $[\alpha]_D^{21}$ -4.8 (c, 0.3 in AcOH aq.).

▶ LD_{50} (mus, ipr) 0.6 mg/kg.

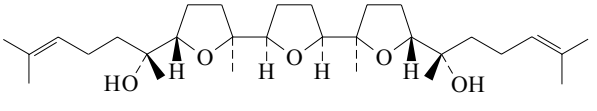
6-De(hydroxymethyl): ***11-Nortetrodotoxin****. 11-Nortetrodotoxin-6S-ol*
[156336-07-1]
$C_{10}H_{15}N_3O_7$ 289.244
Isol. from the fish *Arothron nigropunctatus.*

6-De(hydroxymethyl), 6-epimer: ***6-Epi-11-nortetrodotoxin****. 6-De(hydroxymethyl)-6-epitetrodotoxin. 11-Nortetrodotoxin-6R-ol*
[81520-41-4]
$C_{10}H_{15}N_3O_7$ 289.244
Isol. from *Arothron nigropunctatus*, *Atergatis floridus* and *Fugu* spp. incl. from the puffer fish *Fugu niphobles.* Amorph.

Yakoo, A. *et al., Nippon Kagaku Kaishi*, 1950, **71**, 590 (*isol*)
Tomiie, Y. *et al., Tet. Lett.*, 1963, 2101 (*struct*)
Woodward, R.B. *et al., Pure Appl. Chem.*, 1964, **9**, 49 (*struct*)
Goto, T. *et al., Tetrahedron*, 1965, **21**, 2059 (*isol, ir, pmr, struct*)
Tsuda, K. *et al., Naturwissenschaften*, 1966, **53**, 171 (*rev*)
Furusaki, A. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 3332 (*cryst struct*)
U.S. Pat., 1971, 3 966 934; *CA*, **85**, 87545 (*use*)
Kishi, Y. *et al., J.A.C.S.*, 1972, **94**, 9219 (*synth*)
Yasumoto, T. *et al., Agric. Biol. Chem.*, 1986, **50**, 793-795 (*isol*)
Tetrodotoxin, Saxitoxin and the Molecular Biology of the Sodium Channel, (eds. Kao, C.Y. *et al*), New York Academy of Sciences, 1986, (*book*)
Simidu, U. *et al., Appl. Environ. Microbiol.*, 1987, **53**, 1714-1715 (*occur*)
Yotsu, M. *et al., Toxicon*, 1987, **25**, 225-228 (*isol*)
Yasumoto, T. *et al., J.A.C.S.*, 1988, **110**, 2344-2345 (*derivs, isol, pmr, cmr*)
Endo, A. *et al., Tet. Lett.*, 1988, **29**, 4127-4128 (*6-Epi-11-nortetrodotoxin*)
Khora, S.S. *et al., Tet. Lett.*, 1989, **30**, 4393-4394 (*11-Oxotetrodotoxin*)
Yotsu, M. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 370-371, (*11-Nortetrodotoxin-6S-ol*)
Arakawa, O. *et al., Fish. Sci.*, 1994, **60**, 769-771 (*11-Oxotetrodotoxin, 11-Nortetrodotoxin-6R-ol*)
Yasumoto, T. *et al., J. Toxicol., Toxin Rev.*, 1996, **15**, 81-90 (*rev*)
Kodama, M. *et al., Toxicon*, 1996, **34**, 1101-1105 (*occur*)
Dyakonov, A.L. *et al., Khim. Prir. Soedin.*, 1997, **33**, 297-351; *Chem. Nat. Compd. (Engl. Transl.)*, 1997, **33**, 221-267 (*rev*)
Food Sci. Technol., Seafood and Freshwater Toxins, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*rev*)
Miyazawa, K. *et al., J. Toxicol., Toxin Rev.*, 2001, **20**, 11-33 (*rev, occur*)
Isobe, M. *et al., Tetrahedron*, 2001, **57**, 4543-4558 (*5,11-Dideoxytetrodotoxin, synth*)
Ohyabu, N. *et al., J.A.C.S.*, 2003, **125**, 8798-8805 (*synth*)
Hinman, A. *et al., J.A.C.S.*, 2003, **125**, 11510-11511 (*synth*)
Nishikawa, T. *et al., Pure Appl. Chem.*, 2003, **75**, 251-257 (*11-Deoxytetrodotoxin, synth*)
Yotsu-Yamashita, M. *et al., Toxicon*, 2003, **41**, 893-897 (*11-Oxotetrodotoxin*)
Koert, U. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 5572-5576 (*synth*)
Yotsu-Yamashita, M. *et al., Chem. Res. Toxicol.*, 2005, **18**, 865-871, (*4-S-Cysteinyltetrodotoxin*)
Sato, K. *et al., J.O.C.*, 2005, **70**, 7496-7504 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FOQ000

Teurilene T-279

[96304-92-6]

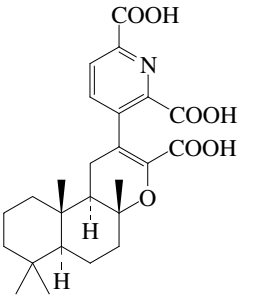


$C_{30}H_{52}O_5$ 492.738
Constit. of red alga *Laurencia obtusa*. Cytotoxic. Cryst. (diisopropyl ether).
Mp 84-85°. $[\alpha]_D^{22}$ 0 (c, 0.37 in $CHCl_3$).

Suzuki, T. *et al., Tet. Lett.*, 1985, **26**, 1329 (*cryst struct*)
Hashimoto, M. *et al., J.O.C.*, 1991, **56**, 2299 (*synth*)

Thallusin T-280

[851369-86-3]



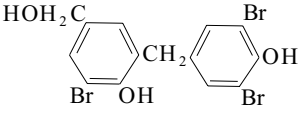
Relative Configuration

$C_{25}H_{31}NO_7$ 457.522
Isol. from a marine bacterium *Cytophaga* sp. YM2-23 obt. from a *Monostroma* sp. Morphogenesis inducer in algae. Amorph. powder.

Matsuo, Y. *et al., Science (Washington, D.C.)*, 2005, **307**, 1598 (*isol, pmr, cmr, cryst struct*)
Gao, X. *et al., Org. Lett.*, 2006, **8**, 2123-2126 (*synth*)

Thelephenol T-281

3,3′,5′-Tribromo-2,4′-dihydroxy-5-hydroxymethyldiphenylmethane
[52193-43-8]

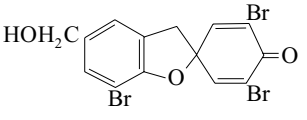


$C_{14}H_{11}Br_3O_3$ 466.951
Isol. from *Thelepus setosus.* Cryst.
Mp 180-182°.

Higa, T. *et al., Tetrahedron*, 1975, **31**, 2379

Thelepin T-282

[52498-93-8]

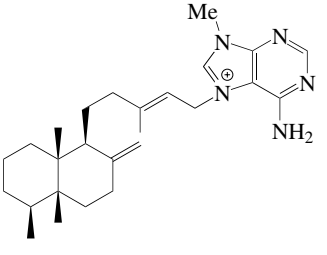


$C_{14}H_9Br_3O_3$ 464.935
Isol. from *Thelepus setosus.* Pale-yellow cryst. (MeOH). Sol. $CHCl_3$.
Mp 202-203° dec. λ_{max} 247 (sh); 257 (ϵ 13180); 280 (sh); 288 (sh) (EtOH) (Derep). λ_{max} 247; 257; 280; 288 (MeOH) (Berdy). λ_{max} 257 (ϵ 1320) (EtOH) (Berdy).

Higa, T. *et al., Tetrahedron*, 1975, **31**, 2379-2381 (*isol*)
Tsuge, O. *et al., Chem. Lett.*, 1984, 1415-1418 (*synth*)

Agelas nakamurai Thelepogane-purine alkaloid T-283

[213749-81-6]



$C_{26}H_{40}N_5$ 422.636

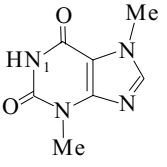
Alkaloid from the sponge *Agelas nakamurai*. Amorph. solid. $[\alpha]_D$ +12.9 (c, 0.18 in MeOH). Closely related to the Agelasines. λ_{max} 215 (log ϵ 4.24); 272 (log ϵ 3.95) (MeOH).

Iwagawa, T. *et al., J. Nat. Prod.*, 1998, **61**, 1310-1312 (*isol, uv, ir, pmr, cmr*)

Theobromine, BAN T-284

*3,7-Dihydro-3,7-dimethyl-1*H*-purine-2,6-dione, 9CI. 3,7-Dimethylxanthine. Diurobromine. Santheose. Thesal. FEMA 3591. Many other names*

[83-67-0]



$C_7H_8N_4O_2$ 180.166

Constit. of tea leaves (*Camellia thea*), *Theobroma cacao* (cocoa), *Cola acuminata*, *Paullinia cupana* and some *Ilex* and *Acer* spp. Adenosine receptor antagonist. Diuretic, cardiac stimulant, arterial dilator. Monoclinic needles.

Mp 351°. Subl. 290. pK_{a1} 1; pK_{a2} 10 (25°). Log P -0.69 (calc).

▶ Human systemic effects by ingestion (CNS and gastrointestinal). LD_{50} (rat, orl) 1265 mg/kg. Exp. reprod. and teratogenic effects (large dose). XH2275000

Perchlorate: Mp 271-273° dec.

1-Hexyl: ***Pentifylline, BAN, INN***. *Cosaldon. Hexyltheobromine. SK 7*

[1028-33-7]

$C_{13}H_{20}N_4O_2$ 264.327

Stabiliser for vitamin preparations. Vasodilator, diuretic agent. Mp 82-83°. Log P 2.59 (uncertain value) (calc).

▶ UO8450000

2-Hydroxy-*form*

O^2*-Me: 3,7-Dihydro-2-methoxy-3,7-dimethyl-6*H*-purin-6-one, 9CI.* ***2-O-Methyltheobromine***

[19143-62-5]

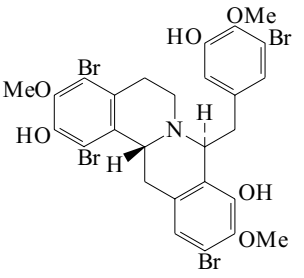
$C_8H_{10}N_4O_2$ 194.193

Constit. of the gorgonian *Echinomuraceae splendens*. λ_{max} 265 (ϵ 8555) (MeOH).

Blout, E.R. *et al., J.A.C.S.*, 1950, **72**, 479 (*ir*)
Lockhart, E.L. *et al., J.A.C.S.*, 1950, **72**, 5328 (*uv*)
Spiteller, G. *et al., Monatsh. Chem.*, 1962, **93**, 632 (*ms*)
Twanmoh, L.-M. *et al., J. Het. Chem.*, 1973, **10**, 187 (*pmr*)
Nicolau, C. *et al., Z. Naturforsch., C*, 1974, **29**, 475 (*cmr*)
Bergmann, F. *et al., J.O.C.*, 1977, **42**, 2470 (*synth*)
Royer, R.F. *et al., Actual. Pharmacol.*, 1982, **191**, 36 (*rev, pharmacol*)
Ueda, T. *et al., Heterocycles*, 1982, **19**, 2291 (*synth*)
Tarka, S.M. *et al., Prog. Clin. Biol. Res.*, 1984, **158**, 9 (*props, isol, biosynth*)
Shively, C.A. *et al., Toxicol. Appl. Pharmacol.*, 1986, **84**, 593 (*metabol, toxicol, rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 688 (*synonyms*)
Atta-ur-Rahman, *et al., The Alkaloids*, 1990, **38**, 230 (*spectral props*)
Fujii, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2833 (*synth, uv, pmr*)
IARC Monog., 1991, **51**, 421 (*rev, tox*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1318
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 751
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2771-2772
Ford, K.A. *et al., Acta Cryst. C*, 1998, **54**, 1980-1983 (*cryst struct*)
Parameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 2002, **41**, 1093-1096 (*2-O-Methyltheobromine*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TEO500

Theoneberine T-285

[145400-57-3]



$C_{27}H_{25}Br_4NO_6$ 779.114

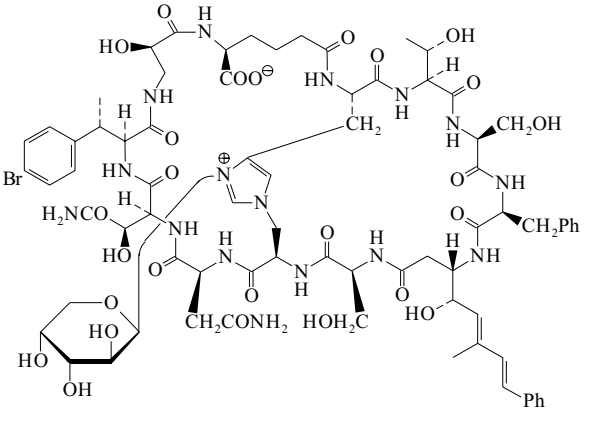
Biogenetically unique isoquinoline alkaloid. Classified as a hybrid between 1-benzylisoquinolines and protoberberines. Alkaloid from the Okinawan marine sponge *Theonella* sp. Exhibits antimicrobial activity against gram-positive bacteria. Also shows cytotoxicity against murine lymphoma L1210 and human epidermoid carcinoma KB cells *in vitro*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

Mp 128°. $[\alpha]_D^{20}$ -53 (c, 0.6 in $CHCl_3$). λ_{max} 286 (ϵ 5300) (MeOH/HCl) (Derep). λ_{max} 300 (ϵ 6800) (MeOH/NaOH) (Derep). λ_{max} 284 (ϵ 5300) (MeOH) (Derep).

Kobayashi, J. *et al., J.O.C.*, 1992, **57**, 6680 (*isol, uv, ir, pmr, cmr, ms, struct*)

Theonegramide T-286

[161017-21-6]



$C_{75}H_{97}BrN_{16}O_{26}$ 1718.587

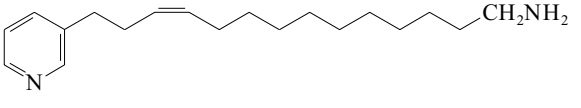
Cyclic peptide antibiotic. The imidazole ring shows charge delocalisation. Isol. from the sponge *Theonella swinhoei*. Antifungal agent. Powder. $[\alpha]_D$ +19 (c, 0.4 in MeCN aq.). Similar to Theonellamide F, T-290. λ_{max} 278 (ϵ 12700); 288 (ϵ 12900); 305 (sh) (ϵ 7100) (MeOH) (Derep).

Bewley, C.A. *et al., J.O.C.*, 1994, **59**, 4849; 1995, **60**, 2644 (*isol, pmr, cmr, struct*)

Theonelladine A T-287

14-(3-Pyridinyl)-11-tetradecen-1-amine, 9CI. 3-(14-Amino-3-tetradecenyl)pyridine

[125289-09-0]



$C_{19}H_{32}N_2$ 288.475

Mol. formula erroneously reported as $C_{20}H_{32}N_2$ in paper.

Alkaloid from the Okinawan marine sponge *Theonella swinhoei*. Exhibits potent antineoplastic activity. Calcium release inducer. λ_{max} 210 (ϵ 12300); 257 (ϵ 3300); 263 (ϵ 3600); 269 (ϵ 2700) (MeOH) (Derep).

1-Aldehyde, oxime (Z-): [291775-83-2]
$C_{19}H_{30}N_2O$ 302.459
Isol. from *Amphimedon* sp. Oxime config. undetermined. λ_{max} 264 (ϵ 3300) (MeOH).

N-*Me:* ***Theonelladine B***
[125289-10-3]
$C_{20}H_{34}N_2$ 302.502
Alkaloid from *Theonella swinhoei*. Exhibits potent antineoplastic activity. Calcium release inducer. Mol. formula erroneously reported as $C_{21}H_{34}N_2$ in paper. λ_{max} 210 (ϵ 12300); 257 (ϵ 3300); 263 (ϵ 3600); 269 (ϵ 2700) (MeOH) (Derep).

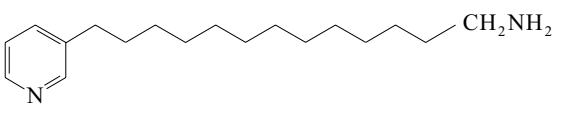
3′,4′-Dihydro, 9′,10′-didehydro, 1-aldehyde, oxime (Z,Z-): [291775-84-3]
$C_{19}H_{30}N_2O$ 302.459
Isol. from *Amphimedon* sp. λ_{max} 264 (ϵ 3200) (MeOH).

11,12-Didehydro: 14-(3-Pyridinyl)-11-tetradecyn-1-amine. 3-(11-Amino-3-tetradecynyl)pyridine. ***Niphatesine A***
[132923-10-5]
$C_{19}H_{30}N_2$ 286.459
Alkaloid from the marine sponge *Niphates* sp. Antineoplastic. Oil. λ_{max} 207 (ϵ 5900); 258 (ϵ 2800); 263 (ϵ 3200); 268 (ϵ 2500) (MeOH) (Berdy).

Kobayashi, J. *et al., J.C.S. Perkin 1*, 1990, 3301-3303 (*isol, uv, pmr, cmr, ms, struct*)
Rao, A.V.R. *et al., J.O.C.*, 1991, **56**, 4545-4547 (*synth*)
Teubner, A. *et al., Annalen*, 1993, 161-165 (*synth*)
Hirano, K. *et al., Chem. Pharm. Bull.*, 2000, **48**, 974-977 (*oximes, isol*)

Theonelladine C T-288

3-Pyridinetridecanamine. 3-(13-Aminotridecyl)pyridine. 3-(3-Pyridyl)tridecylamine
[125289-11-4]



$C_{18}H_{32}N_2$ 276.464
Alkaloid from the Okinawan marine sponge *Theonella swinhoei*. Exhibits potent antineoplastic activity. Calcium release inducer. Obt. mixed with traces of analogues having branched alkyl chains. λ_{max} 210 (ϵ 12300); 257 (ϵ 3300); 263 (ϵ 3600); 269 (ϵ 2700) (MeOH) (Derep).

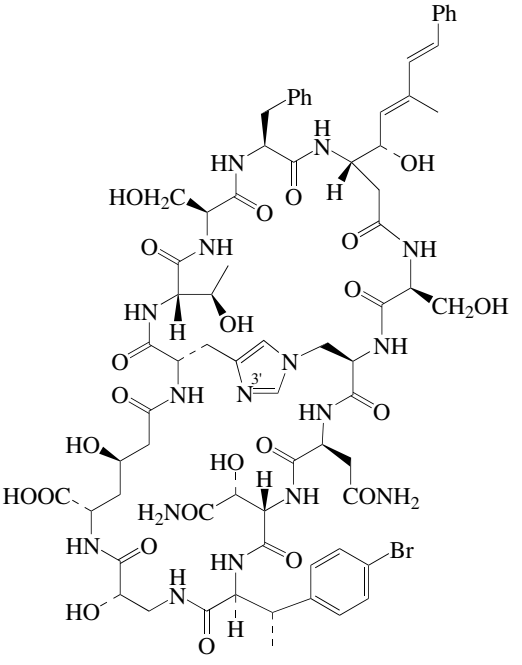
N-*Me:* ***Theonelladine D***
[125289-12-5]
$C_{19}H_{34}N_2$ 290.491
Alkaloid from *Theonella swinhoei*. Exhibits potent antineoplastic activity. Calcium release inducer. Not obt. completely pure. λ_{max} 210 (ϵ 12300); 257 (ϵ 3300); 263 (ϵ 3600); 269 (ϵ 2700) (MeOH) (Derep).

N-*Methoxy:* N-*Methoxy-3-pyridinetridecanamine.* ***Ikimine C***
[131479-32-8]
$C_{19}H_{34}N_2O$ 306.49
Alkaloid from *Niphates* sp. and other sponges. Cytotoxic. Oil. λ_{max} 260 (ϵ 2000); 265 (ϵ 6610); 270 (ϵ 2880) (MeOH) (Derep). λ_{max} 260 (ϵ 1995); 264 (ϵ 6166); 272 (ϵ 3630) (MeOH) (Berdy).

Kobayashi, J. *et al., Tet. Lett.*, 1989, **30**, 4833 (*isol, uv, pmr, cmr, ms, struct*)
Carroll, A.R. *et al., Tetrahedron*, 1990, **46**, 6637 (*Ikimine C*)
Rao, A.V.R. *et al., J.O.C.*, 1991, **56**, 4545 (*synth*)
Teubner, A. *et al., Annalen*, 1993, 161-165 (*synth*)
Wang, Y. *et al., J.O.C.*, 2003, **68**, 3090-3098 (*synth*)

Theonellamide B T-289

[161930-47-8]



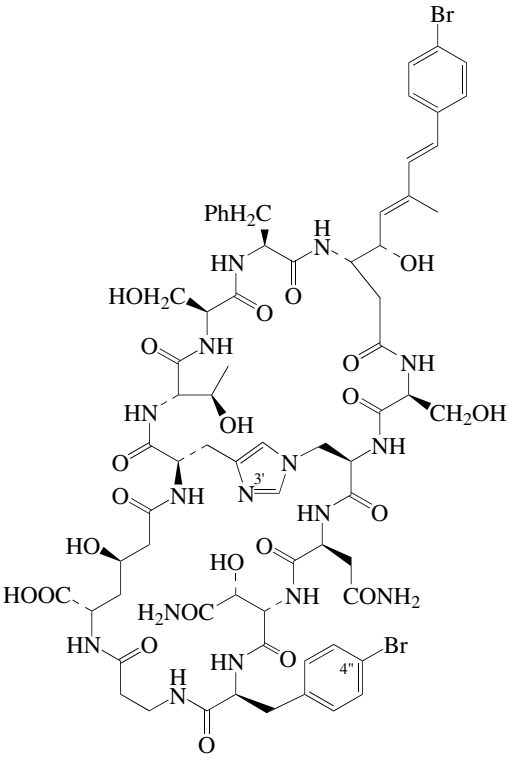
$C_{70}H_{89}BrN_{16}O_{23}$ 1602.471
Isol. from a marine sponge *Theonella* sp. Cytotoxic agent. Powder. Sol. H_2O, butanol, MeOH, DMF; poorly sol. $CHCl_3$, hexane. $[\alpha]_D^{23}$ +6.6 (c, 0.1 in 1-propanol/H_2O (2:1)). λ_{max} 290 (ϵ 9500) (1-propanol/H_2O (2:1)).

$N^{3'}$-*β-D-Galactopyranosyl:* ***Theonellamide A***
[161930-46-7]
$C_{76}H_{99}BrN_{16}O_{28}$ 1764.613
Isol. from a *Theonella* sp. Cytotoxic agent. Powder. Sol. H_2O, butanol, MeOH, DMF; poorly sol. $CHCl_3$, hexane. $[\alpha]_D^{23}$ +23 (c, 0.1 in 1-propanol/H_2O (2:1)). Internal quaternary salt. λ_{max} 288 (ϵ 12000) (1-propanol/H_2O (2:1)).

Matsunaga, S. *et al., J.O.C.*, 1995, **60**, 1177-1181 (*isol, uv, struct*)

Theonellamide F T-290

[119455-31-1]



$C_{69}H_{86}Br_2N_{16}O_{22}$ 1651.34

Isol. from a marine sponge *Theonella* sp. Antifungal agent. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{23}$ -5.5 (c, 0.12 in 1-propanol aq.). λ_{max} 283 (ϵ 24400); 294 (ϵ 24800); 315 (sh) (ϵ 13600) (MeOH assumed, not reported) (Derep).

$N^{3'}$-*β*-L-*Arabinopyranosyl:* ***Theonellamide D***

[161961-75-7]

$C_{74}H_{95}Br_2N_{16}O_{26}$ 1784.464

Isol. from a *Theonella* sp. Cytotoxic agent. Powder. Sol. H_2O, butanol, MeOH, DMF; poorly sol. $CHCl_3$, hexane. $[\alpha]_D^{23}$ +16 (c, 0.1 in 1-propanol aq.). Quaternary nitrogen compd., as internal salt. λ_{max} 290 (ϵ 20000) (1-propanol aq.). λ_{max} 290 (ϵ 20000) (MeOH) (Berdy).

$N^{3'}$-*β*-D-*Galactopyranosyl:* ***Theonellamide E***

[161961-76-8]

$C_{75}H_{97}Br_2N_{16}O_{27}$ 1814.49

Isol. from a *Theonella* sp. Cytotoxic agent. Powder. Sol. H_2O, DMF, butanol, MeOH; poorly sol. $CHCl_3$, hexane. $[\alpha]_D^{23}$ +20 (c, 0.1 in 1-propanol aq.). Internal salt. λ_{max} 292 (ϵ 27000) (1-propanol aq.). λ_{max} 292 (ϵ 27000) (MeOH) (Berdy).

4′′-Debromo: ***Theonellamide C***

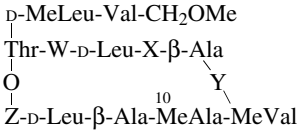
[161930-48-9]

$C_{69}H_{87}BrN_{16}O_{22}$ 1572.444

Isol. from a *Theonella* sp. Cytotoxic agent. Powder. Sol. H_2O, DMF, MeOH, butanol; poorly sol. $CHCl_3$, hexane. Racemic. λ_{max} 292 (ϵ 18000) (1-propanol aq.). λ_{max} 292 (ϵ 18000) (MeOH) (Berdy).

Matsunaga, S. *et al., J.A.C.S.*, 1989, **111**, 2582 (*isol, struct, pmr, cmr*)
Tohdo, K. *et al., Pept. Chem.*, 1993, **31**, 37 (*synth*)
Matsunaga, S. *et al., J.O.C.*, 1995, **60**, 1177 (*Theonellamides C-E*)

Theonellapeptolide T-291



Theonellapeptolide—Ia W = β-Ala, X = MeIle
Y = D-Val, Z = D = MeIle
Ib W = β-Ala, X = MeVal
Y = D-*allo*-Ile, Z = D-MeIle
Ic W = β-Ala, X = MeIle
Y = D-*allo*-Ile, Z = D-MeVal
Id W = β-Ala, X = MeIle
Y = D-*allo*-Ile, Z = D-MeIle
Ie W = Meβ-Ala, X = MeIle
Y = D-*allo*-Ile, Z = D-MeIle

Theonellamine B W = β-Ala, X = MeLeu
Y = D-*allo*-Ile, Z = D-MeIle

Isol. from the marine sponge *Theonella swinhoei*. Inhibit development of the fertilised eggs of the sea urchin *Hemicentrotus pulcherrimus.*

Theonellapeptolide Ia [109767-19-3]

$C_{69}H_{123}N_{13}O_{16}$ 1390.808

Shows immunosuppressive effect. Needles (MeOH aq.). Sol. MeOH. Mp 156-157°. $[\alpha]_D^{20}$ -58 (c, 1.4 in MeOH).

Theonellapeptolide Ib [109767-20-6]

$C_{69}H_{123}N_{13}O_{16}$ 1390.808

Needles (MeOH aq.). Mp 159°. $[\alpha]_D^{20}$ -54 (c, 1.8 in MeOH).

Theonellapeptolide Ic [109767-21-7]

$C_{69}H_{123}N_{13}O_{16}$ 1390.808

Needles (MeOH aq.). Mp 147°. $[\alpha]_D^{20}$ -50 (c, 1.1 in MeOH).

Theonellapeptolide Id [105091-14-3]

[230976-89-9]

$C_{70}H_{125}N_{13}O_{16}$ 1404.835

Shows immunosuppressive effect. Cryst. (MeOH aq.). Mp 168-169°. $[\alpha]_D^{20}$ -68 (MeOH).

10-N-*De-Me:* ***Theonellapeptolide IId***

[161407-71-2]

$C_{69}H_{123}N_{13}O_{16}$ 1390.808

Isol. from *Theonella swinhoei*. Shows immunosuppressive effect. Amorph. solid. $[\alpha]_D$ -27 (c, 1 in MeOH).

33-Demethoxy, 33-methylsulfinyl: ***33-Demethoxy-33-(methylsulfinyl)theonellapeptolide Id***

[246136-21-0]

$C_{70}H_{125}N_{13}O_{16}S$ 1436.901

Isol. from a *Theonella* sp. Amorph. solid. $[\alpha]_D^{25}$ -45 (c, 1 in MeOH).

Theonellapeptolide Ie [109767-22-8]

$C_{71}H_{127}N_{13}O_{16}$ 1418.862

Cryst. (MeOH). Mp 153-155°. $[\alpha]_D^{20}$ -62 (c, 0.2 in MeOH).

33-Demethoxy: ***33-Demethoxytheonellapeptolide Ie***

[245742-46-5]

$C_{70}H_{125}N_{13}O_{15}$ 1388.836

Isol. from a *Theonella* sp. Amorph. solid. $[\alpha]_D^{24}$ -56 (c, 1 in MeOH).

10-N-*De-Me:* ***Theonellapeptolide IIe***

$C_{70}H_{125}N_{13}O_{16}$ 1404.835

Isol. from *Theonella swinhoei.* Amorph. solid. $[\alpha]_D^{30}$ -13.4 (c, 0.6 in $CHCl_3$).

Theonellamine B [105115-91-1]

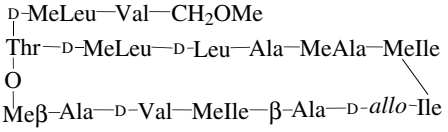
$C_{70}H_{125}N_{13}O_{16}$ 1404.835

Cyclic depsipeptide antibiotic. Isol. from *Theonella* sp. ATP-ase inhibitor. Powder. Sol. MeOH.

Mp 149-151°. $[\alpha]_D^{25}$ -57.2 (c, 1 in MeOH).

Nakamura, H. *et al., Tet. Lett.*, 1986, **27**, 4319-4322 (*Theonellamine B*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1177 (*ms, struct*)
Kitagawa, I. *et al., Tetrahedron*, 1991, **47**, 2169 (*isol, struct*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1410 (*Theonellapeptolide IId*)
Tsuda, M. *et al., Tetrahedron*, 1999, **55**, 10305-10314 (*33-demethoxy derivs*)
Roy, M.C. *et al., Tetrahedron*, 2000, **56**, 9079-9092 (*Theonellapeptolide IIe, activity*)

Theonellapeptolide IIIe **T-292**



$C_{69}H_{127}N_{13}O_{14}$ 1362.841

Isol. from the sponge *Lamellomorpha strongylata*. Plates (Me_2CO aq.).

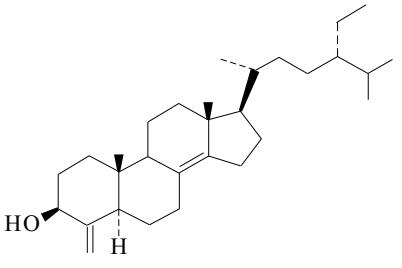
Mp 184-186°. $[\alpha]_D^{22}$ -48.6 (c, 1 in MeOH).

Li, S. *et al., J. Nat. Prod.*, 1998, **61**, 724-728 (*isol, ir, pmr, cmr, ms*)

Theonellasterol **T-293**

4-Methylenestigmast-8(14)-en-3-ol. 24-Ethyl-4-methylenecholest-8(14)-en-3-ol. 4-Methyleneporiferast-8(14)-en-3-ol

[76758-19-5]



$C_{30}H_{50}O$ 426.724

Constit. of the marine sponge *Theonella swinhoei*. Cryst.

Mp 123-124°. $[\alpha]_D^{25}$ +12 ($CHCl_3$).

3-Ketone: 4-Methylenestigmast-8(14)-en-3-one. 24-Ethyl-4-methylenecholest-8(14)-en-3-one. ***Theonellasterone***

[145403-25-4]

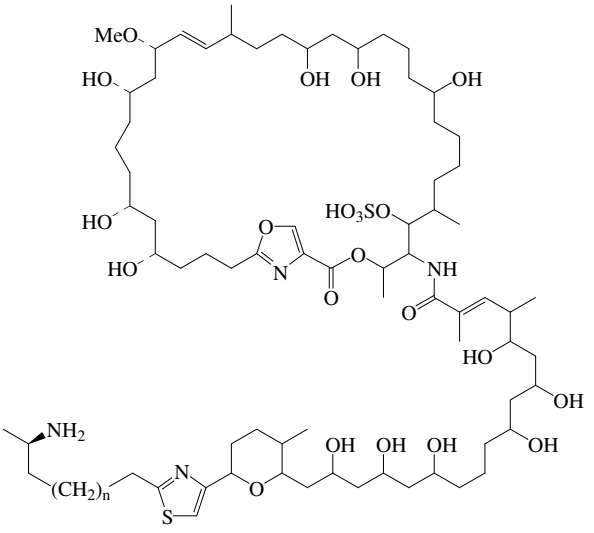
$C_{30}H_{48}O$ 424.709

Constit. of *Theonella swinhoei*. Needles (MeCN).

Mp 99-101°. $[\alpha]_D^{26}$ +34.3 (c, 1.05 in $CHCl_3$).

Kho, E. *et al., J.O.C.*, 1981, **46**, 1836-1839 (*isol, pmr*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1773-1778 (*Theonellasterone*)

Theonezolides **T-294**



Macrolide antibiotics. n = 6,4,8 for Theonezolides A,B,C respectively. Partial stereochem. is known. Isol. from the marine sponge *Theonella* sp. Cytotoxic agents.

Theonezolide A [150243-49-5]

$C_{79}H_{140}N_4O_{22}S_2$ 1562.121

Needles + $3H_2O$. Mp 123°. $[\alpha]_D^{28}$ -8.1 (c, 1.5 in MeOH). λ_{max} 210 (ϵ 22000) (MeOH).

Theonezolide B [157536-46-4]

$C_{77}H_{136}N_4O_{22}S_2$ 1534.067

Cryst. Mp 125°. $[\alpha]_D^{28}$ -8 (c, 1.5 in MeOH). λ_{max} 211 (ϵ 22000) (MeOH).

Theonezolide C [157536-47-5]

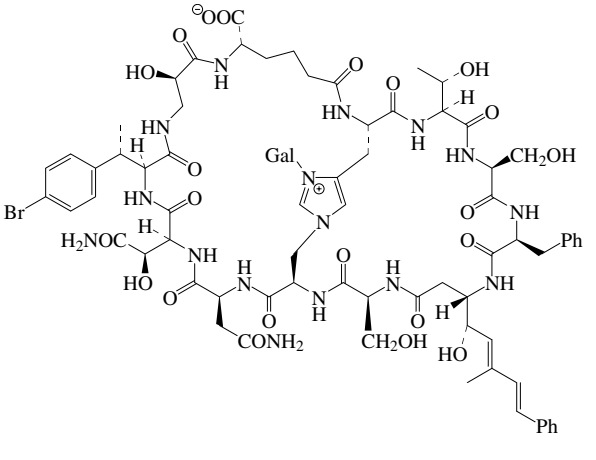
$C_{81}H_{144}N_4O_{22}S_2$ 1590.174

Cryst. Mp 122°. $[\alpha]_D^{28}$ -7.5 (c, 1.5 in MeOH). λ_{max} 211 (ϵ 25000) (MeOH).

Kobayashi, J. *et al., J.A.C.S.*, 1993, **115**, 6661-6665 (*isol, uv, ir, pmr, cmr, ms*)
Kondo, K. *et al., Tetrahedron*, 1994, **50**, 8355-8362 (*isol, uv, ir, pmr, cmr, ms, struct*)
Kobayashi, J. *et al., Heterocycles*, 1998, **49**, 39-42 (*stereochem*)
Sato, M. *et al., Tetrahedron*, 1998, **54**, 4819-4826 (*stereochem*)

Theopalauamide **T-295**

P 951



$C_{76}H_{99}BrN_{16}O_{27}$ 1748.613

Isol. from filamentous bacterial symbionts of the sponge *Theonella swinhoei*. Powder. $[\alpha]_D$ +19 (c, 0.4 in MeOH). Exists as internal quaternary salt. λ_{max} 203 (ϵ 19600); 276 (ϵ 9400); 285 (ϵ 9900); 304 (ϵ 4500) (MeOH). λ_{max} 278; 288 (MeOH) (Berdy).

Conformational isomer: ***Isotheopalauamide***
[204653-16-7]
$C_{76}H_{99}BrN_{16}O_{27}$ 1748.613
Isol. from bacterial symbionts of *Theonella swinhoei*. Powder. $[\alpha]_D$ +35 (c, 0.04 in MeOH).
Schmidt, E.W. *et al., J.O.C.*, 1998, **63**, 1254-1258 (*isol, uv, ir, pmr, cmr*)

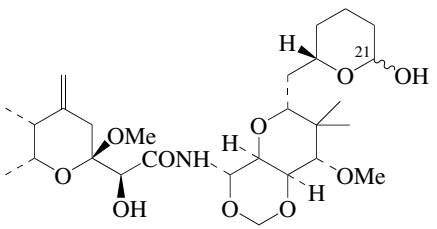
Theopederin I T-296

[252733-51-0]
As Theopederin B, T-298 with
R^1 = H, R^2 = -$CH_2CH(OH)(CH_2)^{21}_3CH{=}^{22}CHCH{=}CHCH{=}$CHCOOH(*R*,*E*,*E*,*E*-)
$C_{32}H_{49}NO_{11}$ 623.739
Isol. from the sponge *Theonella swinhoei*.
$[\alpha]_D^{24}$ +54 (c, 0.08 in MeOH). λ_{max} 300 (ϵ 24000) (MeOH).

21,22-Dihydro: ***Theopederin J***
[252733-64-5]
$C_{32}H_{51}NO_{11}$ 625.755
Isol. from *Theonella swinhoei*.
$[\alpha]_D^{24}$ +48 (c, 0.04 in MeOH). λ_{max} 260 (ϵ 22000) (MeOH).
Tsukamoto, S. *et al., Tetrahedron*, 1999, **55**, 13697-13702

Theopederin A T-297

[141754-55-4]

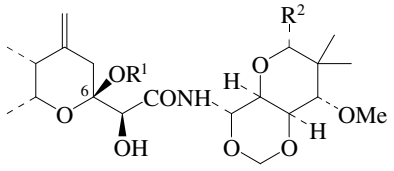


$C_{27}H_{45}NO_{10}$ 543.653
Isol. from the sponge *Theonella* sp. Cytotoxic agent. $[\alpha]_D$ +88.1 (c, 0.1 in $CHCl_3$). Related to Onnamide A, O-107.

21-Ketone (lactone): ***Theopederin C***
[141754-57-6]
$C_{27}H_{43}NO_{10}$ 541.637
Isol. from *Theonella* sp. Cytotoxic agent. $[\alpha]_D$ +172 (c, 0.03 in $CHCl_3$).
Fusetani, N. *et al., J.O.C.*, 1992, **57**, 3828 (*isol, ir, pmr, cmr*)

Theopederin B T-298

[141754-56-5]

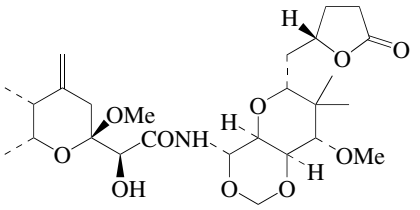


R^1 = Me, R^2 = $CH_2CH(OH)(CH_2)_3COOMe$(*R*-)

$C_{28}H_{47}NO_{11}$ 573.679
Isol. from the sponge *Theonella* sp. Cytotoxic agent. $[\alpha]_D$ +49.1 (c, 0.06 in $CHCl_3$).
Fusetani, N. *et al., J.O.C.*, 1992, **57**, 3828 (*isol, ir, pmr, cmr*)

Theopederin D T-299

[141754-58-7]



$C_{26}H_{41}NO_{10}$ 527.611
Isol. from the sponge *Theonella* sp. Cytotoxic agent. $[\alpha]_D$ +80 (c, 0.04 in $CHCl_3$).
Fusetani, N. *et al., J.O.C.*, 1992, **57**, 3828 (*isol, ir, pmr, cmr*)
Kocienski, P. *et al., J.C.S. Perkin 1*, 2000, 2357-2384 (*synth*)

Theopederin E T-300

[141754-59-8]
As Theopederin B, T-298 with
R^1 = Me, R^2 = –CH_2OH
$C_{22}H_{37}NO_9$ 459.536
Isol. from the sponge *Theonella* sp. Cytotoxic agent. $[\alpha]_D$ +136.7 (c, 0.03 in $CHCl_3$).
Fusetani, N. *et al., J.O.C.*, 1992, **57**, 3828 (*isol, ir, pmr, cmr*)
Simpson, J.S. *et al., J. Nat. Prod.*, 2000, **63**, 704-706 (*isol, pmr, cmr*)

Theopederin F T-301

[252733-06-5]
As Theopederin B, T-298 with
R^1 = Me, R^2 = $CH_2CH(OH)(CH_2)_3CH_2OH$(*R*-)
$C_{27}H_{47}NO_{10}$ 545.669
Isol. from the sponge *Theonella swinhoei*. Antifungal and cytotoxic agent. $[\alpha]_D^{24}$ +32 (c, 0.3 in MeOH).
Tsukamoto, S. *et al., Tetrahedron*, 1999, **55**, 13697-13702

Theopederin G T-302

[252733-29-2]
As Theopederin B, T-298 with
R^1 = H, R^2 = -$CH_2^{17}CH(OH)(CH_2)_3CH{=}CHCH{=}$CHCOOH(*E*,*E*-)
$C_{30}H_{47}NO_{11}$ 597.701
Isol. from the sponge *Theonella swinhoei*.
$[\alpha]_D^{24}$ +45 (c, 0.12 in MeOH). λ_{max} 260 (ϵ 17000) (MeOH).

17-Ketone: ***Theopederin H***
[252733-40-7]
$C_{30}H_{45}NO_{11}$ 595.686
Isol. from *Theonella swinhoei*.
$[\alpha]_D^{24}$ +60 (c, 0.02 in MeOH). λ_{max} 260 (ϵ 21000) (MeOH).

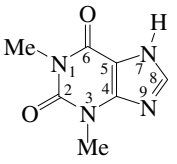
*18,19-Didehydro(*E-*), 6-Me ether:* ***Theopederin L***. *Discalamide B*
[370086-37-6]
$C_{31}H_{47}NO_{11}$ 609.712
Isol. from the sponge *Discodermia* sp. Cytotoxic. Amorph. powder. $[\alpha]_D^{21}$ +34 (c, 0.05 in MeOH). λ_{max} 202 (log ϵ 4.07); 260 (log ϵ 4.1) (MeOH).

*18,19-Didehydro(*E-*), 6,17-di-Me ether:* ***Theopederin K***. *Discalamide A*
[370086-36-5]
$C_{32}H_{49}NO_{11}$ 623.739
Isol. from the sponge *Discodermia* sp. Cytotoxic. Amorph. powder. $[\alpha]_D^{21}$ +90.3 (c, 0.43 in MeOH). λ_{max} 202 (log ϵ 4.23); 254 (log ϵ 4.46) (MeOH).
Tsukamoto, S. *et al., Tetrahedron*, 1999, **55**, 13697-13702 (*isol, pmr, cmr*)
Pat. Coop. Treaty (WIPO), 2001, 01 79 247; *CA*, **135**, 327334k (*Discalamides*)
Paul, G.K. *et al., J. Nat. Prod.*, 2002, **65**, 59-61 (*Theopederins K,L*)

Theophylline, BAN, JAN, USAN T-303

*3,7-Dihydro-1,3-dimethyl-1*H*-purine-2,6-dione, 9CI. 1,3-Dimethylxanthine. Austyn. Elan. Elixophyllin. Euphyllin. Nuelin. Spophyllin retard. Teonova. Theocin. Theodel. Theo-Dur. Theograd. Theolair. Theona P. Theotard. Uniphyllin. Many other names*

[58-55-9]



$C_7H_8N_4O_2$ 180.166

Constit. of tea leaves (*Camellia thea*), *Ilex paraguariensis* and *Paullinia cupana* (Theaceae, Aquifoliaceae, Sapindaceae). Also isol. from the marine sponge *Haliclona* sp. Adenosine receptor antagonist. Smooth muscle relaxant of value in the treatment of bronchial conditions. Antiasthmatic agent. Synergises the antileukaemic acitity of nitrosoureas. Diuretic and cardiac stimulant. Mp 268° Mp 264°. pK_{a1} 1; pK_{a2} 8.6 (25°). Log P -0.06 (uncertain value) (calc).

▶ Adverse effects reported when used therapeutically incl. gastrointestinal and CNS changes. Overdosage can cause death. LD_{50} (rat, orl) 244 mg/kg. Exp. reprod. and teratogenic effects.

XH3850000

N^7-*(2-Deoxy-β-*D*-*erythro*-pentofuranosyl):* ***Aplysidine***

[144096-49-1]

$C_{12}H_{16}N_4O_5$ 296.282

Isol. from the sponge *Aplysina* sp. Adenosine A1 receptor antagonist. Amorph. solid. Sol. H_2O, MeOH. Mp 162°. $[\alpha]_D^{20}$ +17 (c, 0.4 in H_2O). λ_{max} 274 (ϵ 8500) (H_2O) (Berdy). λ_{max} 275 (ϵ 8400) (HCl) (Berdy). λ_{max} 274 (ϵ 8400) (NaOH) (Berdy).

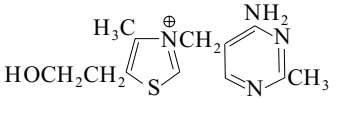
[5967-84-0, 8002-89-9, 49746-06-7, 85531-28-8]

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 214B (*nmr*)
Blout, E.R. *et al., J.A.C.S.*, 1950, **72**, 479 (*ir*)
Spiteller, G. *et al., Monatsh. Chem.*, 1962, **93**, 632 (*ms*)
Twanmoh, L.-M. *et al., J. Het. Chem.*, 1973, **10**, 187 (*pmr*)
Takayama, S. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1200 (*synth, uv*)
Nicolau, C. *et al., Z. Naturforsch., C*, 1974, **29**, 475 (*cmr*)
Cohen, J.L. *et al., Anal. Profiles Drug Subst.*, 1975, **4**, 466 (*rev, ir, pmr, uv, ms, anal*)
Goeber, B. *et al., Pharmazie*, 1978, **33**, 717 (*ms*)
Naqvi, A.A. *et al., J. Appl. Crystallogr.*, 1981, **14**, 464 (*cryst struct*)
Bukowsky, M. *et al., Ann. Intern. Med.*, 1984, **101**, 63 (*rev, pharmacol*)
Weinberger, M. *et al., J. Allergy Clin. Immunol.*, 1984, **73**, 525 (*rev, pharmacol, tox*)
Grant, J.A. *et al., J. Allergy Clin. Immunol.*, 1986, **78**, 669 (*rev, pharmacol*)
Rowe, D.J.F. *et al., Ann. Clin. Biochem.*, 1988, **25**, 4 (*rev, pharmacol, tox, metab*)
Atta-ur-Rahman, *et al., The Alkaloids*, 1990, **38**, 232 (*spectra*)
IARC Monog., 1991, **51**, 391 (*rev, tox*)
Kondo, K. *et al., Tetrahedron*, 1992, **48**, 7145-7148 (*Aplysidine*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1314; 1315; 1319
Ebisuzaki, Y. *et al., Acta Cryst. C*, 1997, **53**, 777-779 (*cryst struct*)
Markham, A. *et al., Drugs*, 1998, **56**, 1081-1091 (*rev*)
Zajac, M.A. *et al., Synth. Commun.*, 2003, **33**, 3291-3297 (*synth, ir, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TEP000; TEP500

Thiamine, BAN, INN T-304

3-[(4-Amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methylthiazolium(1+), 9CI, 8CI. Vitamin B_1. Torulin. Oryzanin. Aneurine. Vitaneurin. Many other names

[70-16-6]



$C_{12}H_{17}N_4OS^{\oplus}$ 265.358

Ubiquitous constit. of biol. materials. Produced by numerous bacterial spp. Used as aq. soln. for fluorimetric detn. of $PO_4^{2\ominus}$ (λ_{max} 440 nm, 5-100 ppb, via molybdatophosphate). Essential vitamin. Sol. H_2O; sl. sol. EtOH. pK_a 5.17. Log P -3.91 (uncertain value) (calc). Labile in acid or alkaline soln. or on heating. In alkaline soln. the thiazolium ring is reversibly opened to thiols. In therapy thiamine can be replaced by various ring-opened analogues, e.g. Benfotiamine.

Chloride: Thiamine monochloride. Thiacrat

[59-43-8]

$C_{12}H_{17}ClN_4OS$ 300.811

Cryst. + $1H_2O$ (H_2O). Mp 120-122° dec., 163-165° dec. (anhyd.). Infrequently encountered, hydrochloride more stable.

▶ XI6550000

Chloride; hydrochloride: ***Thiamine hydrochloride, USAN****. Bewon. Betaxin. Betalin S. Vinothiam. FEMA 3322*

[67-03-8]

$C_{12}H_{18}Cl_2N_4OS$ 337.272

Clinically used vitamin source. Oral or parenterally administered doses. Well tolerated. Plates or cryst. (EtOH). V. sol. H_2O; spar. sol. EtOH; insol. Et_2O, C_6H_6. Mp 248° dec. Mp is not a good criterion of purity.

▶ XI7350000

Nitrate: ***Thiamine mononitrate, USAN***

[532-43-4]

$C_{12}H_{17}N_5O_4S$ 327.363

Clinically used vitamin source. Mp 164-165° Mp 196-200°.

▶ XI7400000

O-*Phosphate, chloride: Monophosphothiamine chloride*

[532-40-1]

$C_{12}H_{18}ClN_4O_4PS$ 380.791

Vitamin B_1 deriv. used clinically. Mp 200°.

O-*Diphosphate:* See Thiamine diphosphate in *The Combined Chemical Dictionary.*

O-*Triphosphate: Thiamine triphosphate. Thiamine triphosphoric acid. TTP*†

[15666-52-1]

$C_{12}H_{20}N_4O_{13}P_3S$ 553.296

Isol. from animal tissues. Cryst. (EtOH aq.). CAS no. refers to chloride.

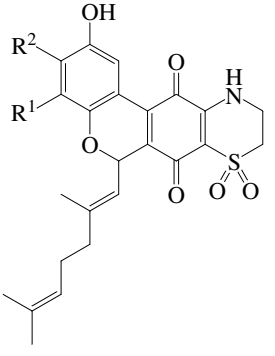
[7019-71-8]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 515C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 647A (*ir*)
Todd, A.R. *et al., J.C.S.*, 1937, 364; 1938, 26 (*synth*)
Karrer, P. *et al., Helv. Chim. Acta*, 1946, **29**, 711 (*phosphate*)
Lenormant, H. *et al., Bull. Soc. Chim. Fr.*, 1954, 375 (*ir, uv*)
Greiling, H. *et al., Nature (London)*, 1958, **13**, 251 (*isol, triphosphate*)
Kotera, K. *et al., Chem. Pharm. Bull.*, 1965, **13**, 440 (*pmr*)
Hesse, M. *et al., Helv. Chim. Acta*, 1967, **50**, 808 (*ms*)
Linnett, P.E. *et al., J.C.S.(C)*, 1967, 796 (*biosynth*)
Pletcher, J. *et al., Acta Cryst. B*, 1972, **28**, 2928 (*cryst struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 2609
Holzbecher, J. *et al., Anal. Chim. Acta*, 1973, **64**, 147 (*detn, P*)
Dwidevi, B.K. *et al., J. Agric. Food Chem.*, 1973, **21**, 54 (*props*)
Gallo, A.A. *et al., J. Biol. Chem.*, 1974, **249**, 1382 (*cmr*)
Thiamine, [Proc. Pap. Discuss. U.S.-Jpn. Semin.], 2nd, Wiley, N.Y., 1976, (*book*)
Oka, Y. *et al., Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley*, 1978, **24**, 124 (*synth*)
Penttinen, H.K. *et al., Methods Enzymol.*, 1979, **62**, 112 (*triphosphate*)
Brown, G.M. *et al., Adv. Enzymol. Relat. Areas Mol. Biol.*, 1982, **53**, 345 (*biosynth*)
Sable, H.Z. *et al., Ann. N.Y. Acad. Sci.*, 1982, **378**, 78; 378; 454 (*book, nmr, cryst struct, conformn*)
Uray, G. *et al., Monatsh. Chem.*, 1982, **113**, 1475 (*synth*)
Davis, R.E. *et al., Adv. Clin. Chem.*, 1983, **23**, 93 (*chemistry*)
Ishida, T. *et al., Acta Cryst. C*, 1984, **40**, 437 (*cryst struct*)
Gubler, C.J. *et al., Handbook of Vitamins*, (Machlin, L.J. Ed.), M. Dekker, New York, 1984, 245 (*rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 2515; 2540; 4574
Al-Rashood, K.A.M. *et al., Anal. Profiles Drug Subst.*, 1989, **18**, 413 (*rev*)
Contant, P. *et al., Helv. Chim. Acta*, 1990, **73**, 1300 (*synth*)
Hu, N. *et al., Acta Cryst. C*, 1992, **48**, 1951 (*cryst struct*)

Bender, D.A. *et al., Nutritional Biochemistry of the Vitamins*, Cambridge University Press, Cambridge, 1992, 128 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1053
Casas, J.S. *et al., Acta Cryst. C*, 1994, **50**, 1265 (*cryst struct, acetate*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 1797
Estramareix, B. *et al., New J. Chem.*, 1996, **20**, 607 (*rev, biosynth*)
Spenser, I.D. *et al., Angew. Chem., Int. Ed.*, 1997, **36**, 1033-1046 (*rev, biosynth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2772-2778 (*rev, use, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TES750; TET300; TET500

Thiaplidiaquinone A T-305

[852872-92-5]



R^1 = $^-CH_2CH{=}C(CH_3)CH_2CH_2CH{=}C(CH_3)_2$ (*E*), R^2 = H

$C_{34}H_{41}NO_6S$ 591.767
Alkaloid from the ascidian *Aplidium conicum*. Antitumour agent.
λ_{max} 354 (ϵ 9300) (MeOH).

Aiello, A. *et al., J. Med. Chem.*, 2005, **48**, 3410-3416 (*isol, pmr, cmr*)

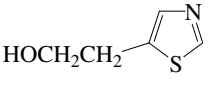
Thiaplidiaquinone B T-306

[852872-93-6]
As Thiaplidiaquinone A, T-305 with
R^1 = H, R^2 = -$CH_2CH{=}C(CH_3)CH_2CH_2CH{=}C(CH_3)_2$(*E*-)
$C_{34}H_{41}NO_6S$ 591.767
Alkaloid from the ascidian *Aplidium conicum*. Antitumour agent.
λ_{max} 324 (ϵ 6300) (MeOH).

Aiello, A. *et al., J. Med. Chem.*, 2005, **48**, 3410-3416 (*isol, pmr, cmr*)

5-Thiazoleethanol, 9CI T-307

2-(5-Thiazolyl)ethanol. 5-(2-Hydroxyethyl)thiazole
[5664-55-1]

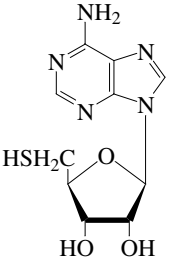


C_5H_7NOS 129.182
Prod. by an unidentified marine bacterium. Bp_{10} 138-141°.

Ulf, H. *et al., Acta Pharm. Suec.*, 1967, **4**, 269-280 (*synth*)
Laasch, H. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

5′-Thioadenosine, 9CI T-308

6-Amino-9-(5-thioribofuranosyl)purine
[67805-97-4]



$C_{10}H_{13}N_5O_3S$ 283.31
Cryst. (H_2O). Mp 75-77°.

S-*Me: 5′*-S-*Methyl-5′-thioadenosine, 9CI, 8CI. Adenine thiomethylpentoside*
[2457-80-9]
$C_{11}H_{15}N_5O_3S$ 297.337
Isol. from yeast and from *Doris verrucosa*. Involved in biological transmethylations. Needles (MeOH aq.).
Mp 213-214°. $[\alpha]_D$ +12.2 (1% H_2SO_4 aq.).
▶ AU7410000

S-*Me, 2′,3′*-O-*isopropylidene:*
$C_{14}H_{19}N_5O_3S$ 337.402
Mp 143°.

S-*Me, tritosyl:* [80860-53-3]
$C_{32}H_{33}N_5O_9S_4$ 759.905
Mp 158-160°.

S-*Me,* S-*oxide(*R-*): 5′-Deoxy-5′-(methylsulfinyl)adenosine, 9CI*
[897-42-7]
[3387-65-3]
$C_{11}H_{15}N_5O_4S$ 313.337
Prod. by *Ganoderma lucidum* (reishi). Platelet aggregation inhibitor. Cryst. Sol. H_2O, MeOH.
Mp 185-187°. $[\alpha]_D^{20}$ -23.5 (c, 1.4 in H_2O). λ_{max} 270 (H_2O) (Berdy).

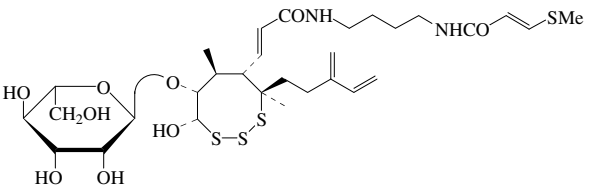
S-*Me,* S-*oxide(*S-*):* [737-74-6]
$C_{11}H_{15}N_5O_4S$ 313.337
Prod. by *Ganoderma lucidum* (reishi). Cryst.
Mp 210-211°. $[\alpha]_D$ -93.3 (c, 1 in H_2O).

S-*(2-Methylpropyl):* [35899-54-8]
$C_{14}H_{21}N_5O_3S$ 339.418
Cryst. (EtOH). Mp 126-128°. $[\alpha]_D^{24}$ 0 (c, 0.85 in MeOH).

3′-Epimer, S-*Me:* ***9-(5-S-Methyl-5-thio-β-D-xylofuranosyl)adenine***
[53458-29-0]
$C_{11}H_{15}N_5O_3S$ 297.337
Isol. from the mollusc *Doris verrucosa*. Glass.
Mp 199-201° (as picrate). $[\alpha]_D^{25}$ -270 (c, 0.39 in Py).

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 219C (*nmr*)
Weygand, F. *et al., Ber.*, 1951, **84**, 633 (*synth*)
Baddiley, J. *et al., J.C.S.*, 1951, 1348 (*synth*)
Satoh, K. *et al., Nature (London)*, 1951, **167**, 238 (*S-Me struct, S-Me tritosyl, S-Me isopropylidene*)
Trauth, O. *et al., Nature (London)*, 1951, **167**, 359 (*S-Me, synth*)
Kuhn, R. *et al., Chem. Ber.*, 1965, **98**, 1699-1704 (*synth*)
Zappia, V. *et al., J. Biol. Chem.*, 1969, **244**, 4499 (*S-Me, biochem*)
Hildesheim, J. *et al., Biochimie*, 1971, **53**, 1067-1071 (S-*2-methylpropyl*)
Montgomery, J.A. *et al., J. Med. Chem.*, 1974, **17**, 1197-1207 (*synth*)
Sugimoto, Y. *et al., Arch. Microbiol.*, 1976, **108**, 175
Borkakoti, N. *et al., Acta Cryst. B*, 1978, **34**, 867 (*S-Me, cryst struct*)
Cimino, G. *et al., Experientia*, 1986, **42**, 1301-1302 (*S-Me, isol, Doris*)
Porcelli, M. *et al., Adv. Exp. Med. Biol.*, 1988, **250**, 219-228 (*3′-epimer-S-Me*)
Porcelli, M. *et al., Biochem. J.*, 1989, **263**, 635-640 (*3′-epimer-S-Me*)
Marriott, J.H. *et al., Tet. Lett.*, 1990, **31**, 7485 (*synth, pmr*)
Robins, M.J. *et al., Can. J. Chem.*, 1991, **69**, 1468 (*S-Me, uv, pmr, cmr, ms*)
Kawagishi, H. *et al., Phytochemistry*, 1993, **32**, 239-241 (*S-Me-S-oxide*)
Pignot, M. *et al., Eur. J. Org. Chem.*, 2000, 549-555 (*synth, pmr, cmr*)

Perophora viridis 1,2,3-Thiocane glycoside T-309



$C_{30}H_{48}N_2O_9S_4$ 708.981

Isol. from the Atlantic tunicate *Perophora viridis*. Pale yellow amorph. solid. $[\alpha]_D^{24}$ +197.3 (c, 0.11 in EtOH). λ_{max} 257 (log ϵ 2.78) (EtOH).

Rezanka, T. *et al., Eur. J. Org. Chem.*, 2002, 2400-2404 (*isol, pmr, cmr, ms*)

1-Thiocarbamoyl-16-thiocyanato-8-hexadecanol T-310

9-Hydroxy-16-thiocyanato-1-hexadecanecarbamothioic acid. 9-Hydroxy-16-thiocyanatohexadecylthiocarbamic acid. ***Thiocyanatin E1***

$NCS(CH_2)_8CH(OH)(CH_2)_7S\text{-}CONH_2$

$C_{18}H_{34}N_2O_2S_2$ 374.611

(ξ)-*form* [720697-78-9]

Isol. from a marine sponge *Oceanapia* sp. Nematocidal agent. Isol. as a mixt. with 16-Thiocarbamoyl-1-thiocyanato-8-hexadecanol, T-311.

Capon, R.J. *et al., J. Nat. Prod.*, 2004, **67**, 1277-1282 (*isol, pmr, cmr, ms*)

16-Thiocarbamoyl-1-thiocyanato-8-hexadecanol T-311

8-Hydroxy-16-thiocyanato-1-hexadecanecarbamothioic acid. 8-Hydroxy-16-thiocyanatohexadecylthiocarbamic acid. ***Thiocyanatin E2***

$NCS(CH_2)_7CH(OH)(CH_2)_8S\text{-}CONH_2$

$C_{18}H_{34}N_2O_2S_2$ 374.611

(ξ)-*form* [720697-80-3]

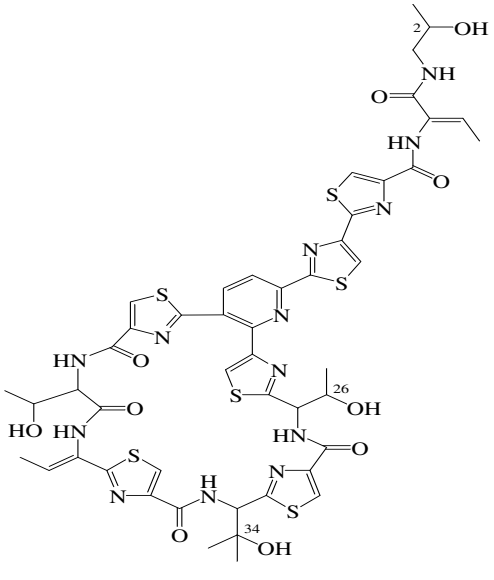
Isol. from a marine sponge *Oceanapia* sp. Nematocidal agent. Viscous oil. Isol. as a mixt. with 1-Thiocarbamoyl-16-thiocyanato-8-hexadecanol, T-310

Capon, R.J. *et al., J. Nat. Prod.*, 2004, **67**, 1277-1282 (*isol, pmr, cmr, ms*)

Thiocillin I T-312

13′,19′-Didehydro-19′-deoxy-28,44-dihydro-41,44-dihydroxymicrococcin P, 9CI

[59979-01-0]



$C_{48}H_{49}N_{13}O_{10}S_6$ 1160.392

Thiopeptide antibiotic. Similar to Micrococcins. Isol. from *Bacillus badius* and *Bacillus cereus*. Active against gram-positive bacteria. Amorph. powder. Sol. DMF, DMSO, THF, $CHCl_3$-MeOH; fairly sol. MeOH, $CHCl_3$, Me_2CO, EtOH; poorly sol. EtOAc, C_6H_6, Et_2O, H_2O, acids. $[\alpha]_D^{24.5}$ +97.7 (c, 2.028 in 90% EtOH aq.). λ_{max} 217 (E1%/1cm 734); 275 (E1%/1cm 326); 348 (E1%/1cm 199) (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 500 - 1500 mg/kg. XK6510000

26-Me ether: ***Thiocillin II***

[59979-02-1]

$C_{49}H_{51}N_{13}O_{10}S_6$ 1174.419

From *Bacillus badius* and *Bacillus cereus*. Amorph. powder. Sol. DMSO, $CHCl_3$-MeOH, THF, DMF; fairly sol. MeOH, EtOH, $CHCl_3$, Me_2CO; poorly sol. EtOAc, H_2O, acids, Et_2O, C_6H_6. $[\alpha]_D^{24.5}$ +93.4 (c, 0.59 in 90% EtOH aq.). λ_{max} 217 (E1%/1cm 705); 278 (E1%/1cm 291); 348 (E1%/1cm 202) (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 400 - 600 mg/kg. XK6520000

34-Me ether: ***Thiocillin III***

[59979-03-2]

$C_{49}H_{51}N_{13}O_{10}S_6$ 1174.419

From *Bacillus badius*. Amorph. powder. Sol. DMF, THF, $CHCl_3$-MeOH, DMSO; fairly sol. MeOH, $CHCl_3$, EtOH, Me_2CO; poorly sol. EtOAc, Et_2O, H_2O, acids, C_6H_6. $[\alpha]_D^{24.5}$ +88 (c, 0.85 in 90% EtOH aq.). λ_{max} 217 (E1%/1cm 729); 275 (E1%/1cm 302); 347 (E1%/1cm 208) (MeOH) (Berdy).

2-Ketone: ***Antibiotic YM 266183***. *YM 266183*

$C_{48}H_{47}N_{13}O_{10}S_6$ 1158.376

Prod. by the marine-derived *Bacillus cereus* QN03323. Active against gram-positive bacteria. Powder. $[\alpha]_D^{25}$ +64.7 (c, 0.37 in MeOH). λ_{max} 213 (ϵ 79830); 290 (sh); 344 (ϵ 14460) (MeOH).

2-Ketone, 26-Me ether: ***Antibiotic YM 266184***. *YM 266184*

$C_{49}H_{49}N_{13}O_{10}S_6$ 1172.403

Prod. by the marine-derived *Bacillus cereus* QN03323. Active against gram-positive bacteria. Powder. $[\alpha]_D^{25}$ +60.9 (c, 0.15 in MeOH). λ_{max} 215 (ϵ 100960); 290 (sh); 346 (ϵ 29350) (MeOH).

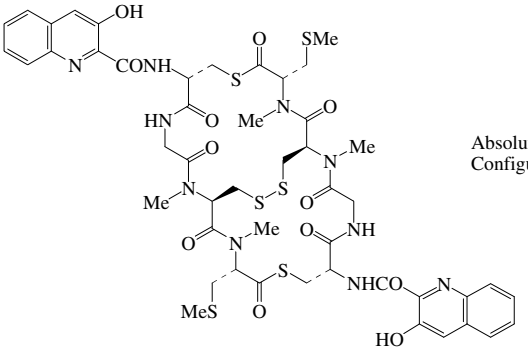
Shoji, J. *et al., J. Antibiot.*, 1976, **29**, 366-374; 1981, **34**, 1126-1136 (*isol, struct*)

Nagai, K. *et al., J. Antibiot.*, 2003, **56**, 123-128; 129-134 (*YM 266183, YM 266184*)

Thiocoraline T-313

PM 93135. Antibiotic PM 93135

[173046-02-1]



Absolute Configuration

$C_{48}H_{56}N_{10}O_{12}S_6$ 1157.426

Depsipeptide antibiotic. Prod. by a marine *Micromonospora* sp. L-13-ACM2-092. Cytotoxic agent. RNA synthesis inhibitor. Weakly inhibits HIV-1 reverse transcriptase. Pale yellow cryst. Mp 266-266.5°. $[\alpha]_D^{25}$ -190.9 (c, 1 in $CHCl_3$). λ_{max} 218 (ϵ 76500); 230 (ϵ 76700); 298 (ϵ 9400); 360 (ϵ 8900) (MeOH).

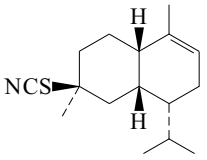
Romero, F. *et al., J. Antibiot.*, 1997, **50**, 734-737 (*isol, props*)

Baz, J.P. *et al., J. Antibiot.*, 1997, **50**, 738-741 (*uv, ir, pmr, cmr*)

Boger, D.L. *et al., J.A.C.S.*, 2001, **123**, 561-568 (*synth, abs config, activity*)

Lombó, F. *et al., ChemBioChem*, 2006, **7**, 366-367 (*biosynth*)

4-Thiocyanato-9-cadinene T-314

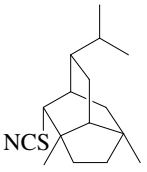


$C_{16}H_{25}NS$ 263.446

(1β,4β*SCN*,6β,7α)-*form* [120475-56-1]
Isol. from sponge *Trachyopsis aplysinoides.*
Cryst.
Mp 67-68°. $[\alpha]_D$ -13.7 (c, 0.27 in $CHCl_3$).
He, H. *et al., J.O.C.*, 1989, **54**, 2511-2514 (*isol, pmr, cmr*)

2-Thiocyanatoneopupukaenane T-315

[137371-79-0]

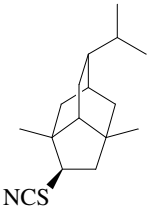


Relative Configuration

$C_{16}H_{25}NS$ 263.446
Rel. config. only known but shown here according to the abs. config. determined for 4-Thiocyanatoneopupukaenane, T-316. Only one stereoisomer apparently known (illus.), descr. as 2β-. Constit. of *Axinyssa aplysinoides* and an unidentified sponge. Antifouling agent, larval settlement inhibitor, crustacean metamorphosis inhibitor. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D$ -71.5 (c, 0.5 in $CHCl_3$) (-31). λ_{max} 240 (1440) (MeOH).
Pham, A.T. *et al., Tet. Lett.*, 1991, **32**, 4843-4846 (*isol, pmr, cmr*)
He, H.-Y. *et al., J.O.C.*, 1992, **57**, 3191-3194 (*isol, pmr, cmr*)
Simpson, J.S. *et al., Aust. J. Chem.*, 1997, **50**, 1123-1127 (*isol, pmr, cmr, ms*)
Srikrishna, A. *et al., J.C.S. Perkin 1*, 2000, 3191-3193 (*synth*)
Uyehara, T. *et al., Tet. Lett.*, 2001, **42**, 699-702 (*synth*)
Srikrishna, A. *et al., Indian J. Chem., Sect. B*, 2003, **42**, 129-134 (*struct*)

4-Thiocyanatoneopupukaenane T-316

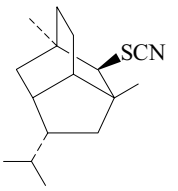
[137441-67-9]



Absolute Configuration

$C_{16}H_{25}NS$ 263.446
Constit. of *Phycopsis terpnis.* Oil. $[\alpha]_D$ -120.5 (c, 1.44 in $CHCl_3$). λ_{max} 240 (ϵ 1440) (MeOH) (Derep).
Pham, A.T. *et al., Tet. Lett.*, 1991, **32**, 4843-4846 (*isol, pmr, cmr*)
Srikrishna, A. *et al., Tet. Lett.*, 1999, **40**, 1035-1038 (*synth*)
Srikrishna, A. *et al., J.O.C.*, 2001, **66**, 4379-4385 (*synth, abs config*)

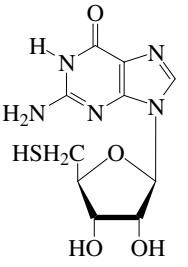
2-Thiocyanatopupukeanane T-317



$C_{16}H_{25}NS$ 263.446
Constit. of *Axinyssa aplysinoides.* Oil. $[\alpha]_D$ +5.8 (c, 0.5 in $CHCl_3$).
He, H.-Y. *et al., J.O.C.*, 1992, **57**, 3191 (*isol, pmr, cmr*)
Simpson, J.S. *et al., Tet. Lett.*, 1998, **39**, 5819-5822 (*biosynth*)

6′-Thioguanosine T-318

6′-Deoxy-6′-mercaptoguanosine

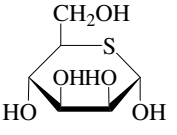


$C_{10}H_{13}N_5O_4S$

S-*Me: 6′-Deoxy-6′-(methylthio)guanosine.* ***Hamiguanosinol***
$C_{11}H_{15}N_5O_4S$ 313.337
Isol. from the sponge *Hamigera hamigera*. Pale yellow powder. $[\alpha]_D^{20}$ +15.8 (c, 0.1 in MeOH). λ_{max} 255; 275 (sh) (MeOH).
Hassan, W. *et al., Mar. Drugs*, 2004, **2**, 88-100 (*isol, pmr, cmr, ms*)

5-Thiomannose T-319

[127854-51-7]



α-D-Pyranose-*form*

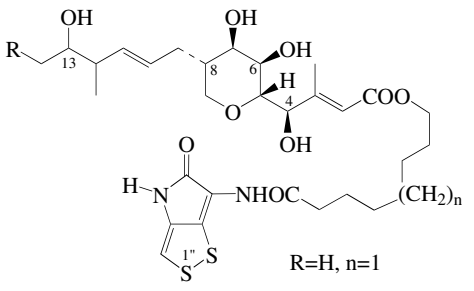
$C_6H_{12}O_5S$ 196.224

D-Pyranose-*form* [110786-41-9]
Constit. of the sponge *Clathria pyramida.* Natural form isol. as a 86:14 mixt. of α- and β-anomers respec.

α-D-Pyranose-*form*
Syrup. $[\alpha]_D$ +49.7 (c, 0.78 in H_2O).
Penta-Ac: 1,2,3,4,6-Penta-O-*acetyl-5-thio-α-D-mannopyranose*
$C_{16}H_{22}O_{10}S$ 406.41
Amorph. Mp 85-87°. $[\alpha]_D^{21}$ +83.1 (c, 1.22 in $CHCl_3$).
[127854-50-6]
Capon, R.J. *et al., Chem. Comm.*, 1987, 1200-1201 (*isol, pmr*)
Yuasa, H. *et al., J. Carbohydr. Chem.*, 1989, **8**, 753-763 (*synth*)

Thiomarinol A T-320

[146697-04-3]



$C_{30}H_{44}N_2O_9S_2$ 640.818

Prod. by the marine bacterium *Alteromonas rava*. Active against gram-positive and -negative bacteria. Inhibitor of isoleucyl transferase and RNA synthetase. Orange cryst. (MeOH). Sol. MeOH, DMSO, DMF, Et_2O; poorly sol. hexane, H_2O. Mp 106-110° dec. $[\alpha]_D^{25}$ +4.3 (c, 1 in MeOH). Related to Pseudomonic acid A. λ_{max} 206 (ϵ 25000); 306 (ϵ 3200); 386 (ϵ 9600) (MeOH/NaOH) (Derep). λ_{max} 214 (ϵ 26000); 300 (ϵ 3500); 387 (ϵ 12000) (MeOH) (Derep). λ_{max} 214; 300; 387 (MeOH/HCl) (Berdy).

1″,1″-Dioxide: ***Thiomarinol B***
[156098-42-9]
$C_{30}H_{44}N_2O_{11}S_2$ 672.816
Prod. by *Alteromonas rava*. Active against gram-positive and -negative bacteria. Inhibitor of isoleucyl transferase and RNA synthetase. Yellow cryst. (MeOH aq.). Sol. MeOH, DMSO, EtOAc, Et_2O, DMF, butanol, 1-propanol; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ +7.7 (c, 1 in propanol). λ_{max} 215 (ϵ 21000); 301 (ϵ 13000); 377 (2900) (MeOH). λ_{max} 221 (ϵ 19000); 301 (ϵ 13000); 377 (ϵ 2900) (MeOH/NaOH) (Berdy).

13-Ketone: ***Thiomarinol F***
[182155-01-7]
$C_{30}H_{42}N_2O_9S_2$ 638.802
Prod. by *Alteromonas rava*. Inhibitor of isoleucyl transferase and RNA synthetase. $[\alpha]_D$ -1.66 (c, 0.8 in MeOH). λ_{max} 210 (ϵ 21200); 300 (ϵ 2600); 385 (ϵ 8500) (MeOH).

4-Deoxy: ***Thiomarinol C***
[156343-39-4]
$C_{30}H_{44}N_2O_8S_2$ 624.818
Prod. by *Alteromonas rava*. Active against gram-positive and -negative bacteria. Inhibitor of isoleucyl transferase and RNA synthetase. Yellow cryst. Sol. MeOH, DMF, Et_2O, EtOAc, DMSO, 1-propanol, butanol; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ -1.4 (c, 1 in MeOH). λ_{max} 215 (ϵ 17000); 300 (ϵ 2700); 388 (9600) (MeOH). λ_{max} 205 (ϵ 49000); 336 (ϵ 8600) (MeOH/NaOH) (Berdy).

4,6-Dideoxy, 8-hydroxy: ***Thiomarinol G***
[194154-33-1]
$C_{30}H_{44}N_2O_8S_2$ 624.818
Prod. by *Alteromonas rava*. λ_{max} 210; 300; 385 (MeOH).

[156098-43-0]

Shiozawa, H. *et al., J. Antibiot.*, 1993, **46**, 1834; 1995, **48**, 907; 1997, **50**, 449-452 (*isol, uv, ir, pmr, cmr, props*)
Gao, X. *et al., J.A.C.S.*, 2005, **127**, 1628-1629 (*synth*)

Thiomarinol D T-321

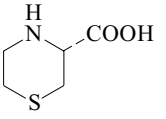
[182154-99-0]
As Thiomarinol A, T-320 with
R = CH_3, n = 1
$C_{31}H_{46}N_2O_9S_2$ 654.844
Stereochemical identity with Thiomarinol A, T-320 not confirmed. Prod. by *Alteromonas rava*. Inhibitor of isoleucyl transferase and RNA synthetase. $[\alpha]_D^{25}$ +1.5 (c, 0.8 in MeOH). λ_{max} 210 (ϵ 20900); 300 (ϵ 2600); 385 (ϵ 8900) (MeOH).
Shiozawa, H. *et al., J. Antibiot.*, 1997, **50**, 449-452 (*isol, uv, ir, pmr, cmr*)

Thiomarinol E T-322

[182155-00-6]
As Thiomarinol A, T-320 with
R = H, n = 3
$C_{32}H_{48}N_2O_9S_2$ 668.871
Stereochemical identity with Thiomarinol A, T-320 not confirmed. Prod. by *Alteromonas rava*. λ_{max} 210; 300; 385 (MeOH).
Shiozawa, H. *et al., J. Antibiot.*, 1997, **50**, 449-452 (*isol, uv, pmr, cmr*)

3-Thiomorpholinecarboxylic acid, 9CI T-323

*Tetrahydro-2*H*-1,4-thiazine-3-carboxylic acid. 1,4-Thiazane-3-carboxylic acid. Deoxychondrine. Chordarine. Perhydro-1,4-thiazine-3-carboxylic acid*
[20960-92-3]



(*R*)–*form*

$C_5H_9NO_2S$ 147.198

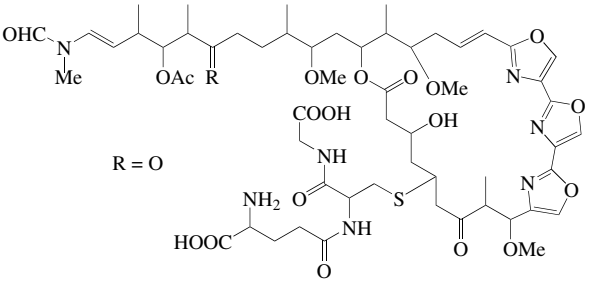
(R)-form
L-form
[65527-54-0]
Isol. from *Heterochordaria abietina*.
Tiny needles (Me_2CO aq.).
Mp 270-271° dec. (sealed tube). $[\alpha]_D^{25.5}$ -54.03 (c, 1.6 in H_2O).
S-*Oxide:* See Chondrine, C-636
S,S-*Dioxide:*
$C_5H_9NO_4S$ 179.196
Cryst. Mp 268-269°. $[\alpha]_D^{40}$ -3.4 (c, 0.005 in $CHCl_3$).

(±)-form
Cryst. (EtOH aq.), prisms (Me_2CO aq.). Mp 263-265° (sealed tube).

Tominaga, F. *et al., J. Biochem. (Tokyo)*, 1963, **54**, 222
Carson, J.F. *et al., J.O.C.*, 1964, **29**, 2203 (*synth, bibl*)
Kogami, Y. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 2963 (*synth*)
Larsson, U. *et al., Acta Chem. Scand.*, 1994, **48**, 517 (*dioxide*)

Thiomycalolide A T-324

[207227-80-3]



$C_{57}H_{81}N_7O_{20}S$ 1216.368
Isol. from a sponge *Mycale* sp. Cytotoxic agent. λ_{max} 238 (MeOH) (Berdy).

Matsunaga, S. *et al., J. Nat. Prod.*, 1998, **61**, 663-666 (*isol, pmr*)

Thiomycalolide B T-325

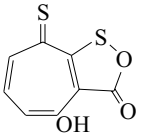
[207227-81-4]
As Thiomycalolide A, T-324 with
R = H, –OOCCH(OMe)CH_2OMe
$C_{62}H_{91}N_7O_{23}S$ 1334.5
Isol. from a sponge *Mycale* sp. Cytotoxic agent. Brownish powder. $[\alpha]_D$ -3.3 (c, 0.1 in MeOH). λ_{max} 238 (ϵ 33500) (MeOH).

Matsunaga, S. *et al., J. Nat. Prod.*, 1998, **61**, 663-666 (*isol, uv, pmr, cmr, ms*)

Thiotropocin T-326

4-Hydroxy-8-thioxocyclohept[c][1,2]oxathiol-3(8H)-one. CB 104. Antibiotic CB 104

[89550-93-6]



$C_8H_4O_3S_2$ 212.25

Prod. by *Pseudomonas* sp. CB-104 and the marine-derived *Caulobacter* sp. PK654. Active against gram-positive and -negative bacteria, fungi and mycoplasmas, esp. in acid soln. Fine orange needles. Sol. MeOH, EtOAc, DMSO, THF; fairly sol. Me_2CO, MeOH, EtOAc; poorly sol. H_2O, hexane, Et_2O. Mp 222-225° dec Mp 300°. λ_{max} 214 (ϵ 25200); 243 (ϵ 12700); 302 (ϵ 18100); 354 (ϵ 7200); 430 (ϵ 2600) (as Na salt) (Derep). λ_{max} 217 (ϵ 25000); 245 (ϵ 11300); 307 (ϵ 16300); 356 (ϵ 6200); 452 (ϵ 2100) (MeOH) (Derep). λ_{max} 210 (ϵ 35000); 356 (ϵ 37000); 460 (ϵ 6800) (MeOH/NaOH) (Berdy).

▶ LD_{50} (mus, orl) 50 - 100 mg/kg. GU4695200

Na salt:

Yellowish-orange powder.

Methyl thioether: Mp 145-150° dec.

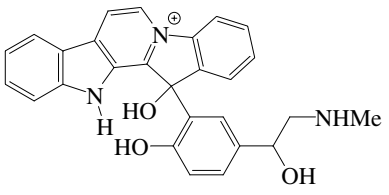
p-*Bromobenzyl thioether:*

Yellowish-green plates. Mp 152° dec.

Kintaka, K. *et al., J. Antibiot.*, 1984, **37**, 1294-1300 (*isol*)
Tsubotani, S. *et al., Tet. Lett.*, 1984, **25**, 419-422 (*isol, uv, ir, pmr, cmr, ms*)
Cane, D.E. *et al., J.A.C.S.*, 1992, **114**, 8479-8483 (*biosynth*)
Kawano, Y. *et al., J. Mar. Biotechnol.*, 1997, **5**, 225-229; 1998, **6**, 49-52 (*isol, activity*)

Thorectandramine T-327

[459165-95-8]



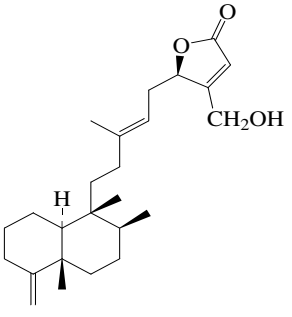
$C_{27}H_{24}N_3O_3^{\oplus}$ 438.505

Quaternary alkaloid isol. from the marine sponge *Thorectandra* sp. Yellow solid (as NH_4 salt). $[\alpha]_D$ +4.9 (c, 0.08 in MeOH) (NH_4 salt). λ_{max} 224 (log ϵ 4.16); 270 (log ϵ 3.97); 338 (log ϵ 3.87); 407 (log ϵ 3.22) (MeOH) (NH_4 salt).

Charan, R.D. *et al., Tet. Lett.*, 2002, **43**, 5201-5204 (*isol, pmr, cmr*)

Thorectandrol A T-328

[346578-57-2]



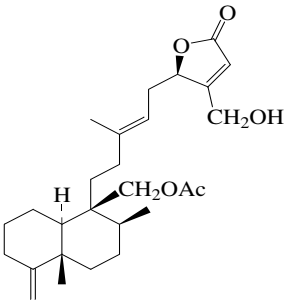
$C_{25}H_{38}O_3$ 386.573

Constit. of a *Thorectandra* sponge. Yellow oil. $[\alpha]_D$ -15 (c, 0.15 in MeOH). λ_{max} 209 (log ϵ 3.94) (MeOH).

Charan, R. D. *et al., J. Nat. Prod.*, 2001, **64**, 661-663 (*isol, pmr, cmr*)

Thorectandrol B T-329

[346578-58-3]



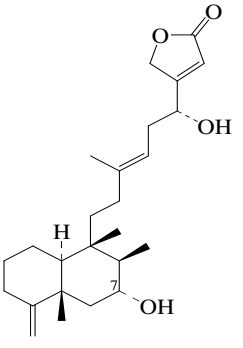
$C_{27}H_{40}O_5$ 444.61

Constit. of a *Thorectandra* sponge. Yellow oil. $[\alpha]_D$ -19.4 (c, 0.07 in MeOH). Error in struct. diag. in ref.

Charan, R.D. *et al., J. Nat. Prod.*, 2001, **64**, 661-663 (*isol, pmr, cmr*)

Thorectandrol E T-330

[425368-64-5]



$C_{25}H_{38}O_4$ 402.573

Constit. of a *Thorectandra* sp. Oil. $[\alpha]_D$ -2.14 (c, 0.14 in MeOH). λ_{max} 206 (log ϵ 3.6) (MeOH).

7-Ac: ***Thorectandrol C***

[425368-59-8]

$C_{27}H_{40}O_5$ 444.61

Constit. of a *Thorectandra* sp. Oil. $[\alpha]_D$ -29 (c, 0.27 in MeOH). λ_{max} 218 (log ϵ 3.6) (MeOH).

7-Deoxy: ***Thorectandrol D***

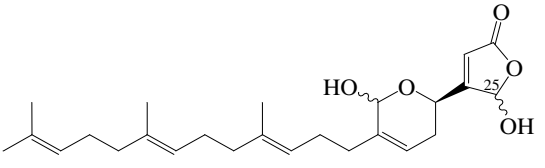
[425368-62-3]

$C_{25}H_{38}O_3$ 386.573

Oil. $[\alpha]_D$ -12.4 (c, 0.13 in MeOH). λ_{max} 213 (log ϵ 3.8) (MeOH).

Charan, R.D. *et al., J. Nat. Prod.*, 2002, **65**, 492-495 (*isol, pmr, cmr*)

Thorectolide T-331



$C_{25}H_{36}O_5$ 416.556

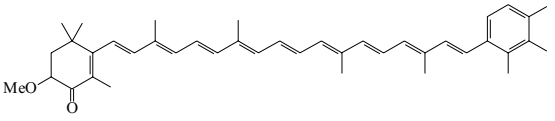
λ_{max} 212 (MeOH) (Berdy).

25-Ac: ***Thorectolide 25-acetate***
$C_{27}H_{38}O_6$ 458.594
Constit. of *Thorectandra excavatus*. Wax. $[\alpha]_D^{23}$ +33 (c, 1 in $CHCl_3$).

Cambie, R.C. *et al., J. Nat. Prod.*, 1988, **51**, 331
Soriente, A. *et al., Eur. J. Org. Chem.*, 2000, 947-953 (*abs config*)

Thorexanthin T-332

3-Methoxy-β,χ-caroten-4-one
[145038-22-8]

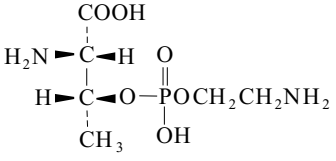


$C_{41}H_{52}O_2$ 576.861
Constit. of *Thorecta horridus*.
$[\alpha]_D^{25}$ -15 (c, 0.03 in $CHCl_3$).

Fattorusso, E. *et al., Z. Naturforsch., B*, 1992, **47**, 1477 (*isol, pmr, cmr*)

Threonine ethanolamine phosphate T-333

Threonine 2-aminoethyl hydrogen phosphate, 9CI



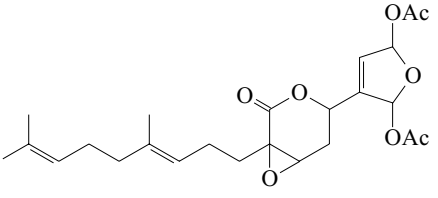
$C_6H_{15}N_2O_6P$ 242.168

(S)-form
L-form
[1935-19-9]
Constit. of fish, e.g. cod/haddock lenses.
Mp 176° dec. $[\alpha]_D$ -37.3 (c, 0.94 in H_2O).

Rosenberg, H. *et al., Biochem. J.*, 1962, **84**, 536 (*isol, synth, ir*)
Porcellati, G. *et al., Comp. Biochem. Physiol.*, 1965, **14**, 413
Allen, A.K. *et al., Comp. Biochem. Physiol.*, 1968, **27**, 695 (*biosynth*)
Rosenberg, H. *et al., Comp. Biochem. Physiol.*, 1968, **27**, 695 (*isol, synth, ir*)
v. Heyningen, R. *et al., Exp. Eye Res.*, 1976, **23**, 29

Thuridillin A T-334

[149992-83-6]

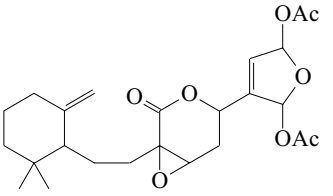


$C_{24}H_{32}O_8$ 448.512
Constit. of mollusc *Thuridilla hopei*. Defensive secretion.
$[\alpha]_D^{25}$ -12.5 (c, 0.4 in $CHCl_3$).

Gavagnin, M. *et al., Gazz. Chim. Ital.*, 1993, **123**, 205 (*isol, pmr, cmr*)

Thuridillin B T-335

[149992-84-7]

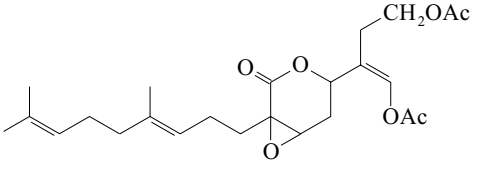


$C_{24}H_{32}O_8$ 448.512
Constit. of the mollusc *Thuridilla hopei*. Defensive agent. $[\alpha]_D^{25}$ -9.4 (c, 0.48 in $CHCl_3$).

Gavagnin, M. *et al., Gazz. Chim. Ital.*, 1993, **123**, 205 (*isol, pmr, cmr*)

Thuridillin C T-336

[149992-85-8]

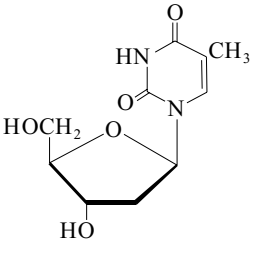


$C_{24}H_{34}O_7$ 434.528
Constit. of *Thuridilla hopei*.
$[\alpha]_D^{25}$ -86 (c, 0.05 in $CHCl_3$).

Gavagnin, M. *et al., Gazz. Chim. Ital.*, 1993, **123**, 205-208 (*isol, pmr, cmr*)

Thymidine, 8CI T-337

*1-(2-Deoxy-β-D-*erythro*-pentofuranosyl)-5-methyl-2,4(1H,3H)-pyrimidinedione, 9CI. 1-(2-Deoxy-β-D-ribofuranosyl)-5-methyluracil. Thymine 2-deoxyriboside. Thymosine†. NSC 21548*
[50-89-5]



$C_{10}H_{14}N_2O_5$ 242.231
Isol. from plant sources, e.g. seedlings of *Phaseolus vulgaris* (kidney bean). Constit. of the starfish *Acanthaster planci*, the marine mollusc *Cryptochiton stelleri* and the sea pen *Pavonaria finmarchica*. A principal constit. of DNA.
Mp 186-187°. $[\alpha]_D$ +18.5 (H_2O). $[\alpha]_D^{25}$ +30.6 (c, 1.0 in H_2O). pK_{a1} 9.8; pK_{a2} 12.9 (25°). λ_{max} 207 (ε 9800); 267 (ε 9700) (no solvent reported) (pH 7.2).

▶ Exp. reprod. and teratogenic effects (large dose), human adverse systemic effects (large dose), exp. antineoplastic agent (and in co-administration with methotrexate. LD_{50} (mus, ipr) 2512 mg/kg. XP2071000

*3′-Ac: 3′-*O*-Acetylthymidine*
[21090-30-2]
$C_{12}H_{16}N_2O_6$ 284.268
Constit. of *Cladiella australis*. Prod. by the marine bacterium strain Bio134.
Mp 176°. $[\alpha]_D^{25}$ -21 (c, 0.4 in $CHCl_3$).

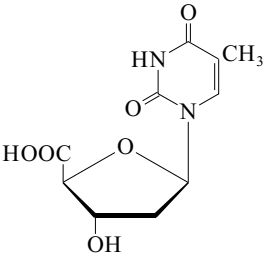
5′-Ac: 5′-O-*Acetylthymidine*
[35898-31-8]
$C_{12}H_{16}N_2O_6$ 284.268
Mp 146°. $[\alpha]_D^{25}$ -9 (c, 0.6 in $CHCl_3$).

[50-88-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 815A; 818A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 370B; 376B (*nmr*)
Fox, J.J. *et al., Adv. Carbohydr. Chem.*, 1959, **14**, 283-380 (*rev*)
Shaw, G. *et al., J.C.S.*, 1959, 50-55 (*synth*)
Lemieux, R.U. *et al., Can. J. Chem.*, 1961, **39**, 110-115; 116-120 (*conformn*)
Ulbricht, T.L.V. *et al., Tet. Lett.*, 1964, 695-698 (*ord*)
Young, D.W. *et al., Acta Cryst. B*, 1969, **25**, 1423-1432 (*cryst struct*)
Gupta, V.S. *et al., Can. J. Chem.*, 1971, **49**, 719-724 (*synth*)
Krugh, T.R. *et al., J.A.C.S.*, 1973, **95**, 4761-4762 (*cmr*)
Davies, D.B. *et al., J.C.S. Perkin 2*, 1975, 1703-1711 (*pmr*)
Komari, T. *et al., Annalen*, 1980, 653-824 (*isol, Acanthaster, ms*)
Mathlouthi, M. *et al., Carbohydr. Res.*, 1984, **134**, 23-38 (*ir, Raman*)
Moyroud, E. *et al., Tetrahedron*, 2000, **56**, 1475-1484 (*synth, pmr, cmr*)
Shaaban, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*3′-Ac, marine, isol*)
Kapustina, I.I. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 109-110 (*Cryptochiton stelleri constit*)
Ahmed, A.F. *et al., J. Chin. Chem. Soc. (Taipei)*, 2006, **53**, 489-494 (*Cladiella acetates*)

Thymidine-5′-carboxylic acid T-338

*1,2-Dideoxy-1-[3,4-dihydro-5-methyl-2,4-dioxo-1(2*H*)-pyrimidinyl]-β-D-*erythro*-pentofuranuronic acid, 9CI*
[3544-99-8]



$C_{10}H_{12}N_2O_6$ 256.215
Constit. of the ascidian *Aplidium fuscum*. Inhibitor of thymidine and thymidylate kinase. Cryst. (H_2O).
Mp 263-265° dec. (250-251°).

Me ester: [50700-64-6]
$C_{11}H_{14}N_2O_6$ 270.241
Mp 247° dec. (237-238°).

Amide: Thymidine-5′-carboxamide
[52995-48-9]
$C_{10}H_{13}N_3O_5$ 255.23
Mp 251-252° dec. (240°).

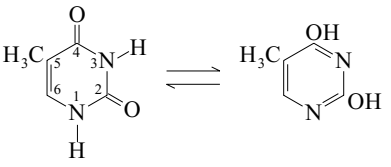
Nitrile: [52995-49-0]
$C_{10}H_{11}N_3O_4$ 237.215
Cryst. Mp 235°.

[37781-47-8]

Moss, G.P. *et al., J.C.S.*, 1963, 1149 (*synth*)
Suck, D. *et al., Biochim. Biophys. Acta*, 1974, **361**, 1 (*cryst struct*)
Baker, J.J. *et al., J. Med. Chem.*, 1974, **17**, 764 (*synth*)
Schinazi, R.F. *et al., J. Med. Chem.*, 1978, **21**, 1141 (*synth*)
Montgomery, J.A. *et al., Nucleic Acids Symp. Ser.*, 1981, **9**, 95 (*synth*)
Dematte, N. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **84**, 11 (*isol*)

Thymine, 8CI T-339

*5-Methyl-2,4(1*H*,3*H*)-pyrimidinedione, 9CI. 4-Hydroxy-5-methyl-2(1*H*)-pyrimidinone, 9CI. 5-Methyluracil. 2,4-Dihydroxy-5-methylpyrimidine. 5-Methyl-2,4-pyrimidinediol*
[65-71-4]
[27942-00-3]



$C_5H_6N_2O_2$ 126.115
Dioxo tautomer predominates in solid, soln. and gas phases. Intermediate tautomers also possible. Component of nucleic acids. Also detected in the free state in bacteria. Used as a 0.25% aq. soln for pptn. sepn. of Hg. Plates (H_2O) or parallelepipeds + H_2O (H_2O). Spar. sol. H_2O (0.6-0.8 g per 100 cm^3).
Mp 326° Mp 340°. pK_{a1} 9.9 (25°).
▶ LD_{50} (mus, orl) 3500 mg/kg. XP2100000
N^1*-(2-Hydroxyethyl):* N^1*-(2-Hydroxyethyl)thymine.* ***Thyminol***
[22441-51-6]
$C_7H_{10}N_2O_3$ 170.168
Isol. from a colonial Zoanthid.
Mp 179-181°. λ_{max} 263 (log ϵ 2.99) (MeOH).

[41935-71-1]

Atta-ur-Rahman, *et al., Nat. Prod. Lett.*, 1999, **13**, 255-261 (*Thyminol*)

Thymosin† T-340

[61512-21-8]
A family of hormone-like peptides. Several thymosins have been isol. and sequenced. Isol. from the thymus gland. Also from perch (*Lateolabrax japonicus*) liver. Regulates immune function. May play a significant part in the initiation of the aging process.

[69521-94-4, 69772-65-2, 77591-33-4, 77642-24-1, 80700-15-8, 80700-16-9, 80893-57-8, 81775-03-3, 81775-04-4, 87397-91-9, 88160-82-1, 89072-27-5, 92480-71-2, 92480-88-1, 113595-86-1, 132821-23-9, 140207-69-8, 141639-18-1]

Goldstein, A.L. *et al., Recent Prog. Horm. Res.*, 1981, **37**, 369 (*rev*)
Oates, K.K. *et al., Trends Pharmacol. Sci.*, 1984, **5**, 347 (*rev*)
Low, T.L.K. *et al., Arch. Biochem. Biophys.*, 1992, **293**, 32 (*isol*)

Thynnin T-341

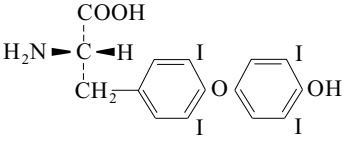
H-Pro-Arg-Arg-Arg-Arg-Glu-Ala-Ser-Arg-Pro-Val-Arg-Arg-Arg-Arg-Arg-Tyr-Arg-Arg-Ser-Thr-Ala-Ala-Arg-Arg-Arg-Arg-Arg-Val-Val-Arg-Arg-Arg-Arg-OH
A mixt. of 4 peptides designated thynnins Y1, Y2, Z1 and Z2. Struct. of Y1 shown, others differ in 1-3 residues. The protamine of tuna fish.

[9063-52-9, 37318-82-4, 50924-08-8, 50924-09-9]

Bretzel, G. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1971, **352**, 1025; 1972, **353**, 933; 1362; 1973, **354**, 543 (*isol, struct*)

Thyroxine, BAN T-342

O-*(4-Hydroxy-3,5-diiodophenyl)-3,5-diiodotyrosine, 9CI. 2-Amino-3-[4-(4-hydroxy-3,5-diiodophenoxy)-3,5-diiodophenyl]propanoic acid. 3-[4-(4-Hydroxy-3,5-diiodophenoxy)]-3,5-diiodophenylalanine. Tetraiodothyronine. T4*



(*S*)*–form*

$C_{15}H_{11}I_4NO_4$ 776.874
^{125}I and ^{131}I labelled compds. are used as radioactive agents.
Log P 3.7 (uncertain value) (calc).

(*R*)-*form*

Dextrothyroxine, BAN. *Deketrol. Many other names*
[51-49-0] Antihyperlipidaemic agent (esp. LDL). Mp 237° dec. $[\alpha]_{Hg}^{21}$ +2.97 (EtOH/NaOH).

Na salt: Dextrothyroxine sodium, INN, USAN. Choloxin
[137-53-1]

▶ Cardiovascular effects reported when used therapeutically. Exp. reprod. and teratogenic effects. XP3582990

(*S*)-*form*

Levothyroxine
[51-48-9]
Isol. from thyroid gland extract and also from proteins of brown algae, *Heterochordaria abietina*, *Undaria pinnatifida*, *Sargassum thunbergii*, *Polysiphonia urceolata*, *Dendrodoa grossularia*, *Porphyra umbilicalis* and *Enteromorpha intestinalis.* Thyromimetic, antihypercholesterolaemic. Marketed drug
Mp 235°. $[\alpha]_{Hg}$ -4.45 (EtOH/NaOH).

▶ Human toxic effects at low oral doses. Exp. reprod. and teratogenic effects. YP2833500

Na salt: Levothyroxine sodium, INN, USAN. Eltroxin. Elthyrone. Euthyrox. Levaxin. Levo-T. Levothroid. Levoxyl. Oroxine. Synthroid. Thyrax. Thyrex. Many other names
[55-03-8]
[25416-65-3]
Triclinic cryst. or cream-coloured powder (as pentahydrate). Mp 207-210° dec. (pentahydrate). $[\alpha]_D^{20}$ -4.4 (c, 3 in EtOH). Component of Liotrix, USAN, Euthroid and Thyrolar.

▶ Adverse human effects when used therapeutically (corresponding with symptoms of hyperthyroidism). LD_{50} (rat, ipr) 20 mg/kg. Exp. reprod. and teratogenic effects. XP3583000

5-Deiodo: O-*(4-Hydroxy-3,5-diiodophenyl)-3-iodotyrosine, 9CI. 3-[4-(4-Hydroxy-3,5-diiodophenoxy)]-3-iodophenylalanine. 2-Amino-3-[4-(4-hydroxy-3,5-diiodophenoxy)-3-iodophenyl]propanoic acid.* ***5-Deiodothyroxine.*** *Triiodothyronine*
[5817-39-0]
$C_{15}H_{12}I_3NO_4$ 650.978
Minor constit. of thyroid extract.

(±)-*form* [300-30-1]
Needles by addn. of AcOH to alk. EtOH aq. soln. V. spar. sol. H_2O; insol. org. solvs.; sol. NH_3 and alc. alkalis.

Me ester:
$C_{16}H_{13}I_4NO_4$ 790.901
Prisms (EtOH aq.). Spar. sol. H_2O most org. solvs. Mp 156°.

Me ester; hydrochloride:
Needles (EtOH/HCl). Mp 221.5°.

N-*Ac:*
$C_{17}H_{13}I_4NO_5$ 818.911
Cryst. (AcOH aq.). Mp 210-215° dec.

N-*Di-Ac, Et ester:*
$C_{21}H_{19}I_4NO_6$ 889.002
Needles. Mp 216-217° (230°).

Me ether, Me ester:
$C_{17}H_{15}I_4NO_4$ 804.928
Mp 224°.

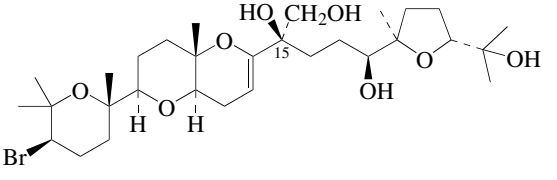
Me ether, N-*Ac, Me ester:*
$C_{19}H_{17}I_4NO_5$ 846.965
Plates (anisole). Mp 208-209° dec.

[6106-07-6, 7019-69-4, 7054-08-2, 8065-29-0, 24486-40-6, 25416-65-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 254A; 254B; 254C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1186B (*nmr*)
Harington, C.R. *et al., Biochem. J.*, 1926, **20**, 293; 1927, **21**, 169; 1928, **22**, 1429; 1436; 1929, **23**, 1178; 1930, **24**, 456; 1934, **28**, 68
Chalmers, J.R. *et al., J.C.S.*, 1949, 3424-3433 (*synth*)
Hems, B.A. *et al., Chem. Ind. (London)*, 1950, 663
Joel, N. *et al., Acta Cryst.*, 1951, **4**, 283 (*cryst struct*)
Coulson, C.B. *et al., Chem. Ind. (London)*, 1953, 997-998 (*occur*)
Coulson, C.B. *et al., CA*, 1954, **48**, 2838 (*isol*)
Roche, J. *et al., Biochim. Biophys. Acta*, 1956, **19**, 308-317 (*5-Deiodothyroxine*)
Nahm, H. *et al., Chem. Ber.*, 1963, **96**, 1 (*synth*)
Amaral, A.D. *et al., CA*, 1972, **77**, 111749 (*occur*)
Post, A. *et al., Anal. Profiles Drug Subst.*, 1976, **5**, 225 (*rev, Na salt, prop, synth, metab*)
Ito, K. *et al., CA*, 1977, **86**, 3897 (*occur*)
Cody, V. *et al., Acta Cryst. B*, 1981, **37**, 1685-1689 (*conformn, cryst struct*)
Hay, I.D. *et al., J. Chromatogr.*, 1981, **226**, 383-390 (*resoln*)
De Mayer, P. *et al., Thyroid Dis.*, 1983, 23 (*detn*)
Dratman, M.B. *et al., Neurol. Neurobiol.*, 1984, **85**, 425 (*use*)
Ong, R.L. *et al., Biochem. Int.*, 1985, **10**, 803-811 (*nmr, conformn*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 3429; 3430
Bell, N.V. *et al., Can. J. Chem.*, 1997, **75**, 873-883 (*synth, biosynth*)
Salamonczyk, G.M. *et al., Tet. Lett.*, 1997, **38**, 6965-6968 (*synth*)
Evans, D.A. *et al., Tet. Lett.*, 1998, **39**, 2937-2940 (*synth*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1497
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LEQ300; TFZ275, R; SKJ300

Thyrsenol A T-343

[188826-89-3]



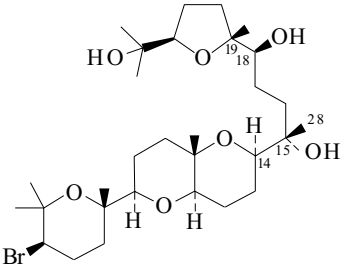
$C_{30}H_{51}BrO_8$ 619.632
Constit. of *Laurencia viridis.* Amorph. solid. $[\alpha]_D^{25}$ +12.9 (c, 0.69 in $CHCl_3$).

15-Epimer: ***Thyrsenol B***
[188826-90-6]
$C_{30}H_{51}BrO_8$ 619.632
Constit. of *Laurencia viridis.* Amorph. solid. $[\alpha]_D^{25}$ -1.1 (c, 0.26 in $CHCl_3$).

Norte, M. *et al., Tetrahedron*, 1997, **53**, 3173-3178 (*isol, pmr, cmr*)

Thyrsiferol T-344

[66873-39-0]



$C_{30}H_{53}BrO_7$ 605.648
Config. at C-14 and C-15 wrongly drawn in early references. Metab. of *Laurencia thyrsifera*. Sol. MeOH, $CHCl_3$.

23-Ac: [96304-95-9]
$C_{32}H_{55}BrO_8$ 647.686
Constit. of *Laurencia obtusa*. Cytotoxic agent. Cryst. (MeOH aq.).
Mp 118-119°. $[\alpha]_D^{29}$ +1.99 (c, 4.4 in $CHCl_4$).

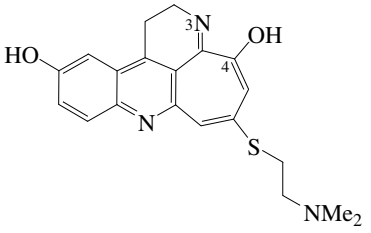
18,19-Diepimer: ***Venustatriol***
[105880-10-2]
$C_{30}H_{53}BrO_7$ 605.648
From *Laurencia venusta*. Antiviral agent. Cryst.
Mp 161.5°. $[\alpha]_D^{20}$ +9.4 (c, 3.2 in $CHCl_3$).

15-Deoxy-15,16-didehydro(Z): See 15-Anhydrothyrsiferol, A-508

Blunt, J.W. *et al., Tet. Lett.*, 1978, 69 (*isol, struct*)
Suzuki, T. *et al., Tet. Lett.*, 1985, **26**, 1329 (*isol*)
Sakami, S. *et al., Tet. Lett.*, 1986, **27**, 4287 (*isol, cryst struct*)
Hashimoto, M. *et al., J.O.C.*, 1990, **55**, 5088 (*synth*)

Tintamine T-345

[211311-10-3]

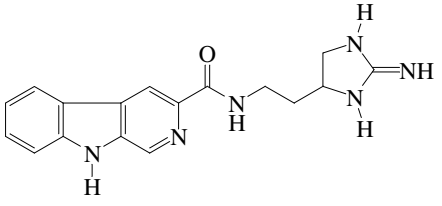


$C_{20}H_{21}N_3O_2S$ 367.471

Numbered by analogy with pyridoacridine alkaloids to which it appears to be related. Tautomeric with the 4-oxo-3*NH*-form. Alkaloid from the tunicate *Cystodytes violatinctus*. λ_{max} 265 (log ϵ 3.68); 308 (log ϵ 3.67) (MeOH) (as di-Ac).

Koren-Goldshlager, G. *et al., J.O.C.*, 1998, **63**, 4601-4603 (*isol, uv, ir, pmr, cmr*)

Tiruchanduramine T-346



$C_{17}H_{18}N_6O$ 322.369

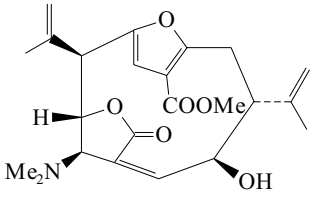
(ξ)-*form*

Alkaloid from the ascidian *Synoicum macroglossum*. α-Glucosidase inhibitor. Semisolid. $[\alpha]_D$ +31 (c, 0.5 in MeOH). λ_{max} 215; 234; 270; 334; 347 (MeOH).

Ravinder, K. *et al., Tet. Lett.*, 2005, **46**, 5475-5478 (*isol, synth, pmr, cmr*)

Tobagolide T-347

[126596-06-3]



$C_{23}H_{29}NO_6$ 415.485

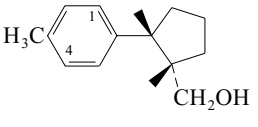
Metab. of *Pseudopterogorgia acerosa*. Cryst.

Mp 165-166°. $[\alpha]_D$ -130.5. λ_{max} 235 (ϵ 4000); 275 (ϵ 2000) (MeOH) (Derep).

Chan, W.R. *et al., J.O.C.*, 1991, **56**, 1773-1776

Tochuinol T-348

1,2-Dimethyl-2-(4-methylphenyl)cyclopentanemethanol, 9CI. 12-Hydroxycuparene



$C_{15}H_{22}O$ 218.338

*Ac: **Tochuinyl acetate***

[111621-35-3]

$C_{17}H_{24}O_2$ 260.375

Constit. of *Tochuina tetraquetra*. Oil. $[\alpha]_D^{25}$ -42.5 (c, 1.09 in CH_2Cl_2).

*1,4-Dihydro, Ac: **Dihydrotochuinyl acetate***

[111621-36-4]

$C_{17}H_{26}O_2$ 262.391

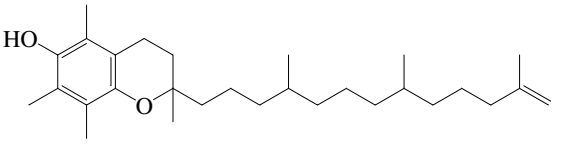
Constit. of *Tochuina tetraquetra*. Oil. $[\alpha]_D^{25}$ -29.3 (c, 1.11 in CH_2Cl_2).

Williams, D.E. *et al., Can. J. Chem.*, 1987, **65**, 2244
Taber, D.F. *et al., J.O.C.*, 1992, **57**, 436 (*synth*)
Srikrishna, A. *et al., Tetrahedron*, 1998, **54**, 8133-8140 (*synth*)
Srikrishna, A. *et al., Tet. Lett.*, 2002, **43**, 151-156 (*synth*)
Paul, T. *et al., ARKIVOC*, 2003, **ix**, 104-114 (*synth*)
Paul, T. *et al., Tet. Lett.*, 2003, **44**, 737-740 (*synth*)
Acherar, S. *et al., Tetrahedron*, 2004, **60**, 5907-5912 (*synth*)

α-Tocomonoenol T-349

Marine derived tocopherol

[205323-14-4]



$C_{29}H_{48}O_2$ 428.697

Constit. of eggs of Pacific salmon *Oncorhynchus keta*.

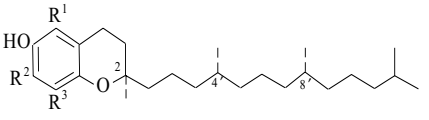
Yamamoto, Y. *et al., J. Nat. Prod.*, 1999, **62**, 1685-1687 (*isol, pmr, cmr*)

α-Tocopherol T-350

3,4-Dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-ol, 9CI. 5,7,8-Trimethyltocol. Vitamin E†. Antisterility vitamin. Ephynal. Syntopherol. Profecundin. E307

[59-02-9]

[364-50-1, 1431-54-5, 2074-53-5, 10191-41-0, 43119-47-7]



$R^1 = R^2 = R^3 = CH_3$

$C_{29}H_{50}O_2$ 430.713

Constit. of many vegetable oils. Dietary supplement and nutrient. Antioxidant, prevents oxidative damage to cell membranes. Possesses antisterility props. Pharmaceutical excipient. Viscous oil, cryst. (MeOH at -35°). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 2.5-3.5°. $Bp_{0.03}$ 140°. $[\alpha]_D^{25}$ +0.65 (EtOH). Log P 12.15 (uncertain value) (calc). Thermostable. λ_{max} 294 (E1%/1cm 71) (MeOH) (Berdy). λ_{max} 292 (EtOH) (Berdy).

► DJ2900000

*Ac: Alfacol. Fertilvit. Tocophrin. **α-Tocopherol acetate**. Vitamin E acetate. Combinal E. Many other names*

[58-95-7]

[54-22-8, 7695-91-2, 52225-20-4]

$C_{31}H_{52}O_3$ 472.75

Vitamin E supplement. Oil. Mp 26.5-27.5°. $Bp_{0.02}$ 205° (bath). $[\alpha]_D^{25}$ +3.03 (c, 5 in EtOH). Log P 12.15 (uncertain value) (calc).

► GP8588000

*3-Carboxypropanoyl: **α-Tocopherol succinate**. Many other names*

[4345-03-3]

$C_{33}H_{54}O_5$ 530.787

Vitamin E supplement. Needles (petrol). Mp 76-77°. Log P 11.82 (uncertain value) (calc).

3-Pyridinecarbonyl: ***α-Tocopherol nicotinate****. Tocopheryl nicotinate. Vitamin E nicotinate. Many other names*
[16676-75-8]
[51898-34-1]
$C_{35}H_{53}NO_3$ 535.809
Vasodilator. Yellow oil or solid. Mp 38°.

p-*Phenylazobenzoyl:*
Cryst. Mp 62-64°. $[\alpha]_{600}$ +6.99 (c, 3.33 in $CHCl_3$).

Ester with polyethylene glycol succinate: ***Tocophersolan, USAN****. Tocofersolan, INN*
[30999-06-5] Vitamin E supplement, antioxidant.

3,4-Didehydro: ***Dehydro-α-tocopherol***
[72420-55-4]
$C_{29}H_{48}O_2$ 428.697
Constit. of *Stemona collinsae*. Oil. $[\alpha]_D^{25}$ -18 (c, 0.1 in MeOH).
λ_{max} 232; 272; 282; 332 (MeOH).

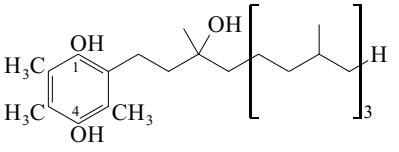
8′,12′-Dihydroxy: [159860-32-9]
$C_{29}H_{50}O_4$ 462.712
Constit. of *Sinularia mayi*. Oil. $[\alpha]_D$ -6 (c, 0.5 in $CDCl_3$).

[1406-66-2, 17407-37-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 330A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1326A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1387B (*ir*)
Baxter, J.G. *et al., J.A.C.S.*, 1943, **65**, 918-924 (*succinate*)
Praill, P.F. *et al., J.C.S.*, 1959, 3100 (*esters*)
Robeson, C.D. *et al., J.A.C.S.*, 1962, **84**, 3196-3197 (*isol*)
Meyer, H. *et al., Helv. Chim. Acta*, 1963, **46**, 650-671; 963-982 (*synth, abs config*)
Fr. Pat., 1968, M6320; *CA*, **74**, 79582 (*nicotinate*)
Nakamura, A. *et al., Chem. Pharm. Bull.*, 1971, **19**, 2318-2324 (*synth*)
Scheppele, S.E. *et al., Lipids*, 1972, **7**, 297-304 (*ms*)
Rudy, B.C. *et al., Anal. Profiles Drug Subst.*, 1974, **3**, 111-126 (*bibl*)
Gatlin, L.A. *et al., Drug Intell. Clin. Pharm.*, 1975, **9**, 655-656 (*Tocophersolan, rev*)
Scott, J.W. *et al., Helv. Chim. Acta*, 1976, **59**, 290-306 (*synth*)
Cohen, N. *et al., J.O.C.*, 1976, **41**, 3505-3511; 1992, **57**, 5783-5785 (*synth, bibl*)
Schultz, G. *et al., Phytochemistry*, 1976, **15**, 1383-1386 (*biosynth*)
Matsuo, M. *et al., Tetrahedron*, 1976, **32**, 229-231 (*pmr*)
Nakamura, T. *et al., J. Nutr. Sci. Vitaminol.*, 1978, **24**, 459-469 (*pharmacol, esters*)
Chan, K.-K. *et al., J.O.C.*, 1978, **43**, 3435-3440 (*synth*)
Igarashi, T. *et al., J. Nutr. Sci. Vitaminol.*, 1979, **25**, 159-173 (*nicotinate, pharmacol*)
Cohen, N. *et al., J.A.C.S.*, 1979, **101**, 6710-6716 (*synth*)
Akkerman, J.M. *et al., J.C.S. Perkin 1*, 1979, 2124-2129 (*synth*)
Urano, S. *et al., Chem. Pharm. Bull.*, 1980, **28**, 1992-1998 (*cmr*)
Olson, G.L. *et al., J.O.C.*, 1980, **45**, 803-805 (*synth*)
Cohen, N. *et al., Helv. Chim. Acta*, 1981, **64**, 1158-1173 (*synth, isom*)
Suzuki, N. *et al., J. Nutr. Sci. Vitaminol.*, 1983, **29**, 93-103 (*nicotinate, metab*)
Ballester-Rodes, M. *et al., Synth. Commun.*, 1984, 14, 515-520 (*nicotinate, synth*)
Burton, G.W. *et al., Acc. Chem. Res.*, 1986, **19**, 194-201 (*rev, props*)
Inoue, S. *et al., J.O.C.*, 1987, **52**, 5495-5497 (*synth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 7835; 7936; 8009
Furuya, T. *et al., Phytochemistry*, 1987, **26**, 2741-2747 (*biosynth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, TGJ050; TGJ060; VSZ450
Hübscher, M. *et al., Helv. Chim. Acta*, 1990, **73**, 782-789; 1068-1086 (*bibl, hplc*)
Bourgeois, C. *et al., Determination of Vitamin E, Tocopherols and Tocotrienols*, Elsevier, 1992, (*book*)
Berger, S. *et al., Annalen*, 1994, 1239-1241 (*cmr*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 12-14
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1994, 494-495 (*8′,12′-Dihydroxy-α-tocopherol, isol*)
Matsui, M. *et al., Bull. Chem. Soc. Jpn.*, 1995, **68**, 3569-3571; 1996, **69**, 137-139 (*synth*)
Chen, C.Y. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2153-2156 (*synth*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1391
Huo, S. *et al., Org. Lett.*, 2001, 3253-3256 (*synth*)
Odinokov, V.N. *et al., ARKIVOC*, 2003, **xiii**, 101-118 (*synth*)
Mazzini, F. *et al., Eur. J. Org. Chem.*, 2004, 4864-4869 (*synth*)
Brem, B. *et al., Phytochemistry*, 2004, **65**, 2719-2729 (*Dehydro-α-tocopherol*)
Tietze, L.F. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 257-259 (*synth*)
Sen, C.K. *et al., Life Sci.*, 2006, **78**, 2088-2098 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TGJ050; TGJ060; VSZ450

α-Tocopherolhydroquinone T-351

α-Tocopheryl hydroquinone
[14745-36-9]



$C_{29}H_{52}O_3$ 448.728
Viscous, golden-yellow oil.

Tri-Ac:
Cryst. Mp 75°.

1,4-Quinone: ***α-Tocopherolquinone****. α-Tocoquinone. Eutrophyl. Ipotensil. Metorena. Tensiopress. Trimina. Vitapressina. D 178. α-Tocopheryl quinone*
[7559-04-8]
$C_{29}H_{50}O_3$ 446.712
Isol. from spinach (*Spinacia oleracea*) chloroplasts, spadix of *Arum maculatum*, green alga *Codium iyengarii* and many other plant sources. Antihypertensive agent. Platelet aggregation inhibitor. Shows cytotoxic and phytotoxic activities. Viscous, golden-yellow oil. $Bp_{0.002}$ 120°. Log P 9.62 (uncertain value) (calc).

▶ DK5170000

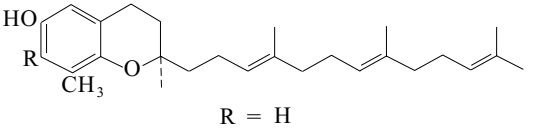
1,4-Quinone, Me ether: ***α-Tocopherolquinone methyl ether***
[137551-40-7]
$C_{30}H_{52}O_3$ 460.739
Constit. of *Psoralea plicata*. Yellow oil. $[\alpha]_D$ +15 (c, 1.2 in $CHCl_3$).

*1,4-Quinone, 11′ξ,14′*S*-dihydroxy:* ***3′,11′,14′-Trihydroxy-α-tocopherolquinone***
$C_{29}H_{50}O_5$ 478.711
Constit. of *Sinularia mayi*. Cryst.
Mp 113-114°. $[\alpha]_D$ -4 (c, 0.34 in $CDCl_3$).

Tishler, M. *et al., J.A.C.S.*, 1941, **63**, 1532 (*struct*)
MacKenzie, J.B. *et al., J. Biol. Chem.*, 1950, **183**, 655 (*props*)
Cairella, M. *et al., Clin. Ter. (Rome)*, 1964, **31**, 278 (*pharmacol*)
Chow, C.K. *et al., Lipids*, 1967, **2**, 390 (*metab*)
Whistace, J. *et al., Biochem. J.*, 1968, **109**, 577 (*biosynth*)
Kleeva, L.P. *et al., Zh. Org. Khim.*, 1968, **4**, 1171 (*synth*)
Rao, G.H.R. *et al., Prog. Lipid Res.*, 1981, **20**, 549 (*pharmacol*)
Rasool, N. *et al., Phytochemistry*, 1991, **30**, 2800 (*α-Tocopherolquinone methyl ether*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1422
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1994, 494 (*3′,11′,14′-Trihydroxy-α-tocopherol quinone*)
Shaik-Ali, M. *et al., Nat. Prod. Sci.*, 2000, **6**, 61-65 (*isol, activity*)

δ-Tocotrienol T-352

*3,4-Dihydro-2,8-dimethyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-2*H*-1-benzopyran-6-ol, 9CI. 2,8-Dimethyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-6-chromanol. 8-Methyltocotrienol*
[25612-59-3]



R = H

$C_{27}H_{40}O_2$ 396.612
Constit. of palm oil and *Iryanthera grandis*. Component of *Sargassum tortile*, settling hormone for hydrocoan larvae. Shows anticancer props. Affects blood lipid profile. Oil. Poorly sol. hexane.

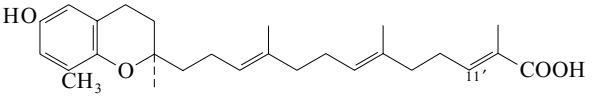
11′,12′-Epoxide: ***Epoxy-δ-tocotrienol***. *δ-Tocotrienol epoxide*
[57576-80-4]
$C_{27}H_{40}O_3$ 412.611
Isol. from the alga *Sargassum tortile.*

5-Formyl: ***5-Formyl-δ-tocotrienol***
[815577-43-6]
$C_{28}H_{40}O_3$ 424.622
Constit. of *Garcinia virgata*. Oil. $[\alpha]_D^{25}$ -11.1 (c, 0.18 in MeOH). λ_{max} 226 (log ϵ 2.1); 241 (log ϵ 2.3); 278 (log ϵ 0.4); 326 (log ϵ 0.4) (MeOH).

7-Formyl: ***7-Formyl-δ-tocotrienol***
[815577-44-7]
$C_{28}H_{40}O_3$ 424.622
Constit. of *Garcinia virgata*.

Dunphy, P.J. *et al., Nature (London)*, 1965, **207**, 521 (*isol*)
Whittle, K.J. *et al., Biochem. J.*, 1966, **100**, 138 (*ir*)
Kato, T. *et al., Chem. Lett.*, 1975, 335 (*Epoxytocotrienol*)
Kato, T. *et al., Experientia*, 1975, **31**, 433-434 (*isol*)
Vieira, P.C. *et al., Phytochemistry*, 1983, **22**, 2281 (*isol, pmr*)
Guthrie, N. *et al., Handbook of Nutraceuticals and Functional Foods*, (ed. Wildman, R.E.C.), CRC Press, 2001, 269-280
Merza, J. *et al., Phytochemistry*, 2004, **65**, 2915-2920 (*Formyltocotrienols*)
Sen, C.K. *et al., Life Sci.*, 2006, **78**, 2088-2098 (*rev*)

δ-Tocotrienoloic acid T-353



(11′*E*)*–form*

$C_{27}H_{38}O_4$ 426.595

(11′*E*)-*form*
Garcinoic acid
[91893-83-3]
Constit. of *Clusia grandiflora*, *Tovomitopsis psychotriifolia* and *Garcinia kola*. Antibacterial agent. Oil.

13′-Aldehyde: ***Garcinal***
$C_{27}H_{38}O_3$ 410.595
Constit. of the seeds of *Garcinia kola*. Pale yellow oil. Racemic. λ_{max} 295 (ϵ 3300) (MeOH).

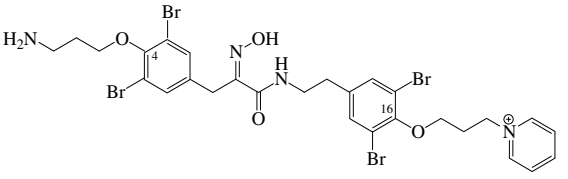
*3,4-Didehydro: 13-(6-Hydroxy-2,8-dimethyl-2*H*-1-benzopyran-2-yl)-2,6,10-trimethyl-2,6,10-tridecatrienoic acid*
$C_{27}H_{36}O_4$ 424.579
Constit. of the brown alga *Desmarestia menziesii*. Pale brown oil (as Me ester). $[\alpha]_D^{25}$ +1.2 (c, 1 in $CHCl_3$) (Me ester). C-2 config. not determined.

*3,4-Didehydro, 13′-alcohol: 2-(13-Hydroxy-4,8,12-trimethyl-3,7,11-tridecatrienyl)-2,8-dimethyl-2*H*-1-benzopyran-6-ol*
$C_{27}H_{38}O_3$ 410.595
Constit. of the brown alga *Desmarestia menziesii*. Pale brown oil (as di-Ac). $[\alpha]_D^{25}$ +1.5 (c, 0.8 in $CHCl_3$) (di-Ac).

(11′*Z*)-*form* [91893-89-9]
Constit. of *Clusia grandiflora*.
Oil. $[\alpha]_D$ -3 (c, 1.2 in $CHCl_3$).

Delle Monache, F. *et al., Gazz. Chim. Ital.*, 1984, **114**, 135 (*isol, pmr, cmr*)
Setzer, W.N. *et al., Planta Med.*, 1995, **61**, 275 (*isol, cmr, props*)
Terashima, K. *et al., Heterocycles*, 1997, **45**, 1559-1566 (*Garcinoic acid, Garcinal*)
Davyt, D. *et al., Nat. Prod. Lett.*, 1997, **9**, 305-312 (*3,4-didehydro derivs*)
Maloney, D.J. *et al., Org. Lett.*, 2005, **7**, 4297-4300 (*synth*)

Tokaradine A T-354



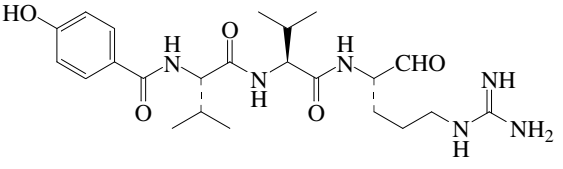
$C_{28}H_{31}Br_4N_4O_4^{\oplus}$ 807.193
Quaternary alkaloid from *Pseudoceratina purpurea*. Amorph. yellow solid. Counterion not specified. λ_{max} 216 (ϵ 21800); 258 (sh) (ϵ 4000) (MeOH).

Regioisomer: ***Tokaradine B***
$C_{28}H_{31}Br_4N_4O_4^{\oplus}$ 807.193
Quaternary alkaloid from *Pseudoceratina purpurea*. Amorph. yellow solid. Has the groups attached to C-4 and C-16 interchanged. Counterion not specified. λ_{max} 214 (ϵ 20600); 258 (sh) (ϵ 3800) (MeOH).

Fusetani, N. *et al., Tetrahedron*, 2001, **57**, 7507-7511

Tokaramide A T-355

[258273-52-8]

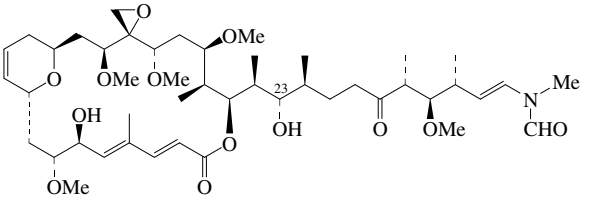


$C_{23}H_{36}N_6O_5$ 476.575
Isol. from the sponge *Theonella* aff. *mirabilis.* Cathepsin B inhibitor. Pale yellow solid. $[\alpha]_D^{29}$ -19 (c, 0.06 in MeOH). λ_{max} 255 (ϵ 5950) (MeOH).

Fusetani, N. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 3397-3402 (*isol, pmr, cmr, activity*)

Tolytoxin T-356

[127999-44-4]



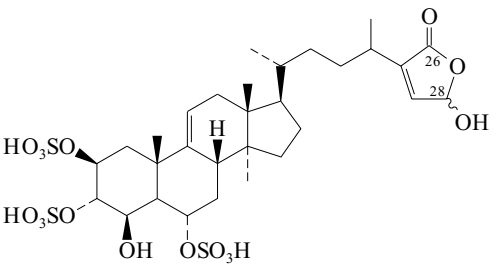
$C_{46}H_{75}NO_{13}$ 850.097
Macrolide antibiotic. Related to Scytophycin A. Isol. from *Tolypothrix conglutinata* var. *colorata* and *Scytonema* spp. Shows antileukaemic props. Antifungal agent and cytotoxin. Amorph. solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 261 (ϵ 27000) (EtOH) (Derep). λ_{max} 264 (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 1.5 mg/kg.

23-Ac: ***23-O-Acetyltolytoxin***. *Tolytoxin 23-acetate*
$C_{48}H_{77}NO_{14}$ 892.135
Isol. from the mollusc *Philinopsis speciosa*. Amorph. solid. $[\alpha]_D^{31}$ -45 (c, 1.36 in MeOH). λ_{max} 208 (ϵ 14100); 212 (ϵ 12900); 269 (ϵ 150); 284 (ϵ 130) (MeOH).

Moore, R.E. *et al., Pure Appl. Chem.*, 1986, **58**, 263-271 (*isol*)
Carmeli, S. *et al., J. Nat. Prod.*, 1990, **53**, 1533 (*pmr, cmr, struct*)
Carmeli, S. *et al., Tet. Lett.*, 1993, **34**, 5571-5574 (*biosynth*)
Nakao, Y. *et al., J.O.C.*, 1998, **63**, 3272-3280 (*23-Acetyltolytoxin*)

Topsentiasterol sulfate A T-357

[157622-57-6]



$C_{30}H_{46}O_{16}S_3$ 758.882
Constit. of a *Topsentia* sp.
$[\alpha]_D$ +48.4 (c, 0.2 in MeOH) (as tri-Na salt).

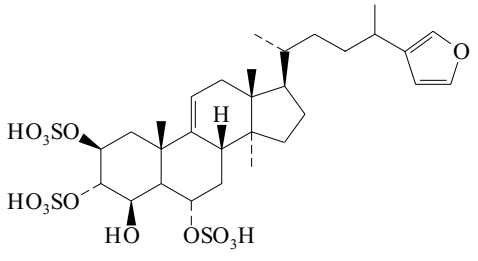
28-Oxo, 26-alcohol: ***Topsentiasterol sulfate B***
[157622-58-7]
$C_{30}H_{46}O_{16}S_3$ 758.882
Constit. of a *Topsentia* sp.
$[\alpha]_D$ +13.1 (c, 0.1 in MeOH) (as tri-Na salt).

28-Deoxy: ***Topsentiasterol sulfate C***
[157622-59-8]
$C_{30}H_{46}O_{15}S_3$ 742.882
Constit. of a *Topsentia* sp.
$[\alpha]_D$ +24.8 (c, 0.1 in MeOH) (as tri-Na salt).

Fusetani, N. *et al., Tetrahedron*, 1994, **50**, 7765-7770 (*isol, pmr, cmr, struct*)

Topsentiasterol sulfate D T-358

[157622-60-1]

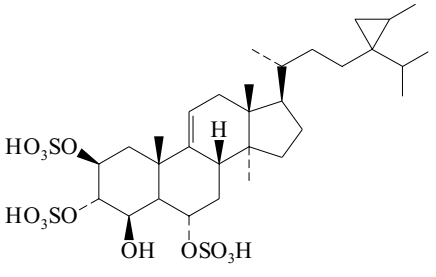


$C_{30}H_{46}O_{14}S_3$ 726.883
Constit. of *Topsentia* sp.
$[\alpha]_D$ +9.3 (c, 0.1 in MeOH) (as tri-Na salt).

Fusetani, N. *et al., Tetrahedron*, 1994, **50**, 7765-7770 (*isol, pmr, cmr, struct*)

Topsentiasterol sulfate E T-359

[157622-61-2]

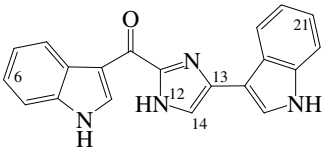


$C_{31}H_{52}O_{13}S_3$ 728.942
Constit. of a *Topsentia* sp.
$[\alpha]_D$ +58.3 (c, 0.1 in MeOH).

Fusetani, N. *et al., Tetrahedron*, 1994, **50**, 7765-7770 (*isol, pmr, cmr, struct*)

Topsentin A T-360

1H-Indol-3-yl[4-(1H-indol-3-yl)-1H-imidazol-2-yl]methanone, 9CI. 4-(3-Indolyl)-2-(3-indolylcarbonyl)imidazole. Deoxytopsentin
[112515-42-1]



$C_{20}H_{14}N_4O$ 326.357
Shows tautomerism of the imidazole ring in soln., tautomer shown predominates. Naming and numbering systems vary. Alkaloid from the Mediterranean sponge *Topsentia genitrix*. Shows weak piscicidal activity.
Mp 290-292°.

13,14-Dihydro: ***Topsentin D***
[122889-35-4]
$C_{20}H_{16}N_4O$ 328.373
Alkaloid from *Topsentia* sp.

6-Hydroxy: ***Topsentin B1***. *Topsentin*
[112515-43-2]
$C_{20}H_{14}N_4O_2$ 342.356
Alkaloid from *Topsentia genitrix* and from the Caribbean deep-sea sponge *Spongosorites* sp. Weak piscicide. Amorph. bright yellow solid.
Mp 270°. λ_{max} 208 (ϵ 1800); 246 (ϵ 5100); 300 (ϵ 3400); 375 (ϵ 3100) (EtOH/KOH) (Derep). λ_{max} 202 (ϵ 41000); 220 (sh) (ϵ 31500); 240 (sh) (ϵ 19200); 280 (ϵ 13500); 378 (ϵ 17300) (95% EtOH) (Derep).

▶ PC4957000

6-Bromo: 6-Bromotopsentin A. ***Isobromodeoxytopsentin***
[223596-72-3]
$C_{20}H_{13}BrN_4O$ 405.253
Alkaloid from *Spongosorites genitrix*. Moderate cytotoxic agent. Amorph. yellow solid.
Mp 225-230°. λ_{max} 213 (log ϵ 4.41); 252 (log ϵ 4.04); 280 (log ϵ 4.06); 375 (log ϵ 4.02) (MeOH).

6-Bromo, 13,14-dihydro: ***Dihydrodeoxybromotopsentin***
[116747-40-1]
$C_{20}H_{15}BrN_4O$ 407.269
Isol. from a sponge tentatively identified as *Spongosorites* sp., also from *Topsentia* sp. and *Rhaphisia lacazei*. Antiviral and anti-tumour agent. Amorph. yellow powder. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{24}$ +198 (c, 2.0 in MeOH). λ_{max} 196 (ϵ 102000); 198 (ϵ 29300); 214 (ϵ 34000); 215 (ϵ 76000); 274 (ϵ 8800); 294 (ϵ 109000); 328 (ϵ 5700); 330 (ϵ 7600) (MeOH) (Berdy).

6-Bromo, 22-hydroxy: ***Isobromotopsentin***
[173220-97-8]
$C_{20}H_{13}BrN_4O_2$ 421.252
Alkaloid from *Spongosorites* sp. Amorph. yellow solid.
Mp 225-228° dec. λ_{max} 207 (ϵ 11150); 284 (ϵ 2900); 415 (ϵ 4260) (EtOH).

21-Bromo: 21-Bromotopsentin A. ***Bromodeoxytopsentin***
[180633-55-0]
$C_{20}H_{13}BrN_4O$ 405.253
Alkaloid from *Spongosorites genitrix* and *Rhaphisia lacazei*. Moderate cytotoxic agent. Amorph. yellow solid.
Mp 240-243°. λ_{max} 209 (log ϵ 4.61); 235 (log ϵ 4.4); 250 (sh) (log ϵ 4.36); 367 (log ϵ 4.17) (MeOH).

21-Bromo, 6-hydroxy: ***Topsentin B2***. *Bromotopsentin*
[112515-44-3]
$C_{20}H_{13}BrN_4O_2$ 421.252
Alkaloid from *Topsentia genitrix, Spongosorites* sp. and another sponge *Hexadella* sp. Shows antitumour and antiviral activity. Weak piscicide. Bright yellow cryst. ($CHCl_3$/MeOH) or yellow-green oil. Sol. MeOH, CH_2Cl_2.
Mp 260° Mp 296-297°. λ_{max} 209 (ϵ 19000); 234 (sh) (ϵ 9700); 300 (ϵ 4200); 375 (ϵ 3500) (EtOH/KOH) (Derep). λ_{max} 208 (ϵ 40000); 237 (ϵ 28800); 254 (sh) (ϵ 22300); 286 (ϵ 15300); 378 (ϵ 17200)

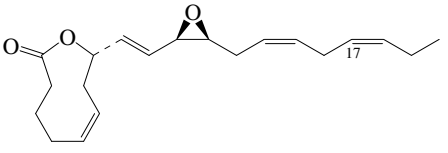
(95% EtOH) (Derep). λ_{max} 208 (ϵ 40000); 237 (ϵ 28800); 286 (ϵ 15300); 328 (ϵ 17200); 382 (ϵ 15500) (EtOH) (Berdy).

6,21-Dibromo: 6,21-Dibromotopsentin A. ***Bromodeoxytopsentin***
$C_{20}H_{12}Br_2N_4O$ 484.149
Alkaloid from the sponge *Spongosorites* sp. Amorph. yellow powder.

6,21-Dibromo, 13,14-dihydro, N^{12}*-Me:* ***Topsentin C***
[128364-30-7]
$C_{21}H_{16}Br_2N_4O$ 500.192
Alkaloid from the Pacific Ocean sponge *Hexadella* sp. Pale yellow powder.

Braekman, J.C. *et al., Bull. Soc. Chim. Belg.*, 1987, **96**, 809-812 (*synth, Topsentin A*)
Bartik, K. *et al., Can. J. Chem.*, 1987, **65**, 2118-2121 (*isol, uv, ir, pmr, cmr, ms, struct, Topsentins A,B,B2*)
Tsujii, S. *et al., J.O.C.*, 1988, **53**, 5446-5453 (*isol, uv, ir, pmr, cmr, ms, synth, Topsentin, Bromotopsentin, Dihydrodeoxybromotopsentin*)
Morris, S.A. *et al., Can. J. Chem.*, 1989, **67**, 677-681 (*isol, uv, ir, pmr, cmr, ms, Topsentin B2*)
Morris, S.A. *et al., Tetrahedron*, 1990, **46**, 715-720 (*Topsentin C*)
Murray, L.M. *et al., Aust. J. Chem.*, 1995, **48**, 2053-2058 (*Isobromotopsentin*)
Achab, S. *et al., Tet. Lett.*, 1996, **37**, 5503-5506 (*synth, Topsentin, Deoxytopsentin, Bromotopsentin*)
Kawasaki, I. *et al., Heterocycles*, 1998, **48**, 1887-1901 (*synth*)
Shin, J. *et al., J. Nat. Prod.*, 1999, **62**, 647-649 (*Bromodeoxytopsentin, Isobromodeoxytopsentin*)
Casapullo, A. *et al., J. Nat. Prod.*, 2000, **63**, 447-451 (*isol*)
Miyake, F.Y. *et al., Org. Lett.*, 2000, **2**, 2121-2123 (*synth*)
Bao, B. *et al., J. Nat. Prod.*, 2005, **68**, 711-715 (*Dibromodeoxytopsentin*)

Topsentolide A_1 T-361



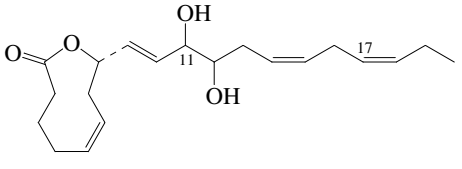
Relative Configuration

$C_{20}H_{28}O_3$ 316.439
Constit. of a *Topsentia* sp. Moderately cytotoxic. Oil. $[\alpha]_D^{24}$ +59.4 (c, 0.11 in MeOH).

17,18-Dihydro: ***Topsentolide A_2***
$C_{20}H_{30}O_3$ 318.455
Constit. of a *Topsentia* sp. Oil. $[\alpha]_D^{24}$ +84.6 (c, 0.27 in MeOH).

Luo, X. *et al., J. Nat. Prod.*, 2006, **69**, 567-571 (*isol, pmr, cmr*)

Topsentolide B_1 T-362



$C_{20}H_{30}O_4$ 334.455
Constit. of a *Topsentia* sp. Moderately cytotoxic. Oil. $[\alpha]_D^{23}$ +38.2 (c, 0.27 in MeOH). Possesses *threo*-config. at C-11/C-12.

17,18-Dihydro: ***Topsentolide B_2***
$C_{20}H_{32}O_4$ 336.47
Constit. of a *Topsentia* sp. Oil. $[\alpha]_D^{23}$ +9.8 (c, 0.27 in MeOH). Possesses *threo*-config.

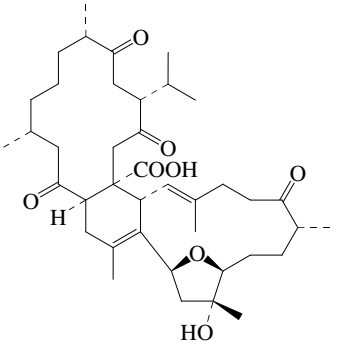
Stereoisomer, 11-Me ether: ***Topsentolide C_1***
$C_{21}H_{32}O_4$ 348.481
Constit. of a *Topsentia* sp. Oil. $[\alpha]_D^{23}$ +40.8 (c, 0.27 in MeOH). Possesses (11ξ,12*S*)-config.

Stereoisomer, 17,18-dihydro: ***Topsentolide B_3***
$C_{20}H_{32}O_4$ 336.47
Constit. of a *Topsentia* sp. Oil. $[\alpha]_D^{24}$ +44.2 (c, 0.06 in MeOH). Possesses *erythro*-config.

Stereoisomer, 17,18-dihydro, 11-Me ether: ***Topsentolide C_2***
$C_{21}H_{34}O_4$ 350.497
Constit. of a *Topsentia* sp. Oil. $[\alpha]_D^{23}$ +14.5 (c, 0.27 in MeOH). Possesses (11ξ,12*S*)-config.

Luo, X. *et al., J. Nat. Prod.*, 2006, **69**, 567-571 (*isol, pmr, cmr*)

Tortuic acid B T-363



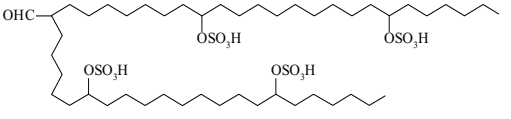
$C_{40}H_{60}O_8$ 668.909

Me ester: ***Methyl tortuate B***
[805230-76-6]
$C_{41}H_{62}O_8$ 682.936
Constit. of *Sarcophyton tortuosum*. Cryst. (EtOH). Mp 229-231°. $[\alpha]_D^{25}$ +84 (c, 0.03 in MeOH).

Zeng, L.-M. *et al., J. Nat. Prod.*, 2004, **67**, 1915-1918 (*isol, pmr, cmr, cryst struct*)

Toxadocial A T-364

[148099-32-5]



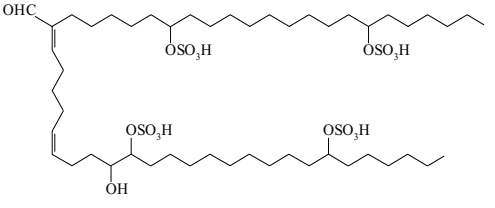
$C_{48}H_{96}O_{17}S_4$ 1073.54
Isol. from the marine sponge *Toxadocia cylindrica*. Thrombin inhibitor. Amorph. solid (as tetra-Na salt). $[\alpha]_D$ -2.2 (c, 1 in MeOH) (tetra-Na salt). CAS nos. refer to tetra-Na salts.

Carboxylic acid: ***Toxadocic acid***
[152574-80-6]
$C_{48}H_{96}O_{18}S_4$ 1089.54
Isol. from *Toxadocia cylindrica*. Thrombin inhibitor. Amorph. solid (as tetra-Na salt). $[\alpha]_D^{23}$ +0.6 (c, 0.36 in MeOH) (tetra-Na salt).

Nakao, Y. *et al., Tet. Lett.*, 1993, **34**, 1511 (*isol, struct*)
Nakao, Y. *et al., Tetrahedron*, 1993, **49**, 11183 (*Toxadocic acid*)

Toxadocial B T-365

[152574-78-2]

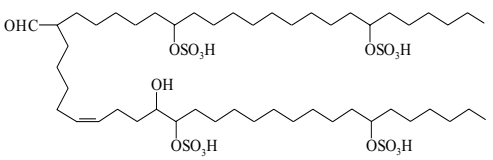


$C_{50}H_{96}O_{18}S_4$ 1113.562
Isol. from the marine sponge *Toxadocia cylindrica*. Thrombin inhibitor. Amorph. solid (as tetra-Na salt). $[\alpha]_D^{23}$ +3.7 (c, 0.2 in MeOH) (tetra-Na salt). CAS no. refers to tetra-Na salt.

Nakao, Y. *et al., Tetrahedron*, 1993, **49**, 11183

Toxadocial C T-366

[152574-79-3]



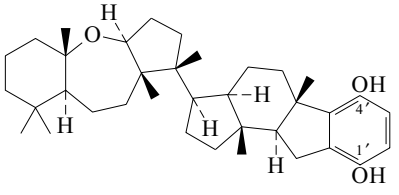
$C_{50}H_{98}O_{18}S_4$ 1115.577

Isol. from the marine sponge *Toxadocia cylindrica*. Thrombin inhibitor. Amorph. solid (as tetra-Na salt). $[\alpha]_D^{23}$ +2.2 (c, 0.2 in MeOH) (tetra-Na salt). CAS no. refers to tetra-Na salt.

Nakao, Y. *et al., Tetrahedron*, 1993, **49**, 11183

Toxicol B T-367

[149764-32-9]



$C_{36}H_{54}O_3$ 534.821

Constit. of *Toxiclona toxius*. Powder. $[\alpha]_D$ -16 (c, 0.004 in MeOH/CH_2Cl_2).

4′-Sulfate: ***Toxicol C***
[149764-33-0]
$C_{36}H_{54}O_6S$ 614.885

Constit. of *Toxiclona toxius*. Oil (as Na salt). $[\alpha]_D$ +21 (c, 0.07 in MeOH) (as Na salt).

1′,4′-Disulfate: ***Toxicol A***
[149764-31-8]
$C_{36}H_{54}O_9S_2$ 694.949

Constit. of *Toxiclona toxius*. Oil (as di-Na salt). $[\alpha]_D$ +35 (c, 1 in MeOH) (Na salt).

Loya, S. *et al., J. Nat. Prod.*, 1993, **56**, 2120 (*isol*)
Isaacs, S. *et al., Tetrahedron*, 1993, **49**, 4275 (*isol, pmr, cmr*)

Anemonia sulcata Toxin T-368

ATX. Sea anemone toxin

Peptides. Isol. from the sea anemone *Anemonia sulcata*. Toxins.

ATX I

Toxin AS I. AS I
[89177-43-5]
[60748-44-9]

Peptide containing 46 amino acid residues and 3 disulfide bonds. λ_{max} 280 (H_2O) (Berdy).

▶ LD_{50} (mus, ipr) 4 mg/kg.

ATX II

Toxin AS II. AS II
[69071-93-8]
[60748-45-0]

Cardiac stimulant. Peptide containing 47 amino acid residues and 3 disulfide bonds. λ_{max} 280 (H_2O) (Berdy).

▶ LD_{50} (mus, ipr) 0.1 mg/kg.

ATX III

Toxin AS III. AS III
[64513-68-4]
[60748-46-1]

Peptide comprising 27 amino acid residues and 2 disulfide bonds. λ_{max} 280 (H_2O) (Berdy).

▶ LD_{50} (mus, ipr) 18 mg/kg.

ATX V

Toxin AS V. AS V

Peptide containing 46 amino acid residues and 3 disulfide bonds. λ_{max} 280 (H_2O).

▶ LD_{50} (mus, ipr) 0.019 mg/kg.

Novak, V. *et al., Toxicon*, 1973, **11**, 411-417 (*isol*)
Beress, L. *et al., FEBS Lett.*, 1975, **50**, 311-314 (*isol*)
Beress, L. *et al., Toxicon*, 1975, **13**, 359-367 (*ATX II, isol*)
Wunderer, G. *et al., Eur. J. Biochem.*, 1976, **68**, 193-198; 1978, **89**, 11-17 (*ATX I, ATX II, struct*)
Wunderer, G. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1976, **357**, 235-240; 1978, **359**, 1193-1201 (*ATX II, struct*)
Martinez, G. *et al., FEBS Lett.*, 1977, **84**, 247-252 (*ATZ III, struct*)
Beress, L. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1977, **358**, 985-988 (*ATX III, struct*)
Schweitz, H. *et al., Biochemistry*, 1981, **20**, 5245-5252 (*isol*)
Schaeffler, J.J. *et al., Biochem. Biophys. Res. Commun.*, 1982, **107**, 272-278 (*ATX V, struct*)
Widmer, H. *et al., Eur. J. Biochem.*, 1988, **171**, 177-192 (*ATX I, soln struct*)
Norton, R.S. *et al., Biochem. J.*, 1993, **293**, 545-551 (*ATX III, soln struct*)
Manoleras, N. *et al., Biochemistry*, 1994, **33**, 11051-11061 (*ATX III, 3D struct*)

Chiropsalmus quadrigatus Toxin T-369

CqTX-A

Protein toxin. Isol. from the box jellyfish *Chiropsalmus quadrigatus*. Potent hemolytic agent.

Nagai, H. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 97-102 (*isol, struct*)

Condylactis gigantea Toxin T-370

Basic protein. Isol. from the sea anemone *Condylactis gigantea*. Shows cytolytic activity.

Bernheimer, A.W. *et al., Arch. Biochem. Biophys.*, 1982, **214**, 840-845 (*isol*)

Radianthus paumotensis Toxin T-371

Peptide complex. Four toxins isol. Structs. of toxins II and III have been reported; each consists of 48 amino acid residues. Isol. from the sea anemone *Radianthus paumotensis*.

Schweitz, H. *et al., Biochemistry*, 1985, **24**, 3554 (*isol*)
Wemmer, D.E. *et al., Biochemistry*, 1986, **25**, 6842 (*struct, Toxin II*)
Pease, J.H.B. *et al., Biochemistry*, 1989, **28**, 2199 (*struct, Toxin III*)

Toxin Ae 1 T-372

Polypeptide containing 54 amino acid residues. Isol. from the sea anemone *Actinia equina*. Toxin; lethal to crabs.

Lin, X.Y. *et al., Toxicon*, 1996, **34**, 57-65 (*isol*)
Minagawa, S. *et al., FEBS Lett.*, 1998, **427**, 149-151 (*isol, props*)

Bunodosoma granulifera Toxin BgK T-373

Peptide containing 37 amino acid residues and 3 disulfide bonds. Isol. from the sea anemone *Bunodosoma granulifera*. Potassium-channel toxin.

Aneiros, A. *et al., Biochim. Biophys. Acta*, 1993, **1157**, 86-92 (*isol*)
Cotton, J. *et al., Eur. J. Biochem.*, 1997, **244**, 192-202 (*struct, synth*)

Entacmaea quadricolor Toxin EnT T-374

Protein. Isol. from the sea anemone *Entacmaea quadricolor*. Shows cytolytic activity.

Samejima, Y. *et al., Toxicon*, 2000, **38**, 259-264 (*isol*)

Radianthus crispus Toxin Rc1 T-375

Polypeptide containing 47 amino acid residues incl. a hydroxyproline residue. Isol. from the sea anemone *Radianthus crispus*. Lethal to crabs.

Shiomi, K. *et al., Fish. Sci.*, 1996, **62**, 629-633 (*isol*)

Carybdea alata Toxins T-376

CaTX

Two protein toxins. CaTX-A contains 463 amino acids. Isol. from the box jellyfish *Carybdea alata*. Potent haemolytic agents.

Nagai, H. *et al., Biochem. Biophys. Res. Commun.*, 2000, **275**, 589-594 (*isol, struct*)

Condylactis aurantiaca Toxins T-377

Four polypeptides containing 49-51 amino acid residues. Isol. from the sea anemone *Condylactis aurantiaca*. Toxic to the shore crab *Carcinus maenas*.

Beress, R. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1976, **357**, 409-414

Radianthus paumotensis Toxins T-378

4 Peptides containing 48 or 49 amino acid residues with 3 intramol. disulfide bonds. Isol. from *Radianthus paumotensis*. Toxins.

Rp II

Contains 48 amino acid residues.

Rp III

The most abundant constituent; comprises 48 amino acid residues.

Schweitz, H. *et al., Biochemistry*, 1985, **24**, 3554-3561 (*isol*)
Wemmer, D.E. *et al., Biochemistry*, 1986, **25**, 6842-6849 (*Rp II, pmr, struct*)
Metrione, R.M. *et al., FEBS Lett.*, 1987, **218**, 59-62 (*Rp III, struct*)
Pease, J.H. *et al., Biochemistry*, 1989, **28**, 2199-2204 (*Rp III, pmr, secondary struct*)

Stichodactyla mertensii Toxins T-379

Two peptides, SmT-1 and SmT-2. Isol. from the venom of the sea anemone *Stichodactyla mertensii*. Cytolysins. Not found in CAS.

Samejima, Y. *et al., Toxicon*, 2000, **38**, 259-264 (*isol, struct*)

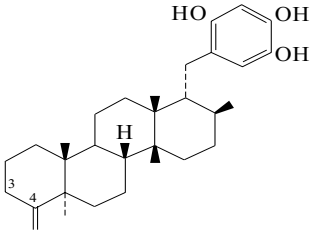
Stichodactyla Toxins SmT T-380

Two polypeptides, SmT-1 and SmT-2. Isol. from the sea anemone *Stichodactyla mertensii*. Cytolysins.

Samejima, Y. *et al., Toxicon*, 2000, **38**, 259-264 (*isol*)

Toxistylide B T-381

[73538-56-4]



$C_{31}H_{46}O_3$ 466.703
Constit. of *Microciona toxystyla*.

Tri-Ac:
Cryst. (EtOH). Mp 226-228°. $[\alpha]_D$ +25 (c, 0.5 in $CHCl_3$).

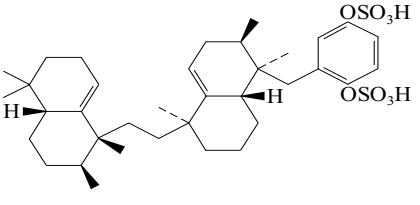
Δ^3-Isomer: ***Toxistylide A***
[73538-57-5]
$C_{31}H_{46}O_3$ 466.703
Constit. of *Microciona toxystyla*.

Δ^3-Isomer, tri-Ac:
Cryst. (MeOH aq.). Mp 193-195°. $[\alpha]_D$ +9.4 (c, 1.0 in $CHCl_3$).

Cimino, G. *et al., Tet. Lett.*, 1979, 3619 (*cryst struct, rel config*)

Toxiusol T-382

[149764-34-1]

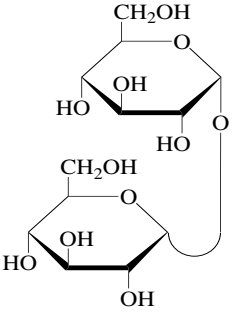


$C_{36}H_{54}O_8S_2$ 678.95
Constit. of *Toxiclona toxius*. HIV reverse transcriptase (HIV-rt) inhibitor. Oil (as di-Na salt).

Loya, S. *et al., J. Nat. Prod.*, 1993, **56**, 2120 (*isol, activity*)
Isaacs, S. *et al., Tetrahedron*, 1993, **49**, 4275 (*isol, pmr, cmr*)

α,α-Trehalose T-383

α-D-Glucopyranosyl-α-D-glucopyranoside, 9CI, 8CI. Mycose. Mushroom sugar. Trehalose
[99-20-7]



$C_{12}H_{22}O_{11}$ 342.299
By-product in industrial fermentations. Occurs in fungi, moulds, ergot, algae, yeast and many insects. *Selaginella lepidophylla* contains the free disaccharide. Found in high concs. in anhydrobiotic organisms, those resistant to dehydration. Probable energy reserve in many organisms and important cellular protectant in drought resistant organisms. Associated with maintenance of the integrity of biol. membranes in organisms subject to severe thermal stresses. Exists in various anhydrous forms and a dihydrate.
Mp 97° (hydrate) Mp 214-216° (anhyd.). $[\alpha]_D^{20}$ +178.3 (H_2O) (hydrate). $[\alpha]_D^{20}$ +199 (H_2O) (anhyd.). Sweet taste. Sweetness = 0.36 × sucrose. Fermented by yeast.

2-Sulfate: [141923-45-7]
$C_{12}H_{22}O_{14}S$ 422.363
Core carbohydrate of the sulfatides of *Mycobacterium tuberculosis*. V. hygroscopic solid (as NH_4 salt).
Mp 150° (browns) (NH_4 salt). $[\alpha]_D^{22}$ +151 (c, 0.6 in MeOH).

6-Phosphate: [4484-88-2]
Prod. by *Streptomyces hygroscopicus, Mycobacterium smegmatis* and yeasts.
$[\alpha]_D$ +185 (H_2O).

2,2′,3,3′,4,4′-Hexa-Ac:
$C_{24}H_{34}O_{17}$ 594.522
Cryst. (EtOH/petrol). Mp 93-96°. $[\alpha]_D^{19}$ +158 ($CHCl_3$).

2,2′,3,3′,4,4′,6-Hepta-Ac: [113842-79-8]
$C_{26}H_{36}O_{18}$ 636.56
Mp 124-126° (EtOH). $[\alpha]_D$ +167.5 (c, 0.7 in $CHCl_3$).

Octa-Ac: [25018-27-3]
$C_{28}H_{38}O_{19}$ 678.597
Mp 100-102°. $[\alpha]_D$ +163 ($CHCl_3$).

6,6′-Dihexadecanoyl: α,α-Trehalose-6,6′-dipalmitate
[3317-99-5]
$C_{44}H_{82}O_{13}$ 819.124
Chord factor analogue.
Mp 158.5-160°. $[\alpha]_D$ +78 (c, 1 in $CHCl_3$).

6,6′-Dimesyl, hexa-Ac: [23089-73-8]
$C_{26}H_{38}O_{21}S_2$ 750.706
Cryst. (EtOH). Mp 168-169.5°. $[\alpha]_D$ +143 (c, 1.6 in $CHCl_3$).

6,6′-Ditosyl: [23235-67-8]
$C_{26}H_{34}O_{15}S_2$ 650.678
Cryst. (MeOH aq.). Mp 106-110°. $[\alpha]_D$ +90 (c, 0.2 in MeOH/$CHCl_3$).

6,6′-Ditosyl, hexa-Ac: [23089-74-9]
$C_{38}H_{46}O_{21}S_2$ 902.901
Cryst. (MeOH). Mp 170-172°. $[\alpha]_D$ +132 (c, 0.5 in $CHCl_3$).

4,6:4′,6′-Di-O-ethylidene:
$C_{16}H_{26}O_{11}$ 394.375
Mp 285° dec. $[\alpha]_D^{23}$ +143 (c, 0.4 in H_2O).

Octa-Me: [25018-29-5]
$C_{20}H_{38}O_{11}$ 454.514
Syrup. $Bp_{0.03}$ 170°. $[\alpha]_D^{20}$ +199.8 (C_6H_6).

6-Trityl, hepta-Ac: [113842-78-7]
$C_{45}H_{50}O_{18}$ 878.879
Mp 203-205° (EtOH). $[\alpha]_D$ +134 (c, 0.7 in $CHCl_3$).

6,6′-Ditrityl, hexa-Ac: [75869-80-6]
$C_{62}H_{62}O_{17}$ 1079.162
Mp 246-248°. $[\alpha]_D$ +112 (c, 1 in $CHCl_3$).

[6138-23-4]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 912C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 196A (*ir*)
Robison, R. *et al., Biochem. J.*, 1928, **22**, 1277 (*synth, phosphate*)
Bredereck, H. *et al., Ber.*, 1930, **63**, 959 (*hexa-Ac*)
Richtmyer, N.K. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 370 (*isol*)
Birch, G. *et al., Adv. Carbohydr. Chem.*, 1963, **18**, 201 (*rev*)
MacDonald, D.L. *et al., Biochim. Biophys. Acta*, 1964, **86**, 390 (*synth, phosphate*)
Birch, G. *et al., J.C.S.(C)*, 1966, 1072 (*synth*)
Birch, G. *et al., Carbohydr. Res.*, 1968, **8**, 411 (*6,6′-dimesyl hexa-Ac, 6,6′-ditosyl hexa-Ac, 6,6′-ditosyl*)
Pazur, J.H. *et al., The Carbohydrates*, (Eds., Pigman, W., *et al*), 2nd edn., Academic Press, 1970, **2A**, 106 (*rev*)
Lapp, D. *et al., J. Biol. Chem.*, 1971, **246**, 4567 (*synth, phosphate*)
Taga, T. *et al., Acta Cryst. B*, 1972, **28**, 3258 (*cryst struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 644 (*occur*)
Usui, T. *et al., J.C.S. Perkin 1*, 1973, 2425 (*conformn, cmr*)
Elbein, A.D. *et al., Adv. Carbohydr. Chem. Biochem.*, 1974, **30**, 227 (*rev*)
Usui, T. *et al., Carbohydr. Res.*, 1974, **33**, 105 (*pmr, config*)
Hough, L. *et al., Pure Appl. Chem.*, 1977, **49**, 1069 (*rev*)
Pfeffer, P.E. *et al., J.A.C.S.*, 1979, **107**, 1265 (*cmr*)
Lee, G.K. *et al., Dev. Food Carbohydr.*, Applied Science Pub., 1980, **2**, 1 (*rev*)
Liav, A. *et al., Carbohydr. Res.*, 1984, **127**, 211 (*2-sulfate*)
Bottle, S. *et al., Chem. Comm.*, 1984, 385 (*dipalmitate*)
Jeffrey, G.A. *et al., Carbohydr. Res.*, 1985, **137**, 21 (*cryst struct*)
Szurmai, Z. *et al., Carbohydr. Res.*, 1987, **164**, 313 (*hepta-Ac, pmr*)
Abbate, S. *et al., Carbohydr. Res.*, 1991, **210**, 1 (*ir, Raman*)
Ronnow, T.E.C.L. *et al., Carbohydr. Res.*, 1994, **260**, 323 (*synth, 6-phosphate, 6,6′-dipho phate*)
Tarelli, E. *et al., Carbohydr. Res.*, 1994, **261**, 25 (*synth, phosphates*)
Hull, S.R. *et al., Carbohydr. Res.*, 1995, **266**, 147-157 (*isol*)
Gilbertson, S.R. *et al., J.O.C.*, 1995, **60**, 6226 (*hexa-Me, hexabenzyl*)
Mueller, J. *et al., Plant Sci. (Limerick, Irel.)*, 1995, **112**, 1 (*rev, occur*)
Gil, A.M. *et al., Spectrochim. Acta A*, 1996, **52**, 1649-1659 (*ir, Raman, pmr, cmr*)
Sussich, F. *et al., Carbohydr. Res.*, 1999, **322**, 113-119 (*bibl*)
Food Chem. News, 2000, **42(42)**, 6; 2001, **43(20)**, 15 (*use*)
Sussich, F. *et al., Carbohydr. Res.*, 2001, **334**, 165-176 (*solution props*)
Akao, K. *et al., Carbohydr. Res.*, 2001, **334**, 233-241 (*ir, props*)
Nagase, H. *et al., Carbohydr. Res.*, 2002, **337**, 167-173 (*polymorphism*)
Wingler, A. *et al., Phytochemistry*, 2002, **60**, 437-440 (*rev, biosynth*)
Haines, A.H. *et al., Carbohydr. Res.*, 2003, **338**, 813-818 (*L-enantiomer*)
Pratt, M.R. *et al., Org. Lett.*, 2003, **5**, 3185-3188 (*synth*)

α,α-Trehalose phosphorylase T-384

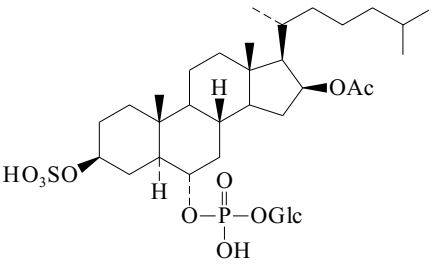
E.C. 2.4.1.64. α,α-Trehalose:phosphate β-D-glucosyltransferase
[37205-59-7]

Hexosyltransferase enzyme. Occurs in many fungi, algae, etc. Catalyses the reversible reaction of α,α-Trehalose, T-383 with orthophosphate to give D-glucose and β-D-glucose 1-phosphate.

Belocopitow, E. *et al., Biochim. Biophys. Acta*, 1970, **198**, 151-154 (*Euglena gracilis*)
Marechal, L.R. *et al., J. Biol. Chem.*, 1972, **247**, 3223-3228 (*Euglena gracilis*)
Wennet, W.J. *et al., Biochim. Biophys. Acta*, 1998, **1425**, 177-188 (*Agaricus bisporus*)
Aisaka, K. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 782-787 (*Catellatospora ferruginea*)
Eis, C. *et al., Biochem. J.*, 1999, **341**, 385-393 (*Schizophyllum commune*)

Tremasterol A T-385

[140866-19-9]



$C_{35}H_{61}O_{15}PS$ 784.898
Isol. from the starfish *Tremaster novaecaledoniae.*
$[\alpha]_D$ +40 (c, 0.5 in MeOH) (as di-Na salt).

6′-Ac: ***Tremasterol C***
[140866-21-3]
$C_{37}H_{63}O_{16}PS$ 826.935
Constit. of *Tremaster novaecaledoniae.* Conts. a 6-acetylglucosyl residue.

2′,3′,4′,6′-Tetra-Ac: ***Tremasterol B***
[140866-20-2]
$C_{43}H_{69}O_{19}PS$ 953.046
Constit. of *Tremaster novaecaledoniae.*

De Riccardis, F. *et al., Tet. Lett.*, 1992, **33**, 1097-1100

5,9-Triacontadienoic acid T-386

$H_3C(CH_2)_{19}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{30}H_{56}O_2$ 448.771

(*Z,Z*)-*form* [130127-72-9]
Isol. from the phospholipids of the sponge *Petrosia pellasarca.*
Carballeira, N.M. *et al., J. Nat. Prod.*, 1990, **53**, 836 (*isol, ms*)

9,23-Triacontadienoic acid T-387

$H_3C(CH_2)_5CH{=}CH(CH_2)_{12}CH{=}CH(CH_2)_7COOH$
$C_{30}H_{56}O_2$ 448.771

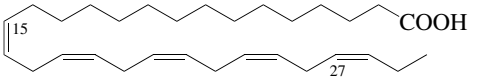
(*Z,Z*)-*form* [150731-83-2]
Isol. from the sponge *Trikentrion loeve.*
Barnathan, G. *et al., Nat. Prod. Lett.*, 1992, **1**, 201-207 (*isol*)

19,23-Triacontadienoic acid T-388

$H_3C(CH_2)_5CH{=}CHCH_2CH_2CH{=}CH(CH_2)_{17}COOH$
$C_{30}H_{56}O_2$ 448.771

(*Z,Z*)-*form* [187657-36-9]
Isol. from the sponges *Haliclona cinerea* and *Trikentrion loeve.*
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol, ms*)
Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*isol, ms*)

15,18,21,24,27-Triacontapentaenoic acid T-389



$C_{30}H_{50}O_2$ 442.724

(*all-Z*)-*form* [71387-74-1]
Metab. of the sponge *Cliona celata.* Also found in sperm of humans and other mammals.

27,28-Dihydro: 15,18,21,24-Triacontatetraenoic acid
[71387-73-0]
$C_{30}H_{52}O_2$ 444.74

Metab. of *Cliona celata*. Also found in sperm of humans and other mammals.

15,16,27,28-Tetrahydro: 18,21,24-Triacontatrienoic acid
[105658-29-5]
$C_{30}H_{54}O_2$ 446.755
Found in sperm of humans and other mammals.

[106575-29-5, 106575-32-0]

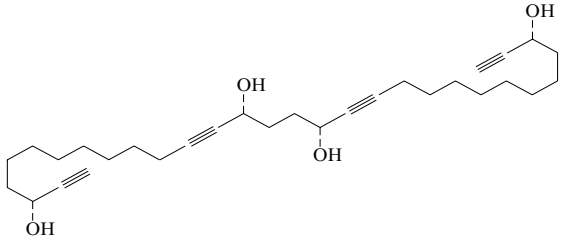
Litchfield, C. *et al., Lipids*, 1979, **14**, 619 (*isol*)
Poulos, A. *et al., Biochem. J.*, 1986, **240**, 891 (*occur, isol*)
Aveldano, M.I. *et al., J. Biol. Chem.*, 1987, **262**, 1180 (*ms*)

5,9,19,23-Triacontatetraenoic acid T-390

$H_3C(CH_2)_5CH{=}CHCH_2CH_2CH{=}CH(CH_2)_8CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$
$C_{30}H_{52}O_2$ 444.74

(all-Z)-form [187657-38-1]
Isol. from the sponge *Haliclona cinerea*.
Joh, Y.G. *et al., Lipids*, 1997, **32**, 13-17 (*isol, ms*)

1,12,18,29-Triacontatetrayne-3,14,17,28-tetrol T-391



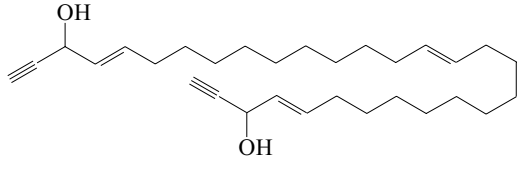
$C_{30}H_{46}O_4$ 470.691

(all-R)-form [155624-58-1]
Isol. from the marine sponge *Petrosia* sp.
Amorph. solid. $[\alpha]_D^{22}$ +10 (c, 0.1 in $CHCl_3$).

14,17-Diketone: 3,28-Dihydroxy-1,12,18,29-triacontatetrayne-14,17-dione
[155624-57-0]
$C_{30}H_{42}O_4$ 466.659
Isol. from *Petrosia* sp. Pale yellow oil. $[\alpha]_D^{22}$ +22 (c, 0.2 in $CHCl_3$).
Ochi, M. *et al., Chem. Lett.*, 1994, 89 (*isol, uv, ir, pmr, cmr, ms*)

4,15,26-Triacontatriene-1,29-diyne-3,28-diol T-392

Duryne
[108641-87-8]



$C_{30}H_{48}O_2$ 440.708
Isol. from the marine sponges *Cribrochalina dura* and *Strongylophora durissima*. Cytotoxic. Solid. Sol. $CHCl_3$; poorly sol. hexane. Mp 44-45°. λ_{max} 224 (ϵ 313); 230 (ϵ 307) (MeOH).

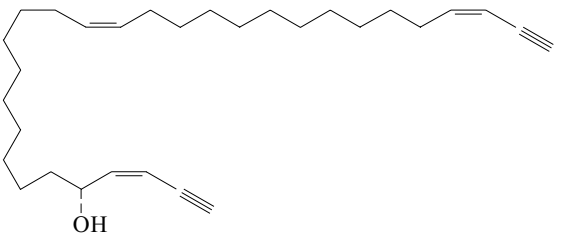
Di-Ac: [111755-80-7]
$C_{34}H_{52}O_4$ 524.782
Isol. from *Cribrochalina dura*. Cytotoxic.

Diketone: 4,15,26-Triacontatriene-1,29-diyne-3,28-dione, 9CI
[111755-81-8]
$C_{30}H_{44}O_2$ 436.676
Isol. from *Cribrochalina dura*. Cytotoxic.

[124918-59-8, 124918-60-1]

Pat. Coop. Treaty (WIPO), 1987, 87 04 703; *CA*, **108**, 621b (*isol*)
Wright, A.E. *et al., Tet. Lett.*, 1987, **28**, 1377-1379 (*isol, ir, ms, pmr, cmr*)
Deshpande, V.H. *et al., Tet. Lett.*, 1989, **30**, 1991-1992 (*synth*)
Shen, Y.C. *et al., J. Nat. Prod.*, 2000, **63**, 1686-1688 (*isol*)

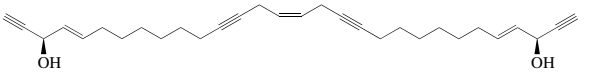
3,15,27-Triacontatriene-1,29-diyn-5-ol T-393



$C_{30}H_{48}O$ 424.709

(3Z, 5S, 15Z, 27Z)-form [155624-60-5]
Isol. from the sponge *Petrosia* sp.
Pale yellow oil. $[\alpha]_D^{20}$ -14 (c, 0.3 in $CHCl_3$). λ_{max} 223 (ϵ 37300) (EtOH).
Ochi, M. *et al., Chem. Lett.*, 1994, 89 (*isol, uv, ir, pmr, cmr, ms*)

4,15,26-Triacontatriene-1,12,18,29-tetrayne-3,28-diol T-394



$C_{30}H_{40}O_2$ 432.645

(3RS,4E,15Z,26E,28SR)-form
Petrosiacetylene A
Isol. from the sponge *Petrosia* sp. Opt. inactive (*meso*-).

4,5-Dihydro: 4,15-Triacontadiene-1,12,18,29-tetrayne-3,28-diol. ***Petrosiacetylene C***
$C_{30}H_{42}O_2$ 434.661
Isol. from *Petrosia* sp. Oil. Exhibits small -ve opt. rotation. Obt. as a mixture of C-28 epimers.

12,13-Dihydro(Z-): 4,12,15,26-Triacontatetraene-1,18,29-triyne-3,28-diol. ***Petrosiacetylene B***
$C_{30}H_{42}O_2$ 434.661
Isol. from *Petrosia* sp. Oil. Exhibits small -ve opt. rotation.

12,12,13,13-Tetrahydro: 4,15,26-Triacontatriene-1,12,29-triyne-3,28-diol. ***Petrosiacetylene D***
$C_{30}H_{44}O_2$ 436.676
Isol. from *Petrosia* sp. Oil. $[\alpha]_D^{25}$ +5.2 (c, 0.3 in MeOH). Obt. as a mixture of C-28 epimers.

(3ξ,4E,15Z,26E,28ξ)-form
Dideoxypetrosynol A
[206554-64-5]
[201990-73-0]
Isol. from the sponge *Petrosia* sp. Cytotoxic agent. Amorph. solid.

4,5-Dihydro: ***Dideoxypetrosynol B***
[206554-66-7]
$C_{30}H_{42}O_2$ 434.661
Isol. from a *Petrosia* sp. Amorph. solid.

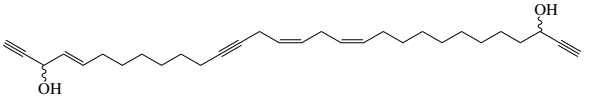
12,13-Dihydro(Z-): ***Dideoxypetrosynol C***
[206554-76-9]
$C_{30}H_{42}O_2$ 434.661
Isol. from a *Petrosia* sp. Pale yellow oil.

(3S,15Z,28S)-form

4,5,26,27-Tetrahydro: 15-Triacontene-1,12,18,29-tetrayne-3,28-diol. ***Dideoxypetrosynol D***
[206554-83-8]
$C_{30}H_{44}O_2$ 436.676
Isol. from a *Petrosia* sp. Amorph. solid. $[\alpha]_D^{23}$ +38 (c, 0.05 in $CHCl_3$).

Seo, Y. *et al., Tetrahedron*, 1998, **54**, 447-462 (*isol, ir, pmr, cmr, ms*)
Kim, J.S. *et al., Tetrahedron*, 1998, **54**, 3151-3158 (*isol, ir, pmr, cmr*)

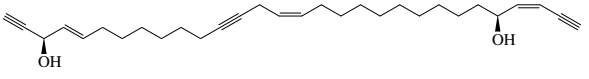
4,15,18-Triacontatriene-1,12,29-triyne-3,28-diol T-395



$C_{30}H_{44}O_2$ 436.676

(3ξ,4*E*,15*Z*,18*Z*,28ξ)-*form*
Dideoxypetrosynol F
[222178-92-9]
Isol. from the sponge *Petrosia* sp. Cytotoxic agent. Amorph. solid.
Kim, J.S. *et al., J. Nat. Prod.*, 1999, **62**, 554-559

4,15,27-Triacontatriene-1,12,29-triyne-3,26-diol T-396



$C_{30}H_{44}O_2$ 436.676

(3*R*,4*E*,15*Z*,26*S*,27*Z*)-*form*
Dideoxypetrosynol E
[222178-91-8]
Isol. from the sponge *Petrosia* sp. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{23}$ +2.6 (c, 0.03 in MeOH). Struct. not fully elucidated. λ_{max} 229 (log ϵ 3.7) (MeOH).
Kim, J.S. *et al., J. Nat. Prod.*, 1999, **62**, 554-559

5,9,21-Triacontatrienoic acid T-397

$H_3C(CH_2)_7CH{=}CH(CH_2)_{10}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$

$C_{30}H_{54}O_2$ 446.755

(*all-Z*)-*form* [200722-43-6]
Isol. from the sponge *Amphimedon* sp.
Oil. λ_{max} 199 (ϵ 7210) (MeOH).
Nemoto, T. *et al., Tetrahedron*, 1997, **53**, 16699-16710 (*isol, uv, pmr, cmr*)

5,9,23-Triacontatrienoic acid T-398

$H_3C(CH_2)_5CH{=}CH(CH_2)_{12}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$

$C_{30}H_{54}O_2$ 446.755

(*all-Z*)-*form* [73768-92-0]
Metab. of numerous sponges incl. *Haliclona* sp., *Amphimedon complanata*, *Aplysina fistularis* and *Chondrilla nucula*.
Me ester:
$C_{31}H_{56}O_2$ 460.782
Isol. from the sponge *Chondrilla nucula*. Elastase inhibitor. Oil.
[89188-22-7]
Litchfield, C. *et al., Lipids*, 1980, **15**, 200
Lankelma, J. *et al., Lipids*, 1983, **18**, 853-858 (*ms*)
Raederstorff, D. *et al., J.O.C.*, 1987, **52**, 2337-2346 (*isol*)
Carballeira, N.M. *et al., Lipids*, 1989, **24**, 229; 1992, **27**, 681 (*isol*)
Barnathan, G. *et al., Lipids*, 1992, **27**, 779 (*isol*)
Barnathan, G. *et al., Nat. Prod. Lett.*, 1992, **1**, 201 (*isol*)
Meyer, M. *et al., Lipids*, 2002, **37**, 1109-1111 (*Me ester, isol*)

5,9,25-Triacontatrienoic acid T-399

$H_3C(CH_2)_3CH{=}CH(CH_2)_{14}CH{=}CHCH_2CH_2CH{=}CH(CH_2)_3COOH$

$C_{30}H_{54}O_2$ 446.755

(*all-Z*)-*form* [150677-61-5]
Isol. from the sponge *Trikentrion loeve.*
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol, ms*)

23-Triacontenoic acid T-400

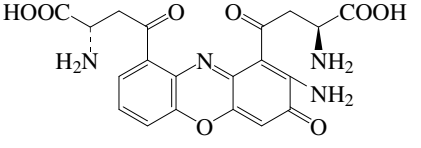
$H_3C(CH_2)_5CH{=}CH(CH_2)_{21}COOH$

$C_{30}H_{58}O_2$ 450.787

(*Z*)-*form* [89022-39-9]
Constit. of the sponge *Trikentrion loeve* and from hamster meibomian gland.
Harvey, D.J. *et al., Biomed. Chromatogr.*, 1989, **3**, 251 (*isol*)
Barnathan, G. *et al., Lipids*, 1996, **31**, 193-200 (*isol, ms*)

α,α′,2-Triamino-γ,γ′,3-trioxo-3*H*-phenoxazine-1,9-dibutanoic acid, 9CI T-401

[105334-59-6]

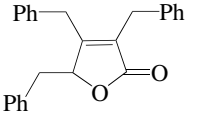


Absolute Configuration

$C_{20}H_{18}N_4O_8$ 442.384
Ommochrome pigment from the eyes and skin of cephalopods *Loligo vulgaris, Sepia officinalis* and *Octopus vulgaris.* Yellow cryst. Insoluble. Closely related to Xanthommatin, X-2. Readily cyclises to Dihydroxanthommatin, D-591. λ_{max} 430 (no solvent reported).
Bolognese, A. *et al., CA*, 1987, **106**, 15949 (*isol*)
Bolognese, A. *et al., J. Het. Chem.*, 1988, **25**, 1243-1246 (*bibl*)

3,4,5-Tribenzyl-2(5*H*)-furanone T-402

*3,4,5-Tris(phenylmethyl)-2(5*H*)-furanone, 9CI.* ***Maculalactone A***



$C_{25}H_{22}O_2$ 354.448

(+)-*form* [184584-40-5]
Isol. from the cyanobacteria *Kyrtuthrix maculans.*
Oil. $[\alpha]_D^{25}$ +70.2 (c, 0.4 in CH_2Cl_2). Partial racemate (90-95% *S*-isomer).
Tsui, W.-Y. *et al., Phytochemistry*, 1996, **43**, 1083-1085 (*isol, ir, pmr, cmr, ms*)
Brown, G.D. *et al., Tetrahedron*, 2004, **60**, 5439-5451 (*synth, abs config*)
Kar, A. *et al., Tetrahedron*, 2005, **61**, 5297-5302 (*synth*)

Tribromoacetaldehyde T-403

Tribromoethanal. Bromal
[115-17-3]
Br_3CCHO

C_2HBr_3O 280.741
Isol. from *Asparagopsis* spp. Formerly used as hypnotic. Yellowish oily liq. Sol. H_2O, EtOH. d_4^{25} 2.67. Bp 174° dec. Bp_9 61°.

Covalent hydrate: 2,2,2-Tribromo-1,1-ethanediol. Bromal hydrate
[507-42-6]
$C_2H_3Br_3O_2$ 298.756
Deliquescent cryst. Sol. H_2O, EtOH, $CHCl_3$. Mp 53.5°.
▶ AB3325000

Hydrate, di-Ac: 1,1,1-Tribromo-2,2-diacetoxyethane. Tribromoethylidene diacetate
$C_6H_7Br_3O_4$ 382.831
Mp 77-78°.

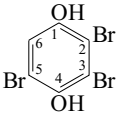
Di-Et acetal: 1,1,1-Tribromo-2,2-diethoxyethane
$C_6H_{11}Br_3O_2$ 354.864
$Bp_{22.5}$ 138-141° (lit. gives a pressure range).
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 478A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 747C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 569A (*ir*)
Schäffer, L. *et al., Ber.*, 1871, **4**, 366 (*synth*)
Org. Synth., 1937, **17**, 18 (*synth*)
Cristol, S.J. *et al., J.A.C.S.*, 1946, **68**, 140 (*di-Ac*)
Jain, S.R. *et al., Tetrahedron*, 1964, **20**, 1589 (*hydrate*)
Fenical, W. *et al., Proc. Int. Seaweed Symp.*, 1977, **9**, 387-400; *CA*, **91**, 14474y (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, THU500

Tribromoacetic acid, 9CI, 8CI T-404

[75-96-7]
Br_3CCOOH
$C_2HBr_3O_2$ 296.741
Monoclinic prisms. Sol. H_2O, EtOH, Et_2O. Mp 131°. Bp 245° dec. pK_a 0.66 (25°, H_2O).
▶ Irritant.
Me ester: [3222-05-7]
$C_3H_3Br_3O_2$ 310.768
d 2.33. Bp_{15} 103°. n_D^{20} 1.5580.
Et ester: [599-99-5]
$C_4H_5Br_3O_2$ 324.794
Constit. of *Asparagopsis armata*. Liq. Bp 178-180° Bp_{73} 148°.
▶ AJ7600000
Chloride: [34718-47-3]
C_2Br_3ClO 315.186
Liq. Bp_{12} 80-82°.
Bromide: [10588-31-5]
C_2Br_4O 359.637
Liq. Bp 210-215° Bp_{12} 88-90°.
Amide: Tribromoacetamide, 9CI
[594-47-8]
$C_2H_2Br_3NO$ 295.756
Isol. from the alga *Wrangelia* sp. Sol. Et_2O, hot EtOH.
Mp 122°. Sublimes.
Nitrile: Tribromoacetonitrile, 9CI. Tribromocyanomethane
[75519-19-6]
C_2Br_3N 277.741
Oil. Sol. EtOH, Et_2O, C_6H_6. Bp 170°.
Anhydride: [41936-89-4]
$C_4Br_6O_3$ 575.466
Solid (CCl_4). Mp 63-64°.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 509B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 793C (*nmr*)
Sadtler Standard C-13 NMR Spectra, 12470 (*cmr*)
Sadtler Standard Proton NMR Spectra, 41588 (*pmr*)
U.S. Pat., 1936, 2 057 964; *CA*, **31**, 112 (*synth*)
Köbrich, G. *et al., Chem. Ber.*, 1968, **101**, 3208 (*synth*)
McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367-374 (*Et ester, isol*)
Parkash, R. *et al., Bull. Chem. Soc. Jpn.*, 1991, **64**, 1443 (*anhydride*)
Márquez, F. *et al., Spectrosc. Lett.*, 1992, **25**, 821 (*ir, Raman*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **7**, 4992-4993 (*bromide, use*)
Kigoshi, H. *et al., Chem. Lett.*, 2004, 98-99 (*amide, isol*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 1040

2,3,5-Tribromo-1,4-benzenediol T-405

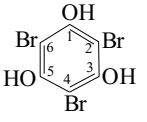
Tribromohydroquinone. Tribromoquinol
[23149-36-2]



$C_6H_3Br_3O_2$ 346.8
Constit. of the acorn worm *Ptychodera flava*. Needles ($CHCl_3$). Mp 136°. Luminescent.
Di-Ac: [23030-35-5]
$C_{10}H_7Br_3O_4$ 430.875
Mp 186-190°.
Sarauw, E. *et al., Annalen*, 1881, **209**, 116 (*synth*)
Terentev, A.P. *et al., Zh. Obshch. Khim.*, 1954, **24**, 1433; *CA*, **49**, 12353e (*synth*)
Higa, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **65**, 525 (*isol*)
Kanakubo, A. *et al., Bioorg. Med. Chem.*, 2005, **13**, 2741-2747 (*isol*)

2,4,6-Tribromo-1,3,5-benzenetriol T-406

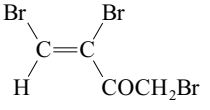
1,3,5-Tribromo-2,4,6-trihydroxybenzene. Tribromophloroglucinol
[3354-82-3]



$C_6H_3Br_3O_3$ 362.8
Constit. of the red alga *Rhabdonia verticillata*. Cryst. + $3H_2O$ (H_2O).
Mp 152-153° anhyd.
▶ SY1400000
Tri-Ac:
$C_{12}H_9Br_3O_6$ 488.911
Needles (EtOH). Mp 181-183°.
Tri-Me ether: 1,3,5-Tribromo-2,4,6-trimethoxybenzene
$C_9H_9Br_3O_3$ 404.88
Needles (EtOH). Mp 145°.
Herzig, K. *et al., Monatsh. Chem.*, 1902, **23**, 577 (*synth*)
Perkin, W.H. *et al., J.C.S.*, 1905, **87**, 855 (*synth*)
Blackman, A.J. *et al., Phytochemistry*, 1982, **21**, 2141 (*isol*)
Kiehlmann, E. *et al., Can. J. Chem.*, 1989, **67**, 335

1,3,4-Tribromo-3-buten-2-one T-407

[55716-02-4]



$C_4H_3Br_3O$ 306.779
(Z)-form [56020-85-0]
Constit. of the red seaweed *Asparagopsis taxiformis*.
Fenical, W. *et al., Tet. Lett.*, 1974, 4463 (*isol*)
Burreson, B.J. *et al., Tet. Lett.*, 1975, 473 (*isol*)

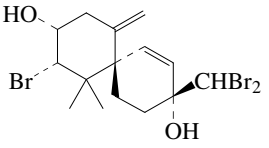
1,4,4-Tribromo-3-buten-2-one T-408

[59228-05-6]
$Br_2C{=}CHCOCH_2Br$
$C_4H_3Br_3O$ 306.779
Constit. of the red seaweed *Asparagopsis taxiformis*.
Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*isol*)

3,4,4-Tribromo-3-buten-2-one T-409

[70442-45-4]
$Br_2C{=}CBrCOCH_3$
$C_4H_3Br_3O$ 306.779
Constit. of the red seaweed *Asparagopsis taxiformis*.
Fenical, W. *et al., Proc. Int. Seaweed Symp.*, 1977, **9**, 387; *CA*, **91**, 14474

10,15,15-Tribromo-1,7(14)-chamigradiene-3,9-diol T-410
Mailiohydrin
[350247-76-6]



$C_{15}H_{21}Br_3O_2$ 473.042
Constit. of a *Laurencia* sp. Oil. $[\alpha]_D$ -9.6 (c, 0.26 in $CHCl_3$).

Francisco, N.E.Y. *et al., J. Nat. Prod.*, 2001, **64**, 790-791 (*isol, pmr, cmr*)

1,1,4-Tribromo-4-chloro-3-buten-2-one T-411
[59228-09-0]
$ClBrC{=}CHCOCHBr_2$
$C_4H_2Br_3ClO$ 341.224
Constit. of the red seaweed *Asparagopsis taxiformis.*

Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*isol*)

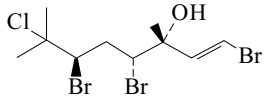
1,3,4-Tribromo-1-chloro-3-buten-2-one T-412
[55716-04-6]
$BrHC{=}CBrCOCHBrCl$
$C_4H_2Br_3ClO$ 341.224
Constit. of the red seaweed *Asparagopsis taxiformis.*

Fenical, W. *et al., Tet. Lett.*, 1974, 4463 (*isol*)

1,4,4-Tribromo-1-chloro-3-buten-2-one T-413
[59228-08-9]
$Br_2C{=}CHCOCHBrCl$
$C_4H_2Br_3ClO$ 341.224
Constit. of the red seaweed *Asparagopsis taxiformis.*

Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*isol*)

1,4,6-Tribromo-7-chloro-3,7-dimethyl-1-octen-3-ol T-414

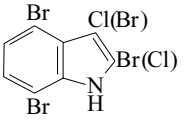


$C_{10}H_{16}Br_3ClO$ 427.4

(1*E*,3*R*,4*R*,6*R*)-*form* [52194-66-8]
Constit. of *Aplysia californica* and *Plocamium cartilagineum.*
Oil. $[\alpha]_D^{20}$ -64 (c, 2.25 in $CHCl_3$).

Faulkner, D.J. *et al., Tet. Lett.*, 1973, 1171-1174 (*isol*)
Willcott, M.R. *et al., Tet. Lett.*, 1973, 3967 (*struct*)
Stallard, M.O. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1974, **49**, 25-35; 37-41 (*isol*)
Mynderse, J.S. *et al., Tetrahedron*, 1975, **31**, 1963 (*isol*)
Faulkner, D.J. *et al., Tetrahedron*, 1977, **33**, 1421-1443

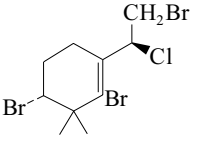
2,4,7(3,4,7)-Tribromo-3(2)-chloro-1*H*-indole, 9CI T-415
[68124-91-4]



$C_8H_3Br_3ClN$ 388.283
Alkaloid from the marine red alga *Rhodophyllis membranacea.*

Brennan, M.R. *et al., Tet. Lett.*, 1978, 1637 (*isol, pmr, struct*)
Ohta, T. *et al., Heterocycles*, 1989, **29**, 1663 (*synth*)

1,6,8-Tribromo-2-chloro-3(8)-ochtodene T-416
2,4-Dibromo-1-(2-bromo-1-chloroethyl)-3,3-dimethylcyclohexene, 9CI
[92632-96-7]



$C_{10}H_{14}Br_3Cl$ 409.385
Metab. of *Ochtodes secundiramea*. Oil. $[\alpha]_D$ +55 (c, 0.74 in $CHCl_3$).

Diastereoisomer:
$C_{10}H_{14}Br_3Cl$ 409.385
Constit. of *Portieria hornemannii*.
$[\alpha]_D$ +125 (c, 1 in $CHCl_3$).

Gerwick, W.H. *et al., Phytochemistry*, 1984, **23**, 1323
Fuller, R.W. *et al., J. Med. Chem.*, 1994, **34**, 4407-4411 (*isol, pmr, cmr*)

1,1,2-Tribromo-4-chloro-1-octen-3-one T-417
[64785-97-3]
$H_3C(CH_2)_3CHClCOCBr{=}CBr_2$
$C_8H_{10}Br_3ClO$ 397.331
Constit. of the seaweed *Delisea fimbriata*.

Rose, A.F. *et al., Tet. Lett.*, 1977, 1847 (*isol, synth, ir, pmr, cmr, ms*)

1,2,4-Tribromo-1-chloro-1-octen-3-one T-418
$H_3C(CH_2)_3CHBrCOCBr{=}CBrCl$
$C_8H_{10}Br_3ClO$ 397.331

(*E*)-*form* [64785-90-6]
Constit. of the seaweed *Bonnemaisonia asparagoides.* Antibacterial agent.

McConnell, O.J. *et al., Tet. Lett.*, 1977, 1851 (*isol, synth, ms*)

1,1,3-Tribromo-3-chloro-2-propanone, 9CI T-419
1,1,3-Tribromo-3-chloroacetone
[55716-01-3]
$Br_2CHCOCHBrCl$
$C_3H_2Br_3ClO$ 329.213
Minor component of the red algae *Asparagopsis taxiformis* and *Falkenbergia rufolanosa.* Liq.

Tetrahydrate:
Solid (EtOH aq.). Mp 64-65°.

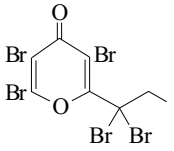
Moore, J.E. *et al., J.A.C.S.*, 1917, **39**, 974 (*synth*)
Fenical, W. *et al., Tet. Lett.*, 1974, 4463 (*isol, glc, ms*)
Bruneau, Y. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1978, **286**, 603
Combaut, G. *et al., Phytochemistry*, 1978, **17**, 1661 (*isol, glc*)

1,1,3-Tribromo-3-chloro-1-propene T-420
[56020-80-5]
$BrCHClCH{=}CBr_2$
$C_3H_2Br_3Cl$ 313.214
Isol. from the alga *Asparagopsis taxiformis.*

Burreson, B.J. *et al., Tet. Lett.*, 1975, 473 (*isol, ms*)
Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*isol*)

2,3,5-Tribromo-6-(1,1-dibromopropyl)-4*H*-pyran-4-one, 9CI T-421

[69267-70-5]

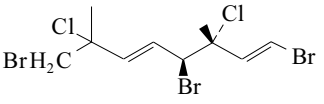


$C_8H_5Br_5O_2$ 532.646

Isol. from *Ptilonia australasica*. Prisms (EtOAc/hexane). Mp 98-99°. λ_{max} 238 (ϵ 15800); 275 (ϵ 11500) (MeOH) (Berdy).

Kazlauskas, R. *et al., Tet. Lett.*, 1978, 3165 (*struct, uv, ir, pmr, ms*)

1,4,8-Tribromo-3,7-dichloro-3,7-dimethyl-1,5-octadiene T-422



$C_{10}H_{13}Br_3Cl_2$ 443.83

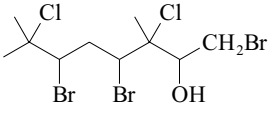
(1E,3R,4S,5E)-form [75207-35-1]

Constit. of *Aplysia californica*. Cryst. (MeOH). Mp 20°.

Ireland, C. *et al., J.O.C.*, 1976, **41**, 2461 (*isol*)
Stierle, D.B. *et al., Tetrahedron*, 1979, **35**, 2855 (*struct*)

1,4,6-Tribromo-3,7-dichloro-3,7-dimethyl-2-octanol, 9CI T-423

[96300-32-2]



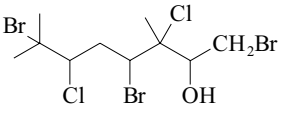
$C_{10}H_{17}Br_3Cl_2O$ 463.861

Constit. of *Plocamium cartilagineum*. Oil.

Blunt, J.W. *et al., Aust. J. Chem.*, 1985, **38**, 319

1,4,7-Tribromo-3,6-dichloro-3,7-dimethyl-2-octanol, 9CI T-424

[96300-31-1]

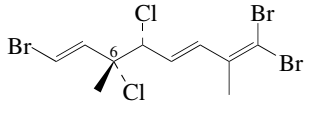


$C_{10}H_{17}Br_3Cl_2O$ 463.861

Constit. of *Plocamium cartilagineum*.

Blunt, J.W. *et al., Aust. J. Chem.*, 1985, **38**, 319

1,1,8-Tribromo-5,6-dichloro-2,6-dimethyl-1,3,7-octatriene T-425



(3*E*,5*R**,6*R**,7*E*)-*form*

$C_{10}H_{11}Br_3Cl_2$ 441.814

(3E,5R*,6R*,7E)-form [57766-80-0]

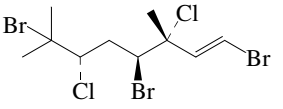
Constit. of the red alga *Plocamium cartilagineum*. $[\alpha]_D^{25}$ +44.1 (c, 1.2 in $CHCl_3$). λ_{max} 257 (pentane).

(3E,5R*,6S*,7E)-form [57766-81-1]

Constit. of *Plocamium cartilagineum*. $[\alpha]_D^{25}$ -34.7 (c, 1.1 in $CHCl_3$). λ_{max} 257 (pentane).

Mynderse, J.S. *et al., Tetrahedron*, 1975, **31**, 1963 (*isol, uv, pmr, ms*)

1,4,7-Tribromo-3,6-dichloro-3,7-dimethyl-1-octene T-426



$C_{10}H_{15}Br_3Cl_2$ 445.846

(1E,3R,4S,6S)-form

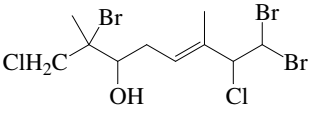
Anverene

[754983-90-9]

Constit. of *Plocamium cartilagineum*. Cryst. $[\alpha]_D^{25}$ -12 (c, 0.25 in $CHCl_3$). λ_{max} 198 (log ϵ 4.74) (no solvent reported).

Ankisetty, S. *et al., J. Nat. Prod.*, 2004, **67**, 1295-1302 (*isol, pmr, cmr, cryst struct, abs config*)

2,8,8-Tribromo-1,7-dichloro-2,6-dimethyl-5-octen-3-ol T-427



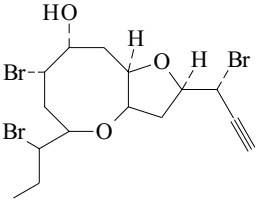
$C_{10}H_{15}Br_3Cl_2O$ 461.845

Ac: [477949-89-6]
$C_{12}H_{17}Br_3Cl_2O_2$ 503.883

Isol. from *Plocamium cartilagineum*. Oil.

Argandoña, V.H. *et al., J. Agric. Food Chem.*, 2002, **50**, 7029-7033 (*isol, pmr, cmr, ms*)

3,6,13-Tribromo-4,10:9,12-diepoxy-14-pentadecyn-7-ol T-428



$C_{15}H_{21}Br_3O_3$ 489.041

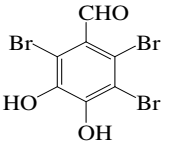
Incorrect struct. originally assigned. Metab. of *Laurencia obtusa*. Oil. $[\alpha]_D^{25}$ -8.2 (c, 0.09 in $CHCl_3$).

Ac: 9-Acetoxy-3,10,13-tribromo-4,7:6,12-diepoxy-1-pentadecyne [94444-25-4]
$C_{17}H_{23}Br_3O_4$ 531.078

Metab. of red alga *Laurencia obtusa*. Mobile oil. $[\alpha]_D$ -29.3 (c, 1.14 in $CHCl_3$).

Gonzalez, A.G. *et al., Tetrahedron*, 1984, **40**, 3443 (*isol*)
Norte, M. *et al., Tetrahedron*, 1989, **45**, 5987 (*struct*)

2,3,6-Tribromo-4,5-dihydroxybenzaldehyde T-429

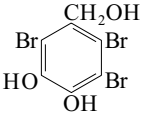


$C_7H_3Br_3O_3$ 374.811
Isol. from the red alga *Symphyocladia latiuscula*. Amorph. yellowish solid.
Mp 134-135°.

Wang, W. *et al., J. Nat. Prod.*, 2005, **68**, 620-622 (*isol, pmr, cmr, ms*)

2,3,6-Tribromo-4,5-dihydroxybenzyl alcohol T-430

3,4,6-Tribromo-5-(hydroxymethyl)-1,2-benzenediol, 9CI
[52897-67-3]



$C_7H_5Br_3O_3$ 376.827
Constit. of *Polysiphonia lanosa*, *Polysiphonia elongata*, *Symphyocladia latiuscula* and *Rhodomela subfusca*. Shows antibiotic props. DPPH radical scavenger. Antioxidant.
Mp 128-130°.

1′,4-Disulfate: [73731-88-1]
$C_7H_5Br_3O_9S_2$ 536.955
Constit. of the red alga *Symphyocladia latiuscula*. Fine needles (as di-Na salt).

1′-Me ether: 3,4,6-Tribromo-5-(methoxymethyl)-1,2-benzenediol, 9CI. 2,3,6-Tribromo-4,5-dihydroxybenzyl methyl ether
[256474-80-3]
$C_8H_7Br_3O_3$ 390.854
Constit. of *Symphyocladia latiuscula*.

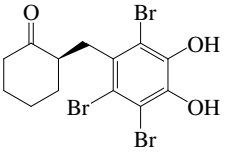
5-Me ether: 2,3,6-Tribromo-4-hydroxy-5-methoxybenzyl alcohol
[73731-89-2]
$C_8H_7Br_3O_3$ 390.853
Mp 152-153°.

4,5-Di-Me ether: 2,3,6-Tribromo-4,5-dimethoxybenzyl alcohol
$C_9H_9Br_3O_3$ 404.88
Mp 122-123°.

Glombitza, K.W. *et al., Planta Med.*, 1974, **25**, 105 (*occur*)
Pedersen, M. *et al., Phytochemistry*, 1978, **17**, 291
Kurata, K. *et al., Chem. Lett.*, 1980, 279 (*1′,4-disulfate*)
Park, H.J. *et al., CA*, 2000, **132**, 134756d (*1′-Me ether*)
Choi, J.S. *et al., J. Nat. Prod.*, 2000, **63**, 1705-1706 (*activity*)
Chung, H.Y. *et al., J. Agric. Food Chem.*, 2001, **49**, 3614-3621 (*1′-Me ether*)

2-(2,3,6-Tribromo-4,5-dihydroxybenzyl)cyclohexanone T-431

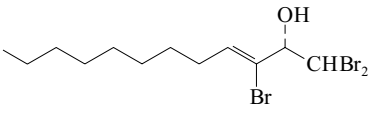
Symphyoketone



$C_{13}H_{13}Br_3O_3$ 456.956

(R)-form
Constit. of the red alga *Symphyocladia latiuscula*. Antioxidant. Amorph. powder. $[\alpha]_D^{23}$ +7.3 (c, 0.11 in MeOH). λ_{max} 236 (sh) (log ϵ 4.09); 260 (sh) (log ϵ 3.34); 287 (sh) (log ϵ 3.3); 296 (log ϵ 3.41) (MeOH).
Choi, J.S. *et al., J. Nat. Prod.*, 2000, **63**, 1705-1706 (*isol, pmr, cmr*)

1,1,3-Tribromo-3-dodecen-2-ol T-432



$C_{12}H_{21}Br_3O$ 421.009

(2S,3Z)-form [145382-73-6]
Constit. of the red alga *Delisea pulchra*.
Yellow oil. $[\alpha]_D$ -40 (c, 0.1 in EtOH).
De Nys, R. *et al., Aust. J. Chem.*, 1992, **45**, 1625 (*isol, pmr, cmr*)

1,1,3-Tribromo-2-heptanol T-433

[69394-11-2]
$H_3C(CH_2)_3CHBrCH(OH)CHBr_2$
$C_7H_{13}Br_3O$ 352.891
Isol. from *Bonnemaisonia hamifera*.

Ac: [69394-13-4]
$C_9H_{15}Br_3O_2$ 394.928
Constit. of *Bonnemaisonia hamifera*.

Jacobsen, N. *et al., Tet. Lett.*, 1978, **19**, 3065-3068 (*isol*)
McConnell, O.J. *et al., Phytochemistry*, 1980, **19**, 233-247 (*isol, ms*)

1,3,3-Tribromo-2-heptanol T-434

[69394-10-1]
$H_3C(CH_2)_3CBr_2CH(OH)CH_2Br$
$C_7H_{13}Br_3O$ 352.891

(ξ)-form
Isol. from *Bonnemaisonia hamifera*.

Ac: [69549-56-0]
$C_9H_{15}Br_3O_2$ 394.928
Constit. of *Bonnemaisonia hamifera*.

Jacobsen, N. *et al., Tet. Lett.*, 1978, **19**, 3065-3068 (*isol*)
McConnell, O.J. *et al., Phytochemistry*, 1980, **19**, 233-247 (*isol, ms*)

1,1,3-Tribromo-2-heptanone T-435

[54899-95-5]
$H_3C(CH_2)_3CHBrCOCHBr_2$
$C_7H_{11}Br_3O$ 350.875
Constit. of red alga *Bonnemaisonia hamifera*.

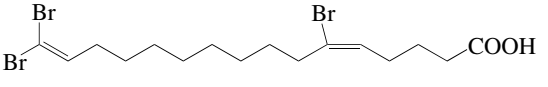
Siuda, J.F. *et al., J.A.C.S.*, 1975, **97**, 937 (*isol, ms*)

1,3,3-Tribromo-2-heptanone T-436

[54899-96-6]
$H_3C(CH_2)_3CBr_2COCH_2Br$
$C_7H_{11}Br_3O$ 350.875
Constit. of red alga *Bonnemaisonia hamifera*.

Siuda, J.F. *et al., J.A.C.S.*, 1975, **97**, 937 (*isol, ms*)

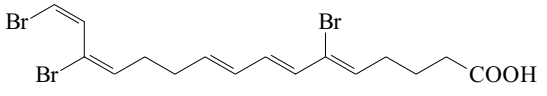
6,16,16-Tribromo-5,15-hexadecadienoic acid T-437



$C_{16}H_{25}Br_3O_2$ 489.084

(E)-form
cis-*form*
[162259-46-3]
Isol. from the sponge *Xestospongia* sp.
Li, Y. *et al., J. Chem. Res., Synop.*, 1995, 126-127 (*isol*)

6,14,16-Tribromo-5,7,9,13,15-hexadecapentaenoic acid T-438

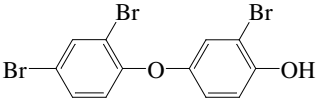


$C_{16}H_{19}Br_3O_2$ 483.037

(5Z,7E,9E,13E,15Z)-form [152543-02-7]
Isol. from the sponge *Oceanapia* sp. λ_{max} 208 (ϵ 4600); 264 (ϵ 11700); 272 (ϵ 14600); 284 (ϵ 11900) (MeOH) (Berdy).
Ichiba, T. *et al., Helv. Chim. Acta*, 1993, **76**, 2814 (*isol, pmr, cmr, uv, ir*)

2,3′,4-Tribromo-4′-hydroxydiphenyl ether T-439

2-Bromo-4-(2,4-dibromophenoxy)phenol, 9CI. ***Corallinaether***



$C_{12}H_7Br_3O_2$ 422.898
Isol. from crustose coralline red algae. Oil.
Kitamura, M. *et al., Chem. Lett.*, 2005, **34**, 1272-1273 (*isol, pmr, cmr*)

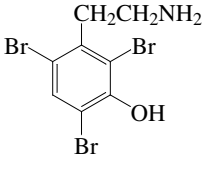
1,1,2-Tribromo-6-hydroxy-1-octen-3-one T-440

$H_3CCH_2CH(OH)CH_2CH_2COCBr{=}CBr_2$
$C_8H_{11}Br_3O_2$ 378.886

(±)-form
Ac: ***6-Acetoxy-1,1,3-tribromo-1-octen-3-one***
[145382-74-7]
$C_{10}H_{13}Br_3O_3$ 420.923
Constit. of the red alga *Delisea pulchra*. Yellow oil.
De Nys, R. *et al., Aust. J. Chem.*, 1992, **45**, 1625

2,4,6-Tribromo-3-hydroxyphenethylamine T-441

3-(2-Aminoethyl)-2,4,6-tribromophenol, 9CI. 2-(2,4,6-Tribromo-3-hydroxyphenyl)ethylamine



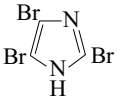
$C_8H_8Br_3NO$ 373.869

Me ether, N-*formyl: 2,4,6-Tribromo*-N-*formyl-3-methoxyphenethylamine.* ***Lutamide A***
[294210-56-3]
$C_{10}H_{10}Br_3NO_2$ 415.907
Alkaloid from the marine bryozoan *Amathia convoluta*. Needles (EtOH).
Mp 105°.

N,O-*Di-Me,* N-*formyl: 2,4,6-Tribromo*-N-*formyl-3-methoxy*-N-*methylphenethylamine.* ***Lutamide C***
[294210-58-5]
$C_{11}H_{12}Br_3NO_2$ 429.933
Alkaloid from the marine bryozoan *Amathia convoluta*. Needles (EtOH).
Mp 69-70°.
Hashima, H. *et al., Bioorg. Med. Chem.*, 2000, **8**, 1757-1766 (*Lutamides*)

2,4,5-Tribromo-1*H*-imidazole, 9CI T-442

Tribromoglyoxaline
[2034-22-2]



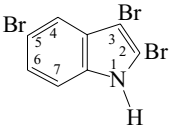
$C_3HBr_3N_2$ 304.766
Isol. from the egg masses of the molluscs *Ceratosoma erinaceum*, *Trophon geversianus* and *Trunculariopsis trunculus.* Silky needles (AcOH).
Mp 221°.

▶ Exp. neurotoxic props. LD_{50} (rat, orl) 34 mg/kg. NI8660000

1-Me: [1003-91-4]
$C_4H_3Br_3N_2$ 318.793
Cryst. (AcOH aq.). Mp 88-89°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 616D (*ir*)
Balaban, E. *et al., J.C.S.*, 1922, 947 (*synth*)
Stensiö, K.-E. *et al., Acta Chem. Scand.*, 1973, **27**, 2179 (*synth*)
Verschoyle, R.D. *et al., Arch. Toxicol.*, 1984, **56**, 109 (*neurotox*)
Iddon, B. *et al., Chem. Comm.*, 1985, 1428 (*deriv, synth*)
Iddon, B. *et al., Tet. Lett.*, 1986, **27**, 1635 (*haz, use*)
Iddon, B. *et al., J.C.S. Perkin 1*, 1987, 1445 (*tox, props*)
O'Connell, J.F. *et al., Synthesis*, 1988, 767 (*synth, ir, pmr*)
Benkendorff, K. *et al., Nat. Prod. Res.*, 2004, **18**, 427-431 (*isol, synth, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, THV450

2,3,5-Tribromo-1*H*-indole, 9CI T-443



$C_8H_4Br_3N$ 353.838

N-*Me:* ***2,3,5-Tribromo-1-methyl-1H-indole***
[70063-25-1]
$C_9H_6Br_3N$ 367.865
Alkaloid from the alga *Laurencia brongniartii* and from *Aplysia dactylomela*. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O.
Mp 120-122°. λ_{max} 228 (ϵ 34000); 282 (ϵ 7300); 290 (ϵ 10000); 297 (ϵ 8000); 300 (sh) (EtOH) (Derep).
Carter, G.T. *et al., Tet. Lett.*, 1978, 4479-4482 (*isol, uv, pmr, ms, struct*)
Liu, Y. *et al., J. Nat. Prod.*, 2002, **65**, 748-749 (*synth*)

2,3,6-Tribromo-1*H*-indole, 9CI T-444

$C_8H_4Br_3N$ 353.838

N-*Me:* ***2,3,6-Tribromo-1-methyl-1H-indole***
[70063-24-0]
$C_9H_6Br_3N$ 367.865
Alkaloid from the alga *Laurencia brongniartii*.
Mp 90.5-91°. λ_{max} 230 (ϵ 39000); 288 (ϵ 10000); 294 (ϵ 10000) (EtOH) (Derep).
Carter, G.T. *et al., Tet. Lett.*, 1978, 4479 (*isol, uv, pmr, cmr, ms, struct*)

2,3,7-Tribromo-1*H*-indole, 9CI T-445

[68234-21-9]

$C_8H_4Br_3N$ 353.838
Alkaloid from the marine red alga *Rhodophyllis membranacea*.
Mp 115-116°.
Brennan, M.R. *et al., Tet. Lett.*, 1978, 1637 (*isol, pmr, struct*)
Erickson, K.L. *et al., Synth. Commun.*, 1981, **11**, 253 (*synth, ir, pmr, ms*)

2,4,6-Tribromo-1*H*-indole, 9CI T-446

[128367-88-4]

$C_8H_4Br_3N$ 353.838

Alkaloid from the Okinawan red alga *Laurencia brongniartii*.

Cryst. (hexane/CCl_4).

Mp 106-113°.

Tanaka, J. *et al., Tetrahedron*, 1989, **45**, 7301 (*isol, ir, pmr, ms, struct*)

3,4,6-Tribromo-1*H*-indole, 9CI T-447

Balanoglossol

[74076-58-7]

$C_8H_4Br_3N$ 353.838

Isol. from *Balanoglossus carnosus*.

Mp 95° (89-90° dec.).

Ac:

$C_{10}H_6Br_3NO$ 395.876

Mp 240-242°.

Higa, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **65**, 525-530 (*isol, pmr, ms, struct*)
Ohta, T. *et al., Heterocycles*, 1987, **26**, 2817-2822 (*synth*)
Martin, P. *et al., Tet. Lett.*, 1987, **28**, 1645-1647 (*synth*)
Higa, T. *et al., Tetrahedron*, 1987, **43**, 1063-1070 (*isol, pmr*)
Martin, P. *et al., Helv. Chim. Acta*, 1988, **71**, 344-347 (*synth, pmr*)

3,5,7-Tribromo-1*H*-indole, 9CI T-448

[59025-61-5]

$C_8H_4Br_3N$ 353.838

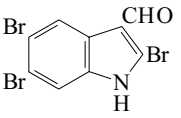
Isol. from the hemichordates *Ptychodera flava laysanica* and *Ptychodera flava*.

Mp 120-122°.

Higa, T. *et al., Heterocycles*, 1976, **4**, 231 (*synth, pmr, ms*)
Higa, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **65**, 525 (*occur*)

2,5,6-Tribromo-1*H*-indole-3-carboxaldehyde T-449

2,5,6-Tribromo-3-formylindole



$C_9H_4Br_3NO$ 381.849

N-*Me: 2,5,6-Tribromo-1-methyl-1*H-*indole-3-carboxaldehyde*

[85908-67-4]

$C_{10}H_6Br_3NO$ 395.875

Alkaloid from the marine bryozoan *Zoobotryon verticillatum*. Delays the metamorphosis in fertilised sea urchin eggs at low concentrations.

Mp 228.5-229.5°. λ_{max} 223 (ϵ 18100); 256 (ϵ 13700); 309 (ϵ 6900) (MeOH) (Berdy).

Ortega, M.J. *et al., J. Nat. Prod.*, 1993, **56**, 633-636 (*isol, uv, ir, pmr, cmr, ms, struct*)

1,3,3-Tribromo-1-iodo-1-propene T-450

[56020-82-7]

$Br_2CHCH{=}CBrI$

$C_3H_2Br_3I$ 404.665

Isol. from the alga *Asparagopsis taxiformis*.

Burreson, B.J. *et al., Tet. Lett.*, 1975, 473 (*isol, ms*)
Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*isol*)

Tribromomethane, 9CI, 8CI T-451

Bromoform. Methyl tribromide

[75-25-2]

$CHBr_3$

$CHBr_3$ 252.731

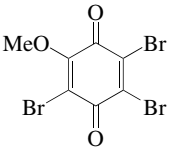
Synth. by bromination of Me_2CO or EtOH in the presence of base. Constit. of the red algae *Asparagopsis* spp. and *Falkenbergia rufolanosa*. Intermed. in org. synth., solvent for waxes, greases and oils. Antitussive; sedative. Heavy liq., non-flammable. d_4^{20} 2.89. Mp 9° (7.7°). Bp 150.3-151.2° (149.5°). n_D^{20} 1.5959. Stabilised by addn. of 4% EtOH. Reacts violently with Me_2CO in presence of base. Federally controlled subst.

▶ Vapour is a lachrymator and respiratory tract irritant. Liquid is a skin irritant. Exp. neoplastic agent. Hepatotoxic. LD_{50} (rat, orl) 1147 mg/kg. OES: long-term 0.5 ppm (Sk). PB5600000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 83B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 123A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 117B (*ir*)
Aldrich Library of NMR Spectra, **1**, 64B (*pmr*)
Soroos, H. *et al., J.A.C.S.*, 1945, **67**, 1642 (*synth*)
Kergomard, A. *et al., Bull. Soc. Chim. Fr.*, 1961, 2360 (*synth*)
Kawaguchi, T. *et al., Acta Cryst. B*, 1972, **28**, 967 (*cryst struct*)
McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367 (*isol*)
Combaut, G. *et al., Phytochemistry*, 1978, **17**, 1661 (*isol*)
Kimura, M. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 2747 (*struct*)
Dostovalova, V.I. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1985, 2467; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1985, 2282 (*cmr*)
Tate, R. *et al., Z. Naturforsch., A*, 1986, **41**, 1091 (*uv*)
IARC Monog., 1991, **52**, 213 (*rev, tox*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 731-735 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 3469 (*tox*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0350
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 172
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BNL000

2,3,5-Tribromo-6-methoxy-1,4-benzoquinone T-452

2,3,5-Tribromo-6-methoxy-2,5-cyclohexadiene-1,4-dione



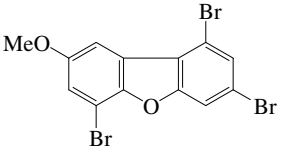
$C_7H_3Br_3O_3$ 374.811

Isol. from *Ptychodera flava laysanica*.

Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 22 (*occur*)

1,3,6-Tribromo-8-methoxydibenzofuran T-453

Corallinafuran



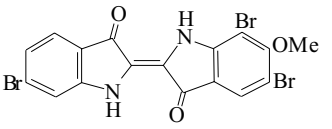
$C_{13}H_7Br_3O_2$ 434.909

Isol. from crustose coralline red algae. Powder.

Kitamura, M. *et al., Chem. Lett.*, 2005, **34**, 1272-1273 (*isol, pmr, cmr*)

5,6′,7-Tribromo-6-methoxyindigotin T-454

[58933-46-3]



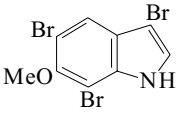
$C_{17}H_9Br_3N_2O_3$ 528.982

Pigment from the marine invertebrate *Ptychodera flava laysanica*. Purple-blue powder.
Mp 300°.

Higa, T. *et al., Heterocycles*, 1976, **4**, 227 (*isol, uv, struct*)

3,5,7-Tribromo-6-methoxy-1*H*-indole, 9CI T-455

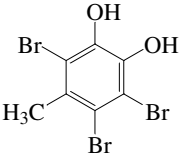
6-Methoxy-3,5,7-tribromoindole
[74076-57-6]



$C_9H_6Br_3NO$ 383.864
Isol. from the hemichordate *Ptychodera flava*.
Mp 110-112°.

Higa, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **65**, 525 (*isol, pmr, ms, struct*)

3,4,6-Tribromo-5-methyl-1,2-benzenediol T-456

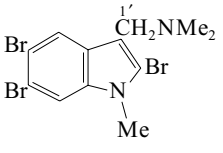


$C_7H_5Br_3O_2$ 360.827
Isol. from the red alga *Symphyocladia latiuscula*. Yellowish amorph. powder.
Mp 126-129°.

Wang, W. *et al., J. Nat. Prod.*, 2005, **68**, 620-622 (*isol, pmr, cmr, ms*)

2,5,6-Tribromo-*N*-methylgramine T-457

*2,5,6-Tribromo-*N,N*,1-trimethyl-1*H*-indole-3-methanamine, 9CI*.
2,5,6-Tribromo-3-(dimethylaminomethyl)-1-methylindole
[64945-29-5]



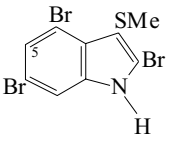
$C_{12}H_{13}Br_3N_2$ 424.96
Alkaloid from the subtropical marine bryozoan *Zoobotryon verticillatum* and *Zoobotryon pellucidum*. Toxic to brine shrimp. Larval settlement inhibitor. Antifouling agent. Cryst. (MeOH). Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 112-113°. λ_{max} 232 (ϵ 46800); 298 (ϵ 9900); 308 (ϵ 9100) (MeOH) (Berdy). λ_{max} 232 (ϵ 46000); 298 (ϵ 9700); 307 (ϵ 9000) (EtOH) (Berdy).

1′-N- *Oxide:* ***2,5,6-Tribromo*-N-*methylgramine* N-*oxide***
[85908-65-2]
$C_{12}H_{13}Br_3N_2O$ 440.959
Alkaloid from *Zoobotryon verticillatum*. Toxic to brine shrimp. Cryst. (MeOH aq.). Sol. MeOH, EtOAc; poorly sol. H_2O.
Mp 116-120° dec. λ_{max} 230 (ϵ 38800); 294 (ϵ 11800); 306 (ϵ 10700) (MeOH) (Berdy).

DaSettino, A. *et al., Chim. Ind. (Milan)*, 1977, **59**, 454; *CA*, **87**, 201244c (*synth*)
Sato, A. *et al., Tet. Lett.*, 1983, **24**, 481-484 (*isol, uv, ir, pmr, cmr, ms, struct, synth*)
Kon-Ya, K. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 2178-2181

2,4,6-Tribromo-3-methylthio-1*H*-indole T-458

[128351-83-7]



$C_9H_6Br_3NS$ 399.931
Isol. from a Taiwanese collection of the red alga *Laurencia brongniartii*. Also found in the Okinawan red alga *Laurencia grevilleana* (possibly synonymous with *Laurencia brongniartii*).

S-*Oxide: 2,4,6-Tribromo-3-(methylsulfinyl)-1*H*-indole*
$C_9H_6Br_3NOS$ 415.931
Isol. from *Laurencia brongniartii*.
Mp 102-104°. λ_{max} 236 (log ϵ 4.7); 312 (log ϵ 4.1) (MeOH).

5-Bromo: ***2,4,5,6-Tetrabromo-3-methylthio-1*H*-indole***
[128351-84-8]
$C_9H_5Br_4NS$ 478.827
Isol. from *Laurencia brongniartii* and *Laurencia grevilleana* (? *Laurencia brongniartii*).

Tanaka, J. *et al., Tetrahedron*, 1989, **45**, 7301-7310 (*Laurencia brongniartii constits*)
El-Gamal, A.A. *et al., J. Nat. Prod.*, 2005, **68**, 815-817 (*S-oxide*)

1,1,3-Tribromo-2-nonanone, 9CI T-459

[66002-51-5]
$H_3C(CH_2)_5CHBrCOCHBr_2$
$C_9H_{15}Br_3O$ 378.929
Isol. from *Bonnemaisonia nootkana*.

Fenical, W. *et al., Proc. Int. Seaweed Symp.*, 1977, **9**, 387-400; *CA*, **91**, 14474y (*isol*)

1,1,2-Tribromo-1-octen-3-ol T-460

[64786-00-1]
$H_3C(CH_2)_4CH(OH)CBr{=}CBr_2$
$C_8H_{13}Br_3O$ 364.902

(±)-form
Oil.
Ac: [186344-78-5]
$C_{10}H_{15}Br_3O_2$ 406.939
Isol. from the alga *Delisea fimbriata*. Oil.

Rose, A.F. *et al., Tet. Lett.*, 1977, 1847-1850 (*synth*)
Cueto, M. *et al., J. Nat. Prod.*, 1997, **60**, 279-281 (*isol, acetate*)

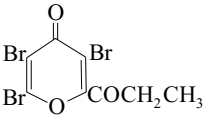
1,1,2-Tribromo-1-octen-3-one T-461

[64785-96-2]
$H_3C(CH_2)_4COCBr{=}CBr_2$
$C_8H_{11}Br_3O$ 362.886
Constit. of the seaweed *Delisea fimbriata*. λ_{max} 220 (ϵ 7000); 283 (ϵ 1080) (MeOH) (Berdy).

Rose, A.F. *et al., Tet. Lett.*, 1977, 1847 (*isol, synth, ir, pmr, cmr, ms*)

2,3,5-Tribromo-6-(1-oxopropyl)-4*H*-pyran-4-one, 9CI T-462

*3,5,6-Tribromo-2-propanoyl-4*H*-pyran-4-one*
[69267-71-6]



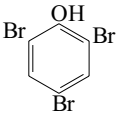
$C_8H_5Br_3O_3$ 388.838

Metab. of *Ptilonia australasica*. Solid.
Mp 155-156°.

Kazlauskas, R. *et al., Tet. Lett.*, 1978, 3165-3168 (*isol, ir, pmr, ms*)

2,4,6-Tribromophenol, 9CI, 8CI T-463

Bromol. Flammex 3BP. Velcide
[118-79-6]
[25376-38-9]



$C_6H_3Br_3O$ 330.801

The synonym Velcide refers to the Na salt. Isol. from a marine acorn worm *Ptychodera flava laysanica*, the green alga *Ulva lactuca*, molluscs and crustaceans. Used as 5-7% soln. in KOH for gravimetric detn. of Pd(*II*) or Pt(*II*) (in NH_3 soln., as $[M(NH_3)_4][OC_6H_2Br_3]_2$). Flavour component of seafood, imparts an intense shrimp-like flavour. Strong antiseptic. Needles (EtOH), prisms (C_6H_6). Sol. alkalis, EtOH, petrol.
Mp 87-89°. Subl. 95-96. λ_{max} 288; 297 (EtOH) (Berdy).
▶ Potent irritant. LD_{50} (rat, orl) 2000 mg/kg. SN1225000

Ac: [607-95-4]
$C_8H_5Br_3O_2$ 372.838
Plates or needles (EtOH). Mp 87°.

Benzoyl: [24003-13-2]
$C_{13}H_7Br_3O_2$ 434.909
Needles (EtOH). Mp 81°.

4-Methylbenzenesulfonyl: [2437-48-1]
$C_{13}H_9Br_3O_3S$ 484.99
Cryst. (EtOH). Mp 113°.

Me ether: 1,3,5-Tribromo-2-methoxybenzene, 9CI. 2,4,6-Tribromoanisole
[607-99-8]
$C_7H_5Br_3O$ 344.828
Constit. of the red alga *Polysiphonia sphaerocarpa*. Needles (EtOH).
Mp 88°.

Et ether: 1,3,5-Tribromo-2-ethoxybenzene, 9CI. 2,4,6-Tribromophenetole
[98437-52-6]
$C_8H_7Br_3O$ 358.855
Prisms (EtOH). Mp 72-73°.

2-Propenyl ether: 1,3,5-Tribromo-2-(2-propenyloxy)benzene, 9CI. Allyl 2,4,6-tribromophenyl ether
[3278-89-5]
$C_9H_7Br_3O$ 370.866
Needles. Mp 77°.

[2666-53-7, 3784-04-1, 78697-30-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1098D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 291B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1034C (*ir*)
Buraway, A. *et al., J.C.S.*, 1952, 2310 (*uv*)
Hutton, H.M. *et al., Can. J. Chem.*, 1962, **40**, 1758 (*cmr*)
Kaemmerer, H. *et al., Spectrochim. Acta A*, 1968, **44**, 2059 (*uv*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 424 (*use*)
Higa, T. *et al., Experientia*, 1975, **62**, 395-396 (*isol*)
Faniran, J.A. *et al., J. Raman Spectrosc.*, 1980, **9**, 73 (*ir, Raman*)
Volkov, V.E. *et al., Zh. Anal. Khim.*, 1981, **36**, 1853 (*detn, Pd, Pt*)
He, C.-H. *et al., Tetrahedron*, 1987, **43**, 1063-1070 (*isol*)
Wang, M.L. *et al., Ind. Eng. Chem. Res.*, 1990, **29**, 522 (*allyl ether, synth*)
Olszanowski, A. *et al., J. Prakt. Chem.*, 1990, **332**, 1093 (*synth*)
Boyle, J.L. *et al., J. Food Sci.*, 1992, **57**, 918-922 (*occur*)
Corgiat, J.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1993, **106**, 83-86 (*Ptychodera bahamensis constit*)
Whitfield, F.B. *et al., J. Agric. Food Chem.*, 1997, **45**, 4398-4405; 1999, **47**, 2367-2373 (*occur*)
Flodin, C. *et al., Phytochemistry*, 1999, **51**, 249-255; 2000, **53**, 77-80 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, THV750

1,1,1-Tribromo-2-propanone, 9CI, 8CI T-464

1,1,1-Tribromoacetone
[3770-98-7]
Br_3CCOCH_3
$C_3H_3Br_3O$ 294.768
Isol. from the alga *Asparagopsis taxiformis*. d_4^{20} 2.33.
Mp 26°. Bp 255° dec. Bp_{14} 128-129°.

Rappe, C. *et al., Ark. Kemi*, 1963, **21**, 503 (*synth*)
Cox, R.A. *et al., Can. J. Chem.*, 1972, **50**, 3242 (*synth, pmr*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)

1,1,3-Tribromo-2-propanone, 9CI, 8CI T-465

1,1,3-Tribromoacetone
[3475-39-6]
$Br_2CHCOCH_2Br$
$C_3H_3Br_3O$ 294.768
Constit. of the red algae *Asparagopsis* spp. and *Falkenbergia rufolanosa*.
Mp 30-30.5°. Bp_{14} 114-116° Bp_9 107-107.5°.

Weygand, F. *et al., Chem. Ber.*, 1949, **82**, 33 (*synth*)
Rappe, C. *et al., Ark. Kemi*, 1963, **21**, 503 (*synth*)
Bruneau, Y. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1978, **286**, 603 (*occur*)

2,3,3-Tribromo-2-propenoic acid, 9CI T-466

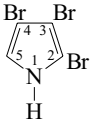
2,3,3-Tribromoacrylic acid, 8CI
[71815-46-8]
$Br_2C{=}CBrCOOH$
$C_3HBr_3O_2$ 308.752
Minor component of the Hawaiian red alga *Asparagopsis taxiformis*. Yellowish hexagonal prisms (heptane).
Mp 119-120°.

Me ester:
$C_4H_3Br_3O_2$ 322.778
Liq. $Bp_{0.8}$ 60°.

Strauss, F. *et al., Ber., B*, 1930, **63**, 1868 (*synth*)
Levas, M. *et al., Bull. Soc. Chim. Fr.*, 1959, 1800 (*synth*)
Castro, C.E. *et al., J.O.C.*, 1965, **30**, 587 (*synth, pmr, ir*)
Roedig, A. *et al., Annalen*, 1967, **710**, 7 (*synth*)
Woolard, F.X. *et al., Phytochemistry*, 1979, **18**, 617 (*isol, synth, glc, Me ester*)

2,3,4-Tribromo-1*H*-pyrrole T-467

[69624-12-0]



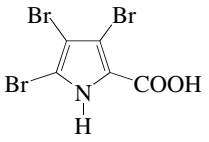
$C_4H_2Br_3N$ 303.778
Isol. from the marine polychaete *Polyphysia crassa* and *Saccoglossus kowalevskii*. Possesses antibacterial and antifeedant activity. Pale yellow oil. Dec. slowly above -18° in soln.

N-*Sulfonic acid:* [162821-17-2]
$C_4H_2Br_3NO_3S$ 383.843
Isol. from *Saccoglossus kowalevskii*. Isol. as Na salt, to which CAS no. refers.

Emrich, R. *et al., J. Nat. Prod.*, 1990, **53**, 703-705 (*isol, pmr, ms, synth*)
Martin, P. *et al., Marine Ecol.: Progr. Ser.*, 1995, **116**, 125-136; *CA*, **122**, 261393 (*1-sulfonic acid*)
John, E.A. *et al., J. Nat. Prod.*, 2004, **67**, 1929-1931 (*synth*)
Kicklighter, C.E. *et al., Limnol. Oceanogr.*, 2004, **49**, 430-441 (*isol, activity*)

3,4,5-Tribromo-1*H*-pyrrole-2-carboxylic acid T-468

[74039-30-8]



$C_5H_2Br_3NO_2$ 347.788
Isol. from an Australian sponge *Axinella* sp. Plates (H_2O).
Mp 192-195°. λ_{max} 258 (ϵ 12800) (MeOH).

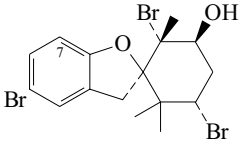
Me ester: [1198-67-0]
$C_6H_4Br_3NO_2$ 361.815
Cryst. (hexane). Mp 212-214°.

N-*Me: 3,4,5-Tribromo-1-methyl-1*H*-pyrrole-2-carboxylic acid*
[150314-26-4]
$C_6H_4Br_3NO_2$ 361.815
Isol. from an *Axinella* sp. Cryst.
Mp 175-176° dec. λ_{max} 254 (ϵ 13700); 272 (ϵ 4400) (MeOH).

Hodge, P. *et al., J.C.S.*, 1965, 459-470 (*synth, ester*)
Tashiro, M. *et al., J. Chem. Res., Synop.*, 1988, 136-137 (*synth*)
Barrow, R.A. *et al., Nat. Prod. Lett.*, 1993, **1**, 243-250 (*isol, synth, cmr*)

Tribromospirocacoxanthene T-469

*2′,5,5′-Tribromo-2′,6′,6′-trimethylspiro[benzofuran-2(3*H*),1′-cyclohexan]-3′-ol*
[132268-25-8]



$C_{16}H_{19}Br_3O_2$ 483.037
Constit. of a *Cacospongia* sp. Oil. $[\alpha]_D$ -32.4 (c, 0.153 in $CHCl_3$).

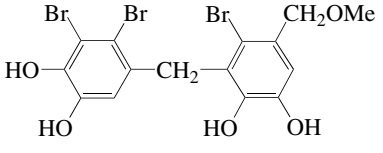
Ac: ***Acetyltribromospirocacoxanthene***
[132244-40-7]
$C_{18}H_{21}Br_3O_3$ 525.074
Constit. of a *Cacospongia* sp. Oil. $[\alpha]_D$ -21.6 (c, 0.473 in $CHCl_3$).

7-Bromo: ***Tetrabromospirocacoxanthene****. 2′,5,5′,7-Tetrabromo-2′,6′,6′-trimethylspiro[benzofuran-2(3*H*),1′-cyclohexan]-3′-ol*
[132244-39-4]
$C_{16}H_{18}Br_4O_2$ 561.933
Constit. of a *Cacospongia* sp. Solid. $[\alpha]_D$ +33.7 (c, 0.601 in $CHCl_3$).

Bali, D.K.L. *et al., Aust. J. Chem.*, 1990, **43**, 2009 (*isol, pmr, cmr*)

2,2′,3-Tribromo-4,5,5′,6′-tetrahydroxy-3′-(methoxymethyl)diphenylmethane T-470

4-Bromo-3-[(2,3-dibromo-4,5-dihydroxyphenyl)methyl]-5-methoxymethyl-1,2-benzenediol, 9CI
[192721-71-4]

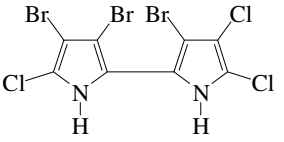


$C_{15}H_{13}Br_3O_5$ 512.977
Isol. from the red alga *Odonthalia corymbifera*. Gum.

Tetra-Ac: [192721-72-5]
Cryst. (MeOH). Mp 195-196°.

Kurata, K. *et al., Phytochemistry*, 1997, **45**, 485-487 (*isol, ir, pmr*)

3,3′,4-Tribromo-4′,5,5′-trichloro-2,2′-bi-1*H*-pyrrole T-471

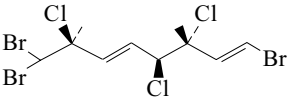


$C_8H_2Br_3Cl_3N_2$ 472.187

N,N′-*Di-Me: 3,3′,4-Tribromo-4′,5,5′-trichloro-1,1′-dimethyl-2,2′-bi-1*H*-pyrrole. DBP-Br_3Cl_3*
[400766-93-0]
$C_{10}H_6Br_3Cl_3N_2$ 500.241
Marine natural product of unknown biogenic origin. Present in marine or freshwater fish, shrimps, seabirds and seal blubber.

Tittlemier, S.A. *et al., Environ. Pollut.*, 2002, **116**, 85-93 (*N,N′-di-Me, occur, detn*)
Tittlemier, S.A. *et al., J. Agric. Food Chem.*, 2004, **52**, 2010-2015 (*N,N′-di-Me, occur, detn*)

1,8,8-Tribromo-3,4,7-trichloro-3,7-dimethyl-1,5-octadiene T-472



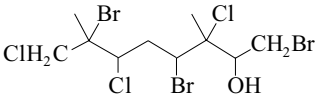
$C_{10}H_{12}Br_3Cl_3$ 478.275

(1E,3R,4S,5E,7S)-form [51212-86-3]
Constit. of *Aplysia californica* and *Plocamium cartilagineum*.
Antifouling agent. Cryst. (MeOH).
Mp 54°. $[\alpha]_D^{23}$ -50.2 (c, 1.0 in $CHCl_3$).

Faulkner, D.J. *et al., J.A.C.S.*, 1973, **95**, 3413-3414 (*cryst struct, isol*)
Mynderse, J.S. *et al., Tetrahedron*, 1975, **31**, 1963 (*isol*)
Faulkner, D.J. *et al., Tetrahedron*, 1977, **33**, 1421-1443
Koñig, G.M. *et al., J. Nat. Prod.*, 1999, **62**, 383-385 (*pmr, cmr*)

1,4,7-Tribromo-3,6,8-trichloro-3,7-dimethyl-2-octanol, 9CI T-473

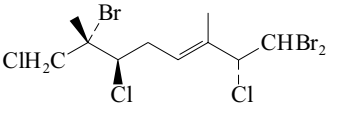
[96300-33-3]



$C_{10}H_{16}Br_3Cl_3O$ 498.306
Constit. of *Plocamium cartilagineum*. Oil.

Blunt, J.W. *et al., Aust. J. Chem.*, 1985, **38**, 319

1,1,7-Tribromo-2,6,8-trichloro-3,7-dimethyl-3-octene T-474



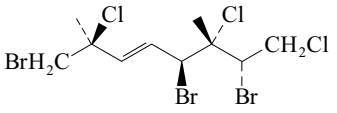
$C_{10}H_{14}Br_3Cl_3$ 480.291

(2R,3E,6R,7S)-form [72994-84-4]
Constit. of *Plocamium cruciferum*.
Cryst. (EtOH).
Mp 60.5-61.5°. $[\alpha]_D^{25}$ +99 (c, 0.0002 in cyclohexane).

Bates, P. *et al., Aust. J. Chem.*, 1979, **32**, 2545

1,5,7-Tribromo-2,6,8-trichloro-2,6-dimethyl-3-octene T-475

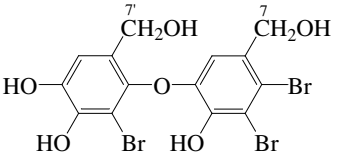
[119903-43-4]



$C_{10}H_{14}Br_3Cl_3$ 480.291
Constit. of *Placamium hamatum*. Cytotoxic agent. Cryst. Mp 92.5-94°. $[\alpha]_D$ -118 (c, 0.017 in $CHCl_3$).

Coll, J.C. *et al., Aust. J. Chem.*, 1988, **41**, 1743 (*isol, cryst struct*)
König, G.M. *et al., Phytochemistry*, 1999, **52**, 1047 (*activity*)

2′,3,4-Tribromo-2,3′,4′-trihydroxy-5,6′-bis(hydroxymethyl)diphenyl ether T-476



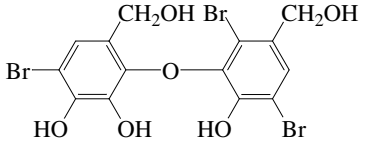
$C_{14}H_{11}Br_3O_6$ 514.949

7,7′-Di-Et ether: 2′,3,4-Tribromo-5,6′-bis(ethoxymethyl)-2,3′,4′-trihydroxydiphenyl ether
$C_{18}H_{19}Br_3O_6$ 571.057
Constit. of the brown alga *Leathesia nana*. Brown powder (Me_2CO).
Mp 153-155°.

Xu, X. *et al., J. Nat. Prod.*, 2004, **67**, 1661-1666 (*isol, pmr, cmr, ms*)

2,4′,5-Tribromo-2′,3′,6-trihydroxy-3,6′-bis(hydroxymethyl)diphenyl ether T-477

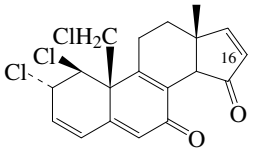
6-Bromo-3-[2,5-dibromo-6-hydroxy-3-(hydroxymethyl)phenoxy]-4-(hydroxymethyl)-1,2-benzenediol



$C_{14}H_{11}Br_3O_6$ 514.949
Isol. from the red alga *Odonthalia corymbifera*. Pale yellow solid. λ_{max} 292 (log ϵ 4.08) (EtOH).

Kurihara, H. *et al., J. Nat. Prod.*, 1999, **62**, 882-884 (*isol, uv, ir, pmr, cmr, ms*)

1,2,19-Trichloroandrosta-3,5,8,16-tetraene-7,15-dione T-478



$C_{19}H_{17}Cl_3O_2$ 383.7

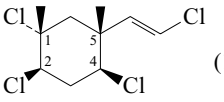
(1β,2α)-*form*
Clionastatin A
[694440-86-3]
Constit. of *Cliona nigricans*.
Amorph. solid. $[\alpha]_D^{25}$ +66 (c, 0.02 in $CHCl_3$). λ_{max} 214 (ϵ 14500); 265 (ϵ 125000); 303 (ϵ 6000) (MeCN).

16-Chloro: 1,2,16,19-Tetrachloroandrosta-3,5,8,16-tetraene-7,15-dione. ***Clionastatin B***
[694440-87-4]
$C_{19}H_{16}Cl_4O_2$ 418.145
Constit. of *Cliona nigricans*.

Fattorusso, E. *et al., Org. Lett.*, 2004, **6**, 1633-1635 (*isol, pmr, cmr*)

1,2,4-Trichloro-5-(2-chloroethenyl)-1,5-dimethylcyclohexane, 9CI T-479

[123805-38-9]



(1*R*,2*R*,4*S*,5*R*)–*form*

$C_{10}H_{14}Cl_4$ 276.031

(1*R*,2*R*,4*S*,5*R*)-*form*
Aplysiaterpenoid A. *Gelidene*
[119945-08-3]
Metab. of *Gelidium sesquipedale*, *Placamium hamatum* and *Aplysia kurodai*. Insecticide. Feeding inhibitor. Cryst. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O.
Mp 86-88° (82°). $[\alpha]_D$ +9.4 (c, 0.01 in $CHCl_3$).

(1*R*,2*S*,4*S*,5*S*)-*form*
Metab. of *Placamium cartilagineum*.
Cryst. (hexane).
Mp 91°.

(1*S*,2*R*,4*R*,5*R*)-*form*
Metab. of *Placamium cartilagineum*.
Cryst. (hexane).
Mp 105°.

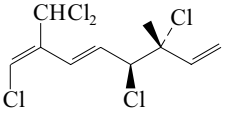
(1*S*,2*R*,4*R*,5*S*)-*form*
Metab. of *Placamium cartilagineum* and *Placamium hamatum*.
Necrotic to soft corals. Antibacterial agent. Oil or cryst. (Me_2CO).

(1*S*,2*R*,4*S*,5*S*)-*form*
Metab. of *Placamium cartilagineum*. Insecticide. Acaricide. Cryst.
Mp 57-58°. $[\alpha]_D^{70}$ +7.7 (c, 1 in $CHCl_3$).

[106621-87-8, 106621-88-9, 106621-89-0, 106621-90-3]

Miyamoto, T. *et al., Annalen*, 1988, 1191-1193 (*Aplysiaterpenoid A, cryst struct*)
Coll, J.C. *et al., Aust. J. Chem.*, 1988, **41**, 1743 (*isol, cryst struct*)
Aazizi, M.A. *et al., J. Nat. Prod.*, 1989, **52**, 829 (*isol, pmr, cmr*)
De Nys, R. *et al., Mar. Biol. (Berlin)*, 1991, **108**, 315 (*activity*)
San-Martin, A. *et al., Phytochemistry*, 1991, **30**, 2165 (*isol, pmr, cmr*)
Rivera, P. *et al., Acta Cryst. C*, 1998, **54**, 816-818 (*(1S,2R,4R,5S)-form, cryst struct*)
König, G.M. *et al., Phytochemistry*, 1999, **52**, 1047 (*isol, activity*)

1,5,6-Trichloro-2-(dichloromethyl)-6-methyl-1,3,7-octatriene, 9CI T-480



(1*E*,3*E*,5*S*,6*R*)–*form*

$C_{10}H_{11}Cl_5$ 308.46

(1*E*,3*E*,5*S*,6*R*)-*form* [57804-31-6]
Isol. from the red alga *Placamium cartilagineum*.
$[\alpha]_D^{25}$ -39.3 (c, 1.1 in $CHCl_3$).

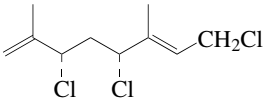
(1*Z*,3*E*,5*R*,6*R*)-*form* [57804-29-2]
Isol. from the red alga *Placamium cartilagineum*, and the tunicate *Clavelina lepadiformis*.
$[\alpha]_D^{25}$ +34.6 (c, 1.6 in $CHCl_3$).

(1*Z*,3*E*,5*S*,6*R*)-*form* [57804-30-5]
Isol. from the red algae *Plocamium cartilagineum* and *Plocamium coccineum* and from the mollusc *Aplysia limacina*.
$[\alpha]_D^{25}$ +5.1 (c, 0.4 in $CHCl_3$).

[93752-45-5, 93752-46-6, 93752-47-7]

Mynderse, J.S. *et al., Tetrahedron*, 1975, **31**, 1963 (*isol*)
Imperato, F. *et al., Experientia*, 1977, **33**, 1273 (*isol*)
De Napoli, L. *et al., Biochem. Syst. Ecol.*, 1984, **12**, 321 (*isol*)
Steffan, B. *et al., Tetrahedron*, 1991, **47**, 8729 (*isol*)

3,5,8-Trichloro-2,6-dimethyl-1,6-octadiene T-481



(3*S*,5*R*,6*E*)-*form*

$C_{10}H_{15}Cl_3$ 241.587

(3*S*,5*R*,6*E*)-*form*
Preplocamene C
[62743-09-3]
Constit. of the red alga *Plocamium violaceum*.

(3*S*,5*S*,6*E*)-*form*
Preplocamene B
[62743-08-2]
Constit. of *Plocamium violaceum*.

Crews, P. *et al., J.O.C.*, 1977, **42**, 2812 (*isol, pmr, ms*)

1,1,2-Trichloroethane, 9CI, 8CI T-482

β-Trichloroethane
[79-00-5]
$ClCH_2CHCl_2$
$C_2H_3Cl_3$ 133.404
Isol. from the alga *Cystoseira barbata*. Industrial solv. Non-flammable, mobile liq. with pleasant odour. Insol. H_2O; misc. most org. solvs. d_4^{20} 1.44.
Mp -35.5° (-36.7°). Bp 113-114° $Bp_{75.900002}$ 49.97°. n_D^{20} 1.4715.
▶ Eye, respiratory tract and severe skin irritant. High vapour conc. narcotic. Prolonged or repeated exposure can damage liver and kidneys. LD_{50} (rat, orl) 836 mg/kg. LD_{50} (rbt, skn) 5377 mg/kg. Exp. carcinogen (large dose). Exp. reprod. effects. KJ3150000

[25323-89-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 85A (*ir*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 85A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 123C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 118B (*ir*)
Sadtler Standard C-13 NMR Spectra, 344 (*cmr*)
Prins, H.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1926, **45**, 80 (*synth*)
Netherlands Pat., 1965, 6 414 743; *CA*, **64**, 590 (*manuf*)
IARC Monog., 1979, **20**, 533; *Suppl.* 7, 73 (*rev, tox*)
Organo-chlorine Solvents, Royal Society of Chemistry, 1986, 131 (*tox, rev*)
Abraham, M.H. *et al., J.C.S. Perkin 2*, 1991, 463 (*pmr, conformn*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 22 (*rev*)
Milkova, T. *et al., Phytochemistry*, 1996, **45**, 93 (*isol*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1244
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TIN000

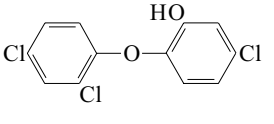
Trichloroethylene, 8CI, INN T-483

Trichloroethene, 9CI. Tri-Clene. Trichloran. Chlorylen. Trilene. R 1120. Many other names
[79-01-6]
$Cl_2C{=}CHCl$
C_2HCl_3 131.388
Manuf. by treatment of tetrachloroethanes with strong base. Prod. by several spp. of macroalgae, one microalga (*Porphyridium purpureum*) and the red alga *Meristiella gelidium*. Industrial solv. for grease, waxes, oils, paints and adhesives etc. Used in manuf. of fluorocarbons. Chain-transfer agent in PVC prodn. Solvent and extractive in the manuf. of foods. Veterinary inhalation anaesthetic. Nonflammable mobile liq. with characteristic odour. Insol. H_2O; misc. EtOH, Et_2O. d_4^{20} 1.46.
Mp -84.8° (-86.8). Bp 86.7° Bp_{60} 20°. n_D^{20} 1.4775. Log P 2.63 (calc). Vp 74 mmHg (25°). Widespread use declining due to toxicity. Resistant to radical homopolym. but undergoes copolym. with some vinyl monomers. Q/e values for copolym., Q 0.010, e +1.29.
▶ Non-flammable, autoignition temp. 410/420°. Eye and severe skin irritant. High vapour conc. narcotic. Prolonged or repeated exposure can damage kidney, liver, heart and lung, and produce skin disorders and conjunctivitis. Probable human carcinogen (IARC 2A). LD_{50} (mus, orl) 2402 mg/kg; LC_{50} (rat, ihl) 25700 ppm (1h exposure). MEL: long-term 100 ppm; short-term 150 ppm (Sk). KX4550000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 101B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 147C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 141D (*ir*)
Alfrey, T. *et al., J. Polym. Sci.*, 1948, **3**, 297-301 (*copolym*)
Breitenbach, J.W. *et al., Monatsh. Chem.*, 1950, **81**, 21-30 (*polymerisability*)
Japan. Pat., 1954, 6874; *CA*, **50**, 2651 (*synth*)
Shikaji, T. *et al., Chem. Eng. (Rugby, Engl.)*, 1970, **77**, 74 (*synth*)
Roberts, J.D. *et al., J.O.C.*, 1974, **39**, 1276-1290 (*cmr*)
Stepanyants, A.U. *et al., Zh. Anal. Khim.*, 1976, **31**, 1770-1774; *J. Anal. Chem. USSR (Engl. Transl.)*, 1976, **31**, 1333-1336 (*pmr*)
Waters, E.M. *et al., J. Toxicol. Environ. Health*, 1977, **2**, 671-707 (*rev*)
IARC Monog., 1979, **20**, 545; *Suppl.* 7, 364; *Suppl.* 6, 530 (*rev, tox*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427-443 (*Q/e values*)
Fielder, R.J. *et al., Toxic. Rev.*, 1982, **6**, (*rev, metab, tox*)
Organo-chlorine Solvents, Royal Society of Chemistry, 1986, 93 (*tox rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 32
McCunney, R.J. *et al., Br. J. Ind. Med.*, 1988, **45**, 122-126 (*human tox*)
Bretherick, L. *et al., Chem. Eng. News*, Dec. 12, 1988, 2 (*haz*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 40-50 (*rev*)
Collen, J.A. *et al., Phyto hemistry*, 1994, **36**, 1197-1202 (*occur*)
Abrahamsson, K. *et al., Limnol. Oceanogr.*, 1995, **40**, 1321-1326 (*occur*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1-423 (*occur*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2826
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1234
IARC Monog. (Web), (*carcinogen*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1245
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, TIO750

2,4,4′-Trichloro-2′-hydroxydiphenyl ether T-484

*5-Chloro-2-(2,4-dichlorophenoxy)phenol, 9CI, 8CI. **Triclosan, BAN, INN, USAN**. Irgasan DP 300. Cloxifenol. Zilesan UW. Irgasan CH 3565. Many other names*
[3380-34-5]



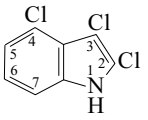
$C_{12}H_7Cl_3O_2$ 289.544
Reported from sponge-associated bacterium *Micrococcus luteus*. Bacteriostatic agent used in soaps, dentifrices and deodorants, low acute toxicity. Off-white cryst. powder or soft agglomerates. Insol. H_2O, sol. org. solvs.
Mp 54-57°. Log P 5.84 (calc). Light-sensitive.
▶ Skin irritant, can cause contact dermatitis. Forms dichlorodibenzo-*p*-dioxins in presence of sunlight or on pyrolysis. KO1100000

Belg. Pat., 1965, 659 636; *CA*, **64**, 2010e (*synth*)
Furia, T.E. *et al., Proc. Annu. Meet., Chem. Spec. Manuf. Assoc.*, 1967, **54**, 131 (*rev, pharmacol*)
Black, J.G. *et al., Toxicology*, 1975, **3**, 33 (*metab*)
Siddiqui, W.H. *et al., J. Environ. Pathol. Toxicol.*, 1979, **2**, 861 (*pharmacol*)
Tulp, M.T.M. *et al., Xenobiotica*, 1979, **9**, 65 (*metab*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 2192
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 805

Bultel-Poncé, V. *et al., J. Mar. Biotechnol.*, 1998, **6**, 233-236 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TIQ000

2,3,4-Trichloro-1*H*-indole, 9CI T-485

[68234-24-2]



$C_8H_4Cl_3N$ 220.484
Alkaloid from the marine red alga *Rhodophyllis membranacea*.

Brennan, M.R. *et al., Tet. Lett.*, 1978, 1637 (*isol, pmr, struct*)

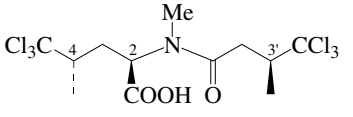
2,3,7-Trichloro-1*H*-indole, 9CI T-486

[68234-18-4]

$C_8H_4Cl_3N$ 220.484
Alkaloid from the marine red alga *Rhodophyllis membranacea*.
Mp 86°.

Brennan, M.R. *et al., Tet. Lett.*, 1978, 1637 (*isol, pmr, struct*)
Erickson, K.L. *et al., Synth. Commun.*, 1981, **11**, 253 (*synth, ir, pmr, ms*)

5,5,5-Trichloro-*N*-methyl-*N*-(4,4,4-trichloro-3-methylbutanoyl)leucine T-487



(2*R*,3'*S*,4*S*)-*form*

$C_{12}H_{17}Cl_6NO_3$ 435.987
Peptide related to Dysidenin, D-1280.

(2*R*,3′*S*,4*S*)-*form*
Isol. from a *Dysidea* sp.
Cryst. ($CHCl_3$).
Mp 140-143°. $[\alpha]_D$ -6.9 (c, 0.03 in $CHCl_3$).

Me ester:
$C_{13}H_{19}Cl_6NO_3$ 450.014
Isol. from a *Dysidea* sp. Cryst. (Et_2O/pentane).
Mp 47-48°. $[\alpha]_D$ -10.5 (c, 0.02 in $CHCl_3$).

4′,5-Bis(dechloro), Me ester:
$C_{13}H_{21}Cl_4NO_3$ 381.125
Isol. from a *Dysidea* sp. Oil. $[\alpha]_D$ -22.2 (c, 0.0003 in $CHCl_3$).

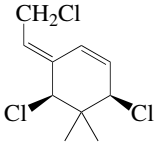
(2*S*,3′*S*,4*S*)-*form*
Isol. from a *Dysidea* sp.
Cryst. ($CHCl_3$).
Mp 129-133°. $[\alpha]_D$ -35.2 (c, 0.04 in $CHCl_3$).

Me ester: Isol. from a *Dysidea* sp.
Cryst. (Et_2O/pentane).
Mp 66-68°. $[\alpha]_D$ -16.1 (c, 0.02 in $CHCl_3$).

Stapleton, B.L. *et al., Tetrahedron*, 2001, **57**, 4603-4607

1,6,8-Trichloro-2,4-ochtodadiene T-488

3,5-Dichloro-6-(2-chloroethylidene)-4,4-dimethylcyclohexene



$C_{10}H_{13}Cl_3$ 239.571
λ_{max} 242 (ϵ 3340) (MeOH) (Berdy).

(2*E*,6*R,8*S**)-*form*** [142439-87-0]
Isol. from the red alga *Portieria hornemanii*.
Oil. $[\alpha]_D$ +71.3 (c, 1 in $CHCl_3$). λ_{max} 242 (ϵ 3340) (CH_2Cl_2).

Fuller, R.W. *et al., J. Med. Chem.*, 1992, **35**, 3007-3011 (*isol, uv, pmr, cmr, ms*)

1,1,3-Trichloro-2-propanone, 9CI, 8CI T-489

1,1,3-Trichloroacetone
[921-03-9]
$Cl_2CHCOCH_2Cl$
$C_3H_3Cl_3O$ 161.414
Constit. of the red alga *Asparagopsis taxiformis*. Bp 172° Bp_{10} 62°.
► LC_{50} (rat, ihl) 390 mg m^{-3} (2h exposure). UC3840000

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 652A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 505C (*ir*)
Wyman, D.P. *et al., J.O.C.*, 1964, **29**, 1956 (*synth, nmr, ir*)
McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367-374 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TII550

1,1,1-Trichloro-5-undecylamine T-490

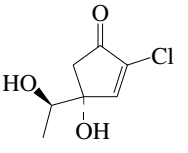
1,1,1-Trichloro-5-undecanamine. 5-Amino-1,1,1-trichloroundecane
$H_3C(CH_2)_5CH(NH_2)(CH_2)_3CCl_3$
$C_{11}H_{22}Cl_3N$ 274.66

(+)-*form*
N-*Ac: 5-Acetamido-1,1,1-trichloroundecane*
[345261-12-3]
$C_{13}H_{24}Cl_3NO$ 316.697
Isol. from the cyanobacterium *Microcoleus lyngbyaceus*. Oil.
$[\alpha]_D$ +60 (c, 0.02 in $CHCl_3$).

Orsini, M.A. *et al., J. Nat. Prod.*, 2001, **64**, 572-577 (*isol, ir, pmr, cmr*)

Trichodenone B T-491

2-Chloro-4-hydroxy-4-(1-hydroxyethyl)-2-cyclopenten-1-one



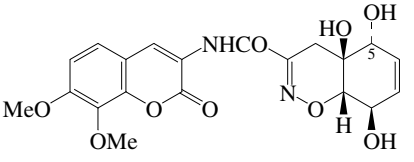
Absolute Configuration

$C_7H_9ClO_3$ 176.599
Prod. by a *Trichoderma harzianum* isol. from the sponge *Halichondria okadai*. Cytotoxic agent. Oil. Sol. MeOH, DMSO, $CHCl_3$, Me_2CO, hexane, EtOAc; poorly sol. H_2O. λ_{max} 227 (log ϵ 3.76) (EtOH).

Amagata, T. *et al., J. Antibiot.*, 1998, **51**, 33-40 (*isol, uv, ir, cd, pmr, cmr*)
Usami, Y. *et al., Synlett*, 1999, 723-724 (*synth, abs config*)

Trichodermamide A T-492

Penicillazine



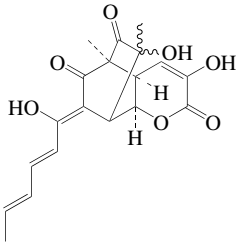
Absolute Configuration

$C_{20}H_{20}N_2O_9$ 432.386
Isol. from the marine-derived fungi *Penicillium* sp. (strain No. 386), *Spicaria elegans* and *Trichoderma virens*. Also prod. by *Aspergillus unilateralis*. Cytotoxic. Needles (Me_2CO).
Mp 258-260° (224-226°). $[\alpha]_D^{15}$ +128 (c, 0.15 in MeOH). $[\alpha]_D^{25}$ -11.9 (c, 2.2 in $CHCl_3$). λ_{max} 250 (sh) (log ϵ 3.98); 334 (log ϵ 4.23) (MeOH). λ_{max} 205 (log ϵ 4.6); 266 (log ϵ 4); 343 (log ϵ 4) ($CHCl_3$).

*5-Deoxy, 5*R*-chloro:* ***Trichodermamide B***
$C_{20}H_{19}ClN_2O_8$ 450.831
Isol. from *Trichoderma virens*. Cytotoxic. Oil. $[\alpha]_D^{15}$ +110.7 (c, 0.15 in MeOH). λ_{max} 252 (log ϵ 3.56); 344 (log ϵ 3.86) (MeOH).

Lin, Y. *et al., Tetrahedron*, 2000, **56**, 9607-9609 (*Penicillazine*)
Garo, E. *et al., J. Nat. Prod.*, 2003, **66**, 423-426 (*Trichoderma, pmr, cmr, cryst struct*)
Liu, R. *et al., Arch. Pharmacal Res.*, 2005, **28**, 1042-1046 (*Spicaria, pmr, cmr, ms*)
Capon, R.J. *et al., Org. Biomol. Chem.*, 2005, **3**, 123-129 (*Aspergillus, isol, struct*)

Trichodermanone A T-493



$C_{19}H_{20}O_7$ 360.363
Prod. by a marine-derived *Trichoderma viride*. Yellowish viscous oil. $[\alpha]_D^{22}$ +51.5 (c, 0.08 in MeOH). λ_{max} 204 (log ϵ 4.1); 250 (log ϵ 4.2); 360 (log ϵ 4.3) (MeOH).

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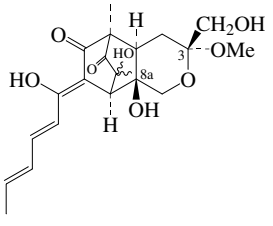
Trichodermanone B T-494



$C_{21}H_{28}O_8$ 408.447
Enolised β-diketone. Prod. by a marine-derived *Trichoderma viride*. Yellowish viscous oil. $[\alpha]_D^{22}$ -203 (c, 0.24 in MeOH). λ_{max} 203 (log ϵ 4.2); 248 (log ϵ 4.2); 360 (log ϵ 4.6) (MeOH).

*8*a*-Epimer:* ***Trichodermanone C***
$C_{21}H_{28}O_8$ 408.447
Prod. by a marine-derived *Trichoderma viride*. Yellowish viscous oil. $[\alpha]_D^{22}$ +251.5 (c, 0.2 in MeOH). λ_{max} 202 (log ϵ 4.4); 248 (log ϵ 4.2); 358 (log ϵ 4.7) (MeOH).

*3,8*a*-Diepimer, O*^{3}*-de-Me:* ***Trichodermanone D***
$C_{20}H_{26}O_8$ 394.421
Prod. by a marine-derived *Trichoderma viride*. Yellowish viscous oil. $[\alpha]_D^{22}$ +265.7 (c, 0.5 in MeOH). λ_{max} 248 (log ϵ 3.8); 360 (log ϵ 4.3) (MeOH).

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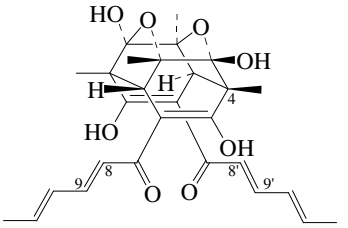
Trichodimerol T-495

BMS 182123. Antibiotic BMS 182123
[145174-90-9]



$C_{28}H_{32}O_8$ 496.556
Dimer of Sorbicillin, S-264. Metab. of *Trichoderma longibrachiatum*, *Penicillium chrysogenum* and the marine-derived *Penicillium terrestre*. β-1,6-Glucan biosynthesis inhibitor. Shows DPPH radical scavenging activity. Pale yellow cryst.
Mp 166-167°. $[\alpha]_D$ -376 (c, 0.26 in MeOH).

8,9-Dihydro: ***Dihydrotrichodimerol***
$C_{28}H_{34}O_8$ 498.572
Prod. by the marine-derived *Penicillium terrestre* and an unidentified fungal strain B00853. Yellow powder.
Mp 82-83° Mp 112-117°. $[\alpha]_D$ +99 (c, 0.01 in MeOH). λ_{max} 241 (log ϵ 3.87); 308 (log ϵ 4.18); 360 (log ϵ 4.22) (MeOH).

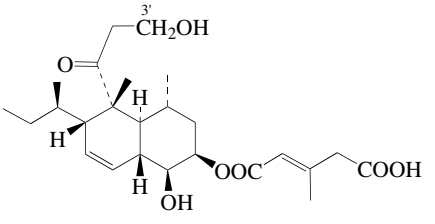
8,8′,9,9′-Tetrahydro: ***Tetrahydrotrichodimerol***
$C_{28}H_{36}O_8$ 500.588
Prod. by the marine-derived *Penicillium terrestre*. Yellow powder.
Mp 40-50°. $[\alpha]_D^{20}$ +190.3 (c, 0.22 in MeOH). λ_{max} 297 (log ϵ 4.27) (MeOH).

4-Demethyl: ***Demethyltrichodimerol***
$C_{27}H_{30}O_8$ 482.529
Metab. of *Trichoderma* sp. USF-2690. Amorph. yellow powder. $[\alpha]_D^{28}$ -278.5 (c, 2 in MeOH). λ_{max} 243 (ϵ 5000); 307 (ϵ 11100); 353 (sh) (ϵ 17700); 363 (ϵ 19800); 373 (sh) (ϵ 17700); 393 (sh) (ϵ 9600) (MeOH). λ_{max} 249 (ϵ 4900); 307 (ϵ 10100); 364 (ϵ 21000) (MeOH/HCl) (Berdy). λ_{max} 254 (ϵ 14100); 278 (ϵ 16000); 379 (ϵ 13800) (MeOH/NaOH) (Berdy).

Andrade, R. *et al., Can. J. Chem.*, 1992, **70**, 2526 (*isol, pmr, cmr, struct*)
Gao, Q. *et al., J. Nat. Prod.*, 1995, **58**, 1817 (*cryst struct*)
Warr, G.A. *et al., J. Antibiot.*, 1996, **49**, 234 (*isol, props*)
Abe, N. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 661-666 (*Demethyltrichodimerol*)
Nicolaou, K.C. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 3555-3559 (*synth*)
Barnes-Seeman, D. *et al., Org. Lett.*, 1999, **1**, 1503-1504 (*synth*)
Nicolaou, K.C. *et al., J.A.C.S.*, 2000, **122**, 3071-3079 (*synth*)
Lee, D. *et al., J. Antibiot.*, 2005, **58**, 615-620 (*Dihydrotrichodimerol*)
Liu, W. *et al., J. Antibiot.*, 2005, **58**, 621-624 (*Dihydrotrichodimerol, Tetrahydrotrichodimerol*)

Trichoharzin T-496

[153888-68-7]



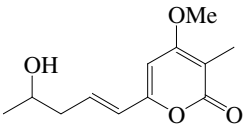
Absolute Configuration

$C_{25}H_{38}O_7$ 450.571
Prod. by *Trichoderma harzianum* found in the sponge *Mycale cecilia*. Cytotoxic. Glassy solid. $[\alpha]_D$ +38 (MeOH). λ_{max} 222 (ϵ 26000) (MeOH) (Derep). λ_{max} 222 (ϵ 26000) (MeOH) (Berdy).

Kobayashi, M. *et al., Tet. Lett.*, 1993, **34**, 7925-7928 (*isol, uv, ir, pmr, cmr*)

Trichopyranone T-497

*6-(4-Hydroxy-1-pentenyl)-4-methoxy-3-methyl-2*H*-pyran-2-one*



$C_{12}H_{16}O_4$ 224.256

Prod. by a marine-derived *Trichoderma viride*. Yellowish viscous oil. $[\alpha]_D^{22}$ -10.3 (c, 0.1 in MeOH). λ_{max} 227 (log ϵ 4); 278 (log ϵ 3.5); 334 (log ϵ 3.5) (MeOH).

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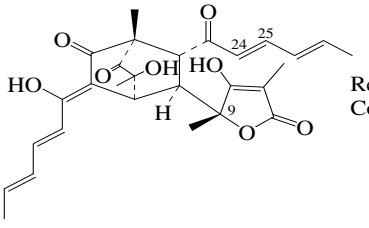
Trichotetronine T-498

[199729-12-9]



Relative Configuration

$C_{28}H_{32}O_8$ 496.556

Oxidised dimer of Sorbicillin, S-264. Prod. by a *Trichoderma* sp. grown on rice, *Trichoderma* sp. USF-2690 and *Trichoderma longibrachiatum* separated from a *Haliclona* sp. sponge. Amorph. yellow powder. $[\alpha]_D$ +456 (c, 0.08 in MeOH) (124.4). λ_{max} 271 (log ϵ 4.58); 291 (log ϵ 4.63); 384 (log ϵ 4.29) (MeOH). λ_{max} 262 (ϵ 23500); 292 (ϵ 24100); 370 (ϵ 23500) (MeOH). λ_{max} 271 (ϵ 38000); 291 (ϵ 42660); 384 (ϵ 19500) (MeOH) (Berdy).

24,25-Dihydro: ***Dihydrotrichotetronine***
[199729-13-0]
$C_{28}H_{34}O_8$ 498.572
Isol. from a *Trichoderma* sp. grown on rice. Pale yellow amorph. powder. $[\alpha]_D$ +354 (c, 0.1 in MeOH). λ_{max} 257 (log ϵ 4.55); 368 (log ϵ 4.6) (MeOH). λ_{max} 257 (ϵ 35900); 368 (ϵ 42660) (MeOH) (Berdy).

9-Epimer: ***Bisorbibutenolide****. Bislongiquinolide*
[194155-78-7]
$C_{28}H_{32}O_8$ 496.556
Prod. by *Penicillium notatum* (GWP A) and *Trichoderma* sp. USF-2690. Amorph. yellow powder. $[\alpha]_D^{27}$ +124.4 (c, 0.5 in MeOH).

Andrade, R. *et al., Aust. J. Chem.*, 1997, **50**, 255-257 (*Bislongiquinolide*)
Shirota, O. *et al., J.C.S. Perkin 1*, 1997, 2961-2964 (*Trichotetronine, Dihydrotrichotetronine*)
Abe, N. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 2120-2126 (*Bisorbibutenolide*)
Sperry, S. *et al., J.O.C.*, 1998, **63**, 10011-10014 (*Bislongiquinolide*)
Nicolaou, K.C. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 3555-3559 (*synth*)
Nicolaou, K.C. *et al., J.A.C.S.*, 2000, **122**, 3071-3079 (*synth*)
Abe, N. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 2090-2099 (*biosynth*)
Hong, R. *et al., Angew. Chem., Int. Ed.*, 2005, **44**, 3478-3481 (*Bisorbibutenolide, synth*)
Maskey, R.P. *et al., J. Nat. Prod.*, 2005, **68**, 865-870 (*isol, pmr, cmr*)

1,14-Tricosadiene T-499

$H_3C(CH_2)_7CH{=}CH(CH_2)_{11}CH{=}CH_2$
$C_{23}H_{44}$ 320.601

(*E*)-*form* [104899-43-6]
Isol. from the green alga *Botryococcus braunii*.

(*Z*)-*form* [104899-38-9]
Isol. from *Botryococcus braunii*.

Metzger, P. *et al., Phytochemistry*, 1986, **25**, 1869; 1993, **33**, 1125 (*isol, pmr, cmr*)

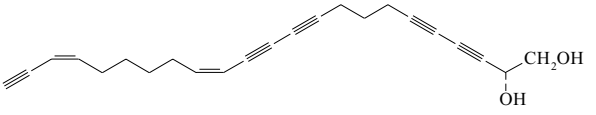
6,8-Tricosadiene-4,19-diynoic acid T-500

$H_3CCH_2CH_2C{\equiv}C(CH_2)_9CH{=}CHCH{=}CHC{\equiv}CCH_2CH_2COOH$
$C_{23}H_{34}O_2$ 342.52

(6*Z*,8*E*)-*form*
Carduusyne A
[158182-75-3]
Constit. of the marine sponge *Phakellia carduus*.
Oil (as Et ester). λ_{max} 265 (ϵ 30900) (MeOH) (as Et ester).

Barrow, R.A. *et al., Aust. J. Chem.*, 1994, **47**, 1901-1918 (*isol, uv, ir, pmr, cmr*)
Charoenying, P. *et al., Tet. Lett.*, 1996, **37**, 1913 (*synth*)

14,20-Tricosadiene-3,5,10,12,22-pentayne-1,2-diol, 9CI T-501



$C_{23}H_{24}O_2$ 332.441
Sol. Me_2CO, $CHCl_3$; poorly sol. H_2O.

(2*R*,14*Z*,20*Z*)-*form*
Siphonodiol
[90934-31-9]
Metab. of sponge *Siphonochalina truncata*. Shows antibacterial activity. HKATP-ase inhibitor. Cryst.
Mp 31-32°. $[\alpha]_D$ -6.7 (c, 0.5 in MeOH). λ_{max} 215 (ϵ 69700); 223 (ϵ 15100); 241 (ϵ 11300); 254 (ϵ 13800); 268 (ϵ 19300); 284 (ϵ 14900) (MeOH).

1-O-*Sulfate:* ***Callyspongin B***
$C_{23}H_{24}O_5S$ 412.506
Metab. of the sponge *Callyspongia truncata*.
$[\alpha]_D^{25}$ +3.1 (c, 0.4 in DMSO). λ_{max} 270 (ϵ 4800); 285 (ϵ 4100) (DMSO).

Di-O-*sulfate:* ***Callyspongin A***
$C_{23}H_{24}O_8S_2$ 492.57
Metab. of *Callyspongia truncata*.
$[\alpha]_D^{25}$ -40.3 (c, 1 in H_2O). λ_{max} 207 (log ϵ 25100); 214 (log ϵ 26800); 253 (log ϵ 7400); 267 (log ϵ 8900); 287 (log ϵ 7100) (H_2O).

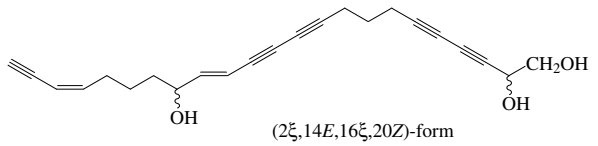
14,15-Dihydro: 20-Tricosene-3,5,10,12,22-pentayne-1,2-diol. ***14,15-Dihydrosiphonodiol***
[111243-22-2]
$C_{23}H_{26}O_2$ 334.457
From *Siphonochalina truncata*. HKATPase inhibitor. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 223 (ϵ 11000) (EtOH) (Derep).

12,13,14,15-Tetrahydro: 12,20-Tricosadiene-3,5,10,22-tetrayne-1,2-diol. ***12,13,14,15-Tetrahydrosiphonodiol***
[111216-68-3]
$C_{23}H_{28}O_2$ 336.473
From *Siphonochalina truncata*. HKATPase inhibitor. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 223 (ϵ 11000) (EtOH) (Derep). λ_{max} 223 (ϵ 19600) (MeOH) (Berdy).

9ξ-Hydroxy: 14,20-Tricosadiene-3,5,10,12,22-pentayne-1,2,9-triol. ***Callytriol A***
$C_{23}H_{24}O_3$ 348.441
Metab. of the sponge *Callyspongia truncata*. Induces metamorphosis in ascidians. Yellow oil. Shows small positive opt. rotn. λ_{max} 209 (ϵ 33600); 216 (ϵ 38400); 254 (ϵ 8600); 268 (ϵ 10600); 284 (ϵ 9000) (EtOH).

Tada, H. *et al., Chem. Lett.*, 1984, 779
Fusetani, N. *et al., Tet. Lett.*, 1987, **28**, 4311 (*isol, struct*)
Uno, M. *et al., J. Nat. Prod.*, 1996, **59**, 1146 (*Callyspongins*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 1997, **60**, 126 (*Callytriol A*)
López, S. *et al., J.O.C.*, 2005, **70**, 6346-6352 (*synth*)

14,20-Tricosadiene-3,5,10,12,22-pentayne-1,2,16-triol T-502



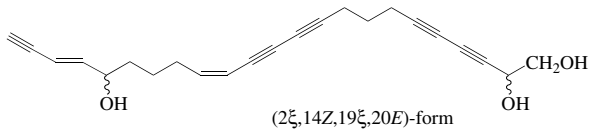
(2ξ,14*E*,16ξ,20*Z*)-form

$C_{23}H_{24}O_3$ 348.441

(2ξ,14*E*,16ξ,20*Z*)-*form*
Callytriol E
[185548-45-2]
Isol. from the sponge *Callyspongia truncata*. Induces metamorphosis in ascidians. Yellow oil. $[\alpha]_D^{25}$ -1.6 (c, 0.05 in MeOH). λ_{max} 207 (ϵ 33000); 214 (ϵ 41900); 253 (ϵ 10000); 268 (ϵ 14700); 284 (ϵ 11600) (EtOH). λ_{max} 207 (ϵ 33800); 214 (ϵ 41900); 253 (ϵ 10000); 267 (ϵ 14700); 287 (ϵ 11600) (EtOH) (Berdy).

(2ξ,14*Z*,16α,20*Z*)-*form*
Callytriol B
[185548-39-4]
Isol. from *Callyspongia truncata*. Induces metamorphosis in ascidians. Yellow oil. $[\alpha]_D^{25}$ +1 (c, 0.08 in MeOH). λ_{max} 205 (ϵ 30500); 214 (ϵ 32300); 253 (ϵ 8200); 268 (ϵ 9300) (EtOH). λ_{max} 205 (ϵ 30500); 214 (ϵ 32300); 253 (ϵ 8200); 268 (ϵ 9300); 284 (ϵ 8800) (EtOH) (Berdy).
Tsukamoto, S. *et al., J. Nat. Prod.*, 1997, **60**, 126-130 (*isol, uv, ir, pmr, cmr*)

14,20-Tricosadiene-3,5,10,12,22-pentayne-1,2,19-triol T-503



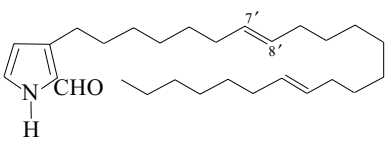
(2ξ,14*Z*,19ξ,20*E*)-form

$C_{23}H_{24}O_3$ 348.441

(2ξ,14*Z*,19ξ,20*E*)-*form*
Callytriol D
[185548-44-1]
Isol. form the sponge *Callyspongia truncata*. Induces metamorphosis in ascidians. Yellow oil. $[\alpha]_D^{25}$ -1.5 (c, 0.03 in MeOH). λ_{max} 207 (ϵ 32700); 215 (ϵ 39700); 253 (ϵ 8100); 268 (ϵ 11800); 283 (ϵ 9400) (EtOH). λ_{max} 207 (ϵ 29800); 214 (ϵ 37300); 253 (ϵ 7300); 267 (ϵ 10500); 283 (ϵ 8300) (EtOH) (Berdy).

(2ξ,14*Z*,19ξ,20*Z*)-*form*
Callytriol C
[185548-40-7]
Isol. from *Callyspongia truncata*. Induces metamorphosis in ascidians. Yellow oil. $[\alpha]_D^{25}$ -4.5 (c, 0.05 in MeOH). λ_{max} 207 (ϵ 32700); 215 (ϵ 39700); 253 (ϵ 8100); 268 (ϵ 11800); 283 (ϵ 9400) (EtOH). λ_{max} 206 (ϵ 32700); 214 (ϵ 39700); 253 (ϵ 8100); 267 (ϵ 11800); 283 (ϵ 9400) (EtOH) (Berdy).
Tsukamoto, S. *et al., J. Nat. Prod.*, 1997, **60**, 126-130 (*isol, uv, ir, pmr, cmr*)

3-(7,16-Tricosadienyl)-1*H*-pyrrole-2-carboxaldehyde, 9CI T-504



$C_{28}H_{47}NO$ 413.685

(*E*,*E*)-*form* [57992-58-2]
Isol. from the marine sponge *Oscarella lobularis*.
7′,8′-Dihydro: ***3-(16-Tricosenyl)-1H-pyrrole-2-carboxaldehyde, 9CI***
[57992-56-0]
$C_{28}H_{49}NO$ 415.701
Isol. from *Oscarella lobularis*.
Cimino, G. *et al., Experientia*, 1975, **31**, 1387 (*isol, uv, pmr, ms, struct*)

17-Tricosenal T-505

$H_3C(CH_2)_4CH{=}CH(CH_2)_{15}CHO$
$C_{23}H_{44}O$ 336.6

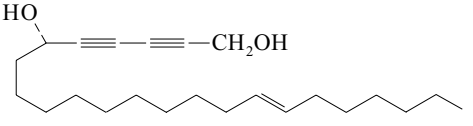
(*Z*)-*form* [140163-47-9]
Constit. of the sponge *Amphimedon compressa*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1992, **55**, 333

1-Tricosene T-506

[18835-32-0]
$H_3C(CH_2)_{20}CH{=}CH_2$
$C_{23}H_{46}$ 322.616
Constit. of the alga *Botryococcus braunii* and various plant spp. incl. *Gardenia tahitensis*.
Fp 41.6. Bp 379° Bp_{10} 222.4°.
Dreisbach, R.R. *et al., Adv. Chem. Ser.*, 1959, **22**, 1 (*props*)
Bessiere, J.M. *et al., Fitoterapia*, 1985, **56**, 62 (*isol*)
MacLeod, G. *et al., Phytochemistry*, 1990, **29**, 1197 (*isol*)
Davis, F. *et al., Macromolecules*, 1991, **56**, 5695 (*synth*)
Metzger, P. *et al., Phytochemistry*, 1993, **33**, 1125 (*isol*)

16-Tricosene-2,4-diyne-1,6-diol, 9CI T-507

[64010-41-9]



$C_{23}H_{38}O_2$ 346.552

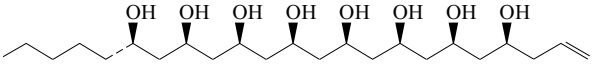
(*R*)-(*Z*)-*form*
18-Hydroxyrenierin 2
Constit. of *Reniera fulva*.
Mp 32°. $[\alpha]_D$ -38 (c, 1.6 in MeOH). λ_{max} 230 (ϵ 354), 243 (330) and 256 nm (200) (MeOH).
Cimino, G. *et al., Tet. Lett.*, 1977, 1325 (*isol, uv, ir, ms*)

16-Tricosene-2,4-diyn-1-ol T-508

[63987-86-0]
$H_3C(CH_2)_5CH{=}CH(CH_2)_{10}C{\equiv}CC{\equiv}CCH_2OH$
$C_{23}H_{38}O$ 330.553

(*Z*)-*form*
Renierin 2
Constit. of *Reniera fulva*.
Mp 35°. λ_{max} 231 (ϵ 354); 242 (ϵ 330); 256 (ϵ 400) (MeOH) (Derep).
Cimino, G. *et al., Tet. Lett.*, 1977, 1325 (*isol, struct*)

1-Tricosene-4,6,8,10,12,14,16,18-octol T-509



$C_{23}H_{46}O_8$ 450.612

(4*S*,6*S*,8*S*,10*S*,12*R*,14*R*,16*R*,18*R*)-*form*

Octa-Me ether: 4,6,8,10,12,14,16,18-Octamethoxy-1-tricosene
[131487-89-3]
$C_{31}H_{62}O_8$ 562.826
Isol. from the blue-green algae *Scytonema mirabile* and *Scytonema burmanicum*.
$[\alpha]_D^{25}$ +5.44 (c, 0.5 in $CHCl_3$).
Mori, Y. *et al., J.O.C.*, 1991, **56**, 631 (*isol, synth, pmr, cmr, abs config*)

10-Tricosenoic acid T-510

$H_3C(CH_2)_{11}CH{=}CH(CH_2)_8COOH$
$C_{23}H_{44}O_2$ 352.599

(*Z*)-*form* [212377-05-4]
Isol. from the sponge *Calyx podatypa*.

[212376-96-0]

Carballeira, N.M. *et al., J. Nat. Prod.*, 1998, **61**, 1049-1052 (*isol, synth*)

15-Tricosenoic acid T-511

$H_3C(CH_2)_6CH{=}CH(CH_2)_{13}COOH$
$C_{23}H_{44}O_2$ 352.599

(*Z*)-*form* [140703-38-4]
Constit. of lipids of human brain. Isol. from the sponge *Calyx podatypa*.
Johnson, D.W. *et al., Lipids*, 1992, **27**, 177-180 (*isol, brain*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 1998, **61**, 1049-1052 (*isol, Calyx*)

16-Tricosenoic acid T-512

$H_3C(CH_2)_5CH{=}CH(CH_2)_{14}COOH$
$C_{23}H_{44}O_2$ 352.599

(*Z*)-*form* [140163-36-6]
Constit. of the sponges *Amphimedon compressa* and *Mycale laevis*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1992, **55**, 333

17-Tricosenoic acid T-513

$H_3C(CH_2)_4CH{=}CH(CH_2)_{15}COOH$
$C_{23}H_{44}O_2$ 352.599

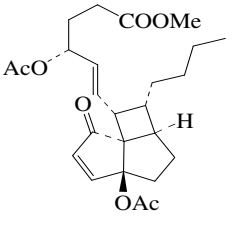
(*Z*)-*form* [140163-37-7]
Constit. of the sponge *Amphimedon compressa*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1992, **55**, 333

18-Tricosenoic acid T-514

$H_3C(CH_2)_3CH{=}CH(CH_2)_{16}COOH$
$C_{23}H_{44}O_2$ 352.599

(*Z*)-*form* [140163-38-8]
Constit. of the sponge *Amphimedon compressa*.
Carballeira, N.M. *et al., J. Nat. Prod.*, 1992, **55**, 333

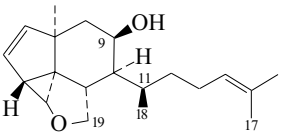
Tricycloclavulone T-515



$C_{25}H_{34}O_7$ 446.539
Prostanoid-related oxylipin. Isol. from *Clavularia viridis*. Oil. $[\alpha]_D^{25}$ +9.7 (c, 0.12 in $CHCl_3$). λ_{max} 205 (ϵ 12800) (EtOH).
Iwashima, M. *et al., J.O.C.*, 2002, **67**, 2977-2981 (*isol, pmr, cmr*)
Ito, H. *et al., J.A.C.S.*, 2004, **126**, 4520-4521 (*synth*)

Tricyclodictyofuran A T-516

[96829-62-8]



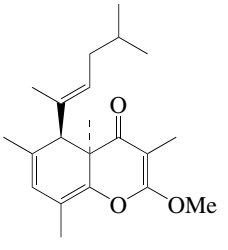
$C_{20}H_{30}O_2$ 302.456
Constit. of brown alga *Dictyota dichotoma*. Oil. $[\alpha]_D^{25}$ +26.7 (c, 1.8 in $CHCl_3$).

9-Deoxy: ***Tricyclodictyofuran B***
[96829-60-6]
$C_{20}H_{30}O$ 286.456
Constit. of *Dictyota dichotoma*. Oil. $[\alpha]_D^{21}$ +25.7 (c, 0.3 in cyclohexane).

9-\Deoxy, 19β-methoxy: ***Tricyclodictyofuran C***
[96829-61-7]
$C_{21}H_{32}O_2$ 316.483
Constit. of *Dictyota dichotoma*. Oil. $[\alpha]_D^{21}$ +27.4 (c, 0.27 in cyclohexane).
Enoki, N. *et al., Tet. Lett.*, 1985, **26**, 1731

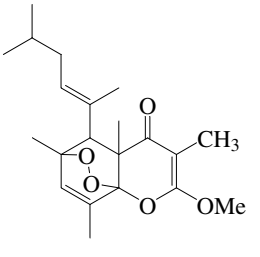
Tridachiahydropyrone T-517

*5-(1,4-Dimethyl-1-pentenyl)-4*a*,5-dihydro-2-methoxy-3,4*a*,6,8-tetramethyl-4*H*-1-benzopyran-4-one, 9CI*
[178180-08-0]



$C_{21}H_{30}O_3$ 330.466
The physical props. of the synth. material do not agree with the natural product. Isol. from the sacoglossan *Tridachia crispata*. Cryst. (hexane). Sol. MeOH, Et_2O, Me_2CO; poorly sol. H_2O. Mp 78-82°. $[\alpha]_D$ -476.1 (c, 0.5 in $CHCl_3$). λ_{max} 217 (ϵ 10840) (MeOH).
Gavagnin, M. *et al., Tet. Lett.*, 1996, **37**, 4259-4262 (*isol, uv, ir, pmr, cmr, ms*)
Jeffery, D.W. *et al., Org. Lett.*, 2005, **7**, 1581-1584 (*synth*)

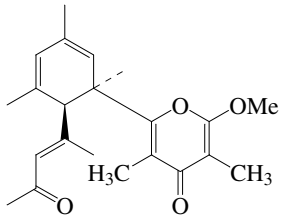
Tridachiahydropyrone B T-518



$C_{21}H_{30}O_5$ 362.465
Isol. from the mollusc *Placobranchus ocellatus*. Glass. Isol. as a mixture with Tridachiahydropyrone C to which data refers. λ_{max} 278 (ϵ 11300) (MeOH).

Z-Isomer: ***Tridachiahydropyrone C***
$C_{21}H_{30}O_5$ 362.465
Isol. from *Placobranchus ocellatus.*
Fu, X. *et al., Tetrahedron*, 2000, **56**, 8989-8993 (*isol*)

Tridachiapyrone I T-519

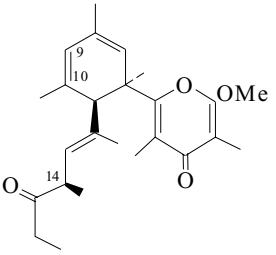


Relative Configuration

$C_{22}H_{28}O_4$ 356.461
Isol. from the mollusc *Placobranchus ocellatus.* Glass. λ_{max} 252 (ϵ 13100) (MeOH).
Fu, X. *et al., Tetrahedron*, 2000, **56**, 8989-8993

Tridachiapyrone A T-520

[99265-40-4]



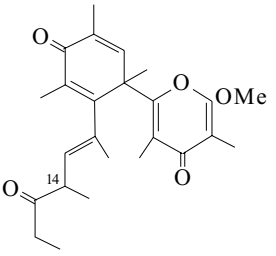
$C_{25}H_{34}O_4$ 398.541
Constit. of *Tridachia crispata*. Oil. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 255 (ϵ 11800) (MeOH) (Berdy).

14-Epimer: ***Isotridachiapyrone A***
[99148-24-0]
$C_{25}H_{34}O_4$ 398.541
Constit. of *Tridachia crispata*. Oil. λ_{max} 253 (ϵ 11900) (MeOH).

9α,10α-Epoxide: ***Tridachiapyrone C***
[99165-16-9]
$C_{25}H_{34}O_5$ 414.541
Constit. of *Tridachia crispata*. Oil. λ_{max} 254 (ϵ 5890) (MeOH) (Derep).
Ksebati, M.B. *et al., J.O.C.*, 1985, **50**, 5637-5642 (*isol, pmr, cmr*)

Tridachiapyrone B T-521

[99148-25-1]

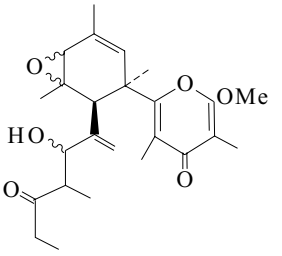


$C_{25}H_{32}O_5$ 412.525
Constit. of *Tridachia crispata*. Oil. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 248 (ϵ 11900); 255 (ϵ 5900) (MeOH) (Derep).

14-Epimer: ***Isotridachiapyrone B***
[99212-17-6]
$C_{25}H_{32}O_5$ 412.525
From *Tridachia crispata*. Oil. λ_{max} 225 (ϵ 7450); 255 (ϵ 5850) (MeOH) (Derep).
Ksebati, M.B. *et al., J.O.C.*, 1985, **50**, 5637-5642 (*isol, pmr, cmr*)

Tridachiapyrone D T-522

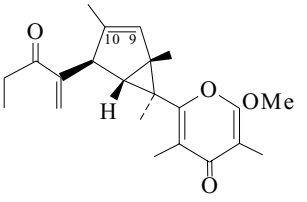
[99148-21-7]



$C_{25}H_{34}O_6$ 430.54
Constit. of *Tridachia crispata*. Cytotoxic. Oil. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 253 (ϵ 6000) (MeOH) (Derep). λ_{max} 255 (ϵ 5900) (MeOH) (Berdy).
Ksebati, M.B. *et al., J.O.C.*, 1985, **50**, 5637

Tridachiapyrone E T-523

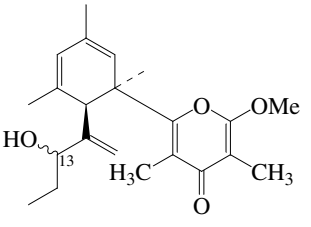
[99148-22-8]



$C_{22}H_{28}O_4$ 356.461
Constit. of *Tridachia crispata*. Oil. λ_{max} 225 (ϵ 7450); 255 (ϵ 5850) (MeOH) (Derep).

9,10α-Dihydro, 9-oxo: ***Tridachiapyrone F***
[99148-23-9]
$C_{22}H_{28}O_5$ 372.46
Constit. of *Tridachia crispata*. Powder. λ_{max} 225 (ϵ 7450); 255 (ϵ 5850) (MeOH) (Derep).
Ksebati, M.B. *et al., J.O.C.*, 1985, **50**, 5637-5642 (*isol*)

Tridachiapyrone G T-524



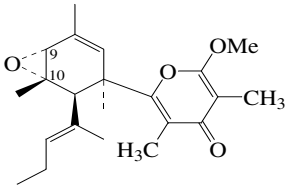
Relative Configuration

$C_{22}H_{30}O_4$ 358.477
Isol. from the mollusc *Placobranchus ocellatus.* Glass. $[\alpha]_D$ +229 (c, 0.16 in CH_2Cl_2). λ_{max} 260 (ϵ 12300) (MeOH).

13-Epimer: ***Tridachiapyrone H***
$C_{22}H_{30}O_4$ 358.477
Isol. from *Placobranchus ocellatus.* Glass. λ_{max} 260 (ϵ 11800) (MeOH).

13-Hydroperoxide: ***Tridachiapyrone J***
$C_{22}H_{30}O_5$ 374.476
Isol. from *Placobranchus ocellatus*. Glass. $[\alpha]_D$ +59.2 (c, 0.56 in CH_2Cl_2). λ_{max} 252 (ϵ 13700) (MeOH).
Fu, X. *et al., Tetrahedron*, 2000, **56**, 8989-8993

Tridachione T-525



(-)-*form*

$C_{22}H_{30}O_4$ 358.477
λ_{max} 255 (ϵ 15000) (MeOH) (Derep).

(-)-*form* [65955-40-0]
Constit. of *Tridachiella diomedea*.
Oil. $[\alpha]_D$ -113.3 (c, 0.06 in $CHCl_3$).

Deepoxy, 9,10-didehydro: ***9,10-Deoxytridachione***
[71725-09-2]
$C_{22}H_{30}O_3$ 342.477
Constit. of *Tridachiella diomedea*. Oil. $[\alpha]_D$ -194.8 (c, 0.27 in $CHCl_3$). λ_{max} 255 (ϵ 15000) (MeOH) (Derep).

Deepoxy, 9,10-didehydro, 6-epimer: ***Iso-9,10-dideoxytridachione***
[153830-33-2]
$C_{22}H_{30}O_3$ 342.477
Constit. of *Elysia timida*. Ichthyotoxin. Oil. $[\alpha]_D$ +5.9 ($CHCl_3$). λ_{max} 253 (ϵ 20200) (MeOH).

(+)-*form*

Deepoxy, 9,10-didehydro: [103665-41-4]
Metab. of mollusc *Elysia chlorotica*.
Oil. $[\alpha]_D$ +400 (c, 0.3 in $CHCl_3$). λ_{max} 255 (ϵ 15000) (MeOH) (Berdy).
Ireland, C. *et al., J.A.C.S.*, 1978, **100**, 1002-1003 (*isol*)
Ireland, C. *et al., Tetrahedron, Suppl.*, No. 1, 1981, 233 (*cryst struct*)
Dawe, R.D. *et al., Tet. Lett.*, 1986, **27**, 2559 (*isol*)
Gavagnin, M. *et al., J. Nat. Prod.*, 1994, **57**, 298-304 (*Iso-9,10-deoxytridachione*)
Moses, J.E. *et al., Chem. Comm.*, 2005, 1687-1689 (*9,10-Deoxytridachione, synth*)

2,4-Tridecadiyn-1-ol T-526

$H_3C(CH_2)_7C{\equiv}CC{\equiv}CCH_2OH$
$C_{13}H_{20}O$ 192.3

Methoxyacetyl: [125906-56-1]
$C_{16}H_{24}O_3$ 264.364
Isol. from the hermatypic corals *Montipora* spp. Shows ichthyotoxicity. Sol. MeOH, Me_2CO. λ_{max} 220 (E1%/1cm 545); 231 (E1%/1cm 647); 243 (E1%/1cm 625); 256 (E1%/1cm 418); 278 (E1%/1cm 417) (MeOH) (Berdy).
Higa, T. *et al., Chem. Lett.*, 1990, 145 (*isol, struct*)

1,5-Tridecanediol T-527

[39516-30-8]
$H_3C(CH_2)_7CH(OH)CH_2CH_2CH_2CH_2OH$
$C_{13}H_{28}O_2$ 216.363

(±)-*form*
Cryst. (petrol). Mp 51-52°.

(ξ)-*form*

5-Me ether: 5-Methoxy-1-tridecanol
$C_{14}H_{30}O_2$ 230.39
Isol. from *Asterias rollestoni*.
Massy-Westropp, R.A. *et al., Aust. J. Chem.*, 1984, **37**, 1303 (*synth, ir, pmr*)
Zhang, L.-X. *et al., Tianran Chanwu Yanjiu Yu Kaifa*, 2005, **17**, 35-37

2-Tridecanone T-528

FEMA 3388
[593-08-8]
$H_3C(CH_2)_{10}COCH_3$
$C_{13}H_{26}O$ 198.348
Isol. from plant oils, e.g. *Schizandra nigra*, palm oil, coconut oil. Also found in American cranberry, blueberry, raspberry, grapefruit, onion, ginger. Ant alarm pheromone. Constit. of male mandibular gland secretions of *Philanthus basilaris* and *Philanthus bicinctus*. Isol. from an arctic marine bacterium. Used as a flavouring essence.
Mp 29°. Bp 260-265° Bp_{16} 160°.
▶Fl. p. 107°.

Oxime:
$C_{13}H_{27}NO$ 213.362
Insol. petrol. Mp 56-57°.

Semicarbazone: Mp 126°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 641C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 498A (*ir*)
Pickard, R.H. *et al., J.C.S.*, 1911, **55**, 45 (*synth*)
Morgan, G.T. *et al., J. Soc. Chem. Ind., London*, 1925, **44**, 108r
Allen, R.R. *et al., Chem. Ind. (London)*, 1965, 1560 (*isol*)
Regnier, F.E. *et al., J. Insect Physiol.*, 1968, **43**, 411
Hajek, M. *et al., Tet. Lett.*, 1974, **36**, 3193 (*synth*)
McDaniel, C.A. *et al., J. Chem. Ecol.*, 1987, **13**, 227
Singh, J. *et al., Indian J. Chem., Sect. B*, 2001, **40**, 386-390 (*synth*)
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*marine isol*)

6-Tridecylamine T-529

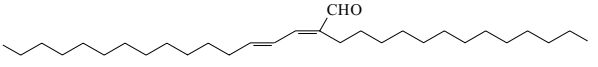
6-Tridecanamine. 1-Pentyloctylamine. 6-Aminotridecane
$H_3C(CH_2)_6CH(NH_2)(CH_2)_4CH_3$
$C_{13}H_{29}N$ 199.379

(ξ)-*form*

N-*Ac: 6-Acetamidotridecane*
[345261-17-8]
$C_{15}H_{31}NO$ 241.416
Isol. from the cyanobacterium *Microcoleus lyngbyaceus*. Cryst.
Orsini, M.A. *et al., J. Nat. Prod.*, 2001, **64**, 572-577 (*isol, ir, pmr, cmr*)

2-Tridecyl-2,4-heptadecadienal T-530

14-Formyl-14,16-nonacosadiene

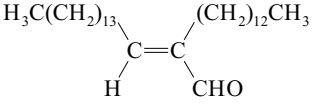


$C_{30}H_{56}O$ 432.772

(2*E*,4*E*)-*form* [169565-73-5]
Constit. of the red alga *Corallina mediterranea*.
De Rosa, S. *et al., Phytochemistry*, 1995, **40**, 995 (*isol, pmr, cmr*)

2-Tridecyl-2-heptadecenal T-531

14-Formyl-14-nonacosene

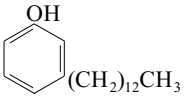


$C_{30}H_{58}O$ 434.788

(*E*)-*form* [112642-50-9]
Constit. of the red algae *Corallina mediterranea, Laurencia obtusa, Laurencia papillosa* and *Laurencia undulata*.
Cryst. λ_{max} 231 (log ϵ 4.02) (MeOH).
Suzuki, M. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 3793 (*isol, struct*)
De Rosa, S. *et al., Phytochemistry*, 1995, **40**, 995-996 (*isol, pmr, cmr, ms*)

3-Tridecylphenol, 9CI T-532

Cardanol $C_{13:0}$
[72424-02-3]



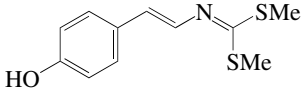
$C_{19}H_{32}O$ 276.461
Isol. from the brown alga *Caulocystis cephalornithos*. Phospholipase Cγ1 inhibitor.
Mp 44-45°.

8′,9′-Didehydro (Z-): 3-(8-Tridecenyl)phenol
$C_{19}H_{30}O$ 274.445
Constit. of *Knema hookeriana*. Oil. λ_{max} 217 (ϵ 5200); 273 (ϵ 1610); 280 (sh) (ϵ 1400) (MeOH).

Durrani, A.A. *et al., J.C.S. Perkin 1*, 1979, 2069 (*synth, pmr*)
Kazlauskas, R. *et al., Aust. J. Chem.*, 1980, **33**, 2097 (*isol*)
Alen, Y. *et al., Z. Naturforsch., C*, 2000, **55**, 300-303 (*8-Tridecenylphenol*)

Tridentatol A T-533

[185548-48-5]



$C_{11}H_{13}NOS_2$ 239.362
Metab. from the marine hydroid *Tridentata marginata*. Amorph. solid. λ_{max} 337 (ϵ 18000) (MeOH).

O-*Sulfate:* ***Tridentatol E***
$C_{11}H_{13}NO_4S_3$ 319.426
Isol. from *Tridentata marginata*. Amorph. solid (as Na salt). λ_{max} 326 (log ϵ 4.41) (MeOH) (Na salt).

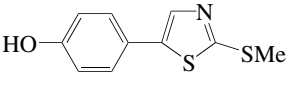
Z-*Isomer:* ***Tridentatol B***
[185548-49-6]
$C_{11}H_{13}NOS_2$ 239.362
Isol. from *Tridentata marginata*. Amorph. solid. λ_{max} 332 (ϵ 11000) (MeOH).

Z-*Isomer,* O-*sulfate:* ***Tridentatol F***
$C_{11}H_{13}NO_4S_3$ 319.426
Isol. from *Tridentata marginata*. Amorph. solid (as Na salt). λ_{max} 325 (log ϵ 3.78) (MeOH) (Na salt).

Lindquist, N. *et al., Tet. Lett.*, 1996, **37**, 9131-9134 (*Tridentatols A,B*)
Lindquist, N. *et al., J. Nat. Prod.*, 2002, **65**, 681-684 (*Tridentatols E,F*)

Tridentatol C T-534

4-[2-(Methylthio)-5-thiazolyl]phenol, 9CI. 2-(4-Hydroxyphenyl)-5-(methylthio)thiazole
[185548-50-9]

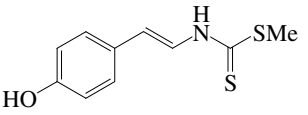


$C_{10}H_9NOS_2$ 223.319
Metab. from the marine hydroid *Tridentata marginata*. Plates. λ_{max} 313 (ϵ 3000) (MeOH).

O-*Sulfate:* ***Tridentatol H***
[439255-40-0]
$C_{10}H_9NO_4S_3$ 303.383
Isol. from *Tridentata marginata*. Amorph. powder (as Na salt).

Lindquist, N. *et al., Tet. Lett.*, 1996, **37**, 9131-9134 (*isol, uv, ir, pmr, cryst struct*)
Jayatilake, G.S. *et al., Org. Lett.*, 1999, **1**, 661-662 (*synth*)
Lindquist, N. *et al., J. Nat. Prod.*, 2002, **65**, 681-684 (*Tridentatol H*)

Tridentatol D T-535



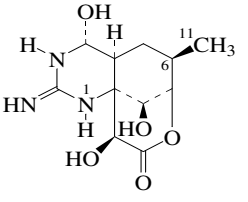
$C_{10}H_{11}NOS_2$ 225.335
Isol. from the marine hydroid *Tridentata marginata*. Amorph. solid. λ_{max} 342 (log ϵ 4.35) (MeOH).

O-*Sulfate:* ***Tridentatol G***
$C_{10}H_{11}NO_4S_3$ 305.399
Isol. from *Tridentata marginata*. Amorph. powder (as Na salt). λ_{max} 289 (sh); 339 (log ϵ 4.32) (MeOH) (Na salt).

Lindquist, N. *et al., J. Nat. Prod.*, 2002, **65**, 681-684 (*isol, pmr, cmr*)

5,6,11-Trideoxytetrodotoxin T-536

[172228-91-0]



$C_{11}H_{17}N_3O_5$ 271.272
Slightly misleading name. In Tetrodotoxin, T-278 the 5-OH is present as an internal acetal. Isol. from the fish *Fugu poecilonotus*.
$[\alpha]_D^{23}$ -17.4 (c, 0.5 in AcOH aq.).
▶ Toxic.

6,N^1-*Dihydroxy:* ***1-Hydroxy-5,11-dideoxytetrodotoxin***
[146689-16-9]
$C_{11}H_{17}N_3O_7$ 303.271
Isol. from the newt *Taricha granulosa* and *Taricha torosa*. Amorph. powder. $[\alpha]_D$ +14.5 (c, 0.3 in AcOH aq.). Misleading synonym. λ_{max} 225 (H_2O) (Berdy).
▶ Neurotoxin.

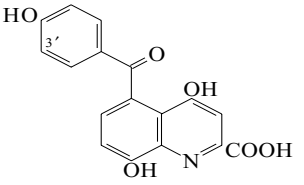
6,11-*Dihydroxy:* ***5-Deoxytetrodotoxin***
$C_{11}H_{17}N_3O_7$ 303.271
Isol. from *Fugu poecilonotus*. Amorph. solid.

4-*Epimer:* ***5,6,11-Trideoxy-4-epitetrodotoxin***
[172339-07-0]
$C_{11}H_{17}N_3O_5$ 271.272
Isol. from *Fugu poecilonotus*.
$[\alpha]_D^{23}$ -60.2 (c, 0.65 in AcOH aq.).
▶ Toxic.

Kotaki, Y. *et al., J.A.C.S.*, 1993, **115**, 827-830 (*1-Hydroxy-5,11-dideoxytetrodotoxin*)
Yotsu-Yamashita, M. *et al., Tet. Lett.*, 1995, **36**, 9329-9332 (*isol, struct*)
Yotsu-Yamashita, M. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 961-963 (*5-Deoxytetrodotoxin*)

Trididemnic acid A T-537

4,8-Dihydroxy-5-(4-hydroxybenzoyl)-2-quinolinecarboxylic acid, 9CI
[142808-50-2]

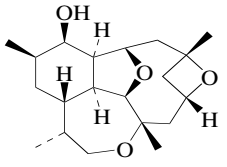


$C_{17}H_{11}NO_6$ 325.277

Alkaloid from the marine ascidian *Trididemnum* sp. Pale yellow solid.

3′-Hydroxy: ***Trididemnic acid B.*** *5-(3,4-Dihydroxybenzoyl)-4,8-dihydroxy-2-quinolinecarboxylic acid, 9CI*
[142808-51-3]
$C_{17}H_{11}NO_7$ 341.276
Alkaloid from *Trididemnum* sp.
Dilip de Silva, E. *et al., Tet. Lett.*, 1992, **33**, 2917-2920 (*isol, pmr, cmr, struct*)

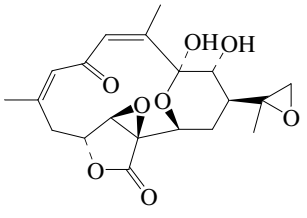
2,9:3,16:5,7-Triepoxy-11-asbestian-11-ol T-538



$C_{20}H_{32}O_4$ 336.47

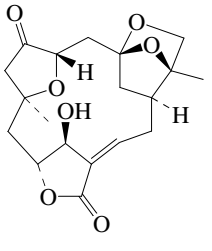
Ac: [153977-18-5]
$C_{22}H_{34}O_5$ 378.508
Constit. of *Briareum asbestinum*. Gum. $[\alpha]_D$ -5.8 (c, 0.1 in $CHCl_3$).
Dookran, R. *et al., Tetrahedron*, 1994, **50**, 1983-1992 (*isol, pmr, cmr*)

3,13:11,12:15,16-Triepoxy-2,3-dihydroxy-6-oxo-4,7-cembradien-20,10-olide T-539



$C_{20}H_{24}O_8$ 392.405
Constit. of *Pseudopterogorgia bipinnata*.
Fenical, W. *et al., J. Nat. Prod.*, 1987, **50**, 1001-1008

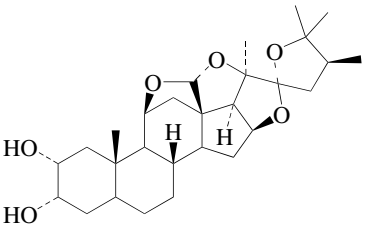
3,15:3,16:5,8-Triepoxy-11-hydroxy-18-nor-6-oxo-12-cembren-20,10-olide T-540



$C_{19}H_{24}O_7$ 364.394

(1*S*,3*S*,5*S*,8*S*,10*R*,11*S*,12*Z*,15*S*)-*form*
Leptocladolide C
[605659-51-6]
Constit. of *Sinularia leptoclados.*
Cryst.
Mp 215-216°. $[\alpha]_D^{25}$ +83 (c, 0.3 in $CHCl_3$).
Ahmed, A.F. *et al., Tetrahedron*, 2003, **59**, 7337-7344 (*isol, pmr, cmr*)

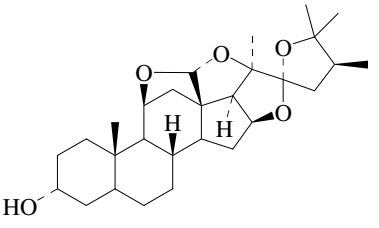
11,18:18,20:22,25-Triepoxy-24-methylfurostane-2,3-diol T-541



$C_{28}H_{42}O_6$ 474.636

(2α,3α,5α,11β,18*R*,22*S*,24*S*)-*form*
2-Ac: [858950-48-8]
$C_{30}H_{44}O_7$ 516.673
Constit. of *Isis hippuris.* Powder.
Mp 236-237°. $[\alpha]_D$ -27 (c, 0.96 in $CHCl_3$).
3-Ac: [858950-46-6]
$C_{30}H_{44}O_7$ 516.673
Constit. of *Isis hippuris.* Powder.
Mp 193-194°. $[\alpha]_D$ -30 (c, 0.83 in $CHCl_3$).
2,3-Di-Ac: [858950-44-4]
$C_{32}H_{46}O_8$ 558.711
Constit. of *Isis hippuris.* Powder.
Mp 252-253°. $[\alpha]_D$ -22 (c, 0.31 in $CHCl_3$).
Chao, C.-H. *et al., J. Nat. Prod.*, 2005, **68**, 880-885 (*Isis hippuris constits*)

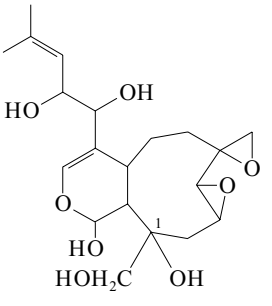
11,18:18,20:22,25-Triepoxy-24-methylfurostan-3-ol T-542



$C_{28}H_{42}O_5$ 458.637

(3α,5α,11β,18*R*,22*S*,24*S*)-*form*
3-Ac: [79858-77-8]
$C_{30}H_{44}O_6$ 500.674
Constit. of *Isis hippuris.* Cryst.
Mp 245.5-247°.
Higa, T. *et al., Tet. Lett.*, 1981, **29**, 2777-2780 (*isol*)
Chao, C.-H. *et al., J. Nat. Prod.*, 2005, **68**, 880-885 (*cryst struct*)

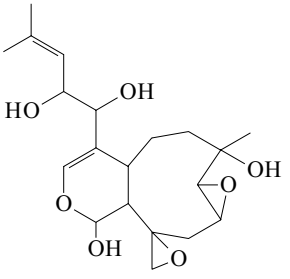
6,20:7,8:17,18-Triepoxy-10(17),13-xenicadiene-1,11,12,18,19-pentol T-543



$C_{20}H_{30}O_8$ 398.452

11,12,18,19-Tetra-Ac: ***19-Acetoxy-11-havannahol***
$C_{28}H_{38}O_{12}$ 566.601
Constit. of *Xenia membranacea*. Amorph. $[\alpha]_D$ +4.5 (c, 0.55 in $CHCl_3$).
Almourabit, A. *et al., J. Nat. Prod.*, 1990, **53**, 894 (*isol, pmr, cmr*)

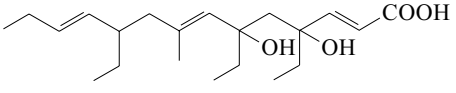
1,19:7,8:17,18-Triepoxy-10(17),13-xenicadiene-6,11,12,18-tetrol **T-544**



$C_{20}H_{30}O_7$ 382.453

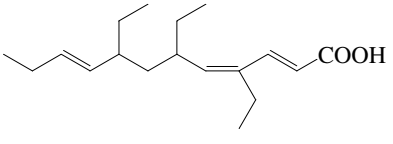
11,12,18-Tri-Ac: ***7-Havannahol***
$C_{26}H_{36}O_{10}$ 508.564
Constit. of *Xenia membranacea*. Amorph. $[\alpha]_D$ +16 (c, 2.27 in $CHCl_3$).
Almourabit, A. *et al., J. Nat. Prod.*, 1990, **53**, 894 (*isol, pmr, cmr*)

4,6,10-Triethyl-4,6-dihydroxy-8-methyl-2,7,11-tetradecatrienoic acid **T-545**
[152821-48-2]



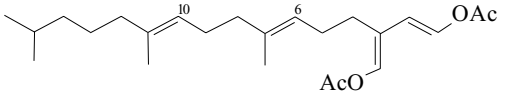
$C_{21}H_{36}O_4$ 352.513
Isol. from the sponge *Plakortis halichondrioides*. Cytotoxic. Oil. $[\alpha]_D$ +4.8 (c, 0.46 in $CHCl_3$).
Rudi, A. *et al., J. Nat. Prod.*, 1993, **56**, 1827 (*isol, pmr*)

4,6,8-Triethyl-2,4,9-dodecatrienoic acid **T-546**
Monotriajaponide A



$C_{18}H_{30}O_2$ 278.434
Isol. from the marine sponge *Monotria japonica*. Selectively lyses starfish oocytes. Viscous oil. $[\alpha]_D$ +63 (c, 0.09 in $CHCl_3$). λ_{max} 271 (log ϵ 4.28) (MeOH).
Yanai, M. *et al., Bioorg. Med. Chem.*, 2003, **11**, 1715-1721 (*isol, pmr, cmr*)

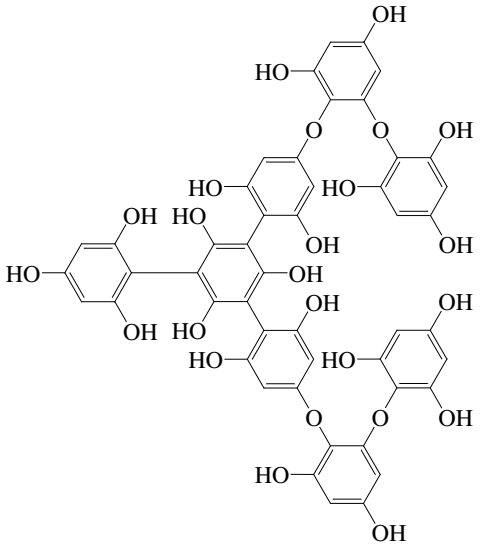
Trifarin **T-547**
1,20-Diacetoxy-1,3(20),6,10-phytatetraene
[69625-34-9]



$C_{24}H_{38}O_4$ 390.562
Constit. of *Caulerpa flexilis*. Oil.

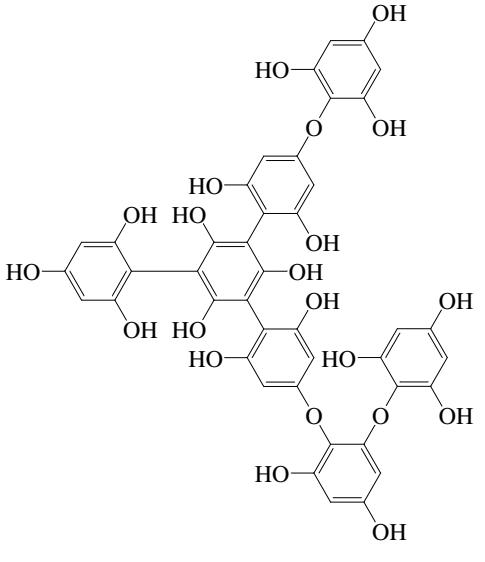
6,7,10,11-Tetrahydro: ***Bisdihydrotrifarin***
$C_{24}H_{42}O_4$ 394.593
Constit. of *Pseudochlorodesmis furcellata*. Feeding deterrent. Oil. $[\alpha]_D^{25}$ +1.6 (c, 0.68 in $CHCl_3$). λ_{max} 250 (ϵ 14500) (MeOH) (Berdy).
Blackman, A.J. *et al., Tet. Lett.*, 1978, 3063 (*isol*)
Paul, V.J. *et al., Phytochemistry*, 1988, **27**, 1011 (*deriv*)

Trifucotetraphlorethol A **T-548**



$C_{48}H_{34}O_{24}$ 994.782
Isol. from *Fucus vesiculosus*.
Japan. Pat., 1983, 58 118 591; *CA*, **100**, 12637 (*occur*)

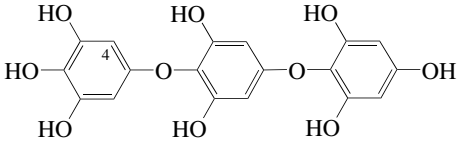
Trifucotriphlorethol A **T-549**



$C_{42}H_{30}O_{21}$ 870.686
Isol. from *Fucus vesiculosus*. Not indexed by CAS.
Preuss, B. *et al., Thesis*, Bonn, 1983,

Trifuhalol A T-550

5-[2,6-Dihydroxy-4-(2,4,6-trihydroxyphenoxy)phenoxy]-1,2,3-benzenetriol, 9CI. Trifuhalol
[51593-97-6]



$C_{18}H_{14}O_{10}$ 390.303

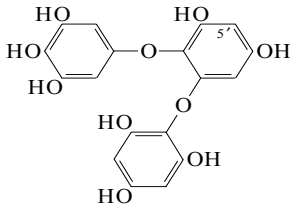
CAS numbering shown. Stable only as per-substituted deriv. Isol. from *Halidrys siliquosa*, *Sargassum muticum* and *Carpophyllum angustifolium*. Shows antibiotic props. Cryst. (MeOH)(as oct-Ac). Mp 117-123° Octa-Ac.

4-Hydroxy: ***Hydroxytrifuhalol A***
[164176-18-5]
$C_{18}H_{14}O_{11}$ 406.302
Constit. of *Sargassum spinuligerum*.

Glombitza, K.W. *et al., Tet. Lett.*, 1973, 4277-4280 (*isol, synth, struct, uv, pmr, cmr*)
Sattler, E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1975, **308**, 813 (*synth*)
Glombitza, K.W. *et al., Phytochemistry*, 1976, **15**, 1279; 1978, **38**, 579 (*isol*)
Keusgen, M. *et al., Phytochemistry*, 1995, **38**, 975 (*2-hydroxy, isol, pmr, cmr, ms*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

Trifuhalol B T-551

5-[2,4-Dihydroxy-6-(2,4,6-trihydroxyphenoxy)phenoxy]-1,2,3-benzenetriol, 9CI. 5-(2,4,6-Trihydroxyphenoxy)-4-(3,4,5-trihydroxyphenoxy)-1,3-benzenediol
[67492-10-8]

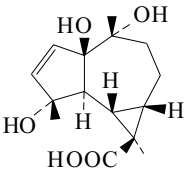


$C_{18}H_{14}O_{10}$ 390.303
Isol. from *Sargassum muticum* (as per-Ac).

5′-Hydroxy: ***Hydroxytrifuhalol B***
[164176-19-6]
$C_{18}H_{14}O_{11}$ 406.302
Constit. of *Sargassum spinuligerum*.

Glombitza, K.W. *et al., Phytochemistry*, 1978, **17**, 579 (*isol, struct*)
Keusgen, M. *et al., Phytochemistry*, 1995, **38**, 975 (*5′-hydroxy, isol, pmr, cmr, ms*)

1,4,10-Trihydroxy-2-aromadendren-12-oic acid T-552



$C_{15}H_{22}O_5$ 282.336

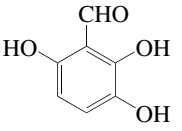
(1β,4α,5α,6β,7β,10α,10α,11β)-*form* [79383-58-7]

Me ester:
$C_{16}H_{24}O_5$ 296.363
Constit. of *Clavularia koellikeri*. Oil. $[\alpha]_D$ -72 (c, 0.52 in $CHCl_3$).

Braekman, J.C. *et al., Tetrahedron*, 1981, **37**, 179-186 (*cryst struct*)

2,3,6-Trihydroxybenzaldehyde, 9CI T-553

[64168-39-4]



$C_7H_6O_4$ 154.122

2-Sulfate: ***Polyclinal***
[136092-30-3]
$C_7H_6O_7S$ 234.186
Constit. of *Polyclinum planum*. Cryst. λ_{max} 232 (ϵ 12000); 264 (ϵ 9300); 368 (ϵ 4200) (MeOH) (Berdy).

2-Me ether: 3,6-Dihydroxy-2-methoxybenzaldehyde
[80832-56-0]
$C_8H_8O_4$ 168.149
Cryst. ($CHCl_3$/petrol). Mp 85-86°.

3,6-Di-Me ether: 2-Hydroxy-3,6-dimethoxybenzaldehyde
[64466-51-9]
$C_9H_{10}O_4$ 182.176
Fine yellow needles (MeOH). Mp 67-67.5° Mp 105-106°.

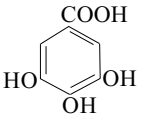
2,3,6-Tri-Me ether: 2,3,6-Trimethoxybenzaldehyde
[5556-86-5]
$C_{10}H_{12}O_4$ 196.202
Mp 20°.

2,3,6-Tri-Me ether, 2,4-dinitrophenylhydrazone:
Cryst. (AcOH). Mp 221° (203°).

Merchant, J.R. *et al., J.C.S.*, 1957, 4142-4143 (*tri-Me ether*)
Shulgin, A.T. *et al., J. Med. Chem.*, 1966, **9**, 445-446 (*tri-Me ether*)
Wriede U., *et al., J.O.C.*, 1987, **52**, 4485-4489 (*3,6-di-Me ether, synth, pmr*)
Lindquist, N. *et al., Experientia*, 1991, **47**, 503-504 (*Polyclinal*)

3,4,5-Trihydroxybenzoic acid T-554

Gallic acid
[149-91-7]



$C_7H_6O_5$ 170.121
Isol. by Scheele in 1786 from fermented galls. Occurs in many tannins. Specific flowering inhibitor in leaves of *Kalanchoe bloesfeldiana*. Used in tanning, as anal. reagent and photographic developer. Used as 2% soln. in Me_2CO for photometric detn. of Nb (in the presence of aniline), Th, Ti, Ce, Cu. Antineoplastic agent, astringent. Possesses bacteriostatic activity. Needles (MeOH or $CHCl_3$); cryst. + $1H_2O$ (H_2O). Sol. Me_2CO, EtOH; spar. sol. H_2O; insol. C_6H_6, $CHCl_3$. Mp 253° dec. (225°, 235-240°). pK_{a1} 3.13; pK_{a2} 8.84; pK_{a3} 12.4 (20°, 0.1*M* KNO_3). Log P 0.43 (calc).

▶ LD_{50} (rbt, orl) 5000 mg/kg. Exp. reprod. effects. LW7525000

Me ester: Methyl 3,4,5-trihydroxybenzoate. Methyl gallate. Gallicin†
[99-24-1]
$C_8H_8O_5$ 184.148
Found in *Koelreuteria paniculata*, *Euphorbia* spp., *Geranium* spp., *Sapium sebiferum*, *Acacia* spp., *Spirogyra* spp., *Rhus glabra* and *Pelargonium sidoides*. Reverse transcriptase inhibitor. Sol. MeOH, EtOH, Me_2CO, dioxan, Py, Et_2O; fairly sol. $CHCl_3$, H_2O; poorly sol. C_6H_6, toluene, hexane, CCl_4. Mp 157°. pK_{a1} 7.88 (25°, 0.1*M* KNO_3). λ_{max} 276 (E1%/1cm 623); 283 (EtOH) (Berdy).

▶ LD_{50} (mus, orl) 1700 mg/kg; LD_{50} (mus, ivn) 470 mg/kg; LD_{50} (mus, ipr) 784 mg/kg. LW8000000

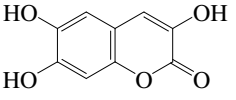
[5995-86-8, 13405-60-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 229B; 232A; 232B; 301A; 301B; 461B (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1142C; 1143A; 1147C; 1148B; 1261B; 1261C; 1352C; 1539C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1332D; 1370B; 1370C; 1419C (*ir*)
Morris, S.G. *et al., J.A.C.S.*, 1946, **68**, 500 (*esters*)
Pearl, I.A. *et al., J.A.C.S.*, 1950, **72**, 1743-1746 (*synth, derivs*)
Van Der Kerk, G.J.M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1951, **70**, 277 (*esters*)
Nakabayashi, T. *et al., CA*, 1955, **49**, 36529 (*Me ester*)
Lajis, N.H. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 609 (*Methyl gallate, bibl*)
Zhu, J. *et al., Synth. Commun.*, 1996, **26**, 2479 (*esters*)

3,6,7-Trihydroxy-2*H*-1-benzopyran-2-one T-555

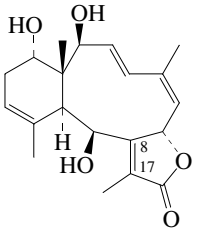
3,6,7-Trihydroxycoumarin
[20759-58-4]



$C_9H_6O_5$ 194.143
Constit. of *Dasycladus vermicularis*. Cryst.
Mp 272-274°.

Fr. Pat., 1968, 1 523 317; *CA*, **72**, 31615v (*synth*)
Menzel, D. *et al., Bot. Mar.*, 1983, **26**, 23
Bailly, F. *et al., Bioorg. Med. Chem.*, 2004, **12**, 5611-5618 (*synth, pmr, cmr*)

2,9,14-Trihydroxy-3,5,8(17),11-briaratetraen-18,7-olide T-556



$C_{20}H_{26}O_5$ 346.422

(2β,3*E*,5*Z*,7α,8α,9β,14α,17α)-*form*

8,17-Epoxide: 8,17-Epoxy-2,9,14-trihydroxy-3,5,11-briaratrien-18,7-olide
$C_{20}H_{26}O_6$ 362.422

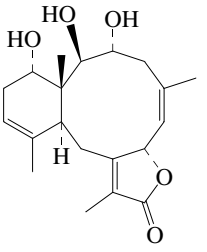
8α,17α-Epoxide, tri-Ac: ***Briaranolide I***
[866087-93-6]
$C_{26}H_{32}O_9$ 488.533
Constit. of a *Briareum* sp. Cryst.
Mp 213-216°. $[\alpha]_D^{25}$ +33.6 (c, 1.1 in $CHCl_3$).

8,17:11,12-Diepoxide: 8,17:11,12-Diepoxy-2,9,14-trihydroxy-3,5-briaradien-18,7-olide
$C_{20}H_{26}O_7$ 378.421

8α,17α:11α,12α-Diepoxide, tri-Ac: ***Briaranolide J***
[866087-94-7]
$C_{26}H_{32}O_{10}$ 504.533
Constit. of a *Briareum* sp. Amorph. solid. $[\alpha]_D^{24}$ +11.8 (c, 1 in $CHCl_3$).

Hoshino, A. *et al., J. Nat. Prod.*, 2005, **68**, 1328-1335 (*Briaranolides*)

2,3,14-Trihydroxy-5,8(17),11-briaratrien-18,7-olide T-557



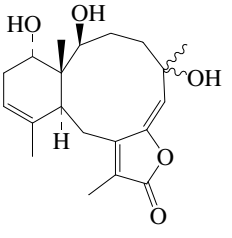
$C_{20}H_{28}O_5$ 348.438

(2β,3α,5*Z*,7α,14α)-*form*

Tri-Ac: ***Brianthein A***. *Briviolide J*
[383366-81-2]
$C_{26}H_{34}O_8$ 474.55
Constit. of *Briareum excavatum*. Amorph. powder. $[\alpha]_D^{20}$ +118.7 (c, 0.4 in EtOH). $[\alpha]_D$ -104 (c, 0.07 in MeOH). λ_{max} 224 (ε 9200) (MeOH).

Aoki, S. *et al., Tetrahedron*, 2001, **57**, 8951-8957 (*Brianthein A*)
Iwagawa, T. *et al., Heterocycles*, 2005, **65**, 2083-2093 (*Briviolide J*)

2,5,14-Trihydroxy-6,8(17),11-briaratrien-18,7-olide T-558



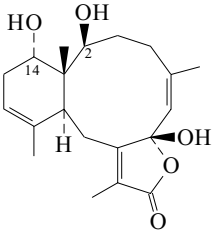
$C_{20}H_{28}O_5$ 348.438

(2β,5ξ,6*E*,14α)-*form*

2-(3-Methylbutanoyl), 14-Ac: [76353-45-2]
$C_{27}H_{38}O_7$ 474.593
Constit. of *Scytalium tentaculatum*. Foam. $[\alpha]_D^{20}$ +63.6 (c, 1.1 in CCl_4). λ_{max} 205 (ε 16300); 220 (ε 1300) (MeOH).

Ravi, B.N. *et al., Aust. J. Chem.*, 1980, **33**, 2307-2316 (*isol, pmr, cmr*)

2,7,14-Trihydroxy-5,8(17),11-briaratrien-18,7-olide T-559



$C_{20}H_{28}O_5$ 348.438

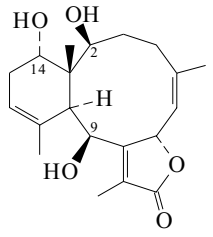
(2β,5*Z*,7β*OH*,14α)-*form*

2,14-Di-Ac: ***Funicolide E***
[171370-69-7]
$C_{24}H_{32}O_7$ 432.513
Constit. of *Funiculina quadrangularis* (Funiculidae).
$[\alpha]_D^{20}$ -61.7 (c, 0.59 in EtOH).

2-Propanoyl, 14-Ac: ***Funicolide B***
[171423-46-4]
$C_{25}H_{34}O_7$ 446.539
Constit. of *Funiculina quadrangularis*.

$[\alpha]_D^{20}$ -45.7 (c, 0.14 in EtOH).
Guierro, A. *et al., Helv. Chim. Acta*, 1995, **78**, 1465 (*isol, pmr, cmr*)

2,9,14-Trihydroxy-5,8(17),11-briaratrien-18,7-olide T-560



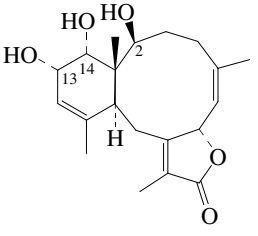
$C_{20}H_{28}O_5$ 348.438

(2β,5*Z*,7α,9β,14α)-*form*

2-Propanoyl, 9,14-di-Ac: ***Funicolide C***
[171370-67-5]
$C_{27}H_{36}O_8$ 488.577
Constit. of *Funiculina quadrangularis.*
$[\alpha]_D^{20}$ +69.4 (c, 0.3 in EtOH).

2-Butanoyl, 14-Ac: ***Briareolide J***
[180283-30-1]
$C_{26}H_{36}O_7$ 460.566
Constit. of *Briareum abestinum*. Amorph. powder. $[\alpha]_D$ +57.8 (c, 0.28 in $CHCl_3$). λ_{max} 235 (log ϵ 3.75) (MeOH).
Guierro, A. *et al., Helv. Chim. Acta*, 1995, **78**, 1465 (*Funicolide C*)
Mootoo, B.S. *et al., Tetrahedron*, 1996, **52**, 9953 (*Briareolide J*)

2,13,14-Trihydroxy-5,8(17),11-briaratrien-18,7-olide T-561



$C_{20}H_{28}O_5$ 348.438

(2β,5*Z*,7α,13α,14α)-*form*

2-Propanoyl, 13,14-di-Ac: ***Anthoptilide E***
[264618-22-6]
$C_{27}H_{36}O_8$ 488.577
Constit. of *Anthoptilum* cf. *kukenthali*. Amorph. solid. $[\alpha]_D^{25}$ +2.2 (c, 0.28 in MeOH). λ_{max} 202 (ϵ 13420); 218 (ϵ 10160) (MeOH).

13-Ketone: 2,14-Dihydroxy-13-oxo-5,8(17),11-briaratrien-18,7-olide
$C_{20}H_{26}O_5$ 346.422

13-Ketone, 2-tigloyl, 14-Ac: ***Anthoptilide A***
[264618-18-0]
$C_{27}H_{34}O_7$ 470.561
Constit. of *Anthoptilum* cf. *kukenthali*. Solid. $[\alpha]_D^{25}$ +92.6 (c, 0.63 in MeOH). λ_{max} 216 (ϵ 20200); 241 (ϵ 15370) (MeOH).

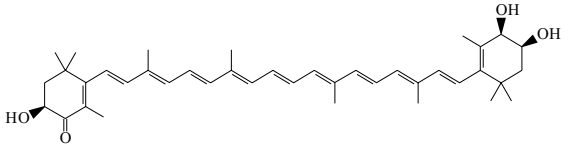
13-Ketone, 2-(2-methylpropanoyl), 14-Ac: ***Anthoptilide B***
[264618-19-1]
$C_{26}H_{34}O_7$ 458.55
Constit. of *Anthoptilum* cf. *kukenthali*. Solid. $[\alpha]_D^{25}$ +59.1 (c, 0.52 in MeOH). λ_{max} 216 (ϵ 18930); 241 (ϵ 15370) (MeOH).

13-Ketone, 2-propanoyl, 14-Ac: ***Anthoptilide C***
[264618-20-4]
$C_{25}H_{32}O_7$ 444.524
Constit. of *Anthoptilum* cf. *kukenthali*. Solid. $[\alpha]_D^{25}$ +17.6 (c, 0.19 in MeOH). λ_{max} 213 (ϵ 16100); 241 (ϵ 13820) (MeOH).

13-Ketone, 2-benzoyl, 14-Ac: ***Anthoptilide D***
[264618-21-5]
$C_{29}H_{32}O_7$ 492.568
Constit. of *Anthoptilum* cf. *kukenthali*. Powder. $[\alpha]_D^{25}$ +104.2 (c, 0.49 in MeOH). λ_{max} 228 (ϵ 7750) (MeOH).
Pham, N.B. *et al., J. Nat. Prod.*, 2000, **63**, 318-321 (*isol, pmr, cmr, cryst struct*)

3,3′,4′-Trihydroxy-β,β-caroten-4-one, 9CI T-562

[25510-19-4]

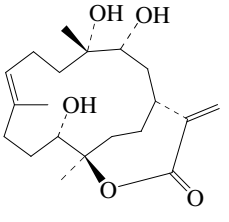


$C_{40}H_{54}O_4$ 598.864

(3*S*,3′*S*,4′*R*)-*form*

Idoxanthin
[97169-13-6]
Isol. from Japanese sandfish and marine fish-eggs. Postulated metab. prod. of Astaxanthin, A-721 in mackerel eggs.
Cryst. (Me_2CO/hexane). λ_{max} 457 (hexane).
Hodler, M. *et al., Chimia*, 1974, **28**, 723 (*synth*)
Matsuno, T. *et al., Nippon Suisan Gakkaishi*, 1983, **49**, 1475 (*isol*)
Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 779; 1995, **111**, 597-605 (*occur, biosynth*)

3,4,11-Trihydroxy-7,15(17)-cembradien-16,12-olide T-563

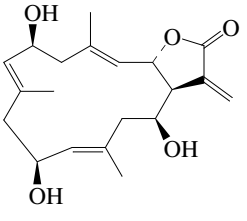


$C_{20}H_{32}O_5$ 352.47

(1*R*,3*R*,4*S*,7*E*,11*S*,12*R*)-*form*

Capillolide
[306997-16-0]
[457633-49-7, 817636536 hydr-at-e]
Constit. of *Sinularia capillosa*, *Sinularia microclavata* and *Sinularia tenella*.
Cryst.
Mp 158-160°. $[\alpha]_D^{25}$ +42.8 (c, 0.05 in EtOH).
Yang, R.-L. *et al., Huaxue Xuebao*, 2000, **58**, 1186-1187 (*isol, pmr, cmr*)
Su, J. *et al., J. Nat. Prod.*, 2000, **63**, 1543-1545 (*isol, pmr, cmr*)
Lin, C.-W. *et al., Chem. Res. Chin. Univ.*, 2002, **18**, 189-191 (*isol, pmr, cmr, cryst struct*)
Zhang, C.-X. *et al., Acta Cryst. E*, 2004, **60**, o1598-o1600 (*cryst struct*)

6,10,14-Trihydroxy-3,7,11,15(17)-cembratetraen-16,2-olide T-564



$C_{20}H_{28}O_5$ 348.438

(1*S*,2*S*,3*E*,6*S*,7*E*,10*S*,11*E*,14*S*)-*form*

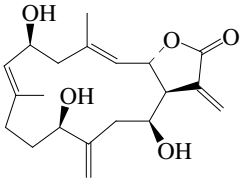
6,10-Di-Ac: [314739-96-3]
$C_{24}H_{32}O_7$ 432.513
Constit. of *Clavularia koellikeri*. Oil. $[\alpha]_D^{25}$ -19.2 (c, 0.19 in $CHCl_3$). λ_{max} 218 (log ϵ 3.48) (EtOH).

10,14-Di-Ac: [314739-97-4]
$C_{24}H_{32}O_7$ 432.513
Constit. of *Clavularia koellikeri*. Oil. $[\alpha]_D^{25}$ -35 (c, 0.12 in $CHCl_3$). λ_{max} 229 (log ϵ 3.39) (EtOH).

Tri-Ac: [314739-95-2]
$C_{26}H_{34}O_8$ 474.55
Constit. of *Clavularia koellikeri*. Oil. $[\alpha]_D^{25}$ -19.5 (c, 0.19 in $CHCl_3$). λ_{max} 208 (log ϵ 4.1) (EtOH).

Iwashima, M. *et al., J. Nat. Prod.*, 2000, **63**, 1647-1652 (*isol, pmr, cmr*)

6,11,14-Trihydroxy-3,7,12(20),15(17)-cembratetraen-16,2-olide T-565



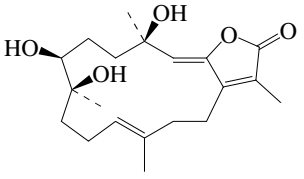
$C_{20}H_{28}O_5$ 348.438

(1*S*,2*S*,3*E*,6*S*,7*E*,11*R*,14*S*)-*form*

Di-Ac: [473700-49-1]
$C_{24}H_{32}O_7$ 432.513
Constit. of *Clavularia koellikeri*. Oil. $[\alpha]_D^{25}$ +28.4 (c, 0.19 in $CHCl_3$). λ_{max} 220 (log ϵ 3.48) (no solvent reported).

Iwashima, M. *et al., J. Nat. Prod.*, 2002, **65**, 1441-1446 (*isol, pmr, cmr*)

4,7,8-Trihydroxy-1(15),2,11-cembratrien-16,2-olide T-566



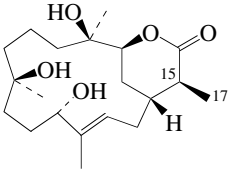
$C_{20}H_{30}O_5$ 350.454

(2*Z*,4*R*,7*S*,8*S*,11*E*)-*form*

Polydactylide
[878665-05-5]
Constit. of *Sinularia polydactyla*.
$[\alpha]_D^{25}$ +11 (c, 0.1 in $CHCl_3$).

Grote, D. *et al., Nat. Prod. Res.*, 2006, **20**, 285-291 (*Polydactylide*)

4,8,11-Trihydroxy-12-cembren-16,3-olide T-567



$C_{20}H_{34}O_5$ 354.486

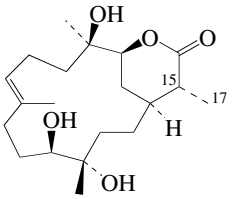
(1*R*,3*S*,4*S*,8*R*,11*R*,12*E*)-*form*

Dihydroflexibilolide
[184169-48-0]
Constit. of *Sinularia flexibilis*.
Needles.
Mp 160-163°. $[\alpha]_D^{27}$ -22 (c, 1 in MeOH).

15,17-Didehydro: 4,8,11-Trihydroxy-12,15(17)-cembradien-16,3-olide. ***Flexibilolide***
[184362-79-6]
$C_{20}H_{32}O_5$ 352.47
Constit. of *Sinularia flexibilis*. Needles.
Mp 178-180°. $[\alpha]_D^{27}$ -40.7 (c, 0.9 in MeOH). λ_{max} 217 (MeOH) (Berdy).

Anjaneyulu, A.S.R. *et al., Nat. Prod. Lett.*, 1996, **9**, 127-135 (*isol, pmr cmr*)
Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 1997, **60**, 9-12 (*isol, pmr, cmr*)

4,11,12-Trihydroxy-7-cembren-16,3-olide T-568



$C_{20}H_{34}O_5$ 354.486

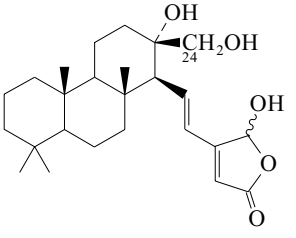
(1*S*,3*S*,4*R*,7*E*,11*R*,12*S*,15*R*)-*form*

Dihydrosinuflexolide
[210706-46-0]
Constit. of *Sinularia flexibilis*.
Cryst.
Mp 165-167°. $[\alpha]_D^{25}$ -3.8 (c, 0.066 in MeOH). λ_{max} 208 (log ϵ 4.4) (MeOH). λ_{max} 208 (ϵ 25120) (MeOH) (Berdy).

15,17-Didehydro: 4,11,12-Trihydroxy-7,15(17)-cembradien-16,3-olide. ***Sinuflexolide***
[210706-45-9]
$C_{20}H_{32}O_5$ 352.47
Constit. of *Sinularia flexibilis*. Cryst.
Mp 172-173°. $[\alpha]_D^{25}$ -8.6 (c, 0.17 in $CHCl_3$). λ_{max} 242 (log ϵ 4.1) (MeOH). λ_{max} 242 (ϵ 12590) (MeOH) (Berdy).

Duh, C.-Y. *et al., J. Nat. Prod.*, 1998, **61**, 844-847 (*isol, pmr, cmr, cryst struct*)

13,24,25-Trihydroxy-15,17-cheilanthadien-19,25-olide T-569



$C_{25}H_{38}O_5$ 418.572

(13α,15*E*,25ξ)-*form*

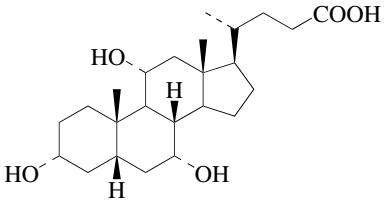
24-Ac: ***Spongianolide A***
[158846-17-4]
$C_{27}H_{40}O_6$ 460.609
Constit. of a *Spongia* sp.
$[\alpha]_D$ -31.9 (c, 1.4 in MeOH). λ_{max} 264 (ϵ 15800) (MeOH) (Derep). λ_{max} 264 (ϵ 15820) (MeOH) (Berdy).

24-(3-Hydroxybutanoyl): ***Spongianolide B***
[158846-18-5]
$C_{29}H_{44}O_7$ 504.662
Constit. of a *Spongia* sp.
$[\alpha]_D$ -25.7 (c, 1.1 in MeOH). λ_{max} 265 (ϵ 14500) (MeOH) (Derep). λ_{max} 265 (ϵ 14545) (MeOH) (Berdy).

He, H. *et al., Tet. Lett.*, 1994, **35**, 7189 (*isol, pmr, cmr*)

Hata, T. *et al., Tet. Lett.*, 1999, **40**, 1731-1734 (*synth*)
Furuichi, N. *et al., Tetrahedron*, 2001, **57**, 8425-8442 (*synth*)

3,7,11-Trihydroxycholan-24-oic acid T-570

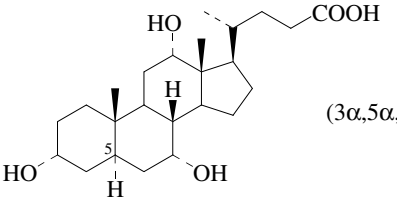


$C_{24}H_{40}O_5$ 408.577

(3α,5β,7α,11α)-*form*

Taurine amide: [203741-20-2]
$C_{26}H_{45}NO_7S$ 515.71
Constit. of bile of sunfish *Mola mola*. Amorph. powder.
$[\alpha]_D^{25}$ +21.8 (c, 1 in MeOH).
Ishida, H. *et al., Chem. Pharm. Bull.*, 1998, **46**, 12-16 (*isol, pmr, cmr*)

3,7,12-Trihydroxycholan-24-oic acid T-571



(3α,5α,7α,12α)-*form*

$C_{24}H_{40}O_5$ 408.577

(3α,5α,7α,12α)-*form*
Allocholic acid
[2464-18-8]
Isol. from many animal sources. Bile acid in penguin (*Pinguinus impennis*) and sturgeon (*Acipenser sturio*).
Cryst. (Me_2CO aq.).
Mp 250-251°. $[\alpha]_D^{25}$ +27.8 (c, 0.75 in MeOH).
Orphan drug designated (2003) for the treatment of inborn errors of synth. and metab. of bile acid and cholesterol

(3α,5β,7α,12α)-*form*
Cholic acid. *Cholalic acid. Cholagit. Colalin. Falkochol. Hypocholate. NSC 6135*
[81-25-4]
Isol. from bile and animal excretions. Widespread primary bile acid found in many spp. Forms many inclusion complexes, has been used as a resolving agent. Choleretic, laxative. Cryst. + 1 H_2O (H_2O or Et_2O aq.). Cryst. + 1EtOH (EtOH).
Mp 197° (anhyd.). $[\alpha]_D^{20}$ +37 (EtOH). pK_{a1} 4.98 (20°). Log P 2.39 (uncertain value) (calc).
▶ LD_{50} (mus, orl) 4950 mg/kg. FZ9350000

[361-09-1, 71781-34-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1057C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 594B (*nmr*)
Anderson, I.G. *et al., Biochem. J.*, 1957, **67**, 323-328; 1962, **85**, 236-242 (*isol, 3α,5β,7α,12α-form, 3α,5α,7α,12α-form, synth, bibl*)
Eneroch, P. *et al., J. Lipid Res.*, 1966, **7**, 524-530 (*ms*)
Leibfritz, D. *et al., J.A.C.S.*, 1973, **95**, 4996-5003 (*cmr*)
Lessinger, L. *et al., Cryst. Struct. Commun.*, 1982, **11**, 1787-1792 (*3α,5β,7α,12α-form, cryst struct*)
Lissel, M. *et al., Z. Naturforsch., B*, 1986, **41**, 367-370 (*3α,5β,7α,12α-form, amide*)
Paternostre, M.T. *et al., Biochemistry*, 1988, **27**, 2668-2677 (*use*)
Nishi, H. *et al., J. Chromatogr.*, 1990, **498**, 313-323 (*use*)
Kirk, D.N. *et al., J.C.S. Perkin 2*, 1990, 1567-1594 (*pmr*)
Iida, T. *et al., Chem. Pharm. Bull.*, 1993, **41**, 763-765 (*3α,5α,7α,12α-form, synth, pmr*)
Lessinger, L. *et al., J. Crystallogr. Spectrosc. Res.*, 1993, **23**, 85-99 (*3α,5β,7α,12α-form, cryst struct*)
Yuri, M. *et al., Chem. Comm.*, 1994, 2325-2326 (*3α,5β,7α,12α-form, biosynth*)
Wahle, M.-C. *et al., Acta Cryst. C*, 1996, **52**, 325-328; 2500-2502 (*3α,5β,7α,12α-form, cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 581-582
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CME750

3,7,23-Trihydroxycholan-24-oic acid T-572

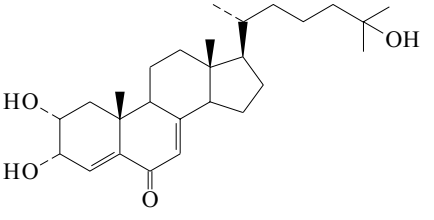
$C_{24}H_{40}O_5$ 408.577

(3α,5β,7α,23*R*)-*form*
β-Phocaecholic acid
[105369-89-9]
Bile acid from the seal, walrus and mallard ducks (*Anas platyrhynchos*).
Cryst. (Me_2CO).
Mp 222-224°. $[\alpha]_D$ +11 ($CHCl_3$).
Me ester:
$C_{25}H_{42}O_5$ 422.604
Mp 110-112°. $[\alpha]_D^{23}$ +8 (c, 1 in $CHCl_3$).

[105369-90-2]

Hammersten, O. *et al., Z. Phys. Chem.*, 1909, **61**, 451; 1910, **68**, 109
Haslewood, G.A.D. *et al., Biochem. J.*, 1961, **78**, 352
Kutner, A. *et al., Steroids*, 1982, **40**, 11 (*synth, esters*)
Jirsa, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **92**, 357-360 (*isol, duck isolate*)

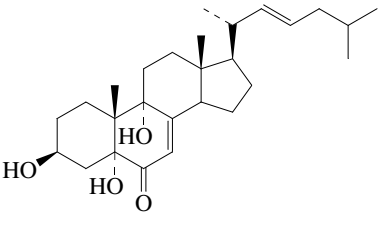
2,3,25-Trihydroxycholesta-4,7-dien-6-one T-573



$C_{27}H_{42}O_4$ 430.626

(2α,3α)-*form*
Diaulusterol B
[105317-87-1]
Constit. of *Diaulula sandiegensis.*
Oil.
25-(3-Hydroxybutanoyl): ***Diaulusterol A***
[105335-04-4]
$C_{31}H_{48}O_6$ 516.717
Constit. of *Diaulula sandiegensis.* Oil.
Williams, D.E. *et al., Can. J. Chem.*, 1986, **64**, 1527 (*isol, pmr, cmr*)
Kubanek, J. *et al., J. Nat. Prod.*, 1999, **62**, 777-779 (*biosynth*)

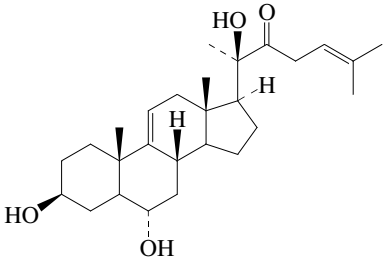
3,5,9-Trihydroxycholesta-7,22-dien-6-one T-574



$C_{27}H_{42}O_4$ 430.626

(3β,5α,9α,22*E*)-*form*
Homaxisterol C_1
[877373-35-8]
Constit. of a *Homaxinella* sp.
Amorph. solid.
Mansoor, T.A. *et al., J. Nat. Prod.*, 2006, **69**, 131-134 (*Homaxisterol C_1*)

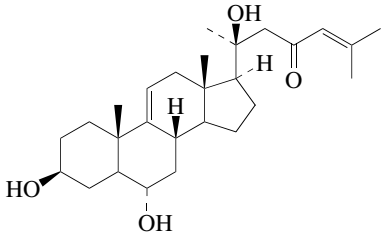
3,6,20-Trihydroxy-9(11),24-cholestadien-22-one T-575



$C_{27}H_{42}O_4$ 430.626

(3β,6α,22*R*)-*form*
6-O-[β-D-Fucopyranosyl-(1→2)-6-deoxy-β-D-glucopyranosyl-(1→4)-[6-deoxy-3-O-methyl-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-O-sulfate: ***Goniopectenoside C***
[326793-70-8]
$C_{57}H_{92}O_{27}S$ 1241.404
Constit. of *Goniopecten demonstrans*. Amorph. powder. $[\alpha]_D$ +6.6 (c, 0.4 in MeOH).
De Marino, S. *et al., Eur. J. Org. Chem.*, 2000, 4093-4098 (*isol, pmr, cmr*)

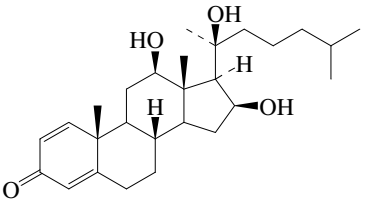
3,6,20-Trihydroxycholesta-9(11),24-dien-23-one T-576



$C_{27}H_{42}O_4$ 430.626

(3β,5α,6α,20*S*)-*form*
6-O-[β-D-Fucopyranosyl-(1→2)-6-deoxy-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate:
Acanthaglycoside A
[84821-12-5]
$C_{56}H_{90}O_{27}S$ 1227.377
Constit. of *Acanthaster planci*. Powder.
Mp 208°. $[\alpha]_D$ -8.7 (H_2O).
6-O-[β-D-Fucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate:
Acanthaglycoside B
[102679-93-6]
$C_{56}H_{90}O_{28}S$ 1243.376
Constit. of *Acanthaster planci*. Powder.
Mp 230° (dec.). $[\alpha]_D$ -7.2 (c, 0.83 in H_2O).
6-O-[β-D-Fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate:
Acanthaglycoside D
[95481-79-1]
$C_{56}H_{90}O_{28}S$ 1243.376
Constit. of *Acanthaster planci*. Powder.
Mp 226-227° (dec.). $[\alpha]_D$ +1.3 (c, 0.83 in H_2O).
Komori, T. *et al., Annalen*, 1983, 37-55 (*isol, pmr, cmr*)
Itakura, Y. *et al., Annalen*, 1986, 499-508 (*Acanthaglycosides*)

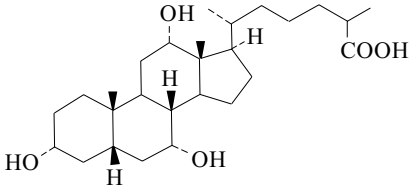
12,16,20-Trihydroxycholesta-1,4-dien-3-one T-577



$C_{27}H_{42}O_4$ 430.626

(12β,16β,20*S*)-*form*
12,16-Di-Ac: ***Nanjiol A***
[473739-38-7]
$C_{31}H_{46}O_6$ 514.701
Constit. of *Nephthea bayeri*. Amorph. powder. $[\alpha]_D^{25}$ +43.8 (c, 0.35 in $CHCl_3$). λ_{max} 242 (log ϵ 4.17) (MeOH).
Shao, Z.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1675-1677 (*isol, pmr, cmr*)

3,7,12-Trihydroxycholestan-26-oic acid T-578



$C_{27}H_{46}O_5$ 450.657

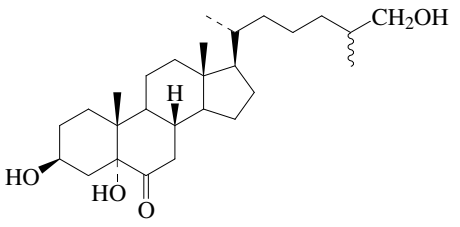
(3α,5β,7α,12α,25*R*)-*form*
3,7,12-Trihydroxycoprostanic acid. ***Coprocholic acid***
[23740-14-9]
Isol. from bile of various species incl. *Alligator mississippiensis*, *Caiman crocodilus*, *Crocodylus niloticus* and frog *Rana catesbiana*.
Cryst. (EtOAc).
Mp 183-184° (180-182°). $[\alpha]_D^{20}$ +28 (MeOH).
Me ester: [23740-21-8]
$C_{28}H_{48}O_5$ 464.684
Cryst. (Et_2O). Mp 153-154°.

(3α,5β,7α,12α,25*S*)-*form* [23047-29-2]
Cryst. (EtOAc or EtOH aq.). Mp 199-201°. $[\alpha]_D^{25}$ +44 (EtOH aq.).
Me ester:
Cryst. (Et_2O/petrol). Mp 160-161°.

[547-98-8, 17708-88-2]

Haslewood, G.A.D. *et al., Biochem. J.*, 1952, **52**, 583-587 (*isol*)
Bridgwater, R.J. *et al., Biochem. J.*, 1956, **64**, 593-599 (*synth*)
Briggs, T. *et al., J.O.C.*, 1970, **35**, 1431-1434 (*synth*)
Kamat, S.Y. *et al., Steroids*, 1972, **20**, 279-294 (*synth*)
Batta, A.K. *et al., J. Lipid Res.*, 1979, **20**, 935-940; 1983, **24**, 94-99 (*isol, cryst struct, config*)
Kurosawa, T. *et al., Steroids*, 1995, **60**, 439-444 (*synth*)

3,5,26-Trihydroxycholestan-6-one T-579



$C_{27}H_{46}O_4$ 434.658

(3β,5α,25ξ)-*form*

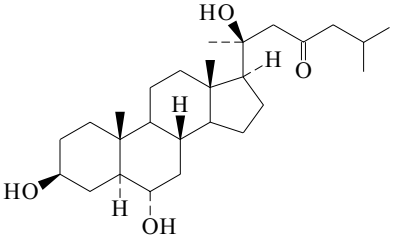
26-Ac: [283605-46-9]
$C_{29}H_{48}O_5$ 476.695
Constit. of *Acalycigorgia inermis.*

26-Carboxylic acid: 3,5-Dihydroxy-6-oxocholestan-26-oic acid

26-Carboxylic acid, Me ester: [283610-20-8]
$C_{28}H_{46}O_5$ 462.668
Constit. of *Acalycigorgia inermis.*

Rho, J.-R. *et al., Bull. Korean Chem. Soc.*, 2000, **21**, 518-520; *CA*, **133**, 102224h (*isol, pmr, cmr*)

3,6,20-Trihydroxycholestan-23-one T-580



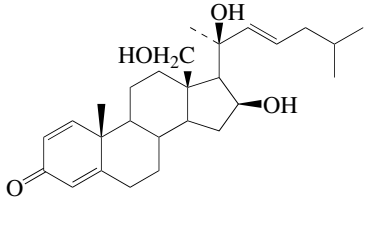
$C_{27}H_{46}O_4$ 434.658

(3β,5α,6α,20*S*)-*form*

3-O-*β*-D-*Glucuronopyranoside, 6-sulfate:* ***Downeyoside J***
[174286-22-7]
$C_{33}H_{54}O_{13}S$ 690.848
Constit. of *Henricia downeyae.*
$[\alpha]_D$ -9.5.

Palagiano, E. *et al., J. Nat. Prod.*, 1996, **59**, 348 (*isol, pmr, cmr*)

16,18,20-Trihydroxycholesta-1,4,22-trien-3-one T-581



$C_{27}H_{40}O_4$ 428.611

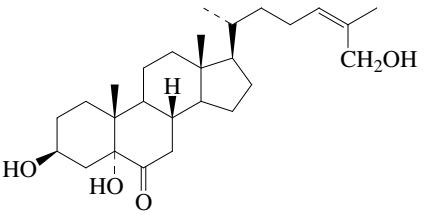
(16β,20*S*,22*E*)-*form* [89837-96-7]
Constit. of *Leptogorgia sarmentosa* and *Antipathes subpinnata*.

1,2-Dihydro: ***16,18,20-Trihydroxycholesta-4,22-dien-3-one***
[89837-98-9]
$C_{27}H_{42}O_4$ 430.626
Constit. of *Leptogorgia sarmentosa* and *Antipathes subpinnata*.

1,2,22,23-Tetrahydro: ***16,18,20-Trihydroxycholest-4-en-3-one***
$C_{27}H_{44}O_4$ 432.642
Constit. of *Antipathes subpinnata.*

Cimino, G. *et al., Experientia*, 1984, **40**, 246
Aiello, A. *et al., Steroids*, 1991, **56**, 513 (*isol, pmr, cmr, struct*)

3,5,26-Trihydroxycholest-24-en-6-one T-582



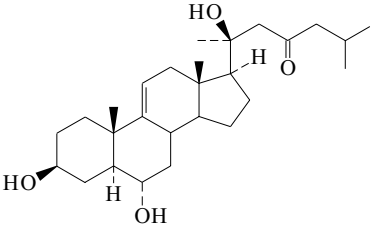
$C_{27}H_{44}O_4$ 432.642

(3β,5α,24*Z*)-*form*

26-Ac: [283605-45-8]
$C_{29}H_{46}O_5$ 474.679
Constit. of *Acalycigorgia inermis.*

Rho, J.-R. *et al., Bull. Korean Chem. Soc.*, 2000, **21**, 518-520; *CA*, **133**, 102224h (*isol, pmr, cmr*)

3,6,20-Trihydroxycholest-9(11)-en-23-one T-583



$C_{27}H_{44}O_4$ 432.642

(3β,5α,6α,20*S*)-*form*

Thornasterol A
[55897-77-3]
Constit. of *Acanthaster planci.*
Amorph. powder.
Mp 168-171°. $[\alpha]_D$ +1 (c, 0.74 in MeOH).

3-O-*Sulfate:* ***3*-O-*Sulfothornasterol A***
[125136-25-6]
[67850-87-7, 170079-89-7]
$C_{27}H_{44}O_7S$ 512.706
Constit. of *Aphelasterias japonica*, *Asterias amurensis* cf. *versicolor*, *Asterias rubens* and *Lethasterias nanimensis chelifera*.
Amorph. powder.
Mp 156-160° (Na salt). $[\alpha]_D$ +1.2 (c, 0.41 in MeOH). Isol. as Na salt to which CAS registry number refers.

3-O-*Sulfate, salt with Salsolinol:* [514828-17-2]
$C_{37}H_{57}NO_9S$ 691.925
Constit. of *Lethasterias nanimensis chelifera*. Amorph. solid.
$[\alpha]_D^{25}$ -2 (c, 0.3 in MeOH).

3-O-*β*-D-*Glucuronopyranoside, 6*-O-*sulfate:* ***Downeyoside F***
[174286-18-1]
$C_{33}H_{52}O_{13}S$ 688.832
Constit. of *Henricia downeyae.*
$[\alpha]_D$ -10.

3-O-*[β*-D-*Fucopyranosyl-(1→2)-α*-L-*arabinopyranosyl-(1→4)-[6-deoxy-β*-D-*glucopyranosyl-(1→2)]-β*-D-*xylopyranosyl-(1→3)-6-deoxy-β*-D-*glucopyranoside], 6*-O-*sulfate:* [865092-62-2]
$C_{55}H_{90}O_{27}S$ 1215.366
Constit. of *Culcita novaeguineae.* Amorph. powder.
Mp 203-204°. $[\alpha]_D^{20}$ +5 (c, 0.21 in MeOH).

6-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Forbeside H***
[130062-45-2]
$C_{44}H_{72}O_{19}S$ 937.107
Isol. from *Asterias forbesi*. Powder (as Na salt).
Mp 188° (Na salt). $[\alpha]_D^{20}$ -4.7 (c, 0.01 in H_2O).

6-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-*xylo-*hexopyranosid-4-uloside], 3*-O-*sulfate:* ***Forbeside G***
[130014-51-6]
$C_{45}H_{72}O_{19}S$ 949.118
Isol. from *Asterias forbesi*. Powder (as Na salt).
Mp 194° (Na salt). $[\alpha]_D^{20}$ -4.7 (c, 0.01 in H_2O).

6-O-*[β-D-Xylopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Cosmasteroside C***
[158243-23-3]
$C_{49}H_{80}O_{23}S$ 1069.223
Constit. of *Cosmasterias lurida*.
$[\alpha]_D$ -7 (MeOH).

6-O-*[β-D-Xylopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-β-D-glucopyranoside], 3*-O-*sulfate:* ***Cosmasteroside D***
[158275-00-4]
$C_{49}H_{80}O_{24}S$ 1085.223
Constit. of *Cosmasterias lurida*.
$[\alpha]_D$ +3.2 (H_2O).

6-O-*[6-Deoxy-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-*xylo-*hexopyranosid-4-uloside], 3*-O-*sulfate:* ***Forbeside F***
[130014-50-5]
$C_{51}H_{82}O_{23}S$ 1095.261
Isol. from *Asterias forbesi*. Powder (as Na salt).
Mp 208° (Na salt). $[\alpha]_D^{20}$ +11.6 (c, 0.01 in H_2O).

6-O-*[β-D-Galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Myxodermoside A***
[130829-34-4]
$C_{50}H_{82}O_{24}S$ 1099.249
Constit. of *Myxoderma platyacanthum*.
$[\alpha]_D$ +3.1 (H_2O).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Ophidianoside F***
[96626-37-8]
$C_{55}H_{90}O_{27}S$ 1215.366
Constit. of *Ophidiaster ophidianus*, *Luidia clathrata*, *Linckia laevigata*, *Oreaster reticulatus*, *Thromidia catalai* and *Cosmasterias lurida*. Antibarnacle agent. $[\alpha]_D$ +0.4 (MeOH).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-β-D-glucopyranoside], 3*-O-*sulfate:* ***Cosmasteroside B***
[158274-99-8]
$C_{55}H_{90}O_{28}S$ 1231.365
Constit. of *Cosmasterias lurida*.
$[\alpha]_D$ +2.8 (MeOH).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Regularoside B***
[100019-23-6]
$C_{56}H_{92}O_{27}S$ 1229.393
Constit. of *Halityle regularis*, *Coscinasterias tenuispina* and *Thromidia catalai*.
$[\alpha]_D$ +4.2 (MeOH).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-*xylo-*hexopyranosid-4-uloside], 3*-O-*sulfate:* ***Forbeside C***
[95481-80-4]
$C_{57}H_{92}O_{27}S$ 1241.404
Isol. from *Asterias forbesi*. Glassy solid (as Na salt).
Mp 180-182° (Na salt).

6-O-*[β-D-Fucopyranosyl-(1→2)-6-deoxy-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Luidiaglycoside B***. *Maculatoside*
[88434-26-8]
$C_{56}H_{92}O_{27}S$ 1229.393
Constit. of *Luidia maculata* and *Linckia laevigata*. Powder.
Mp 207-210° dec. $[\alpha]_D$ +2.7 (MeOH).

6-O-*[β-D-Fucopyranosyl-(1→2)-6-deoxy-β-D-glucopyranosyl-(1→4)-[6-deoxy-3-*O-*methyl-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Goniopectenoside B***
[326793-69-5]
$C_{57}H_{94}O_{27}S$ 1243.419
Constit. of *Goniopecten demonstrans*. Amorph. powder. $[\alpha]_D$ -7.5 (c, 0.2 in MeOH).

6-O-*[β-D-Fucopyranosyl-(1→2)-6-deoxy-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 3*-O-*sulfate:* ***Labidiasteroside A***
[288256-80-4]
$C_{57}H_{94}O_{29}S$ 1275.418
Constit. of *Labidiaster annulatus*.

6-O-*[β-D-Fucopyranosyl-(1→2)-6-deoxy-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Luidiaquinoside***
[528880-40-2]
$C_{57}H_{94}O_{28}S$ 1259.419
Constit. of *Luidia quinaria*. Amorph. powder. $[\alpha]_D$ +3.9 (c, 0.13 in MeOH).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Thornasteroside A***. *Ophidianoside E*
[67849-63-2]
$C_{56}H_{92}O_{28}S$ 1245.392
From *Acanthaster planci*, *Thromidia catalai*, *Pisaster giganteus*, *Luidia clathrata*, *Distolasterias nipon* and *Heliaster helianthus*.
Hypotensive agent. Cryst. (butanol) (as Na salt).
Mp 203-204° (Na salt). $[\alpha]_D^{25}$ -7 (c, 0.5 in H_2O).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-*xylo-*hexopyranosid-4-uloside], 3*-O-*sulfate:* ***Brasiliensoside***
[158243-32-4]
$C_{57}H_{92}O_{28}S$ 1257.403
Constit. of *Echinaster brasiliensis*.
$[\alpha]_D$ +3.9.

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Acanthaglycoside C***
[95531-18-3]
$C_{56}H_{92}O_{28}S$ 1245.392
Constit. of *Acanthaster planci*. Powder.
Mp 225-230° dec. $[\alpha]_D$ -6.4 (c, 0.83 in H_2O).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Pectinioside A***
[106543-01-5]
$C_{57}H_{94}O_{28}S$ 1259.419
Constit. of *Asterina pectinifera*. Amorph. powder.

Mp >° 300 dec. $[\alpha]_D$ -6.6 (c, 0.96 in Py).

6-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-[6-deoxy-β-D-glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Forbeside B****. Glycoside* B_2
[110660-85-0]
$C_{56}H_{92}O_{28}S$ 1245.392
Isol. from *Asterias amurensis* and *Asterias forbesi*. Glassy foam (as Na salt).
Mp 206-208° (Na salt). $[\alpha]_D^{28}$ -2.8 (c, 0.009 in H_2O).

6-O-*[α-L-Arabinofuranosyl-(1→3)-β-D-fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Psilasteroside***
[528880-44-6]
$C_{61}H_{100}O_{32}S$ 1377.508
Constit. of *Psilaster cassiope*. Amorph. powder. $[\alpha]_D$ +4.1 (c, 0.54 in MeOH).

6-O-*[α-L-Arabinopyranosyl-(1→4)-[β-D-fucopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Pectinioside G***
[128885-04-1]
$C_{62}H_{102}O_{32}S$ 1391.535
Constit. of *Asterina pectinifera*.

6-O-*[β-D-Fucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Pectinioside E***
[115185-90-5]
$C_{62}H_{102}O_{32}S$ 1391.535
Constit. of *Asterina pectinifera*. Amorph. powder. Sol. MeOH, H_2O.
Mp 225-230°. $[\alpha]_D^{25}$ -13 (c, 0.16 in H_2O).

6-O-*[β-D-Fucopyranosyl-(1→3)-β-D-fucopyranosyl-(1→2)-6-deoxy-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Marthasteroside*** A_2*. Luidiaglycoside A*
[89383-05-1]
$C_{62}H_{102}O_{31}S$ 1375.535
Constit. of *Marthasterias glacialis* and *Luidia maculata*. Sol. MeOH. $[\alpha]_D$ +6.5 (MeOH).

6-O-*[β-D-Fucopyranosyl-(1→3)-β-D-fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Marthasteroside*** A_1
[88434-24-6]
$C_{62}H_{102}O_{32}S$ 1391.535
Constit. of *Marthasterias glacialis* and *Echinaster brasiliensis*. Sol. MeOH. $[\alpha]_D$ +3.6.

6-O-*[β-D-Fucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)]-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Antarcticoside A***
[181186-45-8]
$C_{63}H_{104}O_{33}S$ 1421.561
Constit. of a starfish (Echinasteridae).
$[\alpha]_D$ +4.8 (MeOH).

6-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-[β-D-galactopyranosyl-(1→3)-6-deoxy-β-D-galactopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Forbeside A****. Versicoside A*
[88434-20-2]
$C_{62}H_{102}O_{33}S$ 1407.534
Isol. from the starfish *Asterias amurensis* ssp. *versicolor* and *Asterias forbesi*. Needles (MeOH aq.) (as Na salt).
Mp 200-203° (198.5-200°) (Na salt). $[\alpha]_D$ -1.7 (c, 0.42 in H_2O).

6-O-*[β-D-Galactopyranosyl-(1→3)-β-D-fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Asteriidoside A***
[214976-27-9]
$C_{63}H_{104}O_{33}S$ 1421.561
Constit. of an Asteriidae starfish.
$[\alpha]_D$ +5.9 (c, 1 in MeOH).

6-O-*[β-D-Galactopyranosyl-(1→4)-[β-D-fucopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Pectinioside F***
[115185-91-6]
$C_{62}H_{102}O_{33}S$ 1407.534
Constit. of *Asterina pectinifera*. Amorph. powder.
Mp 225-230° dec. $[\alpha]_D^{25}$ -5.8 (c, 0.11 in H_2O).

6-O-*[β-D-Galactopyranosyl-(1→4)-[β-D-fucopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Patirioside B***
[129700-54-5]
$C_{63}H_{104}O_{33}S$ 1421.561
Constit. of *Patiria miniata*.
$[\alpha]_D$ +6 (MeOH).

3,6-Di-Ac:
Cryst. (hexane). Mp 158.5-159.5°. $[\alpha]_D^{15}$ +23 (c, 0.1 in MeOH).

(3β,5α,6α,20ξ)-*form*

6-O-*[6-Deoxy-β-D-galactopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate:* ***Laevigatoside***
[96626-38-9]
$C_{56}H_{92}O_{27}S$ 1229.393
Constit. of *Linckia laevigata*.
$[\alpha]_D$ +4.2 (c, 0.8 in MeOH) (as Na salt).

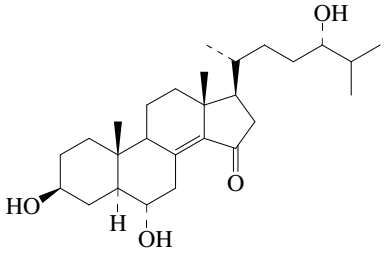
6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-fucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-*xylo-*hexopyranosid-4-uloside 4′-hydrate], 3*-O-*sulfate:* ***Asterosaponin 1****. Ovarian asterosaponin 1*
[77680-78-5]
$C_{57}H_{94}O_{28}S$ 1259.419
Constit. of *Asterias amurensis*. Cryst.
Mp 203-204°. $[\alpha]_D$ +19.3. $[\alpha]_D$ +1.5 (c, 1 in H_2O). $[\alpha]_D$ -2 (c, 0.21 in H_2O).

[89383-05-1, 115225-96-2]

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1978, **26**, 1852-1863; 1864-1873 (*isol*)
Ikegami, S. *et al., Tet. Lett.*, 1979, **20**, 1769-1772 (*Glycoside* B_2)
Okanu, K. *et al., Agric. Biol. Chem.*, 1981, **45**, 805 (*Asterosaponin 1*)
Komori, T. *et al., Annalen*, 1983, 24-36 (*Thornasteroside A*)
Itakura, Y. *et al., Annalen*, 1983, 2079-2091; 1986, 499-508 (*Forbeside A, Acanthaglycoside C*)
Komori, T. *et al., Annalen*, 1983, 2092-2113 (*Luidiaglycosides*)
Bruno, I. *et al., J.C.S. Perkin 1*, 1984, 1875-1883 (*Marthasterosides*)
Riccio, R. *et al., J. Nat. Prod.*, 1985, **48**, 97-101; 756-765 (*Laevigatoside, Regularoside B*)
Riccio, R. *et al., J.C.S. Perkin 1*, 1985, 655-659; 1988, 1337-1347 (*Ophidianosides, Forbeside B, Asterosaponin I*)
Honda, M. *et al., Tet. Lett.*, 1986, **27**, 3369-3372 (*Thornasterol A, struct, synth*)
Noguchi, Y. *et al., Annalen*, 1987, 341-348 (*Pectinioside A*)
Findlay, J.A. *et al., Can. J. Chem.*, 1987, **65**, 1384-1391; 2605-2611; 1990, **68**, 1215-1217 (*Forbesides*)
Dubois, M.A. *et al., Annalen*, 1988, 845-850 (*Pectiniosides E,F*)
Iorizzi, M. *et al., Gazz. Chim. Ital.*, 1990, **120**, 147-153 (*Pectinioside G*)
D'Auria, M.V. *et al., J.C.S. Perkin 1*, 1990, 1019-1023 (*Patirioside B*)
Finamore, E. *et al., J.O.C.*, 1991, **56**, 1146-1153 (*Myxodermoside A*)
Finamore, E. *et al., J. Nat. Prod.*, 1992, **55**, 767-772 (*3-sulfate*)
Iorizzi, M. *et al., J. Nat. Prod.*, 1993, **56**, 2149-2162 (*Brasiliensoside*)
Roccatagliata, A.J. *et al., J. Nat. Prod.*, 1994, **57**, 747-754 (*Cosmasterosides, isol, pmr, cmr*)
De Marino, S. *et al., Gazz. Chim. Ital.*, 1996, **126**, 667-672 (*Antarcticoside A*)
Palagiano, E. *et al., J. at. Prod.*, 1996, **59**, 348-354 (*Downeyoside F*)

De Marino, S. *et al., J. Nat. Prod.*, 1998, **61**, 1319-1327 (*Asteriidoside A*)
De Marino, S. *et al., Eur. J. Org. Chem.*, 2000, 4093-4098 (*Goniopectenoside B*)
Ivanchina, N.V. *et al., J. Nat. Prod.*, 2000, **63**, 1178-1181 (*3-sulfate*)
Diaz de Vivar, M.E. *et al., Molecules*, 2000, **5**, 350-351; *CA*, **133**, 249954e (*Labidiasteroside A*)
De Marino, S. *et al., J. Nat. Prod.*, 2003, **66**, 515-519 (*Luidiaquinoside, Psilasteroside*)
Kicha, A.A. *et al., Tet. Lett.*, 2003, **44**, 1935-1937 (*Lethasterias salt*)
Tang, H.-F. *et al., Planta Med.*, 2005, **71**, 458-463 (*Culcita novaeguineae constit*)

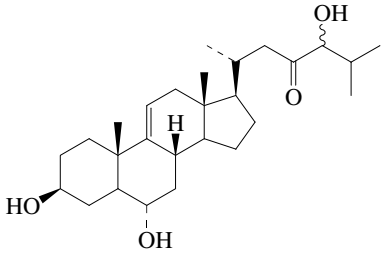
3,6,24-Trihydroxycholest-8(14)-en-15-one T-584



$C_{27}H_{44}O_4$ 432.642

(3β,5α,6α,24*S*)-*form*
Certonardosterol Q₆
[781646-81-9]
Constit. of *Certonardoa semiregularis.*
Cryst.
Wang, W. *et al., J. Nat. Prod.*, 2004, **67**, 1654-1660 (*isol, pmr, cmr*)

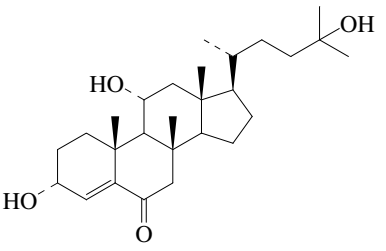
3,6,24-Trihydroxycholest-9(11)-en-23-one T-585



$C_{27}H_{44}O_4$ 432.642

(3β,5α,6α,24ξ)-*form* [290826-07-2]
3-O-*Sulfate:* ***Aphelaketotriol***
[290826-05-0]
$C_{27}H_{44}O_7S$ 512.706
Constit. of *Aphelasterias japonica*. Amorph. powder. $[\alpha]_D$ +12.8 (c, 0.2 in MeOH).
6-O-*(6-Deoxy-4*-O-*sulfo-β-*D*-glucopyranoside), 3*-O-*sulfate:* ***Aphelasteroside C***
[290826-04-9]
$C_{33}H_{54}O_{14}S_2$ 738.913
Constit. of *Aphelasterias japonica*. Amorph. powder. $[\alpha]_D$ +15.4 (c, 1.7 in MeOH).
Ivanchina, N.V. *et al., J. Nat. Prod.*, 2000, **63**, 1178-1181 (*isol, pmr, cmr*)

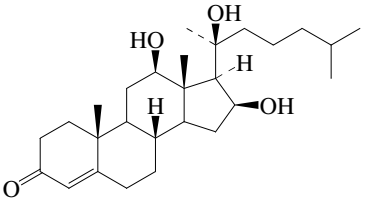
3,11,25-Trihydroxycholest-4-en-6-one T-586



$C_{27}H_{44}O_4$ 432.642

(3α,11α)-*form*
3,11-Di-Ac: [745075-30-3]
$C_{31}H_{48}O_6$ 516.717
Constit. of *Dasystenella acanthina*. Amorph. powder. $[\alpha]_D^{25}$ +62.4 (c, 0.14 in $CHCl_3$). λ_{max} 233 (ε 7170) (MeOH).
Mellado, G.G. *et al., Steroids*, 2004, **69**, 291-299 (*isol, pmr, cmr*)

12,16,20-Trihydroxycholest-4-en-3-one T-587

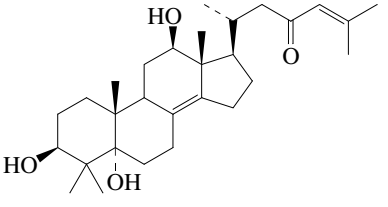


$C_{27}H_{44}O_4$ 432.642

(12β,16β,20*S*)-*form*
12,16-Di-Ac: ***Nanjiol B***
[473739-39-8]
$C_{31}H_{48}O_6$ 516.717
Constit. of *Nephthea bayeri*. Oil. $[\alpha]_D^{25}$ +75.8 (c, 1.02 in $CHCl_3$). λ_{max} 239 (log ε 4.18) (MeOH).
24,25-Didehydro: 12,16,20-Trihydroxycholesta-4,24-dien-3-one
$C_{27}H_{42}O_4$ 430.626
24,25-Didehydro, 12,16-di-Ac: ***Nanjiol D***
[862587-17-5]
$C_{31}H_{46}O_6$ 514.701
Constit. of *Nephthea bayeri*. Amorph. powder. $[\alpha]_D^{25}$ +125 (c, 0.2 in $CHCl_3$). λ_{max} 240 (log ε 4.23) (MeOH).
Shao, Z.Y. *et al., J. Nat. Prod.*, 2002, **65**, 1675-1677 (*Nanjiol B*)
Yan, X.H. *et al., Chin. Chem. Lett.*, 2005, **16**, 356-358 (*Nanjiol D*)

3,5,12-Trihydroxy-4,4-dimethylcholesta-8(14),24-dien-23-one T-588

3,5,12-Trihydroxy-30-norlanosta-8(14),24-dien-23-one



$C_{29}H_{46}O_4$ 458.68

(3β,5α,12β)-*form*

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]: ***Sarasinoside E***

[147769-48-0]

$C_{61}H_{98}N_2O_{27}$ 1291.442

Constit. of *Asteropus sarasinosum*. Protein kinase C inhibitor. Cryst. Sol. MeOH, butanol; fairly sol. $CHCl_3$; poorly sol. H_2O. Mp 193-197°. $[\alpha]_D^{20}$ -8.4 (MeOH).

12-Me ether, 3-O-[β-D-glucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]: ***Sarasinoside F***

[147769-49-1]

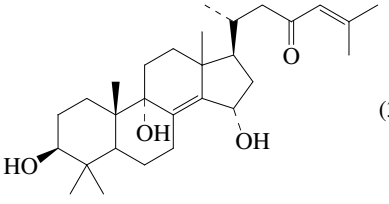
$C_{62}H_{100}N_2O_{27}$ 1305.469

Constit. of *Asteropus sarasinosum*. Cryst. Mp 192-195°. $[\alpha]_D^{20}$ -8.4 (MeOH).

Espada, A. *et al., Tetrahedron*, 1992, **48**, 8685-8696 (*isol, pmr, cmr*)

3,9,15-Trihydroxy-4,4-dimethylcholesta-8(14),24-dien-23-one T-589

3,9,15-Trihydroxy-30-norlanosta-8(14),24-dien-23-one



(3β,15α)-*form*

$C_{29}H_{46}O_4$ 458.68

(3β,15α)-*form*

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]: ***Sarasinoside I_1***

[287977-02-0]

$C_{62}H_{100}N_2O_{28}$ 1321.469

Constit. of *Melophlus isis*. Amorph. solid. Mp 219-222°. $[\alpha]_D^{25}$ -5.3 (c, 0.2 in MeOH). λ_{max} 238 (log ϵ 4.14) (MeOH).

15-Me ether, 3-O-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]: ***Sarasinoside I_2***

[287977-03-1]

$C_{63}H_{102}N_2O_{28}$ 1335.495

Constit. of *Melophlus isis*. Amorph. solid. Mp 216-219°. $[\alpha]_D^{25}$ -6.3 (c, 0.12 in MeOH). λ_{max} 238 (log ϵ 4.06) (MeOH).

(3β,15β)-*form*

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]: ***Sarasinoside H_1***

[287977-00-8]

$C_{62}H_{100}N_2O_{28}$ 1321.469

Constit. of *Melophlus isis*. Amorph. solid. Mp 204-207°. $[\alpha]_D^{25}$ -9 (c, 0.2 in MeOH). λ_{max} 239 (log ϵ 4.18) (MeOH).

15-Me ether, 3-O-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→6)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→2)-[2-acetamido-2-deoxy-β-D-galactopyranosyl-(1→4)]-β-D-xylopyranoside]: ***Sarasinoside H_2***

[287977-01-9]

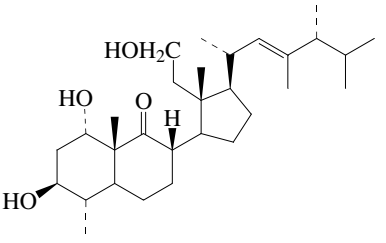
$C_{63}H_{102}N_2O_{28}$ 1335.495

Constit. of *Melophlus isis*. Amorph. solid. Mp 201-203°. $[\alpha]_D^{25}$ -8.9 (c, 0.1 in MeOH). λ_{max} 238 (log ϵ 4.04) (MeOH).

Lee, H.-S. *et al., J. Nat. Prod.*, 2000, **63**, 915-919 (*isol, pmr, cmr*)

1,3,11-Trihydroxy-4,23-dimethyl-9,11-secoergost-22-en-9-one T-590

1,3,11-Trihydroxy-4,23,24-trimethyl-9,11-secocholest-22-en-9-one



$C_{30}H_{52}O_4$ 476.738

(1α,3β,4α,22*E*,24*R*)-*form*

1α-Hydroxy-9(11)-secodinosterol

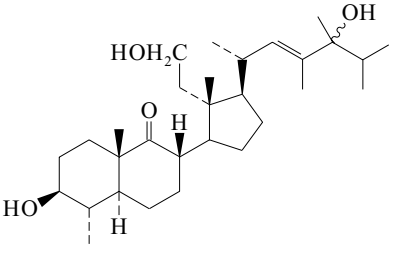
[215929-19-4]

Constit. of *Pseudopterogorgia americana*. Powder. $[\alpha]_D^{25}$ +7 (c, 1.42 in $CHCl_3$).

Rodriguez, A.D. *et al., Tet. Lett.*, 1998, **39**, 7645-7648 (*isol, pmr, cmr*)

3,11,24-Trihydroxy-4,23-dimethyl-9,11-secoergost-22-en-9-one T-591

3,11,24-Trihydroxy-4,23,24-trimethyl-9,11-secocholest-22-en-9-one



$C_{30}H_{52}O_4$ 476.738

(3β,4α,5α,22*E*,24ξ)-*form*

9,11-Seco-24-hydroxydinosterol

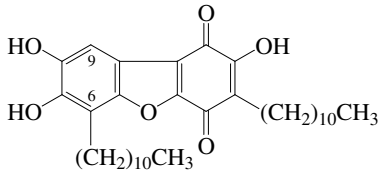
[161236-62-0]

Constit. of *Pseudopterogorgia americana* and an unidentified *Pseudopterogorgia* sp. Gum. $[\alpha]_D$ -11.4 (c, 0.08 in $CHCl_3$). $[\alpha]_D$ +6.8 (c, 2.7 in MeOH).

[161813-71-4]

Miller, S.L. *et al., Tet. Lett.*, 1995, **36**, 1227 (*isol, pmr, cmr*)
He, H. *et al., Tetrahedron*, 1995, **51**, 51 (*isol, pmr, cmr*)

2,7,8-Trihydroxy-3,6-diundecyl-1,4-dibenzofurandione T-592



$C_{34}H_{50}O_6$ 554.765

8-Me ether: 2,7-Dihydroxy-8-methoxy-3,6-diundecyl-1,4-dibenzofurandione
$C_{35}H_{52}O_6$ 568.792
Constit. of the mangrove plant *Aegiceras corniculatum*. Dark red solid ($CHCl_3$).
Mp 65-66°. λ_{max} 220 (log ϵ 3.94); 258 (log ϵ 3.72); 289 (log ϵ 3.55) (MeOH).
Xu, M. *et al., J. Nat. Prod.*, 2004, **67**, 762-766 (*isol, pmr, cmr, ms*)

2,7,8-Trihydroxy-3,9-diundecyl-1,4-dibenzofurandione T-593

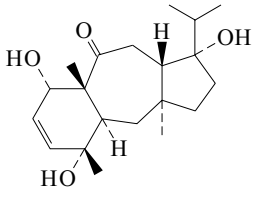
$C_{34}H_{50}O_6$ 554.765

7-Me ether: 2,8-Dihydroxy-7-methoxy-3,9-diundecyl-1,4-dibenzofurandione
$C_{35}H_{52}O_6$ 568.792
Constit. of the mangrove plant *Aegiceras corniculatum*. Dark red solid ($CHCl_3$).
Mp 88-89°. λ_{max} 222 (log ϵ 4.21); 258 (log ϵ 3.8); 295 (log ϵ 3.65) (MeOH).
Xu, M. *et al., J. Nat. Prod.*, 2004, **67**, 762-766 (*isol, pmr, cmr, ms*)

12,13,14-Trihydroxy-4,7,10,16,19-docosapentaenoic acid T-594

[104008-77-7]
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH(OH)CH(OH)CH(OH)CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH_2COOH$
$C_{22}H_{34}O_5$ 378.508
Isol. from the barnacle *Balanus balanoides.*
Song, W.C. *et al., Biochim. Biophys. Acta*, 1990, **1047**, 239-246 (*isol*)

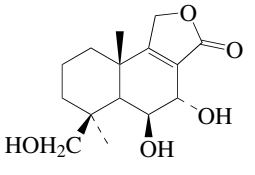
1,4,9-Trihydroxy-2-dolasten-6-one T-595



$C_{20}H_{32}O_4$ 336.47

(1α,4α,9α)-*form* [158962-87-9]
Constit. of *Dictyota bartayresiana*.
$[\alpha]_D$ -150 (c, 0.54 in MeOH).
Rao, C.B. *et al., Phytochemistry*, 1994, **37**, 509-513 (*isol, pmr, cmr*)

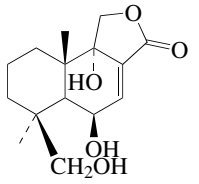
6,7,14-Trihydroxy-8-drimen-12,11-olide T-596



$C_{15}H_{22}O_5$ 282.336

(6β,7α)-*form*
6-(4-Nitrobenzoyl): [204716-03-0]
$C_{22}H_{25}NO_8$ 431.441
Metab. of *Aspergillus versicolor* isol. from the alga *Penicillus capitatus.* Pale yellow solid. $[\alpha]_D$ -11 (c, 0.45 in MeOH). Dec. >200°. λ_{max} 257 (ϵ 21100) (MeOH).
14-(4-Nitrobenzoyl): [204716-06-3]
$C_{22}H_{25}NO_8$ 431.441
Metab. of *Aspergillus versicolor* isol. from *Penicillus capitatus.* Pale yellow solid. $[\alpha]_D$ +15 (c, 0.17 in MeOH). Dec. >230°. λ_{max} 258 (ϵ 7600) (MeOH).
Belofsky, G.N. *et al., Tetrahedron*, 1998, **54**, 1715-1724 (*isol, pmr, cmr*)

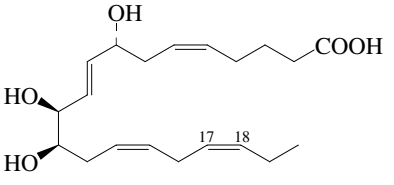
6,9,14-Trihydroxy-7-drimen-12,11-olide T-597



$C_{15}H_{22}O_5$ 282.336

(6β,9α)-*form*
6-(4-Nitrobenzoyl): ***Insulicolide A****. 9,14-Dihydroxy-6-(4-nitrobenzoyloxy)cinnamolide*
[191803-40-4]
$C_{22}H_{25}NO_8$ 431.441
Metab. of *Aspergillus insulicola* and *Aspergillus versicolor* isol. from *Penicillus* spp. Cryst. or pale yellow solid.
Mp 184-185° Mp 193° dec. $[\alpha]_D^{22}$ -360 (c, 0.0025 in EtOH). $[\alpha]_D$ -204 (c, 0.41 in MeOH). λ_{max} 254 (log ϵ 4.17) (no solvent reported). λ_{max} 255 (ϵ 16900) (MeOH) (Berdy).
Rahbaek, L. *et al., J. Nat. Prod.*, 1997, **60**, 811-813 (*isol, pmr, cmr, cryst struct*)
Belofsky, G.N. *et al., Tetrahedron*, 1998, **54**, 1715-1724 (*isol, pmr, cmr*)

8,11,12-Trihydroxyeicosa-5,9,14,17-tetraenoic acid T-598



$C_{20}H_{32}O_5$ 352.47

(5*Z*,8*R*,9*E*,11*S*,12*R*,14*Z*,17*Z*)-*form* [140631-49-8]
Isol. from *Dermasterias imbricata*, *Pycnopodia helianthoides*, *Culcita novaeguinea* and *Nardoa tubercolata*.
17,18-Dihydro: [140631-50-1]
$C_{20}H_{34}O_5$ 354.486
Isol. from *Pycnopodia helianthoides.*
Bruno, I. *et al., Experientia*, 1992, **48**, 114-115 (*isol, pmr, 17,18-dihydro*)

10,11,12-Trihydroxy-5,8,14,17-eicosatetraenoic acid T-599

Trioxilin B₄
[98004-40-1]
[103301-71-9]
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH(OH)CH(OH)CH(OH)CH{=}CHCH_2CH{=}CH(CH_2)_3COOH$
$C_{20}H_{32}O_5$ 352.47
Isol. from the barnacle *Balanus balanoides.*
17,18-Dihydro: See 10,11,12-Trihydroxy-5,8,14-eicosatrienoic acid, T-601
Holland, D.L. *et al., Prostaglandins*, 1985, **29**, 1021-1029 (*isol*)
Song, W.C. *et al., Biochim. Biophys. Acta*, 1990, **1047**, 239-246 (*isol*)

13,14,15-Trihydroxy-5,8,11,17-eicosatetraenoic acid T-600

[131917-09-4]

$H_3CCH_2CH{=}CHCH_2CH(OH)CH(OH)CH(OH)CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_3COOH$

$C_{20}H_{32}O_5$ 352.47

Isol. from the barnacle *Balanus balanoides.*

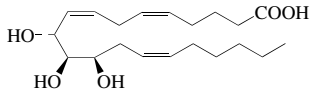
Song, W.C. *et al., Biochim. Biophys. Acta*, 1990, **1047**, 239-246 (*isol*)

10,11,12-Trihydroxy-5,8,14-eicosatrienoic acid T-601

Trioxilin B$_3$

[85589-25-9]

[94161-08-7]



(5*Z*,8*Z*,10*R*,11*R*,12*R*,14*Z*)-*form*

$C_{20}H_{34}O_5$ 354.486

Metab. of arachidonic acid in mammalian blood platelets. Also isol. from *Balanus balanoides.*

(5*Z*,8*Z*,10*R*,11*R*,12*R*,14*Z*)-*form* [150336-79-1]

Me ester: [119119-49-2]

$[\alpha]_D^{20}$ -16.1 (c, 3.2 in $CHCl_3$).

(5*Z*,8*Z*,10*S*,11*R*,12*R*,14*Z*)-*form* [119238-83-4]

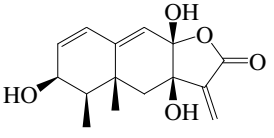
$[\alpha]_D$ +30.2 (c, 1.8 in Me_2CO).

Me ester: [119238-82-3]

$[\alpha]_D^{22}$ +29.2 (c, 2.0 in Me_2CO).

Sun, L.M. *et al., Tet. Lett.*, 1988, **29**, 4237 (*synth, pmr, hplc*)
Wu, W.-L. *et al., J.C.S. Perkin 1*, 1992, 2705 (*synth, pmr, ms*)
Yadav, J.S. *et al., Tet. Lett.*, 1992, **33**, 135-138 (*synth, pmr*)
Wu, W.-L. *et al., J.O.C.*, 1993, **58**, 2760 (*synth*)

3,7,8-Trihydroxy-1,9,11(13)-eremophilatrien-12,8-olide T-602



$C_{15}H_{18}O_5$ 278.304

(3β,7β,8β*OH*)-*form*

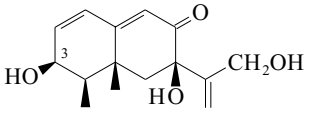
3-O-*(6*S*-Methyl-2*E*,4*E*-octadienoyl):* ***Metabolite A 6651E****. A 6651E*

$C_{24}H_{30}O_6$ 414.497

Prod. by a marine-derived fungus. Pale yellow oil. λ_{max} 275 (log ϵ 4.37) (MeOH).

Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*A 6651E*)

3,7,12-Trihydroxy-1,9,11(13)-eremophilatrien-8-one T-603



$C_{15}H_{20}O_4$ 264.321

(3β,7β)-*form*

3-O-*(6*S*-Methyl-2*E*,4*E*-octadienoyl):* ***Dendryphiellin E***

[121661-42-5]

$C_{24}H_{32}O_5$ 400.514

Metab. of *Dendryphiella salina*. Oil. $[\alpha]_D^{20}$ +166.7 (c, 0.22 in EtOH). Treatment with acidic ethanol gives an artifact Dendryphiellin F.

*3-(4,6-Dimethyl-2*E*,4*E*-octadienoyl), 12-Ac:* ***Emeremophiline***

[312624-82-1]

$C_{27}H_{36}O_6$ 456.578

Metab. of *Emericella aurantio-brunnea*. Amorph. solid.

3-Ketone: 7,12-Dihydroxy-1,9,11(13)-eremophilatriene-3,8-dione. ***Dendryphiellin G***

[121661-44-7]

$C_{15}H_{18}O_4$ 262.305

Metab. of *Dendryphiella salina*. Oil. $[\alpha]_D^{20}$ -11.2 (c, 0.12 in EtOH).

12-Aldehyde: 3,7-Dihydroxy-8-oxo-1,9,11(13)-eremophilatrien-12-al. ***Bipolaroxin***

[100665-30-3]

$C_{15}H_{18}O_4$ 262.305

Metab. of plant-pathogenic fungus *Bipolaris cynodontis*. Phytotoxic agent. Cryst. (EtOH). Sol. MeOH, $CHCl_3$.

Mp 163-165°. $[\alpha]_D^{22}$ +310 (c, 0.24 in $CHCl_3$). λ_{max} 216 (ϵ 3600); 279 (ϵ 9300) (EtOH) (Derep).

12-Aldehyde, 3-O-*(6*S*-methyl-2*E*,4*E*-octadienoyl):* ***KM-01****. Bipolal*

[155112-68-8]

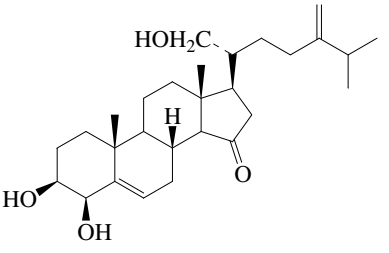
$C_{24}H_{30}O_5$ 398.498

Metab. of *Drechslera avenae* and *Bipolaris* sp. F5206. Brassinolide inhibitor. Cryst.

Mp 108-110°. $[\alpha]_D^{24}$ +364 (c, 1 in EtOH). $[\alpha]_D^{20}$ +472.8 (c, 0.027 in $CHCl_3$). λ_{max} 277 (ϵ 55000) (MeOH) (Derep).

Sugawara, F. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1985, **82**, 8291 (*isol, struct*)
Lidert, Z. *et al., Tet. Lett.*, 1988, **29**, 1347 (*struct, synth*)
Guerriero, A. *et al., Helv. Chim. Acta*, 1989, **72**, 438 (*isol, pmr, cmr*)
Kim, S.-K. *et al., Tet. Lett.*, 1994, **35**, 1731 (*KM-01*)
Watanabe, N. *et al., J. Nat. Prod.*, 1995, **58**, 463 (*Bipolal*)
Kim, S.-K. *et al., Bioorg. Med. Chem.*, 1998, **6**, 1975-1982 (*KM-01*)
Fujimoto, H. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1436-1441 (*Emeremophiline*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine, isol*)

3,4,21-Trihydroxyergosta-5,24(28)-dien-15-one T-604



$C_{28}H_{44}O_4$ 444.653

(3β,4β)-*form*

3-O-*[β-D-Galactopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→4)]-β-D-glucopyranoside]:* ***Mycaloside H***

[593280-57-0]

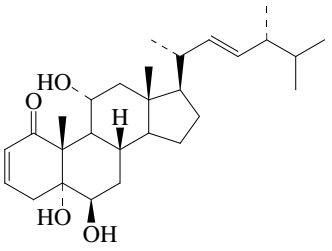
$C_{51}H_{82}O_{23}$ 1063.195

Constit. of *Mycale laxissima* . Solid.

Mp 205-209°. $[\alpha]_D^{25}$ -31.6 (c, 0.3 in MeOH).

Antonov, A.S. *et al., J. Nat. Prod.*, 2003, **66**, 1082-1088 (*isol, pmr, cmr*)

5,6,11-Trihydroxyergosta-2,22-dien-1-one T-605



$C_{28}H_{44}O_4$ 444.653

(5α,6β,11α,22*E*)-*form*

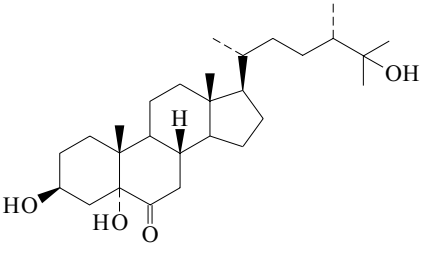
6-Ac: ***Yonarasterol A***
[263764-01-8]
$C_{30}H_{46}O_5$ 486.69
Constit. of the soft coral *Clavularia viridis*. Amorph. solid. $[\alpha]_D^{25}$ -1.1 (c, 0.47 in $CHCl_3$). λ_{max} 226 (log ϵ 3.93) (EtOH).

22,23-Dihydro: 5,6,11-Trihydroxyergost-2-en-1-one
$C_{28}H_{46}O_4$ 446.669

22,23-Dihydro, 6-Ac: ***Yonarasterol B***
[263764-02-9]
$C_{30}H_{48}O_5$ 488.706
Constit. of *Clavularia viridis*. Amorph. solid. $[\alpha]_D^{25}$ +6 (c, 0.4 in $CHCl_3$). λ_{max} 225 (log ϵ 4.04) (EtOH).
Iwashima, M. *et al., Steroids*, 2000, **65**, 130-137 (*isol, pmr, cmr*)

3,5,25-Trihydroxyergostan-6-one T-606

3,5,25-Trihydroxy-24-methylcholestan-6-one

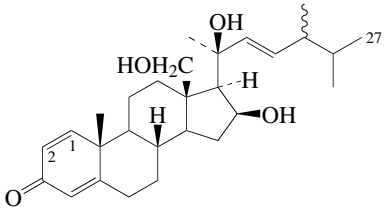


$C_{28}H_{48}O_4$ 448.685

(3β,5α,24*S*)-*form*
Cryst. Mp 257-260°. $[\alpha]_D^{29}$ -38 (c, 0.09 in $CHCl_3$).
25-Ac: [133883-19-9]
$C_{30}H_{50}O_5$ 490.722
Constit. of *Sclerophytum* spp.
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 297 (*isol, pmr, cmr*)

16,18,20-Trihydroxyergosta-1,4,22-trien-3-one, 9CI T-607

16,18,20-Trihydroxy-24-methylcholesta-1,4,22-trien-3-one



$C_{28}H_{42}O_4$ 442.637

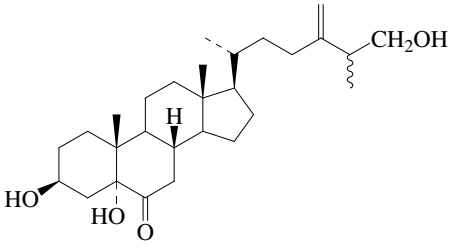
(16β,20*S*,22*E*,24ξ)-*form* [89837-95-6]
Constit. of *Leptogorgia sarmentosa* and *Antipathes subpinnata*.

1,2-Dihydro: ***16,18,20-Trihydroxyergosta-4,22-dien-3-one***.
16,18,20-Trihydroxy-24-methylcholesta-4,22-dien-3-one
[89837-97-8]
$C_{28}H_{44}O_4$ 444.653
From *Leptogorgia sarmentosa* and *Antipathes subpinnata*.

4,5-Dihydro: ***16,18,20-Trihydroxyergosta-1,22-dien-3-one***.
16,18,20-Trihydroxy-24-methylcholesta-1,22-dien-3-one
$C_{28}H_{44}O_4$ 444.653
Constit. of *Antipathes subpinnata*.
Cimino, G. *et al., Experientia*, 1984, **40**, 246
Aiello, A. *et al., Steroids*, 1991, **56**, 513 (*isol, pmr, cmr, struct*)

3,5,26-Trihydroxyergost-24(28)-en-6-one T-608

3,5,26-Trihydroxy-24-methylenecholestan-6-one

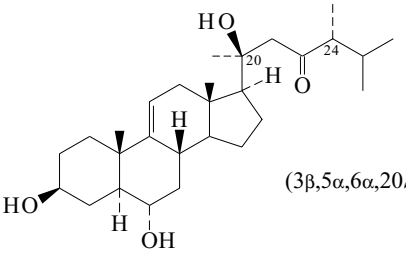


$C_{28}H_{46}O_4$ 446.669

(3β,5α,25ξ)-*form*
26-Ac: [395070-90-3]
[395070-91-4]
$C_{30}H_{48}O_5$ 488.706
Constit. of *Plexaurella grisea*. Amorph. solid. $[\alpha]_D$ -12.2 (c, 0.09 in MeOH).
Rueda, A. *et al., Steroids*, 2001, **66**, 897-904 (*isol, pmr, cmr*)

3,6,20-Trihydroxyergost-9(11)-en-23-one T-609

3,6,20-Trihydroxy-24-methylcholest-9(11)-en-23-one



(3β,5α,6α,20*S*,24*R*)–*form*

$C_{28}H_{46}O_4$ 446.669

(3β,5α,6α,20*S*,24*R*)-*form*
(20S,24R)-Thornasterol B
Constit. of *Asterias amurensis versicolor*. CAS no. not found to 2005.

3-Sulfate: [891511-22-1]
$C_{28}H_{46}O_7S$ 526.733
Constit. of *Asterias amurensis*.
$[\alpha]_D^{25}$ -14.2 (c, 0.5 in MeOH).

3-O-[β-D-Fucopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 6-O-sulfate: [865092-64-4]
$C_{56}H_{92}O_{27}S$ 1229.393
Constit. of *Culcita novaeguineae*. Amorph. powder.
Mp 225-227°. $[\alpha]_D^{20}$ -5 (c, 0.13 in MeOH).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Versicoside C****. Thornasteroside B*
[95481-81-5]
[105499-03-4]
$C_{57}H_{94}O_{28}S$ 1259.419
Constit. of *Asterias amurensis* cf. *versicolor*, *Acanthaster pauci*, *Luidia maculata* and *Coscinasterias tenuispina*. Needles (MeOH aq.).
Mp 224-226° dec. $[\alpha]_D$ -9.6 (c, 0.92 in H_2O).

6-O-*[6-Deoxy-β-D-glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Asteroside C***
[115225-66-6]
$C_{57}H_{94}O_{28}S$ 1259.419
Constit. of *Asterias amurensis*.

6-O-*[β-D-Galactopyranosyl-(1→3)-β-D-fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Versicoside B***
[95481-82-6]
$C_{63}H_{104}O_{33}S$ 1421.561
Constit. of *Asterias amurensis* cf. *versicolor*. Cryst. (MeOH aq.).
Mp 206.5-208°. $[\alpha]_D$ -8.4 (c, 0.45 in H_2O).

3,6-Di-Ac:
Cryst. (hexane). Mp 140-141°.

(3β,5α,6α,20*S*,24*S*)-*form*
(20*S*,24*S*)-Thornasterol B*. 3,6,20-Trihydroxycampest-9(11)-en-23-one*
Constit. of *Acanthaster planci*. CAS no. not found to 2005.

3-O-*Sulfate:* [181229-19-6]
[67850-86-6]
$C_{28}H_{46}O_7S$ 526.733
Constit. of an Antarctic starfish.

3-O-*β-D-Glucuronopyranoside, 6*-O-*sulfate:* ***Downeyoside G***
[174286-19-2]
$C_{34}H_{54}O_{13}S$ 702.859
Constit. of *Henricia downeyae*.
$[\alpha]_D$ -13.4.

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-xylohexos-4-ulopyranoside], 3*-O-*sulfate:* ***24-Methylbrasilienoside***
[181186-50-5]
$C_{58}H_{94}O_{28}S$ 1271.43
Constit. of a starfish (Echinasteridae).
$[\alpha]_D$ +12.5 (MeOH).

6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***24-Methylpectinioside A***
[181034-99-1]
$C_{58}H_{96}O_{28}S$ 1273.446
Constit. of a starfish (Echinasteridae).
$[\alpha]_D$ +12 (MeOH).

6-O-*[β-D-Fucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)]-β-D-glucopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Antarcticoside B***
[181186-46-9]
$C_{64}H_{106}O_{33}S$ 1435.588
Constit. of a starfish (Echinasteridae).
$[\alpha]_D$ +6.1 (MeOH).

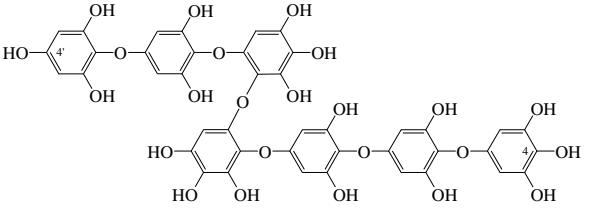
6-O-*[β-D-Fucopyranosyl-(1→3)-β-D-fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3*-O-*sulfate:* ***Acanthaglycoside F***
[95481-83-7]
$C_{63}H_{104}O_{32}S$ 1405.561
Constit. of *Acanthaster planci*. Powder.
Mp 223-228° dec. $[\alpha]_D$ +11.3 (c, 0.9 in H_2O).

3,6-Di-Ac:
Cryst. (hexane). Mp 143-144°. $[\alpha]_D^{15}$ +18 (c, 0.3 in $CHCl_3$).

[55897-78-4, 88494-40-0]

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1978, **26**, 1852-1863 (*Thornasterol B sulfate, isol*)
Itakura, Y. *et al., Annalen*, 1986, 359-373; 499-508 (*Versiciosides, Acanthaglycoside F*)
Riccio, R. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 869-893 (*Thornasteroside B*)
Honda, M. *et al., Tet. Lett.*, 1986, **27**, 3369-3372 (*20S,24R-Thornasterol B, 20S,24S-Thornasterol B, Versicoside C, synth, struct*)
Riccio, R. *et al., J.C.S. Perkin 1*, 1988, 1337-1347 (*Asteroside C*)
De Marino, S. *et al., Gazz. Chim. Ital.*, 1996, **126**, 667-672 (*Antarcticoside B, 24-Methylbrasilienoside, 24-Methylpectinioside*)
Palagiano, E. *et al., J. Nat. Prod.*, 1996, **59**, 348-354 (*Downeyoside G*)
Iorizzi, M. *et al., Tetrahedron*, 1996, **52**, 10997-11012 (*Antarctic starfish constit*)
Tang, H.-F. *et al., Planta Med.*, 2005, **71**, 458-463 (*Culcita novaeguineae constit*)
Liu, H.-W. *et al., J. Chin. Pharm. Sci.*, 2006, **15**, 1-5; *CA*, **145**, 59465w, (*3-sulfate*)

Trihydroxyheptaphlorethol A T-610



$C_{42}H_{30}O_{24}$ 918.685
Constit. of *Carpophyllum angustifolium*. Isol. as the peracetate.

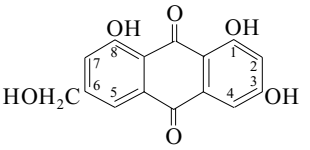
4-O-*(3,4,5-Trihydroxyphenyl):* ***Trihydroxyoctaphlorethol A***
$C_{48}H_{34}O_{27}$ 1042.78
Constit. of *Carpophyllum angustifolium*. Isol. as the peracetate.

4,4′-Bis-O-*(3,4,5-trihydroxyphenyl):* ***Trihydroxynonaphlorethol B***
$C_{54}H_{38}O_{30}$ 1166.876
Constit. of *Carpophyllum angustifolium*. Isol. as peracetate.

Glombitza, K. *et al., Phytochemistry*, 1999, **51**, 1095-1100

1,3,8-Trihydroxy-6-hydroxymethylanthraquinone T-611

Citreorosein*. ω-Hydroxyemodin*
[481-73-2]



$C_{15}H_{10}O_6$ 286.24
Prod. by *Penicillium* spp., *Preussia multispora*, *Zopfiella longicaudata*, *Polygonum cuspidatum*, *Rhamnus nepalensis* and in the lichens *Xanthoria aureola* and the insects *Nipaecoccus aurilanatus* and *Pseudococcus albizziae*. Also in *Preussia multispora* and *Xanthoria aureola*. Also a marine-derived *Gliocladium* sp. T31. cAMP phosphodiesterase inhibitor. Mycotoxin. Yellow-orange needles (EtOH).
Mp 282° Mp 288°. λ_{max} 224 (log ε 4.4); 250 (log ε 4.15); 268 (sh) (log ε 4.12); 295 (log ε 3.95); 440 (log ε 3.92); 455 (log ε 3.9) (EtOH). λ_{max} 221 (ε 25700); 252 (ε 15500); 290 (ε 15500); 438 (ε 9000) (EtOH) (Berdy).

1-Me ether: 1,6-Dihydroxy-3-hydroxymethyl-8-methoxyanthraquinone. ***Questinol***
[35688-09-6]
$C_{16}H_{12}O_6$ 300.267

Metab. of *Penicillium frequentans* and *Chrysosporium merdarium*. Isol. from roots of *Polygonum cuspidatum* (Japanese knotweed). Yellow cryst. (EtOH).
Mp 280-282°.

3-Me ether: 1,8-Dihydroxy-3-hydroxymethyl-6-methoxyanthraquinone. ***Fallacinol****. Teloschistin*
[569-05-1]
$C_{16}H_{12}O_6$ 300.267
Pigment of lichens, e.g. *Protoblastenia incrustans* and *Fulgensia*, *Xanthoria* and *Caloplaca* spp.; and from *Dermocybe cinnabarina*. Shows antifungal activity. Red cryst.
Mp 246-247°. λ_{max} 224; 250; 265; 287; 433; 455 (MeOH) (Berdy).

3-Me ether, 1′-Ac: 3-Acetoxymethyl-1,8-dihydroxy-6-methoxyanthraquinone. ***Fallacinol ω-acetate***
[20194-61-0]
$C_{18}H_{14}O_7$ 342.304
From *Dermocybe cinnabarina*.
Mp 195-196°.

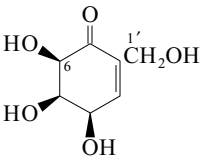
8-Me ether: 1,3-Dihydroxy-6-hydroxymethyl-8-methoxyanthraquinone. ***Carviolin****. Roseopurpurin*
$C_{16}H_{12}O_6$ 300.267
Prod. by *Penicillium carminoviolaceum*, a marine *Penicillium* sp. and *Zopfiella longicaudata*. Mycotoxin. Yellow needles (AcOH).
Mp 286°. λ_{max} 210; 248; 267; 278; 284; 434 (EtOH) (Berdy).

8-Me ether, 1′-Ac: ***Carviolin ω-acetate***
$C_{18}H_{14}O_7$ 342.304
Prod. by *Zopfiella longicaudata*. Orange powder (MeOH).
Mp 249-252°.

1,3-Di-Me ether: 8-Hydroxy-6-hydroxymethyl-1,3-dimethoxyanthraquinone. ***6,8-Di-O-methylcitreorosein****. 1-Hydroxy-3-hydroxymethyl-6,8-dimethoxyanthraquinone, 8CI*
[33982-71-7]
$C_{17}H_{14}O_6$ 314.294
From the wood of *Melanoxylon braunia* (Leguminosae). Orange needles.
Mp 237-239°.

Anslow, W.K. *et al., Biochem. J.*, 1940, **34**, 159 (*isol*)
Howard, B.H. *et al., Biochem. J.*, 1955, **59**, 485 (*uv*)
Bloom, H. *et al., J.C.S.*, 1959, 178 (*ir*)
Gottlieb, O.R. *et al., Phytochemistry*, 1971, **10**, 1379-1383 (*6,8-Di-O-methylcitreorosein*)
Steglich, W. *et al., Chem. Ber.*, 1972, **105**, 2922 (*isol*)
Hirose, Y. *et al., Chem. Pharm. Bull.*, 1982, **30**, 4186 (*synth, pmr*)
Nikaido, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3075 (*props*)
Benfaremo, N. *et al., J.O.C.*, 1985, **50**, 139 (*synth*)
Kalidhar, S.B. *et al., Phytochemistry*, 1989, **28**, 3459-3463 (*pmr*)
Schmidt, R.R. *et al., Synthesis*, 1994, 255 (*synth, pmr*)
Buchanan, M.S. *et al., Aust. J. Chem.*, 1998, **51**, 103-109 (*isol, uv, pmr, cmr*)
Fujimoto, H. *et al., Chem. Pharm. Bull.*, 2004, **52**, 1005-1008 (*Citreorosein, Carviolin, Carviolin acetate*)
Ren, H. *et al., Arch. Pharmacal Res.*, 2006, **29**, 59-63 (*marine, isol*)

4,5,6-Trihydroxy-2-hydroxymethyl-2-cyclohexen-1-one T-612



(4R,5R,6R)–form

$C_7H_{10}O_5$ 174.153

(4R,5R,6R)-form
Gabosine C*. KD 16-U1. Antibiotic KD 16-U1*
[40980-53-8]
Prod. by *Streptomyces cellulosae*.
Needles (EtOAc/EtOH). Sol. H_2O.
Mp 112-113°. $[\alpha]_D^{20}$ -163 (c, 0.5 in H_2O). λ_{max} 229 (ϵ 9500); 311 (ϵ 60) (0.1*N* HCl) (Derep). λ_{max} 218 (ϵ 3900); 265 (ϵ 7600); 300 (sh) (ϵ 3000) (0.1*N* NaOH) (Derep). λ_{max} 229 (ϵ 9500); 311 (ϵ 60) (H_2O) (Derep).

1′-O-(2-Butenoyl): 2-Crotonyloxymethyl-4,5,6-trihydroxy-2-cyclohexenone. ***COTC***
[57449-30-6]
$C_{11}H_{14}O_6$ 242.228
Isol. from *Streptomyces griseosporeus* and *Streptomyces filipinensis*. Glyoxalase I inhibitor, antitumour antibiotic. Needles ($CHCl_3$/MeOH). Sol. H_2O, MeOH, EtOH, DMSO; fairly sol. butanol, EtOAc, butyl acetate; poorly sol. Me_2CO, C_6H_6, $CHCl_3$, Et_2O, hexane.
Mp 181°. $[\alpha]_D^{24}$ -109 (c, 1.5 in EtOH). λ_{max} 213 (ϵ 21800); 310 (ϵ 56) (pH 7 H_2O) (Derep). λ_{max} 211 (ϵ 19400); 312 (ϵ 52) (EtOH) (Derep).
► LD_{50} (mus, ivn) 90 mg/kg. EM9259200

(4R,5R,6S)-form
6-Ac: [36916-29-7]
$C_9H_{12}O_6$ 216.19
Prod. by *Phyllosticta* sp.
Mp 166-168°. $[\alpha]_D$ -181 (c, 1 in EtOH). λ_{max} 221 (ϵ 4400) (EtOH).

6-O-(2-Hydroxy-6-methylbenzoyl): [146475-71-0]
$C_{15}H_{16}O_7$ 308.287
Prod. by a *Phoma* sp. on leaves and stalks of rhubarb. λ_{max} 211 (ϵ 23000); 240 (ϵ 9500); 309 (ϵ 2800) (MeOH) (Berdy).

(4R,5S,6R)-form
Prod. by the marine *Aspergillus varians* KMM 4630.

(4S,5S,6R)-form
Gabosine E
[148154-53-4]
Prod. by *Streptomyces cellulosae* ssp. *griseorubiginosus*. Sol. H_2O. $[\alpha]_D$ +152 (c, 1 in H_2O). λ_{max} 222 (ϵ 22500) (MeOH/HCl) (Derep). λ_{max} 214 (ϵ 22100); 313 (ϵ 14100) (MeOH/NaOH) (Derep). λ_{max} 221 (ϵ 28600) (MeOH) (Derep). λ_{max} 222 (ϵ 22300) (MeOH/HCl) (Berdy).

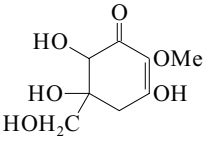
1′-Ac: ***Gabosine D***
[148099-40-5]
$C_9H_{12}O_6$ 216.19
Isol. from *Streptomyces cellulosae* ssp. *griseorubiginosus*.
$[\alpha]_D^{20}$ +86.2 (c, 1 in MeOH).

[53496-14-3]

Nabeta, K. *et al., Agric. Biol. Chem.*, 1971, **35**, 1639-1641; 1975, **39**, 403-407 (*6-Ac*)
Tatsuta, K. *et al., J. Antibiot.*, 1974, **27**, 579 (*isol*)
Takeuchi, T. *et al., J. Antibiot.*, 1975, **28**, 737 (*COTC*)
Chimura, H. *et al., J. Antibiot.*, 1975, **28**, 743 (*COTC*)
Japan. Pat., 1977, 77 71 448; *CA*, **87**, 184080b (*Gabosine C, synth*)
Mirza, S. *et al., Helv. Chim. Acta*, 1985, **68**, 988 (*Gabosine C, synth, uv, ir, pmr*)
Takayama, H. *et al., Tet. Lett.*, 1986, **27**, 5509 (*synth*)
Venkatasubbaiah, P. *et al., J. Nat. Prod.*, 1992, **55**, 639 (*deriv*)
Bach, G. *et al., Annalen*, 1993, 241 (*isol, pmr, cmr*)
Lygo, B. *et al., Tet. Lett.*, 1994, **35**, 4197 (*synth*)
Tatsuta, K. *et al., Tet. Lett.*, 1998, **39**, 401-402 (*synth*)
Tang, Y.-Q. *et al., Eur. J. Org. Chem.*, 2000, 149-153 (*isol*)
Hoefs, R. *et al., Eur. J. Org. Chem.*, 2000, 1883-1887 (*biosynth*)
Huntley, C.F.M. *et al., Tet. Lett.*, 2000, **41**, 2031-2034 (*synth, COTC*)
Smetanina, O.F. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 243-244 (*marine isol*)
Ramana, G.V. *et al., Tet. Lett.*, 2005, **46**, 3049-3051 (*Gabosine C, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, COC825

3,5,6-Trihydroxy-5-(hydroxymethyl)-2-methoxy-2-cyclohexen-1-one, 9CI T-613

Gadusol
[76663-30-4]



$C_8H_{12}O_6$ 204.179

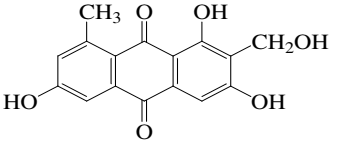
Mycosporine related metabolite. Isol. from the eggs of brine shrimp (*Artemia*), sea urchin, *Pleuronectes platessa* (plaice), *Platichthys flesus* (flounder), *Gadus morhua*, *Melanogrammus aeglefinus* (haddock), *Microstomus kitt* (lemon sole), *Limanda limanda* (common dab), *Hippoglossoides platessa* (long rough dab) and other fish. Amorph. powder (EtOH). Sol. H_2O. Mp 178-179°. Subl.0.03 120. pK_a 4.17 (50% EtOH aq.). λ_{max} 269 (ϵ 12400) (H_2O/HCl) (Derep). λ_{max} 296 (ϵ 22200) (H_2O/NaOH) (Derep). λ_{max} 269 (ϵ 12400) (dil acid) (Derep). λ_{max} 294 (MeOH) (Berdy). λ_{max} 268 (MeOH-HCl) (Berdy).

[105660-63-7]

Chioccara, F. *et al., Bull. Soc. Chim. Belg.*, 1980, **89**, 1101 (*isol, uv, pmr, cmr, ms*)
Grant, P.T. *et al., Tet. Lett.*, 1980, **21**, 4043-4044 (*isol, struct*)
Plack, P.A. *et al., Biochem. J.*, 1981, **199**, 741-747 (*isol, struct, uv, ir, pmr*)
Grant, P.T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 755 (*isol*)

1,3,6-Trihydroxy-2-hydroxymethyl-8-methylanthraquinone T-614

1,3,6-Trihydroxy-2-hydroxymethyl-8-methyl-9,10-anthracenedione



$C_{16}H_{12}O_6$ 300.267

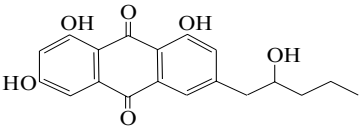
3,6-Di-Me ether: 1-Hydroxy-2-hydroxymethyl-3,6-dimethoxy-8-methylanthraquinone. ***Flavomarin B***
$C_{18}H_{16}O_6$ 328.321
Prod. by a marine-derived *Streptomyces* sp. B1108.

1′,3,6-Tri-Me ether: 1-Hydroxy-3,6-dimethoxy-2-methoxymethyl-8-methylanthraquinone. ***Flavomarin A***
$C_{19}H_{18}O_6$ 342.348
Prod. by a marine-derived *Streptomyces* sp. B1108.

Laatsch, H. *et al., Dissertation*, Univ. of Göttingen, 2005,

1,3,8-Trihydroxy-6-(2-hydroxypentyl)anthraquinone T-615

[52422-02-3]

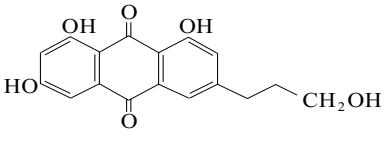


$C_{19}H_{18}O_6$ 342.348
Isol. from the crinoid *Comanthus bennetti* and the starfish *Echinaster echinophorus*. Orange needles. Mp 193-195°.

Bartolini, G.L. *et al., Tetrahedron*, 1973, **29**, 3699-3702 (*isol*)
Utkin, N.K. *et al., Khim. Prir. Soedin.*, (*Engl. transl.* p. 528), 1977, 636 (*isol, pmr, cmr*)

1,3,8-Trihydroxy-6-(3-hydroxypropyl)anthraquinone T-616

1,3,8-Trihydroxy-6-(3-hydroxypropyl)-9,10-anthracenedione. ***ω-Rhodoptilometrin***
[69260-86-2]

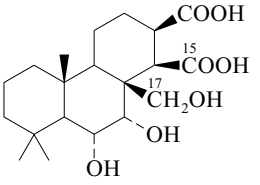


$C_{17}H_{14}O_6$ 314.294

Isol. from starfish *Echinaster echinophorus*. Mp 229-230°.

Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1978, 651-652; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 561 (*isol, uv, pmr, ms*)

6,7,17-Trihydroxy-15,16-isocopalanedioic acid T-617



$C_{20}H_{32}O_7$ 384.469

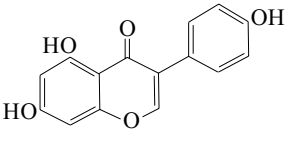
(6α,7α,13α*H*,14α*H*)-*form*

15→17 Lactone, Me ester: ***Dendrillol 4***
[106009-83-0]
$C_{21}H_{32}O_6$ 380.48
Isol. from *Dendrilla rosea*. Woolly cryst.
Mp 235-237°. $[\alpha]_D^{20}$ +40 (c, 1 in $CHCl_3$).

Karuso, P. *et al., Aust. J. Chem.*, 1986, **39**, 1643

4′,5,7-Trihydroxyisoflavone T-618

*5,7-Dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Genistein***†. *Differenol A. Genisteol. Prunetol. Sophoricol. K 254I. NSC 36586*
[446-72-0]



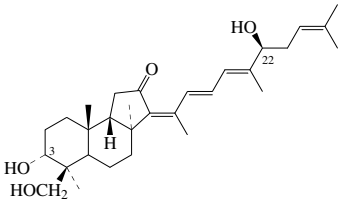
$C_{15}H_{10}O_5$ 270.241
V. widely distributed in the Leguminosae subf. Papilionoideae but also in *Podocarpus spicatus* (Podocarpaceae) and wood of *Prunus* spp. (Rosaceae). The major isoflavone in soy beans and isolated soy protein. Claimed to be prod. by microorganisms *Streptomyces vulgare* and other *Streptomyces* spp., *Aspergillus niger, Mycobacterium phlei* and *Micromonospora halophytica*. Prod. by the marine-derived *Ascochyta salicorniae*. Weak estrogen. Shows insect antifeedant and weak antibacterial activity against *E. coli* and *Xanthomonas oryzae*. Experimentally used as protein kinase inhibitor against protein tyrosine kinases including those activated by epidermal growth factor (EGRF) and platelet derived growth factor (PDGF) receptors. Antioxidant. Claimed antineoplastic preventative activity. Nutriceutical with anti-cancer and bone protective props. Prisms (EtOH aq.).
Mp 301-302° dec. Log P 0.98 (calc). All isolations of isoflavonoids from microorganisms are considered dubious. Methylgenistein, Isogenistin and Methylisogenistin were all impure Genistein.
λ_{max} 261 (ϵ 38500) (MeOH) (Derep).
▶ Exp. reprod. effects (large doses). NR2392000

[52796-14-2]

Wagner, H. *et al., Chem. Ber.*, 1967, **100**, 101 (*synth*)
Markham, K.R. *et al., Phytochemistry*, 1968, **7**, 791 (*isol*)
Ganguly, A.K. *et al., Chem. Ind. (London)*, 1970, 201 (*isol*)
Umezawa, H. *et al., J. Antibiot.*, 1975, **28**, 947 (*isol*)
Wagner, H. *et al., Tet. Lett.*, 1976, 1799 (*cmr*)
Hazeto, T. *et al., J. Antibiot.*, 1979, **32**, 217 (*isol*)
Asahi, K. *et al., J. Antibiot.*, 1981, **34**, 919 (*uv, ir*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Breytenbach, J.C. *et al., J. Nat. Prod.*, 1986, **49**, 1003 (*isol, deriv*)
Jain, A.C. *et al., J.C.S. Perkin 1*, 1986, 215 (*synth*)
Murthy, M.S.R. *et al., Org. Magn. Reson.*, 1986, **24**, 225 (*cmr*)
Goto, *et al., Agric. Biol. Chem.*, 1987, **51**, 3003 (*isol, props, pmr*)
Sekizaki, H. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4876 (*synth, derivs*)
Anyanwutaku, I.O. *et al., J. Nat. Prod.*, 1992, **55**, 1498 (*isol, pmr, cmr, ms*)
Nishiyama, K. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 107 (*synth*)

Wang, T.T. *et al., Carcinogenesis (London)*, 1996, **17**, 271 (*pharmacol*)
Osterhage, C. *et al., J.O.C.*, 2000, **65**, 6412-6417 (*Ascochyta salicorniae isol*)
Balasubramanian, S. *et al., Synth. Commun.*, 2000, **30**, 469-484 (*synth, pmr*)
Hendrich, S. *et al., Handbook of Nutraceuticals and Functional Foods*, (ed. Wildman, R.E.C.), CRC Press, 2001, 55-75 (*occur, metab*)

3,22,29-Trihydroxy-13,15,17(20),24-isomalabaricatetraen-12-one T-619



(3α,13*Z*,15*E*,17(20)*E*,22*S*)-*form*

$C_{30}H_{46}O_4$ 470.691

(3α,13*Z*,15*E*,17(20)*E*,22*S*)-*form*

3-Ac: ***3-Epi-29-hydroxystelliferin A***
[260436-29-1]
$C_{32}H_{48}O_5$ 512.728
Constit. of *Stelletta globostellata*. Yellow solid. $[\alpha]_D^{25}$ -84 (c, 0.22 in MeOH). Error in struct. in ref. λ_{max} 238 (log ε 3.75); 345 (log ε 4.34) (MeOH).

22-Ac: ***Stelliferin G***
[333970-13-1]
$C_{32}H_{48}O_5$ 512.728
Constit. of a *Jaspis* sponge. Yellow solid. $[\alpha]_D^{25}$ -17 (c, 0.02 in MeOH). λ_{max} 232 (log ε 4.13); 342 (log ε 4.43) (MeOH).

3,22-Di-Ac: ***3-Epi-29-hydroxystelliferin E***
[260436-28-0]
$C_{34}H_{50}O_6$ 554.765
Constit. of *Stelletta globostellata*. Yellow solid. $[\alpha]_D^{25}$ -113 (c, 0.69 in MeOH). λ_{max} 234 (log ε 4.27); 339 (log ε 4.55) (MeOH).

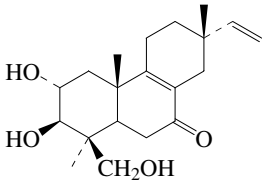
(3β,13*Z*,15*E*,17(20)*E*,22*S*)-*form*

3-Ac: ***29-Hydroxystelliferin A***
[333723-98-1]
$C_{32}H_{48}O_5$ 512.728
Constit. of a *Jaspis* sponge. Yellow solid. $[\alpha]_D^{25}$ -37 (c, 0.1 in MeOH). λ_{max} 232 (log ε 3.77); 348 (log ε 4.04) (MeOH).

3,22-Di-Ac: ***29-Hydroxystelliferin E***
[333723-97-0]
$C_{34}H_{50}O_6$ 554.765
Constit. of a *Jaspis* sp. sponge. Yellow solid. $[\alpha]_D^{25}$ -40 (c, 0.33 in MeOH). λ_{max} 232 (log ε 4.23); 342 (log ε 4.52) (MeOH).

Oku, N. *et al., J. Nat. Prod.*, 2000, **63**, 205-209 (*isol, pmr, cmr*)
Meragelman, K.M. *et al., J. Nat. Prod.*, 2001, **64**, 389-392 (*29-Hydroxystelliferins A and E, Stelliferin G*)

2,3,19-Trihydroxy-8,15-isopimaradien-7-one T-620

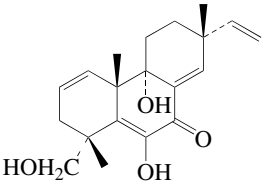


$C_{20}H_{30}O_4$ 334.455

(2α,3β)-*form* [280144-93-6]
Amorph. solid. $[\alpha]_D^{20}$ +31 (c, 0.1 in MeOH). λ_{max} 251 (log ε 4.08) (MeOH).

19-O-*β*-*D*-*Altropyranoside:* ***Virescenoside M***
[281205-10-5]
$C_{26}H_{40}O_9$ 496.597
Metab. of *Acremonium striatisporum* KMM 4401 isol from the sea cucumber *Eupentacta fraudatrix*. Plates (MeOH).
Mp 143-146°. $[\alpha]_D^{20}$ +29 (c, 0.28 in MeOH). λ_{max} 248 (log ε 3.9) (MeOH).
Afiyatullov, S.Sh. *et al., J. Nat. Prod.*, 2000, **63**, 848-850 (*Virescenoside M*)

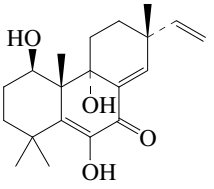
6,9,18-Trihydroxy-1,5,8(14),15-isopimaratetraen-7-one T-621



$C_{20}H_{26}O_4$ 330.423
Enolised α-diketone.

9α-*form*
Libertellenone B
[866413-29-8]
Metab. of a marine-derived *Libertella* sp.
Yellow powder. $[\alpha]_D$ -64.7 (c, 0.973 in MeCN). λ_{max} 216 (log ε 3.62); 263 (log ε 3.57); 317 (log ε 3.8) (MeCN).
Oh, D.-C. *et al., Bioorg. Med. Chem.*, 2005, **13**, 5267-5273 (*Libertellenone B*)

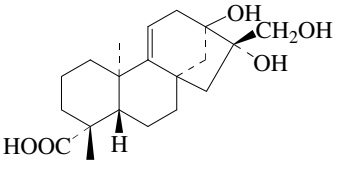
1,6,9-Trihydroxy-5,8(14),15-isopimaratrien-7-one T-622



$C_{20}H_{28}O_4$ 332.439

(1β,9α)-*form*
Libertellenone A
[866413-28-7]
Metab. of a marine-derived *Libertella* sp.
Powder. $[\alpha]_D$ -96.8 (c, 0.133 in MeCN). λ_{max} 216 (log ε 3.55); 266 (log ε 3.45); 322 (log ε 3.67) (MeCN).
Oh, D.-C. *et al., Bioorg. Med. Chem.*, 2005, **13**, 5267-5273 (*Libertellenone A*)

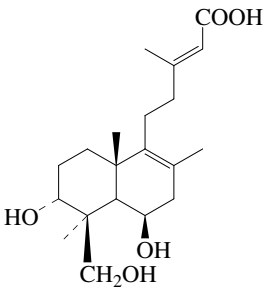
13,16,17-Trihydroxy-9(11)-kauren-19-oic acid T-623



$C_{20}H_{30}O_5$ 350.454

(*ent*-16β*OH*)-*form* [765315-56-8]
Constit. of *Bruguiera gymnorrhiza*.
Amorph. solid. $[\alpha]_D^{20}$ +67.4 (c, 0.5 in $CHCl_3$/MeOH).
Han, L. *et al., J. Nat. Prod.*, 2004, **67**, 1620-1623 (*isol, pmr, cmr*)

3,6,19-Trihydroxy-8,13-labdadien-15-oic acid T-624



$C_{20}H_{32}O_5$ 352.47

(3α,6β,13*E*)-*form* [581798-64-3]
Constit. of *Trimusculus peruvianus*.
Powder. $[\alpha]_D^{25}$ +40 (c, 0.45 in MeOH).

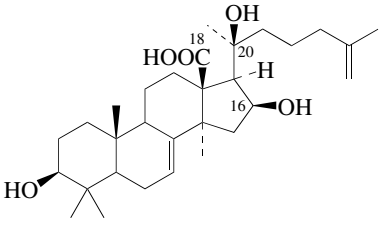
3-Pentanoyl: [581798-65-4]
$C_{25}H_{40}O_6$ 436.587
Constit. of *Trimusculus peruvianus*. Oil. $[\alpha]_D^{25}$ -23 (c, 0.48 in $CHCl_3$).

3,6-Dipentanoyl: [581798-66-5]
$C_{30}H_{48}O_7$ 520.705
Constit. of *Trimusculus peruvianus*. Oil. $[\alpha]_D^{25}$ -36 (c, 0.97 in $CHCl_3$).

3,19-Dipentanoyl: [581798-67-6]
$C_{30}H_{48}O_7$ 520.705
Constit. of *Trimusculus peruvianus*. Oil. $[\alpha]_D^{25}$ -21 (c, 0.85 in $CHCl_3$).

Díaz-Marrero, A.R. *et al., Tetrahedron*, 2003, **59**, 4805-4809 (*isol, pmr, cmr*)

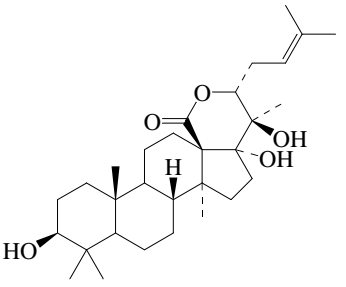
3,16,20-Trihydroxylanosta-7,25-dien-18-oic acid T-625



$C_{30}H_{48}O_5$ 488.706

(3β,5ξ,16β,20*S*)-*form*
18→16-Lactone, 20-Ac, 3-O-*[β-D-glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→2)][6*-O-*sulfo-β-D-glucopyranosyl-(1→4)]-β-D-glucopyranoside]:* ***Psolusoside B***
[113066-18-5]
$C_{56}H_{88}O_{28}S$ 1241.36
Isol. from *Psolus fabricii*. Isol. as Na salt.
Mp 217-220°. $[\alpha]_D^{20}$ -67 (c, 0.1 in Py). CAS number refers to Na salt.
Kalinin, V.I. *et al., Khim. Prir. Soedin.*, 1989, 361-368 (*isol, struct*)

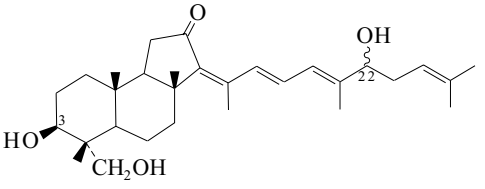
3,17,20-Trihydroxylanost-24-en-18,22-olide T-626



$C_{30}H_{48}O_5$ 488.706

(3β,17α,20*R*,22*R*)-*form*
3-O-*[3*-O-*Methyl-6*-O-*sulfo-β-D-glucopyranosyl-(1→3)-6*-O-*sulfo-β-D-glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-6-deoxy-β-D-glucopyranosyl-(1→2)-4*-O-*sulfo-β-D-xylopyranoside], 20-Ac:* ***Frondoside F***
[349543-47-1]
$C_{61}H_{98}O_{37}S_3$ 1519.621
Constit. of *Cucumaria frondosa*. Cryst.
Mp 251-254° dec. $[\alpha]_D^{23}$ -9.1 (c, 0.00055 in Py aq.).
Yayli, N. *et al., Indian J. Chem., Sect. B*, 2001, **40**, 399-404 (*isol, pmr, cmr*)

3,22,28-Trihydroxy-13,15,17(20),24-malabaricatetraen-12-one T-627

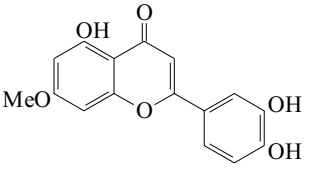


$C_{30}H_{46}O_4$ 470.691

(3β,13*Z*,15*E*,17(20)*E*,22ξ)-*form* [81575-85-1]
3,28-Di-Ac:
$C_{34}H_{50}O_6$ 554.765
Constit. of *Jaspis stellifera*. Foam. $[\alpha]_D^{20}$ -32.7 (c, 1 in $CHCl_3$).
λ_{max} 343 (ε 29100) (MeOH) (Derep).
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 39-50 (*Jaspis stellifera constit*)

3′,4′,5-Trihydroxy-7-methoxyflavone T-628

*2-(3,4-Dihydroxyphenyl)-5-hydroxy-7-methoxy-4*H*-1-benzopyran-4-one, 9CI. Luteolin 7-methyl ether*
[20243-59-8]



$C_{16}H_{12}O_6$ 300.267
Isol. from *Baccharis* spp., *Eremanthus* sp., *Hazardia* sp., *Salvia officinalis* (sage) and *Thymus membranaceus* and other plants.
Yellow prisms (EtOH).
Mp 266-268° Mp 306-308°.

5-O-*β-D-Glucopyranoside:* ***Yuanhuanin***
[83133-14-6]
$C_{22}H_{22}O_{11}$ 462.409
Isol. from *Daphne sericea* and *Daphne genkwa*.

3′-O-β-D-Glucopyranoside: [107140-38-5]
[304902-15-6]
$C_{22}H_{22}O_{11}$ 462.409
Constit. of *Pseudocyclosorus* spp. and *Avicennia marina*. λ_{max} 253; 267; 346 (MeOH).

3′-O-β-D-Galactopyranoside: [304902-16-7]
$C_{22}H_{22}O_{11}$ 462.409
Constit. of *Avicennia marina*. λ_{max} 251; 267; 347 (MeOH).

4′-O-α-L-Rhamnopyranoside: ***Spinoside***
[31159-36-1]
$C_{22}H_{22}O_{10}$ 446.41
Isol. from *Atraphaxis spinosa*. Lemon-yellow needles (MeOH aq.). Mp 179-181°. $[\alpha]_D$ -167.2 (c, 0.16 in MeOH).

5-O-[α-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]: [50675-77-9]
$C_{27}H_{30}O_{15}$ 594.525
Isol. from *Ovidia pillo-pillo*.
Mp 189-192°.

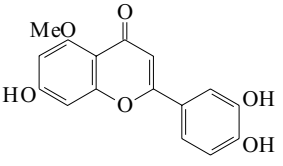
4′-O-[β-D-Glucofuranosyl-(1→6)-β-D-glucopyranoside]: [35128-74-6]
$C_{28}H_{32}O_{16}$ 624.551
Isol. from *Atraphaxis spinosa*. Cryst. (EtOH aq.).
Mp 166-168°. $[\alpha]_D^{22}$ -50.5 (c, 0.1 in MeOH).

4′-O-[β-D-Glucopyranosyl-(1→?)-β-D-glucopyranoside]:
$C_{28}H_{32}O_{16}$ 624.551
Isol. from *Carex nigromarginata*.

Pankajamani, K.S. *et al., J. Indian Chem. Soc.*, 1954, **31**, 565 (*synth*)
Chumbalev, T.K. *et al., Khim. Prir. Soedin.*, 1970, **6**, 626; 1971, **7**, 525; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 639; 1971, **7**, 504 (*Spinoside, glucofuranosylglucopyranoside*)
Brieskorn, C.H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1971, **304**, 557 (*isol*)
Nunez-Alarcon, J. *et al., Phytochemistry*, 1973, **12**, 1451, (*5-xylosylglucoside*)
Ulubelen, A. *et al., Phytochemistry*, 1982, **21**, 801 (*Yuanhuanin*)
Wada, H. *et al., Yakugaku Zasshi*, 1986, **106**, 989 (*3′-glucoside*)
Rettig, J.H. *et al., Biochem. Syst. Ecol.*, 1990, **18**, 393 (*4′-diglucoside*)
Sharaf, M. *et al., Fitoterapia*, 2000, **71**, 274-277 (*3′-glucoside, 3′-galactoside*)

3′,4′,7-Trihydroxy-5-methoxyflavone, 8CI T-629

*2-(3,4-Dihydroxyphenyl)-7-hydroxy-5-methoxy-4*H*-1-benzopyran-4-one, 9CI. Luteolin 5-methyl ether*
[58115-29-0]



$C_{16}H_{12}O_6$ 300.267
Found in seeds of *Medicago varia*; sea grass *Phyllospadix japonica*; wing and bodies of marbled white butterfly *Melanargia galathea*. Also in *Cyperus* spp.

7-O-β-D-Glucopyranoside: [58115-30-3]
$C_{22}H_{22}O_{11}$ 462.409
Isol. from *Juncus* spp.

Morris, S.J. *et al., Tet. Lett.*, 1963, 101 (*isol, uv*)
Williams, C.A. *et al., Biochem. Syst. Ecol.*, 1975, **3**, 181 (*glucoside*)
Takagi, M. *et al., Agric. Biol. Chem.*, 1979, **43**, 2417 (*isol*)
Gehring, E. *et al., Z. Naturforsch., C*, 1980, **35**, 380 (*ms, isol*)
Harborne, J.B. *et al., Phytochemistry*, 1985, **24**, 751 (*isol*)

4′,5,7-Trihydroxy-3′-methoxyflavone, 8CI T-630

*5,7-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Chrysoeriol****. Scoparol. Luteolin 3′-methyl ether*
[491-71-4]
$C_{16}H_{12}O_6$ 300.267
Occurs in many plants in Asteraceae, Cyperaceae, Fabaceae, Hydrophyllaceae, Labiatae, Passifloraceae, Penaeaceae and Scrophulariaceae. Shows antioxidative and antimutagenic activity. Yellow needles (EtOH). Sol. Py; fairly sol. EtOH, EtOAc.
Mp 330-331°. The identity of Scoparol with Chrysoeriol is not confirmed. λ_{max} 252; 270; 346 (MeOH). λ_{max} 241; 249 (sh); 269; 347 (MeOH).

▶ LK9278000

7-O-Sulfate: [60048-90-0]
$C_{16}H_{12}O_9S$ 380.331
Isol. from *Zostera marina*.

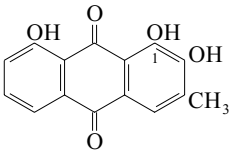
7-O-(2-O-Sulfo-β-D-glucopyranoside): ***Thalassiolin B***
$C_{22}H_{22}O_{14}S$ 542.473
Constit. of the seagrass *Thalassia testudianum*. Inhibitor of HIV integrase. Yellow amorph. solid. $[\alpha]_D$ -72 (c, 0.25 in MeOH). λ_{max} 207 (ε 35800); 251 (ε 16800); 268 (ε 15900); 346 (ε 20600) (MeOH).

[28709-98-0, 38725-01-8, 87861-40-3]

Harborne, J.B. *et al., Biochem. Syst. Ecol.*, 1976, **4**, 37-41 (*7-sulfate*)
Rowley, D.C. *et al., Bioorg. Med. Chem.*, 2002, **10**, 3619-3625 (*Thalassiolin B*)

1,2,8-Trihydroxy-3-methylanthraquinone T-631

Norobtusifolin. 2-Hydroxychrysophanol. 1,2,8-Trihydroxy-3-methyl-9,10-anthracenedione, 9CI



$C_{15}H_{10}O_5$ 270.241
Constit. of the roots of *Hemerocallis fulva* and *Myrsine africana* (Cape myrtle). Orange-red needles (MeOH).
Mp 265° (255°). λ_{max} 208 (log ε 4.19); 235 (log ε 4.05); 258 (log ε 4.11); 426 (log ε 3.73) (EtOH).

2-O-β-D-Glucopyranoside: ***Kwanzoquinone C***
$C_{21}H_{20}O_{10}$ 432.383
Constit. of the roots of *Hemerocallis fulva*. Fine yellow needles.
Mp 233-234°. $[\alpha]_D^{20}$ -46 (c, 0.03 in EtOH). λ_{max} 206 (log ε 4.2); 227 (log ε 4.23); 260 (log ε 4.17); 429 (log ε 3.78) (EtOH).

2-O-(6-O-Malonyl-β-D-glucopyranoside): ***Kwanzoquinone D***
$C_{24}H_{22}O_{13}$ 518.43
Constit. of the roots of *Hemerocallis fulva*. Golden yellow needles.
Mp 174-175°. $[\alpha]_D^{29}$ -313 (c, 0.008 in EtOH). λ_{max} 205 (log ε 4.28); 227 (log ε 4.35); 260 (log ε 4.31); 290 (sh) (log ε 3.91); 430 (log ε 3.96) (EtOH).

1-Me ether: 2,8-Dihydroxy-1-methoxy-3-methylanthraquinone. ***Obtusifolin***†
[477-85-0]
$C_{16}H_{12}O_5$ 284.268
Isol. from seeds of *Cassia obtusifolia* and from *Hemerocallis citrina*. Yellow needles (MeOH).
Mp 237-238°. Not the same as Obtusifolin.

1-Me ether, di-Ac:
$C_{20}H_{16}O_7$ 368.342
Light yellow needles. Mp 187-188°.

1-Me ether, 2-O-β-D-glucopyranoside: ***Glucoobtusifolin***
[120163-18-0]
$C_{22}H_{22}O_{10}$ 446.41
Isol. from seeds of *Cassia obtusifolia* and *Cassia tora*. Platelet aggregation inhibitor. Cryst + $1H_2O$.
Mp 205-206°.

1,2-Di-Me ether: 8-Hydroxy-1,2-dimethoxy-3-methylanthraquinone
[82868-99-3]
$C_{17}H_{14}O_5$ 298.295
Constit. of *Hemerocallis citrina* and the marine worm *Urechis unicinctus*. Orange needles.
Mp 214-215°.

Tri-Me ether: 1,2,8-Trimethoxy-3-methylanthraquinone
$C_{18}H_{16}O_5$ 312.321
Light yellow needles (petrol). Mp 145-146°.

Takido, M. *et al., Chem. Pharm. Bull.*, 1958, **6**, 397 (*isol, struct*)
Takido, M. *et al., CA*, 1965, **62**, 5326f (*Glucoobtusifolin*)
He, X. *et al., CA*, 1982, **97**, 107044x (*isol, di-Me ether*)
Cameron, D.W. *et al., Tet. Lett.*, 1986, **27**, 4999 (*synth*)
Li, X.-H. *et al., J. Nat. Prod.*, 1989, **52**, 660 (*isol, pmr*)
Wong, S.-M. *et al., Phytochemistry*, 1989, **28**, 211-214 (*Glucoobtusifolin*)
Krohn, K. *et al., Annalen*, 1993, 905-909 (*synth, di-Me ether*)
Chang, S. *et al., J. Korean Chem. Soc.*, 1998, **42**, 64-68 (*isol*)
Cichewicz, R.H. *et al., Tetrahedron*, 2002, **58**, 8597-8606 (*isol, pmr, cmr, Kwanzoquinones*)

1,3,6-Trihydroxy-8-methylanthraquinone, 8CI T-632

1,3,6-Trihydroxy-8-methyl-9,10-anthracenedione, 9CI. ***Deoxyerythrolaccin***

[18499-83-7]

$C_{15}H_{10}O_5$ 270.241

Constit. of jalari stick lac (from *Laccifer lacca* and *Austrotachardia acaciae*), also isol. from *Aloe saponaria*. Prod. by the marine-derived *Streptomyces* sp. B1108. Orange needles (MeOH).
Mp 310° dec. λ_{max} 292 (sh); 310 (ϵ 7940); 372 (sh); 510 (ϵ 2510) (MeOH/KOH) (Derep). λ_{max} 265 (sh); 284 (ϵ 15800); 425 (sh); 432 (ϵ 2510) (MeOH) (Derep).

Tri-Ac: [18499-85-9]
$C_{21}H_{16}O_8$ 396.353
Yellow needles (MeOH). Mp 172°.

Mehandale, A.R. *et al., Tet. Lett.*, 1968, 2231 (*isol, synth, ir*)
Yagi, A. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1159 (*isol, ir, uv, pmr*)
Cameron, D.W. *et al., Aust. J. Chem.*, 1978, **31**, 1363 (*synth*)
Roberge, G. *et al., J.C.S. Perkin 1*, 1978, 1041 (*synth*)
Mills, R.J. *et al., Tet. Lett.*, 1984, **25**, 479 (*synth*)
Abdelfattah, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*marine, isol*)

1,3,8-Trihydroxy-6-methylanthraquinone, 8CI T-633

1,3,8-Trihydroxy-6-methyl-9,10-anthracenedione, 9CI. ***Emodin****. Rheum-emodin. Frangula emodin. Archin. Frangulinic acid. Emodol. Alatinone*

[518-82-1]

$C_{15}H_{10}O_5$ 270.241

Present in Cascara sagrada, in aloes and in other plant material. Isol. from *Penicillium* spp., *Aspergillus* spp. and from *Anixiella micropetrusa*. Antimicrobial, antineoplastic agent. Cathartic agent. Shows monoamine oxidase inhibitory activity. Orange or yellow-brown needles (Py aq. or MeOH).
Mp 266-268° (264-265°). Log P 1.8 (calc). λ_{max} 222 (ϵ 35500); 252 (ϵ 18200); 265 (ϵ 18600); 289 (ϵ 21900); 437 (ϵ 12600) (EtOH) (Derep).

▶ LD_{50} (mus, ipr) 35 mg/kg. CB7920600

3-Me ether: 1,8-Dihydroxy-3-methoxy-6-methylanthraquinone. ***Physcion****. Parietin. Methylemodin. Physcic acid. Rheochrysidin. Przewalskinone B*

[521-61-9]

$C_{16}H_{12}O_5$ 284.268

Widely distributed in lichens, e.g. *Parmelia* spp., higher plants, e.g. *Rumex* spp. and prod. by *Aspergillus* and *Penicillium* spp. Also isol. from the marine annelid *Urechis unicintus*. Antimicrobial agent. Possesses cathartic props. Orange needles (EtOAc/petrol). Mp 209-210°. Log P 2.37 (calc). Struct. of Przewalskinone B revised in 1996. λ_{max} 237; 301; 508 (MeOH/NaOH) (Derep). λ_{max} 248; 265; 286; 406; 431 (MeOH) (Derep).

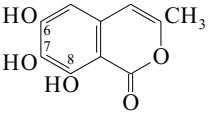
▶ LD_{50} (mus, ipr) 10 mg/kg. CB6720000

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 91D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 88D (*ir*)
Eder, R. *et al., Helv. Chim. Acta*, 1925, **8**, 140 (*bibl*)
Hirose, Y. *et al., Chem. Pharm. Bull.*, 1973, **21**, 2790 (*synth*)
Banville, J. *et al., Can. J. Chem.*, 1974, **52**, 80 (*synth, uv, ir, pmr*)
Fairbairn, J.W. *et al., Pharmacology*, Suppl. 1, 1976, **14**, 1 (*rev*)
Anderson, J.A. *et al., Phytochemistry*, 1986, **25**, 1115 (*biosynth*)
Ahmed, S.A. *et al., Chem. Comm.*, 1987, 883 (*synth*)
Kalidhar, S.B. *et al., Phytochemistry*, 1989, **28**, 2455; 3459 (*pmr*)
Coskun, M. *et al., Phytochemistry*, 1990, **29**, 2018 (*cd, pmr, cmr*)
Schmidt, R.R. *et al., Synthesis*, 1994, 255 (*synth, pmr*)
Chang, S. *et al., J. Korean Chem. Soc.*, 1998, **42**, 64-68 (*3-Me ether, isol, Urechis*)

6,7,8-Trihydroxy-3-methyl-1*H*-2-benzopyran-1-one, 9CI T-634

6,7,8-Trihydroxy-3-methylisocoumarin, 8CI

[33624-51-0]



$C_{10}H_8O_5$ 208.17
Isol. from *Streptomyces mobaraensis*. Cryst. (EtOH).
Mp 234°.

*7-Me ether: 6,8-Dihydroxy-7-methoxy-3-methyl-1*H*-2-benzopyran-1-one, 9CI. 6,8-Dihydroxy-7-methoxy-3-methylisocoumarin, 8CI.* ***Reticulol***

[26246-41-3]
$C_{11}H_{10}O_5$ 222.197
Isol. from *Streptomyces mobaraensis* and *Streptomyces rubrireticulae*. Inhibitor of cyclic nucleotide phosphodiesterase. Cryst. (EtOH). Sol. MeOH, EtOAc, Me_2CO, butanol; fairly sol. $CHCl_3$; poorly sol. H_2O, hexane.
Mp 194°. λ_{max} 245 (ϵ 46800); 275 (ϵ 6920); 337 (ϵ 5250) (MeOH) (Derep). λ_{max} 245 (ϵ 47860); 275 (ϵ 6920); 278 (ϵ 7250); 330 (ϵ 5750); 337 (ϵ 5250) (MeOH) (Berdy). λ_{max} 245 (ϵ 43200); 278 (ϵ 7100); 332 (ϵ 5500) (MeOH/HCl) (Berdy). λ_{max} 245 (ϵ 32700); 255 (ϵ 44300); 310 (ϵ 16500) (MeOH/NaOH) (Berdy).

*6,7-Di-Me ether: 8-Hydroxy-6,7-dimethoxy-3-methyl-1*H*-2-benzopyran-1-one, 9CI. 8-Hydroxy-6,7-dimethoxy-3-methylisocoumarin, 8CI.* ***6-O-Methylreticulol***

[24350-93-4]
$C_{12}H_{12}O_5$ 236.224
Isol. from *Streptomyces mobaraensis*. Constit. of *Wettsteinia inversa*. Cryst. (EtOH).
Mp 199° (178-180°). λ_{max} 241 (log ϵ 4.59); 255 (sh); 278 (sh); 290 (sh); 334 (log ϵ 3.74) (MeOH).

7,8-Methylene, 6-Me ether: 6-Methoxy-3-methyl-7,8-methylenedioxyisocoumarin. ***Inversin***

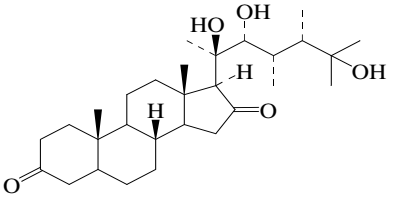
$C_{12}H_{10}O_5$ 234.208
Constit. of *Wettsteinia inversa*. Antiplatelet agent. Cryst. ($CHCl_3$/MeOH).
Mp 197-201°.

*5-Chloro, 7-Me ether: 5-Chloro-6,8-dihydroxy-7-methoxy-3-methyl-1*H*-2-benzopyran-1-one. 5-Chloro-6,8-dihydroxy-7-methoxy-3-methylisocoumarin. 5-Chlororeticulol.* ***Avicennin A***

$C_{11}H_9ClO_5$ 256.642
Isol. from the endophytic fungus of *Avicennia marina*. Needles.
Mp 197-199°. λ_{max} 247 (ϵ 51570); 359 (ϵ 2540) ($CHCl_3$).

Mitscher, L.A. *et al., Experientia*, 1964, **20**, 258 (*isol*)
Lin, J. *et al., Agric. Biol. Chem.*, 1971, **35**, 363 (*isol, uv, ir, ms, pmr*)
Eaton, M.A.W. *et al., Tet. Lett.*, 1971, 1337 (*isol, uv, ir, ms, pmr*)
Furutani, Y. *et al., J. Antibiot.*, 1975, **28**, 558 (*isol, props*)
Umezawa, H. *et al., Agric. Biol. Chem.*, 1977, **41**, 989; 1587 (*biosynth, cmr, props, bibl*)
Kiang, F.-M. *et al., Phytochemistry*, 1994, **37**, 1459 (*Inversin*)
Lin, Y. *et al., Zhongshan Daxue Xuebao Ziran Kexueban*, 2001, **40**, 127-128; *CA*, **135**, 179750 (*Avicennin A*)

20,22,25-Trihydroxy-23-methylergostane-3,16-dione T-635

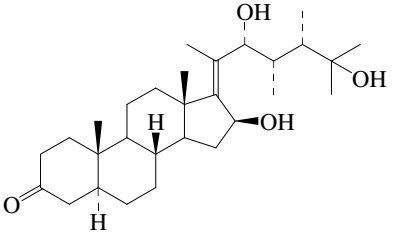


$C_{29}H_{48}O_5$ 476.695

(20*R*,22*R*,23*S*,24*S*)-*form*

22,25-Di-Ac: ***Hippuristerone E***
[549528-38-3]
$C_{33}H_{52}O_7$ 560.77
Constit. of *Isis hippuris*. Powder.
Mp 174-176°. $[\alpha]_D$ -92 (c, 0.1 in $CHCl_3$).
Sheu, J.-H. *et al., J. Nat. Prod.*, 2003, **66**, 917-921 (*isol, pmr, cmr*)

16,22,25-Trihydroxy-23-methylergost-17(20)-en-3-one T-636



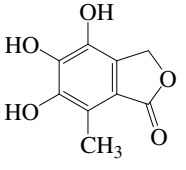
$C_{29}H_{48}O_4$ 460.696

(5α,16β,17(20)*Z*,22*R*,23*S*,24*S*)-*form*

22-Ac: ***Hippuristerone L***
[868395-86-2]
$C_{31}H_{50}O_5$ 502.733
Constit. of *Isis hippuris*. Powder.
Mp 204-205°. $[\alpha]_D$ +9 (c, 1.28 in $CHCl_3$).
Chao, C.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1366-1370 (*Hippuristerone L*)

4,5,6-Trihydroxy-7-methyl-1(3*H*)-isobenzofuranone T-637

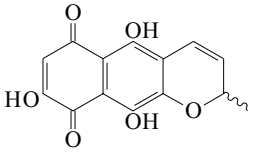
4,5,6-Trihydroxy-7-methylphthalide. ***Epicoccone***



$C_9H_8O_5$ 196.159
Prod. by the marine fungus *Epicoccum* sp. Antioxidant. Cryst.
Mp 249-250°. λ_{max} 217 (log ε 4.1); 273 (log ε 3.6) (no solvent reported).
Abdel-Lateff, A. *et al., Planta Med.*, 2003, **69**, 831-834 (*isol, pmr, cmr*)

5,8,10-Trihydroxy-2-methyl-2*H*-naphtho[2,3-*b*]pyran-6,9-dione, 9CI, 8CI T-638

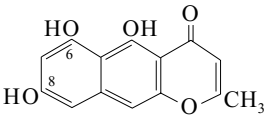
*8-Hydroxy-2-methyl-2*H*-pyrano[3,2-*g*]naphthazarin*
[20052-67-9]



$C_{14}H_{10}O_6$ 274.229
Pigment from the spines of the sea urchin *Echinothrix diadema*. Cryst. (petrol).
Mp 165-172° dec. λ_{max} 292; 340; 488; 564 (sh) ($CHCl_3$).
Moore, R.E. *et al., Tet. Lett.*, 1968, 4581-4583 (*isol, uv, pmr, ms*)

5,6,8-Trihydroxy-2-methyl-4*H*-naphtho[2,3-*b*]pyran-4-one, 9CI T-639

5,6,8-Trihydroxy-2-methylbenzo[g]chromen-4-one. ***Norrubrofusarin***
[3566-98-1]



$C_{14}H_{10}O_5$ 258.23
Isol. from seeds of *Cassia tora* (charota). Orange-red cryst. (dioxan aq.).
Mp 298-299° dec. λ_{max} 225 (log ε 4.43); 278 (log ε 4.65); 329 (log ε 3.43); 415 (log ε 3.73) (EtOH).

*6-Me ether: 5,8-Dihydroxy-6-methoxy-2-methyl-4*H*-naphtho[2,3-b]pyran-4-one, 9CI. 5,8-Dihydroxy-6-methoxy-2-methylbenzo[g]chromen-4-one.* ***6-O-Methylnorrubrofusarin****. Antibiotic TMC 256A$_1$. TMC 256A$_1$*
[3773-18-0]
$C_{15}H_{12}O_5$ 272.257
Prod. by *Aspergillus niger* var. *niger* TC 1629. Isol. from *Comantheria briareus*. Inhibitor of IL-4 signal transduction.
Yellow powder. λ_{max} 224 (log ε 4.42); 253 (log ε 4.42); 276 (log ε 4.61); 326 (log ε 3.4); 405 (log ε 3.81) (MeOH).

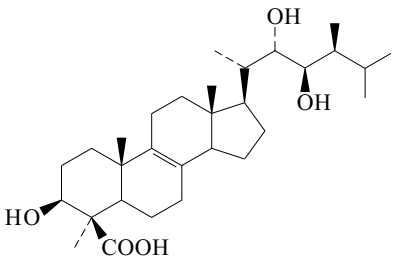
*8-Me ether: 5,6-Dihydroxy-8-methoxy-2-methyl-4*H*-naphtho[2,3-b]pyran-4-one, 9CI. 5,6-Dihydroxy-8-methoxy-2-methylbenzo[g]chromen-4-one.* ***Rubrofusarin***
[3567-00-8]
$C_{15}H_{12}O_5$ 272.257
Pigment from *Fusarium culmorum*. Isol. from *Senna obliqua* and *Comantheria briareus*. Shows *in vivo* anticancer and antimycobacterial activity. Orange needles (MeOH).
Mp 212-214°. λ_{max} 224 (ε 28200); 250; 277 (ε 47600); 325 (ε 3210); 407 (ε 5480) (MeCN) (Derep). λ_{max} 225 (ε 28200); 278 (ε 49700); 328 (ε 3400); 415 (ε 5200) (MeOH) (Berdy).

*5,6-Di-Me ether: 8-Hydroxy-5,6-dimethoxy-2-methyl-4*H*-naphtho[2,3-b]pyran-4-one, 9CI.* ***Comantherin***
[17276-02-7]
$C_{16}H_{14}O_5$ 286.284
Isol. from *Comantheria briareus* and *Comantheria perplexa*. Yellow prisms (MeOH).
Mp 272° dec Mp 285° dec. λ_{max} 225 (log ε 4.5); 248 (log ε 4.59); 274 (log ε 4.66); 331 (log ε 3.5); 351 (sh) (log ε 3.61); 386 (log ε 3.93) (EtOH).

*5,6-Di-Me ether, 8-*O*-sulfate: Comantherin sulfate*
[72246-25-4]
[31665-30-2 (hydrogen sulfate Na salt)]
$C_{16}H_{14}O_8S$ 366.348
Isol. from *Comantheria perplexa*. Yellow powder (as Na salt).
Mp >° 200 (darkens) (Na salt). λ_{max} 222; 259; 316; 384 (H_2O) (Na salt).

Stout, G.H. *et al., Chem. Ind. (London)*, 1961, 289-290 (*Rubrofusarin, cryst struct*)
Shoji, S. *et al., Chem. Pharm. Bull.*, 1967, **15**, 1757-1764 (*Rubrofusarin, synth*)
Kent, R.A. *et al., Aust. J. Chem.*, 1970, **23**, 2325-2335 (*Comantherin, sulfate*)
Ogura, M. *et al., J. Nat. Prod.*, 1977, **40**, 347-351 (*Rubrofusarin, isol*)
Rideout, J.A. *et al., Experientia*, 1979, **35**, 1273-1274 (*Comantherin sulfate*)
Francesconi, K.A. *et al., Aust. J. Chem.*, 1980, **33**, 2781-2784 (*Comantherin, isol*)
Abell, C. *et al., Chem. Comm.*, 1986, 15-17 (*Rubrofusarin, synth*)
Sakurai, M. *et al., J. Antibiot.*, 2002, **55**, 685-692 (*TMC 256A*)
Graham, J.G. *et al., J. Nat. Prod.*, 2004, **67**, 225-227 (*Rubrofusarin, isol, pmr, cmr, cryst struct*)

3,22,23-Trihydroxy-24-methyl-30-nor-8-lanosten-29-oic acid T-640



$C_{30}H_{50}O_5$ 490.722

(3β,22*S*,23*R*,24*S*)-*form*

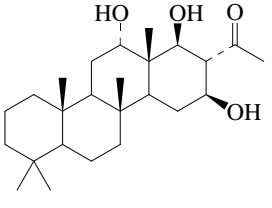
3-O-*β*-D-*Glucopyranoside:* ***Ulososide C***
[454470-27-0]
$C_{36}H_{60}O_{10}$ 652.864
Constit. of an *Ulosa* sp.

3-O-*(2-Acetamido-2-deoxy-β*-D-*glucopyranoside):* ***Ulososide D***
[454470-61-2]
$C_{38}H_{63}NO_{10}$ 693.916
Constit. of an *Ulosa* sp.

3-O-*[β*-D-*Arabinopyranosyl-(1→2)-β*-D-*glucuronopyranoside]:* ***Ulososide E***
[454470-88-3]
$C_{41}H_{66}O_{15}$ 798.963
Constit. of an *Ulosa* sp.

3-O-*[β*-D-*Glucuronopyranosyl-(1→6)-β*-D-*glucopyranoside]:* ***Ulososide A***
[161622-28-2]
$C_{42}H_{68}O_{16}$ 828.99
Constit. of an *Ulosa* sp. Amorph. powder (EtOH aq.) (as di-Na salt).
Mp 191-193° (di-Na salt). $[\alpha]_D$ -4.5 (c, 2.51 in MeOH) (di-Na salt).
Antonov, A.S. *et al., Izv. Akad. Nauk, Ser. Khim.*, 1994, **43**, 1326; *Russ. Chem. Bull. (Engl. Transl.)*, 1994, **43**, 1265 (*Ulososide A*)
Antonov, A.S. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2002, **28**, 183-188 (*Ulososides C-E*)

12,16,18-Trihydroxy-24-methyl-25-nor-24-scalaranone T-641

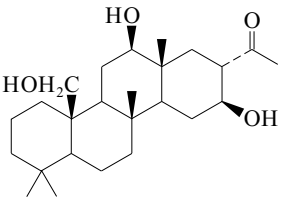


$C_{25}H_{42}O_4$ 406.604

(12α,16β,18β)-*form*

12-Ac: [478364-23-7]
$C_{27}H_{44}O_5$ 448.642
Constit. of a *Phyllospongia* sp. Glass. $[\alpha]_D^{23}$ +27 (c, 0.48 in $CHCl_3$).
Roy, M.C. *et al., J. Nat. Prod.*, 2002, **65**, 1838-1842 (*isol, pmr, cmr*)

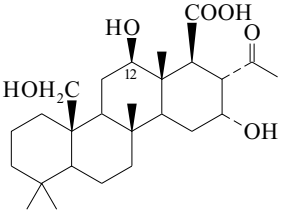
12,16,22-Trihydroxy-24-methyl-25-nor-24-scalaranone T-642



$C_{25}H_{42}O_4$ 406.604

(12β,16β)-*form* [135048-60-1]
Metab. of *Phyllospongia dendyi*.
Cryst. (MeOH).
Mp 288-291°. $[\alpha]_D^{25}$ +6.1 (c, 0.46 in Py).
Rao, C.B. *et al., J. Nat. Prod.*, 1991, **54**, 364-371 (*isol, pmr, cmr*)

12,16,22-Trihydroxy-24-methyl-24-oxo-25-scalaranoic acid T-643



(12β,16α)–*form*

$C_{26}H_{42}O_6$ 450.614

(12β,16α)-*form*

25→12-Lactone: 16,22-Dihydroxy-24-methyl-24-oxo-25,12-scalaranolide
[142780-27-6]
$C_{26}H_{40}O_5$ 432.599
Constit. of *Lendenfeldia frondosa*. Shows antiinflammatory props.
Amorph. solid (as di-Ac). $[\alpha]_D$ +12 (c, 1 in $CHCl_3$) (di-Ac).

(12β,16β)-*form* [804531-46-2]
Constit. of *Lendenfeldia* spp.
Oil.

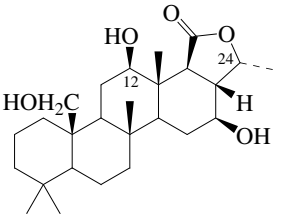
Me ester: [804531-45-1]
$C_{27}H_{44}O_6$ 464.641
Constit. of *Lendenfeldia frondosa* and other *Lendenfeldia* spp. Oil or amorph. solid (as di-Ac). $[\alpha]_D$ +45 (c, 1 in $CHCl_3$) (di-Ac).

22-Ac, Me ester: [804531-47-3]
$C_{29}H_{46}O_7$ 506.678
Constit. of *Lendenfeldia* spp. Oil.

25→12 Lactone:
$C_{26}H_{40}O_5$ 432.599
Constit. of a *Lendenfeldia* sp. Cryst. (DMF/MeCN).
Mp 279-280°. $[\alpha]_D^{21}$ +46.8 (c, 1 in MeOH).

25→12 Lactone, 22-Ac:
$C_{28}H_{42}O_6$ 474.636
Constit. of a *Lendenfeldia* sp. Cryst. (EtOAc/petrol).
Mp 244-246°. $[\alpha]_D^{21}$ +27.7 (c, 1 in $CHCl_3$).
Kazlauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 51-59 (*isol, pmr, cmr*)
Alvi, K.A. *et al., J. Nat. Prod.*, 1992, **55**, 859 (*isol, pmr, cmr*)
Chill, L. *et al., Tetrahedron*, 2004, **60**, 10619-10626 (*isol, pmr, cmr*)

12,16,22-Trihydroxy-24-methyl-25,24-scalaranolide T-644



(12β,16β,24α)-*form*

$C_{26}H_{42}O_5$ 434.615

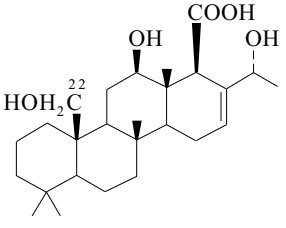
(12β,16β,24α)-*form* [452956-74-0]
Constit. of *Lendenfeldia frondosa*.
Solid. $[\alpha]_D$ +42.1 (c, 0.076 in CH_2Cl_2).

(12β,16β,24β)-*form* [135048-58-7]
Constit. of *Lendenfeldia frondosa* and *Phyllospongia dendyi*.
Cryst. (Et_2O).
Mp 313-316°. $[\alpha]_D^{25}$ +15.8 (c, 0.9 in Py).

22-Ac: [81575-78-2]
$C_{28}H_{44}O_6$ 476.652
Constit. of a *Lendenfeldia* sp. Cryst. (MeOH).
Mp 270-271°.

Kazlauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 51-59 (*22-Ac, isol, struct*)
Rao, C.B. *et al., J. Nat. Prod.*, 1991, **54**, 364-371 (*Phyllospongia dendyi constit*)
Alvi, K.A. *et al., J. Nat. Prod.*, 1992, **55**, 859-865 (*12β,16β,24β-form*)
Stessman, C.C. *et al., J. Nat. Prod.*, 2002, **65**, 1183-1186 (*12β,16β,24α-form*)

12,22,24-Trihydroxy-24-methyl-16-scalaren-25-oic acid T-645



$C_{26}H_{42}O_5$ 434.615

(12β,24*R*)-*form*

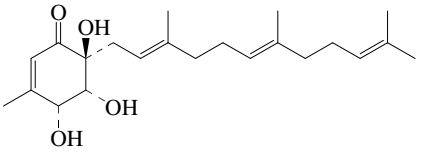
25→12 Lactone: 22,24-Dihydroxy-24-methyl-16-scalaren-25,12-olide. ***Sednolide***
[85337-14-0]
$C_{26}H_{40}O_4$ 416.6
Constit. of *Chromodoris sedna*. Cryst.
Mp 268-272°.

25→12 Lactone, 22-Ac: ***Acetylsednolide***
[85337-15-1]
$C_{28}H_{42}O_5$ 458.637
Constit. of *Chromodoris sedna*. Oil.

24-Ketone, 25→12 lactone: ***22-Hydroxy-24-methyl-24-oxo-16-scalaren-25,12-olide***
[452956-75-1]
$C_{26}H_{38}O_4$ 414.584
Constit. of *Lendenfeldia frondosa*. Solid. $[\alpha]_D$ +18 (c, 0.22 in CH_2Cl_2).

Hochlowski, J.E. *et al., J.O.C.*, 1983, **48**, 1738-1740 (*Sednolide, Acetylsednolide*)
Stessman, C.C. *et al., J. Nat. Prod.*, 1982, **65**, 1183-1186 (*Lendenfeldia frondosa constit*)

4,5,6-Trihydroxy-3-methyl-6-(3,7,11-trimethyl-2,6,10-dodecatrienyl)-2-cyclohexen-1-one T-646



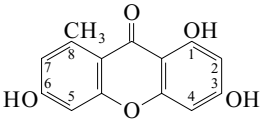
Relative Configuration

$C_{22}H_{34}O_4$ 362.508
Prod. by a marine-derived *Penicillium* sp. Unstable yellow oil. $[\alpha]_D$ -2.1 (c, 0.3 in $CHCl_3$). λ_{max} 203 (log ϵ 4.2); 238 (log ϵ 4) (MeOH).

Li, X. *et al., J. Nat. Prod.*, 2003, **66**, 1499-1500 (*isol, pmr, cmr*)

1,3,6-Trihydroxy-8-methylxanthone T-647

*1,3,6-Trihydroxy-8-methyl-9*H*-xanthen-9-one, 9CI.* ***Norlichexanthone***
[20716-98-7]



$C_{14}H_{10}O_5$ 258.23
Isol. from lichen *Lecanora reuteri* and *Penicillium patulum*. Prod. by the marine fungus *Wardomyces anomalus*. Active against *Clostridium welchii*. Yellow prisms (EtOH aq. or Et_2O).
Mp 285-290° (274-275°). λ_{max} 241 (ϵ 36500); 311 (ϵ 22500) (EtOH) (Berdy).

1-Me ether: 3,6-Dihydroxy-1-methoxy-8-methylxanthone. ***Antibiotic F 483A****. F 483A*
[176204-30-1]
$C_{15}H_{12}O_5$ 272.257
Prod. by a *Penicillium* sp. Antitumour agent. λ_{max} 239; 312 (MeOH) (Berdy).

3-Me ether: 1,6-Dihydroxy-3-methoxy-8-methylxanthone. ***Griseoxanthone C***
[3569-83-3]
$C_{15}H_{12}O_5$ 272.257
Metab. of *Penicillium patulum* and *Aspergillus versicolor*.
Intermed. in biosynth. of Griseofulvin. Pale yellow needles (EtOAc/petrol).
Mp 257-258° (253-255°).

6-Me ether: 1,3-Dihydroxy-6-methoxy-8-methylxanthone. ***6-O-Methylnorlichexanthone***
[22938-77-8]
$C_{15}H_{12}O_5$ 272.257
Isol. from lichens. Yellow cryst. (Py).
Mp 260-263°.

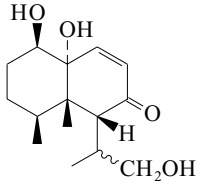
6-Me ether, di-Ac: Mp 196-197°.

3,6-Di-Me ether: 1-Hydroxy-3,6-dimethoxy-8-methylxanthone. ***Lichexanthone***
[15222-53-4]
$C_{16}H_{14}O_5$ 286.284
Prod. by *Parmelia formosana, Pertusaria sulphurata*, *Anthocleista djalonensis* and *Aspidosperma formosanum*. Constit. of *Ruprechtia tangarana*. Yellow cryst. ($CHCl_3$/cyclohexane or Me_2CO aq.).
Mp 187-188°. λ_{max} 242 (ϵ); 251 (sh) (ϵ); 267 (sh) (ϵ); 306 (ϵ); 340 (sh) (ϵ) (EtOH) (Derep).

McMaster, W.J. *et al., J.C.S.*, 1960, 4628-4631 (*3-Me ether*)
Jayalakshmi, V. *et al., Indian J. Chem.*, 1974, **12**, 441-443 (*Griseoxanthone C, synth*)
Broadbent, D. *et al., Phytochemistry*, 1975, **14**, 2082 (*isol, ir, uv, pmr, ms*)
Harris, C.M. *et al., J.A.C.S.*, 1976, **98**, 5380-5386; 1977, **99**, 1631-1637 (*Griseoxanthone C, Lichexanthone, synth, ir, uv, pmr, ms*)
Kingston, D.G.I. *et al., Phytochemistry*, 1976, **15**, 1037-1039 (*Griseoxanthone C, isol*)

Ruben, F.G.M. *et al., Phytochemistry*, 1976, **15**, 1093-1095 (*Lichexanthone, isol, uv, ir, pmr, ms*)
Okorie, D.A. *et al., Phytochemistry*, 1976, **15**, 1799-1800 (*Lichexanthone, isol, ir, uv, pmr, ms*)
Elix, J.A. *et al., Aust. J. Chem.*, 1978, **31**, 145-155 (*Lichexanthone, synth*)
Sundholm, E.G. *et al., Tetrahedron*, 1978, **34**, 577-586 (***synth, pmr, cmr***)
Sandifer, R.M. *et al., J.O.C.*, 1981, **46**, 2260-2267 (*Norlichexanthone, synth*)
Japan. Pat., 1996, 96 12 666; *CA*, **124**, 315162n (*Antibiotic F483A*)
Abdel-Lateff, A. *et al., J. Nat. Prod.*, 2003, **66**, 706-708 (*isol, pmr, cmr*)
Pettit, G.R. *et al., J. Nat. Prod.*, 2003, **66**, 1065-1069 (*Lichexanthone, cryst struct*)
Mutanyatta, J. *et al., Phytochemistry*, 2003, **62**, 797-804 (*isol, pmr, cmr*)

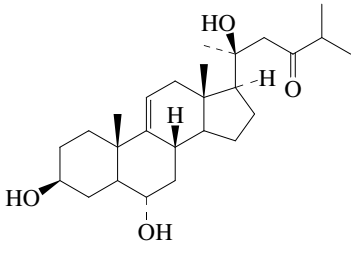
1,10,12-Trihydroxy-8-nardosinen-7-one T-648



$C_{15}H_{24}O$ 220.354

(1β,10α,11ξ)-*form*
Parathylone
[147658-99-9]
Constit. of *Paralemnalia thyrsoides.*
Needles.
Mp 108.5-109.5°. $[\alpha]_D$ -16 (c, 0.05 in MeOH).
Su, J.-Y. *et al., J. Nat. Prod.*, 1993, **56**, 288 (*isol, pmr, cmr*)

3,6,20-Trihydroxy-24-norcholest-9(11)-en-23-one T-649

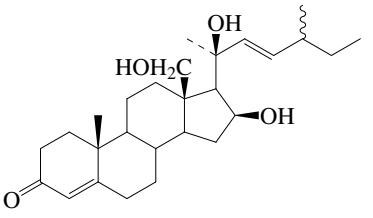


$C_{26}H_{42}O_4$ 418.615

(3β,5α,6α,20*S*)-*form*
24-Northornasterol A
6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate:* ***Ophidianoside B***
[97165-89-4]
$C_{55}H_{90}O_{28}S$ 1231.365
Constit. of *Ophidiaster ophidianus* and *Hacelia attenuata.*
$[\alpha]_D$ +2.8 (MeOH).
6-O-*[β-D-Fucopyranosyl-(1→2)-β-D-xylopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 3-sulfate:* ***Ophidianoside C.***
Attenuatoside D
[97165-90-7]
$C_{54}H_{88}O_{27}S$ 1201.339
Constit. of *Ophidiaster ophidianus* and *Hacelia attenuata.*
$[\alpha]_D$ -2.9 (MeOH).
Minale, L. *et al., Gazz. Chim. Ital.*, 1984, **114**, 151-158 (*isol, pmr, cmr*)
Riccio, R. *et al., J.C.S. Perkin 1*, 1985, 655-660 (*isol, pmr, cmr*)

16,18,20-Trihydroxy-27-norergosta-4,22-dien-3-one T-650

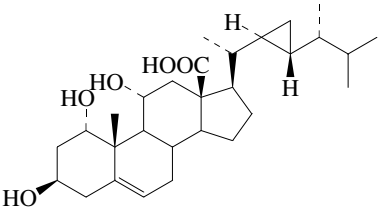
16,18,20-Trihydroxy-24-methyl-27-norcholesta-4,22-dien-3-one



$C_{27}H_{42}O_4$ 430.626

(16β,20*S*,22*E*,24ξ)-*form* [89837-99-0]
Isol. from *Leptogorgia sarmentosa.*
Cimino, G. *et al., Experientia*, 1984, **40**, 246

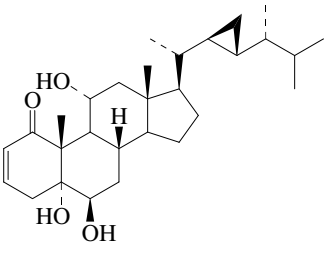
1,3,11-Trihydroxy-23-norgorgost-5-en-13-oic acid T-651



$C_{29}H_{46}O_5$ 474.679

(1α,3β,11α)-*form*
1,11-Dihydroxy-23-demethylgorgosterol-13-carboxylic acid
[97190-41-5]
Isol. from *Sinularia dissecta.*
Jagodzinska, B.M. *et al., J.O.C.*, 1985, **50**, 2988

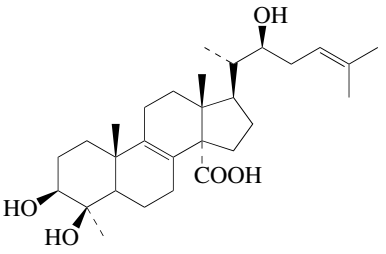
5,6,11-Trihydroxy-33-norgorgost-2-en-1-one T-652



$C_{29}H_{46}O_4$ 458.68

(5α,6β,11α,22*R*,23*R*,24*R*)-*form*
6-Ac: ***Yonarasterol C***
[263764-03-0]
$C_{31}H_{48}O_5$ 500.717
Constit. of *Clavularia viridis.* Amorph. solid. $[\alpha]_D^{25}$ +10.4 (c, 0.09 in $CHCl_3$). λ_{max} 225 (log ϵ 3.94) (EtOH).
Iwashima, M. *et al., Steroids*, 2000, **65**, 130-137 (*isol, pmr, cmr*)

3,4,22-Trihydroxy-29-norlanosta-8,24-dien-30-oic acid T-653

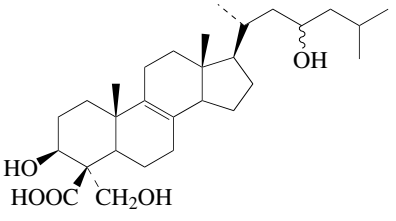


$C_{29}H_{46}O_5$ 474.679

(3β,4β,22*S*)-*form* [220543-68-0]
Oil.

3-O-*[β-D-Galactopyranosyl-(1→4)-α-L-arabinopyranosyl-(1→2)-β-D-galactopyranoside]:* ***Ectyoplaside A***
[220605-04-9]
$C_{46}H_{74}O_{19}$ 931.079
Constit. of *Ectyoplasia ferox*. Amorph. solid. $[\alpha]_D^{25}$ +3 (c, 0.002 in MeOH).
Cafieri, F. *et al., Eur. J. Org. Chem.*, 1999, 231-238 (*isol, pmr, smr*)

3,23,28-Trihydroxy-30-norlanost-8-en-29-oic acid T-654

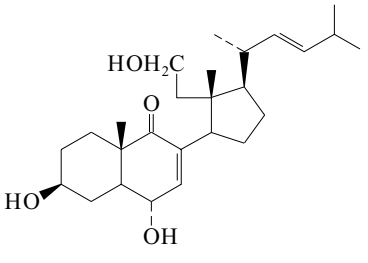


$C_{29}H_{48}O_5$ 476.695

(3β,23ξ)-*form*

*3-(*N-*Acetyl-β-D-glucosaminide):* ***Uloside B***
[209344-56-9]
$C_{37}H_{61}NO_{10}$ 679.89
Constit. of an *Ulosa* sp. Cryst.
Mp 196-198°. $[\alpha]_D$ +33 (c, 0.1 in MeOH).
Antonov, A.S. *et al., Tet. Lett.*, 1998, **39**, 3807-3808 (*isol, pmr, cmr*)

3,6,11-Trihydroxy-24-nor-9,11-secocholesta-7,22-dien-9-one T-655



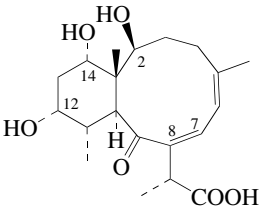
$C_{26}H_{42}O_4$ 418.615

(3β,6α,22*E*)-*form*

11-Ac: [147879-65-0]
$C_{28}H_{44}O_5$ 460.653
Constit. of *Gersemia fruticosa*. Shows cytotoxicity against cancer cell lines. Oil. $[\alpha]_D^{22}$ +23 (c, 0.17 in MeOH). λ_{max} 239 (ε 4000) (EtOH) (Derep).

11-Aldehyde: ***3,6-Dihydroxy-24-nor-9-oxo-9,11-secocholesta-7,22-dien-11-al***
$C_{26}H_{40}O_4$ 416.6
Constit. of *Gersemia fruticosa*. Oil. λ_{max} 239 (EtOH).
Koljak, R. *et al., Tet. Lett.*, 1993, **34**, 1985 (*isol, pmr, cmr*)
Lopp, A. *et al., Steroids*, 1994, **59**, 274-281 (*activity*)
Koljak, R. *et al., Tetrahedron*, 1998, **54**, 179-186 (*aldehyde*)

2,12,14-Trihydroxy-9-oxo-5,7-briaradien-18-oic acid T-656



$C_{20}H_{30}O_6$ 366.453

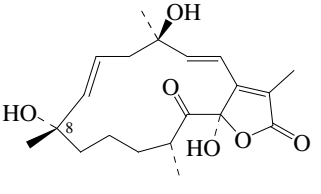
2-Butanoyl, 14-Ac, Me ester: ***Briareolate ester G***
[180283-27-6]
$C_{27}H_{40}O_8$ 492.608
Constit. of *Briareum asbestinum*. Toxic to brine shrimp. Cryst. (Me_2CO/petrol).
Mp 99.5-101°. $[\alpha]_D$ -121.7 (c, 0.23 in $CHCl_3$). Config. of the 7,8-double bond is uncertain. λ_{max} 232 (log ε 3.74); 288 (log ε 3.67) (MeOH).

7β,8α-Epoxide, 2-butanoyl, 14-Ac, Me ester: Briareolate ester D
[180283-24-3]
$C_{27}H_{40}O_9$ 508.608
Constit. of *Briareum asbestinum*. Toxic to brine shrimp. Cryst. (EtOAc/petrol).
Mp 160-163°. $[\alpha]_D$ -120 (c, 0.2 in $CHCl_3$).

7β,8α-Epoxide, 2-butanoyl, 12,14-di-Ac, Me ester: ***Briareolate ester E***
[180283-25-4]
$C_{29}H_{42}O_{10}$ 550.645
Constit. of *Briareum asbestinum*. Amorph. powder. $[\alpha]_D$ -74.7 (c, 0.28 in $CHCl_3$).

7β,8α-Epoxide, 2,12-dibutanoyl, 14-Ac, Me ester: ***Briareolate ester F***
[180283-26-5]
$C_{31}H_{46}O_{10}$ 578.698
Constit. of *Briareum asbestinum*. Amorph. powder. $[\alpha]_D$ -62.1 (c, 0.29 in $CHCl_3$).
Mootoo, B.S. *et al., Tetrahedron*, 1996, **52**, 9953-9962 (*isol, pmr, cmr, cryst struct*)

4,8,14-Trihydroxy-13-oxo-1(15),2,6-cembratrien-16,14-olide T-657

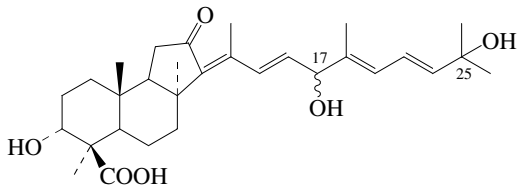


$C_{20}H_{28}O_6$ 364.438

(2*E*,4*R*,6*E*,8*S*,12*R*,14*R*)-*form*

8-Hydroperoxide: 8-Hydroperoxy-4,14-dihydroxy-13-oxo-1(15),2,6-cembratrien-16,14-olide. ***Uprolide L***
[461441-42-9]
$C_{20}H_{28}O_7$ 380.437
Constit. of *Eunicea pinta*. Oil. $[\alpha]_D^{25}$ +42.5 (c, 0.4 in $CHCl_3$). λ_{max} 270 (ε 8600) (MeOH).
Shi, Y.-P. *et al., J. Nat. Prod.*, 2002, **65**, 1232-1241 (*isol, pmr, cmr*)

3,17,25-Trihydroxy-12-oxo-13,15,20(22),23-isomalabaricatetraen-29-oic acid T-658

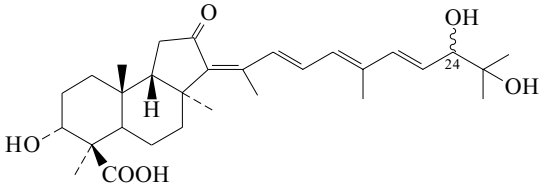


$C_{30}H_{44}O_6$ 500.674

(3α,13*E*,15*E*,20(22)*E*,23*E*)-*form*

17,25-Di-Me ether, 3-Ac: ***Globostellatic acid E***
[282524-62-3]
[282524-61-2]
$C_{34}H_{50}O_7$ 570.765
Constit. of a *Jaspis* sp. Yellow amorph. solid (as Me ester). $[\alpha]_D^{25}$ -23.8 (c, 0.4 in $CHCl_3$) (Me ester). λ_{max} 235 (log ϵ 4.1); 340 (log ϵ 4.8) (MeOH) (Me ester).
Zampella, A. *et al., J. Nat. Prod.*, 2000, **63**, 943-946 (*isol, pmr, cmr*)

3,24,25-Trihydroxy-12-oxo-13,15,17(20),22-isomalabaricatetraen-29-oic acid T-659



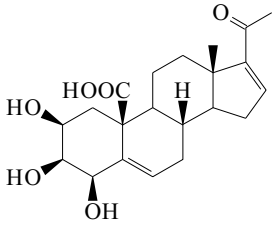
$C_{30}H_{44}O_6$ 500.674

(3α,13*Z*,15*E*,17(20)*E*,22*E*,24ξ)-*form*

24-Me ether: ***Globostellatic acid D***
[175669-13-3]
$C_{31}H_{46}O_6$ 514.701
Constit. of *Stelletta globostellata*. Yellow amorph. solid. $[\alpha]_D^{23}$ +135.7 (c, 1.1 in MeOH). Genus name sometimes incorr. given as Stellata. λ_{max} 257 (ϵ 9800); 368 (ϵ 27000) (MeOH). λ_{max} 257 (ϵ 9800); 368 (ϵ 27000) (MeOH) (Berdy).

24-Me ether, 3-Ac: ***Globostellatic acid C***
[175669-12-2]
$C_{33}H_{48}O_7$ 556.738
Constit. of *Stelletta globostellata*. Yellow amorph. solid. $[\alpha]_D^{23}$ +15.2 (c, 0.82 in MeOH). λ_{max} 257 (ϵ 9200); 368 (ϵ 25000) (MeOH). λ_{max} 257 (ϵ 9200); 368 (ϵ 25000) (MeOH) (Berdy).
Ryu, G. *et al., J. Nat. Prod.*, 1996, **59**, 512 (*isol, pmr, cmr*)

2,3,4-Trihydroxy-20-oxopregna-5,16-dien-19-oic acid T-660

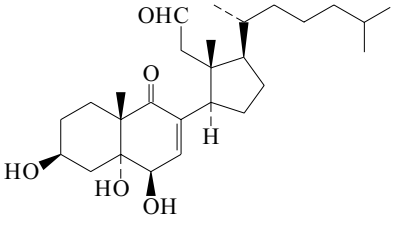


$C_{21}H_{28}O_6$ 376.449

(2β,3β,4β)-*form*

19→2 Lactone: 3,4-Dihydroxy-20-oxopregna-5,16-dien-19,2-olide
[147253-29-0]
$C_{21}H_{26}O_5$ 358.433
Constit. of a *Strongylophora* sponge.
$[\alpha]_D$ -130 (c, 1.5 in $CHCl_3$). λ_{max} 204 (ϵ 10620) (MeOH) (Berdy). λ_{max} 260 (ϵ 2280) (EtOH) (Berdy).
Corgiat, J.M. *et al., Tetrahedron*, 1993, **49**, 1557 (*isol, pmr, cmr*)

3,5,6-Trihydroxy-9-oxo-9,11-secocholest-7-en-11-al T-661



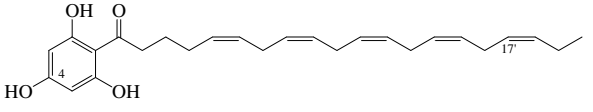
$C_{27}H_{44}O_5$ 448.642

(3β,5α,6β)-*form*

3-Ac: [159728-16-2]
$C_{29}H_{46}O_6$ 490.679
Constit. of *Spongia officinalis*. Cryst. ($CHCl_3$/petrol). Mp 164-165°. $[\alpha]_D$ -52.5 (c, 0.3 in $CHCl_3$).
Adinolfi, R. *et al., J. Nat. Prod.*, 1994, **57**, 1220 (*isol, pmr, cmr, synth*)

1-(2,4,6-Trihydroxyphenyl)-5,8,11,14,17-eicosapentaen-1-one, 9CI T-662

2-(5,8,11,14,17-Eicosapentaenoyl)-1,3,5-benzenetriol. 2-(5,8,11,14,17-Eicosapentaenoyl)phloroglucinol



$C_{26}H_{34}O_4$ 410.552

(all-Z)-form [79553-90-5]
Constit. of the brown algae *Zonariaturneriana*, *Zonaria diesingiana*, *Zonaria farlowii*, *Zonaria tournefortii* and *Distromium decumbens*.
Pale yellow oil. λ_{max} 314 (ϵ) (MeOH/NaOH) (Derep). λ_{max} 287 (ϵ 21100) (MeOH) (Derep).

4-Me ether: 1-(2,6-Dihydroxy-4-methoxyphenyl)-5,8,11,14,17-eicosapentaen-1-one, 9CI
[83147-38-0]
$C_{27}H_{36}O_4$ 424.579
Constit. of *Distromium decumbens*, *Zonaria farlowii* and other *Zonaria* spp. Light yellow oil. Sol. MeOH, HCl; poorly sol. H_2O, hexane. λ_{max} 286 (ϵ 16000) (MeOH).

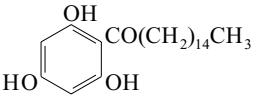
*17′,18′-Dihydro, 17′*R*-hydroxy: 17-Hydroxy-1-(2,4,6-trihydroxyphenyl)-5,8,11,14-eicosatetraen-1-one*
[82461-10-7]
$C_{26}H_{36}O_5$ 428.567
Constit. of *Zonariaturneriana* and *Distromium decumbens*. Pale yellow oil. λ_{max} 314 (ϵ) (MeOH/NaOH) (Derep). λ_{max} 287 (ϵ 21100) (MeOH) (Derep).

*$\Delta^{13'}$-Isomer(*E*-), 15′*S*-hydroxy: 15-Hydroxy-1-(2,4,6-trihydroxyphenyl)-5,8,11,13,17-eicosapentaen-1-one*
[82427-74-5]
$C_{26}H_{34}O_5$ 426.552
Constit. of *Zonaria tournefortii*. Pale yellow oil. $[\alpha]_D$ +8.3 (c, 1 in EtOH). λ_{max} 232 (log ϵ 4.57); 287 (log ϵ 4.25) (EtOH).
Amico, V. *et al., Phytochemistry*, 1981, **20**, 1451-1453; 1982, **21**, 739-741 (*isol, pmr, cmr*)
Gerwick, W. *et al., Phytochemistry*, 1982, **21**, 633-637 (*isol, pmr, cmr*)

Blackman, A.J. *et al., J. Nat. Prod.*, 1988, **51**, 158-160 (*isol*)
Kusumi, T. *et al., Tet. Lett.*, 1994, **35**, 3127-3128 (*dihydro-17-hydroxy*)

1-(2,4,6-Trihydroxyphenyl)-1-hexadecanone, 9CI T-663

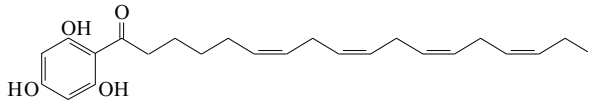
2-Hexadecanoyl-1,3,5-benzenetriol
[82461-11-8]



$C_{22}H_{36}O_4$ 364.524
Constit. of *Virola elongata* and the brown alga *Lobophora papenfussi*.

Gerwick, W. *et al., Phytochemistry*, 1982, **21**, 633 (*isol*)
Kato, M.J. *et al., Phytochemistry*, 1990, **29**, 1799 (*isol*)

1-(2,4,6-Trihydroxyphenyl)-6,9,12,15-octadecatetraen-1-one, 9CI T-664



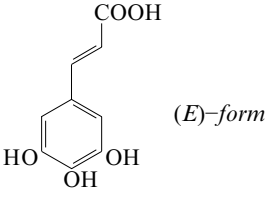
$C_{24}H_{32}O_4$ 384.514

(all-Z)-form [77464-68-7]
Isol. from the brown algae *Cystophora* spp.
Oil.

Kaslauskas, R. *et al., Aust. J. Chem.*, 1981, **34**, 439 (*isol, uv, ir, pmr, cmr, ms*)

3-(3,4,5-Trihydroxyphenyl)-2-propenoic acid T-665

3-(3,4,5-Trihydroxyphenyl)acrylic acid. 3,4,5-Trihydroxycinnamic acid
[6093-59-0]



(*E*)–*form*

$C_9H_8O_5$ 196.159
Does not appear to have been found in nature in the free state despite extensive searches.

(E)-form
Needles + $1H_2O$ (H_2O) becoming anhyd. at 120°. Mp 207-208° dec. CAS no. not found 8-14 Cl.

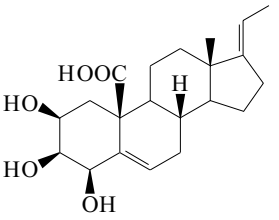
3,5-Di-Me ether, isopropyl ester: Isopropyl sinapate
[389141-49-5]
$C_{14}H_{18}O_5$ 266.293
Constit. of the marine brown alga *Spatoglossum variabile*. Oil. λ_{max} 282 (log ϵ 4.6) ($CHCl_3$).

3,5-Di-Me ether, butyl ester: Butyl sinapate
[475211-36-0]
$C_{15}H_{20}O_5$ 280.32
Isol. from the marine brown alga *Spatoglossum variabile*. Yellow oil. λ_{max} 313 (log ϵ 5.07) ($CHCl_3$).

[54976-67-9]

Hayat, S. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1297-1299 (*Butyl sinapate, Isopropyl sinapate*)

2,3,4-Trihydroxypregna-5,17-dien-19-oic acid T-666

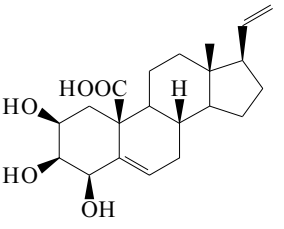


$C_{21}H_{30}O_5$ 362.465

(2β,3β,4β,17(20)E)-form
19→2 Lactone: 3,4-Dihydroxypregna-5,17-dien-19,2-olide
[147253-27-8]
$C_{21}H_{28}O_4$ 344.45
Constit. of a *Strongylophora* sponge. Cryst. $[\alpha]_D$ -82 (c, 1.2 in $CHCl_3$).

Corgiat, J.M. *et al., Tetrahedron*, 1993, **49**, 1557 (*isol, pmr, cmr, cryst struct*)

2,3,4-Trihydroxypregna-5,20-dien-19-oic acid T-667

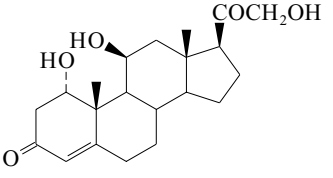


$C_{21}H_{30}O_5$ 362.465

(2β,3β,4β)-form
19→2 Lactone: 3,4-Dihydroxypregna-5,20-dien-19,2-olide
[147253-28-9]
$C_{21}H_{28}O_4$ 344.45
Constit. of a *Strongylophora* sponge.
$[\alpha]_D$ -96 (c, 5 in $CHCl_3$).

Corgiat, J.M. *et al., Tetrahedron*, 1993, **49**, 1557 (*isol, pmr, cmr*)

1,11,21-Trihydroxypregn-4-ene-3,20-dione, 9CI T-668



$C_{21}H_{30}O_5$ 362.465

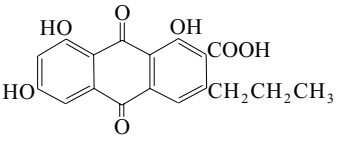
(1α,11β)-form
1α-Hydroxycorticosterone. 1α,11β,21-Trihydroxyprogesterone
[10163-49-2]
Obt. from the perivisceral fluid of the elasmobranch *Raja radiata* (a cartilaginous fish). Cryst. (Me_2CO/hexane). Mp 201-202°. $[\alpha]_D$ +159.5 ($CHCl_3$).

1,21-Di-Ac: [16852-52-1]
$C_{25}H_{34}O_7$ 446.539
Mp 182-183°.

Idler, D.R. *et al., Steroids*, 1967, **9**, 457 (*isol, uv, ir*)
Kime, D.E. *et al., J.C.S. Perkin 1*, 1975, 2371 (*isol, synth, ir, ms*)

1,6,8-Trihydroxy-3-propylanthraquinone-2-carboxylic acid T-669

9,10-Dihydro-1,6,8-trihydroxy-9,10-dioxo-3-propyl-2-anthracenecarboxylic acid, 9CI. ***Ptilometric acid***
[15979-76-7]



$C_{18}H_{14}O_7$ 342.304
Constit. of the crinoids *Ptilometra australis* and *Tropiometra afra*.
Red needles (AcOH).
Mp 298-299°. λ_{max} 228 (ϵ 34500); 277 (ϵ 29240); 313 (ϵ 9700); 444 (ϵ 14860) (EtOH).

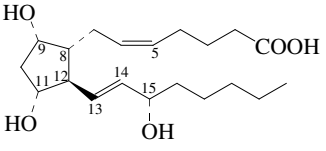
6-O-Sulfate: Ptilometric acid 6-sulfate
[557112-75-1]
$C_{18}H_{14}O_{10}S$ 422.369
Constit. of *Tropiometra afra macrodiscus* and *Oxycomanthus japonicus*. Reddish cryst. λ_{max} 225 (ϵ 11270); 262 (ϵ 11240); 435 (ϵ 4660) (MeOH aq.).

Tri-Ac:
Orange-yellow needles (MeOH). Mp 194-195°.

Tri-Me ether, Me ester: [15939-13-6]
Yellow needles (C_6H_6 or MeOH). Mp 155-156° (after cooling, has Mp 169-170°).

Powell, V.H. *et al., Aust. J. Chem.*, 1967, **20**, 541-553 (*uv, struct*)
Matsuno, T. *et al., Chem. Pharm. Bull.*, 1972, **20**, 1079-1082 (*isol*)
Lam, J.K.K. *et al., J.C.S. Perkin 1*, 1974, 1417-1421 (*synth*)
Banville, J. *et al., J.O.C.*, 1976, **41**, 3018-3020 (*synth, pmr*)
Takahashi, D. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1609-1612 (*6-sulfate, isol, pmr, cmr, ms*)

9,11,15-Trihydroxyprosta-5,13-dienoic acid, 9CI T-670



(5*Z*,8*R*,9*S*,11*R*,12*R*,13*E*,15*S*)-form

$C_{20}H_{34}O_5$ 354.486
Log P 1.38 (calc).

(5*Z*,8*R*,9*S*,11*R*,12*R*,13*E*,15*S*)-*form*

(9α,11α,15α)-(5Z,13E)-form. Prostaglandin $F_{2\alpha}$. $PGF_{2\alpha}$. ***Dinoprost, BAN, INN, JAN.*** *Cyclosin. Many other names*
[551-11-1]
Common naturally occurring mammalian prostaglandin. Also prod. by a variety of marine algae and invertebrates, such as *Phascolosoma japonica*, *Haliotis ovina*, *Crenomytilus grayanus*, *Modiolus difficilis*, *Stichopus japonicus*, *Distolasterias nipon* and *Halocynthia aurantium*. Abortifacient, oxytocic and smooth muscle stimulant. Oil or solid.
Mp 25-35°. $[\alpha]_D^{25}$ +23.5 (c, 1 in THF).
▶ Gastrointestinal effects reported when used therapeutically. Human and exp. teratogen. Human and exp. reprod. effects (low doses). LD_{50} (rat, orl) 1170 mg/kg. UK8020000

9-Ac, Me ester: [55022-57-6]
$C_{23}H_{38}O_6$ 410.55
Constit. of the gorgonian coral *Plexaura homomalla*.

11-Ac: [74728-08-8]
$C_{22}H_{36}O_6$ 396.523
Isol. from the soft coral *Lobophytum depressum*.

11-Ac, Me ester: [74728-06-6]
$C_{23}H_{38}O_6$ 410.55
Isol. from *Lobophytum depressum*. Cryst. (hexane).
Mp 55°.

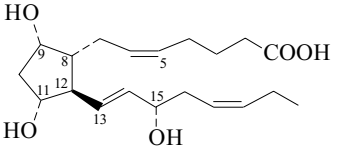
11-Ac, 1,15-lactone: [132541-84-5]
$C_{22}H_{34}O_5$ 378.508
Isol. from the nudibranch *Tethys fimbria*.

[33854-16-9, 53275-58-4]

Carmely, S. *et al., Tet. Lett.*, 1980, **21**, 875-878 (*Lobophytum depressum constits*)
Stehle, R.G. *et al., Methods Enzymol.*, 1982, **86**, 436-458 (*rev*)
Groweiss, A. *et al., J. Nat. Prod.*, 1990, **53**, 222-223 (*Plexaura homomalla constit*)
Cimino, G. *et al., J.O.C.*, 1991, **56**, 2907-2911 (*Tethys fimbria constit*)
Karotchenko, O.D. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1999, **35**, 612-615 (*$F_{2\alpha}$, marine, occur*)

9,11,15-Trihydroxyprosta-5,13,17-trienoic acid, 9CI T-671

7-[3,5-Dihydroxy-2-(3-hydroxy-1,5-octadienyl)cyclopentyl]-5-heptenoic acid, 8CI



$C_{20}H_{32}O_5$ 352.47

(5*Z*,9*S*,11*R*,13*E*,15*S*,17*Z*)-*form*

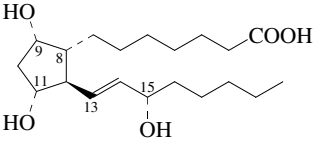
(9α,11α,15α)-(5Z,13E,17Z)-form. Prostaglandin $F_{3\alpha}$. $PGF_{3\alpha}$
[745-64-2]
Biosynth. from eicosapentaenoic acid.
Viscous oil. $[\alpha]_D^{26}$ +29.6 (c, 0.54 in THF).

1,15-Lactone, 11-Ac: [132618-68-9]
$C_{22}H_{32}O_5$ 376.492
Constit. of the nudibranch *Tethys fimbria*.

Corey, E.J. *et al., J.A.C.S.*, 1971, **93**, 1490 (*synth*)
Cimino, G. *et al., J.O.C.*, 1991, **56**, 2907-2911 (*isol, deriv*)
Di Marzo, V. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1992, **101**, 99-104

9,11,15-Trihydroxyprost-13-enoic acid T-672

3,5-Dihydroxy-2-(3-hydroxy-1-octenyl)cyclopentaneheptanoic acid, 8CI



(8*R*,9*S*,11*R*,13*E*,15*S*)-*form*

$C_{20}H_{36}O_5$ 356.501

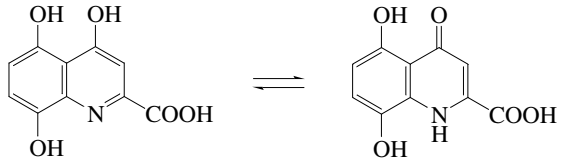
(8*R*,9*S*,11*R*,13*E*,15*S*)-*form*

Prostaglandin $F_{1\alpha}$. $PGF_{1\alpha}$. *Prostaglandin* F_1
[745-62-0]
Constit. of sheep prostate gland. Found in *Oncorhynchus mykiss* (rainbow trout), *Anguilla anguilla* (European eel) and *Teleogryllus commodus* (Australian field cricket). Stimulates rabbit duodenum *in vitro*. Cryst.
Mp 102-103°.
▶ GY4569700

Brown, J.A. *et al., CA*, 1992, **116**, 125324 (*PGF1α, occur*)

4,5,8-Trihydroxy-2-quinolinecarboxylic acid T-673

1,4-Dihydro-5,8-dihydroxy-4-oxo-2-quinolinecarboxylic acid, 9CI
[115525-96-7]

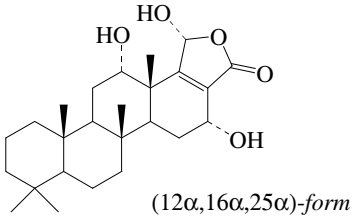


$C_{10}H_7NO_5$ 221.169

Depicted as the quinolone tautomer which prob. predominates in soln. Pigment from the Antarctic sponge *Dendrilla membranosa*. Exhibits antimicrobial activity. Yellow solid. Sol. H_2O. Mp 295-300° dec. λ_{max} 236 (ϵ 16300); 258 (ϵ 13300); 280 (sh) (ϵ 6550); 353 (ϵ 4250) (H_2O at pH 10) (Derep). λ_{max} 232 (ϵ 17100); 250 (ϵ 14600); 270 (sh) (ϵ 6550); 331 (ϵ 3900); 347 (ϵ 3080) (H_2O) (Derep). λ_{max} 232 (ϵ 17100); 250 (ϵ 14600); 331 (ϵ 3900); 347 (ϵ 3080) (H_2O) (Berdy).

Molinski, T.F. *et al., Tet. Lett.*, 1988, **29**, 2137 (*isol, uv, ir, pmr, ms, struct*)

12,16,25-Trihydroxy-17-scalaren-24,25-olide T-674



(12α,16α,25α)-*form*

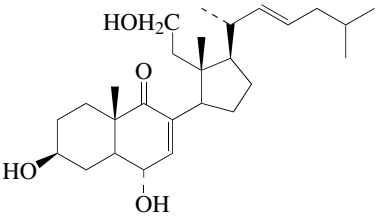
$C_{25}H_{38}O_5$ 418.572

(12α,16α,25α)-*form*
12-Ac: [705279-72-7]
$C_{27}H_{40}O_6$ 460.609
Constit. of *Hyrtios erectus*. Cryst.
Mp 220-222°. $[\alpha]_D^{25}$ +81.46 (c, 0.205 in MeOH).

(12β,16α,25α)-*form*
Hyrtiolide
[302324-59-0]
Constit. of *Hyrtios erectus*.
Amorph. solid. $[\alpha]_D^{25}$ +6 (c, 0.43 in $CHCl_3$). λ_{max} 212 (log ϵ 3.76) (MeOH).
16-Me ether, 12-Ac: [508193-32-6]
$C_{28}H_{42}O_6$ 474.636
Constit. of a *Spongia* sp.
$[\alpha]_D^{24}$ -6.5 (c, 0.12 in $CHCl_3$). λ_{max} 204 (log ϵ 3.4) (MeOH).

(12β,16β,25α)-*form*
Sesterstatin 6
[864532-50-3]
Constit. of *Hyrtios erecta*.
Cryst.
Mp 253-255°. $[\alpha]_D^{24}$ +11.3 (c, 0.08 in $CHCl_3$).
Miyaoka, H. *et al., J. Nat. Prod.*, 2000, **63**, 1369-1372 (*isol, pmr, cmr*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 2003, **66**, 438-440 (*16-Me ether 12-Ac*)
Qiu, Y. *et al., J. Nat. Prod.*, 2004, **67**, 921-924 (*12-Ac*)
Pettit, G.R. *et al., J. Nat. Prod.*, 2005, **68**, 1253-1255 (*Sesterstatin 6*)

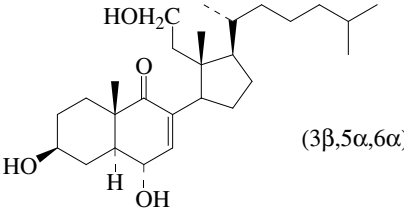
3,6,11-Trihydroxy-9,11-secocholesta-7,22-dien-9-one T-675



$C_{27}H_{44}O_4$ 432.642

(3β,5α,6α,22*E*)-*form*
11-Ac: [201800-58-0]
$C_{29}H_{46}O_5$ 474.679
Constit. of *Gersemia fruticosa*. Oil. λ_{max} 239 (EtOH).
Koljak, R. *et al., Tetrahedron*, 1998, **54**, 179-186 (*isol, pmr, cmr*)

3,6,11-Trihydroxy-9,11-secocholest-7-en-9-one T-676



(3β,5α,6α)-*form*

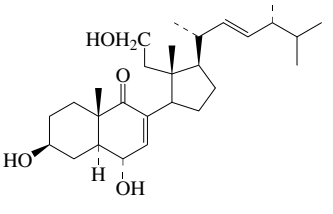
$C_{27}H_{46}O_4$ 434.658

(3β,5α,6α)-*form* [143625-39-2]
Constit. of *Spongia officinalis* and *Subergorgia suberosa*.
Needles ($CHCl_3$/MeOH) or amorph. powder. $[\alpha]_D^{20}$ -7 (c, 0.24 in $CHCl_3$). λ_{max} 240 (ϵ 3460) (MeOH).

(3β,5α,6β)-*form*
Aplidiasterol A
[646487-23-2]
Constit. of *Aplidium conicum*.
$[\alpha]_D$ -15.2 (c, 0.002 in MeOH).
Migliuolo, A. *et al., Steroids*, 1992, **57**, 344-347 (*isol, pmr, cmr*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 418-423 (*isol, pmr, cmr*)
Aknin, M. *et al., Steroids*, 1998, **63**, 575-578 (*isol, pmr, cmr*)
Aiello, A. *et al., Steroids*, 2003, **68**, 719-723 (*Aplidiasterol A*)

3,6,11-Trihydroxy-9,11-secoergosta-7,22-dien-9-one T-677

3,6,11-Trihydroxy-24-methyl-9,11-secocholesta-7,22-dien-9-one



(3β,5α,6α,22*E*,24*R*)-*form*

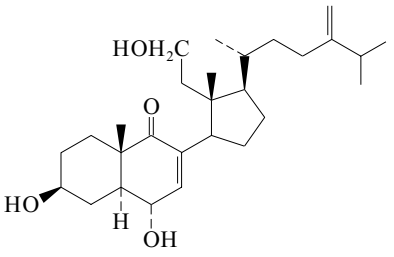
$C_{28}H_{46}O_4$ 446.669

(3β,5α,6α,22*E*,24*R*)-*form* [219517-49-4]
Constit. of *Subergorgia suberosa*.

(3β,5α,6α,22*E*,24*S*)-*form* [219517-48-3]
Constit. of *Subergorgia suberosa*.
Aknin, M. *et al., Steroids*, 1998, **63**, 575-578 (*isol, pmr, cmr*)

3,6,11-Trihydroxy-9,11-secoergosta-7,24(28)-dien-9-one T-678

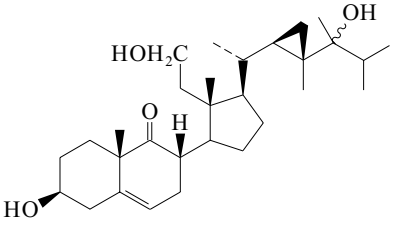
3,6,11-Trihydroxy-24-methylene-9,11-secocholest-7-en-9-one



$C_{28}H_{46}O_4$ 446.669

(3β,5α,6α)-*form* [143625-40-5]
Constit. of *Spongia officinalis* and *Sinularia hirta*.
Amorph. powder.
Mp 162-164°. $[\alpha]_D^{20}$ +9 (c, 0.24 in $CHCl_3$). $[\alpha]_D^{30}$ +28 (c, 0.5 in Py).
λ_{max} 240 (ϵ 3659) (MeOH).
Migliuolo, A. *et al., Steroids*, 1992, **57**, 344-347 (*isol, pmr, cmr, ms*)
Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 144-147 (*isol*)

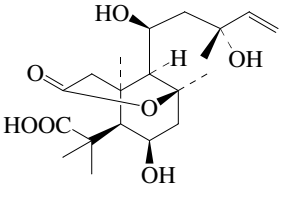
3,11,24-Trihydroxy-9,11-secogorgost-5-en-9-one T-679



$C_{30}H_{50}O_4$ 474.723

(3β,24ξ)-*form* [161441-78-7]
Constit. of a *Pseudopterogorgia* sp.
Powder. $[\alpha]_D$ +1.5 (c, 1.2 in MeOH).
He, H. *et al., Tetrahedron*, 1995, **51**, 51 (*isol, pmr, cmr*)

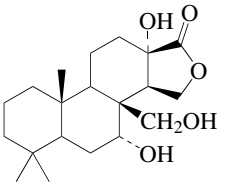
6,11,13-Trihydroxy-2,3-seco-14-labden-2,8-olid-3-oic acid T-680



$C_{20}H_{32}O_7$ 384.469

(*ent*-5β*H*,8α,9β*H*,11*R*,13*S*)-*form*
Rhizophorin A
[350986-07-1]
Constit. of *Rhizophora macronata*.
Cryst. ($CHCl_3$/MeOH).
Mp 242-243°. $[\alpha]_D^{25}$ +128 (c, 0.2 in $CHCl_3$).
Anjaneyulu, A.S.R. *et al., Nat. Prod. Lett.*, 2001, **15**, 13-19 (*isol, pmr, cmr*)

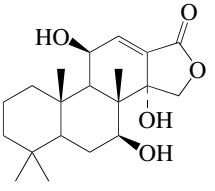
7,13,17-Trihydroxy-16-spongianone T-681



$C_{20}H_{32}O_5$ 352.47

(7α,13α)-*form*
7,17-Di-Ac: ***Aplyroseol 16***
[200437-68-9]
$C_{24}H_{36}O_7$ 436.544
Constit. of *Aplysilla rosea*. Gum.
Taylor, W.C. *et al., Aust. J. Chem.*, 1997, **50**, 895-902 (*isol, pmr, cmr*)

7,11,14-Trihydroxy-12-spongien-16-one T-682

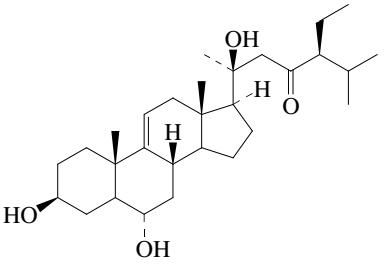


$C_{20}H_{30}O_5$ 350.454

(7β,11β,14α)-*form*
7,11-Di-Ac: ***Dorisenone A***
[178179-98-1]
$C_{24}H_{34}O_7$ 434.528
Constit. of *Chromodoris obsoleta*. Needles (MeOH).
Mp 255-257°. $[\alpha]_D^{28}$ +188.2 (c, 1.4 in $CHCl_3$). λ_{max} 218 (ϵ 8000) (EtOH). λ_{max} 218 (ϵ 8000) (MeOH) (Berdy).
Miyamoto, T. *et al., Tetrahedron*, 1996, **52**, 8187-8198 (*isol, pmr, cmr*)

3,6,20-Trihydroxystigmast-9(11)-en-23-one T-683

24-Ethyl-3,6,20-trihydroxycholest-9(11)-en-23-one



$C_{29}H_{48}O_4$ 460.696

(3β,5α,6α,20*S*,24*S*)-*form* [106521-62-4]
Sapogenin from *Asterina pectinifera*.
Amorph. powder.
Mp 185-188°. $[\alpha]_D$ +27.8 (c, 0.4 in $CHCl_3$).
6-O-[β-D-Fucopyranosyl-(1→3)-β-D-fucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-[β-D-quinovopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-β-D-quinovopyranoside], 3-sulfate: ***Pectinioside C***
[113322-00-2]
$C_{64}H_{106}O_{32}S$ 1419.588
Constit. of *Asterina pectinifera*. Amorph. powder. Sol. MeOH, H_2O.
Mp 230-235° (dec.). $[\alpha]_D$ +5.38 (c, 0.275 in MeOH).
Noguchi, Y. *et al., Annalen*, 1987, 341-348 (*isol, pmr, cmr*)

Dubois, M.-A. *et al., Annalen*, 1988, 495-500 (*Pectinioside C*)
Honda, M. *et al., Annalen*, 1990, 547-553 (*stereochem*)

3,28,33-Trihydroxy-4-tritriacontene-1,29,31-triyn-16-one T-684

$HC{\equiv}CCH(OH)CH{=}CH(CH_2)_{10}CO(CH_2)_{11}CH(OH)C{\equiv}CC{\equiv}CCH_2OH$

$C_{33}H_{52}O_4$ 512.771

Position of oxo-group not certain.

(-)-(*E*)-*form*

Pellynone

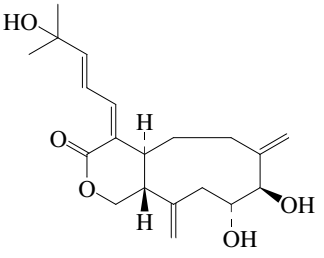
[186248-13-5]

Isol. from the sponge *Pellina triangulata*.

$[\alpha]_D$ -9 (c, 0.4 in $CHCl_3$).

Fu, X. *et al., Tetrahedron*, 1997, **53**, 799 (*isol, ir, pmr, cmr*)

7,8,14-Trihydroxy-1(19),6(20),10,12-xenicatetraen-17,18-olide T-685



$C_{20}H_{28}O_5$ 348.438

(7β,8α,10*Z*)-*form*

7-Hydroxyxeniolide F. *9-Hydroxyxeniolide F*

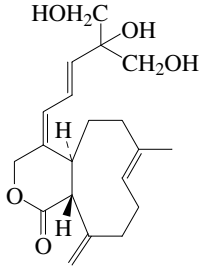
[437710-62-8]

Constit. of a *Xenia* soft coral.

Amorph. solid. $[\alpha]_D^{25}$ +38.3 (c, 0.05 in CH_2Cl_2). λ_{max} 223 (log ϵ 3.55); 271 (log ϵ 3.49) (MeOH).

Anta, C. *et al., J. Nat. Prod.*, 2002, **65**, 766-768 (*isol, pmr, cmr*)

14,15,16-Trihydroxy-1(19),6,10,12-xenicatetraen-18,17-olide T-686



$C_{20}H_{28}O_5$ 348.438

(6*E*,10*E*,12*E*)-*form*

Xeniatriol

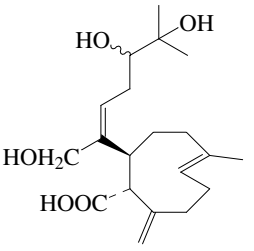
[251343-63-2]

Constit. of a *Xenia* sp.

Oil. $[\alpha]_D^{28}$ -14 (c, 0.8 in $CHCl_3$). λ_{max} 244 (ϵ 9600) (EtOH).

Miyaoka, H. *et al., Tetrahedron*, 1999, **55**, 12977-12982 (*isol, pmr, cmr*)

13,14,17-Trihydroxy-1(19),6,10-xenicatrien-18-oic acid T-687



$C_{20}H_{32}O_5$ 352.47

(6*E*,10*E*,13ξ)-*form*

17-Ac, Me ester: ***Umbellacin F***

[871483-38-4]

$C_{23}H_{36}O_6$ 408.534

Constit. of *Xenia umbellata*. Amorph. solid. $[\alpha]_D^{25}$ -30 (c, 0.1 in $CHCl_3$).

6,7-Epoxide: 6,7-Epoxy-13,14,17-trihydroxy-1(19),10-xenicadien-18-oic acid

$C_{20}H_{32}O_6$ 368.469

6α,7α-Epoxide, 17-Ac, Me ester: ***Umbellacin H***

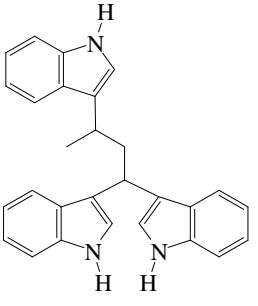
[871483-42-0]

$C_{23}H_{36}O_7$ 424.533

Constit. of *Xenia umbellata*. Amorph. solid. $[\alpha]_D^{25}$ +46 (c, 0.1 in $CHCl_3$).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2006, **69**, 338-341

1,1,3-(Tri-1*H*-indol-3-yl)butane T-688



$C_{28}H_{25}N_3$ 403.526

(ξ)-*form* [639079-45-1]

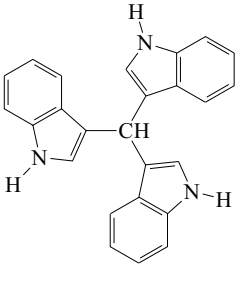
Isol. from the marine bacterium *Vibrio parahaemolyticus* Bio249. Yellowish solid. λ_{max} 276 (sh) (log ϵ 4); 282 (log ϵ 4.03); 290 (log ϵ 3.99) (MeOH).

Veluri, R. *et al., J. Nat. Prod.*, 2003, **66**, 1520-1523 (*isol, pmr, cmr, ms*)

Tri-1*H*-indol-3-ylmethane T-689

*3,3′,3″-Methylidynetris-1*H*-indole, 9CI*

[518-06-9]



$C_{25}H_{19}N_3$ 361.445

Isol. from the marine bacterium *Vibrio parahaemolyticus* Bio249. Cryst. (MeOH).
Mp 244-246°. λ_{max} 248 (sh) (log ϵ 3.56); 283 (log ϵ 3.32); 388 (log ϵ 3.65) (MeOH).

*N,N′,N″-Tri-Me: Tris(1-methyl-3-indolyl)methane. 3,3′,3″-Methylidynetris[1-methyl-1*H*-indole]*
[27065-95-8]
$C_{28}H_{25}N_3$ 403.526
Cryst. (Py). Mp 268-270°.

Harley-Mason, J. *et al., Biochem. J.*, 1952, **51**, 430 (*synth*)
Bergman, J. *et al., J. Het. Chem.*, 1971, **8**, 329; 1985, **22**, 341 (*synth, deriv*)
Akgün, E. *et al., J. Het. Chem.*, 1983, **20**, 1303 (*synth, ir, pmr*)
Koshima, H. *et al., J. Het. Chem.*, 2002, **39**, 1089-1091 (*synth, ir, pmr*)
Veluri, R. *et al., J. Nat. Prod.*, 2003, **66**, 1520-1523 (*isol, pmr, cmr*)

Triiodoacetaldehyde T-690

Iodal
[5703-34-4]
I_3CCHO
C_2HI_3O 421.743

Poorly characterised, both as a nat. prod. and synthetically. Claimed isol. from seaweed.

Masuda, E. *et al., J. Phys. Soc. Jpn.*, 1935, **55**, 625
Brown, M.G. *et al., J.C.S.*, 1956, 2283

Triiodomethane, 9CI, 8CI T-691

Iodoform
[75-47-8]
CHI_3
CHI_3 393.732

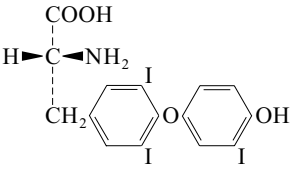
Produced by *Asparagopsis taxiformis*. Disinfectant. Commercially available. Powerful antiseptic. Yellow hexagonal plates (Me_2CO), with characteristic disagreeable odour. Sol. org. solvs., pract. insol. H_2O. d_4^{20} 4.1.
Mp 119-120°. Log P 3.54 (calc). Dec. slowly in light, steam-volatile.

▶ Eye, skin and respiratory tract irritant. LD_{50} (rat, orl) 355 mg/kg. OES: long-term 0.6 ppm; short-term 1 ppm. PB7000000

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 82C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 84A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 117C (*ir*)
Sadtler Standard C-13 NMR Spectra, 8410 (*cmr*)
Datta, R.L. *et al., J.A.C.S.*, 1917, **39**, 441 (*synth*)
Seelye, R.N. *et al., J. Chem. Educ.*, 1959, **36**, 572 (*rev*)
Weiner, P.H. *et al., J. Phys. Chem.*, 1971, **75**, 3971 (*pmr*)
Neto, N. *et al., J. Phys. Chem.*, 1973, **58**, 5661 (*ir*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 266 (*use*)
Iwata, Y. *et al., CA*, 1976, **85**, 54917 (*cryst struct*)
Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*isol, ms, pmr*)
Anders, M.W. *et al., Drug Metab. Dispos.*, 1978, **6**, 556 (*metab*)
Anderson, A. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1985, **82**, 99 (*props, Raman*)
Tate, R. *et al., Z. Naturforsch., A*, 1986, **41**, 1091 (*uv*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 972
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2825-2827 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 734
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IEP000

3,3′,5-Triiodothyronine T-692

O-*(4-Hydroxy-3-iodophenyl)-3,5-diiodotyrosine, 9CI. 3-[4-(4-Hydroxy-3-iodophenoxy)-3,5-diiodophenyl]alanine. 3′-Deiodothyroxine. Triothyrone. Many other names*
[327-86-6]



(*R*)–*form*

$C_{15}H_{12}I_3NO_4$ 650.978
Log P 2.87 (uncertain value) (calc).
^{125}I and ^{131}I labelled compds. are used as radioactive agents; Triomet-125 and Tri-Thyrotope.

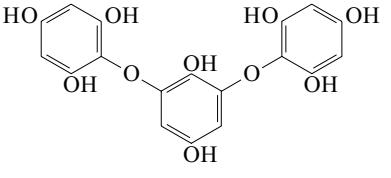
(*S*)-*form*
L-*form*. ***Liothyronine, BAN, INN, USAN***. *T_3. Many other names*
[6893-02-3]
Occurs in marine organisms such as *Heterochordaria abeitina*, *Undaria pinnatifida*, *Sargassum thunbergii*, *Polysiphonia urceolata*. Thyroid hormone.
Mp 236-237° dec. $[\alpha]_D^{30}$ +21.5 (c, 4.75 in EtOH/1*M* HCl).
▶ Exp. reprod. and teratogenic effects. AY6750000

[20196-64-9, 24359-14-6]

Ito, K. *et al., CA*, 1977, **86**, 3897 (*occur*)

Triisofuhalol T-693

2,2′-[(2,5-Dihydroxy-1,3-phenylene)bis(oxy)]bis[1,3,5-benzenetriol], 9CI
[94513-70-9]

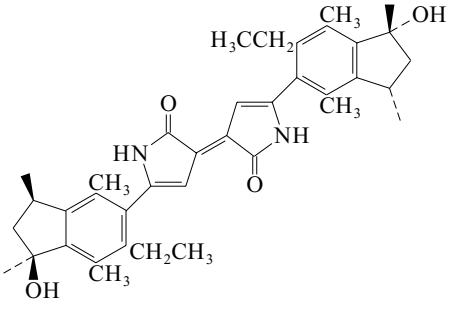


$C_{18}H_{14}O_{10}$ 390.303
Constit. of the alga *Chorda filum*. Isol. as octa-Ac.

Grosse-Damhues, J. *et al., Phytochemistry*, 1984, **23**, 2639 (*isol*)

Trikendiol T-694

[158734-27-1]



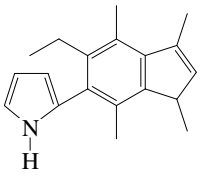
$C_{38}H_{46}N_2O_4$ 594.792
Red pigment from the sponge *Trikentrion loeve*. Cryst. (Me_2CO). Mp 160-162°. $[\alpha]_D$ +102 (c, 0.02 in $CHCl_3$). λ_{max} 210 (ϵ 37400); 265 (ϵ 8050); 337 (sh); 510 (ϵ 8360) (MeOH assumed, not reported) (Derep).

Loukaci, A. *et al., Tet. Lett.*, 1994, **35**, 6869 (*isol, uv, pmr, cmr, struct*)

Trikentramine T-695

*2-(5-Ethyl-1,3,4,7-tetramethyl-1*H*-inden-6-yl)-1*H*-pyrrole, 9CI*

[129536-24-9]



$C_{19}H_{23}N$ 265.397

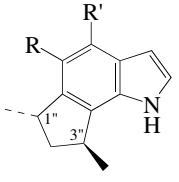
Alkaloid from the Senegalese sponge *Trikentrion loeve*. Cryst. (hexane).

Mp 145°. $[\alpha]_D^{27}$ +175 (c, 0.81 in $CHCl_3$). λ_{max} 209 (ϵ 21300); 222 (ϵ 39700); 271 (ϵ 10700) (no solvent reported).

Aknin, M. *et al., Tet. Lett.*, 1990, **31**, 2979 (*isol, uv, pmr, cmr, cryst struct*)

Trikentrin A T-696

4-Ethyl-1,6,7,8-tetrahydro-6,8-dimethylcyclopent[g]indole, 9CI



(1"*R*,3"*S*)-*form*

R = H, R' = CH_2CH_3

$C_{15}H_{19}N$ 213.322

(1″*R*,3″*S*)-*form*

(+)-cis-*form*

[107368-92-3]

Isol. from *Trikentrion flabelliforme*. Possesses antimicrobial activity. Unstable oil which darkens on storage. Sol. MeOH, $CHCl_3$. $[\alpha]_D$ +48 (c, 2.47 in $CHCl_3$). λ_{max} 241 (ϵ 11350); 271 (ϵ 11200) (MeOH) (Berdy).

(1″*S*,3″*S*)-*form*

(+)-trans-*form*

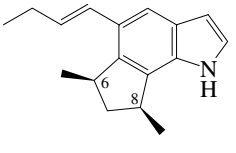
[107438-53-9]

Isol. from the marine sponge *Trikentrion flabelliforme*. Possesses antimicrobial activity. Stable oil which cryst. on standing. Sol. MeOH, $CHCl_3$. $[\alpha]_D$ +23.3 (c, 1.0 in $CHCl_3$). λ_{max} 222 (ϵ 68400); 271 (ϵ 12600) (MeOH) (Berdy).

Capon, R.J. *et al., Tetrahedron*, 1986, **42**, 6545 (*isol, uv, ir, pmr, cmr, ms, struct*)
Macleod, J.K. *et al., Tet. Lett.*, 1988, **29**, 391 (*synth, pmr, cis-Trikentrin A*)
Muratake, H. *et al., Chem. Pharm. Bull.*, 1994, **42**, 854 (*abs config, bibl*)
Huntley, R.J. *et al., Org. Lett.*, 2006, **8**, 3403-3406 (*synth*)

Trikentrin B T-697

5-(1-Butenyl)-1,6,7,8-tetrahydro-6,8-dimethylcyclopent[g]indole, 9CI



(6*R*,8*S*)-*form*

$C_{17}H_{21}N$ 239.36

CAS numbering shown. Isol. as an inseparable mixt. of *cis*- and *trans*-Trikentrin B's. Shows antimicrobial activity. Unstable oil which darkens on storage. $[\alpha]_D$ -13 (c, 1.97 in $CHCl_3$). λ_{max} 249 (ϵ 24200); 275 (ϵ 8800) (MeOH) (Derep).

(6*R*,8*S*)-*form*

cis-*form*

[107438-54-0]

Isol. from the marine sponge *Trikentrion flabelliforme*.

(6*S*,8*S*)-*form*

trans-*form*

[107368-93-4]

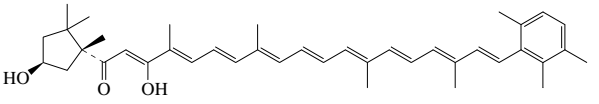
Isol. from *Trikentrion flabelliforme*.

Capon, R.J. *et al., Tetrahedron*, 1986, **42**, 6545 (*isol, uv, ir, pmr, cmr, ms, struct*)
Muratake, H. *et al., Chem. Pharm. Bull.*, 1994, **42**, 854 (*abs config, bibl*)
MacLeod, J.K. *et al., Aust. J. Chem.*, 1998, **51**, 177-187 (*synth, pmr, cmr*)
Jackson, S.K. *et al., Org. Lett.*, 2005, **7**, 1215-1218 (*synth*)
Huntley, R.J. *et al., Org. Lett.*, 2006, **8**, 3403-3406 (*synth*)

Trikentriophidin T-698

3,8-Dihydroxy-κ,ϕ-caroten-6-one, 9CI

[76332-64-4]



$C_{40}H_{52}O_3$ 580.849

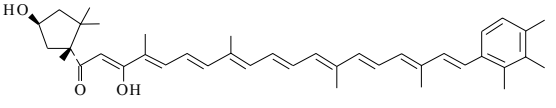
Constit. of *Microciona prolifera*.

Litchfield, C. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **66**, 359-365 (*isol, pmr, ms*)

Trikentriorhodin T-699

3,8-Dihydroxy-κ,χ-caroten-6-one

[55906-76-8]



$C_{40}H_{52}O_3$ 580.849

Constit. of *Trikentrion helium* and *Tedania digitata*.

Aguilar-Martinez, M. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 1247 (*isol, ir, uv, ms*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1977, **60**, 2780 (*isol, uv, pmr, ms*)
Chopra, A.K. *et al., J.C.S. Perkin 1*, 1988, 1371 (*synth*)

Trimethylamine oxide, 8CI T-700

N,N-*Dimethylmethanamine* N-*oxide, 9CI. Trimethyloxamine. Triox*

[1184-78-7]

$Me_3N^{\oplus}–O^{\ominus}$

C_3H_9NO 75.11

Widely distrib. in animal tissues, esp. fish. Oxidising agent used in synthesis. Cleaves Si–C bonds. Large cryst. (DMF). Sol. H_2O, MeOH.

Mp 224-226° dec. Hygroscopic.

▶ Potentially explosive.

Dihydrate: [62637-93-8]

Cryst. (H_2O). Mp 96°.

▶ YH2850000

Hydrochloride: [7651-88-9]

Needles (EtOH). Sol. H_2O, hot MeOH. Mp 218°.

Hydroiodide: [81752-56-9]

Prisms (EtOH). Sol. H_2O, EtOH. Mp 130° dec.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 299B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 480B (*nmr*)
Dunstan, W.R. *et al., J.C.S.*, 1899, **75**, 792 (*synth*)
Caron, A. *et al., Acta Cryst.*, 1964, **17**, 102 (*cryst struct*)
Craig, J.C. *et al., J.O.C.*, 1970, **35**, 1721 (*synth, props*)
Bravo, R. *et al., Org. Magn. Reson.*, 1973, **5**, 357 (*pmr*)
Olah, G.A. *et al., J.O.C.*, 1978, **43**, 2268 (*cmr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 507; 1981, **9**, 31; 489; 1982, **10**, 423; 1986, **12**, 533; 1988, **13**, 325 (*use*)

Harmon, K.M. *et al., J. Mol. Struct.*, 1982, **78**, 43 (*ir*)
Beugelmans, R. *et al., Can. J. Chem.*, 1985, **63**, 725 (*use*)
Chastanet, J. *et al., J.O.C.*, 1985, **50**, 2910 (*use*)
Sakurai, H. *et al., Tet. Lett.*, 1986, **27**, 75 (*use*)
Soderquist, J.A. *et al., Tet. Lett.*, 1986, **27**, 3961 (*synth*)
Mak, T.C.W. *et al., J. Mol. Struct.*, 1988, **178**, 169 (*dihydrate, cryst struct*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **7**, 5197-5201 (*use*)
Knoelker, H.-J. *et al., J. Prakt. Chem.*, 1996, **338**, 190 (*use*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1236
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1281
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TLE100; TLE250

(2-Trimethylammonioethyl)phosphonic acid betaine T-701

N,N,N-*Trimethyl-2-phosphonoethanaminium hydroxide, inner salt, 9CI. Phosphonyldeoxycholine*

[14596-57-7]

$Me_3N^{\oplus}CH_2CH_2PO_3H^{\ominus}$

$C_5H_{14}NO_3P$ 167.144

Constit. of the sea anemone *Anthopleura xanthogrammica*.

Needles (EtOH).

Mp 252° dec. Hygroscopic.

Myers, T.C. *et al., J.O.C.*, 1957, **22**, 180 (*synth*)
Rosenthal, A.F. *et al., J.A.C.S.*, 1958, **80**, 5240 (*synth*)
Kittredge, J.S. *et al., Biochemistry*, 1967, **6**, 289 (*isol, synth, ir, pmr*)
Kittredge, J.S. *et al., Comp. Biochem. Physiol.*, 1969, **29**, 859 (*biosynth*)
Richard, H. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1974, **278**, 1275 (*pmr, conformn*)

Trimethylarsine, 9CI T-702

Arsenic trimethyl. Gosio gas

[593-88-4]

$AsMe_3$

C_3H_9As 120.026

Metab. prod. from microbial action on many arsenicals. Found in v. low levels in some species of deep-sea crustaceans. Ligand for most heavy metals. Liq. with unpleasant penetrating odour.

Mp 55°. Bp 70°. Complexes readily with BH_3 and B trihalides; also with As, and Sb halides, (inorganic and organic). Absorbs O_2 from air → Trimethylarsine oxide.

▶ Highly toxic. Spontaneously flammable in air. CH8800000

Oxide: See Trimethylarsine oxide in *The Combined Chemical Dictionary.*

Sulfide: See Trimethylarsine sulfide in *The Combined Chemical Dictionary.*

Selenide: See Trimethylarsine selenide in *The Combined Chemical Dictionary.*

Fluorine complex (1:1): See Difluorotrimethylarsorane in *The Combined Chemical Dictionary.*

Chlorine complex (1:1): See Dichlorotrimethylarsorane in *The Combined Chemical Dictionary.*

Bromine complex (1:1): See Dibromotrimethylarsorane in *The Combined Chemical Dictionary.*

BBr_3 complex (1:1): [52827-82-4]
$C_3H_9AsBBr_3$ 370.549
Solid. Mp 245°.

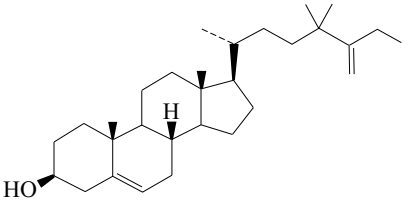
BI_3 complex (1:1): [55042-21-2]
$C_3H_9AsBI_3$ 511.55
Solid. Mp 274-275°. Slowly dec. in $CHCl_3$ → $Me_3AsI^{\oplus}I^{\ominus}$.

AsI_3 complex (1:1): [26459-38-1]
$C_3H_9As_2I_3$ 575.661
Solid. Mp 140-144° dec.

Summers, J.C. *et al., Inorg. Chem.*, 1970, **9**, 862 (*complexes*)
Svergun, V.I. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1970, 482; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1970, 442 (*nqr*)
Kostyanovskii, R.G. *et al., Org. Mass Spectrom.*, 1972, **6**, 1183 (*ms*)
Fournier, L. *et al., Synth. React. Inorg. Met.-Org. Chem.*, 1972, **2**, 53 (*synth*)
Dewar, M.I.S. *et al., J.C.S. Dalton*, 1973, 2381 (*As-75 nmr*)
Durig, J.R. *et al., Inorg. Chem.*, 1974, **13**, 2306 (*ir, Raman, microwave, BH_3 complex*)
Durand, M. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1974, **71**, 847 (*pmr*)
Denniston, M.L. *et al., J. Inorg. Nucl. Chem.*, 1974, **36**, 2175 (*B complexes, pmr, B-11 nmr*)
Elbel, S. *et al., J.C.S. Faraday 2*, 1974, **70**, 555 (*pe*)
Baliman, G. *et al., Helv. Chim. Acta*, 1975, **58**, 1913 (*cmr*)
Mente, D.C. *et al., Inorg. Chem.*, 1975, **14**, 1862 (*B complexes, ir, Raman, ms*)
Efremov, E.A. *et al., Zh. Fiz. Khim.*, 1975, **49**, 1844; *CA*, **83**, 183571
Rojhantalab, H. *et al., Spectrochim. Acta A*, 1976, **32**, 947 (*ir, Raman*)
Beagley, B. *et al., J. Mol. Struct.*, 1977, **38**, 229 (*struct*)
Durand, M. *et al., J.C.S. Dalton*, 1977, **37**, 57 (*B complexes, pmr, B-11 nmr*)
Apel, J. *et al., Z. Anorg. Allg. Chem.*, 1979, **453**, 28 (*nmr*)
Gushikem, Y. *et al., J.C.S. Dalton*, 1980, 2016 (*B complexes, ir, Raman*)
McKean, D.C. *et al., Spectrochim. Acta A*, 1982, **38**, 113 (*ir*)
Blom, R. *et al., Acta Chem. Scand., Ser. A*, 1983, **37**, 595 (*ed, struct*)
Gleiter, R. *et al., Chem. Ber.*, 1983, **116**, 3745 (*pe*)
Whitfield, F.B. *et al., Chem. Ind. (London)*, 1983, 786 (*isol*)
Edmonds, J.S. *et al., J.C.S. Perkin 1*, 1983, 2375 (*pmr, cmr*)
Chadha, R.K. *et al., J. Crystallogr. Spectrosc. Res.*, 1985, **15**, 53 (*B complexes, cryst struct*)
Chehaybar, J.M. *et al., Inorg. Chim. Acta*, 1986, **112**, 209 (*B complexes, pmr, B-11 nmr*)
Fischer, M. *et al., Chemtronics*, 1988, **3**, 156 (*uv*)
Organomet. Synth., 1988, **4**, 582 (*synth*)
Ismail, K. *et al., Pertanika J. Trop. Agric. Sci.*, 1988, **11**, 437 (*synth*)
Watkins, C.L. *et al., Magn. Reson. Chem.*, 1989, **27**, 616 (*pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TLH150
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 396

24,24,27-Trimethylcholesta-5,25-dien-3-ol T-703

25-Ethyl-24-methyl-27-norergosta-5,25-dien-3-ol, 9CI



$C_{30}H_{50}O$ 426.724

3β-*form*

Durissimasterol

[81306-61-8]

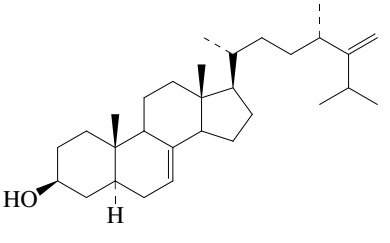
Constit. of the sponge *Strongylophora durissima*.

Cryst. Mp 142-143°. $[\alpha]_D^{20}$ -36 (c, 0.006 in $CHCl_3$).

Li, L.N. *et al., Tet. Lett.*, 1981, **22**, 4639

24,26,26-Trimethylcholesta-7,25(27)-dien-3-ol T-704

25-(1-Methylethyl)-27-norergosta-7,25-dien-3-ol, 9CI



Absolute Configuration

$C_{30}H_{50}O$ 426.724

(3β,5α,24*S*)-*form*

Pulchrasterol

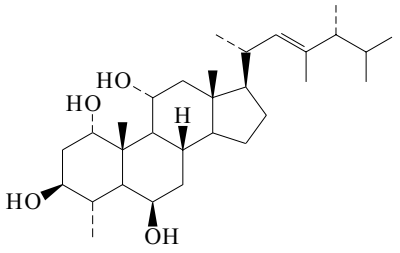
[87307-28-6]

Constit. of *Aciculites pulchra*. Cryst. (MeOH). Mp 130-131°.

$[\alpha]_D^{20}$ +7 (c, 0.2 in $CHCl_3$).

Crist, B.V. *et al., J.O.C.*, 1983, **48**, 4472-4479 (*isol, synth, abs config*)

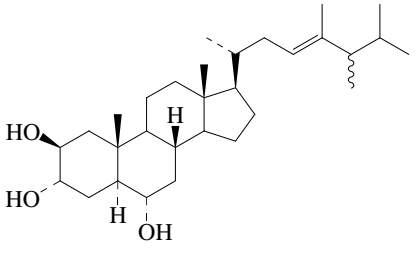
4,23,24-Trimethylcholest-22-ene-1,3,6,11-tetrol T-705
4,23-Dimethylergost-22-ene-1,3,6,11-tetrol



$C_{30}H_{52}O_4$ 476.738

(1α,3β,5α,6β,11α,24*R*)-*form*
Acerosterol
[145940-74-5]
Constit. of *Pseudopterogorgia acerosa*.
Needles.
Mp 118-120°. $[\alpha]_D$ -3.3 (c, 0.04 in MeOH).
John, L.M.D. *et al., J. Nat. Prod.*, 1993, **56**, 144 (*isol, pmr, cmr*)

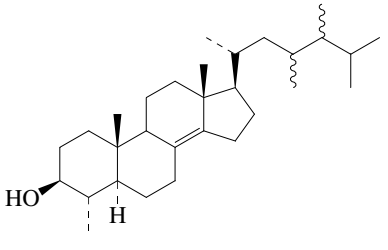
24,26,26-Trimethylcholest-23-ene-2,3,6-triol T-706
25-(1-Methylethyl)-27-norergost-23-ene-2,3,6-triol, 9CI. 26,26-Dimethylergost-23-ene-2,3,6-triol



$C_{30}H_{52}O_3$ 460.739

(2β,3α,5α,6α,23*E*,25ξ)-*form*
26-Norsokotrasterol
Tri-O-*sulfate:* [117675-14-6]
$C_{30}H_{52}O_{12}S_3$ 700.932
Constit. of *Trachyopsis halichondroides*.
Makarieva, T.N. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1988, **24**, 312-315 (*isol*)

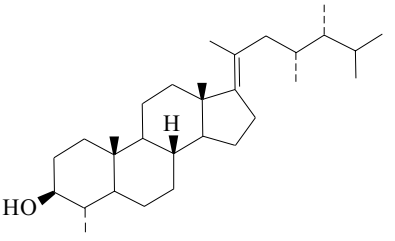
4,23,24-Trimethylcholest-8(14)-en-3-ol T-707
4,23-Dimethylergost-8(14)-en-3-ol



$C_{30}H_{52}O$ 428.74
Tentative identification. May be the 4-methylstigmastane isomer.

(3β,4α,5α,23ξ,24ξ)-*form* [106395-84-0]
[116260-56-1]
Identified in lipids of the dinoflagellate *Prorocentrum balticum*.
Volkman, J.K. *et al., Phytochemistry*, 1999, **52**, 659-668

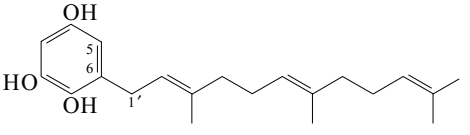
4,23,24-Trimethylcholest-17(20)-en-3-ol T-708
4,23-Dimethylergost-17(20)-en-3-ol, 9CI



$C_{30}H_{52}O$ 428.74

(3β,4α,17*E*,23*R*,24*R*)-*form*
Peridinosterol
[77617-71-1]
Constit. of *Peridinium foliaceum* and *Peridinium balticum*.
Component of lipids of *Prorocentrum* spp. dinoflagellates.
Cryst. Mp 196-200°. $[\alpha]_D$ +3 ($CHCl_3$). A steroid detected in *Prorocentrum cordatum* was identified as the $\Delta^{24(28)}$-isomer. This was probably Peridinosterol.
Swanson, W. *et al., Tet. Lett.*, 1980, **21**, 4663-4666 (*isol, cryst struct*)
Ginèr, J.-L. *et al., J.O.C.*, 1991, **56**, 2357 (*biosynth*)
Volkman, J.K. *et al., Phytochemistry*, 1999, **52**, 659-668 (*occur, dinoflagellates*)

6-(3,7,11-Trimethyl-2,6,10-dodecatrienyl)-1,2,4-benzenetriol T-709
6-Farnesyl-1,2,4-trihydroxybenzene



$C_{21}H_{30}O_3$ 330.466
Constit. of *Phacelia campanularia* and *Phacelia pedicellata*. Yellow oil.

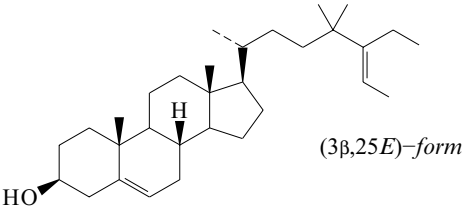
4-Ac: [144599-01-9]
$C_{23}H_{32}O_4$ 372.503
Constit. of *Chroogomphus rutilus*. Cytotoxic. λ_{max} 281 (ϵ 2262) (EtOH) (Berdy).

2-Me ether: 2-Methoxy-6-(3,7,11-trimethyl-2,6,10-dodecatrienyl)-1,4-benzenediol
$C_{22}H_{32}O_3$ 344.493
Constit. of *Thorecta choanoides*. Yellow oil.

1,4-Quinone, 2-Me ether: 2-Methoxy-6-(3,7,11-trimethyl-2,6,10-dodecatrienyl)-1,4-benzoquinone
$C_{22}H_{30}O_3$ 342.477
Constit. of *Thorecta choanoides*. Yellow oil.

Reynolds, G.W. *et al., Phytochemistry*, 1986, **25**, 1617
Piattelli, M. *et al., Planta Med.*, 1992, **58**, 383 (*4-Ac*)
Bonny, M.L. *et al., J. Nat. Prod.*, 1994, **57**, 539 (*isol, pmr, cmr*)

24,26,27-Trimethylergosta-5,25-dien-3-ol T-710
24,24,26,27-Tetramethylcholesta-5,25-dien-3-ol



(3β,25*E*)–*form*

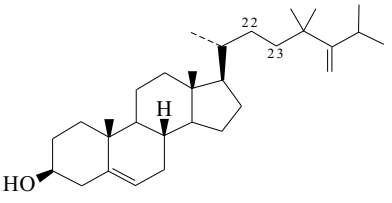
$C_{31}H_{52}O$ 440.751

(3β,25*E*)-*form*
Isoxestospongesterol
[78516-63-9]
Constit. of *Xestospongia* spp. and *Strongylophora durissima*.
Cryst.
Mp 117-118°. $[\alpha]_D^{28}$ -34.2 (c, 0.1 in $CHCl_3$).

(3β,25*Z*)-*form*
Xestospongesterol
[78516-64-0]
Constit. of *Xestospongia* spp. and *Strongylophora durissima*.
Cryst.
Mp 133-134°. $[\alpha]_D^{28}$ -46.6 (c, 0.07 in $CHCl_3$).
Li, L.N. *et al., J.A.C.S.*, 1981, **103**, 3606-3608 (*isol, pmr*)

24,27,27-Trimethylergosta-5,25-dien-3-ol T-711

24,24,26,26-Tetramethylcholesta-5,25(27)-dien-3-ol

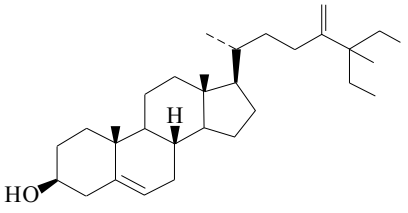


$C_{31}H_{52}O$ 440.751

3β-*form*
Metab. of a *Halichondria* sp.
Ac:
Cryst. (EtOAc). Mp 139-141°. $[\alpha]_D^{20}$ -35.5 (c, 0.5 in $CHCl_3$).
*22,23-Didehydro(*E-*): 24,24,26,26-Tetramethylcholesta-5,22,25(27)-trien-3-ol*
$C_{31}H_{50}O$ 438.735
From a *Halichondria* sp.
22,23-Didehydro, Ac:
Cryst. (EtOAc). Mp 170-172°. $[\alpha]_D^{20}$ -29 (c, 0.8 in $CHCl_3$).
Shubina, L.K. *et al., Khim. Prir. Soedin.*, 1985, **21**, 232; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 217
Ilyin, S.G. *et al., J. Nat. Prod.*, 1992, **55**, 232-236 (*didehydro, cryst struct*)

25,26,27-Trimethylergosta-5,24(28)-dien-3-ol T-712

25,25-Diethyl-27-norergosta-5,24(28)-dien-3-ol, 9CI. 24-Methylene-25,26,27-trimethylcholest-5-en-3-ol

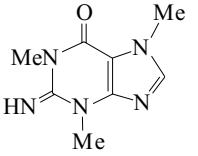


$C_{31}H_{52}O$ 440.751

3β-*form*
25-Methylxestosterol
[78355-28-9]
Constit. of a *Xestospongia* sp.
Cryst. (MeOH).
Mp 143°. $[\alpha]_D^{20}$ -27 (c, 0.76 in $CHCl_3$).
Li, L.N. *et al., J.O.C.*, 1981, **46**, 3867-3870 (*isol*)

1,3,7-Trimethylguanine T-713

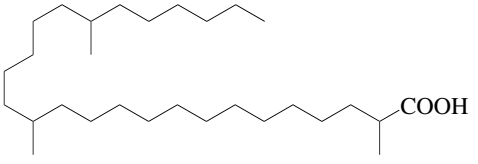
*1,2,3,7-Tetrahydro-2-imino-1,3,7-trimethyl-6*H*-purin-6-one, 9CI*
[110025-83-7]



$C_8H_{11}N_5O$ 193.208
Isol. from *Eudistoma maculosum* and *Latrunculia brevis*. Pale-yellow needles (MeOH/Et_2O).
Mp 192-194°. λ_{max} 213 (ϵ 7900); 288 (ϵ 1600) (pH 13) (Derep). λ_{max} 264 (ϵ 2000) (pH 7) (Derep).
Perry, N.B. *et al., J. Nat. Prod.*, 1987, **50**, 307-308 (*isol, uv, pmr, cmr, ms*)
Berry, Y. *et al., Nat. Prod. Res.*, 2006, **20**, 479-483 (*isol, pmr, cmr, ms*)

2,14,20-Trimethylhexacosanoic acid T-714

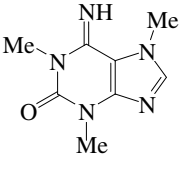
[132970-71-9]



$C_{29}H_{58}O_2$ 438.776
Isol. from *Botryococcus braunii*.
Metzger, P. *et al., Phytochemistry*, 1991, **30**, 185-191 (*isol*)

1,3,7-Trimethylisoguanine T-715

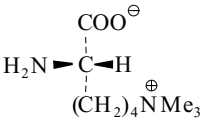
*1,3,6,7-Tetrahydro-6-imino-1,3,7-trimethyl-2*H*-purin-2-one, 9CI*
[290821-46-4]



$C_8H_{11}N_5O$ 193.208
Isol. from a New Zealand ascidian *Pseudodistoma* sp. Constit. of the cuticular wax of *Osmunda regalis*. Light tan oil. λ_{max} 214 (log ϵ 3.6); 288 (log ϵ 3.4) (MeOH).
Copp, B.R. *et al., J. Nat. Prod.*, 2000, **63**, 1168-1169 (*isol, pmr, cmr, uv*)

6-*N*-Trimethyllysine betaine T-716

*5-Amino-5-carboxy-*N,N,N*-trimethyl-1-pentanaminium hydroxide inner salt, 9CI. Laminine. Lysine δ-betaine*
[2408-79-9]
[7622-29-9, 19253-88-4]



$C_9H_{20}N_2O_2$ 188.269

(*S*)-*form*
L-form
[23284-33-5]
Amino acid present in the green alga *Enteromorpha intestinalis* and the brown algae *Laminaria angustata* and *Heterochordaria abietina*; also from the seaweed *Petalonia fascia*, the seeds of

Reseda luteola, histones and rat testis. Intermed. in biosynth. of carnitine and γ-butyrobetaine. Cell proliferation stimulant. Antihypertensive and hypocholesterolemic agent.

▶ LD_{50} (mus, ivn) 394 mg/kg.

Hydrochloride (1:2): Mp 220-250° approx. dec. $[\alpha]_D$ +15.7 (c, 0.05 in 0.1*M* HCl). Variable Mp. Crystallises with difficulty.

Dioxalate:
Needles (EtOH). Mp 122-124°. $[\alpha]_D^{18}$ +10.8 (c, 5 in H_2O).

(±)-*form*
Mp 260-261° (240°) (as hydrochloride).

Enger, R. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1930, **191**, 103-111 (*synth*)
Birkofer, L. *et al., Naturwissenschaften*, 1964, **55**, 37 (*isol*)
Takemoto, T. *et al., Yakugaku Zasshi*, 1964, **84**, 1176-1179; 1180-1182; 1965, **85**, 843-845; *CA*, **62**, 7858; **64**, 3964 (*isol*)
Larsen, P.O. *et al., Acta Chem. Scand.*, 1968, **22**, 1369 (*isol*)
Takagi, N. *et al., Yakugaku Zasshi*, 1970, **90**, 899-902; *CA*, **73**, 127782u (*isol*)
Cox, R.A. *et al., Biochem. J.*, 1973, **136**, 1083-1090; 1974, **142**, 699-701 (*biosynth*)
Cox, R.A. *et al., Biochim. Biophys. Acta*, 1974, **362**, 403-413 (*biosynth*)
Jackson, R.L. *et al., Biochem. Biophys. Res. Commun.*, 1977, **77**, 723-729 (*isol*)
Paik, W.K. *et al., Anal. Biochem.*, 1978, **90**, 262-272 (*synth*)
Hertzberg, T. *et al., Acta Chem. Scand., Ser. B*, 1986, **40**, 387-389 (*synth, pmr, bibl*)

N′,N″,N‴-Trimethyl-*N*-(3-methyl-2,4-dodecadienoyl)spermidine T-717

N-*[3-[[4-(Dimethylamino)butyl]methylamino]propyl]-3-methyl-2,4-dodecadienamide. 2,7,14-Trimethyl-2,7,11-triaza-13,15-tricosadien-12-one*

$H_3C(CH_2)_6CH{=}CHC(CH_3){=}^{2'}CHCONH(CH_2)_3N$-$NMe(CH_2)_4NMe_2$

$C_{23}H_{45}N_3O$ 379.628

(2′*E*,4′*E*)-*form* [583850-68-4]
Isol. from a *Sinularia* sp.
Oil.

4′,5′-Dihydro: N-*[3-[[4-(Dimethylamino)butyl]methylamino]propyl]-3-methyl-2-dodecenamide. 1-(Dimethylamino)-5,12-dimethyl-5,9-diazaheneicos-11-en-10-one.* N′,N″,N‴-*Trimethyl*-N-*(3-methyl-2-dodecenoyl)spermidine. 2,7,14-Trimethyl-2,7,11-triaza-13-tricosen-12-one*
[73710-47-1]
$C_{23}H_{47}N_3O$ 381.644
Isol. from *Sinularia brongersmai*.

(2′*Z*,4′*E*)-*form* [583850-67-3]
Isol. from a soft coral *Sinularia* sp.
Pale yellow oil (rapidly darkens on standing).

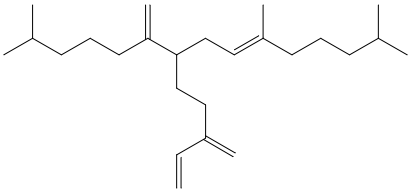
4′,5′-Dihydro: [81419-45-6]
Isol. from the soft coral *Sinularia brongersmai*. Cytotoxic agent. Pale yellow oil. Rapidly darkens on standing. Obt. as a 9:1 mixt. with its dihydro deriv.

2′,3′,4′,5′-Tetrahydro: **N′,N″,N‴-*Trimethyl*-N-*(3-methyldodecanoyl)-spermidine***. N-*[3-[[4-(Dimethylamino)butyl]methylamino]propyl]-3-methyldodecanamide. 2,7,14-Trimethyl-2,7,11-triaza-12-tricosanone*
[73710-48-2]
$C_{23}H_{49}N_3O$ 383.66
Minor constit. of *Sinularia brongersmai*. Cytotoxic.

Schmitz, F.J. *et al., Tet. Lett.*, 1979, 3387 (*isol, ir, pmr, ms, struct, Sinularia brongersmai constits*)
Chantrapromma, K. *et al., Tet. Lett.*, 1980, **21**, 2605 (*synth, ir, pmr, ms*)
Kazlauskas, R. *et al., Aust. J. Chem.*, 1982, **35**, 69-75 (*isol, pmr, cmr, ms, struct, synth*)
Ojika, M. *et al., Biosci., Biotechnol., Biochem.*, 2003, **67**, 1410-1412 (*2′E,4′E-form, 2′Z,4′E-form, isol, pmr, cmr*)

2,6,14-Trimethyl-10-methylene-9-(3-methylene-4-pentenyl)-6-pentadecene T-718

[348614-48-2]

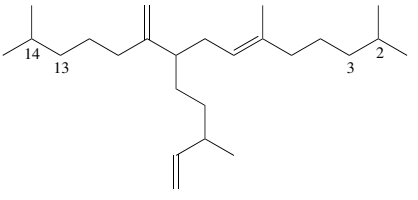


$C_{25}H_{44}$ 344.623
Constit. of *Haslea ostrearia*.

Allard, W.G. *et al., Phytochemistry*, 2001, **56**, 795-800 (*isol, pmr, cmr*)

2,6,14-Trimethyl-10-methylene-9-(3-methyl-4-pentenyl)-6-pentadecene T-719

[178992-70-6]



$C_{25}H_{46}$ 346.638
Isol. from *Haslea ostrearia*.

2,3-Didehydro: ***2,6,14-Trimethyl-10-methylene-9-(3-methyl-4-pentenyl)-2,6-pentadecadiene***
[178992-69-3]
[235094-60-7]
$C_{25}H_{44}$ 344.623
Isol. from *Haslea ostrearia*.

2,3,13,14-Tetradehydro: ***2,6,14-Trimethyl-10-methylene-9-(3-methyl-4-pentenyl)-2,6,13-pentadecatriene***
[178992-71-7]
$C_{25}H_{42}$ 342.607
Isol. from *Haslea ostrearia*.

Belt, S.T. *et al., Tet. Lett.*, 1996, **37**, 4755-4758 (*isol, pmr, cmr*)
Johns, L. *et al., Phytochemistry*, 2000, **53**, 607-611 (*isol*)
Allard, W.G. *et al., Phytochemistry*, 2001, **56**, 765-800 (*isol, ms, bibl*)

N′,N″,N‴-Trimethyl-*N*-(5-methyl-2,4-tetradecadienoyl)spermidine T-720

N-*[3-[[4-(Dimethylamino)butyl]methylamino]propyl]-5-methyl-2,4-tetradecadienamide, 9CI. 2,7,16-Trimethyl-2,7,11-triaza-13,15-pentacosadien-12-one*

$H_3C(CH_2)_8C(CH_3){=}CHCH{=}CHCONH(CH_2)_3N$-$Me(CH_2)_4NMe_2$

$C_{25}H_{49}N_3O$ 407.682

(2*E*,4*E*)-*form* [583850-70-8]
Isol. from the soft coral *Sinularia* sp. Cytotoxic. Oil.

(2*Z*,4*E*)-*form* [583850-69-5]
Isol. from a *Sinularia* sp. Cytotoxic. Oil.

Ojika, M. *et al., Biosci., Biotechnol., Biochem.*, 2003, **67**, 1410-1412 (*isol, pmr, cmr*)

N′,N″,N‴-Trimethyl-*N*-(5-methyl-3-tetradecenoyl)-spermidine T-721

N-*[3-[[4-(Dimethylamino)butyl]methylamino]propyl]-5-methyl-3-tetradecenamide. 2,7,16-Trimethyl-2,7,11-triaza-14-pentacosen-12-one*

$H_3C(CH_2)_8CH(CH_3)CH{=}CHCH_2CONH(CH_2)_3N$-$Me(CH_2)_4NMe_2$

$C_{25}H_{51}N_3O$ 409.697

(*3′E*,5′ξ)-*form* [129722-93-6]
Isol. from the soft coral *Sinularia* sp. Cytotoxic agent. Oil. $[\alpha]_D$ +7 (c, 0.2 in CH_2Cl_2). λ_{max} 200 (MeOH).
Choi, Y.-H. *et al., J. Nat. Prod.*, 1997, **60**, 495-496

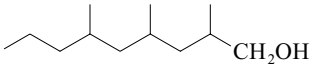
Trimethyl[3-(methylthio)propyl]ammonium(1+), 8CI T-722
N,N,N-*Trimethyl-3-(methylthio)-1-propanaminium(1+), 9CI. TA Toxin A*
[61672-50-2]
$MeSCH_2CH_2CH_2NMe_3^{\oplus}$
$C_7H_{18}NS^{\oplus}$ 148.292
Isol. from the reef shell *Marmarostoma argyrostoma* and the turban shell *Turbo argyrostoma*.
Mp 223-225° (as iodide).

S-*Me: 3-(Dimethylsulfonio)*-N,N,N-*trimethylpropanaminium(2+), 9CI*
[61672-51-3]
$C_8H_{21}NS^{2\oplus}$ 163.327
Isol. from *Marmarostoma argyrostoma*.
Mp 246° (as diiodide).

[14617-80-2, 54289-29-1]

Kirchner, F.D. *et al., J.A.C.S.*, 1955, **77**, 4599 (*synth*)
Tadashi, S. *et al., Yakugaku Zasshi*, 1964, **84**, 1012; *CA*, **62**, 6552g (*synth*)
Yasumoto, T. *et al., Nippon Suisan Gakkaishi*, 1974, **40**, 217; *CA*, **80**, 129589e (*isol*)
Yasumoto, T. *et al., Rinsho Eiyo*, 1976, **49**, 115; *CA*, **86**, 84458s (*isol*)

2,4,6-Trimethyl-1-nonanol T-723
[83474-29-7]



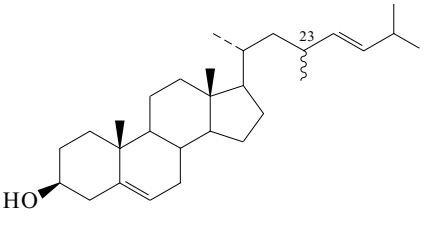
$C_{12}H_{26}O$ 186.337

O-*Sulfate:* [133084-59-0]
$C_{12}H_{26}O_4S$ 266.401
Isol. from the sea cucumber *Cucumaria frondosa*. Amorph. solid (as Na salt).
Mp 180-190° (Na salt). $[\alpha]_D$ -0.6 (c, 0.015 in $CHCl_3$).

[20265-58-1]

Fr. Pat., 1953, 1 045 726; *CA*, **52**, 11888d (*synth*)
Kuwahara, Y. *et al., Agric. Biol. Chem.*, 1982, **46**, 2283 (*synth*)
Findlay, J.A. *et al., J. Nat. Prod.*, 1991, **54**, 302-304 (*isol, sulfate*)

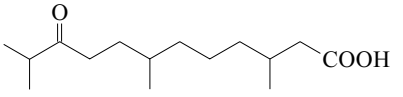
23,26,26-Trimethyl-27-norcholesta-5,24-dien-3-ol T-724
23-(3-Methyl-1-butenyl)-5-cholen-3-ol, 9CI



$C_{29}H_{48}O$ 412.698

(3β,24*E*)-*form*
Echissaposterol
[92264-13-6]
Isol. from the gorgonian *Echinogorgia pseudossapo.*
Su, J. *et al., CA*, 1984, **101**, 148308f (*isol, pmr, cmr, ir*)

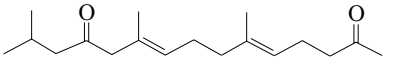
3,7,11-Trimethyl-10-oxododecanoic acid, 9CI T-725
10-Oxo-1-farnesanoic acid
[137761-18-3]



$C_{15}H_{28}O_3$ 256.384
Constit. of *Caulerpa racemosa*. Oil. $[\alpha]_D^{32}$ +1.96 (c, 0.24 in $CHCl_3$). The (3*R*,7*RS*)- stereoisomer has been synthesised but the abs. config. of the nat. prod. does not appear to be known.

Anjaneyulu, A.S.R. *et al., Phytochemistry*, 1991, **30**, 3041 (*isol, pmr, cmr*)
Li, Y. *et al., Synth. Commun.*, 1997, **27**, 4341-4348 (*(3R,4RS)-form, synth, ir, pmr, ms*)

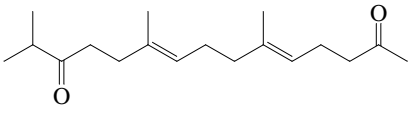
6,10,14-Trimethyl-5,9-pentadecadiene-2,12-dione, 9CI T-726



$C_{18}H_{30}O_2$ 278.434

(*E,E*)-*form* [84321-90-4]
Constit. of *Sargassum micracanthum*.
Liq.
Shizuri, Y. *et al., Phytochemistry*, 1982, **21**, 1808

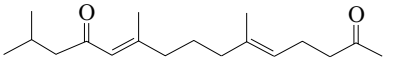
6,10,14-Trimethyl-5,9-pentadecadiene-2,13-dione, 9CI T-727
[66067-36-5]



$C_{18}H_{30}O_2$ 278.434

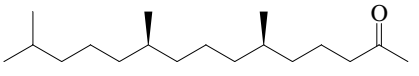
(*E,E*)-*form* [81373-95-7]
Isol. from *Cystophora moniliformis.*
Oil.
Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 171-182 (*isol, pmr, cmr, ms*)
Li, Y. *et al., Synth. Commun.*, 1994, **24**, 117-121 (*synth, pmr, ms*)

6,10,14-Trimethyl-5,10-pentadecadiene-2,12-dione, 9CI T-728
[71802-03-4]



$C_{18}H_{30}O_2$ 278.434
Constit. of *Sargassum micracanthum*. Liq.
Shizuri, Y. *et al., Phytochemistry*, 1982, **21**, 1808

6,10,14-Trimethyl-2-pentadecanone T-729
Phytone
[502-69-2]



$C_{18}H_{36}O$ 268.482

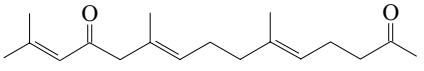
Widespread in plant spp. Present in marine organisms such as the sponge *Spheciospongia vagabunda*, green alga *Caulerpa taxifolia* and crab *Carcinus maenus*. Bp_1 135-137°.

(6*R*,10*R*)-*form* [16825-16-4]
$[\alpha]_D^{25}$ +0.59 (c, 4.4 in Et_2O).

[22571-87-5, 57760-55-1, 96093-84-4, 125354-91-8]

Rao, C.B. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 264-265; 605-606 (*isol, bibl, marine sources*)
Tori, M. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 2669 (*synth*)
Enzell, C.R. *et al., Mass Spectrom. Rev.*, 1986, **5**, 39 (*ms*)
Kulkarni, S.N. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 685 (*synth*)
Baglai, A.K. *et al., J. Chem. Eng. Data*, 1988, **33**, 512 (*props*)
Suga, T. *et al., J.O.C.*, 1989, **54**, 3390 (*synth, cmr, cd, glc*)
Mignani, G. *et al., Tet. Lett.*, 1990, **31**, 5161 (*synth*)
Xiao, D. *et al., Fenxi Huaxue*, 2004, **32**, 1621-1623; *CA*, **143**, 23210 (*Spheciospongia vagabunda constit*)

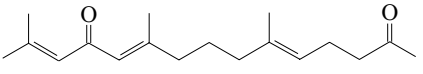
6,10,14-Trimethyl-5,9,13-pentadecatriene-2,12-dione T-730



$C_{18}H_{28}O_2$ 276.418

(*E,E*)-*form* [71802-00-1]
Constit. of the brown alga *Sargassum micracanthum*.
Kusumi, T. *et al., Chem. Lett.*, 1979, 1181 (*isol, pmr, ms*)

6,10,14-Trimethyl-5,10,13-pentadecatriene-2,12-dione T-731

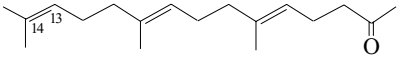


$C_{18}H_{28}O_2$ 276.418

(*E,E*)-*form* [71802-01-2]
Constit. of the brown alga *Sargassum micracanthum*.
Kusumi, T. *et al., Chem. Lett.*, 1979, 1181 (*isol, pmr, ms*)

6,10,14-Trimethyl-5,9,13-pentadecatrien-2-one, 9CI T-732

[762-29-8]

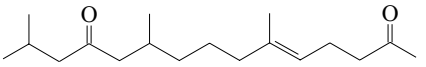


$C_{18}H_{30}O$ 262.434

(5*E*,9*E*)-*form*
Farnesylacetone
[1117-52-8]
Present in various plants, e.g. tobacco, tomato. Isol. from brown alga *Sargassum micracanthum*. n_D^{20} 1.4816. Other stereoisomers also prepd.
Semicarbazone: Mp 81-82°.
*13*R*,14-Epoxide: 6,10-Dimethyl-12-(3,3-dimethyloxiranyl)-5,9-dodecadien-2-one, 9CI*. ***Farnesylacetone epoxide***
[66067-35-4]
$C_{18}H_{30}O_2$ 278.434
Constit. of *Cystophora moniliformis*. Anticonvulsant. Oil. $[\alpha]_D$ -3.2 (c, 1 in $CHCl_3$).
▶ JR1782000

Isler, O. *et al., Helv. Chim. Acta*, 1958, **41**, 786 (*synth*)
Laats, K. *et al., CA*, 1969, **70**, 106666g; 1975, **83**, 97600v (*synth*)
Kazlauskas, R. *et al., Experientia*, 1978, **34**, 156 (*epoxide*)
Ferezou, J.-P. *et al., Helv. Chim. Acta*, 1978, **61**, 669 (*biosynth*)
Kosumi, T. *et al., Chem. Lett.*, 1979, 1181-1184 (*Sargassum constit*)
Enzell, C.R. *et al., Mass Spectrom. Rev.*, 1986, **5**, 39 (*ms*)

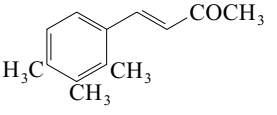
6,10,14-Trimethyl-5-pentadecene-2,12-dione T-733



$C_{18}H_{32}O_2$ 280.45

(*E*)-*form* [71802-02-3]
Constit. of the brown alga *Sargassum micracanthum*.
Oil.
Kusumi, T. *et al., Chem. Lett.*, 1979, 1181 (*isol*)
Shizuri, Y. *et al., Phytochemistry*, 1982, **21**, 1808

4-(2,3,4-Trimethylphenyl)-3-buten-2-one, 9CI T-734

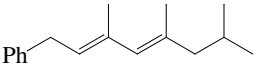


$C_{13}H_{16}O$ 188.269

(*E*)-*form* [122602-80-6]
Isol. from the sponge *Tedania ignis*.
Mp 70-71°. Bp_3 125-130°. Data given is for synth. prod. of unspecified config, prob. (*E*-).
Yamaguchi, M. *et al., Bull. Chem. Soc. Jpn.*, 1960, **33**, 1560 (*synth*)
Dillman, R.L. *et al., J. Nat. Prod.*, 1991, **54**, 1056 (*isol, uv, pmr, cmr*)

3,5,7-Trimethyl-1-phenyl-2,4-octadiene T-735

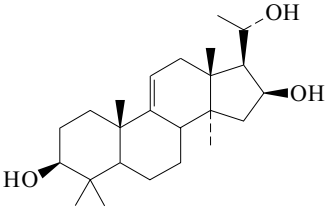
(3,5,7-Trimethyl-2,4-octadienyl)benzene, 9CI



$C_{17}H_{24}$ 228.377

(2ξ,4ξ)-*form* [74096-87-0]
Isol. from a *Plakortis* sp.
Stierle, D.B. *et al., J.O.C.*, 1980, **45**, 3396-3401 (*isol, pmr*)

4,4,14-Trimethylpregn-9(11)-ene-3,16,20-triol T-736

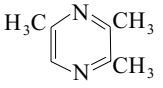


$C_{24}H_{40}O_3$ 376.578

(3β,16β,20*S*)-*form*
16,20-Di-Ac: ***Nemogenin***
[123134-07-6]
$C_{28}H_{44}O_5$ 460.653
Genin from *Duasmodactyla kurilensis*. Cryst.
Mp 238-240°. $[\alpha]_D^{20}$ +91 (c, 1 in $CHCl_3$).
Avilov, S.A. *et al., Khim. Prir. Soedin.*, 1989, **25**, 359; *Chem. Nat. Compd. (Engl. Transl.)*, 309 (*isol, pmr, cmr*)

Trimethylpyrazine, 9CI T-737

FEMA 3244
[14667-55-1]



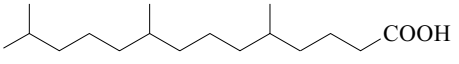
$C_7H_{10}N_2$ 122.169
Urinary signalling pheromone in tree shrews *Tupaia belangeri* and pine vole *Microtus pinetorum*. Isol. from an arctic marine bacterium. Flavouring ingredient. Liq. with roast coffee odour. Bp_{735} 171-172°. pK_{a1} 2.65; pK_{a2} -3.6 (25°, H_2O). Steam-volatile. Odour threshold 9000ppb in H_2O.

▶ LD_{50} (rat, orl) 806 mg/kg. UQ3907000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 841B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 401A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1558B (*ir*)
Das, B.K. *et al., J. Indian Chem. Soc.*, 1968, **45**, 1075 (*uv*)
Bus, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1973, **92**, 123 (*ir*)
Calabretta, P.J. *et al., Cosmet. Perfum.*, 1975, **90**, 74 (*synth*)
Gumbley, S.J. *et al., J. Het. Chem.*, 1985, **22**, 1143 (*props*)
von Stralendorff, F. *et al., J. Chem. Ecol.*, 1987, **13**, 655
Boyer, M.L. *et al., J. Chem. Ecol.*, 1989, **15**, 649
Dickschat, J.S. *et al., Chem. Biodiversity*, 2005, **2**, 318-353 (*marine isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TME270

5,9,13-Trimethyltetradecanoic acid T-738

1,2,20-Trinor-3-phytanoic acid
[22008-57-7]



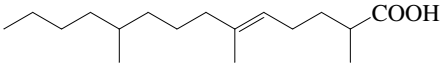
$C_{17}H_{34}O_2$ 270.454
Constit. of the sponge *Cinachyrella alloclada* and fish oils. Also found in oil shales. $Bp_{1.5}$ 154-155°.

[10236-12-1, 42763-81-5, 57689-30-2, 86747-04-8]

Karrer, P. *et al., Helv. Chim. Acta*, 1948, **31**, 1505 (*synth*)
Lukes, R. *et al., Chem. Listy*, 1957, **51**, 330; 568 (*synth*)
Rowland, R.L. *et al., J.A.C.S.*, 1957, **79**, 5007 (*synth*)
Ratanayake, W.M.N. *et al., Lipids*, 1989, **24**, 630-637 (*occur, fish oil*)
Rane, S.S. *et al., Bioorg. Med. Chem.*, 1993, **1**, 399 (*synth*)
Barnathan, G. *et al., Nat. Prod. Lett.*, 1993, **3**, 113 (*isol*)

2,6,10-Trimethyl-5-tetradecenoic acid T-739

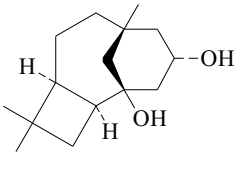
[79605-27-9]



$C_{17}H_{32}O_2$ 268.439
Constit. of the sponge *Aplysina fistularis*.

Walkup, R.D. *et al., Lipids*, 1981, **16**, 631-646 (*isol*)

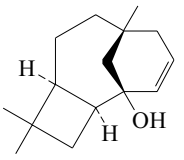
4,11,11-Trimethyltricyclo[6.3.1.0^{2,5}]dodecane-6,8-diol T-740



$C_{15}H_{26}O_2$ 238.369
Constit. of a *Eurypon* sp. Oil. $[\alpha]_D$ -10 (c, 0.002 in $CHCl_3$).

Kernan, M.R. *et al., J. Nat. Prod.*, 1990, **53**, 1353 (*isol, pmr, cmr*)

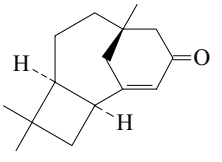
4,11,11-Trimethyltricyclo[6.3.1.0^{2,5}]dodec-6-en-8-ol T-741



$C_{15}H_{24}O$ 220.354
Constit. of a *Eurypon* sp. Cryst. (hexane).
Mp 115°. $[\alpha]_D$ -6.1 (c, 0.03 in $CHCl_3$).

Kernan, M.R. *et al., J. Nat. Prod.*, 1990, **53**, 1353 (*isol, pmr, cmr*)

4,11,11-Trimethyltricyclo[6.3.1.0^{2,5}]dodec-7-en-6-one T-742

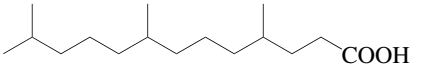


$C_{15}H_{22}O$ 218.338
Constit. of a *Eurypon* sp. Oil.

Kernan, M.R. *et al., J. Nat. Prod.*, 1990, **53**, 1353 (*isol, pmr, cmr*)

4,8,12-Trimethyltridecanoic acid T-743

1,2,3,20-Tetranor-4-phytanoic acid
[10339-73-8]

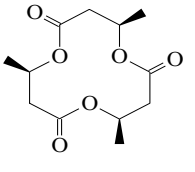


$C_{16}H_{32}O_2$ 256.428
Constit. of *Cinachyrella* spp. and *Callyspongia fallax*. Metab. of 1-Phytanoic acid, P-379. Present in fish oils.

Ratanayake, W.M.N. *et al., Lipids*, 1989, **24**, 630-637 (*occur, fish oil*)
Barnathan, G. *et al., Nat. Prod. Lett.*, 1993, **3**, 113 (*isol, ms*)
Carballeira, N.M. *et al., J. Nat. Prod.*, 2001, **64**, 620-623 (*isol*)

4,8,12-Trimethyl-1,5,9-trioxacyclododecane-2,6,10-trione T-744

Tris-β-butyrolactone. ***Pinnatifolide***



(*R,R,R*)–*form*

$C_{12}H_{18}O_6$ 258.271
Trimer of 3-Hydroxybutanoic acid, readily obt. by thermal treatment of the polymer.

(R,R,R)-form [139629-08-6]
Solid. Mp 110-110.5°. $[\alpha]_D$ -33.9 (c, 1.005 in $CHCl_3$).

(S,S,S)-form [139629-09-7]
Metab. of the red alga *Laurencia pinnatifida*. Active against gram-positive bacteria.

(RS,RS,RS)-form
rac-*form*
[139629-10-0]
Mp 67-67.5°.

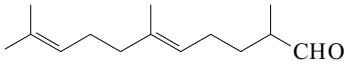
(*RS,RS,SR*)-*form*
rac-epi-*form*
[139683-17-3]
Cryst. (Et_2O/pentane). Mp 104-104.5°.

[85407-33-6, 153063-01-5, 153063-02-6]

Ahmad, V.U. *et al., Pak. J. Sci. Ind. Res.*, 1991, **34**, 161 (*isol*)
Seebach, D. *et al., Angew. Chem., Int. Ed.*, 1992, **31**, 434 (*synth, ir, pmr, cmr, cryst struct*)
Riddell, F.G. *et al., Helv. Chim. Acta*, 1993, **76**, 915 (*cmr, struct*)
Plattner, D.A. *et al., Helv. Chim. Acta*, 1993, **76**, 2004 (*synth, cryst struct*)

2,6,10-Trimethyl-5,9-undecadienal T-745

[54082-68-7]



$C_{14}H_{24}O$ 208.343
Used in perfumery.

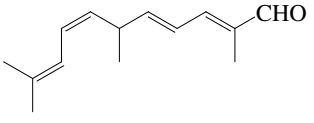
(*E*)-*form* [55903-90-7]
Constit. of the nudibranch *Anisodoris nobilis.*
Sweet smelling oil.

[58001-86-8, 60507-24-6]

Fr. Pat., 1974, 2 216 263; *CA*, **84**, 44468 (*synth*)
Gora, J. *et al., Perfum. Flavor.*, 1980, **5**, 31 (*synth*)
Gustafson, K. *et al., Tetrahedron*, 1985, **41**, 1101 (*isol, pmr*)

2,6,10-Trimethyl-2,4,7,9-undecatetraenal T-746

1-Nor-3,5,8,10-farnesatetraen-2-al



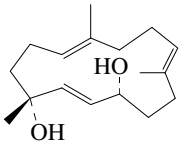
$C_{14}H_{20}O$ 204.311

(3*E*,5*E*,8*Z*)-*form* [340013-39-0]
Constit. of *Plexaurella grisea*.
Oil. $[\alpha]_D^{25}$ +294 (c, 0.16 in $CHCl_3$). λ_{max} 239 (ϵ 15200) (MeOH).

8,9-Dihydro: ***2,6,10-Trimethyl-2,4,9-undecatrienal****. 1-Nor-3,5,10-farnesatrien-2-al*
$C_{14}H_{22}O$ 206.327
Constit. of *Plexaurella grisea*.

Rueda, A. *et al., J. Nat. Prod.*, 2001, **64**, 401-405 (*isol, pmr, cmr*)

15,16,17-Trinor-2,7,11-cembratriene-1,4-diol T-747



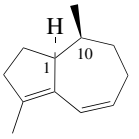
$C_{17}H_{28}O_2$ 264.407

(1*R*,2*E*,4*R*,7*E*,11*E*)-*form*
Chabrolol A
[356558-94-6]
Constit. of *Nephthea chabroli*.
Cryst. (hexane).
Mp 124-125°. $[\alpha]_D^{25}$ +109 (c, 1.48 in $CHCl_3$).

Zhang, W.-H. *et al., Tet. Lett.*, 2001, **42**, 4681-4685 (*isol, pmr, cmr, cryst struct*)

11,12,13-Trinor-4,6-guaiadiene T-748

*2,3,3a,4,5,6-Hexahydro-1,4-dimethylazulene, 9CI. 2,8-Dimethylbicyclo[5.3.0]deca-5,7-diene. 1,4-Dimethyl-2,3,3*a*,4,5,6-hexahydroazulene*



(1α,10β)-*form*

$C_{12}H_{18}$ 162.274

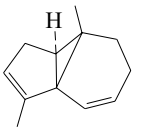
(1α,10β)-*form*
Clavukerin A
[87687-54-5]
Constit. of soft corals *Clavularia koellikeri* and *Cespitularia* sp.
Ichthyotoxin. Oil. $[\alpha]_D^{20}$ -53 ($CHCl_3$). λ_{max} 246 (ϵ 10400) (MeOH) (Derep). λ_{max} 244 (ϵ 21000) (MeOH) (Berdy).

(1β,10β)-*form* [85209-83-2]
Constit. of a *Cespitularia* sp.
Oil. $[\alpha]_D$ -50.8 (c, 0.95 in $CHCl_3$).

Bowden, B.F. *et al., Aust. J. Chem.*, 1983, **36**, 211-214 (*isol*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2160; 1984, **32**, 1667 (*isol, cryst struct*)
Asaoka, M. *et al., Chem. Lett.*, 1991, 1295-1302 (*synth*)
Kim, S.K. *et al., J.O.C.*, 1991, **56**, 6829 (*synth*)
Honda, T. *et al., J.C.S. Perkin 1*, 1994, 3305 (*synth*)
Shimiza, I. *et al., Tet. Lett.*, 1994, **35**, 1905 (*synth*)
Lee, E. *et al., Tet. Lett.*, 1996, **37**, 5929 (*synth*)
Friese, J.C. *et al., Tet. Lett.*, 2002, **43**, 2683-2685 (*synth*)
Grimm, E.L. *et al., Pure Appl. Chem.*, 2003, **75**, 231-234 (*synth*)
Blay, G. *et al., J. Nat. Prod.*, 2006, **69**, 1234-1236 (*synth*)

11,12,13-Trinor-3,6-myliadiene T-749

Inflatene. Trinoranastreptene. Clavukerin B
[90940-32-2]



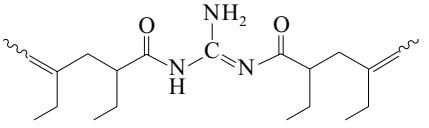
$C_{12}H_{16}$ 160.258
Identity of all samples (esp. abs. config.) not certain. Metabolite of *Clavularia inflata* var. *luzoniana*. Ichthyotoxin. Oil. $[\alpha]_D$ +130 (c, 1.63 in $CHCl_3$).

[86160-98-7]

Takeda, R. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 1265-1266 (*Trinoranastreptene*)
Kobayashi, J. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1667-1670 (*Clavukerin B*)
Izac, R.R. *et al., Tet. Lett.*, 1984, **25**, 1325-1328 (*Inflatene*)

Triophamine T-750

N,N′-*Bis(2,4-diethyl-4-hexenyl)guanidine*
[81256-25-9]

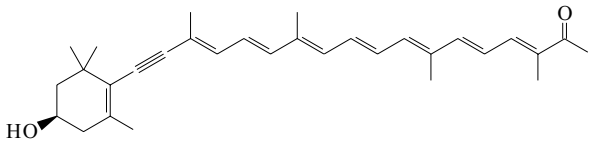


$C_{21}H_{37}N_3O_2$ 363.542
Isol. from skin extracts of the dorid nudibranch *Triopha catalinae.*
Light yellow oil. $[\alpha]_D$ -7 (c, 1.7 in MeOH). λ_{max} 214 (ϵ 14500) (MeOH/HCl) (Derep). λ_{max} 232 (ϵ 10000) (KOH) (Derep). λ_{max} 251 (ϵ 12000) (MeOH) (Derep).

Gustafson, K. *et al., J.O.C.*, 1982, **47**, 2167-2169 (*isol, uv, pmr, cmr, ms, struct*)
Piers, E. *et al., Can. J. Chem.*, 1984, **62**, 1 (*synth*)

Triophaxanthin T-751

18-(4-Hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-3,7,12,16-tetramethyl-3,5,7,9,11,13,15-octadecaheptaen-17-yn-2-one, 9CI. 3-Hydroxy-7,8-didehydro-7′,8′-dihydro-7′-apo-β-caroten-8′-one
[36020-91-4]

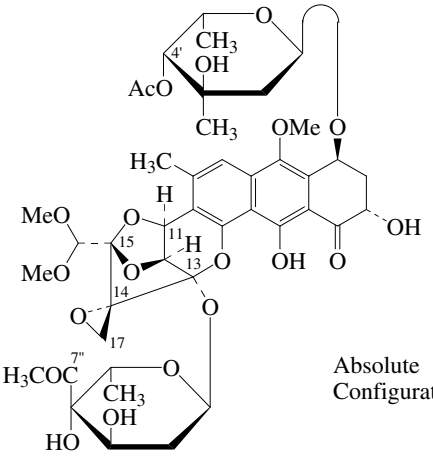


$C_{31}H_{40}O_2$ 444.656
Isol. from the nudibranch *Triopha carpenteri*.
Mp 182-183°. CD: ΔE_{240} -5.2 (Et_2O/pentane/EtOH). λ_{max} 447 (Et_2O). λ_{max} 420; 445; 473 (hexane).

McBeth, J.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1972, **41**, 55 (*isol*)
Matsuno, T. *et al., J. Nat. Prod.*, 1985, **48**, 606-613 (*synth*)
Haugan, J.A. *et al., Acta Chem. Scand.*, 1997, **51**, 1096-1103 (*synth, ir, pmr, cmr, uv, ms*)

Trioxacarcin A, 9CI T-752

DC 45A. Antibiotic DC 45A
[81552-36-5]



Absolute Configuration

$C_{42}H_{52}O_{20}$ 876.861
Isol. from *Streptomyces ochraceus*, *Streptomyces bottropensis* and the marine *Streptomyces* sp. B8652. Active against gram-positive and -negative bacteria and tumours. Yellow powder + $2H_2O$. Sol. MeOH, $CHCl_3$; fairly sol. C_6H_6, H_2O, Et_2O; poorly sol. hexane. Mp 177-183° dec. $[\alpha]_D^{25}$ -15.3 (c, 1 in EtOH). λ_{max} 233 (ϵ 29100); 271 (ϵ 40100); 399 (ϵ 12200) (MeOH) (Derep). λ_{max} 240; 272; 415; 440 (MeOH/NaOH) (Berdy).

▶ LD_{50} (mus, ipr) 1 mg/kg. YJ9410000

*Aglycone: **Trioxacarcin A_2**. Trioxacarcinone A, 9CI. DC $45A_2$. Antibiotic DC $45A_2$*
[81552-35-4]
$C_{25}H_{26}O_{12}$ 518.473
From *Streptomyces bottropensis*. Active against gram-positive and -negative bacteria, fungi and tumours. Yellow powder. Sol. MeOH, EtOAc; fairly sol. $CHCl_3$, Et_2O, H_2O; poorly sol. hexane. Mp 152-158° dec. $[\alpha]_D^{25}$ +97.5 (c, 0.5 in $CHCl_3$). λ_{max} 231; 270; 402 (MeOH) (Berdy).

▶ LD_{50} (mus, ivn) 14 mg/kg , LD_{50} (mus, ipr) 5.5 mg/kg. YJ9500000

*O^{13}-Deglycosyl: **Trioxacarcin A_1**. DC $45A_1$. Antibiotic DC $45A_1$*
[85797-12-2]
$C_{34}H_{40}O_{16}$ 704.68
From *Streptomyces bottropensis*. Active against gram-positive and -negative bacteria, fungi and tumours. Yellow powder. Sol. MeOH, $CHCl_3$; fairly sol. C_6H_6, Et_2O; poorly sol. H_2O, hexane. Mp 184-186° dec. $[\alpha]_D^{25}$ +103 (c, 0.5 in $CHCl_3$). λ_{max} 235; 270; 400 (MeOH) (Berdy). λ_{max} 233 (ϵ 29100); 271 (ϵ 40100); 399 (ϵ 12200) (MeOH/HCl) (Berdy). λ_{max} 240; 272; 415; 440 (MeOH/NaOH) (Berdy).

▶ LD_{50} (mus, ivn) 0.375 mg/kg , LD_{50} (mus, ipr) 0.375 mg/kg. YJ9410500

*4′-O-De-Ac: **Trioxacarcin D***
$C_{40}H_{50}O_{19}$ 834.824
Prod. by *Streptomyces* sp. B8652. Yellow solid. $[\alpha]_D^{20}$ +20 (c, 0.57 in MeOH). λ_{max} 270 (log ϵ 4.54); 396 (log ϵ 4.05) (MeOH).

*7″-Alcohol: **Trioxacarcin C**. 7″-Deoxo-7″-hydroxytrioxacarcin A, 9CI. DC $45B_2$. Antibiotic DC $45B_2$*
[81781-28-4]
$C_{42}H_{54}O_{20}$ 878.877
Isol. from *Streptomyces ochraceus*, *Streptomyces bottropensis* and *Streptomyces* sp. B8652. Active against gram-positive and -negative bacteria and tumours. Yellow powder + $2H_2O$. Sol. MeOH, $CHCl_3$; fairly sol. C_6H_6, Et_2O, H_2O; poorly sol. hexane. Mp 181-182° dec. $[\alpha]_D^{25}$ -10 (c, 0.2 in EtOH). λ_{max} 233 (ϵ 29100); 271 (ϵ 40100); 399 (ϵ 12200) (MeOH) (Derep). λ_{max} 230; 268; 398 (MeOH aq.) (Berdy). λ_{max} 238; 272; 415; 440 (MeOH/NaOH) (Berdy).

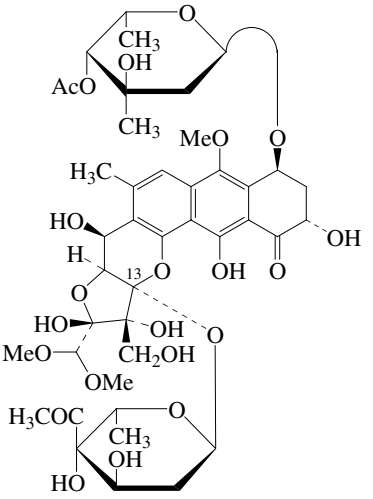
▶ LD_{50} (mus, ipr) 2 mg/kg , LD_{50} (mus, ivn) 1 mg/kg. YJ9411100

*14,17-Deepoxy, 14S,17-dihydroxy: **Trioxacarcin B**. DC $45B_1$. Antibiotic DC $45B_1$*
[81534-36-3]
$C_{42}H_{54}O_{21}$ 894.876
From *Streptomyces ochraceus*, *Streptomyces bottropensis* and *Streptomyces* sp. B8652. Weakly active against gram-positive bacteria, and tumours. Yellow powder + $2H_2O$. Sol. H_2O, $CHCl_3$, MeOH; fairly sol. Me_2CO, EtOAc; poorly sol. Et_2O, hexane. Mp 193-194° dec. $[\alpha]_D^{25}$ -122.7 (c, 1 in $CHCl_3$). λ_{max} 233 (ϵ 29100); 271 (ϵ 40100); 399 (ϵ 12200) (MeOH) (Derep). λ_{max} 238 (ϵ 29000); 272 (ϵ 23200); 415 (ϵ 15500); 440 (ϵ 16000) (MeOH/NaOH) (Berdy).

▶ LD_{50} (mus, ipr) 100 mg/kg. YJ9411000

Tomita, F. *et al., J. Antibiot.*, 1981, **34**, 1519-1524; 1525-1530 (*isol, props*)
Japan. Pat., 1983, 83 65 293; *CA*, **99**, 156836 (*isol, props*)
Maskey, R.P. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 1281-1283 (*abs config*)
Maskey, R.P. *et al., J. Antibiot.*, 2004, **57**, 771-779 (*isol, pmr, abs config, activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TMO775

Trioxacarcin F T-753



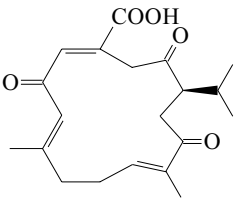
$C_{42}H_{56}O_{22}$ 912.891
Prod. by the marine-derived *Streptomyces* sp. B8652. Yellow solid.

*O^{13}-Deglycosyl: **Trioxacarcin E***
$C_{34}H_{44}O_{18}$ 740.711
Prod. by *Streptomyces* sp. B8652. Yellow solid.

Maskey, R.P. *et al., J. Antibiot.*, 2004, **57**, 771-779 (*isol, pmr, cmr*)

2,6,13-Trioxo-4,7,11-cembratrien-18-oic acid T-754

Sarcoic acid



$C_{20}H_{26}O_5$ 346.422

Me ester: ***Methyl sarcoate***
[135729-26-9]
$C_{21}H_{28}O_5$ 360.449
Constit. of *Sarcophyton glaucum*. λ_{max} 207 (ϵ) (MeOH) (Derep).
Ishitsuka, M.O. *et al., Tet. Lett.*, 1991, **32**, 2917 (*isol, pmr, cmr*)
Ichige, T. *et al., Tet. Lett.*, 2005, **46**, 1263-1267 (*synth*)

2,4,6-Triphenyl-1-hexene, 8CI T-755

1,1′,1″-(1-Methylene-1,3,5-pentanetriyl)trisbenzene, 9CI. ST-1
[18964-53-9]
$H_2C{=}CPhCH_2CHPhCH_2CH_2Ph$
$C_{24}H_{24}$ 312.454

(±)-*form*
Trimer of Styrene.
Yellow viscous oil.

(ξ)-*form*
Constit. of the starfish *Pteraster militaris*. Metab. of the fungus *Phellinus pini*.
Staudinger, H. *et al., Annalen*, 1935, **517**, 35-53 (*synth*)
Mayo, F.R. *et al., J.A.C.S.*, 1968, **90**, 1289-1295 (*synth, ir*)
Saido, K. *et al., Eur. Polym. J.*, 1984, **20**, 1061-1065 (*synth*)
Yayli, N. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 556-561 (*isol*)
Ayer, W.A. *et al., Phytochemistry*, 1996, **42**, 1321-1324 (*isol, pmr, cmr*)
Kawamura, Y. *et al., Shokuhin Eisegaku Zasshi*, 1998, **39**, 110-119; 390-398; *CA*, **129**, 4008w; **130**, 251409n (*detn*)
Ohyama, K. *et al., Environ. Health Perspect.*, 2001, **109**, 699-703 (*tox*)

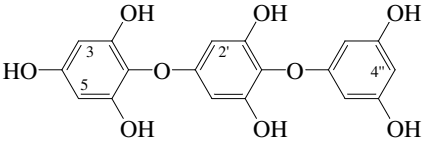
1,3,5-Triphenyl-1-pentanone T-756

[123200-56-6]
$PhCH_2CH_2CHPhCH_2COPh$
$C_{23}H_{22}O$ 314.426
Constit. of the starfish *Pteraster militaris*. Cryst. (EtOH).
Mp 80-81°.

Hydrazone: [123200-57-7]
$C_{23}H_{24}N_2$ 328.456
Pale yellow liq.
Schreck, V.A. *et al., Aust. J. Chem.*, 1989, **42**, 375 (*synth, pmr, cmr*)
Yayli, N. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 556 (*isol*)

Triphlorethol A T-757

2-[4-(3,5-Dihydroxyphenoxy)-3,5-dihydroxyphenoxy]-1,3,5-benzenetriol, 9CI. 2,2′,4,6,6′-Pentahydroxy-1′-(3,5-dihydroxyphenoxy)-diphenyl ether. Triphloroethol A
[81757-68-8]



$C_{18}H_{14}O_9$ 374.303
Numbering systems vary. Constit. of *Cystophora congesta* and other brown algae. Amorph. solid.
Mp 151-153°.

Hepta-Ac: [81757-70-2]
Prisms (2-propanol). Mp 138-139°.

2′-Bromo: ***2[B]-Bromotriphlorethol A***
[256448-60-9 (per-Ac)]
$C_{18}H_{13}BrO_9$ 453.199
Isol. from *Cystophora retroflexa*. Isol. as per-Ac.

2″-Bromo: ***2[D]-Bromotriphlorethol A***
[256448-61-0 (per-Ac)]
$C_{18}H_{13}BrO_9$ 453.199
Isol. from *Cystophora retroflexa*. Isol. as per-Ac.

3-Bromo: ***Bromotriphlorethol A1***
[94513-65-2]
[94513-66-3]
$C_{18}H_{13}BrO_9$ 453.199
Constit. of *Cystophora congesta*. Bright red solid (hepta-Ac).

4″-Bromo: ***Bromotriphlorethol A2***
[94513-67-4]
[94513-68-5 (hepta-Ac)]
$C_{18}H_{13}BrO_9$ 453.199
Constit. of *Cystophora congesta*. Bright red solid (as hepta-Ac).

2′,2″-Dibromo: ***2[B],2[D]-Dibromotriphlorethol A***
[256448-62-1 (per-Ac)]
$C_{18}H_{12}Br_2O_9$ 532.095
Isol. from *Cystophora retroflexa*. Isol. as per-Ac.

2″,3-Dibromo: ***2[D],3[A1]-Dibromotriphlorethol A***
[256448-68-7 (per-Ac)]
$C_{18}H_{12}Br_2O_9$ 532.095
Isol. from *Cystophora retroflexa*. Isol. as per-Ac.

2″-Chloro, 3-bromo: ***3[A1]-Bromo-2[D]-chlorotriphlorethol A***
[256448-69-8 (per-Ac)]
$C_{18}H_{12}BrClO_9$ 487.644
Isol. from *Cystophora retroflexa*. Isol. as per-Ac.

3-Chloro, 4″-bromo: ***3[A1]-Chloro-4[D]-bromotriphlorethol A***
[256448-66-5 (per-Ac)]
$C_{18}H_{12}BrClO_9$ 487.644
Isol. from *Cystophora retroflexa*. Isol. as per-Ac.

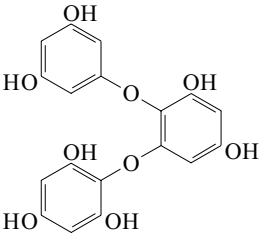
2′,4″-Dichloro: ***2[B],4[D]-Dichlorotriphlorethol A***
[256448-67-6 (per-Ac)]
$C_{18}H_{12}Cl_2O_9$ 443.193
Isol. from *Cystophora retroflexa*. Isol. as per-Ac.

3,4″-Dichloro: ***3[A1],4[D]-Dichlorotriphlorethol A***
[256448-65-4 (per-Ac)]
$C_{18}H_{12}Cl_2O_9$ 443.193
Isol. from *Cystophora retroflexa*. Isol. as per-Ac.

3,5-Dichloro: ***3[A1],5[A1]-Dichlorotriphlorethol A***
[256448-64-3 (per-Ac)]
$C_{18}H_{12}Cl_2O_9$ 443.193
Isol. from *Cystophora retroflexa*. Isol. as per-Ac.
Gregson, R.P. *et al., Aust. J. Chem.*, 1982, **35**, 649 (*isol, pmr, cmr*)
Koch, M. *et al., Phytochemistry*, 1984, **23**, 2633-2637 (*bromo derivs*)
Sailler, B. *et al., Nat. Toxins*, 1999, **7**, 57-62 (*halogenated derivs*)
Sailler, B. *et al., Phytochemistry*, 1999, **50**, 869-881 (*isol*)

Triphlorethol B T-758

2-[2-(3,5-Dihydroxyphenoxy)-3,5-dihydroxyphenoxy]-1,3,5-benzenetriol, 9CI. Triphloroethol B
[79005-83-7]



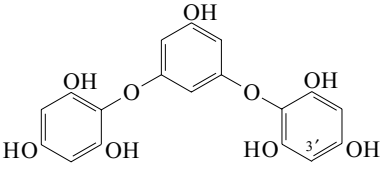
$C_{18}H_{14}O_9$ 374.303
Constit. of the brown algae *Ecklonia kurome*, *Ecklonia stolonifera*, *Cytoseira baccata* and *Carpophyllum angustifolium*. Shows anti-

trypsin and antiplasmin activities. Oil.

Glombitza, K.W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1981, **314**, 602-608 (*isol*)
Fukuyama, Y. *et al., Chem. Lett.*, 1985, 739 (*isol*)
Nakayama, Y. *et al., Agric. Biol. Chem.*, 1989, **53**, 3025 (*props*)
Glombitza, K.W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

Triphlorethol C **T-759**

2,2′-[(5-Hydroxy-1,3-phenylene)bis(oxy)]bis[1,3,5-benzenetriol], 9CI. Triphloroethol C
[61237-22-7]



$C_{18}H_{14}O_9$ 374.303
Constit. of the alga *Laminaria ochroleuca*.

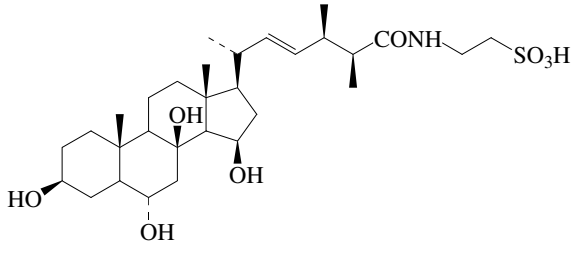
Hepta-Ac:
Cryst. (2-propanol). Mp 68-71°.

3′-Chloro: ***Chlorotriphlorethol C***
[63245-30-7]
$C_{18}H_{13}ClO_9$ 408.748
Constit. of *Laminaria ochroleuca*. CAS no. refers to hepta-Ac.

Glombitza, K.W. *et al., Phytochemistry*, 1976, **15**, 1082 (*isol*)
Glombitza, K.W. *et al., Phytochemistry*, 1977, **16**, 796 (*Chlorotriphlorethol C*)

Triseramide **T-760**

[791849-66-6]

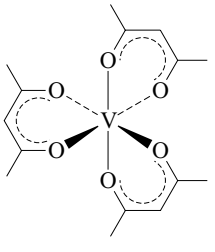


$C_{30}H_{51}NO_8S$ 585.801
Constit. of the starfish *Astropecten triseriatus*. Cryst. (MeOH). Mp 182-183.5°. $[\alpha]_D$ +13.4 (c, 1.7 in MeOH).

Levina, E.V. *et al., Dokl. Biochem. Biophys. (Engl. Transl.)*, 2004, **396**, 171-173; *CA*, **141**, 408790g

Tris(2,4-pentanedionato-*O,O′*)vanadium, 11CI **T-761**

Tris(acetylacetonato)vanadium(III). *Vanadium*(III) *acetylacetonate*
[13476-99-8]

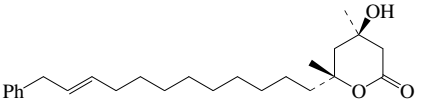


$C_{15}H_{21}O_6V$ 348.269
Octahedral. Synth. from $VCl_3.6H_2O$ or VCl_3 with acac in EtOH in the presence of a base; by electrochem. oxidn. of a V anode in the presence of acac; or by reducing $V(acac)_4$ with zinc. Present in the marine organism *Phallusia nigra*. Commercially available; subject of a large number of patents for use as a catalyst for alkene polym., epoxidation, cross-linking and hydrocracking. Brown solid.
Mp 184°. Paramagnetic; μ_{eff} = 2.60μ_B (20K); 2.87μ_B (300K). Epr: $g_{\parallel}$ = 1.96, $g_{\perp}$ = 1.78. ΔH_f° -1522.8 kJ mol^{-1}.
▶ Toxic.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1278C (*ir*)
Machin, D.J. *et al., J.C.S.(A)*, 1967, 1498 (*magnetism*)
Morosin, B. *et al., Acta Cryst. B*, 1969, **25**, 1354 (*cryst struct*)
Dilli, S. *et al., Aust. J. Chem.*, 1976, **29**, 2369 (*synth, thermal props*)
Gregson, A.K. *et al., Inorg. Chem.*, 1978, **17**, 1216 (*magnetism*)
Van Dam, H. *et al., J. Electron Spectrosc. Relat. Phenom.*, 1979, **17**, 353 (*pe*)
Grobe, J. *et al., Z. Naturforsch., B*, 1984, **39**, 808 (*electrochem synth*)
Boyd, P.D.W. *et al., J.C.S. Dalton*, 1986, 887 (*synth, uv-vis*)
Frank, P. *et al., J. Inorg. Biochem.*, 2001, **86**, 635-648 (*occur, Phallusia*)
Frank, P. *et al., Coord. Chem. Rev.*, 2003, **237**, 31-39 (*occur, Phallusia*)

Trisphaerolide A **T-762**

Tetrahydro-4-hydroxy-4,6-dimethyl-6-(12-phenyl-10-dodecenyl)-2H-pyran-2-one



Relative Configuration

$C_{25}H_{38}O_3$ 386.573
Isol. from the sponge *Erylus trisphaerus*. Amorph. solid. $[\alpha]_D^{27}$ -5.3 (c, 0.32 in MeOH).

Van Altena, I. *et al., J. Nat. Prod.*, 2003, **66**, 561-563 (*isol, pmr, cmr, ms*)

1,3,5-Trithiane, 9CI **T-763**

s-*Trithiane, 8CI. Tris(methylene sulfide). 1,3,5-Trithiacyclohexane. Trithioformaldehyde*
[291-21-4]
$C_3H_6S_3$ 138.278
Trimer of Methanethial. Isol. from various marine organisms; and as a food flavour component. Reagent for aldehyde synth. *via* carbanion formn. Needles (AcOH).
Mp 220°.
▶ Eye and skin irritant. LD_{50} (mus, ipr) 250 mg/kg. YL8225000
S,S,S′,S′,S″,S″-Hexaoxide: [2125-34-0]
$C_3H_6O_6S_3$ 234.275
Cryst. powder. Insol. H_2O, org. solvs.; sol. alkalis. Mp 340°.
▶ YL8400000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 273B (*ir*)
Richtzenhain, H. *et al., Chem. Ber.*, 1953, **86**, 142 (*synth*)
El-Hewehi, Z. *et al., J. Prakt. Chem.*, 1963, **21**, 286 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 564 (*use*)
Asai, M. *et al., Spectrochim. Acta A*, 1978, **34**, 695 (*ir*)
Holzmann, G. *et al., Org. Mass Spectrom.*, 1982, **17**, 165 (*ms*)
Cervellati, R. *et al., J. Mol. Struct.*, 1984, **117**, 247 (*microwave*)
Arens, G. *et al., Chem. Ber.*, 1986, **119**, 3631 (*hexaoxide*)
Bencze, Z. *et al., Acta Chem. Scand.*, 1989, **43**, 953 (*struct*)
Blunt, J.W. *et al., New J. Chem.*, 1990, **14**, 761 (*rev, occur*)
Edema, J.J.H. *et al., Inorg. Chim. Acta*, 1993, **207**, 263 (*conformn*)
Roux, M.V. *et al., J.O.C.*, 2001, **66**, 5343-5351 (*thermodynamic data*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TLS500

1,2,4-Trithiolane, 9CI **T-764**

1,2,4-Trithiacyclopentane
[289-16-7]

$C_2H_4S_3$ 124.252
Constit. of *Acacia pulchella* and *Parkia speciosa*. Also isol. from the alga *Chondria californica* and the mushroom *Lentinus edodes*.

Excretion prod. of *Ochromonas danica*. Component of mushroom flavour. Pale yellow liq. Poorly sol. hexane. Bp_{10} 102-103° Bp_3 78-79°.

1-Oxide: [58966-91-9]
$C_2H_4OS_3$ 140.251
Constit. of the red alga *Chondria californica*. Oil.

4-Oxide: [58966-90-8]
$C_2H_4OS_3$ 140.251
Constit. of *Chondria californica*. Needles (hexane/$CHCl_3$). Mp 76-77°.

Morita, K. *et al., Chem. Pharm. Bull.*, 1967, **15**, 988 (*synth*)
Tjan, S.B. *et al., Tetrahedron*, 1972, **28**, 3489 (*synth, ms*)
Wratten, S.J. *et al., J.O.C.*, 1976, **41**, 2465 (*isol oxides*)
Gmelin, R. *et al., Phytochemistry*, 1981, **20**, 2521 (*isol*)
Holzmann, G. *et al., Org. Mass Spectrom.*, 1982, **17**, 165 (*ms*)
Juettner, F. *et al., Phytochemistry*, 1982, **21**, 2185 (*isol*)
Borseth, D.G. *et al., J.A.C.S.*, 1984, **106**, 841 (*struct*)
Chen, C.C. *et al., J. Agric. Food Chem.*, 1986, **34**, 830 (*isol*)

1,24-Tritriacontadiene T-765

$H_3C(CH_2)_7CH{=}CH(CH_2)_{21}CH{=}CH_2$
$C_{33}H_{64}$ 460.869

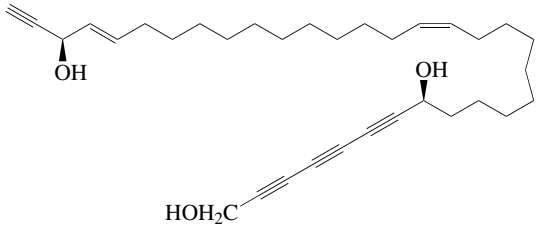
(Z)-form [211238-25-4]
Isol. from the haptophyte *Isochrysis galbana*.
Rieley, G. *et al., Lipids*, 1998, **33**, 617-625 (*isol*)

2,24-Tritriacontadiene T-766

$H_3C(CH_2)_7CH{=}CH(CH_2)_{20}CH{=}CHCH_3$
$C_{33}H_{64}$ 460.869

(Z,Z)-form [211238-29-8]
Isol. from the haptophyte *Emiliania huxleyi*.
Rieley, G. *et al., Lipids*, 1998, **33**, 617-625 (*isol*)

17,29-Tritriacontadiene-2,4,6,32-tetrayne-1,8,31-triol T-767



$C_{33}H_{48}O_3$ 492.74

(8S,17Z,29E,31R)-form
Triangulyne B
[182314-02-9]
Isol. from the sponge *Pellina triangulata*. Cytotoxic agent. Powder. $[\alpha]_D$ -14 (c, 0.8 in $CHCl_3$). λ_{max} 204 (log ϵ 2.35); 226 (log ϵ 3.2); 256 (log ϵ 2.7) (MeOH). λ_{max} 204 (ϵ 3160); 226 (ϵ 1584); 256 (ϵ 500) (MeOH) (Berdy).
Dai, J.-R. *et al., J. Nat. Prod.*, 1996, **59**, 860-865 (*isol, uv, ir, pmr, cmr, ms*)

18,29-Tritriacontadiene-2,4,20,32-tetrayne-1,6,31-triol T-768

$HC{\equiv}CCH(OH)CH{=}CH(CH_2)_7C{\equiv}CCH{=}CH(CH_2)_{11}CH(OH)C{\equiv}CC{\equiv}CCH_2OH$
$C_{33}H_{48}O_3$ 492.74

(-)-(18Z,29E)-form
Pellynol C
[186248-11-3]
Isol. from the sponge *Pellina triangulata*. Exhibits cytotoxic activity to human cell lines. $[\alpha]_D$ -11.2 (c, 2.4 in $CHCl_3$).
Fu, X. *et al., Tetrahedron*, 1997, **53**, 799 (*isol, ir, pmr, cmr*)
Rashid, M.A. *et al., Nat. Prod. Lett.*, 2000, **14**, 387-392 (*isol, activity*)

17,29-Tritriacontadiene-2,4,32-triyne-1,6,31-triol, 9CI T-769

Melyne A
[115276-17-0]
$HC{\equiv}CCH(OH)CH{=}CH(CH_2)_{10}CH{=}CH(CH_2)_{10}CH(OH)C{\equiv}CC{\equiv}CCH_2OH$
$C_{33}H_{52}O_3$ 496.772
Isol. from *Xestospongia* sp.
$[\alpha]_D$ -8 (c, 5.0 in $CHCl_3$). λ_{max} 230 (ϵ 360); 240 (ϵ 330); 255 (ϵ 200) (MeOH) (Derep).

17,18-Didehydo: 29-Tritriacontene-2,4,17,32-tetrayne-1,6,31-triol. ***Pellynol F***
$C_{33}H_{50}O_3$ 494.756
Isol. from a *Theonella* and *Pellina sp.* Exhibits cytotoxic activity to human cell lines.

16-Hydroxy: 17,29-Tritriacontadiene-2,4,32-triyne-1,6,16,31-tetrol. ***Pellynol G***
$C_{33}H_{52}O_4$ 512.771
Isol. from a *Theonella* sp.

16-Oxo: 1,6,31-Trihydroxy-17,29-tritriacontadiene-2,4,32-triyn-16-one. ***Pellynol H***
$C_{33}H_{50}O_4$ 510.756
Isol. from a *Theonella* sp.

[115296-96-3]

Quinoa, E. *et al., Tet. Lett.*, 1988, **29**, 2037 (*isol, struct*)
Fu, X. *et al., J. Nat. Prod.*, 1999, **62**, 1336-1338 (*Pellynols*)
Rashid, M.A. *et al., Nat. Prod. Lett.*, 2000, **14**, 387-392 (*Pellynol F, isol, activity*)

18,29-Tritriacontadiene-2,4,32-triyne-1,6,31-triol T-770

$HC{\equiv}CCH(OH)CH{=}CH(CH_2)_9CH{=}CH(CH_2)_{11}CH(OH)C{\equiv}CC{\equiv}CCH_2OH$
$C_{33}H_{52}O_3$ 496.772

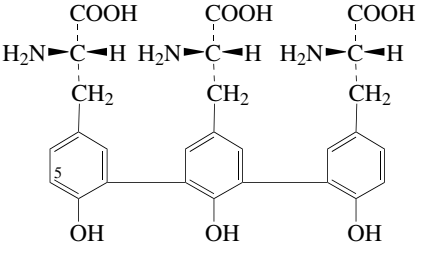
(-)-(18Z,29E)-form
Pellynol A
[186248-09-9]
Isol. from the sponges *Pellina triangulata* and *Haliclona* sp. Exhibits cytotoxic activity to human cell lines. $[\alpha]_D$ -8.5 (c, 1 in $CHCl_3$).

31-Ketone: 28,33-Dihydroxy-4,15-tritriacontadien-1,29,31-triyn-3-one. ***Halicynone A***
$C_{33}H_{50}O_3$ 494.756
Isol. from the sponge *Haliclona* sp. Oil. $[\alpha]_D$ +68.6 (c, 0.03 in $CHCl_3$). λ_{max} 228; 254 (MeOH).

Fu, X. *et al., Tetrahedron*, 1997, **53**, 799-814 (*isol, ir, pmr, cmr*)
Rashid, M.A. *et al., Nat. Prod. Lett.*, 2000, **14**, 387-392 (*isol, activity*)
Zhou, G.-X. *et al., Mar. Drugs*, 2003, **1**, 46-53 (*Halicynone A*)

Trityrosine T-771

[1064-50-2]



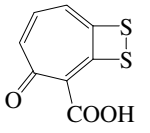
$C_{27}H_{29}N_3O_9$ 539.541
Isol. from the embryo of the sea urchin *Hemicentrotus pulcherrimus* and larvae of *Sarcophaga bullata*. Protein crosslinking agent.

5-Bromo: ***5-Bromotrityrosine***
[59985-26-1]
$C_{27}H_{28}BrN_3O_9$ 618.437
Isol. from the exocuticle of the crab *Cancer pagurus*. Protein crosslinking agent.

Welinder, B.S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **53**, 529-533 (*5-Bromotrityrosine*)
Sugumaran, M. *et al., Biochemistry*, 1982, **21**, 6509-6515 (*isol*)
Sakura, S. *et al., Photochem. Photobiol.*, 1984, **40**, 731-734 (*uv, fluorescence*)
Nomura, K. *et al., Biochemistry*, 1990, **29**, 4525-4534 (*isol*)
Skaff, O. *et al., J.O.C.*, 2005, **70**, 7353-7363 (*synth*)

Tropodithietic acid T-772

*4-Oxo-4*H*-3-cycloheptadithietecarboxylic acid*

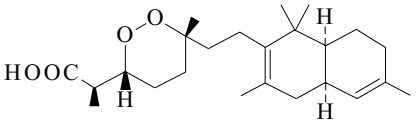


$C_8H_4O_3S_2$ 212.25
Prod. by the marine-derived *Ruegeria* sp. strain T5. Orange solid. Dec. at 220-229°. λ_{max} 216 (log ϵ 4.36); 303 (log ϵ 4.16); 354 (log ϵ 3.67); 448 (log ϵ 3.08) (MeOH). λ_{max} 210 (log ϵ 4.3); 303 (log ϵ 4.19); 355 (log ϵ 3.69); 452 (log ϵ 3.04) (MeOH/HCl). λ_{max} 219 (log ϵ 4.45); 307 (log ϵ 4.11); 445 (log ϵ 3.16) (MeOH/NaOH).

Liang, L. *et al., Dissertation*, Univ. of Göttingen, 2003, (*isol, uv, ir, pmr, cmr, ms, biosynth, cryst struct*)

Trunculin A T-773

[105969-64-0]

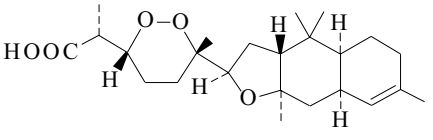


$C_{24}H_{38}O_4$ 390.562
Constit. of *Latrunculia brevis*. Cryst. (MeOH aq.) (as Me ester). Mp 66.5-67.5° (Me ester). $[\alpha]_D$ +158.3 (c, 1.02 in $CHCl_3$) (Me ester).

Capon, R.J. *et al., J.O.C.*, 1987, **52**, 339 (*cryst struct*)

Trunculin B T-774

[105969-65-1]

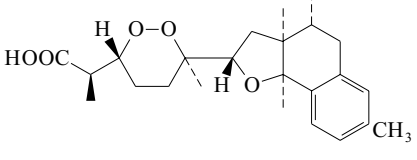


$C_{24}H_{38}O_5$ 406.561
Constit. of *Latrunculia brevis*. Cryst. (MeOH aq.) (as Me ester). Mp 91-93° (Me ester). $[\alpha]_D$ +13.1 (c, 1.54 in $CHCl_3$) (Me ester).

Capon, R.J. *et al., J.O.C.*, 1987, **52**, 339 (*cryst struct*)

Trunculin C T-775

[132410-38-9]



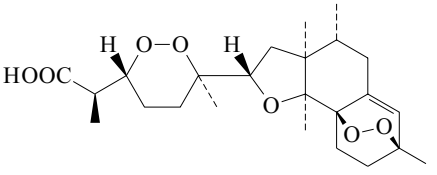
$C_{24}H_{34}O_5$ 402.53

Me ester: [132410-35-6]
$C_{25}H_{36}O_5$ 416.556
Constit. of a *Latrunculia* sp. Cryst.
Mp 138°. $[\alpha]_D$ -46 (c, 0.34 in $CHCl_3$).

He, H.-Y. *et al., J.O.C.*, 1991, **56**, 2112 (*isol, pmr, cmr, cryst struct*)

Trunculin D T-776

[132410-40-3]



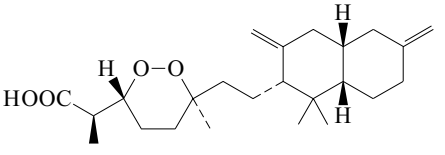
$C_{24}H_{36}O_7$ 436.544

Me ester: [132410-36-7]
$C_{25}H_{38}O_7$ 450.571
Constit. of a *Latrunculia* sp. Oil. $[\alpha]_D$ -24 (c, 1.28 in $CHCl_3$).

He, H.-Y. *et al., J.O.C.*, 1991, **56**, 2112 (*isol, pmr, cmr*)

Trunculin E T-777

[132410-39-0]

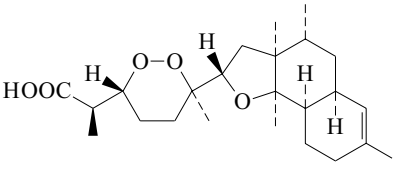


$C_{24}H_{38}O_4$ 390.562
Constit. of a *Latrunculia* sp. Cryst.
Mp 103°. $[\alpha]_D$ -69 (c, 1.2 in $CHCl_3$).

He, H.-Y. *et al., J.O.C.*, 1991, **56**, 2112 (*isol, pmr, cmr*)

Trunculin F T-778

[147391-81-9]

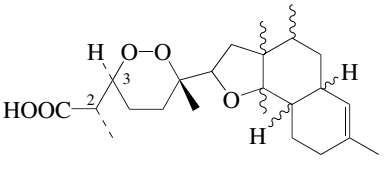


$C_{24}H_{38}O_5$ 406.561
Constit. of *Latrunculia conulosa*. Unstable oil. $[\alpha]_D$ -27.7 (c, 2.68 in $CHCl_3$) (Me ester).

Butler, M.S. *et al., Aust. J. Chem.*, 1993, **46**, 1363 (*isol, pmr, cmr*)

Trunculin H T-779

[213740-51-3]

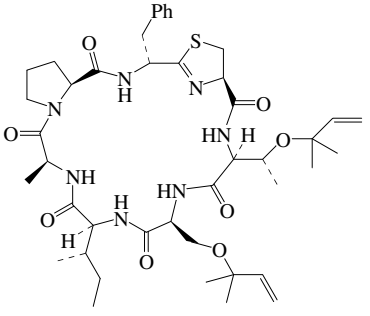


$C_{24}H_{38}O_5$ 406.561
Constit. of a *Latrunculia* sp. Yellow oil (as Me ester). $[\alpha]_D$ +56.2 (c, 0.7 in $CHCl_3$) (Me ester).

2,3-Diepimer: ***Trunculin I***
[213740-52-4]
$C_{24}H_{38}O_5$ 406.561
Constit. of a *Latrunculia* sp. Yellow oil (as Me ester). $[\alpha]_D$ -1.4 (c, 0.4 in $CHCl_3$) (Me ester).
Ovenden, S.P.B. *et al., Aust. J. Chem.*, 1998, **51**, 573-579 (*isol, pmr, cmr*)

Trunkamide A T-780

[181758-83-8]

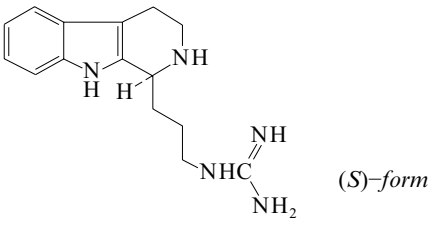


Absolute Configuration

$C_{43}H_{63}N_7O_8S$ 838.079
Cyclic heptapeptide. Isol. from an ascidian *Lissoclinum* sp. Shows promising antitumour activity. Oil. $[\alpha]_D$ -231 (c, 0.06 in $CHCl_3$). λ_{max} 248 (ϵ 14300) (EtOH).
Carroll, A.R. *et al., Aust. J. Chem.*, 1996, **49**, 659-667 (*isol, uv, ir, pmr, cmr, ms*)
PCT Int. Appl., 1997, 1997 039 025; *CA*, **127**, 290919m
Wipf, P. *et al., J.O.C.*, 2000, **65**, 1037-1049 (*synth, abs config*)
Caba, J.M. *et al., J.O.C.*, 2001, **66**, 7568-7574 (*synth*)
Salvatella, X. *et al., J.O.C.*, 2003, **68**, 211-215 (*pmr, struct*)
McKeever, B. *et al., Tetrahedron*, 2003, **59**, 2713-2727 (*synth*)

Trypargine T-781

*3-[(2,3,4,9-Tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-yl)propyl]guanidine, 9CI. 1-(3-Guanidinopropyl)-1,2,3,4-tetrahydro-β-carboline*



(*S*)–*form*

$C_{15}H_{21}N_5$ 271.364

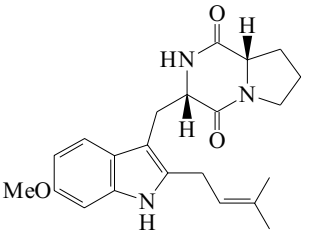
(S)-form [82054-21-5]
[82372-68-7]
Obt. from the skin of the African frog *Kassina senegalensis.* Needles (as hydrochloride).
Mp 204-207° (hydrochloride). $[\alpha]_D^{15}$ +37.2 (c, 0.54 in MeOH) (hydrochloride).
▶ Highly toxic.

(±)-*form* [82264-57-1]
[82264-58-2, 82264-59-3]
Alkaloid from a *Eudistoma* sp.
Pale yellow prisms (MeOH/Et_2O) (as hydrochloride).
Mp 202-206° (hydrochloride).

1,2-Didehydro: ***Trypargimine***
[228113-43-7]
$C_{15}H_{19}N_5$ 269.349
Alkaloid from a *Eudistoma* sp. Light yellow solid. λ_{max} 206 (log ϵ 4.5); 236 (log ϵ 4.3); 254 (log ϵ 4); 316 (log ϵ 4.3); 348 (log ϵ 3.9) (MeOH).
Akizawa, T. *et al., Biomed. Res.*, 1982, **3**, 232-234 (*isol, pmr, cmr, ms*)
Shimizu, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 909-914; 3453-3456; 4529-4533 (*synth, resoln, spectra*)
Shimizu, M. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1313-1325 (*synth, cryst struct, abs config*)
Van Wagoner, R.M. *et al., J. Nat. Prod.*, 1999, **62**, 794-797 (*Trypargimine*)

Tryprostatin A T-782

[171864-80-5]

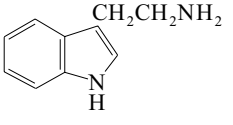


$C_{22}H_{27}N_3O_3$ 381.474
Prod. by the marine-derived *Aspergillus fumigatus.* Mammalian cell cycle inhibitor. Mycotoxin. Microtubule polym. inhibitor. Pale yellow cryst. Sol. MeOH, EtOAc, Me_2CO.
Mp 120-123°. $[\alpha]_D^{27}$ -69.7 (c, 0.7 in $CHCl_3$). Related to Fumitremorgin C, F-131. λ_{max} 227 (ϵ 24540); 270 (ϵ 5450); 297 (ϵ 6590) (MeOH).

Demethoxy: ***Tryprostatin B***
[179936-52-8]
$C_{21}H_{25}N_3O_2$ 351.447
Prod. by the marine-derived *Aspergillus fumigatus.* Cell cycle progression and microtubule polym. inhibitor. Mycotoxin. Pale yellow cryst. Sol. MeOH, Me_2CO, EtOAc.
Mp 102-105°. $[\alpha]_D^{27}$ -71.1 (c, 0.6 in $CHCl_3$). λ_{max} 226 (23780); 277 (8690); 298 (sh) (7180) (MeOH).
Cui, C.-B. *et al., J. Antibiot.*, 1995, **48**, 1382; 1996, **49**, 527; 534 (*isol, uv, ir, props*)
Gan, T. *et al., J.O.C.*, 1997, **62**, 9298-9304 (*synth*)
Kondoh, M. *et al., J. Antibiot.*, 1998, **51**, 801-804 (*activity*)
Zhao, S. *et al., Tet. Lett.*, 1998, **39**, 7009-7012 (*synth*)
Schkeryantz, J.M. *et al., J.A.C.S.*, 1999, **121**, 11964-11975 (*synth*)
Cardoso, A.S. *et al., Tet. Lett.*, 2000, **41**, 3611-3613 (*Tryprostatin B, synth*)
Wang, B. *et al., Tet. Lett.*, 2001, **42**, 1463-1466 (*Tryprostatin B, synth*)
Caballero, E. *et al., J.O.C.*, 2003, **68**, 6944-6951 (*Tryprostatin B, synth*)

Tryptamine T-783

*1*H*-Indole-3-ethanamine, 9CI. 3-(2-Aminoethyl)indole. 2-(3-Indolyl)ethylamine*
[61-54-1]



$C_{10}H_{12}N_2$ 160.218
Occurs widely in plants, esp. *Acacia* spp., *Lens esculenta* (lentil) and *Prosopis juliflora* (Leguminosae) and the fungi *Panaeolus foenisicii* and *Coprinus micaceus* (glistening ink cap). Also obt. from the gorgonian *Paramuricea chamaeleon*. Shows psychotropic effects. Needles (petrol). V. spar. sol. Et_2O, $CHCl_3$, C_6H_6.
Mp 118°. $Bp_{0.15}$ 137°. pK_{a1} -6.31; pK_{a2} 10.2 (25°). Log P 1.27 (calc).
▶ LD_{50} (rat, ipr) *ca.* 223 mg/kg. NL4020000

Hydrochloride: [343-94-2]
Needles (EtOH/EtOAc). Mp 248°.
▶ LD_{50} (mus, ipr) 197 mg/kg. NL4375000

N^b-*Ac:* ***N^b-Acetyltryptamine***
[1016-47-3]
$C_{12}H_{14}N_2O$ 202.255
Alkaloid from leaves of *Prosopis nigra*. Prod. by *Cytophaga marinoflava* sp. AM13.1 and marine-derived fungus isol. from *Gracilaria verrucosa*.
Mp 77°.

N^b-*(3-Methylbutanoyl):* ***Madugin***
[179027-43-1]
$C_{15}H_{20}N_2O$ 244.336
Alkaloid from the leaves of *Clausena indica*. Prod. by *Cytophaga marinoflava* sp. AM13.1. Oil. λ_{max} 224; 274 (sh); 283; 292 (Et_2O).

N^b-*(3-Methyl-2Z-dodecenoyl):* N^b-*(3-Methyl-2-dodecenoyl)tryptamine.* ***Granulatamide A***
[881417-85-2]
$C_{23}H_{34}N_2O$ 354.534
Constit. of *Eunicella granulata*. Cytotoxic. Pale yellow oil.

N^b-*(3,5-Dimethyl-2Z,4E-dodecadienoyl):* N^b-*(3,5-Dimethyl-2,4-dodecadienoyl)*. ***Granulatamide B***
[881417-94-3]
$C_{24}H_{34}N_2O$ 366.545
Constit. of *Eunicella granulata*. Cytotoxic. Pale yellow oil.

N^b-*(7S-Methoxy-4E-tetradecenoyl):* N-*(7-Methoxy-4-tetradecenoyl)tryptamine.* ***Hermitamide B***
$C_{25}H_{38}N_2O_2$ 398.587
Alkaloid from *Lyngbya majuscula*. Cytotoxic agent. Pale yellow oil. $[\alpha]_D^{26}$ -4.5 (c, 0.1 in $CHCl_3$). λ_{max} 224 (ϵ 13600); 282 (ϵ 3600); 292 (ϵ 3000) (EtOH).

[54268-28-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 660C; 660D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 131C (*nmr*)
Ewins, A.J. *et al., J.C.S.*, 1911, **99**, 270-273 (*synth*)
White, E.P. *et al., N.Z. J. Sci. Technol., Sect. B*, 1944, **25**, 137-162; 1951, **33**, 54-60; 1957, **38**, 718-725 (*isol, occur*)
Cohen, L.A. *et al., J.A.C.S.*, 1960, **82**, 2184-2187 (*pmr*)
Jackson, A.H. *et al., J.C.S.*, 1965, 3498-3500 (*synth, struct*)
Kametani, T. *et al., Synthesis*, 1972, 475 (*synth*)
Wakahara, A. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 2481-2486 (*cryst struct*)
Cimino, G. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1978, **61**, 361-362 (*isol*)
Morales-Rios, M.S. *et al., Magn. Reson. Chem.*, 1987, **25**, 377-395 (*cmr*)
Riemer, B. *et al., Phytochemistry*, 1997, **45**, 337-341 (*Madugin*)
Tan, L.T. *et al., J. Nat. Prod.*, 2000, **63**, 952-955 (*Hermitamide B*)
Li, Y. *et al., Arch. Pharmacal Res.*, 2003, **26**, 21-23 (N^b-*Ac, marine, isol*)
Shabaan, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*Cytophaga marinoflava derivs*)
Reyes, F. *et al., J. Nat. Prod.*, 2006, **69**, 668-670 (*Granulatamides*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AJX000; AJX250

Tryptophylvalylvalylglycylaspartylvalylglutamine T-784

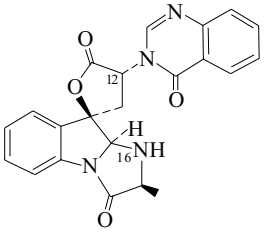
[157724-13-5]
H-Trp-^{2}Val-Val-Gly-Asp-Val-Gln-OH
$C_{37}H_{55}N_9O_{11}$ 801.895
Isol. from the annelid *Perinereis vancaurica*.

2-Methionine analogue: Tryptophylmethionylvalylglycylaspartylvalylglutamine
[157724-14-6]
$C_{37}H_{55}N_9O_{11}S$ 833.961
Isol. from *Perinereis vancaurica*.

Takahashi, T. *et al., Pept. Chem.*, 1993, **31**, 169-174 (*isol*)
Takahashi, T. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1995, **110**, 297-304 (*isol, struct*)

Tryptoquivaline F T-785

Fumitremorgin F. FTF
[61897-89-0]



$C_{22}H_{18}N_4O_4$ 402.409
Isol. from *Aspergillus fumigatus*. Tremorgenic toxin. Fine needles (MeOH).
Mp 277° dec. $[\alpha]_D^{15.5}$ -109 (c, 0.006 in $CHCl_3$). λ_{max} 226 (ϵ 33400); 303 (ϵ 2800); 315 (ϵ 2200) (MeOH) (Berdy).
▶ Toxic.

N-*Ac:* [61897-90-3]
Needles (MeOH). Mp 280-283° dec. $[\alpha]_D^{12}$ -116 (c, 0.12 in $CHCl_3$).

N^{16}-*Hydroxy:* ***Tryptoquivaline H***. *Fumitremorgin H. FTH*
[61949-67-5]
$C_{22}H_{18}N_4O_5$ 418.408
Isol. from *Aspergillus fumigatus*. Tremorigen. Fine needles (MeOH).
Mp 274° dec. $[\alpha]_D^{11}$ -155 (c, 0.02 in Me_2CO). λ_{max} 226 (ϵ 33100); 303 (ϵ 3100); 315 (ϵ 2500) (MeOH) (Berdy).
▶ Toxic.

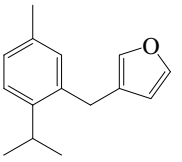
N^{16}-*Hydroxy,* O-*Ac:* [61897-88-9]
Prisms ($MeOH/CH_2Cl_2$). Mp 231-234°. $[\alpha]_D^{16.5}$ +243 (c, 0.0095 in Me_2CO).

12-Epimer: ***Tryptoquivaline J***. *FTJ*
[66212-51-9]
$C_{22}H_{18}N_4O_4$ 402.409
Isol. from *Aspergillus fumigatus*. Tremorigen. Fine needles (Me_2CO/MeOH).
Mp 254-258° dec. $[\alpha]_D^{14}$ +135 (c, 0.024 in Me_2CO). λ_{max} 225 (ϵ 41000); 302 (ϵ 3900); 310 (ϵ 3100) (MeOH) (Berdy).
▶ Toxic.

Yamazaki, M. *et al., Chem. Pharm. Bull.*, 1978, **26**, 111-117 (*isol, uv, ir, pmr, ms*)
Afiyatullov, S.S. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2005, **41**, 236-238 (*Tryptoquivaline J, marine isol*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 440; 444; 448

Tsitsikammafuran T-786

3-[5-Methyl-2-(1-methylethyl)phenylmethyl]furan
[321310-28-5]

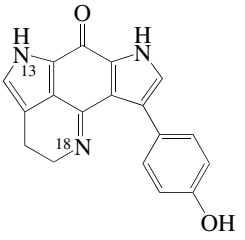


$C_{15}H_{18}O$ 214.307
Constit. of a South African *Dysidea* sponge.

McPhail, K.L. *et al., Tetrahedron*, 2000, **56**, 9391-9396 (*isol, pmr, cmr, synth*)

Tsitsikammamine A T-787

[183114-86-5]



$C_{18}H_{13}N_3O_2$ 303.32
Related to Wakayin, W-11. Alkaloid from the South African latrunculid sponge *Tsitsikamma flavus* and another sponge. Cytotoxic. Exhibits antimicrobial activity. λ_{max} 242; 317; 377 (MeOH) (Berdy).

N^{13}-*Me:* ***Tsitsikammamine B***
[183114-88-7]
$C_{19}H_{15}N_3O_2$ 317.346
Alkaloid from *Tsitsikamma flavus* and a marine sponge. Cytotoxic. Exhibits antimicrobial activity. λ_{max} 242; 317; 374 (MeOH) (Berdy).

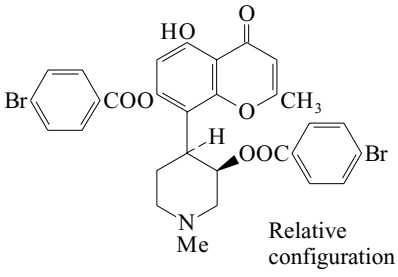
N^{18}-*Hydroxy:* ***Tsitsikammamine A*** $\mathbf{N^{18}}$***-oxime***
$C_{18}H_{14}N_3O_3^{\oplus}$ 320.327
Alkaloid from *Tsitsikamma flavus*. Bright orange-red solid.

N^{18}-*Hydroxy,* N^{13}-*Me:* ***Tsitsikammamine B*** $\mathbf{N^{18}}$***-oxime***
$C_{19}H_{16}N_3O_3^{\oplus}$ 334.354
Alkaloid from *Tsitsikamma flavus*. Bright orange-red solid.

Hooper, G.J. *et al., Tet. Lett.*, 1996, **37**, 7135-7138 (*isol, uv, ir, pmr, cmr*)
Antunes, E.M. *et al., J. Nat. Prod.*, 2004, **67**, 1268-1276 (*oximes*)

Tubastraine T-788

[114216-90-9]

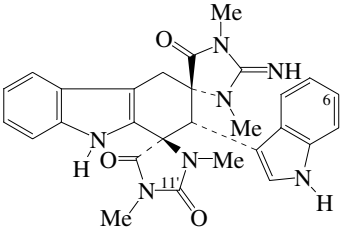


$C_{30}H_{25}Br_2NO_7$ 671.338
Alkaloid from the non-symbiotic marine coral *Tubastrea micrantha*. Glassy compd.
Mp 122°. First chromone isol. from a marine invertebrate. Possibly derived from dietary sources.

Alam, M. *et al., Heterocycles*, 1988, **27**, 719 (*isol, ir, pmr, cmr, ms, struct*)

Tubastrindole C T-789

[524067-26-3]



$C_{28}H_{27}N_7O_3$ 509.566
Alkaloid from a stony coral *Tubastrea* sp.
$[\alpha]_D$ -20 (c. 0.04 in MeOH).

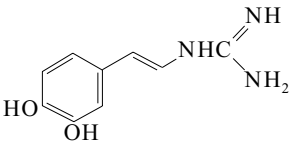
11′-Imide: ***Tubastrindole B***
[524067-25-2]
$C_{28}H_{28}N_8O_2$ 508.582
Alkaloid from a *Tubastrea* sp.
$[\alpha]_D$ -26 (c, 0.07 in MeOH).

6-Bromo, 11′-imide: ***Tubastrindole A***
[524067-24-1]
$C_{28}H_{27}BrN_8O_2$ 587.478
Alkaloid from a *Tubastrea* sp.
$[\alpha]_D$ -38 (c, 0.13 in MeOH). λ_{max} 284 (ϵ 2800); 294 (ϵ 2100) (no solvent reported).

Iwagawa, T. *et al., Tet. Lett.*, 2003, **44**, 2533-2535 (*isol, pmr, cmr*)

Tubastrine T-790

2-[(3,4-Dihydroxyphenyl)ethenyl]guanidine, 9CI. 3,4-Dihydroxy-β-guanidinostyrene. β-(Aminoiminomethyl)amino-3,4-dihydroxystyrene
[107585-47-7]



$C_9H_{11}N_3O_2$ 193.205
Constit. of the coral *Tubastrea aurea*. Shows antiviral props. Light yellow solid. Sol. Me_2CO, MeOH; fairly sol. EtOAc; poorly sol. H_2O.
Mp 173-175°. λ_{max} 222 (ϵ 14500); 287 (ϵ 18500); 304 (ϵ 14000) (MeOH) (Berdy).

3′-Deoxy: ***3′-Deoxytubastrine***
[160525-08-6]
$C_9H_{11}N_3O$ 177.205
Alkaloid from the Australian marine sponge *Spongosorites* sp. Shows modest antibiotic activity. Oil (as monohydrochloride trihydrate). Unnamed in the paper. CAS no. refers to the monohydrochloride. λ_{max} 219 (ϵ 13000); 282 (ϵ 19000); 289; 308 (EtOH) (Berdy).

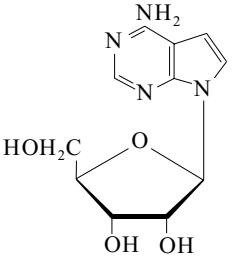
1,2-Dihydro: ***7,8-Dihydrotubastrine***
$C_9H_{13}N_3O_2$ 195.221
Alkaloid from the sponge *Petrosia* cf. *contignata*. Brown viscous oil. λ_{max} 222 (ϵ 3900); 284 (ϵ 1900) (MeOH).

4′-Deoxy, 1,2-dihydro: ***4-Deoxy-7,8-dihydrotubastrine***
$C_9H_{13}N_3O$ 179.221
Isol. from the sponge *Petrosia* cf. *contignata*. Brown viscous oil. λ_{max} 214 (ϵ 4700); 274 (ϵ 1400) (MeOH).

Sakai, R. *et al., Chem. Lett.*, 1987, 127 (*isol*)
Urban, S. *et al., Aust. J. Chem.*, 1994, **47**, 2279 (*3′-Deoxytubastrine*)
Sperry, S. *et al., J. Nat. Prod.*, 1998, **61**, 859-861 (*Dihydrotubastrines*)

Tubercidin T-791

*7-Ribofuranosyl-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-amine, 9CI. 4-Amino-7-ribofuranosyl-7*H*-pyrrolo[2,3-*d*]pyrimidine, 8CI. 7-Deazaadenosine. Sparsomycin A. B 79D. NSC 56408. U 10071. XK 101-1. Antibiotic B 79D. Antibiotic XK 101-1*
[69-33-0]



$C_{11}H_{14}N_4O_4$ 266.256
Nucleoside antibiotic. Isol. from *Streptomyces tubercidus*. Major cytotoxin of *Tolypothrix byssoidea*. Also prod. by *Micromonospora chalcea tubercidica*. Constit. of the sponge *Caulospongia biflabellata*. Antitumour, antifungal and antiviral agent. Nucleoside transporter substrate. Cryst.
Mp 247° dec. $[\alpha]_D^{17}$ -67 (50% AcOH). pK_a 5.3. λ_{max} 227 (ϵ 25000); 272 (ϵ 12200) (dil HCl) (Derep). λ_{max} 270 (ϵ 12100) (dil. NaOH) (Derep). λ_{max} 270 (ϵ 12100) (H_2O) (Derep).
▶ LD_{50} (rat, orl) 16 mg/kg. UY8870000

5′-O-Sulfamoyl: ***Antibiotic SF 2494****. SF 2494*
[114746-65-5]
$C_{11}H_{15}N_5O_6S$ 345.335
From *Streptomyces mirabilis.* Herbicide.

5′-Deoxy: ***5′-Deoxytubercidin***
[41107-17-9]
$C_{11}H_{14}N_4O_3$ 250.257
Isol. from *Didemnum voeltzkowi*. Cryst. (EtOH/C_6H_6).
Mp 203-207°. $[\alpha]_D^{23}$ -70.3 (c, 0.48 in DMSO). λ_{max} 270 (ϵ 12700) (MeOH).

5′-α-D-Glucopyranosyl: ***Tubercidin 5′-α-D-glucopyranose***
[117456-78-7]
$C_{17}H_{24}N_4O_9$ 428.398
Found in *Plectonema radiosum* and *Tolypothrix distorta*. Cytotoxic. Antifungal. Sol. H_2O. $[\alpha]_D^{25}$ +10 (c, 0.01 in H_2O). λ_{max} 268 (ϵ 9300) (H_2O) (Derep).

5-Bromo, 5′-deoxy: ***5-Bromo-5′-deoxytubercidin, 9CI***
[95931-82-1]
$C_{11}H_{13}BrN_4O_3$ 329.153
Isol. from *Didemnum voeltzkowi*.

5-Iodo, 5′-deoxy: ***5′-Deoxy-5-iodotubercidin***
[85209-84-3]
$C_{11}H_{13}IN_4O_3$ 376.153
Constit. of *Hypnea valentiae* and *Didemnum voleltzowi*. Smooth muscle relaxant, hypothermic agent, inhibitor of adenosine kinase.
Cryst. (Py).
Mp 227-228° dec. $[\alpha]_D^{25}$ -55 (c, 0.2 in MeOH).

1′-Epimer, 5-iodo, 5′-deoxy: [85209-85-4]
$C_{11}H_{13}IN_4O_3$ 376.153
Constit. of *Hypnea valentiae* and *Didemnum voleltzowi*. Muscle relaxant. Pale yellow gum.

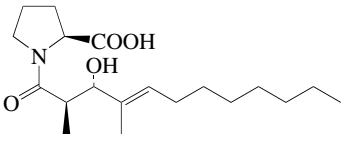
2′-Epimer: Aratubercidin. Ara Tb
[64526-34-7]
$C_{11}H_{14}N_4O_4$ 266.256
Shows antiviral props. Mp 125-126°. $[\alpha]_D^{24}$ +6.9 (c, 0.5 in DMF).

▶ UY8820000

Anzai, K. *et al., J. Antibiot., Ser. A*, 1957, **10**, 201-204 (*isol*)
Mizuno, Y. *et al., J.O.C.*, 1963, **28**, 3329-3331 (*struct, uv, config*)
Smulson, M.E. *et al., J. Biol. Chem.*, 1967, **242**, 2872-2876 (*biosynth*)
Tolman, R.L. *et al., J.A.C.S.*, 1969, **91**, 2102-2108 (*synth, uv, ir, nmr*)
Abola, J. *et al., Acta Cryst. B*, 1973, **29**, 697-703 (*cryst struct*)
Chenon, M.-T. *et al., J.A.C.S.*, 1975, **97**, 4627-4636 (*pmr, cmr*)
Robbins, M.J. *et al., Can. J. Chem.*, 1977, **55**, 1260 (*Aratubercidin*)
Ektova, L.V. *et al., Bioorg. Khim.*, 1978, **4**, 1250-1255; *Sov. J. Bioorg. Chem. (Engl. Transl.)*, 1978, **4**, 907-910 (*synth*)
Fukushima, K. *et al., J. Antibiot.*, 1978, **31**, 377-378 (*ms*)
Japan. Pat., 1978, 78 124 685; *CA*, **90**, 136241v (*isol*)
Uzawa, J. *et al., Org. Magn. Reson.*, 1979, **12**, 612-615 (*cmr*)
Seela, F. *et al., Angew. Chem., Int. Ed.*, 1981, **20**, 97 (*Aratubercidin*)
Kazlauskas, R. *et al., Aust. J. Chem.*, 1983, **36**, 165-170 (*5-iodo-5′-deoxy, 1′-epimer 5-iodo-5′-deoxy*)
Barchi, J.J. *et al., Phytochemistry*, 1983, **22**, 2851-2852 (*isol*)
Seela, F. *et al., Annalen*, 1984, 1972-1980 (*synth, cmr*)
Yoo, J.C. *et al., J. Liq. Chromatogr.*, 1984, **7**, 151-158 (*hplc*)
Bergstrom, D.E. *et al., J. Med. Chem.*, 1984, **27**, 285-292 (*props*)
Cook, A.F. *et al., Nucleosides Nucleotides*, 1984, **3**, 401-411 (*5-Bromo-5′-deoxytubercidin, 5-iodo-5′-deoxy, synth*)
Ramasamy, K. *et al., Tet. Lett.*, 1987, **28**, 5107-5110 (*synth*)
Iwata, M. *et al., CA*, 1988, **109**, 3509 (*SF2494*)
Stewart, J.B. *et al., J. Antibiot.*, 1988, **41**, 1048-1056 (*5′-glucosyl*)
Isono, K. *et al., J. Antibiot.*, 1988, **42**, 1711-1739 (*rev*)
Reddy, A.M. *et al., J. Het. Chem.*, 1990, **27**, 1297-1305 (*ms*)
Plagemann, P.G. *et al., Biochem. Pharmacol.*, 1991, **42**, 247-252 (*pharmacol*)
Mitchell, S.S. *et al.,* J. Nat. Prod., 1996, **59**, 1000-1001 (*5′-deoxy, 5-bromo-5′-deoxy, 5-iodo-5′-doxy*)
Biabani, M.F. *et al., Pharm. Biol.*, 2002, **40**, 302-303 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, TNY500

Tumonoic acid A T-792

N-*(3-Hydroxy-2,4-dimethyl-4-dodecenoyl)proline*

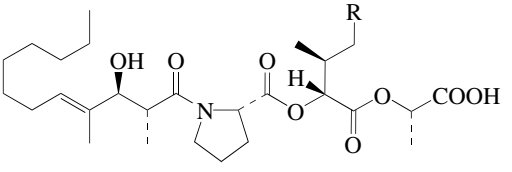


$C_{19}H_{33}NO_4$ 339.474
Isol. from a cyanobacterial assemblage of *Lyngbya majuscula* and *Schizothrix calcicola*. Pale yellow oil. $[\alpha]_D$ -79 (c, 1.1 in $CHCl_3$).

Me ester:
$C_{20}H_{35}NO_4$ 353.501
Isol. from *Lyngbya majuscula* and *Schizothrix calcicola*. Pale yellow oil. $[\alpha]_D$ -51 (c, 1.3 in $CHCl_3$).

Harrigan, G.G. *et al., J. Nat. Prod.*, 1999, **62**, 464-467 (*isol, pmr, cmr, ms*)

Tumonoic acid B T-793



R = CH_3

$C_{28}H_{47}NO_8$ 525.681
Acyclic depsipeptide. Isol. from a cyanobacterial assemblage of *Lyngbya majuscula* and *Schizothrix calcicola*. Pale yellow oil. $[\alpha]_D$ -14 (c, 1.6 in $CHCl_3$).

Me ester:
$C_{29}H_{49}NO_8$ 539.708
Isol. from *Lyngbya majuscula* and *Schizothrix calcicola*. Pale yellow oil. $[\alpha]_D$ -76 (c, 1 in $CHCl_3$).

Harrigan, G.G. *et al., J. Nat. Prod.*, 1999, **62**, 464-467 (*isol, pmr, cmr, ms*)

Tumonoic acid C T-794

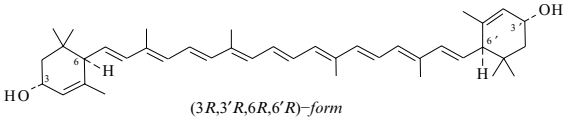
As Tumonoic acid B, T-793 with
R = H

$C_{27}H_{45}NO_8$ 511.654
Acyclic depsipeptide. Isol. from a cyanobacterial assemblage of *Lyngbya majuscula* and *Schizothrix calcicola*. Pale yellow oil. $[\alpha]_D$ -35 (c, 1.2 in $CHCl_3$).

Harrigan, G.G. *et al., J. Nat. Prod.*, 1999, **62**, 464-467 (*isol, pmr, cmr, ms*)

Tunaxanthin T-795

ϵ,ϵ-Carotene-3,3′-diol
[12738-95-3]



(3R,3′R,6R,6′R)–form

$C_{40}H_{56}O_2$ 568.881
Isol. in various pigments of fish and crustaceans.

(3R,3′R,6R,6′R)-form
Tunaxanthin F. Lactucaxanthin
[78306-12-4]

Monoketone: ***3′-Hydroxy-ϵ,ϵ-caroten-3-one***
[102679-34-5]
$C_{40}H_{54}O_2$ 566.865
Isol. from *Thunnus obesus* and *Acanthochiton defilippi*.

(3R,3′R,6R,6′S)-form
Tunaxanthin H
[97673-78-4]
Monoketone: [112923-80-5]
Isol. from *Thunnus obesus.*

(3R,3′R,6S,6′S)-form
Tunaxanthin C. Oxyxanthin 58
[71697-13-7]
Monoketone: [97169-06-7]
Isol. from dolphin eggs (presumably from a dietary source).

(3R,3′S,6R,6′R)-form
Tunaxanthin I*. Chiriquixanthin A*
[63597-82-0]
Also isol. from the skin of *Atelopus chiriquiensis.*

(3R,3′S,6R,6′S)-form
Tunaxanthin E
[82915-90-0]

(3R,3′S,6S,6′R)-form
Tunaxanthin D
[82915-89-7]

(3R,3′S,6S,6′S)-form
Tunaxanthin B. Oxyxanthin 51
[72274-50-1]
Monoketone: [97112-40-8]
Isol. from dolphin eggs (from a dietary source). λ_{max} 415; 438; 468 (petrol).

(3S,3′S,6R,6′R)-form
Tunaxanthin J*. Chiriquixanthin B*
[63597-83-1]
Also isol. from skin of *Atelopus chiriquiensis.*

(3S,3′S,6R,6′S)-form
Tunaxanthin G
[97746-99-1]

(3S,3′S,6S,6′S)-form
Tunaxanthin A. Oxyanthin 4S
[71697-14-8]
Diketone: See ϵ,ϵ-Carotene-3,3′-dione, C-134
Monoketone: Isol. from *Thunnus obesus* and *Acanthochiton defilippi.*
[82915-92-2, 83148-14-5]

Bingham, A. *et al., Chem. Comm.*, 1977, 96 (*Chiriquixanthins*)
Ronneberg, H. *et al., Acta Chem. Scand., Ser. B*, 1978, **32**, 621 (*struct, pmr, ms, uv, cd, abs config*)
Vecchi, M. *et al., Helv. Chim. Acta*, 1982, **65**, 1050 (*pmr, hplc*)
Matsuno, T. *et al., CA*, 1983, **100**, 85953u; 1984, **101**, 207845d (*isol*)
Miki, W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 195 (*biosynth*)
Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 779 (*ketones*)
Ikuno, Y. *et al., J. Chromatogr.*, 1985, **328**, 387 (*hplc*)
Ikuno, Y. *et al., Nippon Suisan Gakkaishi*, 1987, **53**, 1893-1896; *CA*, **108**, 91899n (*monoketones*)
Tsushima, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **93**, 665-671 (*monoketones*)

Tunicate gonadotrophin-releasing hormones T-796

Tunicate GnRH
5-OxoPro-His-Trp-Ser-Asp-Tyr-Phe-Lys-Pro-Gly-NH_2
Struct. of GnRH-I shown. Isol. from the tunicate *Chelyosoma productum.*

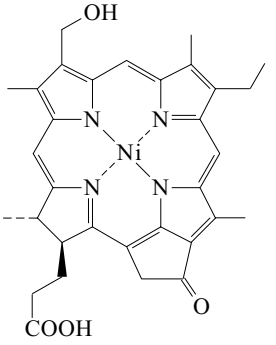
Tunicate GnRH-I [182620-73-1]
$C_{60}H_{75}N_{15}O_{15}$ 1246.344

Tunicate GnRH-II [196863-62-4]
$C_{50}H_{68}N_{16}O_{12}S$ 1117.253
Disulfide-linked dimer; CAS no. and formula refer to monomer.

Powell, J.F. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1996, **93**, 10461-10464 (*isol*)

Tunichlorin T-797

*Nickel(*II*) 2-devinyl-2-hydroxymethylpyrophaeophorbide*
[114571-91-4]

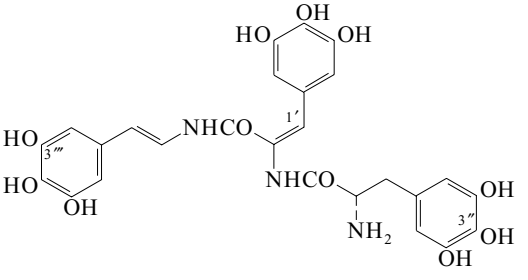


$C_{32}H_{32}N_4NiO_4$ 595.319
The first Ni chlorin isol. from a living organism. Pigment of *Trididemnum solidum*; also isol. from *Dolabella auricularia*. Blue-green. Artifact of hydrol. of numerous long-chain acyltunichlorins (C_{14}-C_{22}), 28 of which were characterised by ms in *T. solideum*. λ_{max} 389; 416; 641 (MeOH) (Berdy). λ_{max} 389 (ϵ 33900); 416 (ϵ 42000); 641 (ϵ 43000) (CH_2Cl_2) (Berdy).

Rinehart, K.L. *et al., J. Nat. Prod.*, 1985, **51**, 1-696 (*isol, ms*)
Bible, K.C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1988, **85**, 4582-4586 (*isol, pmr, cmr, ms*)
Rinehart, K.L. *et al., Pure Appl. Chem.*, 1989, **61**, 525-528 (*isol*)
Pettit, G.R. *et al., J. Nat. Prod.*, 1993, **56**, 1981-1984 (*isol, Dolabella*)
Sings, H.L. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1996, **93**, 10560-10565 (*acyltunichlorins*)

Tunichrome An1 T-798

[116050-17-0]



$C_{26}H_{25}N_3O_{11}$ 555.497
Isol. from the tunicate *Ascidia nigra*. Blood pigment which selectively accumulates vanadium. λ_{max} 210 (ϵ 68000); 245 (sh); 285 (sh); 340 (ϵ 19600) (MeOH) (Derep).

1′Z-Isomer: ***Tunichrome B1***
[97689-87-7]
$C_{26}H_{25}N_3O_{11}$ 555.497
Isol. from *Ascidia nigra*. Sol. MeOH. Dec. in air on warming. λ_{max} 210 (ϵ 68000); 245 (sh); 285 (sh); 340 (ϵ 19600) (MeOH) (Derep).

3″-Deoxy: ***Tunichrome An2***
[115982-31-5]
$C_{26}H_{25}N_3O_{10}$ 539.498
Isol. from *Ascidia nigra*. λ_{max} 210 (ϵ 68000); 245 (sh); 285 (sh); 340 (ϵ 19600) (MeOH) (Derep).

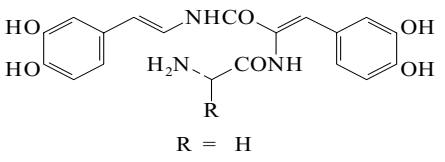
1′Z-Isomer, 3″-deoxy: [133695-74-6]
$C_{26}H_{25}N_3O_{10}$ 539.498
Isol. from *Ascidia nigra*. Unstable.

3″,3‴-Dideoxy: ***Tunichrome An3***
[115982-32-6]
$C_{26}H_{25}N_3O_9$ 523.498
Isol. from *Ascidia nigra*. λ_{max} 210 (ϵ 68000); 245 (sh); 285 (sh); 340 (ϵ 19600) (MeOH) (Derep).

1′Z-Isomer, 3′′,3′′′-dideoxy: [133695-75-7]
$C_{26}H_{25}N_3O_9$ 523.498
Isol. from *Ascidia nigra*. Unstable.
Bruening, R.C. *et al., J.A.C.S.*, 1985, **107**, 5298-5300 (*Tunichrome B1*)
Bruening, R.C. *et al., J. Nat. Prod.*, 1986, **49**, 193 (*Tunichrome B1*)
Oltz, E.M. *et al., J.A.C.S.*, 1988, **110**, 6162-6172 (*isol*)
Horenstein, B.A. *et al., J.A.C.S.*, 1989, **111**, 6242 (*synth*)
Kim, D. *et al., Chem. Comm.*, 1991, 9 (*isol*)
He, X. *et al., Experientia*, 1992, **48**, 367 (*biosynth*)

Tunichrome Mm 1 T-799

*Glycyl-α,β-didehydro-*N*-[2-(3,4-dihydroxyphenyl)ethenyl]-3-hydroxytyrosinamide*
[115982-33-7]



R = H

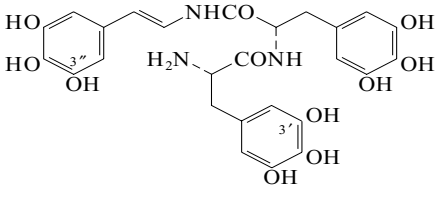
$C_{19}H_{19}N_3O_6$ 385.376
Isol. from the tunicate *Molgula manhattensis*. Readily chelates vanadium. λ_{max} 210 (ϵ 68000); 245 (sh); 285 (sh); 340 (ϵ 19600) (MeOH) (Derep).
Oltz, E.M. *et al., J.A.C.S.*, 1988, **110**, 6162-6172 (*isol*)

Tunichrome Mm 2 T-800

[115982-34-8]
As Tunichrome Mm 1, T-799 with
R = $-CH_2CH(CH_3)_2$
$C_{23}H_{27}N_3O_6$ 441.483
Isol. from the tunicate *Molgula manhattensis*. Readily chelates vanadium. λ_{max} 210 (ϵ 68000); 245 (sh); 285 (sh); 340 (ϵ 19600) (MeOH) (Derep).
Oltz, E.M. *et al., J.A.C.S.*, 1988, **110**, 6162-6172 (*isol*)
Kim, D. *et al., Tet. Lett.*, 1990, **31**, 7119 (*synth*)
Paik, Y.S. *et al., Arch. Pharmacal Res.*, 1992, **15**, 269 (*complexes*)

Tunichrome Pm 1 T-801

*3,5-Dihydroxy-L-tyrosyl-3,5-dihydroxy-*N*-[2-(3,4,5-trihydroxyphenyl)ethenyl]-L-tyrosinamide, 9CI*
[137824-58-9]

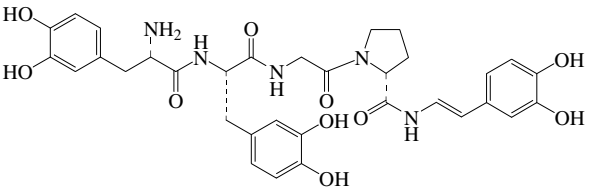


$C_{26}H_{27}N_3O_{11}$ 557.513
Isol. from the tunicate *Phallusia mammillata*. Readily chelates vanadium. λ_{max} 210 (ϵ 68000); 245 (sh); 285 (sh); 340 (ϵ 19600) (MeOH) (Derep). λ_{max} 301 (MeOH) (Berdy).

3′-Deoxy: ***Tunichrome Pm 2***
[137824-59-0]
$C_{26}H_{27}N_3O_{10}$ 541.513
Isol. from *Phallusia mammillata*. Readily chelates vanadium. λ_{max} 210 (ϵ 68000); 245 (sh); 285 (sh); 340 (ϵ 19600) (MeOH) (Derep). λ_{max} 301 (MeOH) (Berdy).

3′′-Deoxy: ***Tunichrome Pm 3***
[137844-97-4]
$C_{26}H_{27}N_3O_{10}$ 541.513
Isol. from *Phallusia mammillata*. Readily chelates vanadium. λ_{max} 210 (ϵ 68000); 245 (sh); 285 (sh); 340 (ϵ 19600) (MeOH) (Derep).
Bayer, E. *et al., Angew. Chem., Int. Ed.*, 1992, **31**, 52-54 (*isol*)

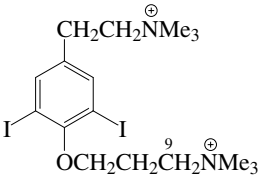
Tunichrome Sp 1 T-802



$C_{33}H_{37}N_5O_{10}$ 663.683
Isol. from the hemocytes of *Styela plicata*. Powder. λ_{max} 227; 280; 311 (no solvent reported).
Tincu, J.A. *et al., J. Nat. Prod.*, 2002, **65**, 377-378 (*isol, pmr*)

Turbotoxin A T-803

[245128-77-2]
[245128-78-3]



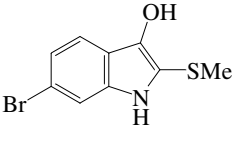
$C_{17}H_{30}I_2N_2O^{2\oplus}$ 532.246
Alkaloid from the Japanese gastropod *Turbo marmorata*. Acetylcholinesterase inhibitor. Isol. as the bis(trifluoroacetate). λ_{max} 226 (ϵ 19000); 239 (sh) (ϵ 9500); 275 (sh) (ϵ 2000) (MeOH) (bistrifluoroacetate).

N^9*-De-Me:* ***Turbotoxin B***
[245128-79-4]
[245128-80-7]
$C_{16}H_{27}I_2N_2O^{\oplus}$ 517.211
Alkaloid from *Turbo marmorata*. Isol. as the bis(trifluoroacetate). λ_{max} 225 (ϵ 11000); 239 (sh) (ϵ 5500); 279 (sh) (ϵ 1500) (MeOH) (bistrifluoroacetate).
Kigoshi, H. *et al., Tetrahedron*, 2000, **56**, 9063-9070 (*isol, synth, uv, pmr, cmr*)

Turritoxins T-804

Two methionine-rich peptides. Isol. from the venoms of the turrid marine snails *Polystira albida* and *Gemmula periscelida*. Neurotoxins.
Lopez-Vera, E. *et al., Toxicon*, 2004, **43(4)**, 365-374 (*isol*)

Tyrindoxol T-805



C_9H_8BrNOS 258.138
Mp 118-120° dec. (Ag salt).

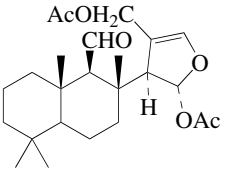
O-*Sulfate: Tyroxindyl sulfate*
[74626-31-6]
$C_9H_8BrNO_4S_2$ 338.203
Constit. of *Dicathais orbita*, *Mancinella keineri*, *Murex* spp. and other molluscs. Precursor of 6,6′-Dibromoindigotin, D-268.
Yellow leaflets + $1H_2O$ (as Ag salt).
Mp 118-120° dec. (Ag salt).

S,S-*Dioxide,* O-*sulfate:*
$C_9H_8BrNO_6S_2$ 370.201
Isol. from *Murex trunculus*, other *Murex* spp. and *Purpura haemastoma*.

Baker, J.T. *et al., Tet. Lett.*, 1968, 43 (*isol, pmr, struct*)
Fouquet, H. *et al., Angew. Chem., Int. Ed.*, 1971, **10**, 816-817 (*isol*)
Baker, J.T. *et al., Tet. Lett.*, 1976, 1233-1234 (*occur*)
Cooksey, C.J. *et al., Molecules*, 2001, **6**, 736-769 (*rev*)

Tyrinnal T-806

[213203-64-6]

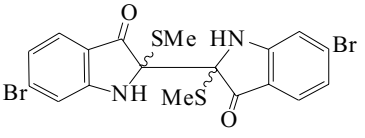


$C_{24}H_{36}O_6$ 420.545
Constit. of *Tyrinna nobilis*. Oil. $[\alpha]_D^{25}$ -14.7 (c, 0.3 in $CHCl_3$).

Fontana, A. *et al., J. Nat. Prod.*, 1998, **61**, 1027-1029 (*isol, pmr, cmr*)

Tyriverdin T-807

2,2′-Bis(methylthio)-6,6′-dibromoindigotin



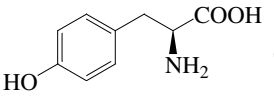
$C_{18}H_{14}Br_2N_2O_2S_2$ 514.261
Mixt. of stereoisomers, Tyriverdins A and B. Prob. artifacts derived from Tyrindoxol, T-805. Isol. from the hypobronchial glands of the gastropod *Thais clavigera*. Also isol. from *Nucella lapilus*. Intermed. in the formation of 6,6′-Dibromoindigotin, D-268. Light-sensitive light green solid; unstable in soln. λ_{max} 237 (log ϵ 4.37); 252 (log ϵ 4.51); 275 (log ϵ 4.08); 350 (log ϵ 3.41); 402 (log ϵ 3.46); 598 (log ϵ 2.85) (MeOH). λ_{max} 255; 280; 366; 400; 595 ($CHCl_3$).

[11051-34-6, 75714-79-3]

Christophersen, C. *et al., Tet. Lett.*, 1977, 1747 (*struct*)
Christophersen, C. *et al., Tetrahedron*, 1978, **34**, 2779 (*synth, uv, ir, pmr*)
Fujise, Y. *et al., Chem. Lett.*, 1980, 631 (*isol, uv, ir, pmr, cmr, struct*)
Cooksey, C.J. *et al., Molecules*, 2001, **6**, 736-769 (*rev*)

Tyrosine, 9CI, 8CI T-808

α-Amino-4-hydroxybenzenepropanoic acid. 2-Amino-3-(4-hydroxyphenyl)propanoic acid. 4-Hydroxy-α-aminohydrocinnamic acid.
p-*Tyrosine. 3*-p-*Hydroxyphenyl-α-alanine. Tyr*
[55520-40-6]



(*S*)-*form*

$C_9H_{11}NO_3$ 181.191

(*S*)-*form*

L-form. FEMA 3736
[60-18-4]
Widely distributed in plant and animal proteins.
Needles (H_2O). Almost insol. H_2O (0.05 g/100 g at 25°).
Mp 290-295° dec. (slow heat) Mp 314-318° dec. approx. (rapid heat). $[\alpha]_D^{20}$ -11.8 (c, 4.0 in 5*M* HCl) (opt. pure). $[\alpha]_D$ -9.01 (11.6% KOH). pK_{a1} 2.2; pK_{a2} 9.11; pK_{a3} 10.07 (phenolic OH). Isoelectric point 5.66. Bitter taste.
▶ Exp. reprod. and teratogenic effects (large doses). YP2275600

N-*(4,6*R-*Dimethyl-2*E,*4*E-*dodecadienoyl), Me ester:* ***Gymnastatin H***
[229334-21-8]
$C_{24}H_{35}NO_4$ 401.545
Prod. by *Gymnascella dankaliensis* isol. from the sponge *Halichondria japonica*.

[16978-66-8, 36546-50-6, 81158-85-2, 126060-58-0]

Amagata, T. *et al., CA*, 1999, **131**, 129789s (*Gymnastatin H*)

Tyrosylarginylisoleucinamide T-809

H-Tyr-Arg-Ile-NH_2
$C_{21}H_{35}N_7O_4$ 449.552

L-L-L-*form*

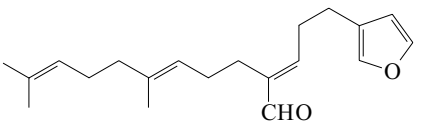
Antho-RI amide II
[139026-55-4]
Isol. from the sea anemone *Anthopleura elegantissima*. Neuropeptide.

N^1-*(2-Hydroxy-3-phenylpropanoyl)*(S-*):* N-*(3-Phenyllactoyl)tyrosylarginylisoleucinamide.* ***Antho-RI amide I***
[139026-54-3]
$C_{30}H_{43}N_7O_6$ 597.713
Isol. from *Anthopleura elegantissima*. Neurotransmitter. Sol. H_2O, MeOH. Neuropeptide.

Nothacker, H.P. *et al., Peptides (N.Y.)*, 1991, **12**, 1165-1173 (*isol, struct*)
McFarlane, I.D. *et al., Proc. R. Soc. London, B*, 1993, **253**, 183-188 (*isol*)

Udoteafuran U-1

1,20-Epoxy-1,3(20),6,10,14-phytapentaen-19-al
[77256-96-3]

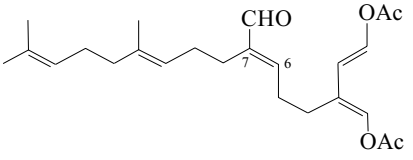


$C_{20}H_{28}O_2$ 300.44
Constit. of *Udotea flabellum*. Oil.

Nakatsu, T. *et al., J.O.C.*, 1981, **46**, 2435

Udoteal U-2

1,20-Diacetoxy-1,3(20),6,10,14-phytapentaen-19-al
[82309-29-3]



$C_{24}H_{34}O_5$ 402.53
Isol. from *Udotea flabellum*. Feeding deterrent. Oil.

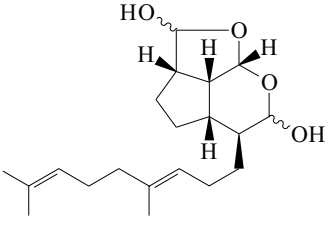
6,7-Dihydro: 1,20-Diacetoxy-1,3(20),10,14-phytatetraen-19-al.
6,7-Dihydroudoteal
$C_{24}H_{36}O_5$ 404.545
Metabolite of *Penicillus dumetosus*. Possesses antibacterial and antifungal props. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{25}$ +0.7 (c, 1.3 in $CHCl_3$). λ_{max} 250 (ϵ 5800) (MeOH) (Berdy).

6Z-Isomer: ***Udoteal B***
[312909-19-6]
$C_{24}H_{34}O_5$ 402.53
Constit. of *Udotea petiolata* and *Elysia translucens*. Oil. λ_{max} 236 (ϵ 1038); 253 (ϵ 1039) (hexane).

Paul, V.J. *et al., Phytochemistry*, 1982, **21**, 468 (*isol, struct*)
Paul, V.J. *et al., Tetrahedron*, 1984, **40**, 2913 (*deriv*)
Gavagnin, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1994, **108**, 107-115 (*isol*)
Iliopoulou, D. *et al., Nat. Prod. Lett.*, 2000, **14**, 373-378 (*Udoteal B*)

Udoteatrial U-3

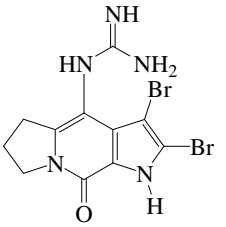
[77256-95-2]



$C_{20}H_{32}O_4$ 336.47
Constit. of *Udotea flabellum*. Oil.

Nakatsu, T. *et al., J.O.C.*, 1981, **46**, 2435 (*isol, struct*)
Whitesell, J.K. *et al., J.O.C.*, 1983, **48**, 1556 (*synth*)
Ge, Y. *et al., Tetrahedron*, 1993, **49**, 10555 (*synth, abs config*)
Tai, H.-M. *et al., J. Chin. Chem. Soc. (Taipei)*, 1995, **42**, 821 (*synth*)
Chang, M.-Y. *et al., Tetrahedron*, 2004, **60**, 1581-1585 (*synth*)

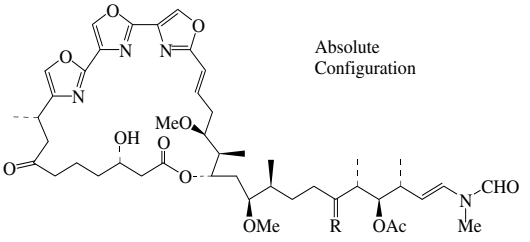
Ugibohlin U-4



$C_{11}H_{11}Br_2N_5O$ 389.049
Isol. from the marine sponge *Axinella carteri*. Amorph. solid. λ_{max} 208 (log ϵ 3.83); 240 (log ϵ 4.25); 242 (log ϵ 4.27); 269 (log ϵ 3.6) (MeOH).

Goetz, G.H. *et al., J. Nat. Prod.*, 2001, **64**, 1581-1582 (*isol, pmr, cmr*)

Ulapualide U-5



Ulapualide A R = O
Ulapualide B R = H, $OCOCH(OMe)CH_2OMe$

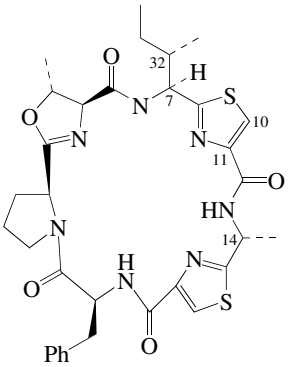
Ulapualide A [100045-73-6]
$C_{46}H_{64}N_4O_{13}$ 881.031
Isol. from *Hexabranchus sanguineus* egg masses. Shows antitumour and antifungal props. Oil. $[\alpha]_D^{21}$ -43.3 (c, 0.3 in MeOH). λ_{max} 246 (ϵ 34000) (MeOH) (Derep).

Ulapualide B [100045-74-7]
$C_{51}H_{74}N_4O_{16}$ 999.163
Isol. from *Hexabranchus sanguineus* egg masses. Shows antitumour and antifungal props. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{25}$ -21.7 (c, 0.138 in MeOH). λ_{max} 246 (ϵ 33000) (MeOH) (Derep).

Roesener, J.A. *et al., J.A.C.S.*, 1986, **108**, 846-847 (*isol, pmr*)
Chattopadhyay, S.K. *et al., J.C.S. Perkin 1*, 2000, 2415-2428; 2429-2454 (*synth, config*)
Allingham, J.S. *et al., Org. Lett.*, 2004, **6**, 597-599 (*cryst struct, abs config*)

Ulicyclamide, 9CI U-6

[74839-81-9]



$C_{33}H_{39}N_7O_5S_2$ 677.847

Numbering systems differ. The closely related Lissoclinamides are numbered differently from Ulicyclamide in CAS. Stereochem. given here is tentative as it is not completely clear in the lit. Isol. from the marine tunicate *Lissoclinum patella*. Cytotoxic. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ +35.7 (c, 2.3 in CH_2Cl_2). λ_{max} 248 (ϵ 7900) (MeOH) (Derep).

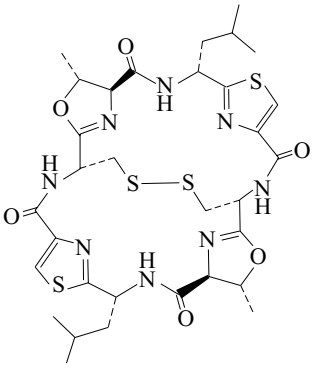
7,14-Diepimer, 10,11α-dihydro: ***Lissoclinamide 3***
[87393-59-7]
[121209-52-7]
$C_{33}H_{41}N_7O_5S_2$ 679.863
Isol. from *Lissoclinum patella*. Sol. $CHCl_3$, MeOH; poorly sol. H_2O. λ_{max} 248 (ϵ 7900) (MeOH) (Derep).

7,32-Diepimer, 10,11α-dihydro: ***Lissoclinamide 2***
[87393-58-6]
$C_{33}H_{41}N_7O_5S_2$ 679.863
Isol. from *Lissoclinum patella*.

Ireland, C. *et al., J.A.C.S.*, 1980, **102**, 5688-5691 (*isol, uv, ir, pmr, ms*)
Wasylyk, J.M. *et al., J.O.C.*, 1983, **48**, 4445-4449 (*isol, ir, pmr, cmr, ms, struct, derivs*)
Schmidt, U. *et al., Angew. Chem., Int. Ed.*, 1985, **24**, 569-571 (*synth*)
Sugiura, T. *et al., Tet. Lett.*, 1987, **28**, 2251-2254 (*synth*)

Ulithiacyclamide U-7

[74847-09-9]



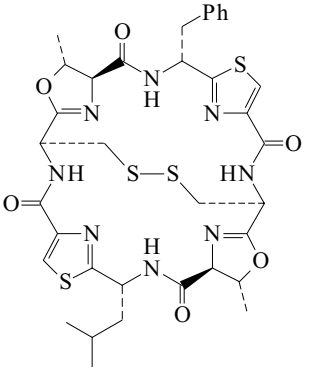
Absolute configuration

$C_{32}H_{42}N_8O_6S_4$ 762.998
Isol. from the marine tunicate *Lissoclinum patella* and from an unidentified sp. of ascidian collected from Rodda Reef, Queensland, Australia. Shows selective metal binding props. Cytotoxic agent. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane. $[\alpha]_D^{25}$ +62.4 (c, 2.9 in CH_2Cl_2). λ_{max} 247 (ϵ 7000) (MeOH) (Derep).

Ireland, C. *et al., J.A.C.S.*, 1980, **102**, 5688-5691 (*uv, ir, pmr, cmr, ms, struct*)
Hamamoto, Y. *et al., Chem. Comm.*, 1983, 323-324 (*occur*)
Biskupiak, J.E. *et al., J.O.C.*, 1983, **48**, 2302-2304 (*abs config*)
Kato, S. *et al., Tet. Lett.*, 1986, **27**, 2653-2656 (*synth*)
Schmidt, U. *et al., Tet. Lett.*, 1986, **27**, 3495-3496 (*synth*)
Ishida, T. *et al., J.O.C.*, 1989, **54**, 5337-5343 (*pmr, conformn*)
Morris, L.A. *et al., Tetrahedron*, 2001, **57**, 3185-3197 (*activity*)

Ulithiacyclamide B U-8

[122759-67-5]

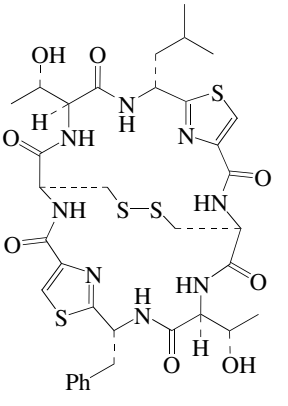


$C_{35}H_{40}N_8O_6S_4$ 797.015
Isol. from the ascidian *Lissoclinum patella*. Potent cytotoxin. Amorph. solid. $[\alpha]_D^{24.5}$ +117 (c, 0.17 in MeOH). λ_{max} 202 (ϵ 154897); 235 (ϵ 63291) (MeOH) (Berdy).

Williams, D.E. *et al., J. Nat. Prod.*, 1989, **52**, 732-739 (*isol, uv, ir, pmr, cmr, ms, struct*)

Ulithiacyclamide E U-9

[218916-92-8]

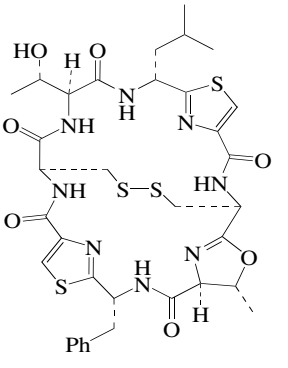


$C_{35}H_{44}N_8O_8S_4$ 833.045
Isol. from the ascidian *Lissoclinum patella*. Amorph. solid. $[\alpha]_D$ +4.9 (c, 0.8 in MeOH).

Fu, X. *et al., J. Nat. Prod.*, 1998, **61**, 1547-1551 (*isol, ir, pmr, cmr, ms*)

Ulithiacyclamide F U-10

[218916-93-9]



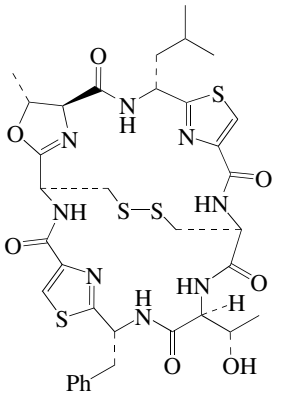
$C_{35}H_{42}N_8O_7S_4$ 815.03

Isol. from the ascidian *Lissoclinum patella*. Amorph. solid. $[\alpha]_D$ +29.6 (c, 0.27 in MeOH).

Fu, X. *et al., J. Nat. Prod.*, 1998, **61**, 1547-1551 (*isol, ir, pmr, cmr*)

Ulithiacyclamide G U-11

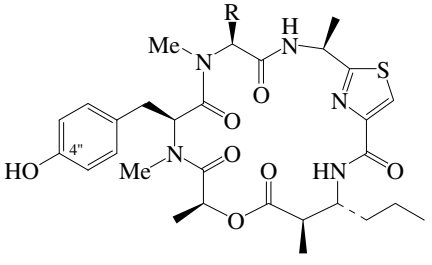
[218916-94-0]



$C_{35}H_{42}N_8O_7S_4$ 815.03
Isol. from the ascidian *Lissoclinum patella*. Amorph. solid. $[\alpha]_D$ +25.6 (c, 0.18 in MeOH).

Fu, X. *et al., J. Nat. Prod.*, 1998, **61**, 1547-1551 (*isol, ir, pmr, cmr, ms*)

Ulongamide B U-12



R = $CH(CH_3)_2$

$C_{32}H_{45}N_5O_7S$ 643.803
Isol. from a Palauan *Lyngbya* sp. Amorph. solid. $[\alpha]_D^{25}$ +10 (c, 0.1 in MeOH). λ_{max} 201 (log ϵ 4.24); 230 (log ϵ 3.87) (MeOH).

4″-Deoxy: ***Ulongamide A***
$C_{32}H_{45}N_5O_6S$ 627.803
Isol. from a Palauan *Lyngbya* sp. Amorph. solid. $[\alpha]_D^{25}$ +12 (c, 0.73 in MeOH). λ_{max} 201 (log ϵ 4.25); 230 (log ϵ 3.88) (MeOH).

Luesch, H. *et al., J. Nat. Prod.*, 2002, **65**, 996-1000 (*isol, pmr, cmr*)

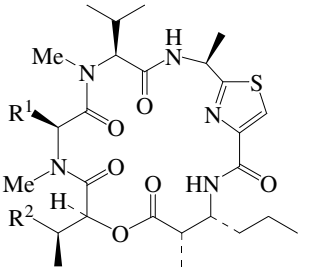
Ulongamide C U-13

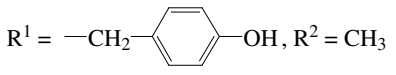
As Ulongamide B, U-12 with
R = CH_2Ph

$C_{36}H_{45}N_5O_7S$ 691.847
Isol. from a Palauan *Lyngbya* sp. Amorph. solid. $[\alpha]_D^{25}$ +9 (c, 0.33 in MeOH). λ_{max} 202 (log ϵ 4.54); 230 (log ϵ 4.12) (MeOH).

Luesch, H. *et al., J. Nat. Prod.*, 2002, **65**, 996-1000 (*isol, pmr, cmr*)

Ulongamide D U-14





$C_{34}H_{49}N_5O_7S$ 671.856
Isol. from a Palauan *Lyngbya* sp. Amorph. solid. $[\alpha]_D^{25}$ +22 (c, 0.12 in MeOH). λ_{max} 201 (log ϵ 4.24); 230 (log ϵ 3.89) (MeOH).

Luesch, H. *et al., J. Nat. Prod.*, 2002, **65**, 996-1000 (*isol, pmr, cmr*)

Ulongamide E U-15

As Ulongamide D, U-14 with
R^1 = CH_2Ph-4OH, R^2 = CH_2CH_3

$C_{35}H_{51}N_5O_7S$ 685.883
Isol. from a Palauan *Lyngbya* sp. Amorph. solid. $[\alpha]_D^{25}$ +20 (c, 0.4 in MeOH). λ_{max} 202 (log ϵ 4.24); 230 (log ϵ 3.89) (MeOH).

Luesch, H. *et al., J. Nat. Prod.*, 2002, **65**, 996-1000 (*isol, pmr, cmr*)

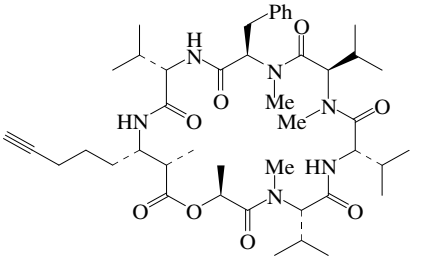
Ulongamide F U-16

As Ulongamide D, U-14 with
R^1 = $CH(CH_3)_2$, R^2 = CH_2CH_3

$C_{31}H_{51}N_5O_6S$ 621.84
Isol. from a Palauan *Lyngbya* sp. Amorph. solid. $[\alpha]_D^{25}$ +25 (c, 0.2 in MeOH). λ_{max} 202 (log ϵ 3.85); 230 (log ϵ 3.5) (MeOH).

Luesch, H. *et al., J. Nat. Prod.*, 2002, **65**, 996-1000 (*isol, pmr, cmr*)

Ulongapeptin U-17



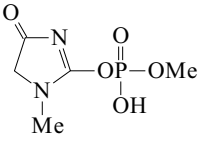
Absolute Configuration

$C_{44}H_{68}N_6O_8$ 809.057
Depsipeptide antibiotic. Isol. from a Palauan *Lyngbya* sp. Cytotoxic. Amorph. powder. $[\alpha]_D^{21}$ -16 (c, 0.4 in MeOH). λ_{max} 204 (log ϵ 3.84) (MeOH).

Williams, P.G. *et al., J. Nat. Prod.*, 2003, **66**, 651-654 (*isol, pmr, cmr*)

Ulosantoin U-18

[145644-07-1]

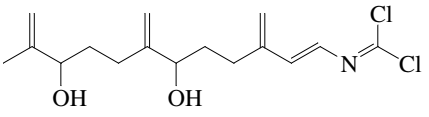


$C_5H_9N_2O_5P$ 208.11

Exists as zwitterion. Isol. from the sponge *Ulosa ruetzleri*. Shows marked insecticidal activity. Acetylcholinesterase inhibitor. Cryst. (Me_2CO/isooctane).
Mp 127-128°. λ_{max} 224 (ϵ 5000) (MeOH) (Derep).

Van Wagenen, B.C. *et al., J.O.C.*, 1993, **58**, 335-337 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)

Ulosin B U-19

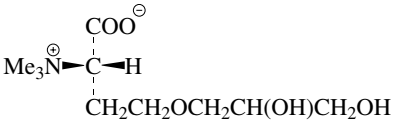


$C_{16}H_{23}Cl_2NO_2$ 332.269
Constit. of *Ulosa spongia*. Oil. $[\alpha]_D^{23}$ +20.9 (c, 0.07 in $CHCl_3$). λ_{max} 283 (log ϵ 4.4) (MeOH).

Kehraus, S. *et al., J. Nat. Prod.*, 2001, **64**, 939-941 (*isol, pmr, cmr*)

Ulvaline U-20

1-Carboxy-3-(2,3-dihydroxypropoxy)-N,N,N-*trimethyl-1-propanaminium inner salt, 9CI*. O-*(1-Glyceryl)*-N,N,N-*trimethylhomoserine*
[56323-09-2]
[66807-99-6]



$C_{10}H_{21}NO_5$ 235.28
Isol. from the marine plant *Monostroma nitidum* and the mushroom *Lampteromyces japonicus*. Diacyl derivs are isol. from numerous marine sources incl. algae and bryophytes. Shows hypocholesterolaemic activity.

Eichenberger, W. *et al., FEBS Lett.*, 1978, **88**, 201-204 (*isol*)
Vaskovskii, V.E. *et al., Lipids*, 1991, **26**, 254-256 (*isol*)
Fushiya, S. *et al., Nat. Med. (Tokyo)*, 1997, **51**, 558 (*isol*)

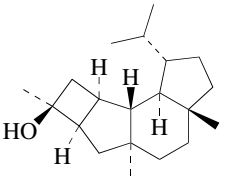
Ulvan U-21

Polysaccharide composed of partially sulfated Rha, Xyl and glucuronic acid. Isol. from cell walls of marine green algae *Ulva rigida*, *Ulva pertusa* and *Ulva lactuca*. Shows cytotoxic props. Antioxidant.

Ray, B. *et al., Carbohydr. Res.*, 1995, **274**, 313-318
Lahaye, M. *et al., Carbohydr. Res.*, 1996, **283**, 161-173
Kaeffer, B. *et al., Planta Med.*, 1999, **65**, 527-531 (*isol, activity*)
Qi, H. *et al., Bioorg. Med. Chem. Lett.*, 2006, **16**, 2441-2445 (*activity*)

Umabanol U-22

[191927-14-7]

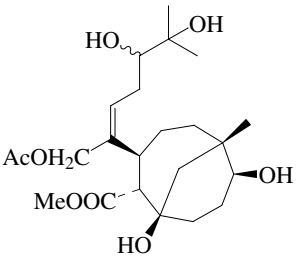


$C_{20}H_{34}O$ 290.488
Constit. of *Epipolasis kushimotoensis*.
$[\alpha]_D$ -78 (c, 0.1 in $CHCl_3$).

Tanaka, J. *et al., Chem. Lett.*, 1997, 489-490 (*isol, pmr, cmr*)

Umbellacin I U-23

[871483-43-1]

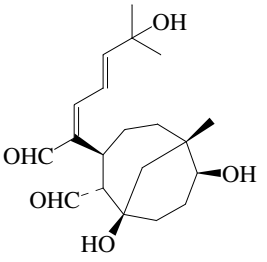


$C_{23}H_{38}O_8$ 442.548
Constit. of *Xenia umbellata*. Amorph. solid. $[\alpha]_D^{25}$ -30 (c, 0.2 in $CHCl_3$).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2006, **69**, 338-341

Umbellacin A U-24

[871483-31-7]

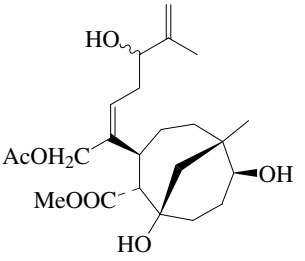


$C_{20}H_{30}O_5$ 350.454
Constit. of *Xenia umbellata*. Oil. $[\alpha]_D^{25}$ -36 (c, 0.2 in $CHCl_3$). λ_{max} 235 (log ϵ 4.26) (MeOH).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2006, **69**, 338-341

Umbellacin B U-25

[871483-33-9]

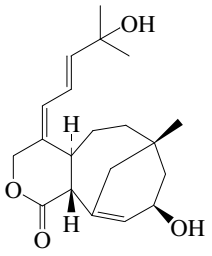


$C_{23}H_{36}O_7$ 424.533
Constit. of *Xenia umbellata*. Amorph. solid. $[\alpha]_D^{25}$ -28 (c, 0.3 in $CHCl_3$).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2006, **69**, 338-341

Umbellacin C U-26

[871483-35-1]

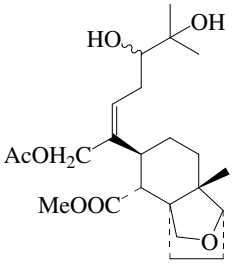


$C_{20}H_{28}O_4$ 332.439
Constit. of *Xenia umbellata*. Oil. $[\alpha]_D^{25}$ +12 (c, 0.2 in $CHCl_3$).
λ_{max} 228 (log ϵ 4.12) (MeOH).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2006, **69**, 338-341

Umbellacin D U-27

[871483-36-2]

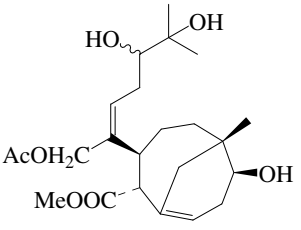


$C_{23}H_{36}O_7$ 424.533
Constit. of *Xenia umbellata*. Amorph. solid. $[\alpha]_D^{25}$ +36 (c, 0.1 in $CHCl_3$).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2006, **69**, 338-341

Umbellacin E U-28

[871483-37-3]

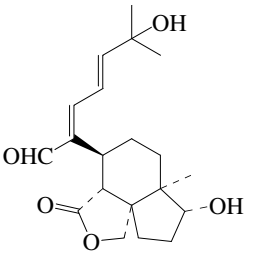


$C_{23}H_{36}O_7$ 424.533
Constit. of *Xenia umbellata*. Amorph. solid. $[\alpha]_D^{25}$ +32 (c, 0.2 in $CHCl_3$).

El-Gamal, A.A.H. *et al., J. Nat. Prod.*, 2006, **69**, 338-341

Umbellactal U-29

[865361-56-4]

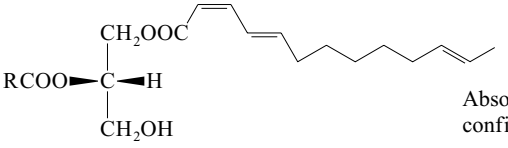


$C_{20}H_{28}O_5$ 348.438
Constit. of *Xenia umbellata*. Oil. $[\alpha]_D^{25}$ -30 (c, 0.1 in $CHCl_3$).

El-Gamal, A.A.H. *et al., Tet. Lett.*, 2005, **46**, 6095-6096 (*Umbellactal*)

Umbraculumin A U-30

Glycerol 2-(3-methyl-2-butenoate) 1-(2,4,11-tridecatrienoate)
[116944-99-1]



Absolute configuration

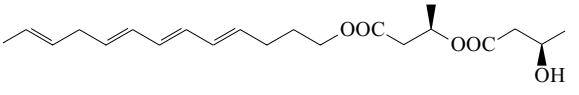
R = —CH=C(CH$_3$)$_2$

$C_{21}H_{32}O_5$ 364.481
Constit. of mollusc *Umbraculum mediterraneum*. Ichthyotoxin. Sol. MeOH, Et_2O; fairly sol. hexane. $[\alpha]_D$ -24.3 (c, 0.8 in $CHCl_3$). λ_{max} 214 (ϵ 14700); 263 (ϵ 21300) (hexane) (Derep). λ_{max} 214 (ϵ 14680); 263 (ϵ 21250) (hexane) (Berdy).

Cimino, G. *et al., Tet. Lett.*, 1988, **29**, 3613-3616 (*isol*)
De Madeiros, E.F. *et al., J.C.S. Perkin 1*, 1991, 2725 (*synth, abs config*)

Umbraculumin B U-31

[123444-54-2]



$C_{21}H_{32}O_5$ 364.481
Isol. from the skin extracts of the mollusc *Umbraculum mediterraneum*. λ_{max} 259 (ϵ 26000); 268 (ϵ 36000); 279 (ϵ 28000) (hexane) (Derep).

Cimino, G. *et al., Tet. Lett.*, 1989, **30**, 1147-1148 (*isol, struct*)

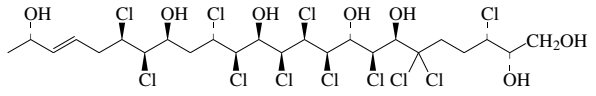
Umbraculumin C U-32

Glycerol 2-(3-methylthio-2-propenoate) 1-(2,4,11-tridecatrienoate)
[116963-50-9]

$C_{20}H_{30}O_5S$ 382.52
Constit. of mollusc *Umbraculum mediterraneum*. Ichthyotoxin. Sol. MeOH, Et_2O; fairly sol. hexane. $[\alpha]_D$ +7 (c, 0.5 in $CHCl_3$). λ_{max} 267 (ϵ 35500) (hexane) (Derep).

Cimino, G. *et al., Tet. Lett.*, 1988, **29**, 3613-3616 (*isol, struct*)
De Madeiros, E.F. *et al., J.C.S. Perkin 1*, 1991, 2725 (*synth, abs config*)

3,6,6,8,10,11,12,14,15,18,19-Undecachloro-21-tetracosene-1,2,7,9,13,17,23-heptol U-33



$C_{24}H_{37}Cl_{11}O_7$ 827.532

(2*S*,3*S*,7*R*,8*S*,9*R*,10*R*,11*S*,12*S*,13*R*,14*R*,15*S*,17*S*,18*R*,19*R*,23*S*)-*form*

23-O-*Hexadecanoyl, 17*-O-*sulfate:*
$C_{40}H_{67}Cl_{11}O_{11}S$ 1146.008
Isol. from the toxic mussel *Mytilus galloprovincialis*. Cytotoxic.
$[\alpha]_D^{25}$ +120.2 (c, 0.005 in MeOH).

7-Deoxy, 23-O-*hexadecanoyl, 17*-O-*sulfate:*
$C_{40}H_{67}Cl_{11}O_{10}S$ 1130.009
Isol. from the toxic mussel *Mytilus galloprovincialis*. Cytotoxic.
$[\alpha]_D$ +84.1 (c, 0.001 in MeOH).

Ciminiello, P. *et al., J.A.C.S.*, 2002, **124**, 13114-13120 (*isol, pmr, cmr*)
Ciminiello, P. *et al., Tetrahedron*, 2004, **60**, 7093-7098 (*isol, pmr, cmr*)

1,4-Undecadiene, 9CI U-34

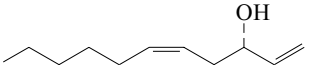
[53786-93-9]
$H_3C(CH_2)_5CH{=}CHCH_2CH{=}CH_2$
$C_{11}H_{20}$ 152.279
Constit. of ginseng oil (*Panax ginseng*) and of Chinese traditional medicine, Gaoben (*Ligusticum* sp.).

(*E*)-*form* [55976-13-1]
$Bp_{0.2}$ 37-38°. n_D^{20} 1.4385.

(*Z*)-*form* [55976-14-2]
Used in synthetic flavour components.
Bp_{10} 66-67°.

Lynd, R.A. *et al., Synthesis*, 1974, 658 (*synth*)
Eisch, J.J. *et al., J.O.C.*, 1976, **41**, 2214 (*synth, ir, pmr*)
Uchida, K. *et al., J.O.C.*, 1976, **41**, 2215 (*synth, ir, pmr, ms*)
Bosshardt, H. *et al., Helv. Chim. Acta*, 1980, **63**, 2393 (*synth, use, ir, pmr, ms*)
Kim, K.R. *et al., Chromatographia*, 1982, **15**, 559 (*ms*)
Hoshi, M. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 2855 (*synth, pmr, ms, ir*)
Arase, A. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 209 (*synth, use, pmr, ir*)

1,5-Undecadien-3-ol U-35



$C_{11}H_{20}O$ 168.278

(3*S*,5*Z*)-*form*
Dictyoprolenol
[81703-01-7]
Constit. of *Dictyopteris* spp.

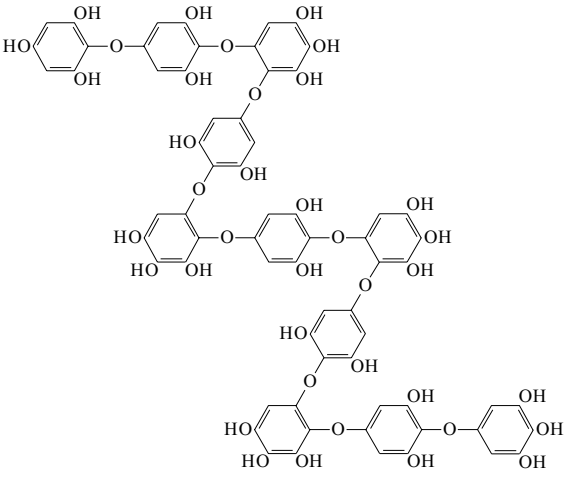
Ac: ***Dictyoprolene***
[72538-16-0]
$C_{13}H_{22}O_2$ 210.316
Odoriferous constit. of brown alga *Dictyopteris prolifera*. Liq.
$[\alpha]_D^{27}$ +13 (c, 1.30 in $CHCl_3$).

[56722-23-7, 77188-82-0]

Yamada, K. *et al., Tetrahedron*, 1986, **42**, 3775-3780 (*struct, synth*)
Yamamoto, Y. *et al., Z. Naturforsch., C*, 1999, **54**, 1027-1032; 2001, **56**, 6-12 (*isol, synth, biosynth*)
Wallner, A. *et al., Tetrahedron: Asymmetry*, 2003, **14**, 2427-2432 (*synth, pmr, cmr*)

Undecafuhalol A U-36

[138530-43-5]



$C_{66}H_{46}O_{38}$ 1447.067
Constit. of the brown algae *Bifurcaria bifurcata*, *Landsburgia quercifolia*, *Carpophyllum angustifolium* and *Sargassum spinuligerum*.

Glombitza, K.-W. *et al., Phytochemistry*, 1976, **15**, 1279; 1981, **20**, 1373-1379; 1995, **38**, 987-995 (*isol, pmr, struct*)
Li, S.M. *et al., Bot. Mar.*, 1991, **34**, 455 (*isol*)
Glombitza, K.-W. *et al., J. Nat. Prod.*, 1999, **62**, 1238-1240 (*isol*)

3-Undecanone U-37

[2216-87-7]
$H_3C(CH_2)_7COCH_2CH_3$
$C_{11}H_{22}O$ 170.294
Constit. of *Dacrydium* sp., *Dictyopteris* sp. , also *Ophrys* sp., *Commiphora rostrata* and other plants. Alarm pheromone for various ant spp. Bp 227° Bp_{11} 104-106°.

Semicarbazone:
Cryst. (EtOH). Mp 90°.

Pickard, R.H. *et al., J.C.S.*, 1913, **103**, 1936; 1946 (*synth*)
Collman, J.P. *et al., J.A.C.S.*, 1972, **94**, 1788 (*synth*)
Mekhliev, L.F. *et al., CA*, 1977, **86**, 43139 (*synth*)
Tamaru, Y. *et al., Tet. Lett.*, 1985, **26**, 5529 (*synth*)
Boland, W. *et al., Tet. Lett.*, 1987, **28**, 307 (*isol*)
Pelter, A. *et al., Tet. Lett.*, 1989, **30**, 5643 (*synth*)
Trehan, I.R. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 396 (*synth, ir*)
Trehan, J.R. *et al., J. Indian Chem. Soc.*, 1997, **74**, 500-501 (*synth*)

Scyliorhinus canicula Undecapeptide U-38

[149756-79-6]
H-Lys-Pro-Arg-Pro-Gly-Gln-Phe-Phe-Gly-Leu-Met-NH_2
$C_{60}H_{93}N_{17}O_{12}S$ 1276.567
Constit. of the brain of the dogfish *Scyliorhinus canicula*. Possesses substance P-like immunoreactivity.

Waugh, D. *et al., Eur. J. Biochem.*, 1993, **214**, 469-474 (*struct, activity*)

1,3,5,8-Undecatetraene U-39

[38533-54-9]
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH{=}CHCH{=}CH_2$
$C_{11}H_{16}$ 148.247

(3*E*,5*E*,8*Z*)-*form* [50277-31-1]
Occurs in pineapples, *Cucumis melo* (cantaloupe), *Dictyopteris plagiogramma* and *Dictyopteris australis*.

(3*E*,5*Z*,8*Z*)-*form*
Finavarrene
[29837-19-2]

Constit. of the essential oil of algae of the genera *Dictyopteris*, *Dictyosiphon* and *Spermatochnus*. Also occurs in the peel of mandarin and tangerine oranges and pineapple. Smelling principle of the gametes of the brown algae *Spermatochnus paradoxus*. Sperm attractant of the marine brown alga *Ascophyllum nodosum*. Liq. Sol. Et_2O, hexane; poorly sol. H_2O. n_D^{14} 1.5285. λ_{max} 257; 266; 277 (EtOH) (Berdy).

(3Z,5E,8Z)-form

n_D^{14} 1.5304.

Pettus, J.A. *et al., Chem. Comm.*, 1970, 1093-1094 (*isol, struct*)
Moore, R.E. *et al., J.O.C.*, 1974, **39**, 2201-2207 (*3E,5E,8Z-form, 3E,5Z,8Z-form, occur*)
Moore, R.E. *et al., Acc. Chem. Res.*, 1977, **10**, 40-47 (*rev*)
Mueller, D.G. *et al., Naturwissenschaften*, 1981, **68**, 478-480 (*isol*)
Janicke, L. *et al., Angew. Chem., Int. Ed.*, 1982, **21**, 643-653 (*rev*)
Marner, F.-J. *et al., Annalen*, 1982, 579-584 (*synth, spectra*)
Mueller, D.G. *et al., Science (Washington, D.C.)*, 1982, **218**, 1119-1120 (*Finavarrene, isol, activity*)
Berger, R.C. *et al., J. Agric. Food Chem.*, 1985, **33**, 232-235 (*3E,5Z,8Z-form, 3E,5E,8Z-form, occur*)
Stratmann, K. *et al., Tetrahedron*, 1993, **49**, 3755-3766 (*biosynth*)
Beaulieu, J.C. *et al., J. Agric. Food Chem.*, 2001, **49**, 1345-1352 (*3E,5E,8Z-form, occur*)
Naef, R. *et al., J. Essent. Oil Res.*, 2001, **13**, 154-157 (*occur*)
Yamamoto, Y. *et al., Z. Naturforsch., C*, 2001, **56**, 8-12 (*occur*)

2,4,6,8-Undecatetraene U-40

[31699-37-3]

$H_3CCH_2CH{=}CHCH{=}CHCH{=}CHCH{=}CHCH_3$

$C_{11}H_{16}$ 148.247

(2Z,4Z,6E,8Z)-form

Giffordene

[109138-61-6]

Odoriferous substance from the brown alga *Giffordia mitchellae*. Liq. The (2*E*,4*E*,6*E*,8*Z*), (2*E*,4*Z*,6*E*,8*Z*), (2*E*,4*Z*,6*E*,8*E*), (2*Z*,4*E*,6*E*,8*Z*) and (2*Z*,4*Z*,6*E*,8*E*) isomers also occur in minor amts. λ_{max} 277 (sh) (ϵ 22100); 289 (ϵ 41400); 302 (ϵ 60000); 316 (ϵ 51400) (MeOH).

[109138-60-5, 109138-62-7, 109138-63-8, 109138-64-9, 109138-65-0]

Boland, W. *et al., Helv. Chim. Acta*, 1987, **70**, 1025-1040 (*isol, synth, uv, pmr, cmr, ms*)

1,3,5-Undecatriene U-41

[16356-11-9]

$H_3C(CH_2)_4CH{=}CHCH{=}CHCH{=}CH_2$

$C_{11}H_{18}$ 150.263

(3E,5E)-form [19883-29-5] Bp_{10} 100-105°.

(3E,5Z)-form

Galbanolene. *Cystophorene*

[51447-08-6]

Occurs in Galbanum extract (*Ferula galbaniflua*). Pheromone of the algae *Cystophora siliquosa* and *Dictyopteris* sp. Bp_{10} 100-105°.

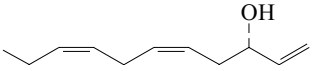
(3Z,5Z)-form [19883-26-2]

Oil. Bp_6 100°. Thermally unstable.

Chretien-Bessiere, Y. *et al., Bull. Soc. Chim. Fr.*, 1967, 97 (*isol*)
Teisseire, P. *et al., Recherches*, 1967, **16**, 5 (*synth*)
Cowie, J.S. *et al., J.C.S. Perkin 1*, 1972, 2197-2201 (*synth*)
Moore, R.E. *et al., J.O.C.*, 1974, **39**, 2201 (*isol*)
Naef, F. *et al., Helv. Chim. Acta*, 1975, **58**, 1016 (*synth*)
Giraudi, E. *et al., Tet. Lett.*, 1983, **24**, 489 (*synth, pmr*)
Hayashi, T. *et al., Tet. Lett.*, 1983, **24**, 2665 (*synth*)
Müller, D.G. *et al., Naturwissenschaften*, 1985, **72**, 97-99 (*Cystophorene, isol*)
Block, E. *et al., J.A.C.S.*, 1986, **108**, 4568 (*synth, bibl*)
Ratovelomanana, V. *et al., Bull. Soc. Chim. Fr.*, 1987, 174 (*synth, ir, cmr, ms, bibl*)
Andreini, B.P. *et al., Tetrahedron*, 1987, **43**, 4591 (*synth, pmr, ir, ms*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 415 (*rev, tox*)
Tsuboi, S. *et al., Bull. Chem. Soc. Jpn.*, 1990, **63**, 1888 (*synth*)
Tellier, F. *et al., Tetrahedron*, 1991, **47**, 7767 (*synth*)
Alexakis, A. *et al., Synth. Commun.*, 1992, **22**, 1839 (*synth*)
Solladie, G. *et al., Synlett*, 1993, 548 (*synth*)
Huynh, C. *et al., Synth. Commun.*, 1994, **24**, 2273 (*Galbanolene, synth, ir, pmr, cmr, ms*)
Alami, M. *et al., Tetrahedron*, 1995, **51**, 1209 (*synth*)

1,5,8-Undecatrien-3-ol U-42

Neodictyoprolenol



$C_{11}H_{18}O$ 166.263

(3S,5Z,8Z)-form

Constit. of *Dictyopteris* spp.

Ac: ***Neodictyoprolene***

[73276-42-3]

$C_{13}H_{20}O_2$ 208.3

Odoriferous constit. of brown alga *Dictyopteris prolifera*. Liq. $[\alpha]_D^{22}$ +20 (c, 1.00 in $CHCl_3$).

Yamada, K. *et al., Tetrahedron*, 1986, **42**, 3775-3780 (*struct, synth*)
Yamamoto, Y. *et al., Z. Naturforsch., C*, 1999, **54**, 1027-1032; 2001, **56**, 6-12 (*synth, biosynth*)

1-Undecen-3-one U-43

[42832-47-3]

$H_3C(CH_2)_7COCH{=}CH_2$

$C_{11}H_{20}O$ 168.278

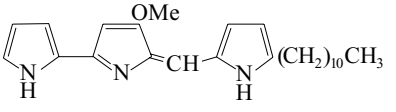
Minor constit. of *Dictyopteris plagiogramma*. Unstable oil.

Roller, P. *et al., Chem. Comm.*, 1971, 503 (*isol*)
Stetter, H. *et al., Chem. Ber.*, 1978, **111**, 431 (*synth*)

Undecylprodigiosin U-44

Undecylprodiginine. Prodigiosin 25c

[13129-81-2]



$C_{25}H_{35}N_3O$ 393.571

Isol. from *Streptomyces* spp., *Nocardia pelletieri* and *Streptoverticillium rubrireticuli*. Antimalarial agent. Weakly active against gram-positive bacteria. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O, acids, bases. Exhibits dimorphism. λ_{max} 273 (ϵ 3640); 297 (ϵ 6900); 362 (ϵ 5000); 500 (sh) (ϵ 31500); 530 (ϵ 75900) (MeOH/HCl) (Derep). λ_{max} 285 (ϵ 6050); 325 (ϵ 4850); 467 (ϵ 30600) (MeOH/KOH) (Derep). λ_{max} 273 (ϵ 3640); 297 (ϵ 6900); 362 (ϵ 5000); 500 (sh) (ϵ 31500); 530 (ϵ 75900) (HCl salt) (Derep). λ_{max} 502 (ϵ 40500); 530 (ϵ 100500) (MeOH) (Berdy). λ_{max} 230 (ϵ 4500); 290 (ϵ 10500); 500 (ϵ 57000); 525 (ϵ 107000) (MeOH-HCl) (Berdy). λ_{max} 290 (ϵ 10500); 460 (ϵ 42200) (MeOH-NaOH) (Berdy).

▶ LD_{50} (mus, ivn) 26.7 mg/kg.

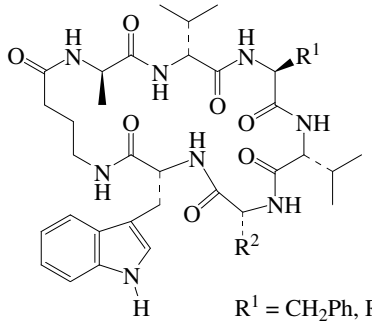
Hydrochloride: [15377-21-6]

Red needles (heptane). Mp 76-78° Mp 106-107° (dimorph.).

[14960-80-6, 52340-48-4, 56247-02-0]

Gerber, N.N. *et al., J. Antibiot.*, 1971, **24**, 636; 1975, **28**, 194; *Appl. Microbiol.*, **30**, 807 (*isol*)
Wasserman, H.H. *et al., Tetrahedron*, 1976, **32**, 1851 (*isol, uv, ir, pmr, struct*)
D'Alessio, R. *et al., Synlett*, 1996, 513 (*synth*)
Fürstner, A. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 3582-3603 (*rev*)

Unguisin A U-45



$R^1 = CH_2Ph$, $R^2 = CH_3$

$C_{40}H_{54}N_8O_7$ 758.916
Prod. by the marine-derived fungus *Emericella unguis.* Amorph. solid. λ_{max} 219 (log ϵ 4.49); 274 (log ϵ 3.63); 281 (log ϵ 3.65); 290 (log ϵ 3.58) (EtOH).

Malmstrom, J. *et al., J. Nat. Prod.*, 1999, **62**, 787-789 (*isol, uv, cd, pmr, cmr*)

Unguisin B U-46

As Unguisin A, U-45 with
$R^1 = CH_2CH(CH_3)_2$, $R^2 = CH_3$

$C_{37}H_{56}N_8O_7$ 724.899
Prod. by the marine-derived fungus *Emericella unguis.* Amorph. solid. λ_{max} 220 (log ϵ 4.42); 274 (log ϵ 3.57); 280 (log ϵ 3.6); 290 (log ϵ 3.53) (EtOH).

Malmstrom, J. *et al., J. Nat. Prod.*, 1999, **62**, 787-789 (*isol, uv, cd, pmr, cmr*)

Unguisin C U-47

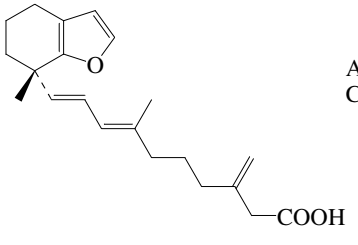
As Unguisin A, U-45 with
$R^1 = CH_2Ph$, $R^2 = CH_2OH$

$C_{40}H_{54}N_8O_8$ 774.915
Prod. by the marine-derived fungus *Emericella unguis.* Amorph. solid. Unguisin D was prod. by directed biosynth. on addition of L-leucine to the culture medium. λ_{max} 219 (log ϵ 4.49); 274 (log ϵ 3.63); 281 (log ϵ 3.65); 290 (log ϵ 3.58) (EtOH).

Malmstrom, J. *et al., Phytochemistry*, 2002, **60**, 869-872 (*isol, uv, pmr, cmr, cd*)

Untenic acid U-48

[141718-52-7]



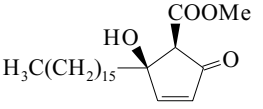
Absolute Configuration

$C_{21}H_{28}O_3$ 328.45
Isol. from an Okinawan sponge. Calcium-ATPase activator. Oil. $[\alpha]_D^{25}$ +1.6 (c, 10.5 in $CHCl_3$). λ_{max} 242 (log ϵ 4.35) (EtOH).

Shoji, N. *et al., Aust. J. Chem.*, 1992, **45**, 793-795 (*isol, pmr, cmr*)

Untenone A U-49

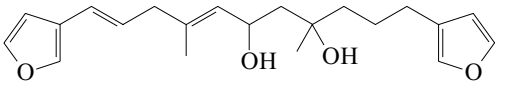
Methyl 2-hexadecyl-2-hydroxy-5-oxo-3-cyclopentene-1-carboxylate, 9CI
[149970-41-2]



$C_{23}H_{40}O_4$ 380.567
Isol. from the sponge *Plakortis* sp. Oil. $[\alpha]_D^{19}$ +0.2 (c, 2.1 in $CHCl_3$). λ_{max} 215 (ϵ 8800) (MeOH) (Derep). λ_{max} 215 (ϵ 8800) (MeOH) (Berdy).

Ishibashi, M. *et al., Tet. Lett.*, 1993, **34**, 3749 (*isol*)
Takeda, K. *et al., Synlett*, 1994, 178 (*synth*)
Asami, M. *et al., Tet. Lett.*, 1995, **36**, 1893 (*synth*)
Miyaoka, H. *et al., Tetrahedron*, 1995, **51**, 8749 (*synth*)
Al-Busafi, S. *et al., Tet. Lett.*, 2000, **41**, 3467-3470 (*synth*)

Untenospongin A U-50



$C_{21}H_{28}O_4$ 344.45

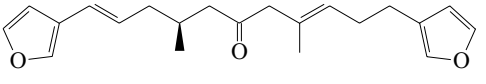
(+)-*form* [270250-15-2]
Constit. of a *Hippospongia* sp.
$[\alpha]_D^{20}$ +4.5. λ_{max} 208 (ϵ 21000); 226 (sh) (MeOH).

(-)-*form* [124666-36-0]
Constit. of a *Hippospongia* sp. Coronary vasodilator. Oil. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{25}$ -3 (c, 1.8 in $CHCl_3$). λ_{max} 208 (ϵ 21200); 226 (EtOH) (Berdy).

Umeyama, A. *et al., Aust. J. Chem.*, 1989, **42**, 459-462 (*(-)-form, isol, activity*)
Guo, Y. *et al., Chin. Chem. Lett.*, 2000, **11**, 327-330 (*(+)-form, isol*)

Untenospongin C U-51

[149298-04-4]

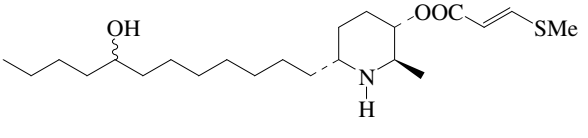


$C_{21}H_{26}O_3$ 326.435
Constit. of *Hippospongia* sp. Oil. $[\alpha]_D^{20}$ -9.3 (c, 1 in $CHCl_3$). λ_{max} 212 (ϵ 23600); 222 (EtOH) (Berdy).

Kobayashi, J. *et al., Chem. Pharm. Bull.*, 1993, **41**, 381 (*isol, pmr, cmr*)

Uoamine A U-52

[356550-05-5]



$C_{22}H_{41}NO_3S$ 399.637
Alkaloid from the ascidian *Aplidium uouo.* Oil. $[\alpha]_D$ +5 (c, 0.16 in $CHCl_3$). λ_{max} 275 (ϵ 10740) (EtOH).

Z-Isomer: ***Uoamine B***
[356550-06-6]
$C_{22}H_{41}NO_3S$ 399.637
Alkaloid from *Aplidium uouo.* Oil. $[\alpha]_D$ +8 (c, 0.15 in $CHCl_3$). λ_{max} 283 (ϵ 1372) (EtOH).

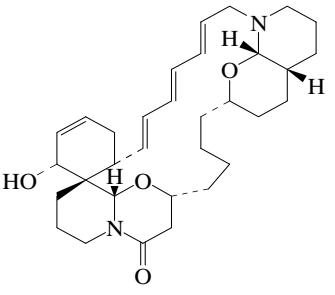
McCoy, M.C. *et al., J. Nat. Prod.*, 2001, **64**, 1087-1089 (*Uoamines A,B, isol, pmr, cmr, uv*)

UpI **U-53**

Basic protein; MW approx. 28kDa. Isol. from the sea anemone *Urticina piscivora*. Potent cardiac stimulator.

Cline, E.I. *et al., Pharmacol. Res.*, 1995, **32**, 309-314 (*isol*)

Upenamide **U-54**



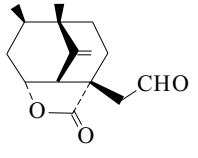
$C_{32}H_{46}N_2O_4$ 522.726

Alkaloid from the Indonesian sponge *Echinochalina* sp. Amorph. solid. $[\alpha]_D$ -9.4 (c, 2.3 in MeOH).

Jimenez, J.I. *et al., J.O.C.*, 2000, **65**, 8465-8469

Upial **U-55**

[72378-77-9]



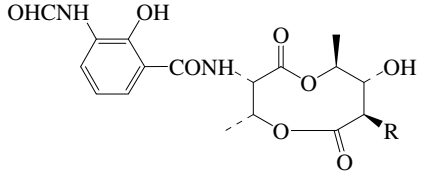
$C_{15}H_{20}O_3$ 248.321

Constit. of *Dysidea fragilis*. Oil. $[\alpha]_D^{25}$ +92.6 (c, 0.27 in $CHCl_3$).

Schulte, G. *et al., J.O.C.*, 1980, **45**, 552
Taschner, M.J. *et al., J.A.C.S.*, 1985, **107**, 5570-5572 (*synth*)
Nagaoka, H. *et al., Tetrahedron*, 1994, **50**, 661 (*synth*)

Urauchimycin A **U-56**

[148163-07-9]



Absolute Configuration

R = $CH_2CH(CH_3)CH_2CH_3$

$C_{22}H_{30}N_2O_8$ 450.488

Macrolide antibiotic. Related to Antimycin A, A-566. Prod. by a marine *Streptomyces* sp. Ni-80. Phytotoxic. Antifungal agent. Sol. MeOH, EtOAc, $CHCl_3$, EtOH; poorly sol. H_2O. $[\alpha]_D^{26}$ +46.7 (c, 0.03 in MeOH). λ_{max} 225; 343 (EtOH) (Derep).

Imamura, N. *et al., J. Antibiot.*, 1993, **46**, 241-246 (*isol, struct, props*)
Hayashi, K.-I. *et al., J. Antibiot.*, 1999, **52**, 325-328 (*abs config*)

Urauchimycin B **U-57**

[148163-08-0]

As Urauchimycin A, U-56 with

R = $CH_2CH_2CH(CH_3)_2$

$C_{22}H_{30}N_2O_8$ 450.488

Macrolide antibiotic. Related to Antimycin A, A-566. Prod. by a marine *Streptomyces* sp. Ni-80 and *Streptomyces* sp. isolate B1751. Antifungal agent. Sol. MeOH, EtOAc, EtOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{26}$ +50 (c, 0.1 in MeOH). λ_{max} 225; 343 (EtOH) (Derep).

Imamura, N. *et al., J. Antibiot.*, 1993, **46**, 241-246 (*isol, struct, props*)
Yao, C.B.F. *et al., Z. Naturforsch., B*, 2006, **61**, 320-325 (*isol, pmr, cmr*)

Urauchimycin C **U-58**

As Urauchimycin A, U-56 with

R = $-CH_2CH_3$

$C_{19}H_{24}N_2O_8$ 408.407

Prod. by the marine-derived *Streptomyces* sp. isolate B1751. Pale yellow solid. λ_{max} 278 (log ϵ 3.46); 321 (log ϵ 3.3) (MeOH).

Yao, C.B.F. *et al., Z. Naturforsch., B*, 2006, **61**, 320-325 (*isol, pmr, cmr, ms*)

Urauchimycin D **U-59**

As Urauchimycin A, U-56 with

R = CH_3

$C_{18}H_{22}N_2O_8$ 394.38

Prod. by the marine-derived *Streptomyces* sp. isolate B1751. Yellow solid. $[\alpha]_D^{20}$ +53 (c, 0.1 in Me_2CO). λ_{max} 201 (log ϵ 4.02); 221 (log ϵ 3.77); 348 (log ϵ 2.99) (MeOH).

Yao, C.B.F. *et al., Z. Naturforsch., B*, 2006, **61**, 320-325 (*isol, pmr, cmr, ms*)

Urea, 9CI, 8CI, USAN **U-60**

Carbamide. Ureaphil. E927b

[57-13-6]

H_2NCONH_2

CH_4N_2O 60.055

Manuf. on large scale from NH_3 and CO_2 at high pressure. Constit. of all vertebrate tissues and of many invertebrates. Found esp. in urine. Also occurs in many plants in traces and in larger amounts in fungi. Fertiliser, cattle feed supplement, also used in manuf. of urea-formaldehyde resins. Forms clathrates (inclusion complexes) with hydrocarbons, useful in petrochemicals industry. Important industrial chemical, USA production in 2002 7.33 million tonnes. Diuretic, dermatic, keratolytic and antiseptic agent. Polymer with formaldehyde (Polynoxylin, BAN, INN) used as a topical antibacterial and antifungal agent. Tetragonal needles or prisms with faint salty taste (H_2O or EtOH). V. sol. H_2O; sol. MeOH, EtOH; insol. $CHCl_3$, C_6H_6.

Mp 133-135°. pK_a 0.1 (21°). Log P -2.11 (calc). Aq. solns hydrol. v. slowly to ammonium carbamate then to NH_3 and CO_2. Weak base.

▶ Irritant to skin, eyes, respiratory tract and mucous membranes. Human reprod. effects (abortifacient), exp. reprod. effects. LD_{50} (rat, orl) 8471 mg/kg. YR6250000

Hydrochloride: [506-89-8]

Plates or faintly yellow, deliquescent cryst. Sol. H_2O. Mp 145° dec.

[1433-11-0, 17687-37-5, 21351-39-3]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 670B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 799C (*ir*)
Reifer, J. *et al., J. Biol. Chem.*, 1949, **178**, 715 (*occur*)
Witanowski, M. *et al., Tetrahedron*, 1976, **32**, 2127 (*nmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **23**, 548 (*rev, bibl*)
Swawinathan, S. *et al., Acta Cryst. B*, 1984, **40**, 300 (*cryst struct*)

Urechistachykinins **U-61**

Leu-Arg-Gln-Ser-Gln-Phe-Val-Gly-Ser-Arg-NH_2

Struct. of Urechistachykinin I shown. Isol. from the echiuroid worm *Urechis unicinctus*. Neuropeptides.

Urechistachykinin I

LRQSQFVGSR amide

[149097-03-0]

$C_{50}H_{85}N_{19}O_{14}$ 1176.34

Urechistachykinin II
AAGMGFFGAR amide
[149097-04-1]
$C_{44}H_{66}N_{14}O_{10}S$ 983.159

Urechistachykinin III
AAPSGFFGAR amide
[331456-26-9]
$C_{45}H_{66}N_{14}O_{11}$ 979.104

Urechistachykinin IV
AAYSGFFGAR amide
[331456-27-0]
$C_{49}H_{68}N_{14}O_{12}$ 1045.163

Urechistachykinin V
APSMGFFGAR amide
[331456-28-1]
$C_{47}H_{70}N_{14}O_{11}S$ 1039.223

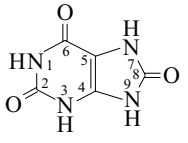
Urechistachykinin VI
APHMRFYGSR amide
[331456-29-2]
$C_{54}H_{81}N_{19}O_{12}S$ 1220.42

Urechistachykinin VII
APKMGFFGAR amide
[331456-30-5]
$C_{50}H_{77}N_{15}O_{10}S$ 1080.319

Ikeda, T. *et al., Biochem. Biophys. Res. Commun.*, 1993, **192**, 1-6 (*Urechistachykinins I-III*)
Kawada, T. *et al., Peptides (N.Y.)*, 2000, **21**, 1777-1783 (*Urechistachykinins IV-VII*)

Uric acid, 8CI U-62

*7,9-Dihydro-1*H*-purine-2,6,8(3*H*)-trione, 9CI. 2,6,8-Trihydroxypurine. 2,6,8(1*H*,3*H*,9*H*)-Purinetrione*
[69-93-2]



$C_5H_4N_4O_3$ 168.112

Exists in several tautomeric forms. Chief end-product of purine metab. Constit. of urine of carnivorous animals, bird excrement (guano), excrement of reptiles, insects etc. Produced by *Mamestra brassicae*. Present in small amts. in higher plants, esp. seeds. Prod. by marine bacterium strain Cr 11 from *Crassostrea gigas* and by a range of microorganisms from fish and shellfish. Sperm-release pheromone of *Platynereis dumerilii*. Odourless, tasteless, rhombic prisms or plates. Sol. alkalis, glycerol; spar. sol. min. acids; v. spar. sol. H_2O; insol. EtOH, Et_2O. pK_a 5.75; pK_{a2} 10.6. Dec. without melting.

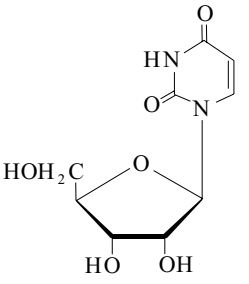
▶ Exp. reprod. effects (male). May evolve HCN when heated. YU7050080

[1198-77-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 710A; 710C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 214C; 215A (*nmr*)
Fischer, E. *et al., Ber.*, 1897, **30**, 559-573; 1899, **32**, 2721-2735 (*synth*)
Traube, W. *et al., Ber.*, 1900, **33**, 1371-1386; 3035-3056 (*synth*)
Lifschitz, C. *et al., Isr. J. Chem.*, 1968, **6**, 827-831 (*ms*)
Weiner, I.M. *et al., CA*, 1975, **82**, 28926 (*rev, bibl*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **23**, 608 (*rev, bibl*)
Takao, T. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1780-1783 (*isol, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, UVA400

Uridine U-63

*1-β-D-Ribofuranosyl-2,4(1*H*,3*H*)-pyrimidinedione, 9CI. 1-β-D-Ribofuranosyluracil, 8CI. NSC 20256*
[58-96-8]
[26287-69-4]



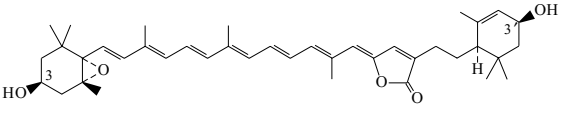
$C_9H_{12}N_2O_6$ 244.204
Prepd. by hydrol. of yeast nucleic acid. Widely distributed in nature.
Mp 165°. $[\alpha]_D^{20}$ +4 (c, 2 in H_2O). λ_{max} 205 (ε 9800); 261 (ε 10100) (pH 7.3).
▶ LD_{50} (mus, ipr) 4335 mg/kg. YR1450000

[19817-91-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 815B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 371B (*nmr*)
Fox, J.J. *et al., Adv. Carbohydr. Chem.*, 1959, **14**, 283 (*rev*)
Biemann, K. *et al., J.A.C.S.*, 1962, **84**, 2005 (*ms*)
Ulbricht, T.L.V. *et al., Tet. Lett.*, 1964, 695 (*ord*)
Green, E.A. *et al., Chem. Comm.*, 1971, 53 (*cryst struct*)
Krugh, T.R. *et al., J.A.C.S.*, 1973, **95**, 4761 (*cmr*)
Belikova, A.M. *et al., Tetrahedron*, 1973, **29**, 2277 (*conformn, pmr*)
Basic Princ. Nucleic Acid Chem., (Ts'O, P.O.P., Ed.), Academic Press, 1974, **1**, (*rev*)
Kikugawa, K. *et al., Chem. Pharm. Bull.*, 1975, **23**, 35 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1425
Moyroud, E. *et al., Tetrahedron*, 1999, **55**, 1277-1284 (*L-form, synth, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, UVJ000

Uriolide U-64

5,6-Epoxy-5,6,7′,8′-tetrahydro-3,3′,11′-trihydroxy-β,ε-caroten-19′-oic acid γ-lactone, 9CI. 5,6-Epoxy-3,3′-dihydroxy-5,6,7′,8′-tetrahydro-β,ε-caroten-11′,19′-olide
[101527-89-3]



$C_{40}H_{54}O_5$ 614.864
Abs. config. postulated biogenetically. Isol. from eukaryotic ultraplankton clones (Prasinophyceae). λ_{max} 448; 472 (Me_2CO).

3-Ketone: ***3′-Dehydrouriolide***
$C_{40}H_{52}O_5$ 612.848
Constit. of *Bathycoccus prasinos*.

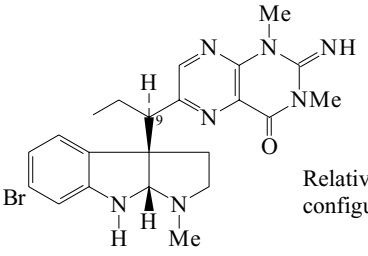
Deepoxy: ***Deepoxyuriolide***
$C_{40}H_{54}O_4$ 598.864
Constit. of clone IIA2. Has double bond in place of epoxide.

3′-Deoxy, 3′,4′-didehydro: ***Anhydrouriolide***
$C_{40}H_{52}O_4$ 596.848
Constit. of *Mantoniella squamata* and *Micromonas pulsilla*.

Foss, P. *et al., Phytochemistry*, 1986, **25**, 119
Egeland, E.S. *et al., Phytochemistry*, 1995, **40**, 515 (*derivs*)

Urochordamine A U-65

[151756-66-0]



Relative configuration

$C_{22}H_{26}BrN_7O$ 484.398

Alkaloid from the tunicates *Ciona savignyi* and *Botrylloides* sp. Promotes larvae settlement and metamorphosis in the tunicate. Exhibits antibacterial activity. $[\alpha]_D$ +11.7 (c, 0.263 in $CHCl_3$). λ_{max} 211 (ϵ 33100); 253 (ϵ 20000); 313 (ϵ 4170); 357 (ϵ 5500) (MeOH) (Derep).

9-Epimer: ***Urochordamine B***
[151851-37-5]
$C_{22}H_{26}BrN_7O$ 484.398
Alkaloid from *Ciona savignyi* and *Botrylloides* sp. Shows antibacterial activity. Metamorphosis promoter and larval settlement inhibitor. $[\alpha]_D$ -36.6 (c, 0.174 in $CHCl_3$). λ_{max} 211 (ϵ 33100); 253 (ϵ 20000); 313 (ϵ 4170); 357 (ϵ 5500) (MeOH) (Derep).

Tsukamoto, S. *et al., Tet. Lett.*, 1993, **34**, 4819-4822 (*isol, uv, ir, pmr, cmr, struct*)

Urotensin I U-66

[9047-54-5]

A 41 amino acid peptide homologous and analogous to mammalian corticotropin-releasing factors. Isol. from the urophysis, the hormone storage-secretion organ of the caudal neurosecretory system of teleost fishes, e.g. *Cyprinus carpio* (carp), *Catostomus commersoni* (white sucker) and *Platichthys flesus* (flounder). Neuropeptide exhibiting potent hypotensive activity (mammals and birds) and corticotropin-releasing activity (fish and mammals).

[83930-33-0, 84133-52-8, 128086-95-3, 131359-76-7]

Ichikawa, T. *et al., Peptides (N.Y.)*, 1982, **3**, 859-867 (*isol, struct, Cyprinus constit*)
Lederis, K. *et al., Can. J. Biochem. Cell Biol.*, 1983, **61**, 602-614 (*isol, struct*)
Osakada, F. *et al., Pept. Chem.*, 1983, 267 (*synth*)
Lederis, K. *et al., Recent Prog. Horm. Res.*, 1985, **41**, 553-576 (*rev*)
Conlon, J.M. *et al., Peptides (N.Y.)*, 1990, **11**, 895 (*isol, Platichthys constit*)

Oncorhynchus mykiss Urotensin II U-67

GGNSECFWKYCV
[152344-00-8]
Gly-Gly-Asn-Ser-Glu-Cys-Phe-Trp-Lys-Tyr-Cys-Val
$C_{62}H_{83}N_{15}O_{18}S_2$ 1390.559

Peptide hormone. Reduced form shown. Isol. from brain of the rainbow trout *Oncorhynchus mykiss*.

Waugh, D. *et al., Gen. Comp. Endocrinol.*, 1993, **92**, 419-427 (*isol*)

Scyliorhinus canicula Urotensin II U-68

[141546-63-6]

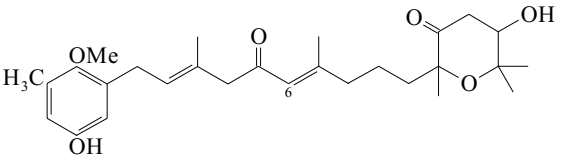
Asn-Asn-Phe-Ser-Asp-Cys-Phe-Trp-Lys-Tyr-Cys-Val

$C_{70}H_{90}N_{16}O_{19}S_2$ 1523.709

Peptide hormone. Reduced form shown. Isol. from the spinal cord of the common dogfish *Scyliorhinus canicula*; from brain of the river lamprey *Lampetra fluviatilis*, the sea lamprey *Petromyzon marinus*, and the longnose skate *Raja rhina*.

Conlon, J.M. *et al., Neuroendocrinology*, 1992, **55**, 230-235 (*isol, dogfish*)
Waugh, D. *et al., Gen. Comp. Endocrinol.*, 1993, **92**, 419-427; 1995, **99**, 323-332 (*isol, lamprey, skate*)

Usneoidol E U-69



$C_{28}H_{40}O_6$ 472.62
Constit. of *Cystoseira usneoides*.
$[\alpha]_D^{24}$ -16.47 (c, 0.17 in $CHCl_3$). λ_{max} 220 (ϵ 20400); 276 (ϵ 7660) (MeOH) (Berdy).

6Z-Isomer: ***Usneoidol Z***
$C_{28}H_{40}O_6$ 472.62
Constit. of *Cystoseira usneoides*.
$[\alpha]_D^{24}$ +3.66 (c, 0.24 in $CHCl_3$). λ_{max} 222 (ϵ 15300); 278 (ϵ 6800) (MeOH) (Berdy).

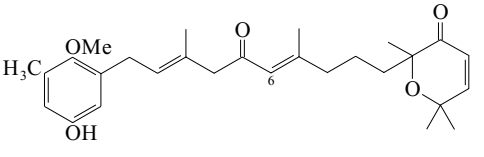
14-Deoxy, 13,14-didehydro: ***Usneoidone E***
[139955-81-0]
$C_{28}H_{38}O_5$ 454.605
Constit. of *Cystoseira usneoides*. Oil. $[\alpha]_D^{24}$ -3.1 (c, 1.7 in $CHCl_3$). λ_{max} 226 (ϵ 24061); 280 (ϵ 3476) (MeOH) (Berdy).

6Z-Isomer, 14-deoxy, 13,14-didehydro: ***Usneoidone Z***
[140147-79-1]
$C_{28}H_{38}O_5$ 454.605
Constit. of *Cystoseira usneoides*. Oil. $[\alpha]_D^{24}$ -6.1 (c, 0.3 in $CHCl_3$). λ_{max} 222 (ϵ 29490); 280 (ϵ 4706) (MeOH) (Berdy).

[142902-56-5, 143004-42-6]

Urones, J.G. *et al., Phytochemistry*, 1992, **31**, 179; 2105 (*isol, pmr, cmr*)

Usneoidone U-70



(6*E*)–*form*

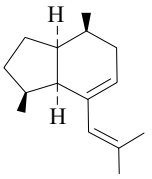
$C_{28}H_{38}O_5$ 454.605

(6*E*)-*form*
Constit. of *Cystoseira usneoides*.
Oil. $[\alpha]_D^{24}$ -3.1 (c, 1.7 in $CHCl_3$).

(6*Z*)-*form*
Constit. of *Cystoseira usneoides*.
Oil. $[\alpha]_D^{24}$ -6.1 (c, 0.3 in $CHCl_3$).

Urones, J.G. *et al., Phytochemistry*, 1992, **31**, 179 (*isol, pmr, cmr*)

6(8),7(11)-Valerenadiene V-1

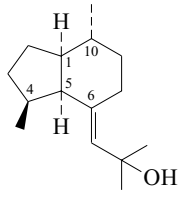


Absolute configuration

$C_{15}H_{24}$ 204.355

(1α,4β,5α,10β)-*form*
Anhydrovalerenol
[84249-44-5]
Constit. of a soft coral, family Xeniidae.
Oil. $[\alpha]_D$ -150 ($CHCl_3$). The name anhydrovalerenol is misleading.
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 3431

6-Valerenen-11-ol V-2



(1α,4β,5α,6*E*,10β)–*form*

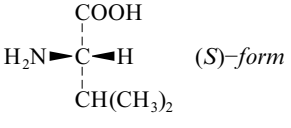
$C_{15}H_{26}O$ 222.37

(1α,4β,5α,6*E*,10β)-*form*
Isovalerenenol
[84249-42-3]
Constit. of soft coral, family Xeniidae.
Semisolid. $[\alpha]_D$ +45 ($CHCl_3$).

(1α,4β,5α,6*Z*,10β)-*form*
Valerenenol
[84249-43-4]
Constit. of a soft coral, family Xeniidae.
Oil. $[\alpha]_D$ +123 ($CHCl_3$).
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 3431 (*isol, pmr, cmr, cryst struct*)
Tori, M. *et al., Tetrahedron*, 1996, **52**, 9999 (*synth*)

Valine V-3

2-Amino-3-methylbutanoic acid, 9CI. 2-Aminoisovaleric acid. Val
[7004-03-7]



(*S*)–*form*

$C_5H_{11}NO_2$ 117.147
▶ YV9355500

(*R*)-*form*
D-form
[640-68-6]
Residue present in microbial cell walls and in antibiotics, e.g. actinomycins.
Plates (EtOH aq.). Sol. H_2O.
Mp 156-157.5° (293° dec. sealed tube). $[\alpha]_D^{25}$ -6.1 (H_2O). $[\alpha]_D^{20}$ -28.8 (c, 1 in 5*M* HCl) (100% op).
▶ YV9360000

(*S*)-*form*
L-form
[72-18-4]
Widely distributed in nature as one of the principal protein amino acids. Dietary supplement. Plates (EtOH aq.). Sol. H_2O (8.85 g per 100 cm^3 at 25°); spar. sol. EtOH.
Mp 315° dec. (sealed tube). $[\alpha]_D^{20}$ +6.3 (H_2O). $[\alpha]_D^{20}$ +23.4 (1*M* HCl). $[\alpha]_D^{20}$ +27.6 (6*M* HCl). pK_{a1} 2.32; pK_{a2} 9.62 (NH_2). Isoelectric point 5.96. Bitter taste.
▶ YV9361000

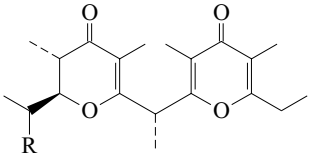
N-*Tri-Me, betaine:* [53948-31-5]
$C_8H_{17}NO_2$ 159.228
Isol. from *Callista brevisiphonata* and *Atrina pectinata*.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 573B; 573C; 573D; 674A; 674B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 872B; 872C; 1071B; 1071C (*nmr*)
Sadtler Standard C-13 NMR Spectra, 4424 (*cmr*)
Adams, R. *et al., J.A.C.S.*, 1934, **56**, 2093 (*resoln*)
Barrow, F. *et al., J.C.S.*, 1935, 410 (*abs config*)
Org. Synth., Coll. Vol., 3, 1955, 848 (*synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, (Chapter 41), Wiley, N.Y., 1961, **3**, (*rev*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Aruldhas, G. *et al., Spectrochim. Acta A*, 1967, **23**, 1345 (*pmr*)
Pachler, K.G.R. *et al., Spectrochim. Acta A*, 1968, **24**, 1311 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 2348 (*occur*)
Armstrong, F.B. *et al., Chem. Comm.*, 1974, 351 (*biosynth*)
Oguri, T. *et al., Chem. Pharm. Bull.*, 1975, **23**, 167 (*synth*)
Shiraiwa, T. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 2234 (*resoln*)
Ullmann's Encycl. Ind. Chem., 5th edn., VCH, Weinheim, 1985, **A2**, 57 (*rev*)
Kulik, W. *et al., Biomed. Mass Spectrom.*, 1988, **15**, 419 (*ms*)
Dalhus, B. *et al., Acta Chem. Scand.*, 1996, **50**, 544-545 (*cryst struct, L-form*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VBP000; VBU000

Valitocin V-4

8-L-Valineoxytocin, 9CI
[3275-87-4]
H-Cys-Tyr-Ile-Gln-Asn-Cys-Pro-Val-Gly-NH_2
Reduced form shown. Isol. from the spiny dogfish (*Squalus acanthias*). Neurohypophysial hormone.
[30635-16-6]
Acher, R. *et al., Eur. J. Biochem.*, 1972, **29**, 12 (*isol*)

Vallartanone A V-5

[122947-98-2]



R = CH_3

$C_{21}H_{30}O_4$ 346.466
Abs. config. confirmed for Vallartanone B but not A (1996). Metab. of the pulmonate mollusc *Siphonaria maura*. Cryst. Mp 69°. $[\alpha]_D$ -176 (c, 0.68 in $CHCl_3$). λ_{max} 215 (ε 12300); 264 (ε 28500) (MeOH) (Derep). λ_{max} 215 (ε 12896); 264 (ε 28510) (MeOH) (Berdy).
Manker, D.C. *et al., J.O.C.*, 1989, **54**, 5374 (*isol, pmr, cmr*)
Arimoto, H. *et al., Tetrahedron*, 1996, **52**, 13901 (*abs config*)

Vallartanone B V-6

[122947-99-3]
As Vallartanone A, V-5 with
R = H
$C_{20}H_{28}O_4$ 332.439
Metab. of the pulmonate mollusc *Siphonaria maura*. Fish antifeedant. Oil. $[\alpha]_D$ -133 (c, 0.59 in $CHCl_3$). λ_{max} 215 (ε 12300); 264 (ε 28500) (MeOH) (Derep).

Manker, D.C. *et al., J.O.C.*, 1989, **54**, 5374-5377 (*isol, pmr, cmr*)
Arimoto, H. *et al., Tetrahedron*, 1996, **52**, 13901 (*synth, abs config*)

Vanabins V-7

Vanadium-associated proteins

Two cysteine- and lysine-rich proteins, Vanabin 1 and Vanabin 2 which contain 87 and 91 amino acids. Isol. from the ascidian *Ascidia sydneiensis samea*. Vanadium binding proteins.

Ueki, T. *et al., Biochim. Biophys. Acta*, 2003, **1626**, 43-50; **1630**, 64-70 (*isol*)
Michibata, H. *et al., Coord. Chem. Rev.*, 2003, **237**, 41-51 (*rev*)
Fukui, K. *et al., J.A.C.S.*, 2003, **125**, 6352-6353
Hamada, T. *et al., J.A.C.S.*, 2005, **127**, 4216-4222 (*Vanabin 2, soln struct*)

Vanadium V-8

[7440-62-2]

V

V 50.942

Atomic No. 23. Ground state electron config. [Ar]$3d^3 4s^2$. 9 Isotopes have been reported of which 2 are natural. Discovered by A.M. del Rio (Mexico City) in 1801, and 'rediscovered' by N .G. Sefström (Sweden) in 1831. Metal prep. reasonably pure by H.E. Roscoe in 1867. Abundance: 136 ppm (earth's crust), 0.002 ppm (sea water). Bcc struct. Important minerals are vanadinite and carnotite. Also found in some crude oils. Extraction is usually by forming $NaVO_3$ with alkali and reduction with Al or with ferrosilicon (to yield Fe/V alloys). Pure metal obt. from VCl_3 VCl_5, + H_2, or Mg; or from V_2O_5 + Ca, Al, C; or by electrolysis of fused halides. Accumulated by many organisms in various ionic forms and as complexes (up to 1.45% in blood of some marine worms, e.g *Ascidia ceratodes*). Used in steels to impart wear resistance and high temp. strength. Biological activity uncertain. Essential trace element. Silvery metal, comparatively soft and ductile when pure. Corrosion resistant (oxide film). Resistant to fused alkalis, attacked by hot conc. mineral acids.

Mp 1915° (1890°). Bp 3380° (3350°). Reacts with Cl_2 at 180°. At high temps. reacts with most non metals.

▶ Human poison by subcutaneous route. Flammable and highly reactive when in finely divided form. YW1355000

Vanadium 47 [14867-38-0]

Radioactive, $t_{½}$ 32.6 min. Prod. from ^{45}Sc (α,2n), ^{47}Ti (p,n), ^{46}Ti (d,n), or ^{47}Ti (d,2n). I = -3/2. Decays by orbital electron capture or $\beta^{\oplus}$ emission to ^{47}Ti.

Vanadium 48 [14331-97-6]

Radioactive, $t_{½}$ 15.98 d. Prod. by ^{45}Sc (α,n), ^{48}Ti (p,n), ^{48}Ti (d,2n), or ^{50}Cr (d,α). Also obt. by proton spallation in ZnO targets (commercial production route). I = +4; μ = +2.01 μ_N. Decays by $\beta^{\ominus}$ emission to ^{48}Ti.

Vanadium 49 [14392-01-9]

Radioactive, $t_{½}$ 337 d. Prod. by ^{52}Cr (p,α), or ^{48}Ti (d,n). Also obt. by proton spallation in ZnO targets (commercial production route). I = -7/2; μ = +4.47 μ_N. Decays by orbital electron capture to ^{49}Ti.

Vanadium 50 [14391-89-0]

Stable. Natural abundance 0.2502-0.2487 atom %. I = +6; μ = +3.34745 μ_N. Nmr relative sensitivity (^{1}H=1.00) 0.0555; receptivity (^{13}C=1.00) 0.755.

Vanadium 51

Stable. Natural abundance 99.7513-99.9498 atom %. Preferred iostope for nmr spectroscopy.
I = -7/2; μ = +5.1574 μ_N. Nmr relative sensitivity (^{1}H=1.00) 0.38; receptivity (^{13}C=1.00) 2150.

Vanaium 52 [14681-50-6]

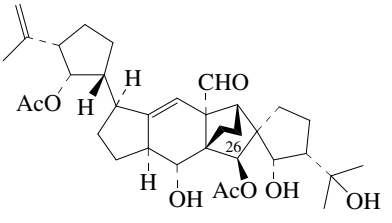
Radioactive, $t_{½}$ 3.75 min. Prod. from ^{51}V (n,γ), or by bombardment of Ti with α-particles. I = +3. Decays by $\beta^{\ominus}$ emission to ^{52}Cr.

[14782-33-3, 15121-26-3, 22537-31-1, 22541-76-0, 22541-77-1]

Mellor Compr. Treat. Inorg. Theor. Chem., 1929, **9**, 714 (*rev, bibl*)
Weeks, M.E. *et al., Discovery of the Elements*, J. Chem. Educ., 6th Edn., 1956, 339 (*history*)
Gmelin Handbook Inorg. Chem., Syst. No. 48, 1968, **A1, A2**, (*rev, bibl*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **3**, 491 (*rev*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **3**, 1407 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **23**, 673 (*rev, bibl*)
Thornhill, D.H. *et al., Future Heavy Crude Tar Sands, Int. Conf., 2nd, 1982 (1984)*, 1982, 1277 (*V in crude oil*)
Granger, P. *et al., NMR Newly Accessible Nucl. 1983*, (Ed. Laszlo, P.), Academic Press, N.Y., 1983, **2**, 385 (*V-51 nmr*)
Kustin, K. *et al., Struct. Bonding (Berlin)*, 1983, **53**, 139 (*accum in marine organisms*)
Amer-Amezaga, S. *et al., Ing. Quim. (Madrid)*, 1984, **16**, 75 (*solvent extrn*)
Boyd, D.W. *et al., Inorg. Biochem.*, 1984, **6**, 311 (*rev, biochem*)
Greenwood, N.N. *et al., Chemistry of the Elements*, Pergamon, Oxford, 1986, 1138 (*rev*)
Morrell, B.G. *et al., Environ. Geochem. Health*, 1986, **8**, 14 (*uptake by plants*)
Wever, R. *et al., Adv. Inorg. Chem.*, 1990, **35**, 81 (*rev, bibl*)
Emsley, J. *et al., The Elements*, 3rd edn., Clarendon Press, 1998, 222; 252
Frank, P. *et al., Coord. Chem. Rev.*, 2003, **237**, 31-39 (*occur, marine organisms*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1468 (*haz*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VCP000

Vannusal A V-9

[230288-21-8]



Relative Configuration

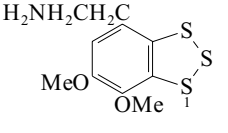
$C_{34}H_{48}O_8$ 584.748
Isol. from *Euplotes vannus*. Cryst. (H_2O).
Mp 95°. $[\alpha]_D^{20}$ -17 (c, 0.3 in MeOH). λ_{max} 229 (sh) (ε 6600); 304 (ε 1300) (MeOH).

26-O-*De-Ac:* ***Vannusal B***
[230288-22-9]
$C_{32}H_{46}O_7$ 542.711
Isol. from *Euplotes vannus*. Amorph. powder. λ_{max} 229 (ε 5100); 301 (ε 1100) (MeOH).

Guella, G. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 1134-1136

Varacin A V-10

6,7-Dimethoxy-4-benzotrithioleethanamine, 9CI
[162857-71-8]



$C_{10}H_{13}NO_2S_3$ 275.416
Alkaloid from the Far Eastern ascidian *Polycitor* sp.

1-S-*Oxide:* ***Varacin B***
[162901-84-0]
$C_{10}H_{13}NO_3S_3$ 291.416
From *Polycitor* sp.

3-S-*Oxide:* ***Varacin C***
[162857-72-9]
$C_{10}H_{13}NO_3S_3$ 291.416
From *Polycitor* sp.

Ac:
Exhibits potent antifungal and antimicrobial activity. Thin yellow cryst. (MeOH). Mp 140-142°.

*Ac, 1-*S*-oxide:*
Exhibits potent antifungal and antimicrobial activity. Thin yellow cryst. (MeOH). Mp 131-133°.

*Ac, 3-*S*-oxide:*
Exhibits potent antifungal and antimicrobial activity. Thin yellow cryst. (MeOH). Mp 70-73°.

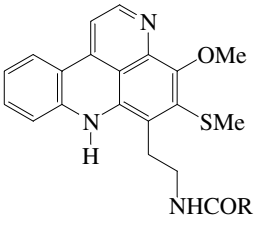
5-(Methylthio): 6-(2-Aminoethyl)-3,4-dimethoxy-5-(methylthio)-benzotrithiane. ***5-(Methylthio)varacin A***
$C_{11}H_{15}NO_2S_4$ 321.509
Isol. from a *Lissoclinum* sp. Protein kinase C inhibitor. Not in CA. λ_{max} 211 (ϵ 34800); 240 (ϵ 21000); 271 (ϵ 14700) (MeOH) (Berdy).

5-(Methylthio), N,N-*di-Me: 6,7-Dimethoxy*-N,N-*dimethyl-5-(methylthio)-4-benzotrithioleethanamine. 6-(2-Aminoethyl)-3,4-dimethoxybenzotrithiane*
$C_{13}H_{19}NO_2S_4$ 349.563
Isol. from *Lissoclinum japonicum*. Protein kinase C inhibitor. Pale yellow oil (as trifluoroacetate). λ_{max} 209 (ϵ 15900); 238 (ϵ 7410); 277 (ϵ 5960) (MeOH).

Campagnone, R.S. *et al., Tetrahedron*, 1994, **50**, 12785-12792 (*methylthio derivs*)
Makarieva, T.N. *et al., J. Nat. Prod.*, 1995, **58**, 254 (*isol, ir, pmr, ms, struct*)
Lee, A.H.F. *et al., J.A.C.S.*, 2002, **124**, 13972-13973 (*Varacin C, synth*)

Varamine A V-11

[122093-14-5]



R = CH_2CH_3

$C_{22}H_{23}N_3O_2S$ 393.509
Alkaloid from the tunicate *Lissoclinum vareau*. Cytotoxic agent (about 1 order of magnitude more toxic than the cystodytins which lack the thiomethyl group). Topoisomerase inhibitor. Orange solid. Sol. MeOH, $CHCl_3$. λ_{max} 224 (ϵ 24400); 228 (sh); 240 (sh); 263 (sh); 280 (sh); 291 (ϵ 31100); 339 (ϵ 20400); 359 (ϵ 4520); 376 (ϵ 4640); 527 (ϵ 5670); 552 (sh) (pH 2) (Derep). λ_{max} 232 (ϵ 31500); 275 (ϵ 25800); 292 (sh); 324 (sh); 382 (ϵ 3530); 464 (ϵ 5170); 494 (sh) (MeOH) (Derep).

▶ Toxic.

Molinski, T.F. *et al., J.O.C.*, 1989, **54**, 4256-4259 (*isol, uv, ir, pmr, cmr, ms, struct*)

Varamine B V-12

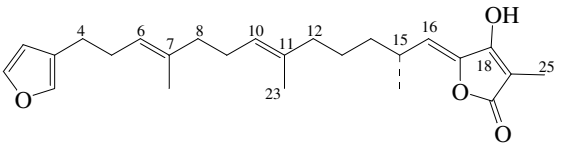
[122093-16-7]
As Varamine A, V-11 with
R = CH_3

$C_{21}H_{21}N_3O_2S$ 379.482
Alkaloid from the tunicate *Lissoclinum vareau*. Cytotoxic agent. Topoisomerase inhibitor. Orange solid. Sol. MeOH, $CHCl_3$. λ_{max} 224 (ϵ 24400); 228 (sh); 240 (sh); 263 (sh); 280 (sh); 291 (ϵ 31100); 339 (ϵ 20400); 359 (ϵ 4520); 376 (ϵ 4640); 527 (ϵ 5670); 552 (sh) (pH 2) (Derep). λ_{max} 232 (ϵ 31500); 275 (ϵ 25800); 292 (sh); 324 (sh); 382 (ϵ 3530); 464 (ϵ 5170); 494 (sh) (MeOH) (Derep). λ_{max} 234 (ϵ 25900); 274 (ϵ 21400); 382 (ϵ 3040); 462 (ϵ 4320) (MeOH/HCl) (Berdy). λ_{max} 223 (ϵ 20570); 294 (ϵ 27400); 311 (ϵ 17300); 379 (ϵ 4190); 529 (ϵ 4720) (MeOH/HCl) (Berdy).

▶ Toxic.

Molinski, T.F. *et al., J.O.C.*, 1989, **54**, 4256-4259 (*isol, uv, ir, pmr, cmr, struct*)

Variabilin† V-13



(6*E*,10*E*,15*R*,16*Z*)-*form*

$C_{25}H_{34}O_4$ 398.541
Different numbering system used in lit. The original Variabilin isol. was the (15*S*,16*Z*)-stereoisomer.

(6*E*,10*E*,15*R*,16*Z*)-*form*
*18*R-*Variabilin*
[181781-60-2]
Isol. from sponges *Ircinia felix* and *Hypselodoris capensis*. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{30}$ +36 (c, 0.96 in $CHCl_3$).

18-Sulfate: [183593-68-2]
$C_{25}H_{34}O_7S$ 478.605
Constit. of an *Ircinia* sp. Ichthyotoxin. Amorph. powder. $[\alpha]_D$ +10.6 ($CHCl_3$). λ_{max} 272 (ϵ 18000) (MeOH).

18-Hexadecanoyl: [191158-73-3]
$C_{41}H_{64}O_5$ 636.954
Constit. of *Ircinia felix*.

18-(10-Methylhexadecanoyl): [191158-75-5]
$C_{42}H_{66}O_5$ 650.98
Constit. of *Ircinia felix*.

18-(14-Methylhexadecanoyl): [191158-78-8]
$C_{42}H_{66}O_5$ 650.98
Constit. of *Ircinia felix*.

18-(15-Methylhexadecanoyl): [191158-77-7]
$C_{42}H_{66}O_5$ 650.98
Constit. of *Ircinia felix*.

18-Octadecanoyl: [191158-81-3]
$C_{43}H_{68}O_5$ 665.007
Constit. of *Ircinia felix*.

18-(9Z-Octadecenoyl): [191158-80-2]
$C_{43}H_{66}O_5$ 662.991
Constit. of *Ircinia felix*.

*18-*O*-(11-Methyloctadecanoyl):* [181134-64-5]
$C_{44}H_{70}O_5$ 679.034
Constit. of *Ircinia felix*. λ_{max} 266 (ϵ 10000) (MeOH) (Derep). λ_{max} 262 (MeOH) (Berdy).

18-(2,11-Dimethyloctadecanoyl): [191158-82-4]
$C_{45}H_{72}O_5$ 693.061
Constit. of *Ircinia felix*.

18-(22-Methyl-5Z,9Z-tricosadienoyl): [191158-69-7]
$C_{49}H_{76}O_5$ 745.136
Constit. of *Ircinia felix*.

18-(5Z,9Z-Tetracosadienoyl): [191158-71-1]
$C_{49}H_{76}O_5$ 745.136
Constit. of *Ircinia felix*.

(6*E*,10*E*,15*S*,16*E*)-*form* [114761-90-9]
Constit. of a *Sarcotragus* sp.
Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. λ_{max} 256 (ϵ 12700) (MeOH) (Berdy). λ_{max} 250 (ϵ 13300); 310 (ϵ 7600) (MeOH/NaOH) (Berdy).

Me ether: ***18*-O-*Methylvariabilin***
[880342-91-6]
$C_{26}H_{36}O_4$ 412.568
Constit. of an *Ircinia* sp.

(6*E*,10*E*,15*S*,16*Z*)-*form* [51847-87-1]
Isol. from the sponge *Ircinia strobilina* and a *Sarcotragus* sp. Plant phytoalexin with antibiotic props. Oil. $[\alpha]_D$ -4 (c, 1 in $CHCl_3$).

λ_{max} 255 (ϵ 12700) (MeOH). λ_{max} 250 (ϵ 13300); 308 (ϵ 7600) (MeOH/NaOH).

Me ether: Constit. of *Ircinia oros.*
Oil. $[\alpha]_D^{20}$ -40.8 (c, 0.7 in $CHCl_3$).

4-Hydroxy: ***5-Hydroxyvariabilin***
[119309-44-3]
$C_{25}H_{34}O_5$ 414.541
Constit. of an *Ircinia* sp. λ_{max} 266 (ϵ 10000) (MeOH) (Berdy).

4-Oxo: ***5-Oxovariabilin***
[119328-95-9]
$C_{25}H_{32}O_5$ 412.525
Constit. of an *Ircinia* sp.

*Δ^{11}-Isomer(*Z-*):* [114728-09-5]
$C_{25}H_{34}O_4$ 398.541
Constit. of a *Sarcotragus* sp. Oil. $[\alpha]_D$ -4.4 (c, 0.9 in $CHCl_3$).

6,7-Dihydro, 7-hydroxy: ***8-Hydroxyvariabilin***
[82124-11-6]
$C_{25}H_{36}O_5$ 416.556
Constit. of a *Sarcotragus* and *Ircinia* spp. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ -24.5 (c, 0.22 in MeOH). λ_{max} 253 (ϵ 10000) (MeOH) (Berdy). λ_{max} 248 (ϵ 1000); 308 (ϵ 7000) (MeOH/NaOH) (Berdy).

*4-Oxo, Δ^7-isomer(*E-*):* ***5-Oxo-8(10)*E*-variabilin***
[119328-94-8]
$C_{25}H_{32}O_5$ 412.525
Constit. of an *Ircinia* sp.

*Δ^7(*E-*), Δ^{11}-Isomer, 4-oxo:* ***5-Oxo-8(10)*E,*13(15)*E-*variabilin***
[119328-96-0]
$C_{25}H_{32}O_5$ 412.525
Constit. of an *Ircinia* sp.

18-Deoxy: ***18-Deoxyvariabilin***. *22-Deoxyvariabilin*
[133084-62-5]
$C_{25}H_{34}O_3$ 382.542
Constit. of a *Thorecta* sp. and *Hypselodoris capensis.* Oil. $[\alpha]_D^{23}$ -73 (c, 0.2 in $CHCl_3$).

18-Deoxy, 25-hydroxy: ***22-Deoxy-23-hydroxymethylvariabilin***
[211946-79-1]
$C_{25}H_{34}O_4$ 398.541
Constit. of *Hypselodoris capensis.* Yellow oil. $[\alpha]_D^{23}$ +18 (c, 0.31 in $CHCl_3$).

(6*E*,10*Z*,15*S*,16*Z*)-*form* [192884-69-8]
Constit. of *Ircinia oros.*
$[\alpha]_D^{20}$ -33.1 (c, 0.7 in $CHCl_3$) (as Me ether).

18-Sulfate: [183593-69-3]
Constit. of *Ircinia* spp. Ichthyotoxin. Amorph. powder. $[\alpha]_D$ +10.6 ($CHCl_3$). Cited to have the same phys. props as 18*R*-Variabilin sulfate. This may be an error. λ_{max} 272 (ϵ 18000) (MeOH).

Me ether: Constit. of *Ircinia oros.*
Oil. $[\alpha]_D$ -33.1 (c, 0.7 in $CHCl_3$). λ_{max} 263 (ϵ 12100) (EtOH).

*Δ^{11}-Isomer(*Z-*), Me ether:*
$C_{26}H_{36}O_4$ 412.568
Constit. of *Ircinia oros.* Oil. $[\alpha]_D^{20}$ -47.2 (c, 0.9 in $CHCl_3$).
λ_{max} 263 (ϵ 13600) (EtOH).

(6*E*,10*Z*,15*R*,16*Z*)-*form* [157809-55-7]
Constit. of *Ircinia dendroides.*
Oil.

*Δ^7-Isomer (7*E-*):* [86153-63-1]
$C_{25}H_{34}O_4$ 398.541
Constit. of *Ircinia dendroides.* Oil.

(6*Z*,10*Z*,15ξ,16*Z*)-*form* [86257-87-6]
Constit. of *Ircinia dendroides.*
Oil.

Faulkner, D.J. *et al., Tet. Lett.*, 1973, 3821 (*isol, uv, ir, nmr, struct*)
Rothberg, I. *et al., Tet. Lett.*, 1975, 769 (*isol, ir, uv, nmr, struct*)
González, A. *et al., J. Nat. Prod.*, 1983, **46**, 256-261 (*Ircinia dendroides constits*)
Barrow, C.J. *et al., J. Nat. Prod.*, 1988, **51**, 275-281 (*Sarcotragus constit*)
Barrow, C.J. *et al., J. Nat. Prod.*, 1988, **51**, 1294-1298 (*Ircinia constit*)
Kernan, M.R. *et al., J. Nat. Prod.*, 1991, **54**, 265 (*22-Deoxyvariabilin*)
Ishibashi, M. *et al., Nat. Prod. Lett.*, 1993, **3**, 189 (*abs config*)
Capon, R.J. *et al., Nat. Prod. Lett.*, 1994, **4**, 51 (*abs config*)
Martinez, A. *et al., Nat. Prod. Lett.*, 1995, **6**, 281-284 (*11-Methyloctadecanoyl*)
De Rosa, S. *et al., Nat. Prod. Lett.*, 1996, **8**, 245-251 (*sulfates*)
Martinez, A. *et al., Chem. Pharm. Bull.*, 1997, **45**, 181-184 (*isol, pmr, cmr*)
Höller, U. *et al., J. Nat. Prod.*, 1997, **60**, 832-835 (*Ircinia oros constit*)
Martinez, A. *et al., Lipids*, 1997, **32**, 565-569 (*isol, esters*)
McPhail, K. *et al., J. Nat. Prod.*, 1998, **61**, 961-964 (*22-Deoxy-23-hydroxymethylvariabilin*)
Höller, U. *et al., Dissertation*, Univ. of Braunschweig, 1999, (*Ircinia oros Me ethers*)
Chau, V.M. *et al., Tap Chi Hoa Hoc*, 2005, **43**, 499-502; *CA*, **144**, 327940r (*Ircinia Me ester*)

Variceramides V-14

$H_3C(CH_2)_nCOCH(OH)CH(CH_2OH)NHCO(CH_2)_{20}CH_3$
Isol. from the marine sponge *Ircinia variabilis.*

Variceramide 1 [128733-00-6]
$C_{41}H_{81}NO_4$ 652.095
Has n=14.

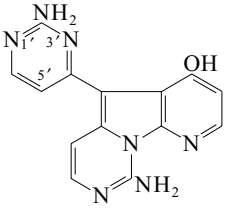
Variceramide 2 [128733-01-7]
$C_{40}H_{79}NO_4$ 638.068
Has n=13.

Variceramide 3 [128733-02-8]
$C_{39}H_{77}NO_4$ 624.042
Has n=12.

Cafieri, F. *et al., Annalen*, 1990, 1141-1142 (*isol, pmr, ms*)

Variolin B V-15

[156790-85-1]



$C_{14}H_{11}N_7O$ 293.287
Alkaloid from the Antarctic sponge *Kirkpatrickia varialosa*. Possesses antitumour and antiviral props. Yellow prisms (TFA aq.). Fairly sol. MeOH, DMSO; poorly sol. H_2O.
Mp 45° dec. λ_{max} 221 (ϵ 14100); 324 (ϵ 3900); 404 (ϵ 9100); 422 (ϵ 8400) (MeOH) (Berdy). λ_{max} 213 (ϵ 15500); 311 (ϵ 4400); 394 (ϵ 6300) (MeOH-HCl) (Berdy).

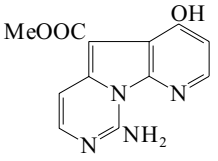
3′,4′,5′,6′-Tetrahydro, $N^{3'}$-Me: ***$N^{3'}$-Methyltetrahydrovariolin B***
[155205-63-3]
$C_{15}H_{17}N_7O$ 311.346
From *Kirkpatrickia varialosa*. Shows antifungal activity and moderate cytotoxicity. Light yellow solid. Fairly sol. MeOH, DMSO.
Mp 226° dec. $[\alpha]_D$ -22.4 (c, 3.5 in MeOH). λ_{max} 256 (ϵ 9680); 311 (ϵ 8660); 324 (ϵ 9885); 351 (ϵ 6995); 367 (ϵ 6840); 385 (ϵ 3190) (MeOH) (Berdy).

5′-Hydroxy, 1′-Me (zwitterion): ***Variolin A***
[155416-43-6]
$C_{15}H_{13}N_7O_2$ 323.313
Alkaloid from *Kirkpatrickia varialosa*. Weakly cytotoxic. Red solid. Fairly sol. MeOH, DMSO; poorly sol. H_2O.
Mp 196° dec. Unstable in base. λ_{max} 254 (ϵ 8945); 315 (ϵ 5375); 469 (ϵ 14570) (MeOH) (Berdy).

Perry, N.B. *et al., Tetrahedron*, 1994, **50**, 3987-3982 (*isol, uv, ir, pmr, cmr, cryst struct*)
Trimurtulu, G. *et al., Tetrahedron*, 1994, **50**, 3993-4000 (*$N^{3'}$-Methyltetrahydrovariolin B, Variolin A*)
Molina, P. *et al., Tet. Lett.*, 2002, **43**, 1005-1007 (*synth*)
Ahaidar, A. *et al., J.O.C.*, 2003, **68**, 10020-10029 (*synth*)
Anderson, R.J. *et al., J.O.C.*, 2005, **70**, 6204-6212 (*synth*)

Variolin D V-16

[156790-86-2]



$C_{12}H_{10}N_4O_3$ 258.236

Possibly an artifact. Alkaloid from the Antarctic sponge *Kirkpatrickia varialosa*. Fairly sol. MeOH, DMSO. Mp 248°. λ_{max} 226 (ϵ 11700); 240 (ϵ 14700); 246 (ϵ 14800); 368 (ϵ 12000); 388 (ϵ 9700) (MeOH) (Berdy).

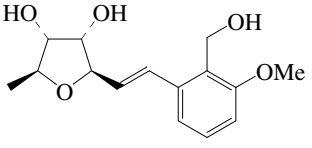
Perry, N.B. *et al., Tetrahedron*, 1994, **50**, 3987 (*isol, uv, ir, pmr, cmr, struct*)

Variolysin V-17

Protein, lacking methionine and cysteine. Isol. from the sea anemone *Pseudactinia varia*. Shows haemolytic activity.

Bernheimer, A.W. *et al., Toxicon*, 1984, **22**, 183-191 (*isol*)

Varitriol V-18



Absolute Configuration

$C_{15}H_{20}O_5$ 280.32

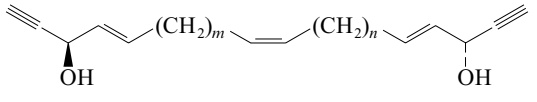
Isol. from the marine-derived *Emericella variecolor*. Cytotoxic. Oil. $[\alpha]_D^{25}$ +18.5 (c, 2.3 in MeOH). λ_{max} 204 (log ϵ 4.64); 260 (log ϵ 4.05); 296 (log ϵ 3.49) (EtOH).

Malmstrom, J. *et al., J. Nat. Prod.*, 2002, **65**, 364-367 (*isol, pmr, cmr*)
Clemens, R.T. *et al., Chem. Comm.*, 2006, 2720-2721 (*synth, abs config*)

Vasculyne V-19

4,?,39-Tritetracontatriene-1,42-diyne-3,41-diol

[172520-40-0]



$m + n = 31$

$C_{43}H_{74}O_2$ 623.056

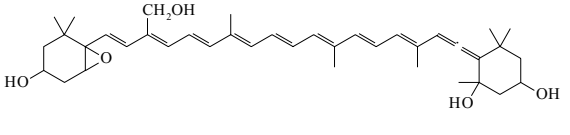
Isol. from the sponge *Cribrochalina vasculum*. Cytotoxic agent. Powder. $[\alpha]_D$ -24 (c, 0.2 in $CDCl_3$). Incorrect name in CA. λ_{max} 206 (log ϵ 3.2); 239 (log ϵ 2.1); 244 (log ϵ 2.1) (MeOH).

Dai, J.-R. *et al., J. Nat. Prod.*, 1996, **59**, 88-89 (*isol*)

Vaucheriaxanthin V-20

6,7-Didehydro-5′,6′-epoxy-5,5′,6,6′-tetrahydro-β,β-carotene-3,3′,5,19′-tetrol

[29789-80-8]



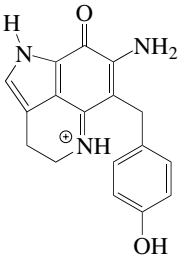
$C_{40}H_{56}O_5$ 616.879

Pigment from *Vaucheria* and *Botrydium* spp. λ_{max} 418, 436 and 466 (EtOH).

Nitsche, H. *et al., Z. Naturforsch., C*, 1973, **28**, 641

Veiutamine V-21

[188010-55-1]



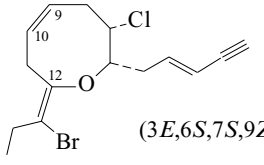
$C_{17}H_{16}N_3O_2^{\oplus}$ 294.332

Alkaloid from the Fijian sponge *Zyzzya fuliginosa*. Potent *in vitro* cytotoxin. Green solid (as trifluoroacetate). λ_{max} 246; 344; 550 (MeOH). λ_{max} 228; 330; 470 (MeOH/KOH).

Venables, D.A. *et al., Tet. Lett.*, 1997, **38**, 721 (*isol, uv, ir, pmr, cmr, struct*)
Moro-oka, Y. *et al., Tet. Lett.*, 1999, **40**, 1713-1716 (*synth, pmr, cmr*)

Venustin V-22

*8-(1-Bromopropylidene)-3-chloro-3,4,7,8-tetrahydro-2-(2-penten-4-ynyl)-2*H*-oxocin, 9CI. 13-Bromo-7-chloro-6,12-epoxy-3,9,12-pentadecatrien-1-yne*



(3*E*,6*S*,7*S*,9*Z*,12*Z*)–*form*

$C_{15}H_{18}BrClO$ 329.663

(3*E*,6*S*,7*S*,9*Z*,12*Z*)-*form*

3*E*-Venustin. *Venustin B*

[75443-71-9]

Constit. of red alga *Laurencia venusta*.

Cryst. (hexane).

Mp 77-78°. $[\alpha]_D^{25}$ -78 (c, 1.2 in $CHCl_3$).

9α,10α-Epoxide: ***3*E*-Epoxyvenustin***. *Venustin A*

[75410-75-2]

$C_{15}H_{18}BrClO_2$ 345.663

Constit. of *Laurencia venusta*. Cryst. (hexane).

Mp 94-95°. $[\alpha]_D^{27}$ -40 (c, 0.81 in $CHCl_3$).

(3*Z*,6*S*,7*S*,9*Z*,12*Z*)-*form*

3Z-Venustin

[86747-07-1]

Constit. of *Laurencia venusta*.

$[\alpha]_D^{20}$ -103 (c, 1.14 in $CHCl_3$).

9α,10α-Epoxide: ***3Z-Epoxyvenustin***

[86747-06-0]

$C_{15}H_{18}BrClO_2$ 345.663

From *Laurencia venusta*. Cryst. (hexane).

Mp 72-73°. $[\alpha]_D^{20}$ -44.1 (c, 1.00 in $CHCl_3$).

(3*Z*,6*R*,7*R*,9*Z*,12*E*)-*form*

Rhodophytin

[53472-38-1]

Constit. of *Laurencia oppositiclada*.

$[\alpha]_D^{25}$ -141.5 (c, 6.85 in hexane). Configs. in ref. incorrectly drawn.

(3*E*,6*R*,7*R*,9*Z*,12*E*)-*form*

trans-*Rhodophytin*

[75443-81-1]

Constit. of *Laurencia* spp.

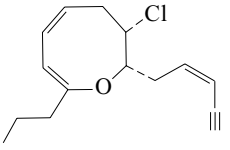
Oil.

Fenical, W. *et al., J.A.C.S.*, 1974, **96**, 5580-5581 (*Rhodophytin*)
Suzuki, M. *et al., Chem. Lett.*, 1980, 1177-1180; 1983, 779-782 (*Venustin B, isol, cryst struct*)

Howard, B.M. *et al., Tetrahedron*, 1980, **36**, 171-176 (*Rhodophytin*)
Norte, M. *et al., Tetrahedron*, 1991, **47**, 9411-9418 (*abs config*)

Venustinene V-23

[86702-74-1]

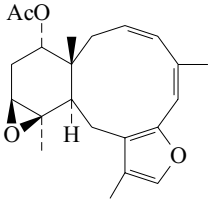


$C_{15}H_{19}ClO$ 250.767
Constit. of red alga *Laurencia venusta*. Cryst. (MeOH aq.). Mp 38-39°. $[\alpha]_D^{23}$ -184 (c, 1.00 in $CHCl_3$).

Suzuki, M. *et al., Chem. Lett.*, 1983, 779

Verecynarmin A V-24

[110600-68-5]

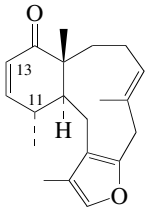


$C_{22}H_{28}O_4$ 356.461
Constit. of *Armina maculata* and *Veretillum cynomorium*. Foam. Mp 127-135°. $[\alpha]_D^{20}$ -255.7 (c, 1.13 in EtOH).

Guerriero, A. *et al., Helv. Chim. Acta*, 1987, **70**, 984-991 (*isol*)

Verecynarmin B V-25

[114915-32-1]



$C_{20}H_{26}O_2$ 298.424
Constit. of *Armina maculata* and *Veretillum cynomorium*. Foam. $[\alpha]_D^{20}$ -95.6 (c, 1.7 in EtOH). λ_{max} 205 (ϵ 11300); 223 (ϵ 13700) (EtOH).

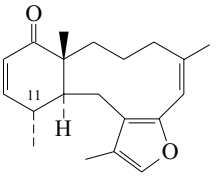
11β-Hydroxy: ***Verecynarmin C***
[114915-33-2]
$C_{20}H_{26}O_3$ 314.424
Constit. of *Armina maculata* and *Veretillum cynomorium*. Foam. $[\alpha]_D$ -0.9 (EtOH). λ_{max} 207 (ϵ 11200); 220 (ϵ 12000) (EtOH).

11β-Hydroxy, 13-chloro: ***Verecynarmin D***
[114915-34-3]
$C_{20}H_{25}ClO_3$ 348.868
Constit. of *Armina maculata* and *Veretillum cynomorium*. Platelets (hexane/EtOAc).
Mp 108-112°. $[\alpha]_D^{20}$ +27.3 (c, 1.3 in EtOH). λ_{max} 204 (ϵ 9400); 233 (ϵ 11100) (EtOH).

Guerriero, A. *et al., Helv. Chim. Acta*, 1988, **71**, 472-485 (*isol, uv, ir, pmr, cmr, ms*)

Verecynarmin F V-26

[128049-13-8]



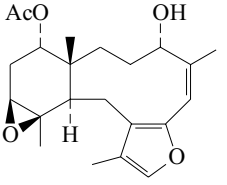
$C_{20}H_{26}O_2$ 298.424
Constit. of *Armina maculata* and *Veretillum cynomorium*. Oil. $[\alpha]_D$ -197.5 (c, 0.27 in EtOH).

11β-Hydroxy: ***Verecynarmin E***
[128022-75-3]
$C_{20}H_{26}O_3$ 314.424
Constit. of *Armina maculata* and *Veretillum cynomorium*. Foam. $[\alpha]_D$ -184.1 (c, 0.62 in EtOH).

Guerriero, A. *et al., Helv. Chim. Acta*, 1990, **73**, 277-283 (*isol, pmr, cmr*)

Verecynarmin G V-27

[128049-14-9]

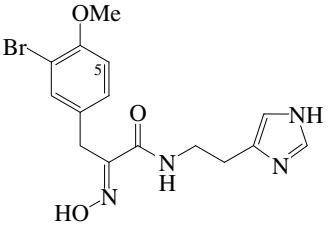


$C_{22}H_{30}O_5$ 374.476
Constit. of *Armina maculata* and *Veretillum cynomorium*. Oil. $[\alpha]_D$ -46.7 (c, 0.23 in EtOH).

Guerriero, A. *et al., Helv. Chim. Acta*, 1990, **73**, 277 (*isol, pmr, cmr*)

Verongamine V-28

[150036-88-7]



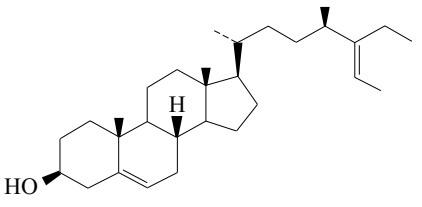
$C_{15}H_{17}BrN_4O_3$ 381.228
Alkaloid from the marine sponge *Verongula gigantea*. Specific histamine H_3-receptor antagonist. Yellow semi-solid or oil. λ_{max} 206 (ϵ 33600); 280 (ϵ 3040); 388 (ϵ 630) (MeOH) (Berdy).

5-Bromo: ***5-Bromoverongamine***
[218931-98-7]
$C_{15}H_{16}Br_2N_4O_3$ 460.124
Metab. of the sponge *Pseudoceratina* sp. Shows antifouling props. Oil. λ_{max} 207 (ϵ 44140) (MeOH).

Mierzwa, R. *et al., J. Nat. Prod.*, 1994, **57**, 175-177 (*isol, uv, ir, pmr, cmr, struct*)
Wasserman, H.H. *et al., J.O.C.*, 1998, **63**, 5581-5586 (*synth*)
Thirionet, I. *et al., Nat. Prod. Lett.*, 1998, **12**, 209-214 (*5-Bromoverongamine, activity*)
Boehlow, T.R. *et al., J.O.C.*, 2001, **66**, 3111-3118 (*synth*)

Verongulasterol V-29

24-(1-Ethyl-1-propenyl)-26,27-dinorcholest-5-en-3-ol, 9CI.
24,26,27-Trimethylcholesta-5,25-dien-3-ol
[70284-74-1]

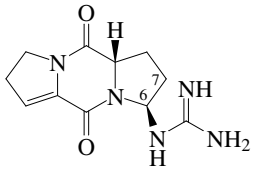


$C_{30}H_{50}O$ 426.724
Constit. of the sponge *Verongula cauliformis*. Cryst.
Mp 101-102°. $[\alpha]_D^{21}$ -14.7 (c, 0.102 in $CHCl_3$).

Kokke, W.C.M.C. *et al., Helv. Chim. Acta*, 1979, **62**, 1310 (*isol, struct*)
Lavanchy, A. *et al., Org. Mass Spectrom.*, 1980, **15**, 355 (*ms*)
Catalan, C.A.N. *et al., Tetrahedron*, 1985, **41**, 1073 (*synth*)

Verpacamide C V-30

*3-(Aminoiminomethyl)-1,2,3,7,8,9*a*-hexahydro-5*H*,10*H*-dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione*

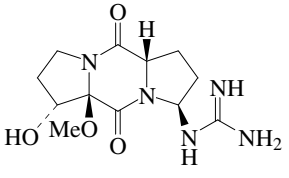


Relative Configuration

$C_{11}H_{15}N_5O_2$ 249.272
Alkaloid from *Axinella vaceleti*. Amorph. solid (as formate salt).
$[\alpha]_D^{24}$ +17.4 (c, 0.15 in H_2O) (formate salt).

Vergne, C. *et al., Org. Lett.*, 2006, **8**, 2421-2424 (*isol, pmr, cmr*)

Verpacamide D V-31



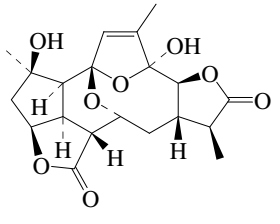
Relative Configuration

$C_{12}H_{19}N_5O_4$ 297.313
Alkaloid from *Axinella vaceleti*. Amorph. solid (as formate salt).

Vergne, C. *et al., Org. Lett.*, 2006, **8**, 2421-2424 (*isol, pmr, cmr*)

Verrillin V-32

[302953-27-1]

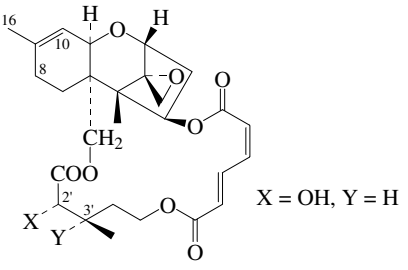


$C_{20}H_{24}O_8$ 392.405
Constit. of *Pseudopterogorgia bipinnata*. Gum. $[\alpha]_D^{24}$ +225 (c, 0.2 in $CHCl_3$). λ_{max} 206 (ϵ 7200) (MeOH).

Rodríguez, A.D. *et al., J.O.C.*, 2000, **65**, 5839-5842 (*isol, pmr, cmr*)

Verrucarin A V-33

Muconomycin A. VER-A. 397 Y
[3148-09-2]



X = OH, Y = H

$C_{27}H_{34}O_9$ 502.56
Trichothecene antibiotic. Prod. by *Myrothecium verrucaria* and a marine-derived *Acremonium neo-caledoniae*. Inhibitor of protein synth. in fungi. Antineoplastic and insecticide. Cryst.
Mp 330°. $[\alpha]_D$ +260 ($CHCl_3$). $[\alpha]_D$ +208 (dioxan). Log P -0.93 (uncertain value) (calc). λ_{max} 260 (ϵ 17800) (MeOH or EtOH) (Derep).

▶ Skin irritant. LD_{50} (rat, ivn) 0.87 mg/kg. WH1316810

O-*Ac:*
Needles (Me_2CO/Et_2O). Mp 212-215°. $[\alpha]_D^{23}$ +132.5 (c, 1.18 in $CHCl_3$).

2′,3′-Didehydro: ***Dehydroverrucarin A***
$C_{27}H_{32}O_9$ 500.544
Isol. from *Myrothecium roridum*. Shows similar activity to that of Verrucarin A. Needles (Me_2CO/Et_2O). Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 233-240°. $[\alpha]_D^{25}$ +118 ($CHCl_3$). λ_{max} 260 (ϵ 23000) (EtOH) (Berdy).

8-Hydroxy: 8-Hydroxyverrucarin A
[74608-63-2]
$C_{27}H_{34}O_{10}$ 518.56
Semisynthetic. Antileukaemic agent. Cryst. (Me_2CO/hexane). Poorly sol. hexane.
Mp 300°. $[\alpha]_D^{25}$ +229 (c, 1.37 in MeOH).

16-Hydroxy: 16-Hydroxyverrucarin A
[74516-64-6]
$C_{27}H_{34}O_{10}$ 518.56
Semisynthetic. Antileukaemic agent. Cryst. (Me_2CO/hexane).
Mp 300°. $[\alpha]_D^{25}$ +169 (c, 1.65 in MeOH).

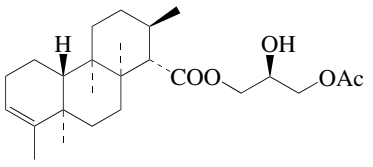
▶ YX9823000

16-Hydroxy, 9,10-epoxide: 9,10-Epoxy-16-hydroxyverrucarin A
[87532-32-9]
$C_{27}H_{34}O_{11}$ 534.559
Semisynthetic. Antileukaemic agent.
Mp 294-298°.

Tamm, Ch. *et al., Helv. Chim. Acta*, 1962, **45**, 1726; 1963, **46**, 1786 (*isol*)
Zurcher, W. *et al., Helv. Chim. Acta*, 1966, **49**, 2594 (*isol, deriv*)
McPhail, A.T. *et al., J.C.S.(C)*, 1966, 1394 (*cryst struct*)
Müller, B. *et al., Helv. Chim. Acta*, 1975, **58**, 453; 471 (*biosynth*)
Breitenstein, W. *et al., Helv. Chim. Acta*, 1975, **58**, 1172 (*nmr*)
Jarvis, B.B. *et al., J. Med. Chem.*, 1980, **23**, 1054; 1984, **27**, 239 (*derivs*)
Still, W.C. *et al., J.O.C.*, 1981, **46**, 5242 (*synth*)
Mohr, P. *et al., Helv. Chim. Acta*, 1982, **65**, 1412 (*synth*)
McDougal, P.G. *et al., Diss. Abstr. Int., B*, 1983, **43**, 3245 (*synth*)
Trichothecenes - Chemical, Biological and Toxicological Aspects, (ed., Ueno, Y.), Elsevier, 1983, (*tox, rev*)
Kemppainen, B.W. *et al., Food Chem. Toxicol.*, 1987, **25**, 379 (*toxicol*)
Laurent, D. *et al., Planta Med.*, 2000, **66**, 63-66 (*Acremonium, isol*)
Liu, J.Y. *et al., J. Appl. Microbiol.*, 2006, **10**, 195-202 (*marine, isol, pmr, cmr*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 247
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MRV500

Verrucosin 2 V-34

[188405-39-2]



$C_{25}H_{40}O_5$ 420.588

Constit. of *Doris verrucosa*. Protein kinase C activator. Morphogenetic hydra tentacle regeneration agent. Tumour promoter. Amorph. solid.

Gavagnin, M. *et al., Tetrahedron*, 1997, **53**, 1491-1504 (*isol, pmr, cmr*)

Verrucotoxin V-35

VTX

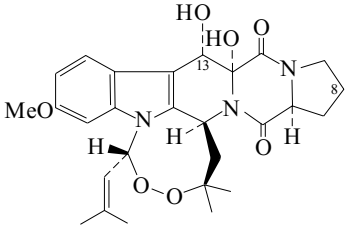
[162629-06-3]

Glycoprotein. MW approx. 322000, comprising 4 subunits, 2 alpha (83000) and 2 beta (78000). Isol. from the venom of the stonefish *Synanceia verrucosa*. Cardiotoxic.

Garnier, P. *et al., Toxicon*, 1995, **33**, 143-145; 1997, **35**, 47-55 (*isol, tox*)
Garnier, P. *et al., Biochim. Biophys. Acta*, 1997, **1337**, 1-5 (*partial struct*)
Khoo, H.E. *et al., Clin. Exp. Pharmacol. Physiol.*, 2002, **29**, 802-806 (*rev*)

Verruculogen V-36

[12771-72-1]



$C_{27}H_{33}N_3O_7$ 511.574

Isol. from *Penicillium* spp., *Aspergillus caespitosus* and *Aspergillus fumigatus*. Tremorgenic toxin. Plates (C_6H_6/EtOH).
Mp 233-235° dec. $[\alpha]_D$ -27.7 ($CHCl_3$). λ_{max} 224; 294 (MeOH) (Berdy). λ_{max} 226 (ϵ 47500); 277 (ϵ 11000); 295 (ϵ 9750) (EtOH) (Berdy).

▶ LD_{50} (mus, ipr) 2.4 mg/kg. JH4920000

O^{13}-3-Methyl-2-butenyl: ***Fumitremorgin A***

[12626-18-5]

$C_{32}H_{41}N_3O_7$ 579.692

Tremorgenic toxin from *Aspergillus fumigatus*. Prisms (MeOH). Sol. MeOH, $CHCl_3$, C_6H_6; poorly sol. H_2O.
Mp 206-209°. $[\alpha]_D^{10}$ +61 (Me_2CO). λ_{max} 225; 275; 295 (MeOH) (Berdy). λ_{max} 226 (ϵ 31700); 277 (ϵ 5300); 296 (ϵ 4900) (EtOH) (Berdy).

▶ LD_{50} (mus, ivn) .185 mg/kg. JH5000000

8β-Acetoxy: ***Acetoxyverruculogen***

[81657-39-8]

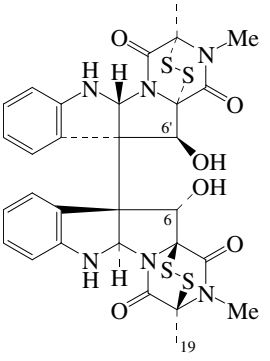
$C_{29}H_{35}N_3O_9$ 569.61

Tremorgenic metab. of *Penicillium verruculosum*.
Mp 217-218° dec.

Fayos, J. *et al., J.A.C.S.*, 1974, **96**, 6785 (*uv, pmr, cryst struct, cd*)
Eickman, N. *et al., Tet. Lett.*, 1975, 1051 (*cryst struct*)
Yamazaki, M. *et al., Chem. Pharm. Bull.*, 1980, **28**, 245 (*isol, uv, ir, pmr, ms, cd*)
Day, J.B. *et al., J. Gen. Microbiol.*, 1980, **117**, 405 (*isol*)
Uramoto, M. *et al., Heterocycles*, (Spec. Issue), 1982, **17**, 349 (*isol, deriv*)
Afiyatullov, S.S. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2004, **40**, 615-617 (*isol, pmr, cmr, ms*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 357; 368; 374

Verticillin A V-37

[32164-16-2]



Absolute Configuration

$C_{30}H_{28}N_6O_6S_4$ 696.852

Epidithiodioxopiperazine-type antibiotic. Isol. from *Verticillium* sp. TM759, *Gliocladium* sp. SCF1168 and a marine *Penicillium* sp. CNC-350. Shows cytotoxic activity, mycotoxin. Yellow needles (Py). Sol. MeOH, dioxan, $CHCl_3$, Py; poorly sol. H_2O, hexane.
Mp 202-217° dec. $[\alpha]_D$ +703.7. $[\alpha]_D$ +727 (dioxan). λ_{max} 203 (ϵ 50100); 240 (sh) (ϵ 14100); 301 (ϵ 5370) (Ac_2O/MeOH) (Derep). λ_{max} 306 (ϵ 6300) (dioxan) (Berdy).

▶ LD_{50} (mus, ipr) 7.6 mg/kg. YY1830000

6-Deoxy: ***11-Deoxyverticillin A***

[240480-95-9]

$C_{30}H_{28}N_6O_5S_4$ 680.852

Isol. from a marine *Penicillium* sp. CNC-350. Cytotoxic. Yellow cryst. (CH_2Cl_2/MeOH).

6,6′-Dideoxy: ***11,11′-Dideoxyverticillin A***

[240480-94-8]

$C_{30}H_{28}N_6O_4S_4$ 664.853

Isol. from a marine *Penicillium* sp. CNC-350. Cytotoxic. Solid. $[\alpha]_D$ +624.1.

19-Hydroxy: ***Verticillin B***

[52212-86-9]

$C_{30}H_{28}N_6O_7S_4$ 712.851

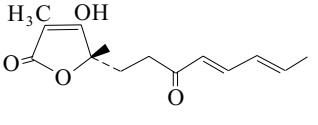
From *Verticillium* sp. TM759. Pale-yellow prisms ($CHCl_3$). Sol. MeOH, $CHCl_3$, dioxan, Py; poorly sol. H_2O, Et_2O, hexane.
Mp 254-256° dec. $[\alpha]_D$ +704.7 (c, 0.493 in dioxan). λ_{max} 306 (ϵ 5600) (dioxan) (Berdy).

Katagiri, K. *et al., J. Antibiot., Ser. B*, 1970, **23**, 420-422 (*isol*)
Minato, H. *et al., J.C.S. Perkin 1*, 1973, 1819-1825 (*isol, ir, pmr, ms, cd, struct, Verticillin B*)
Son, B.W. *et al., Nat. Prod. Lett.*, 1999, **13**, 213-222 (*Deoxyverticillin A, Dideoxyverticillin A*)
Liu, F. *et al., Acta Cryst. E*, 2006, **62**, 974-976 (*cryst struct*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 606

Vertinolide V-38

*4-Hydroxy-3,5-dimethyl-5-(3-oxo-4,6-octadienyl)-2(5*H*)-furanone, 9CI. 3-Hydroxy-2,4-dimethyl-7-oxo-2,8,10-dodecatrien-1,4-olide*

[79950-84-8]



$C_{14}H_{18}O_4$ 250.294

Tetronic acid deriv. Isol. from *Verticillium intertextum* and a marine-derived *Trichoderma viride*. Mycotoxin. Cryst. (Me_2CO). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 149.2-152.3° dec. $[\alpha]_D^{20}$ -25 (c, 0.05 in $CHCl_3$). λ_{max} 229 (ϵ 14400); 272 (ϵ 25300) (no solvent reported) (Derep). λ_{max} 261

(ϵ 36900) (MeOH/NaOH) (Derep). λ_{max} 230 (ϵ 9900); 270 (ϵ 28500) (MeOH) (Derep). λ_{max} 231; 278 (MeOH) (Berdy).

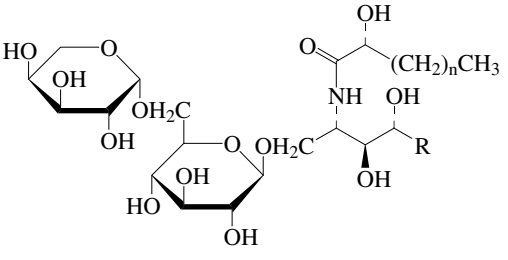
Ac: [82224-92-8]
Mp 83.2-85.5°. $[\alpha]_D^{20}$ -42.5 (c, 0.04 in $CHCl_3$).

Me ether: [82224-91-7]
Needles (Et_2O/pentane). Mp 59-61.5°. $[\alpha]_D^{20}$ -13.2 (c, 0.1 in $CHCl_3$).

1′ξ-Hydroxy: ***5-Hydroxyvertinolide***
$C_{14}H_{18}O_5$ 266.293
Isol. from *Trichoderma longibrachiatum*. Amorph. solid. $[\alpha]_D$ -64 (c, 0.1 in MeOH). λ_{max} 230 (sh); 263 (ϵ 13000); 359 (ϵ 900) (MeOH).

Trifonov, L. *et al., Tetrahedron*, 1982, **38**, 397 (*isol, struct*)
Takaiwa, A. *et al., Agric. Biol. Chem.*, 1983, **47**, 429 (*abs config*)
Wrobel, J.E. *et al., J.O.C.*, 1983, **48**, 3761 (*synth*)
Desmaele, D. *et al., Tetrahedron*, 1992, **48**, 2925 (*synth*)
Matsuo, K. *et al., Heterocycles*, 1996, **43**, 2553 (*synth*)
Andrade, R. *et al., Aust. J. Chem.*, 1997, **50**, 255 (*5-Hydroxyvertinolide*)
Matsuo, K. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1620-1625 (*synth*)
Abdel-Lateff, A. *et al., Dissertation*, Univ. of Bonn, 2004, (*marine, isol*)

Vesparioside V-39



n = 21 or 22

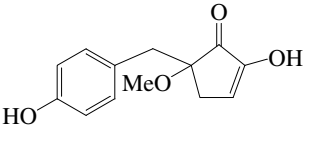
R = $-(CH_2)_{13}CH_3$,
$-(CH_2)_{11}CH(CH_3)CH_2CH_3$,
$-(CH_2)_{12}CH(CH_3)_2$ *or*
$-(CH_2)_{15}CH_3$

Diglycosylceramide complex. Isol. from the sponge *Spheciospongia vesparia*. Amorph. solid. $[\alpha]_D^{25}$ -12 (c, 0.1 in MeOH).

Costantino, V. *et al., Eur. J. Org. Chem.*, 2005, 368-378 (*isol, pmr, cmr, ms*)

Vidalenolone V-40

2-Hydroxy-5-[(4-hydroxyphenyl)methyl]-5-methoxy-2-cyclopenten-1-one

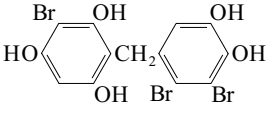


$C_{13}H_{14}O_4$ 234.251
Isol. from the red alga *Vidalia* sp. Oil. $[\alpha]_D^{25}$ -95 (c, 0.31 in MeOH). λ_{max} 209 (log ϵ 4.5); 224 (log ϵ 4.54); 266 (log ϵ 4.08) (MeOH).

Yoo, H.-D. *et al., J. Nat. Prod.*, 2002, **65**, 51-53

Vidalol A V-41

[137182-39-9]



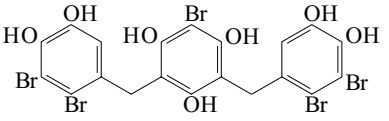
$C_{13}H_9Br_3O_5$ 484.923

Constit. of *Vidalia obtusaloba*. Solid.

Wiemer, D.F. *et al., Experientia*, 1991, **47**, 851 (*isol, pmr, cmr*)

Vidalol B V-42

[137182-40-2]

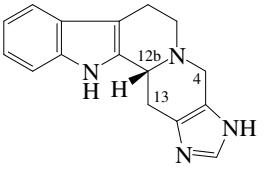


$C_{20}H_{13}Br_5O_7$ 764.838
Constit. of *Vidalia obtusaloba*. Solid.

Wiemer, D.F. *et al., Experientia*, 1991, **47**, 851 (*isol, pmr, cmr*)

Villagorgin A V-43

*4,6,7,12,12*b*,13-Hexahydro-1*H*-imidazo[4,5-*g*]indolo[2,3-*a*]quinazoline, 9CI*
[152606-59-2]



$C_{16}H_{16}N_4$ 264.329
CAS numbering shown.

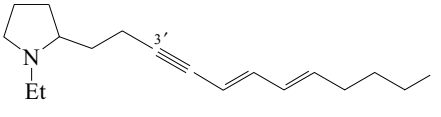
(R)-form
Alkaloid from the gorgonian *Villogorgia rubra*. Shows calmodulin-related antagonist activity. Red amorph. solid. $[\alpha]_D^{20}$ +7.8. Genus name incorrectly given as Villagorgia. λ_{max} 224 (ϵ 25600); 280 (ϵ 52409) (MeOH) (Berdy).

*4,*N*,12*b*,13-Dehydro:* ***1,6,7,12-Tetrahydroimidazo[4,5-g]indolo[2,3-a]quinolizin-5-ium, 9CI. Villagorgin B***
[152606-60-5]
$C_{16}H_{13}N_4^{\oplus}$ 261.305
Alkaloid from the gorgonian *Villogorgia rubra*. Red amorph. solid. Counterion not specified. λ_{max} 228; 244; 280; 338 (MeOH) (Berdy). λ_{max} 222; 242; 332 (MeOH/HCl) (Berdy).

Espada, A. *et al., Tet. Lett.*, 1993, **34**, 7773-7776 (*isol, uv, ir, pmr, cmr, ms, struct*)
Grazul, R.M. *et al., Nat. Prod. Lett.*, 1994, **5**, 187 (*Villagorgin B, synth*)

Villatamine A V-44

2-(5,7-Dodecadien-3-ynyl)-1-ethylpyrrolidine
[168434-14-8]



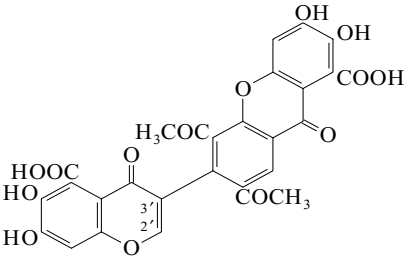
$C_{18}H_{29}N$ 259.434
Alkaloid from the predatory flatworm *Prostheceraeus villatus* and its tunicate prey *Clavelina lepadiformis*. Oil. $[\alpha]_D$ +49 (MeOH). *Prostheceraeus villatus* appears to be an Authors' misspelling of *P. vittatus*. λ_{max} 266 (ϵ 18700) (MeOH) (Berdy).

*3′,4′*E*, 7′,8′-Tetrahydro: 2-(3,5-Dodecadienyl)-1-ethylpyrrolidine.* ***Villatamine B***
[168434-15-9]
$C_{18}H_{33}N$ 263.465
Alkaloid from *Prostheceraeus villatus* and *Clavelina lepadiformis*. Exhibits significant *in vitro* cytotoxicity against human cancer cells. Oil. $[\alpha]_D$ +15 (MeOH). λ_{max} 230 (ϵ 19500) (MeOH) (Berdy).

Kubanek, J. *et al., Tet. Lett.*, 1995, **36**, 6189-6192 (*isol, uv, pmr, cmr, struct*)

Vinaxanthone V-45

Ro 09-1450. Antibiotic Ro 09-1450. 411F. Xanthone 411F
[133293-89-7]



$C_{28}H_{16}O_{14}$ 576.426
Prod. by *Penicillium glabrum* and *Penicillium vinaceum*. Phospholipase C and semaphorin inhibitor. Exhibits CD-4-binding props. Pale yellow cryst. + $^1/_2H_2O$ (EtOAc).
Mp 280°. λ_{max} 230 (ϵ 29500); 280 (ϵ 16800); 350 (ϵ 16100) (MeOH/NaOH) (Derep). λ_{max} 230 (ϵ 29800); 280 (ϵ 19300); 320 (ϵ 16800); 380 (sh) (MeOH) (Derep).

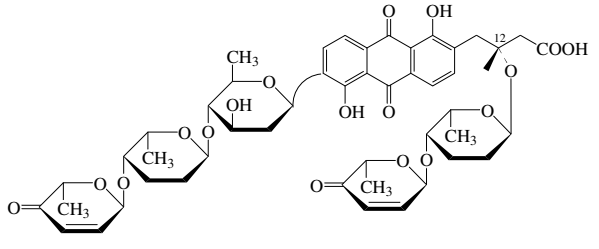
7′,8′-Di-Me ether, di-Me ester: ***Chaetocyclinone C***
$C_{32}H_{24}O_{14}$ 632.533
Prod. by the marine-derived *Chaetomium* sp. Gö 100/2.

2′,3′-Dihydro: ***Xanthone 411J****. 411J*
[145349-94-6]
$C_{28}H_{18}O_{14}$ 578.442
Prod. by *Penicillium glabrum*. Shows CD4-binding activity. Yellow powder.

Aoki, M. *et al., Tet. Lett.*, 1991, **32**, 4737-4740 (*isol, pmr, cmr*)
Wrigley, S.K. *et al., Pure Appl. Chem.*, 1994, **66**, 2383-2386 (*isol*)
Kumagai, K. *et al., J. Antibiot.*, 2003, **56**, 610-616 (*isol, pmr, cmr, activity*)
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*Chaetocyclinone C*)

Vineomycin B_2 V-46

OS 4742B_2. Antibiotic OS 4742B_2
[66198-33-2]



$C_{49}H_{58}O_{18}$ 934.986
Anthraquinone antibiotic. Prod. by *Streptomyces malensis*. Active against gram-positive bacteria, sarcoma cells and tumours. Yellow amorph. powder. Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane. Mp 128-131°. $[\alpha]_D^{26}$ +30.8 (c, 0.5 in $CHCl_3$). λ_{max} 231 (ϵ 41700); 258 (ϵ 33900); 286 (ϵ 7080); 296 (ϵ 7762); 426 (ϵ 11200); 444 (ϵ 11200) (EtOH) (Derep). λ_{max} 230 (E1%/1cm 421); 258 (E1%/1cm 226); 294 (E1%/1cm 76); 427 (E1%/1cm 107); 440 (E1%/1cm 107) (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 100 - 150 mg/kg. CB9653360

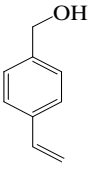
*12-*O*-Deglycosyl:* ***Vineomycin C***
[288104-96-1]
$C_{37}H_{42}O_{14}$ 710.73
Prod. by *Streptomyces* sp. Yellow powder.
Mp 123-162°. $[\alpha]_D$ +110 (c, 1 in $CHCl_3$). λ_{max} 231; 258; 290; 442 (MeOH).

[80928-52-5]

Omura, S. *et al., J. Antibiot.*, 1977, **30**, 908 (*isol*)
Imamura, N. *et al., J. Antibiot.*, 1981, **34**, 1517; 1982, **35**, 602 (*biosynth*)
Danishefsky, S.J. *et al., J.A.C.S.*, 1985, **107**, 1285 (*aglycone*)
Tius, M.A. *et al., J.A.C.S.*, 1991, **113**, 5775 (*synth, bibl*)
Bolitt, V. *et al., J.A.C.S.*, 1991, **113**, 6320 (*synth*)
Matsumoto, T. *et al., J.A.C.S.*, 1991, **113**, 6982 (*synth*)
Alvi, K.A. *et al., J. Antibiot.*, 2000, **53**, 496-501 (*Vineomycin C*)

4-Vinylbenzyl alcohol V-47

4-Ethenylbenzenemethanol, 9CI. 4-(Hydroxymethyl)styrene
[1074-61-9]



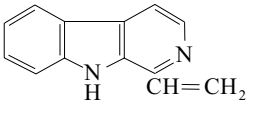
$C_9H_{10}O$ 134.177
Constit. of the soft coral *Cladiella australis*. Cryst. or oil.
Mp 24°. Bp_4 100-101°. Polymerises on standing.

Ac: [1592-12-7]
$C_{11}H_{12}O_2$ 176.215
Oil. Bp_4 97-99°.

Emerson, W.S. *et al., J.A.C.S.*, 1947, **69**, 1905-1906 (*synth*)
Abramo, J.G. *et al., J.O.C.*, 1961, **26**, 2671-2673 (*synth*)
Bamford, C.H. *et al., Polymer*, 1973, **14**, 330-332 (*synth, Ac*)
Arad-Yellin, R. *et al., React. Polym.*, 1989, **11**, 21-27 (*synth, pmr*)
Remmas, M. *et al., Makromol. Chem.*, 1990, **191**, 1277-1285 (*synth*)
Ahmed, A.F. *et al., J. Chin. Chem. Soc. (Taipei)*, 2006, **53**, 489-494 (*isol, pmr, cmr*)

1-Vinyl-β-carboline V-48

*1-Ethenyl-9*H*-pyrido[3,4-*b*]indole, 9CI.* ***Pavettine***
[20127-60-0]



$C_{13}H_{10}N_2$ 194.235
Alkaloid from *Pavetta lanceolata* (Rubiaceae), the bryozoans *Cribricellina cribraria* and *Costaticella hastata* and from *Soulamea raxinifolia* and *Pavetta lanceolata*. Yellowish cryst.
Mp 167-169°.

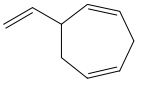
N-*Methoxy:* **N-*Methoxy-1-vinyl-β-carboline***
[69355-01-7]
$C_{14}H_{12}N_2O$ 224.262
Alkaloid from *Picrasma excelsa* (Jamaican quassiawood) (Simaroubaceae).
Mp 185-190° dec.

*7-Bromo: 7-Bromo-1-ethenyl-9*H*-pyrido[3,4-*b*]indole. 7-Bromo-1-vinyl-β-carboline.* ***Plakortamine B***
$C_{13}H_9BrN_2$ 273.132
Alkaloid from the sponge *Plakortis nigra*. Cytotoxic. Yellow oil.
λ_{max} 214 (ϵ 32000) (no solvent reported).

Jordaan, A. *et al., J. S. Afr. Chem. Inst.*, 1968, **21**, 22 (*isol, uv, ir, pmr, ms, synth*)
Wagner, H. *et al., Tet. Lett.*, 1978, 2777 (*deriv*)
Blackman, A.J. *et al., J. Nat. Prod.*, 1987, **50**, 494-496 (*isol, Costaticella*)
Bracher, F. *et al., Annalen*, 1992, 1315 (*synth, ir, pmr, cmr, ms*)
Rocca, P. *et al., Tetrahedron*, 1993, **49**, 3325 (*synth, ir, pmr, cmr*)
Sandler, J.S. *et al., J. Nat. Prod.*, 2002, **65**, 1258-1261 (*Plakortamine B*)

6-Vinyl-1,4-cycloheptadiene V-49

6-Ethenyl-1,4-cycloheptadiene, 9CI
[92340-53-9]



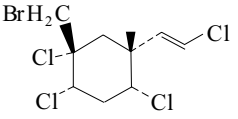
C_9H_{12} 120.194

Constit. of the brown alga *Cutleria multifida*.

Keitel, J. *et al., Helv. Chim. Acta*, 1990, **73**, 2101-2112 (*isol, synth, pmr, cmr, ms*)

Violacene V-50

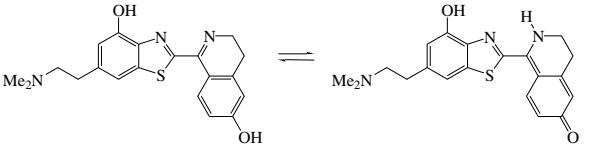
1-(Bromomethyl)-1,2,4-trichloro-5-(2-chloroethenyl)-5-methylcyclohexane, 9CI
[54279-01-5]



$C_{10}H_{13}BrCl_4$ 354.928
Constit. of *Plocamium violaceum* and *Microcladia* spp. Cryst. Sol. MeOH, Et_2O; poorly sol. H_2O.
Mp 71-71.5°.

Mynderse, J.S. *et al., J.A.C.S.*, 1974, **96**, 6771 (*isol*)
Crews, P. *et al., J.O.C.*, 1978, **43**, 116 (*struct*)
v. Engen, D. *et al., Tet. Lett.*, 1978, 29 (*cryst struct*)

Violatinctamine V-51

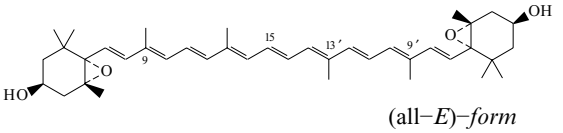


$C_{20}H_{21}N_3O_2S$ 367.471
Alkaloid from *Cystodytes* cf. *violatinctus*. Orange oil.

Chill, L. *et al., Tet. Lett.*, 2004, **45**, 7925-7928 (*isol*)

Violaxanthin V-52

5,6:5′,6′-Diepoxy-5,5′,6,6′-tetrahydro-β,β-carotene-3,3′-diol. Zeaxanthin diepoxide. Violeaxanthin. C.I. Natural Yellow 27



(all–*E*)–*form*

$C_{40}H_{56}O_4$ 600.88

(all-*E*)-*form* [126-29-4]
Constit. of many plants including *Viola tricolor*. Found in brown and green algae.
Red cryst. (MeOH).
Mp 208°. $[\alpha]_D^{20}$ +38 ($CHCl_3$).

3,3′-Dibutanoyl: [637041-45-3]
$C_{48}H_{68}O_6$ 741.062
Constit. of *Mangifera indica* (mango).

15,15′-Didehydro: [122346-90-1]
$C_{40}H_{54}O_4$ 598.864
Synthetic. Shining orange cryst. (Et_2O/hexane). Mp 138-144°.

Monodeoxy: 5,5′,6,6′-Diepoxy-5,5′,6,6′-tetrahydro-β,β-caroten-3-ol, 9CI. Cryptoxanthin diepoxide
[2086-87-5]
$C_{40}H_{56}O_3$ 584.881
Prepared by oxidn. of Cryptoxanthin; isol. from the algae of Xanthophyceae, *Eriobotrya japonica* (loquat) fruit and *Prunus persica* fruit (peach mesocarp during ripening). Cryst. (C_6H_6/petrol). Mp 194°. λ_{max} 473; 503 (CS_2). λ_{max} 415; 438; 468 (no solvent reported). λ_{max} 442; 472 (EtOH).

(9*Z*,9′*Z*)-*form*
Di-cis-*neoviolaxanthin A*
[101627-35-4]
Constit. of *Viola tricolor*.
Orange cryst.
Mp 202°.

(9*Z*,13*Z*)-*form*
Di-cis-*violaxanthin D*
[101627-32-1]
From *Viola tricolor*.
Orange cryst.
Mp 111°.

(9*Z*,13′*Z*)-*form*
Di-cis-*neoviolaxanthin B*
[101627-34-3]
From *Viola tricolor*.
Red cryst.
Mp 135°.

(9*Z*,15*Z*)-*form*
Di-cis-*violaxanthin C*
[101627-33-2]
From *Viola tricolor*.
Red cryst.
Mp 87°.

(13*Z*)-*form* [75715-58-1]
From *Viola tricolor*.
Bright yellow plates (C_6H_6/petrol).
Mp 108°. λ_{max} 337 (log ϵ 4.77); 419 (log ϵ 4.91); 445 (log ϵ 5.06); 475 (log ϵ 5) (C_6H_6).

(15*Z*)-*form* [24620-97-1]
From *Viola tricolor*.
Yellow cryst. (C_6H_6/petrol).
Mp 109°. λ_{max} 337 (log ϵ 4.77); 423 (log ϵ 4.83); 448 (log ϵ 4.98); 479 (log ϵ 4.91) (C_6H_6).

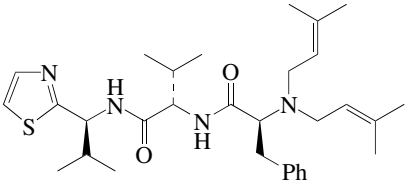
(9*Z*)-*form*
9-cis-*Violaxanthin*
[26927-07-1]

3,3′-Dibutanoyl: [637041-46-4]
$C_{48}H_{68}O_6$ 741.062
Constit. of *Mangifera indica* (mango).

de Ville, T.E. *et al., Chem. Comm.*, 1969, 1311 (*abs config*)
Stransky, H. *et al., Arch. Microbiol.*, 1970, **71**, 164 (*isol, deoxy*)
Banthorpe, D.V. *et al., J.C.S. Perkin 1*, 1972, 1769 (*biosynth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, no. 1842 (*occur*)
Koreeda, N. *et al., J.A.C.S.*, 1973, **95**, 239 (*abs config*)
Sapozhnikov, D.I. *et al., Pure Appl. Chem.*, 1973, **35**, 47 (*rev*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97 (*cmr*)
Lessertois, D. *et al., Phytochemistry*, 1978, **17**, 411 (*isol, deoxy*)
Molnár, P. *et al., Phytochemistry*, 1980, **19**, 623 (*mono-cis isomers*)
Molnár, P. *et al., Acta Chim. Hung.*, 1983, **112**, 477 (*cmr*)
Molnár, P. *et al., Phytochemistry*, 1986, **25**, 195 (*isol*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 259 (*bibl*)
Acemoglu, M. *et al., Helv. Chim. Acta*, 1988, **71**, 931 (*synth*)
Baumeler, A. *et al., Helv. Chim. Acta*, 1992, **75**, 773 (*15,15′-didehydro*)
Pott, I. *et al., Phytochemistry*, 2003, **64**, 825-829 (*dibutanoyl esters*)
Molnár, P. *et al., Helv. Chim. Acta*, 2004, **87**, 11-27 (*synth*)

Virenamide A V-53

[176666-59-4]



$C_{31}H_{46}N_4O_2S$ 538.796

Peptide antibiotic. Isol. from the ascidian *Diplosoma virens*. Cytotoxic agent. Oil. $[\alpha]_D$ -341 (c, 0.1 in $CHCl_3$). λ_{max} 203 (ϵ 7700); 237 (ϵ 4300) (EtOH).

N-*Deprenyl:* ***Virenamide D***

[193264-93-6]

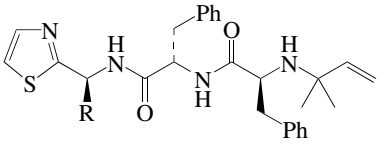
$C_{26}H_{38}N_4O_2S$ 470.678

Isol. from the ascidian *Diplosoma virens*. Oil. $[\alpha]_D$ -65 (c, 0.07 in $CHCl_3$). λ_{max} 202 (ϵ 13700); 239 (ϵ 3050) (MeOH).

Carroll, A.R. *et al., J.O.C.*, 1996, **61**, 4059-4061 (*isol, uv, ir, pmr, cmr, ms*)
Feng, Y. *et al., Aust. J. Chem.*, 1997, **50**, 337-339 (*Virenamide D*)

Virenamide B V-54

[176666-60-7]



R = $CH(CH_3)_2$

$C_{30}H_{38}N_4O_2S$ 518.722

Peptide antibiotic. Isol. from the ascidian *Diplosoma virens*. Cytotoxic agent. Oil. $[\alpha]_D$ -775 (c, 0.1 in $CHCl_3$). λ_{max} 209 (ϵ 13600); 240 (ϵ 4500) (EtOH).

Carroll, A.R. *et al., J.O.C.*, 1996, **61**, 4059-4061 (*isol, uv, ir, pmr, cmr, ms*)
Moody, C.J. *et al., J.O.C.*, 1999, **64**, 8715-8717 (*synth*)

Virenamide C V-55

[176666-61-8]

As Virenamide B, V-54 with

R = $-CH_2Ph$

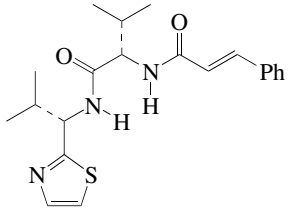
$C_{34}H_{38}N_4O_2S$ 566.766

Peptide antibiotic. Isol. from the ascidian *Diplosoma virens*. Cytotoxic agent. Oil. $[\alpha]_D$ -634 (c, 0.05 in $CHCl_3$). λ_{max} 202 (ϵ 10900); 240 (ϵ 4800) (EtOH).

Carroll, A.R. *et al., J.O.C.*, 1996, **61**, 4059-4061 (*isol, uv, ir, pmr, cmr, ms*)

Virenamide E V-56

[193264-95-8]



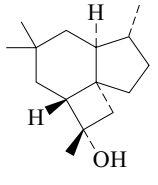
$C_{21}H_{27}N_3O_2S$ 385.529

Isol. from the ascidian *Diplosoma virens*. Oil. $[\alpha]_D$ -40 (c, 0.04 in $CHCl_3$). λ_{max} 216 (ϵ 12700); 222 (ϵ 10800); 274 (ϵ 14150) (MeOH).

Fang, Y. *et al., Aust. J. Chem.*, 1997, **50**, 337-339 (*isol, uv, ir, pmr, cmr, ms*)

Viridianol V-57

[158204-40-1]

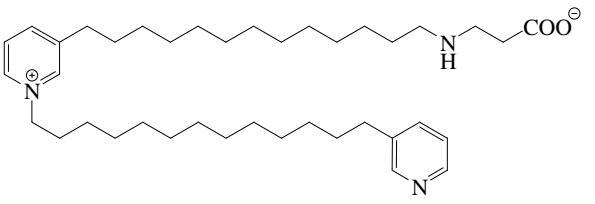


$C_{15}H_{26}O$ 222.37

Constit. of *Laurencia viridis*. A cyclised precapnellane. Amorph. solid. $[\alpha]_D^{25}$ +4.5 (c, 0.15 in $CHCl_3$).

Norte, M. *et al., Tet. Lett.*, 1994, **35**, 4607 (*isol, pmr, cmr*)

Viscosaline V-58



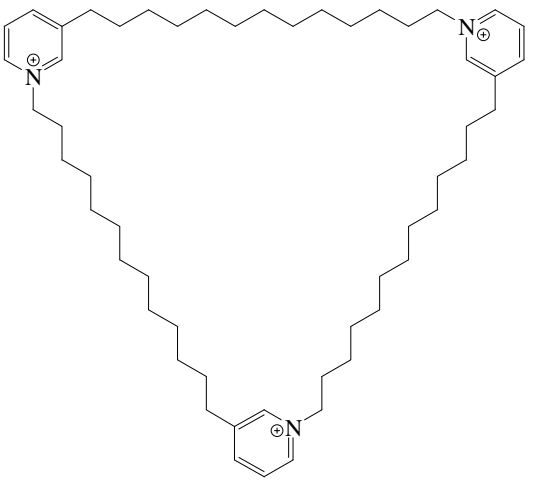
$C_{39}H_{65}N_3O_2$ 607.961

Alkaloid from the sponge *Haliclona viscosa*. CAS no. not found CA 141. λ_{max} 204; 264 (MeOH).

Volk, C.A. *et al., Org. Biomol. Chem.*, 2004, **2**, 1827-1830 (*isol, pmr, cmr*)

Viscosamine V-59

[606136-89-4]



$C_{54}H_{90}N_3^{\oplus}$ 781.325

Related to Cyclostellettamines, C-1065. Alkaloid from the sponge *Haliclona viscosa*. Solid (as trifluoroacetate). λ_{max} 203; 267 (MeOH) (TFA salt).

Volk, C. *et al., Org. Lett.*, 2003, **5**, 3567-3569 (*isol, pmr, cmr, ms*)

Vitellogenesis inhibiting hormone V-60

VIH

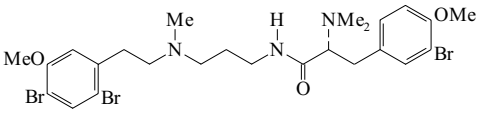
[138360-48-2]

Peptide of the crustacean hyperglycemic hormone family. Two isoforms have been isol. each displaying the same sequence of 77 amino acid residues. Isol. from sinus glands of the lobster *Homarus americanus*.

Soyez, D. *et al., Neuropeptides (Edinburgh)*, 1991, **20**, 25 (*isol*)

Vitilevuamide V-61

[191681-63-7]



$C_{77}H_{114}N_{14}O_{21}S$ 1603.895

Isol. from the ascidians *Didemnum cucculiferum* and *Polysyncraton lithostrotum*. Antitumour agent. Inhibits polymn. of tubulin dimers to microtubules. Amorph. solid. Genus name erroneously given as Polysyncranton. λ_{max} 230 (ϵ 2032) (MeOH).

Pat. Coop. Treaty (WIPO), 1998, 98 13 063; *CA*, **128**, 275065g (*isol, pmr, cmr*)

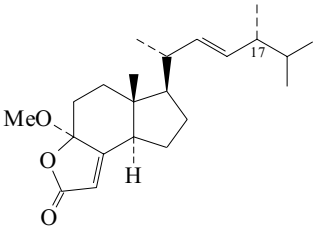
Fernandez, A.M. *et al., Pure Appl. Chem.*, 1998, **70**, 2130-2140 (*isol, pmr, cmr*)

Edler, M.C. *et al., Biochem. Pharmacol.*, 2002, **63**, 707-715 (*activity*)

Volemolide V-62

17-Methylincisterol

[125974-96-1]



$C_{22}H_{34}O_3$ 346.509

Constit. of the edible chichitake mushroom (*Lactarius volemus*) and from the sponge *Dictyonella incisa*. Needles. Mp 61-62°. $[\alpha]_D^{23}$ +215 (c, 0.1 in $CHCl_3$).

17-Epimer: [126060-08-0]

$C_{22}H_{34}O_3$ 346.509

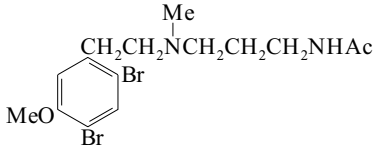
Isol. from *Dictyonella incisa*.

Ciminiello, P. *et al., J.A.C.S.*, 1990, **112**, 3505-3509 (*isol, uv, ir, pmr, cmr, ms, 17epimer*)

Kobata, K. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1542-1544 (*isol, pmr, cmr*)

Volutamide A V-63

[176181-95-6]

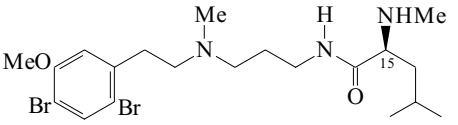


$C_{15}H_{22}Br_2N_2O_2$ 422.159

Alkaloid from the Atlantic bryozoan *Amathia convoluta*. Feeding deterrent to hydroid larvae. Oil. Sol. MeOH, butanol. λ_{max} 285 (ϵ 4200); 292 (ϵ 4100) (MeOH) (Berdy).

Montanari, A.M. *et al., Tetrahedron*, 1996, **52**, 5371-5380 (*isol, uv, ir, pmr, cmr, ms, struct*)

Volutamide B V-64



$C_{20}H_{33}Br_2N_3O_2$ 507.308

(S)-form [176181-96-7]

Alkaloid from the Atlantic bryozoan *Amathia convoluta*. Exhibits antifeedant activity to hydroid larvae. Oil. Sol. MeOH, butanol. $[\alpha]_D$ 0 (c, 0.053 in MeOH). λ_{max} 287 (ϵ 1600); 292 (ϵ 1500) (MeOH) (Berdy).

N^{15}-*Me:* ***Volutamide C***

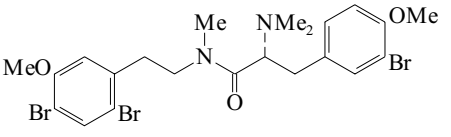
[176181-97-8]

$C_{21}H_{35}Br_2N_3O_2$ 521.334

From *Amathia convoluta*. Exhibits antifeedant activity to hydroid larvae. Oil. Sol. MeOH, butanol. $[\alpha]_D$ 0 (c, 0.032 in MeOH). λ_{max} 285 (ϵ 2100); 293 (ϵ 1900) (MeOH) (Berdy).

Montanari, A.M. *et al., Tetrahedron*, 1996, **52**, 5371-5380 (*isol, uv, ir, pmr, cmr, ms, cd, struct*)

Volutamide D V-65



$C_{22}H_{27}Br_3N_2O_3$ 607.179

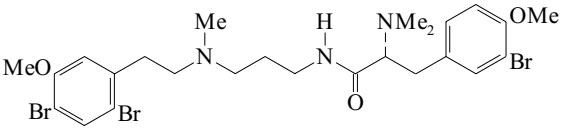
Sol. MeOH, butanol. λ_{max} 287 (ϵ 3500) (MeOH) (Berdy).

(R)-form [176182-10-8]

Alkaloid from the Atlantic bryozoan *Amathia convoluta*. Feeding deterrent to hydroid larvae, shows antiinflammatory props. Cryst. (MeOH). $[\alpha]_D$ -12.9 (c, 0.010 in MeOH). Abs. config. not certain.

Montanari, A.M. *et al., Tetrahedron*, 1996, **52**, 5371 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)

Volutamide E V-66



$C_{25}H_{34}Br_3N_3O_3$ 664.274

Sol. MeOH, butanol.

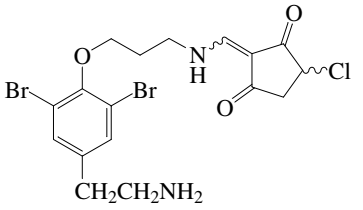
(R)-form [176182-11-9]

Alkaloid from the Atlantic bryozoan *Amathia convoluta*. Feeding deterrent to hydroid larvae, shows antiinflammatory props. Oil. $[\alpha]_D$ -15.8 (c, 0.014 in MeOH). Abs. config. not certain. λ_{max} 287 (ϵ 3800) (MeOH).

Montanari, A.M. *et al., Tetrahedron*, 1996, **52**, 5371-5380 (*isol, uv, ir, pmr, cmr, struct*)

Waianaeamine A W-1

[256472-04-5]

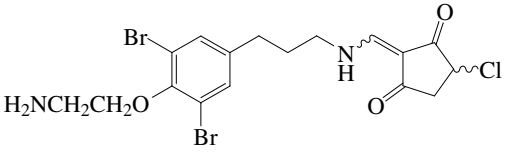


$C_{17}H_{19}Br_2ClN_2O_3$ 494.609
Alkaloid from an undescribed Verongid sponge.
$[\alpha]_D^{27}$ +2.6 (c, 0.23 in MeOH). λ_{max} 209 (log ϵ 4.36); 310 (log ϵ 3.89) (MeOH).

Lacy, C. *et al., J. Nat. Prod.*, 2000, **63**, 119-121 (*isol, pmr, cmr, uv*)

Waianaeamine B W-2

[256472-05-6]

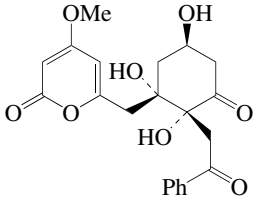


$C_{17}H_{19}Br_2ClN_2O_3$ 494.609
Alkaloid from an undescribed Verongid sponge.
$[\alpha]_D^{27}$ -20.9 (c, 0.07 in MeOH). λ_{max} 209 (log ϵ 4.31); 309 (log ϵ 3.84) (MeOH).

Lacy, C. *et al., J. Nat. Prod.*, 2000, **63**, 119-121 (*isol, pmr, cmr, uv*)

Wailupemycin A W-3

[178179-95-8]

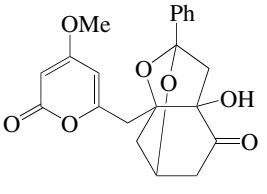


$C_{21}H_{22}O_8$ 402.4
Prod. by *Streptomyces maritimus.* Active against gram-negative bacteria. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O, hexane.
$[\alpha]_D$ +30 (c, 0.4 in MeOH). λ_{max} 208 (ϵ 18600); 251 (ϵ 13540); 272 (ϵ 12250) (MeOH).

Sitachitta, N. *et al., Tetrahedron*, 1996, **52**, 8073 (*isol, uv, ir, pmr, cmr, ms*)

Wailupemycin B W-4

[178179-96-9]

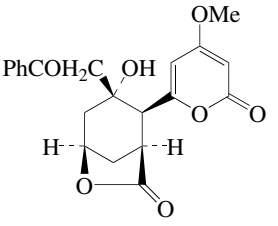


$C_{21}H_{20}O_7$ 384.385
Prod. by *Streptomyces maritimus.*
$[\alpha]_D$ +77.7 (c, 0.7 in MeOH). λ_{max} 208 (ϵ 17660); 279 (ϵ 6830) (MeOH).

Sitachitta, N. *et al., Tetrahedron*, 1996, **52**, 8073-8080 (*isol, uv, ir, pmr, cmr, ms*)
Kirsch, S.F. *et al., Chem. Eur. J.*, 2005, **11**, 7007-7023 (*synth*)

Wailupemycin C W-5

[178179-97-0]

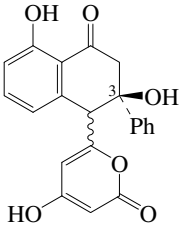


$C_{21}H_{20}O_7$ 384.385
Prod. by *Streptomyces maritimus.*
$[\alpha]_D$ +16 (c, 1 in MeOH). λ_{max} 207; 239; 281 (MeOH).

Sitachitta, N. *et al., Tetrahedron*, 1996, **52**, 8073 (*isol, uv, ir, pmr, cmr, ms*)

Wailupemycin D W-6

[297745-74-5]



Relative Configuration

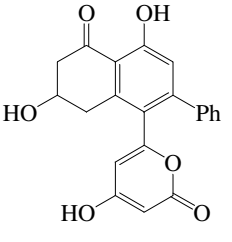
$C_{21}H_{16}O_6$ 364.354
Prod. by *Streptomyces maritimus.*
$[\alpha]_D^{25}$ -5.9 (c, 0.05 in MeOH).

3-Epimer: ***Wailupemycin E***
[426816-65-1]
$C_{21}H_{16}O_6$ 364.354
Prod. by *Streptomyces maritimus.*
$[\alpha]_D$ -19.9 (c, 0.36 in MeOH). λ_{max} 215 (log ϵ 3.56); 255 (log ϵ 3.25); 333 (log ϵ 1.86) (MeOH).

Piel, J. *et al., J.A.C.S.*, 2000, **122**, 5415-5416 (*isol*)
Moore, B.S. *et al., J. Nat. Prod.*, 2002, **65**, 1956-1962 (*rev, biosynth*)
Xiang, L.K. *et al., Org. Lett.*, 2002, **4**, 957-960 (*isol, pmr, cmr*)

Wailupemycin F W-7

[426816-67-3]

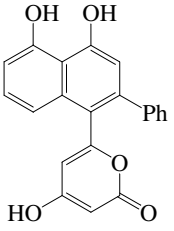


$C_{21}H_{16}O_6$ 364.354
Prod. by *Streptomyces maritimus.*
$[\alpha]_D$ +3.5 (c, 0.36 in MeOH). λ_{max} 239 (log ϵ 3.79); 281 (log ϵ 3.53); 338 (log ϵ 3.33) (MeOH).

Moore, B.S. *et al., J. Nat. Prod.*, 2002, **65**, 1956-1962 (*rev, biosynth*)
Xiang, L.K. *et al., Org. Lett.*, 2002, **4**, 957-960 (*isol, pmr, cmr*)

Wailupemycin G W-8

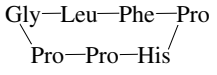
*6-(4,5-Dihydroxy-2-phenyl-1-naphthalenyl)-4-hydroxy-2*H*-pyran-2-one*
[426264-58-6]



$C_{21}H_{14}O_5$ 346.339
Prod. by *Streptomyces maritimus*. λ_{max} 215 (log ϵ 3.59); 250 (log ϵ 3.53); 340 (log ϵ 3.18) (MeOH).

Moore, B.S. *et al., J. Nat. Prod.*, 2002, **65**, 1956-1962 (*rev, biosynth*)
Xiang, L.K. *et al., Org. Lett.*, 2002, **4**, 957-960 (*isol, pmr, cmr*)

Wainunuamide W-9

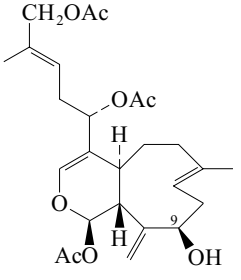


$C_{38}H_{51}N_9O_7$ 745.877
Cyclic peptide antibiotic. Isol. from the Fijian sponge *Stylotella aurantium*. Weak cytotoxic agent. Oil. $[\alpha]_D^{25}$ -64.1 (c, 0.01 in MeOH). λ_{max} 279 (ϵ 3167) (MeOH).

Tabudravu, J. *et al., Tet. Lett.*, 2001, **42**, 9273-9276

Waixenicin B W-10

[95230-64-1]



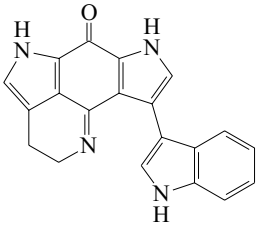
$C_{26}H_{36}O_8$ 476.566
Metabolite of the soft coral *Anthelia edmondsoni*. Cryst.
Mp 124-125°. $[\alpha]_D$ +17.5 (c, 0.27 in MeOH). λ_{max} 224 (ϵ 1160) (acidic MeOH) (Derep). λ_{max} 221 (ϵ 2600); 284 (ϵ 368) (base in MeOH) (Derep).

9-Deoxy: ***Waixenicin A***
[95230-65-2]
$C_{26}H_{36}O_7$ 460.566
Metabolite of *Anthelia edmondsoni*. Oil. $[\alpha]_D$ +62.7 (c, 0.35 in MeOH). λ_{max} 221 (ϵ 2600); 284 (ϵ 368) (base in MeOH) (Derep). λ_{max} 224 (ϵ 1160) (acidic MeOH) (Derep).

Coval, S.J. *et al., Tetrahedron*, 1984, **40**, 3823 (*cryst struct*)

Wakayin W-11

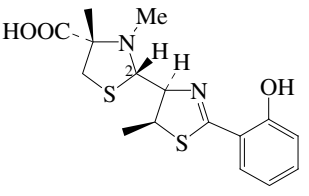
*2,3,5,7-Tetrahydro-9-(1*H*-indol-3-yl)-6*H*-dipyrrolo[4,3,2-*de*:2′,3′-*h*]quinolin-6-one, 9CI*
[134781-25-2]



$C_{20}H_{14}N_4O$ 326.357
Related to Tsitsikammamine A, T-787. Alkaloid from the ascidian *Clavelina* sp. Cytotoxic agent. Exhibits antimicrobial activity. Topoisomerase inhibitor. λ_{max} 226 (ϵ 24600); 299 (ϵ 14000); 413 (ϵ 5100); 474 (ϵ 4600) (MeOH/KOH) (Derep). λ_{max} 222 (ϵ 33500); 243 (ϵ 28200); 311 (ϵ 15000) (MeOH) (Derep). λ_{max} 226 (ϵ 24600); 270 (ϵ 14000); 412 (ϵ 5100); 473 (ϵ 4600) (MeOH/NaOH) (Berdy).

Copp, B.R. *et al., J.O.C.*, 1991, **56**, 4596-4597 (*isol, uv, ir, pmr, cmr, struct*)

Watasemycin A W-12

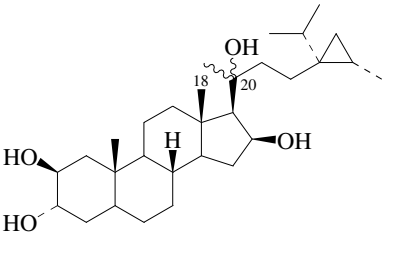


$C_{16}H_{20}N_2O_3S_2$ 352.478
Related to Thiazostatin A. Prod. by the marine-derived *Streptomyces* sp. TP-A0597. Active against gram-positive and -negative bacteria. Pale yellow powder.
Mp 62-65°. $[\alpha]_D^{28}$ +20.5 (c, 0.2 in $CHCl_3$). λ_{max} 212 (log ϵ 4.17); 252 (log ϵ 3.78); 319 (log ϵ 3.45) (MeOH).

2-Epimer: ***Watasemycin B***
$C_{16}H_{20}N_2O_3S_2$ 352.478
Prod. by *Streptomyces* sp. TP-A0597. Active against gram-positive and -negative bacteria. Pale yellow powder.
Mp 58-60°. $[\alpha]_D^{28}$ -2.5 (c, 0.2 in $CHCl_3$). λ_{max} 216 (log ϵ 4.21); 286 (log ϵ 3.87); 322 (log ϵ 3.85) (MeOH).

Sasaki, T. *et al., J. Antibiot.*, 2002, **55**, 249-255 (*isol, uv, pmr, cmr*)

Weinbersterol A W-13



$C_{30}H_{52}O_4$ 476.738

2,3-Disulfate: ***Weinbersterol disulfate A***
[134515-53-0]
$C_{30}H_{52}O_{10}S_2$ 636.867
Constit. of *Petrosia weinbergi*. Antiviral. Cryst. (MeOH aq./$CHCl_3$). Mp 182°. $[\alpha]_D$ +20 (c, 1.75 in MeOH).

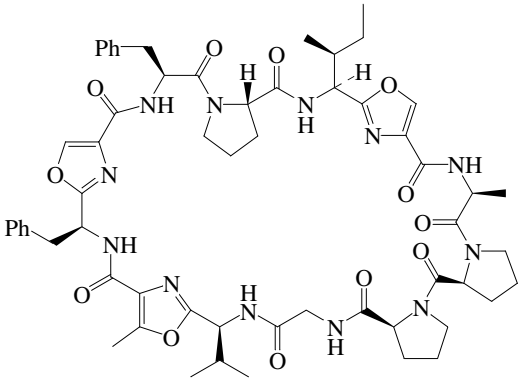
20-Deoxy, 18-hydroxy: Weinbersterol B
$C_{30}H_{52}O_4$ 476.738

20-Deoxy, 18-hydroxy, 2,3-disulfate: ***Weinbersterol disulfate B***
[134515-54-1]
$C_{30}H_{52}O_{10}S_2$ 636.867
Constit. of *Petrosia weinbergi*.
Mp 191°. $[\alpha]_D$ +32 (c, 0.1 in MeOH).

Sun, H.H. *et al., Tetrahedron*, 1991, **47**, 1185-1190 (*isol, pmr*)
Giner, J.L. *et al., Steroids*, 1999, **64**, 820-824 (*config*)

Wewakazole W-14

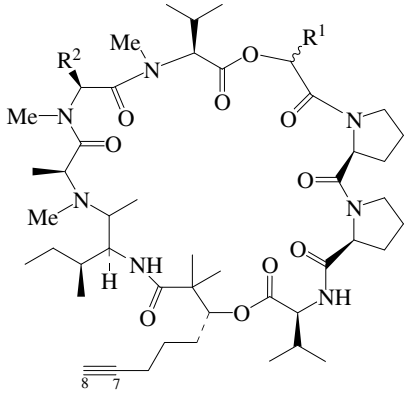
[494798-69-5]



$C_{59}H_{72}N_{12}O_{12}$ 1141.291
Isol. from a *Lyngbya majuscula*. Glassy oil. $[\alpha]_D^{21}$ -46.8 (c, 0.41 in MeOH). λ_{max} 213 (log ϵ 4.55); 221 (log ϵ 4.39) (MeOH).

Nogle, L.M. *et al., Org. Lett.*, 2003, **5**, 3-6 (*isol, pmr, cmr*)

Wewakpeptin A W-15



Absolute Configuration

R^1 = -CH(CH$_3$)$_2$ (*S*), R^2 = -CH(CH$_3$)$_2$

$C_{52}H_{85}N_7O_{11}$ 984.284
Isol. from *Lyngbya semiplena*. Cytotoxic. Amorph. solid. $[\alpha]_D^{26}$ -45 (c, 0.4 in $CHCl_3$). λ_{max} 216 (log ϵ 4.6) (MeOH).

7,8-Tetrahydro: ***Wewakpeptin B***
$C_{52}H_{89}N_7O_{11}$ 988.315
Isol. from *Lyngbya semiplena*. Cytotoxic. Amorph. solid. $[\alpha]_D^{26}$ -53 (c, 0.47 in $CHCl_3$). λ_{max} 215 (log ϵ 4.6) (MeOH).

Han, B. *et al., J.O.C.*, 2005, **70**, 3133-3139 (*isol, pmr, cmr, ms*)

Wewakpeptin C W-16

As Wewakpeptin A, W-15 with
R^1 = -CH$_2$Ph(*R*-), R^1 = CH$_3$

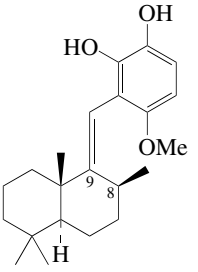
$C_{54}H_{81}N_7O_{11}$ 1004.274
Isol. from *Lyngbya semiplena*. Amorph. solid. $[\alpha]_D^{26}$ -56 (c, 0.27 in $CHCl_3$). λ_{max} 220 (log ϵ 4.5) (MeOH).

7,8-Tetrahydro: ***Wewakpeptin D***
$C_{54}H_{85}N_7O_{11}$ 1008.306
Isol. from *Lyngbya semiplena*. Amorph. solid. $[\alpha]_D^{26}$ -65 (c, 0.6 in $CHCl_3$). λ_{max} 221 (log ϵ 4.5) (MeOH).

Han, B. *et al., J.O.C.*, 2005, **70**, 3133-3139 (*isol, pmr, cmr*)

Wiedendiol B W-17

Sch 50680
[162341-31-3]



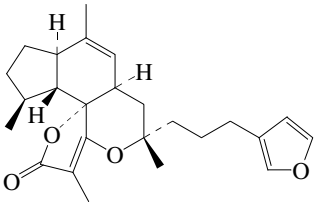
$C_{22}H_{32}O_3$ 344.493
Isol. from the sponge *Xestospongia wiedenmayeri*. Inhibits cholesteryl ester transfer protein. $[\alpha]_D^{21}$ -41 ($CHCl_3$). λ_{max} 199 (ϵ 41400); 288 (ϵ 16100); 325 (ϵ 9400) (heptane).

Δ^8-Isomer: ***Wiedendiol A***. *Sch 50679*
[162341-30-2]
$C_{22}H_{32}O_3$ 344.493
Isol. from *Xestospongia wiedenmayeri*. Inhibits cholesteryl ester transfer protein. $[\alpha]_D^{21}$ +121 ($CHCl_3$). λ_{max} 201 (ϵ 17700); 288 (ϵ 640) (heptane).

[169529-04-8, 169529-05-9]

Coval, S.J. *et al., Bioorg. Med. Chem. Lett.*, 1995, **5**, 605-610 (*isol, pmr, cmr*)
Chackalamannil, S. *et al., Tet. Lett.*, 1995, **36**, 5315-5318 (*synth*)
Bernet, A. *et al., Helv. Chim. Acta*, 2006, **89**, 784-796 (*synth*)

Wistarin W-18



(+)-*form*

$C_{25}H_{32}O_4$ 396.525

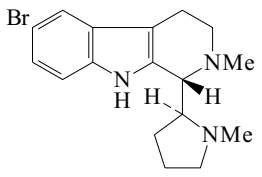
(+)-*form* [83995-04-4]
Constit. of *Ircinia wistarii*.
$[\alpha]_D^{20}$ +130 (c, 0.25 in CH_2Cl_2).

(-)-*form* [253661-83-5]
Constit. of an *Ircinia* sp.
Oil. $[\alpha]_D$ -112.2 (c, 0.7 in $CHCl_3$).

Gregson, R.P. *et al., J. Nat. Prod.*, 1982, **45**, 412
Coll, J.C. *et al., J. Nat. Prod.*, 1997, **60**, 1178-1179 (*cmr*)
Uenishi, J. *et al., J.O.C.*, 1997, **62**, 1691 (*synth*)
Fontana, A. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 3869-3872 (*(-)-form*)

Wolficene W-19

[117021-06-4]



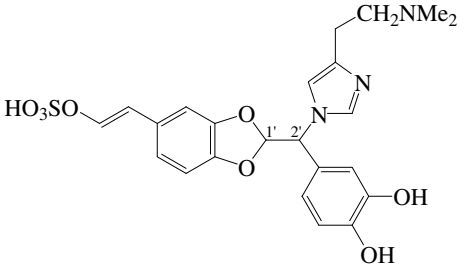
Absolute configuration

$C_{31}H_{52}$ 424.752
Metab. of *Botryococcus braunii*.

Huang, Z. *et al., J.O.C.*, 1988, **53**, 5390 (*isol, pmr, ms*)

Wondonine A W-20

[336825-31-1]



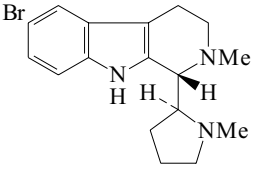
$C_{23}H_{25}N_3O_8S$ 503.532
Isol. from the association of sponges, *Jaspis* sp. and *Poecillastra wondoensis*. Yellow gum (as Na salt). $[\alpha]_D^{25}$ -4.8 (c, 0.12 in MeOH) (Na salt). λ_{max} 210 (log ϵ 4.16); 264 (log ϵ 3.94) (MeOH) (Na salt).

Diastereomer: ***Wondonine B***
[336825-33-3]
$C_{23}H_{25}N_3O_8S$ 503.532
Isol. from the association of sponges, *Jaspis* sp. and *Poecillastra wondoensis*. Yellow gum (as Na salt). $[\alpha]_D^{25}$ +3.6 (c, 0.2 in MeOH) (Na salt). λ_{max} 211 (log ϵ 4.23); 264 (log ϵ 3.25) (MeOH) (Na salt).

Shin, J. *et al., Tet. Lett.*, 2001, **42**, 1965-1968 (*Wondonines A,B*)

Woodinine W-21

[116339-96-9]



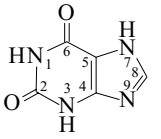
Absolute configuration

$C_{17}H_{22}BrN_3$ 348.285
Alkaloid from the ascidian *Eudistoma fragum*.
Mp 112-113°. $[\alpha]_D$ -38 (c, 0.6 in MeOH). $[\alpha]_D^{23}$ -80.8 (c, 0.6 in MeOH) (synthetic). λ_{max} 230 (ϵ 38000); 291 (ϵ 8510); 300 (sh) (ϵ 7080) (EtOH) (Derep).

Debitus, C. *et al., J. Nat. Prod.*, 1988, **51**, 799 (*isol, uv, pmr, cmr, ms, cd, struct*)
McNulty, J. *et al., Tet. Lett.*, 1991, **32**, 4875 (*synth, abs config*)
Mahboobi, S. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1992, **325**, 249; 1993, **326**, 33 (*synth, pmr, abs config*)
McNulty, J. *et al., J.C.S. Perkin 1*, 1994, 1329 (*synth*)
Mahboobi, S. *et al., J. Nat. Prod.*, 1997, **60**, 587 (*pmr, cmr, cryst struct*)

Xanthine, 8CI X-1

*3,7-Dihydro-1*H*-purine-2,6-dione, 9CI. 2,6-Dihydroxypurine. 2,6-Purinediol*
[69-89-6]



7H–form

$C_5H_4N_4O_2$ 152.112

Exists mainly as 7*H*-dioxo-form in aq. solns. with small amount of 9*H*-dioxo-form. Found in potatoes, coffee beans, etc. Cryst. Mp 350°. pK_{a1} 7.7; pK_{a2} 11.94 (20°). pK_{a1} 0.8; pK_{a2} 7.45; pK_{a3} 11.13 (20°).

▶ LD_{50} (mus, ipr) 500 mg/kg. ZD7700000

7H-form

7-(2-Deoxy-β-D-ribofuranosyl): **N^7-*2′-Deoxypseudoxanthosine***
[35912-09-5]
$C_{10}H_{12}N_4O_5$ 268.229
Constit. of the starfish *Asterias rollestoni*.
Mp 176-178°.

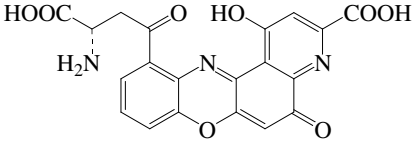
*7-Me: 3,7-Dihydro-7-methyl-1*H*-purine-2,6-dione, 9CI. Heteroxanthine. 7-Methylxanthine*
[552-62-5]
[28109-92-4]
$C_6H_6N_4O_2$ 166.139
Found in urine, sugar cane and other biol. sources, a urinary metab. of caffeine in man. Needles (H_2O).
Mp 380° dec.

▶ ZD8925000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 709C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 213C; 214A (*nmr*)
Elion, G.B. *et al., J.O.C.*, 1962, **27**, 2478-2491 (*3-Me*)
Lister, J.H. *et al., Chem. Heterocycl. Compd.*, (Weissberger, A. *et al*, Ed.), 1971, (*rev*)
Takayama, S. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1200-1202 (*3-Me, synth*)
Tanabe, T. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 3224-3226 (*3-Me*)
Coxon, B. *et al., J.O.C.*, 1977, **42**, 3132-3140 (*cmr*)
Saha, S.K. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 325-327 (*ms*)
Sponer, J. *et al., Struct. Chem.*, 1995, **6**, 281-286 (*tautom*)
Lindsay, B.S. *et al., J. Nat. Prod.*, 1999, **62**, 1573-1575 (*3-Me, isol, pmr, cmr, ms*)
Li, G.-Q. *et al., J. Chin. Pharm. Sci.*, 2004, **13**, 81-86 (*2′-Deoxypseudoxanthosine*)

Xanthommatin X-2

*α-Amino-3-carboxy-1-hydroxy-γ,5-dioxo-5*H*-pyrido[3,2-*a*]phenoxazine-11-butanoic acid, 9CI. Urechochrome*
[521-58-4]



$C_{20}H_{13}N_3O_8$ 423.338

(S)-form

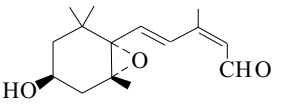
Insect metab. found in secretions of *Vanessa urticae* and in eyes of grasshoppers and blowflies (*Calliphora erythrocephala*). Also obt. from eggs of the marine worm *Urechis caupo*.
Yellow-brown powder.

Dihydro: See Dihydroxanthommatin, D-591

Butenandt, A. *et al., Annalen*, 1954, **586**, 217-228; **588**, 106-116; **590**, 75-90 (*isol, struct, synth*)
Linzen, B. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1959, **314**, 12-14 (*isol*)
Butenandt, A. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1960, **321**, 258-275
Linzen, B. *et al., Adv. Insect Physiol.*, 1974, **10**, 117-246 (*biosynth*)
Kayser, H. *et al., Compr. Insect Physiol. Biochem. Pharmacol.*, 1985, **10**, 367-415 (*rev*)
Martel, R.R. *et al., J. Biol. Chem.*, 1991, **266**, 21392-21398 (*bibl*)

Xanthoxin X-3

Xanthoxal
[8066-07-7]



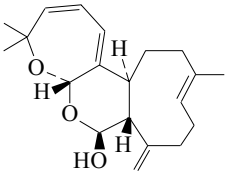
$C_{15}H_{22}O_3$ 250.337
Photooxidn. prod. of violaxanthin and related substances. Constit. of several marine and higher plants. Plant growth inhibitor. Germination inhibitor. Precursor of Abscisic acid, A-27.
Mp 85-86°. $[\alpha]_D$ -56 ($CHCl_3$). λ_{max} 280 (MeOH) (Berdy).

*9*E*-Isomer:* **t-*Xanthocin***
$C_{15}H_{22}O_3$ 250.337
Constit. of several marine and higher plants.

Burden, R.S. *et al., Tet. Lett.*, 1970, 4071 (*isol, struct*)
Oritani, T. *et al., Agric. Biol. Chem.*, 1973, **37**, 1215 (*synth*)
Kienzle, F. *et al., Helv. Chim. Acta*, 1978, **61**, 2616 (*synth*)
Kobayashi, M. *et al., Agric. Biol. Chem.*, 1990, **54**, 2723 (*bibl*)
Sakai, K. *et al., Tetrahedron*, 1992, **48**, 8229 (*synth*)
Milborrow, B.V. *et al., Phytochemistry*, 1997, **44**, 977 (*rev*)
Kuba, M. *et al., Chem. Lett.*, 2002, 1248-1249 (*synth*)

Xeniaacetal X-4

14,17:17,18-Diepoxy-1(19),6,10,12-xenicatetraen-18-ol
[82490-37-7]



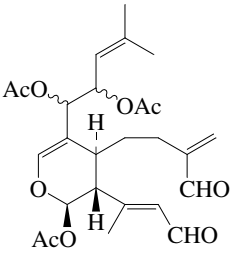
$C_{20}H_{28}O_3$ 316.439
Constit. of *Xenia crassa*. Cryst. (MeCN).
Mp 144-147°.

[88586-18-9]

Bowden, B.F. *et al., Aust. J. Chem.*, 1982, **35**, 997

Xeniacindial X-5

Xenicinedial
[182806-36-6]

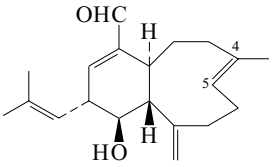


$C_{26}H_{34}O_9$ 490.549
Constit. of a *Xenia* sp. Oil. $[\alpha]_D$ +15 (c, 0.03 in MeOH). λ_{max} 243 (ε 13100) (no solvent reported).

Iwagawa, T. *et al., Tetrahedron*, 1996, **52**, 13121-13128 (*isol, pmr, cmr, ms*)

Xeniafaraunol A X-6

[161162-29-4]

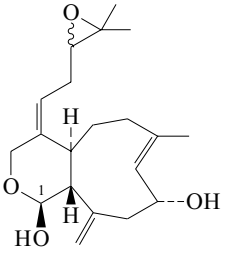


$C_{20}H_{28}O_2$ 300.44
Constit. of *Xenia faraunensis*. Glass. $[\alpha]_D$ +5 (c, 0.01 in $CHCl_3$).

4α,5α-Epoxide: ***Xeniafaraunol B***
[161162-30-7]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Xenia faraunensis* and *Xenia florida*. Oil. $[\alpha]_D$ -73 (c, 0.04 in MeOH). λ_{max} 245 (log ϵ 4.2) (MeOH).
Kashman, Y. *et al., Tet. Lett.*, 1994, **35**, 8855-8858 (*Xeniafaraunol A*)
Iwagawa, T. *et al., J. Nat. Prod.*, 2000, **63**, 468-472 (*Xeniafaraunol B*)

Xenialactol D X-7

[88526-73-2]

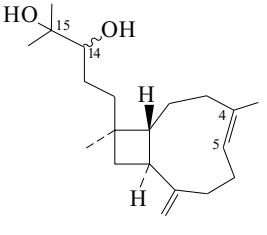


$C_{20}H_{30}O_4$ 334.455
Isol. from soft corals *Xenia obscuronata* and *Xenia lilielae*. Viscous oil.

1-Ketone: ***Xeniolide E***
[88514-06-1]
$C_{20}H_{28}O_4$ 332.439
Trace constit. of *Xenia obscuronata*. Air-sensitive.
Groweiss, A. *et al., Tetrahedron*, 1983, **20**, 3385

4,8(19)-Xeniaphylladiene-14,15-diol X-8

Xeniaphyllandiol
[74176-02-6]



$C_{20}H_{34}O_2$ 306.487
Constit. of soft corals *Xenia macrospiculata* and *Xenia obscuronata*. Oil.

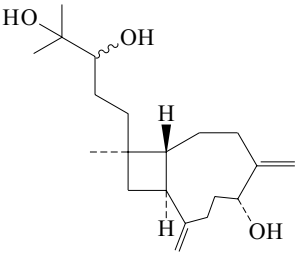
14-Ac: [74176-03-7]
$C_{22}H_{36}O_3$ 348.525
Constit. of *Xenia* spp. Oil. $[\alpha]_D^{25}$ -2 (c, 1.7 in $CHCl_3$).

4β,5β-Epoxide: 4,5-Epoxy-8(19)-xeniaphyllene-14,15-diol.
Epoxyxeniaphyllandiol
[88514-05-0]
$C_{20}H_{34}O_3$ 322.487
Isol. from *Xenia macrospiculata*, *Xenia obscuronata* and *Xenia lilielae*. Oil. $[\alpha]_D^{25}$ +31 (c, 0.9 in $CHCl_3$).

4,5-Epoxide, 14-Ac: [74176-04-8]
$C_{22}H_{36}O_4$ 364.524
Constit. of *Xenia* spp. Oil. $[\alpha]_D^{25}$ +11 (c, 1.6 in $CHCl_3$).
Kashman, Y. *et al., J.O.C.*, 1980, **45**, 3814
Groweiss, A. *et al., Tetrahedron*, 1983, **39**, 3385

4(18),8(19)-Xeniaphylladiene-5,14,15-triol X-9

Xeniaphyllantriol
[88514-02-7]

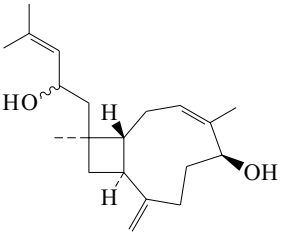


$C_{20}H_{34}O_3$ 322.487
Trace constit. of soft coral *Xenia obscuronata*. Oil. $[\alpha]_D^{25}$ +17 (c, 0.85 in $CHCl_3$). *ca.* 90% pure.

Groweiss, A. *et al., Tetrahedron*, 1983, **39**, 3385 (*isol, ir, ms, pmr, cmr*)

2,8(19),14-Xeniaphyllatriene-5,13-diol X-10

Xeniaphyllenol B
[88514-04-9]

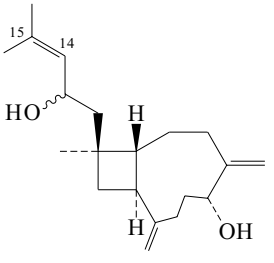


$C_{20}H_{32}O_2$ 304.472
Isol. from soft coral *Xenia macrospiculata*. Oil. $[\alpha]_D^{25}$ -47 (c, 1.1 in $CHCl_3$).

Groweiss, A. *et al., Tetrahedron*, 1983, **39**, 3385 (*isol, ir, ms, pmr, cmr*)

4(18),8(19),14-Xeniaphyllatriene-5,13-diol X-11

Xeniaphyllenol C
[88514-03-8]



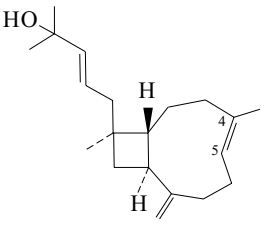
$C_{20}H_{32}O_2$ 304.472
Trace constit. of soft coral *Xenia macrospiculata*.

Groweiss, A. *et al., Tetrahedron*, 1983, **39**, 3385 (*isol, ir, ms, pmr, cmr*)

4,8(19),13-Xeniaphyllatrien-15-ol X-12

Isoxeniaphyllenol

[68651-47-8]



$C_{20}H_{32}O$ 288.472

Probable stereochem. shown following other closely related compds. Constit. of *Xenia* spp. Oil. $[\alpha]_D^{25}$ -13 (c, 0.5 in $CHCl_3$).

4,5-Epoxide: [74176-01-5]

$C_{20}H_{32}O_2$ 304.472

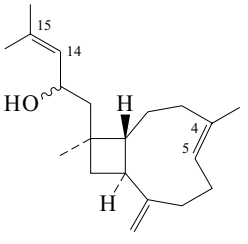
Constit. of *Xenia* spp. Oil. $[\alpha]_D^{25}$ +6 (c, 1.6 in $CHCl_3$). Prob. 4β,5β-.

Kashman, Y. *et al., J.O.C.*, 1980, **45**, 3814 (*isol, struct*)

4,8(19),14-Xeniaphyllatrien-13-ol X-13

Xeniaphyllenol. *Xeniaphyllenol A*

[68612-42-0]



$C_{20}H_{32}O$ 288.472

Constit. of *Xenia macrospiculata*, *Xenia obscuronata* and *Xenia lilielae*. Cryst. (CCl_4/petrol).

Mp 50-52°. $[\alpha]_D^{25}$ -2 (c, 1.5 in $CHCl_3$).

4,5-Epoxide: 4,5-Epoxy-8(19),14-xeniaphylladien-13-ol. ***Xeniaphyllenol oxide***

[68612-41-9]

$C_{20}H_{32}O_2$ 304.472

Isol. from *Xenia macrospiculata*, *Xenia obscuronata* and *Xenia lilielae*. Noncryst.

4,5:14,15-Diepoxide: ***4,14-Diepoxyxeniaphyllenol A***

$C_{20}H_{32}O_3$ 320.471

Isol. from *Xenia lilielae*. Oil. $[\alpha]_D^{25}$ +23 (c, 1.1 in $CHCl_3$).

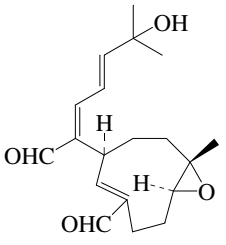
[88586-17-8]

Groweiss, A. *et al., Tet. Lett.*, 1978, 2205

Groweiss, A. *et al., Tetrahedron*, 1983, **39**, 3385

Xenibellal X-14

[861695-50-3]



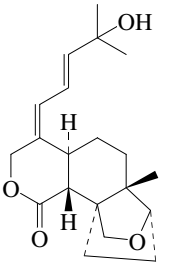
$C_{19}H_{26}O_4$ 318.412

Constit. of *Xenia umbellata*. Oil. $[\alpha]_D^{25}$ +12 (c, 0.1 in $CHCl_3$).

El-Gamal, A.A.H. *et al., Tet. Lett.*, 2005, **46**, 4499-4500 (*Xenibellal*)

Xenibellol A X-15

[852630-00-3]



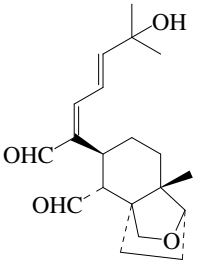
$C_{20}H_{28}O_4$ 332.439

Constit. of *Xenia umbellata*. Oil. $[\alpha]_D^{25}$ +18 (c, 0.1 in $CHCl_3$).

El-Gamal, A.A.H. *et al., Org. Lett.*, 2005, **7**, 2023-2025 (*Xenibellol A*)

Xenibellol B X-16

[852630-01-4]

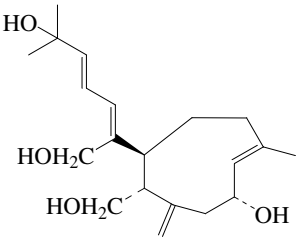


$C_{20}H_{28}O_4$ 332.439

Constit. of *Xenia umbellata*. Oil. $[\alpha]_D^{25}$ +15 (c, 0.1 in $CHCl_3$).

El-Gamal, A.A.H. *et al., Org. Lett.*, 2005, **7**, 2023-2025 (*Xenibellol B*)

1(19),6,10,12-Xenicatetraene-8,14,17,18-tetrol X-17



$C_{20}H_{32}O_4$ 336.47

(6*E*,8α,10*Z*,12*E*)-*form*

8,17,18-Tri-Ac: ***Isoxeniatriacetate***

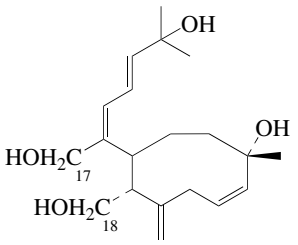
[663154-58-3]

$C_{26}H_{38}O_7$ 462.582

Constit. of a *Xenia* sp. Oil. $[\alpha]_D^{27}$ -196 (c, 0.55 in $CHCl_3$). λ_{max} 244 (ϵ 29000) (MeOH).

Miyaoka, H. *et al., Heterocycles*, 2003, **61**, 189-196 (*isol, pmr, cmr, abs config*)

1(19),7,10,12-Xenicatetraene-6,14,17,18-tetrol X-18



$C_{20}H_{32}O_4$ 336.47

(6α,7*Z*,10*E*,12*E*)-*form*

17-Hexadecanoyl: ***Azamilide F***
[177080-86-3]
$C_{36}H_{62}O_5$ 574.883
Constit. of *Xenia* sp. Oil. $[\alpha]_D$ +128.6 (c, 0.005 in MeOH). λ_{max} 241 (ϵ 25000) (MeOH).

17-Hexadecanoyl, 18-Ac: ***Azamilide B***
[177080-82-9]
$C_{38}H_{64}O_6$ 616.92
Constit. of *Xenia* sp.
$[\alpha]_D$ +99 (c, 0.05 in MeOH). λ_{max} 240 (ϵ 16000) (MeOH).

17-Octadecanoyl: ***Azamilide E***
[177080-85-2]
$C_{38}H_{66}O_5$ 602.936
Constit. of *Xenia* sp. Oil. $[\alpha]_D$ +81.8 (c, 0.067 in MeOH). λ_{max} 241 (ϵ 25000) (MeOH).

17-Octadecanoyl, 18-Ac: ***Azamilide A***
[177080-81-8]
$C_{40}H_{68}O_6$ 644.974
Constit. of *Xenia* sp. Oil. $[\alpha]_D$ +77.1 (c, 0.07 in MeOH). λ_{max} 240 (ϵ 25000) (MeOH).

17-Nonadecanoyl, 18-Ac: ***Azamilide C***
[177080-83-0]
$C_{41}H_{70}O_6$ 659
Constit. of *Xenia* sp. Oil. $[\alpha]_D$ +68.3 (c, 0.07 in MeOH). λ_{max} 240 (ϵ 14000) (MeOH).

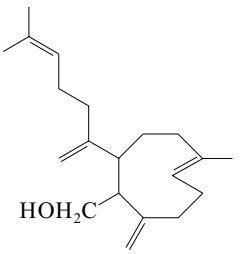
17-Eicosanoyl, 18-Ac: ***Azamilide D***
[177080-84-1]
$C_{42}H_{72}O_6$ 673.027
Constit. of *Xenia* sp. Oil. $[\alpha]_D$ +100 (c, 0.07 in MeOH). λ_{max} 240 (ϵ 24000) (MeOH).

(6α,7*Z*,10*Z*,12*E*)-*form*

17-Hexadecanoyl, 18-Ac: ***Azamilide G***
[177313-82-5]
$C_{38}H_{64}O_6$ 616.92
Constit. of *Xenia* sp. Oil. $[\alpha]_D$ +100 (c, 0.07 in MeOH). λ_{max} 241 (ϵ 23000) (MeOH).

Iwagawa, T. *et al., Bull. Chem. Soc. Jpn.*, 1996, **69**, 1309-1312 (*isol, pmr, cmr*)

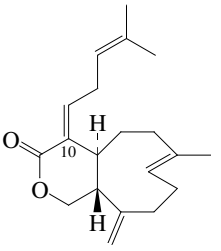
1(19),6,10(17),13-Xenicatetraen-18-ol X-19



$C_{20}H_{32}O$ 288.472

Ac: ***Corabohcin***
[80388-45-0]
$C_{22}H_{34}O_2$ 330.509
Constit. of *Corallium* spp. Oil. $[\alpha]_D^{27}$ -169 (c, 0.7 in $CHCl_3$).
Schwartz, R.E. *et al., Tetrahedron*, 1981, **37**, 2725

1(19),6,10,13-Xenicatetraen-17,18-olide X-20



(10*E*)-*form*

$C_{20}H_{28}O_2$ 300.44

(10*E*)-*form*

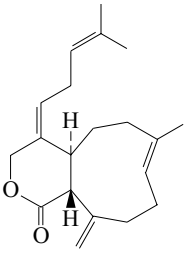
Coraxeniolide C'
[80388-46-1]
Constit. of *Corallium* spp.
Oil. $[\alpha]_D^{26}$ +85 (c, 1 in $CHCl_3$). λ_{max} 214 (ϵ 7760) (MeOH) (Derep).

(10*Z*)-*form*

Coraxeniolide C
[80433-14-3]
Constit. of *Corallium* spp.
Cryst.
Mp 68-69°. $[\alpha]_D^{25}$ +113 (c, 1.24 in $CDCl_3$). λ_{max} 214 (ϵ 7760) (MeOH) (Derep).
Schwartz, R.E. *et al., Tetrahedron*, 1981, **37**, 2725

1(19),6,10,13-Xenicatetraen-18,17-olide X-21

Deoxyxeniolide B
[167386-51-8]



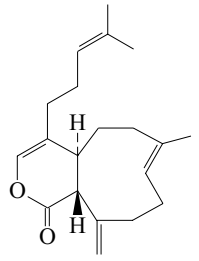
$C_{20}H_{28}O_2$ 300.44
Constit. of the coelenterate *Xenia elongata*. Amorph. solid.
Mp 40-42°. $[\alpha]_D^{27}$ -22.4 (c, 0.96 in $CHCl_3$). Misleading trivial name as Xeniolide B has two OH groups; see 8,14-Dihydroxy-1(19),6,10,12-xenicatetraen-18,17-olide, D-856.

13ξ,14-Epoxide: 13,14-Epoxy-1(19),6,10-xenicatrien-18,17-olide. ***9-Deoxyxeniolide***
[479067-60-2]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Xenia umbellata*. Oil. $[\alpha]_D^{25}$ +16.8 (c, 0.46 in $CHCl_3$). λ_{max} 206 (log ϵ 3.98) (MeOH).

6α,7α:13ξ,14-Diepoxide: 6,7:13,14-Diepoxy-1(19),10-xenicadien-18,17-olide. ***9-Deoxy-7,8-epoxyxeniolide E***
[479067-61-3]
$C_{20}H_{28}O_4$ 332.439
Constit. of *Xenia umbellata*. Oil. $[\alpha]_D^{25}$ +20.6 (c, 0.23 in $CHCl_3$). λ_{max} 204 (log ϵ 3.76) (MeOH).
Miyamoto, T. *et al., J. Nat. Prod.*, 1995, **58**, 924
Duh, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1882-1885 (*epoxides*)

1(19),6,10(17),13-Xenicatetraen-18,17-olide X-22

Acalycigorgin C
[147318-41-0]

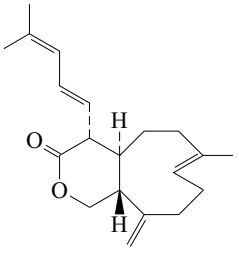


$C_{20}H_{28}O_2$ 300.44
Constit. of an *Acalycigorgia* sp. Oil. $[\alpha]_D^{21}$ +40.3 (c, 0.28 in $CHCl_3$). λ_{max} 235 (ϵ 7000) (MeOH) (Derep).

Ochi, M. *et al., Heterocycles*, 1993, **36**, 41; 1994, **38**, 151 (*isol, pmr, cmr*)

1(19),6,11,13-Xenicatetraen-17,18-olide X-23

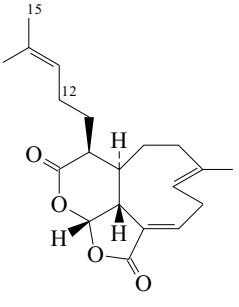
Arboxeniolide I. *Coraxenolide D′*
[80388-44-9]



$C_{20}H_{28}O_2$ 300.44
Constit. of *Paragorgia arborea*. Cryst. (heptane).
Mp 132-134°. $[\alpha]_D^{25}$ -89 (c, 0.69 in Et_2O). Coraxeniolide D′ is a semisynth. prod. λ_{max} 238 (ϵ 12900) (MeOH) (Derep).

Schwartz, R.E. *et al., Tetrahedron*, 1981, **37**, 2725 (*Coraxeniolide D′*)
D'Ambrosio, M. *et al., Z. Naturforsch., C*, 1984, **39**, 1180

1(9),6,13-Xenicatriene-17,18:19,18-diolide X-24



$C_{20}H_{26}O_4$ 330.423

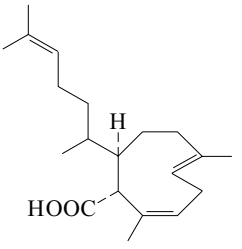
(1(9)*E*,6*E*)-*form*
Constit. of *Dictyota prolificans*.
Oil. $[\alpha]_D^{21}$ -346 (c, 1 in $CHCl_3$).

12,15-Didehydro: ***1(9),6,12,14-Xenicatetraene-17,18:19,18-diolide***
$C_{20}H_{24}O_4$ 328.407
Constit. of *Dictyota prolificans*. Oil. $[\alpha]_D^{21}$ -234 (c, 1 in $CHCl_3$).

Ravi, B.N. *et al., Aust. J. Chem.*, 1982, **35**, 121

1(9),6,13-Xenicatrien-18-oic acid X-25

Dilophic acid
[108864-15-9]

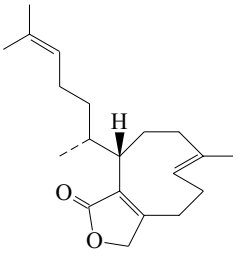


$C_{20}H_{32}O_2$ 304.472
Constit. of *Dilophus guineensis*. Ichthyotoxin. Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{25}$ -116 (c, 2.35 in $CHCl_3$). λ_{max} 228 (ϵ 440) (MeOH) (Berdy).

Schlenk, D. *et al., Phytochemistry*, 1987, **26**, 1081

1,6,13-Xenicatrien-18,19-olide X-26

Neodictyolactone
[89199-91-7]

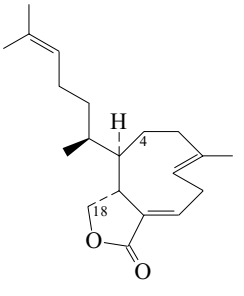


$C_{20}H_{30}O_2$ 302.456
Constit. of brown alga *Pachydictyon coriaceum* and *Dictyota linearis*.
$[\alpha]_D$ -43.4 (c, 0.29 in $CHCl_3$). λ_{max} 220 (ϵ 7800) (MeOH) (Derep).

Ishitsuka, M. *et al., Chem. Lett.*, 1984, 151
Siamopoulou, P. *et al., Phytochemistry*, 2004, **65**, 2025-2030 (*isol, pmr, cmr*)

1(9),6,13-Xenicatrien-19,18-olide X-27

Dictyolactone
[70552-63-5]



$C_{20}H_{30}O_2$ 302.456
Constit. of *Aplysia depilans*. Vasopressin V1 receptor antagonist. Norepinephrine antagonist. Cryst. (hexane).
Mp 64-65°. $[\alpha]_D^{25}$ -165 (c, 0.94 in MeOH). λ_{max} 226 (ϵ 4771) (MeOH) (Berdy).

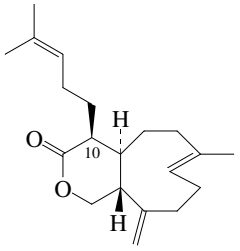
18β-Acetoxy: ***18-Acetoxydictyolactone***
$C_{22}H_{32}O_4$ 360.492
Constit. of *Pachydictyon coriaceum*.

4β-Acetoxy: ***4β-Acetoxy-1(9),6,13-xenicatrien-19,18-olide.***
4-Acetoxydictyolactone
$C_{22}H_{32}O_4$ 360.492

Constit. of *Dictyota dichotoma*. Oil. Sol. MeOH, hexane; poorly sol. H_2O. $[\alpha]_D$ -224 (c, 0.86 in $CHCl_3$). λ_{max} 220 (ϵ 8500) (EtOH) (Derep).

Finer, J. *et al., J.O.C.*, 1979, **44**, 2044 (*isol, cryst struct*)
Ishitsuka, M. *et al., Chem. Lett.*, 1984, 151 (*18-Acetoxydictyolactone*)
Ishitsuka, M.O. *et al., J.O.C.*, 1988, **53**, 5010 (*4ß-Acetoxydictyolactone*)

1(19),6,13-Xenicatrien-17,18-olide X-28



10α*H-form*

$C_{20}H_{30}O_2$ 302.456

10α*H-form* [127524-58-7]
Constit. of *Paragorgia arborea*.
Mp 32-34°. $[\alpha]_D^{25}$ +32 (c, 0.1 in $CHCl_3$).

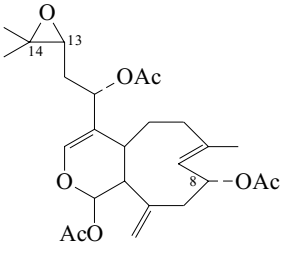
6α,7α-Epoxide: 6,7-Epoxy-1(19),13-xenicadien-17,18-olide.
Acalycixeniolide F
[259658-06-5]
$C_{20}H_{30}O_3$ 318.455
Constit. of *Acalycigorgia inermis*. Gum. $[\alpha]_D^{25}$ +46.8 (c, 0.1 in MeOH).

10β*H-form*
Acalycigorgin E
[153660-22-1]
Constit. of an *Acalycigorgia* sp.
Amorph. solid. $[\alpha]_D^{21}$ +51.4 (c, 0.16 in $CHCl_3$).

Stonik, V.A. *et al., Khim. Prir. Soedin.*, 1990, **26**, 125-126; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 103-104 (*Paragorgia arborea constit, isol, pmr, cmr*)
Ochi, M. *et al., Heterocycles*, 1994, **38**, 151-158 (*Acalycigorgin E*)
Rho, J.R. *et al., J. Nat. Prod.*, 2000, **63**, 254-257 (*Acalycixeniolide F*)

Xeniculin X-29

[68612-43-1]



$C_{26}H_{36}O_8$ 476.566
Constit. of *Xenia macrospiculata*. Cryst. (C_6H_6/petrol).
Mp 112-113°. $[\alpha]_D^{25}$ -3 (c, 1.7 in $CHCl_3$).

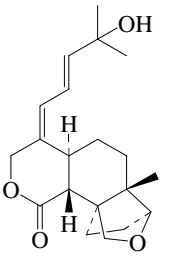
8-Deacetoxy, 13,14-deepoxy: [74175-94-3]
$C_{24}H_{34}O_5$ 402.53
Constit. of *Xenia* spp. Oil.

8-Deacetoxy, 13,14-deepoxy, 6,7-epoxide: [74175-95-4]
$C_{24}H_{34}O_6$ 418.529
Constit. of *Xenia* spp. Oil.

Groweiss, A. *et al., Tet. Lett.*, 1978, 2205 (*isol*)
Kashman, Y. *et al., J.O.C.*, 1980, **45**, 3814 (*isol*)

Xeniolactone A X-30

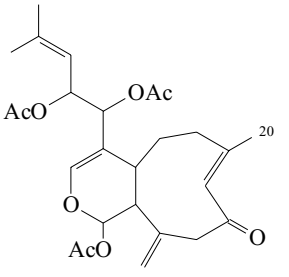
[861676-57-5]



$C_{20}H_{28}O_4$ 332.439
Constit. of *Xenia florida*. Amorph. powder. $[\alpha]_D$ +44 (c, 0.8 in CH_2Cl_2).

Shen, Y.-C. *et al., Tet. Lett.*, 2005, **46**, 4793-4796 (*Xeniolactone A*)

Xenione X-31



$C_{26}H_{34}O_8$ 474.55
Constit. of *Xenia membranacea*. Amorph.

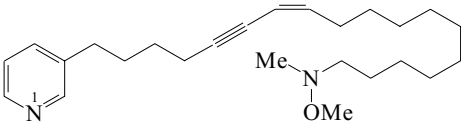
Stereoisomer:
$C_{26}H_{34}O_8$ 474.55
Constit. of *Xenia membranacea*. Amorph.

20-Acetoxy: ***18-Acetoxyxenione***
$C_{28}H_{36}O_{10}$ 532.586
Constit. of *Xenia membranacea*.

Almourabit, A. *et al., J. Nat. Prod.*, 1990, **53**, 894 (*isol, pmr*)

Xestamine A X-32

N-*Methoxy*-N-*methyl-18-(3-pyridinyl)-11-octadecen-13-yn-1-amine, 9CI*
[131985-15-4]



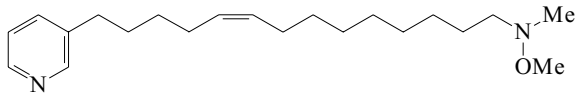
$C_{25}H_{40}N_2O$ 384.604
Isol. from the marine sponges *Xestospongia wiedenmayeri* and *Calyx podotypa*. Oil. λ_{max} 260 (ϵ 2500); 265 (ϵ 3100); 270 (ϵ 2000) (MeOH) (Derep). λ_{max} 227 (ϵ 12200); 257 (ϵ 2100); 263 (ϵ 2400); 269 (ϵ 1600) (MeOH) (Berdy).

N^1-*Me:* ***Xestamine F***
[136945-78-3]
$C_{26}H_{43}N_2O^{\oplus}$ 399.638
Alkaloid from the sponge *Calyx podatypa*. Oil. No counterion specified, presumably chloride. λ_{max} 226; 257; 269 (MeOH) (Berdy).

Sakemi, S. *et al., J. Nat. Prod.*, 1990, **53**, 995 (*isol, struct*)
Stierle, D.B. *et al., J. Nat. Prod.*, 1991, **54**, 1134 (*Xestamine F*)

Xestamine B X-33

N-*Methoxy*-N-*methyl-14-(3-pyridinyl)-9-tetradecen-1-amine, 9CI*
[131985-16-5]

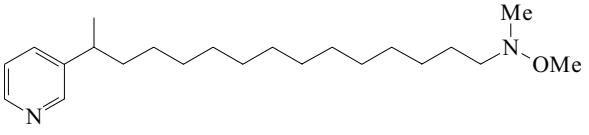


$C_{21}H_{36}N_2O$ 332.528
Alkaloid from the marine sponge *Xestospongia wiedenmayeri*. Oil. λ_{max} 260 (ϵ 2500); 265 (ϵ 3100); 270 (ϵ 2000) (MeOH) (Derep). λ_{max} 205 (ϵ 9700); 257 (ϵ 4300); 262 (ϵ 4900); 269 (ϵ 3700) (MeOH) (Berdy).

Sakemi, S. *et al., J. Nat. Prod.*, 1990, **53**, 995 (*isol, struct*)

Xestamine C X-34

N-*Methoxy*-N,ξ-*dimethyl-3-pyridinetetradecanamine, 9CI*
[131985-17-6]

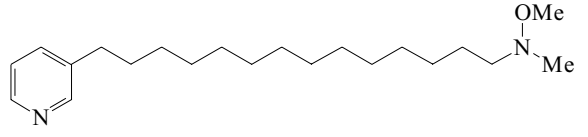


$C_{22}H_{40}N_2O$ 348.571
Alkaloid from the marine sponge *Xestospongia wiedenmayeri*. Oil. $[\alpha]_D^{20}$ -12.9 (c, 0.34 in MeOH). λ_{max} 260 (ϵ 2500); 265 (ϵ 3100); 270 (ϵ 2000) (MeOH) (Derep). λ_{max} 205 (ϵ 5200); 256 (ϵ 2700); 262 (ϵ 3100); 269 (ϵ 2300) (MeOH) (Berdy).

Sakemi, S. *et al., J. Nat. Prod.*, 1990, **53**, 995 (*isol, struct*)

Xestamine D X-35

N-*Methoxy*-N-*methyl-3-pyridinetetradecanamine, 9CI*
[136945-76-1]



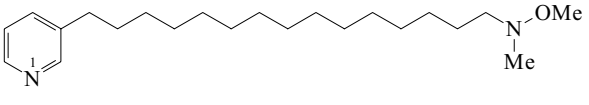
$C_{21}H_{38}N_2O$ 334.544
Alkaloid from the sponge *Calyx podatypa*. Obt. as a mixt. with Xestamine E. λ_{max} 226 (ϵ 8000); 257 (ϵ 2200); 262 (ϵ 2500); 269 (ϵ 2800) (MeOH) (Berdy).

N^1-*Me:* ***Xestamine G***
[136945-79-4]
$C_{22}H_{41}N_2O^{\oplus}$ 349.579
Alkaloid from the sponge *Calyx podatypa*. Obt. as a mixt. with Xestamine H. λ_{max} 226; 257; 269 (MeOH) (Berdy).

Stierle, D.B. *et al., J. Nat. Prod.*, 1991, **54**, 1134 (*isol, pmr, cmr, struct*)
Wang, Y. *et al., J.O.C.*, 2003, **68**, 3090-3098 (*synth*)

Xestamine E X-36

N-*Methoxy*-N-*methyl-3-pyridinepentadecanamine*
[136945-77-2]



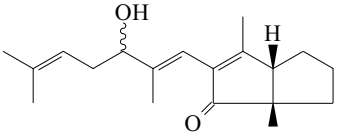
$C_{22}H_{40}N_2O$ 348.571
Alkaloid from the sponge *Calyx podatypa*. Obt. as a mixt. with Xestamine D. λ_{max} 226; 257; 269 (MeOH) (Berdy).

N^1-*Me:* ***Xestamine H***
[136945-80-7]
$C_{23}H_{43}N_2O^{\oplus}$ 363.605
Alkaloid from the sponge *Calyx podatypa*. Obt. as a mixt. with Xestamine G. λ_{max} 226; 257; 269 (MeOH) (Berdy).

Stierle, D.B. *et al., J. Nat. Prod.*, 1991, **54**, 1134 (*isol, pmr, cmr, struct*)

Xestenone X-37

[118169-37-2]

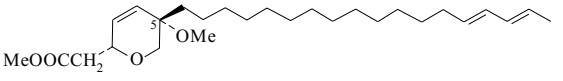


$C_{19}H_{28}O_2$ 288.429
Constit. of sponge *Xestospongia vanilla*. Clear oil. $[\alpha]_D$ 0 (c, 1.0 in MeOH). Positive Cotton effect.

Northcote, P.T. *et al., Tet. Lett.*, 1988, **29**, 4357 (*struct*)

Xestin A X-38

[104532-58-3]



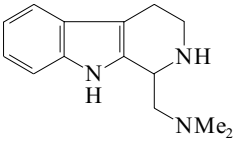
$C_{27}H_{46}O_4$ 434.658
Isol. from *Xestospongia* sp. Potent cytotoxin. Cryst. (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 55-56°. $[\alpha]_D^{20}$ +26.5 (c, 0.37 in CH_2Cl_2). λ_{max} 227 (ϵ 29000) (MeOH) (Derep).

5-Epimer: ***Xestin B***
[104597-39-9]
$C_{27}H_{46}O_4$ 434.658
Isol. from *Xestospongia* sp. Cytotoxin. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ +19.6 (c, 0.11 in CH_2Cl_2). λ_{max} 227 (ϵ 29000) (MeOH) (Derep).

Quinoa, E. *et al., J.O.C.*, 1986, **51**, 4260 (*isol, struct*)

Xestoamine X-39

[145237-04-3]

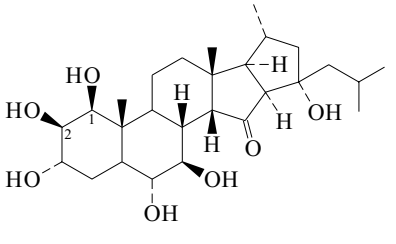


$C_{14}H_{19}N_3$ 229.324
Alkaloid from the New Caledonian sponge *Xestospongia* sp. Amorph. Opt. inactive.

Quirion, J.-C. *et al., J. Nat. Prod.*, 1992, **55**, 1505 (*isol, ir, pmr, cmr, ms, struct*)

Xestobergsterol B X-40

[141272-44-8]



$C_{27}H_{44}O_7$ 480.64

Constit. of *Xestospongia bergquistia*. Potent inhibitor of histamine release. Amorph. powder.

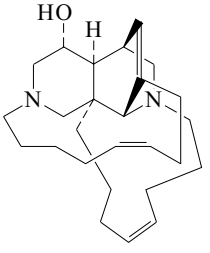
1,2-Dideoxy: ***Xestobergsterol A***
[141272-45-9]
$C_{27}H_{44}O_5$ 448.642
Isol. from *Xestospongia bergquistia*. Potent inhibitor of histamine release. Phospholipase C inhibitor. Antiasthmatic agent. Amorph. powder.

1-Deoxy: ***Xestobergsterol C***
$C_{27}H_{44}O_6$ 464.641
Constit. of an *Ircinia* sp. Powder. $[\alpha]_D^{22}$ -18.6 (c, 0.38 in MeOH).

Shoji, N. *et al., J.O.C.*, 1992, **57**, 2996-2997 (*Xestobergsterols A,B*)
Kobayashi, J. *et al., J. Nat. Prod.*, 1995, **58**, 312-318 (*Xestobergsterol C, abs config*)
Jung, M.E. *et al., Org. Lett.*, 1999, **1**, 1671-1674 (*synth*)
Jung, M. E. *et al., Tetrahedron*, 2001, **57**, 1449-1481 (*synth*)
Nakamura, A. *et al., Tet. Lett.*, 2005, **46**, 6373-6376 (*synth*)

Xestocyclamine A X-41

[151232-83-6]

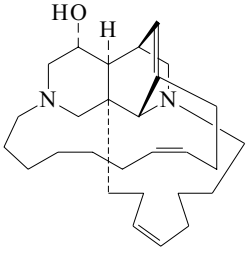


$C_{26}H_{40}N_2O$ 396.615
Alkaloid from the marine sponge *Xestospongia* sp. Protein kinase C inhibitor. $[\alpha]_D$ -13.5 (c, 0.019 in MeOH).

Rodríguez, J. *et al., J.A.C.S.*, 1993, **115**, 10436 (*isol, ir, pmr, cmr, ms*)
Rodríguez, J. *et al., Tet. Lett.*, 1994, **35**, 4719 (*struct*)

Xestocyclamine B X-42

[157207-89-1]

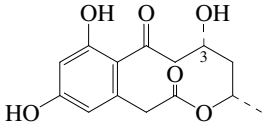


$C_{28}H_{44}N_2O$ 424.668
Alkaloid from the sponge *Xestospongia* sp. Protein kinase inhibitor.

Rodriguez, J. *et al., Tet. Lett.*, 1994, **35**, 4719 (*isol, pmr, cmr, struct*)

Xestodecalactone B X-43

*4,5,6,7-Tetrahydro-6,9,11-trihydroxy-4-methyl-2*H*-3-benzoxecin-2,8(1*H*)-dione, 9CI*



Probable Absolute Configuration

$C_{14}H_{16}O_6$ 280.277
Related to Sporostatin. Prod. by *Penicillium* cf. *montanense* isol. from the sponge *Xestospongia exigua*. Powder. $[\alpha]_D$ +17.3 (c, 3.1 in MeOH). λ_{max} 208; 218 (sh); 240 (sh); 288; 300 (MeOH).

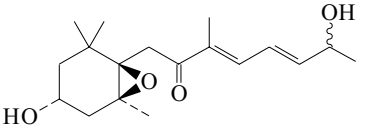
3-Deoxy: ***Xestodecalactone A***
$C_{14}H_{16}O_5$ 264.277
Prod. by *Penicillium* cf. *montanense* isol. from *Xestospongia exigua*. Powder. $[\alpha]_D$ +28.3 (c, 0.31 in MeOH). Possesses *R*-config. λ_{max} 208; 218 (sh); 263; 300 (MeOH).

3-Epimer: ***Xestodecalactone C***
$C_{14}H_{16}O_6$ 280.277
Prod. by *Penicillium* cf. *montanense* isol. from *Xestospongia exigua*. Powder. $[\alpha]_D$ +22.5 (c, 0.15 in MeOH). λ_{max} 208; 218 (sh); 240 (sh); 288; 300 (MeOH).

Edrada, R.A. *et al., J. Nat. Prod.*, 2002, **65**, 1598-1604 (*isol, cd, pmr, cmr, ms*)
Bringmann, G. *et al., Tet. Lett.*, 2004, **45**, 2829-2831 (*Xestodecalactone A, synth*)

Xestodiol X-44

[112727-21-6]

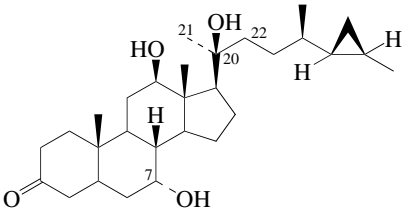


$C_{18}H_{28}O_4$ 308.417
Constit. of the sponge *Xestospongia vanilla*. Oil. $[\alpha]_D$ -27 (c, 0.5 in MeOH).

Northcote, P.T. *et al., J. Nat. Prod.*, 1987, **50**, 1174

Xestokerol B X-45

[151484-66-1]



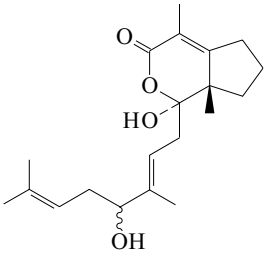
$C_{29}H_{48}O_4$ 460.696
Constit. of a *Xestospongia* sp. Amorph. powder.
Mp 218-221°. $[\alpha]_D^{21}$ -5.2 (c, 1.1 in MeOH).

*7-Deoxy, 21,22*R*-dihydroxy:* ***Xestokerol A***
[151484-65-0]
$C_{29}H_{48}O_5$ 476.695
Constit. of a *Xestospongia* sp. Needles.
Mp 200-202°. $[\alpha]_D^{21}$ +30 (c, 1.1 in MeOH). Opt. rotn. refers to an oily sample.

Kobayashi, J. *et al., J. Nat. Prod.*, 1993, **56**, 1350-1355 (*isol, pmr, cmr*)
Miyaoka, H. *et al., Tetrahedron*, 1997, **53**, 5403-5412 (*abs config*)

Xestolide X-46

[123231-47-0]



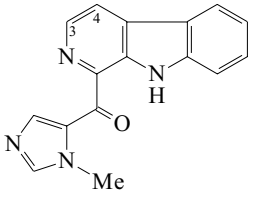
$C_{20}H_{30}O_4$ 334.455
Constit. of *Xestospongia vanilla*. Oil.

Northcote, P.T. *et al., Can. J. Chem.*, 1989, **67**, 1359 (*isol, pmr, cmr*)

Xestomanzamine A X-47

*(1-Methyl-1*H*-imidazol-5-yl)-9*H*-pyrido[3,4-*b*]indol-1-ylmethanone, 9CI*

[164301-25-1]



$C_{16}H_{12}N_4O$ 276.297

Alkaloid from the Okinawan marine sponge *Xestospongia* sp. Yellow needles ($CHCl_3$/MeOH). Mp 185-186°. λ_{max} 221 (ϵ 7400); 257 (ϵ 1700); 300 (ϵ 3900); 395 (ϵ 1600) (MeOH) (Berdy).

N-*De-Me:* **N-*Demethylxestomanzamine A***

[581782-69-6]

$C_{15}H_{10}N_4O$ 262.27

Alkaloid from an Indonesian sponge. Yellow powder. Mp 192° dec. λ_{max} 218; 258; 298; 356; 395 (MeOH).

3,4-Dihydro: ***Xestomanzamine B***

[164301-24-0]

$C_{16}H_{14}N_4O$ 278.313

Alkaloid from *Xestospongia* sp. Exhibits weak cytotoxicity against KB cells. Yellow oil. λ_{max} 222 (ϵ 27200); 270 (ϵ 10300); 298 (ϵ 16500); 388 (ϵ 4500) (MeOH) (Berdy).

Kobayashi, M. *et al., Tetrahedron*, 1995, **51**, 3727-3736 (*isol, uv, ir, pmr, cmr, cryst struct, Xestomanzamine B*)
Molina, P. *et al., Tet. Lett.*, 1996, **37**, 9353-9356 (*synth, Xestomanzamine B*)
Panosyan, F.B. *et al., Can. J. Chem.*, 2001, **79**, 1110-1114 (*synth*)
Burm, B.E.A. *et al., Heterocycles*, 2001, **55**, 495-503 (*synth, Xestomanzamine B*)
Rao, K.V. *et al., J. Nat. Prod.*, 2003, **66**, 823-828 (*N-Demethylxestomanzamine A*)

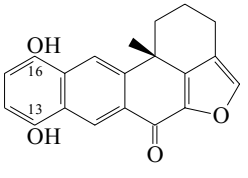
Xestomycin X-48

$C_{23}H_{32}N_2O_9$ 480.514

Saframycin-type antibiotic. Isol. from *Xestospongia* sp. Antibacterial agent. Yellow powder. $[\alpha]_D$ -56 (MeOH). λ_{max} 212; 267; 347 (MeOH).

Gulavita, N.K. *et al., CA*, 1992, **117**, 230454q (*isol*)

Xestoquinol X-49



$C_{20}H_{16}O_4$ 320.344

16-Sulfate: ***Xestoquinol 16-sulfate***

[143380-39-6]

$C_{20}H_{16}O_7S$ 400.408

Constit. of *Xestospongia sapra*. DNA topoisomerase I inhibitor. $[\alpha]_D^{25}$ +27 (c, 0.56 in MeOH). λ_{max} 225 (ϵ 40000); 274 (ϵ 2000); 310 (ϵ 13000); 399 (ϵ 5200) (MeOH) (Berdy).

13-Me ether, 16-sulfate: ***13-O-Methylxestoquinol 16-sulfate***

$C_{21}H_{18}O_7S$ 414.435

Constit. of a *Xestospongia* sp. Yellowish powder. $[\alpha]_D^{23}$ +28 (c, 0.19 in MeOH). λ_{max} 223 (log ϵ 4.5); 273 (log ϵ 4.1); 310 (log ϵ 4); 331 (log ϵ 4) (MeOH).

13,14,15,16-Tetrahydro: ***13,14,15,16-Tetrahydroxestoquinol***

[113830-95-8]

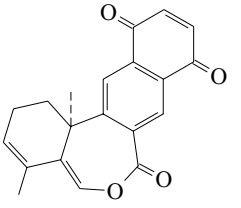
$C_{20}H_{20}O_4$ 324.376

Isol. from the sponge *Adocia* sp. Solid. Mp 224-229°. λ_{max} 233 (sh) (ϵ 7000); 254 (ϵ 7200); 304 (ϵ 13600) (EtOH) (Derep).

Schmitz, F.J. *et al., J.O.C.*, 1988, **53**, 3922 (*Tetrahydroxestoquinol*)
Kobayashi, J. *et al., J. Nat. Prod.*, 1992, **55**, 994 (*isol, pmr, cmr*)
Cao, S. *et al., Bioorg. Med. Chem.*, 2005, **13**, 999-1003 (*13-Methylxestoquinol sulfate*)

Xestoquinolide A X-50

[151171-18-5]



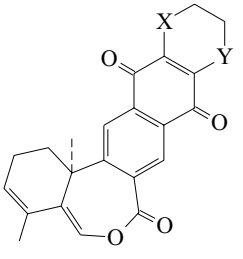
$C_{20}H_{16}O_4$ 320.344

Constit. of *Xestospongia* cf. *carbonaria*. Yellow powder. $[\alpha]_D$ +32. λ_{max} 216; 234 (sh); 245; 325 (MeOH) (Derep).

Alvi, K.A. *et al., J.O.C.*, 1993, **58**, 4871 (*isol, pmr, cmr*)

Xestoquinolide B X-51

[151247-69-7]



X,Y = −NH−,−SO_2 −

$C_{22}H_{19}NO_6S$ 425.461

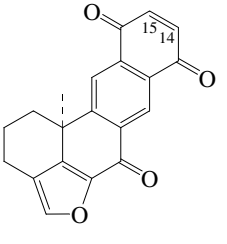
2 Possible isomeric structs. not yet distinguished. Constit. of *Xestospongia* cf. *carbonaria*. Yellow powder. λ_{max} 211; 242; 272; 304 (MeOH) (Derep).

Alvi, K.A. *et al., J.O.C.*, 1993, **58**, 4871 (*isol, pmr, cmr*)

Xestoquinone X-52

*2,3-Dihydro-12*b*-methyl-1*H*-benzo[6,7]phenanthro[10,1-*bc*]furan-6,8,11(12*bH*)-trione, 9CI*

[97743-96-9]



$C_{20}H_{14}O_4$ 318.328

Constit. of sponge *Xestospongia sapra* and *Adocia* sp. Shows cardiotonic activity. Inhibitor of protein tyrosine kinase and topoisomerase I. Yellow powder. Sol. MeOH, $CHCl_3$, C_6H_6, MeCN; poorly sol. H_2O.

Mp 212-214° dec. $[\alpha]_D^{25}$ +17.2 (c, 1.16 in CH_2Cl_2). λ_{max} 217 (ϵ 14400); 252 (ϵ 14400); 259 (sh) (ϵ 13600); 296 (ϵ 8020); 340 (ϵ 4280) (MeCN) (Derep). λ_{max} 216 (ϵ 19900); 251 (ϵ 21400); 294 (ϵ 13700) (MeOH) (Berdy).

14-Methoxy: ***14-Methoxyxestoquinone***
[169387-74-0]
$C_{21}H_{16}O_5$ 348.354
Isol. from a *Xestospongia* sp. Topoisomerase II inhibitor. Inhibitor of protein tyrosine kinase. Yellow solid. $[\alpha]_D$ +13.1 (c, 3.1 in $CHCl_3$). λ_{max} 272 (ϵ 21400) (MeOH).

15-Methoxy: ***15-Methoxyxestoquinone***
[169387-75-1]
$C_{21}H_{16}O_5$ 348.354
Isol. from a *Xestospongia* sp. Topoisomerase II inhibitor. Yellow solid. λ_{max} 272 (ϵ 21400) (MeOH).

14-Hydroxy, 15-chloro: ***15-Chloro-14-hydroxyxestoquinone***
[169387-76-2]
$C_{20}H_{13}ClO_5$ 368.772
Isol. from a *Xestospongia* sp. Topoisomerase II inhibitor. Yellow solid. $[\alpha]_D$ +29.6 (c, 2.8 in $CHCl_3$). λ_{max} 266 (ϵ 76140) (MeOH).

15-Hydroxy, 14-chloro: ***14-Chloro-15-hydroxyxestoquinone***
[169387-77-3]
$C_{20}H_{13}ClO_5$ 368.772
Isol. from a *Xestospongia* sp. Topoisomerase II inhibitor. Yellow solid. λ_{max} 266 (ϵ 76140) (MeOH).

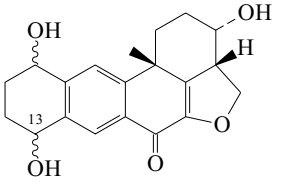
14-(2-Sulfoethylamino): ***Secoadociaquinone B***
[169387-73-9]
$C_{22}H_{19}NO_7S$ 441.461
Isol. from a *Xestospongia* sp. Topoisomerase II inhibitor. Orange solid. $[\alpha]_D$ +30.3 (c, 1.1 in MeOH). Isol. pure. λ_{max} 258 (ϵ 11100) (MeOH).

15-(2-Sulfoethylamino): ***Secoadociaquinone A***
[169387-72-8]
$C_{22}H_{19}NO_7S$ 441.461
Isol. from a *Xestospongia* sp. Topoisomerase II inhibitor. Orange solid. Obt. as a mixt. with Secoadociaquinone B. λ_{max} 258 (ϵ 11100) (MeOH).

Nakamura, H. *et al., Chem. Lett.*, 1985, 713-716 (*isol*)
Harada, N. *et al., J.O.C.*, 1990, **55**, 3158-3163; 1994, **59**, 6606-6613 (*synth, abs config*)
Kanematsu, K. *et al., Tet. Lett.*, 1991, **32**, 4761-4764 (*synth*)
Alvi, K.A. *et al., J.O.C.*, 1993, **58**, 4871-4880 (*14-methoxy, isol, activity*)
Concepcion, G.P. *et al., J. Med. Chem.*, 1995, **38**, 4503-4507 (*isol, uv, ir, pmr, cmr, derivs, activity*)
Maddaford, S.P. *et al., J.A.C.S.*, 1996, **118**, 10766-10773 (*synth*)
Miyazaki, F. *et al., Tetrahedron*, 1998, **54**, 13073-13078 (*synth*)
Wipf, P. *et al., Org. Biomol. Chem.*, 2005, **3**, 2053-2061 (*rev*)

Xestosaprol B X-53

[143380-66-9]



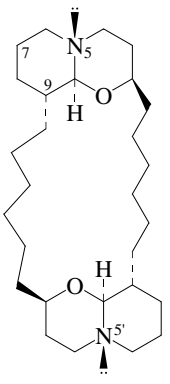
$C_{20}H_{22}O_5$ 342.391
Constit. of *Xestospongia sapra*. Yellow solid. $[\alpha]_D^{28}$ +49 (c, 0.22 in MeOH). λ_{max} 214 (ϵ 14000); 268 (ϵ 6500); 285 (ϵ 5900) (MeOH) (Berdy).

13-Ketone: ***Xestosaprol A***
[143380-40-9]
$C_{20}H_{20}O_5$ 340.375
Constit. of *Xestospongia sapra*. Yellow solid. $[\alpha]_D^{27}$ -42 (c, 0.35 in MeOH). λ_{max} 248 (ϵ 22000); 326 (ϵ 6300) (MeOH) (Berdy).

Kobayashi, J. *et al., J. Nat. Prod.*, 1992, **55**, 994 (*isol, pmr, cmr*)

Xestospongin A X-54

Araguspongine D
[88840-02-2]



Absolute Configuration

$C_{28}H_{50}N_2O_2$ 446.715
The abs. configs. of Xestospongins A and C and Araguspongine B were revised in 1998. The work suggested that the abs. configs. of the other nat. prods. in the series required revision. Araguspongine D was found to be partially racemic Xestospongin A. Isol. from the marine sponge *Xestospongia exigua* and from an Okinawan *Xestospongia* sp. Shows vasodilator props. Cryst. (Et_2O).
Mp 135-136°. $[\alpha]_D$ +6.9 (c, 0.84 in $CHCl_3$) (+ 10). Related to Petrosine, P-287.

7S-Hydroxy: ***7S-Hydroxyxestospongin A***
$C_{28}H_{50}N_2O_3$ 462.715
Isol. from *Xestospongia* sp. Cryst. (Me_2CO).
Mp 166-167°. $[\alpha]_D$ +4.7 (c, 0.25 in $CHCl_3$).

5,9-Diepimer: ***Xestospongin C***. *Araguspongine E*
[88903-69-9]
$C_{28}H_{50}N_2O_2$ 446.715
Isol. from *Xestospongia exigua*. Calcium channel blocker. Inositol triphosphate Ins(1,4,5)P_3 receptor antagonist. Shows vasodilator props. Cryst. (Et_2O). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 149-150°. $[\alpha]_D$ -2.4 (c, 0.54 in $CHCl_3$). Struct. of Araguspongine E revised in 1998.

5,9-Diepimer, 9-hydroxy: ***Xestospongin D***. *Araguspongine A*
[88840-00-0]
$C_{28}H_{50}N_2O_3$ 462.715
Isol. from *Xestospongia exigua* and *Haliclona* sp. Also isol. as racemate from sponge *Niphates* sp. Shows vasodilator props, human cancer cell inhibitory and antimicrobial activity. Cryst. (Et_2O). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.
Mp 156-157°. $[\alpha]_D$ +18.43 (c, 1.08 in $CHCl_3$).

5,9-Diepimer, 9-hydroxy, N^5*-oxide:* ***Araguspongine K***
$C_{28}H_{50}N_2O_4$ 478.714
Alkaloid from *Xestospongia exigua*. Needles. $[\alpha]_D^{25}$ +2.6 (c, 0.35 in $CHCl_3$).

2,2′,5,5′-Tetraepimer: ***Araguspongine M***
$C_{28}H_{50}N_2O_2$ 446.715
Alkaloid from the sponge *Neopetrosia exigua*.
$[\alpha]_D$ -4.6 (c, 0.5 in $CHCl_3$).

5,5′,9,9′-Tetraepimer: ***Araguspongine B***
[123000-02-2]
$C_{28}H_{50}N_2O_2$ 446.715
Alkaloid from an Okinawan sponge *Xestospongia* sp. Shows vasodilator activity. Somatostatin inhibitor. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Isol. as racemate, both enantiomers characterised. Abs. config. indicated refers to (-)-form ($[\alpha]_D$ -15°). Abs. config. revised in 1998.

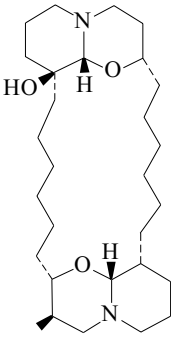
[123000-03-3, 123000-06-6, 123000-07-7, 123048-14-6]

Nakagawa, M. *et al., Tet. Lett.*, 1984, **25**, 3227 (*ir, pmr, cmr, struct, cryst struct*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1676 (*isol, ir, pmr, cmr, struct, abs config*)

Hoye, T.R. *et al., J.A.C.S.*, 1994, **116**, 2617 (*synth*)
Pettit, G.R. *et al., Bioorg. Med. Chem. Lett.*, 1996, **6**, 1313 (*isol, cryst struct, rac-Xestospongin D*)
Gafni, J. *et al., Neuron*, 1997, **19**, 723-733 (*Xestospongin C, pharmacol*)
Kobayashi, M. *et al., Heterocycles*, 1998, **47**, 195-203 (*pmr, cmr, ms, struct*)
Schultz, A.G. *et al., J.A.C.S.*, 1998, **120**, 8259-8260 (*synth, abs config*)
Matzanke, N. *et al., Org. Prep. Proced. Int.*, 1998, **30**, 3-51 (*rev, synth*)
Moon, S.-S. *et al., J. Nat. Prod.*, 2002, **65**, 249-254 (*Xestospongin D, abs config, 7-Hydroxyxestospongin A*)
Orabi, K.Y. *et al., J. Nat. Prod.*, 2002, **65**, 1782-1785 (*Araguspongines A,K*)
Liu, H. *et al., Mar. Drugs*, 2004, **2**, 154-163 (*Araguspongine M*)

Xestospongin B X-55

[88840-01-1]



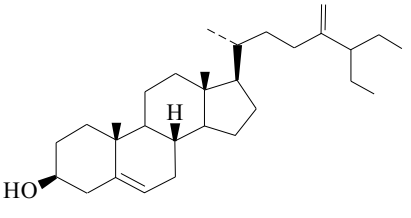
$C_{29}H_{52}N_2O_3$ 476.741
Isol. from the marine sponge *Xestospongia exigua*. Shows vasodilator props. Cryst. (Et_2O).
Mp 179-181°. $[\alpha]_D$ +7.1 (c, 0.91 in $CHCl_3$).

Demethyl: ***Demethylxestospongin B***
$C_{28}H_{50}N_2O_3$ 462.715
Alkaloid from a New Caledonian sponge *Xestospongia* sp.
Amorph. $[\alpha]_D^{20}$ +6 (c, 0.8 in $CHCl_3$).

Nakagawa, M. *et al., Tet. Lett.*, 1984, **25**, 3227 (*ir, pmr, cmr, struct*)
Quirion, J.-C. *et al., J. Nat. Prod.*, 1992, **55**, 1505 (*Demethylxestospongin B*)

Xestosterol X-56

24-(1-Ethylpropyl)-26,27-dinorcholesta-5,24-dien-3-ol. 26,27-Dimethylergosta-5,24(28)-dien-3-ol. 26,27-Dimethyl-24-methylene-cholest-5-en-3-ol. Albidasterol
[71031-58-8]



$C_{30}H_{50}O$ 426.724
Constit. of *Xestospongia muta*. Also from *Nephthea albida*. Cryst. (Me_2CO aq.).
Mp 123.5-125°. $[\alpha]_D^{20}$ -33 ($CHCl_3$).

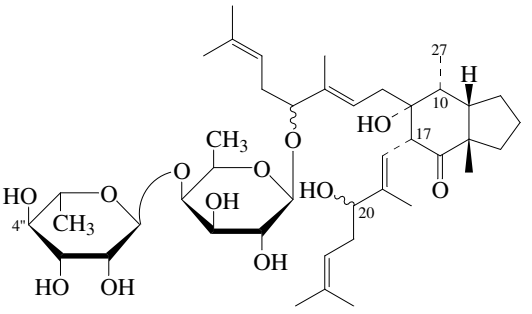
3-O-*(18-Bromo-9*E*,17*E*-octadecadiene-7,15-diynoyl):* [247155-95-9]
$C_{48}H_{71}BrO_2$ 759.992
Constit. of *Xestospongia testudinaria*. Powder. $[\alpha]_D^{25}$ -7.8 (c, 0.19 in CH_2Cl_2). λ_{max} 228 (ϵ 19300); 237 (ϵ 20800); 250 (ϵ 12900) (hexane).

3-O-*(18-Bromo-9*E*,17*E*-octadecadiene-5,7,15-triynoyl):* [247155-96-0]
$C_{48}H_{67}BrO_2$ 755.96
Constit. of *Xestospongia testudinaria*. Powder. $[\alpha]_D^{25}$ -2.6 (c, 0.25 in CH_2Cl_2). λ_{max} 232 (ϵ 8500); 239 (ϵ 9200); 245 (ϵ 8200) (CH_2Cl_2).

Kokke, W.C.M.C. *et al., J.O.C.*, 1979, **44**, 3385
Stoilov, I.L. *et al., Tet. Lett.*, 1986, **27**, 4821 (*biosynth*)
Pham, N.B. *et al., J. Nat. Prod.*, 1999, **62**, 1439-1442 (*esters*)

Xestovanin A X-57

[121541-66-0]



$C_{42}H_{68}O_{12}$ 764.992
Constit. of *Xestospongia vanilla*. Glass. $[\alpha]_D$ -42 (c, 0.3 in MeOH).

20-O-*α-L-Rhamnopyranoside:* ***Xestovanin B***
[137415-09-9]
$C_{48}H_{78}O_{16}$ 911.135
Constit. of *Xestospongia vanilla*. Oil. $[\alpha]_D$ -45.5 (c, 0.3 in MeOH).

10,27-Didehydro: ***Dehydroxestovanin A***
[137443-14-2]
$C_{42}H_{66}O_{12}$ 762.976
Constit. of *Xestospongia vanilla*. Pale yellow glass. $[\alpha]_D$ -45 (c, 0.8 in MeOH).

*10,27-Didehydro, 4″-*O*-α-L-rhamnopyranosyl:* ***Dehydroxestovanin C***
[137443-15-3]
$C_{48}H_{76}O_{16}$ 909.119
Constit. of *Xestospongia vanilla*. Glass. $[\alpha]_D$ -24.6 (c, 0.08 in MeOH).

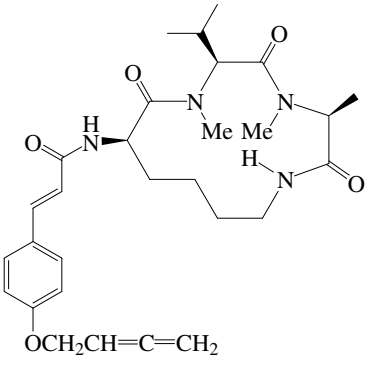
*4″-*O*-α-L-Rhamnopyranosyl:* ***Xestovanin C***
[137415-10-2]
$C_{48}H_{78}O_{16}$ 911.135
Constit. of *Xestospongia vanilla*. Glass. $[\alpha]_D$ -25 (c, 0.2 in MeOH).

17-Epimer, 10,27-didehydro: ***Epidehydroxestovanin A***
[137493-31-3]
$C_{42}H_{66}O_{12}$ 762.976
Constit. of *Xestospongia vanilla*. Pale yellow glass. $[\alpha]_D$ -3.8 (c, 3.8 in MeOH).

Northcote, P.T. *et al., J.A.C.S.*, 1989, **111**, 6276-6280 (*isol, pmr, cmr*)
Morris, S.A. *et al., Can. J. Chem.*, 1991, **69**, 1352 (*isol, pmr, cmr*)

Xyloallenolide A X-58

[329901-31-7]

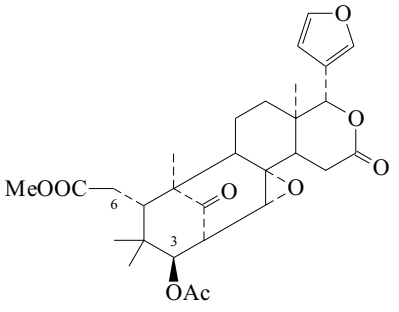


$C_{29}H_{40}N_4O_5$ 524.659
Isol. from *Xylaria* sp. No. 2508. Cryst.
Mp 82-85°. $[\alpha]_D^{25}$ -34.6 (c, 0.06 in $CHCl_3$). λ_{max} 217 (ϵ 38000); 291 (ϵ 29000) ($CHCl_3$).

Lin, Y. *et al., Tet. Lett.*, 2001, **42**, 449-451 (*isol, ir, pmr, cmr, uv*)

Xylocarpin X-59

[26808-27-5]



$C_{29}H_{36}O_9$ 528.598
Constit. of the seeds of *Xylocarpus granatum* and the fruits of *Ruagea glabra*. Shows antifeedant activity on *Spodoptera frugiperda* larvae. Cryst. (C_6H_6).
Mp 213-214°. $[\alpha]_D$ -88 ($CHCl_3$).

*6*R-*Hydroxy,* O-*de-Ac, 3*-O-*propanoyl:* ***Swietemahonin A***
[121825-44-3]
$C_{30}H_{38}O_{10}$ 558.624
Constit. of *Swietenia mahagoni*. Antagonist of platelet activating factor. Needles (EtOAc/diisopropyl ether).
Mp 174-174.5°. $[\alpha]_D$ -12.2 ($CHCl_3$).

*6*R-*Hydroxy,* O-*de-Ac, 3*-O-*tigloyl:* ***Swietemahonin E***
[121825-42-1]
$C_{32}H_{40}O_{10}$ 584.662
Constit. of *Swietenia mahagoni*. Antagonist of PAF. Needles (EtOAc/diisopropyl ether).
Mp 151-152°. $[\alpha]_D$ -20.7 ($CHCl_3$).

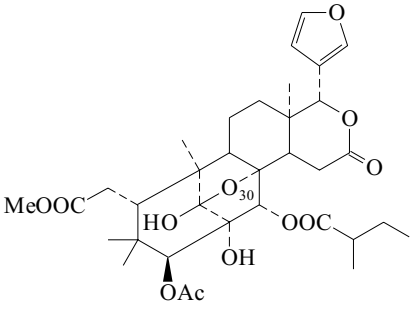
3-O-*De-Ac, 3*-O-*(2-methylpropanoyl):* ***Ruageanin A***
$C_{31}H_{40}O_9$ 556.652
Constit. of *Ruagea glabra* (Meliaceae). Shows antifeedant activity on *Spodoptera frugiperda* larvae. Amorph. solid.
$[\alpha]_D^{25}$ -63.9 (c, 0.74 in $CHCl_3$).

2-Hydroxy: ***Ruageanin C***
$C_{29}H_{36}O_{10}$ 544.597
Constit. of *Ruagea glabra*. Cryst. (MeOH).
Mp 217.5-219°. $[\alpha]_D^{25}$ -15.9 (c, 0.64 in $CHCl_3$).

3-O-*De-Ac, 3*-O-*tigloyl, 2-hydroxy:* ***Ruageanin B***
$C_{32}H_{40}O_{10}$ 584.662
Constit. of *Ruagea glabra*. Shows antifeedant activity on *Spodoptera frugiperda* larvae. Cryst. (MeOH/EtOAc).
Mp 227-229°. $[\alpha]_D^{25}$ -17.7 (c, 0.52 in $CHCl_3$).

Okorie, D.A. *et al., J.C.S.(C)*, 1970, 211 (*props, isol*)
Kodota, S. *et al., Tet. Lett.*, 1989, **30**, 1111 (*Swietemahonins*)
Mootoo, B.S. *et al., J. Nat. Prod.*, 1996, **49**, 544 (*Ruageanins, activity*)

Xyloccensin I X-60

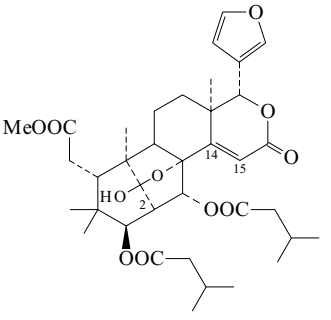


$C_{34}H_{46}O_{12}$ 646.73
Constit. of *Xylocarpus granatum* and *Xylocarpus moluccensis*. Needles (MeOH).
Mp 223-225°. $[\alpha]_D$ -105 (c, 0.06 in CH_2Cl_2).

30-O-*Deacyl, 30*-O-*(2-methylpropanoyl):* ***Xyloccensin J***
[139535-99-2]
$C_{33}H_{44}O_{12}$ 632.703
Constit. of *Xylocarpus granatum* and *Xylocarpus moluccensis*. Needles (MeOH).
Mp 213-215°. $[\alpha]_D$ -106 (c, 0.09 in CH_2Cl_2).
Alvi, K.A. *et al., Tetrahedron*, 1991, **47**, 8943 (*isol, pmr, cmr*)

Xyloccensin A X-61

[62660-19-9]



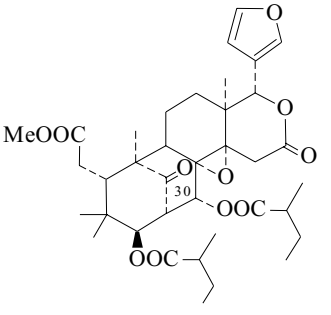
$C_{37}H_{50}O_{11}$ 670.795
Constit. of *Xylocarpus moluccensis*. Cryst. (MeOH).
Mp 221-223°.

14,15-Dihydro: ***Xyloccensin B***
[62660-20-2]
$C_{37}H_{52}O_{11}$ 672.811
Constit. of *Xylocarpus moluccensis*. Cryst. (MeOH).
Mp 154-160°.

2-Hydroxy: ***Xyloccensin D***. *2-Hydroxyxyloccensin A*
[62660-21-3]
$C_{37}H_{50}O_{12}$ 686.795
Constit. of *Xylocarpus moluccensis*. Cryst. (MeOH).
Mp 212-215°.

2-Hydroxy, 14,15-dihydro: ***Xyloccensin F***. *2-Hydroxyxyloccensin B*
[62660-22-4]
$C_{37}H_{52}O_{12}$ 688.811
Constit. of *Xylocarpus moluccensis*. Cryst.
Mp 237-239°.
Connolly, J.D. *et al., J.C.S. Perkin 1*, 1976, 1993

Xyloccensin G X-62

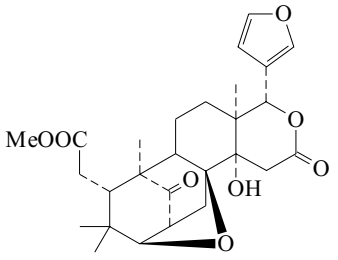


$C_{37}H_{50}O_{11}$ 670.795
Constit. of timber of *Xylocarpus moluccensis*. Cryst. (MeOH/CH_2Cl_2).
Mp 225-230°. Occurs as mixt. of isobutyrate and 2-methylbutyrate esters.

30-Deacyloxy: ***Xyloccensin H***
$C_{32}H_{42}O_9$ 570.678
Isol. from *Xylocarpus moluccensis*. Cryst. (MeOH/CH_2Cl_2).
Mp 200-205°.
Taylor, D.A.H. *et al., Phytochemistry*, 1983, **22**, 1297

Xyloccensin K X-63

[173693-50-0]

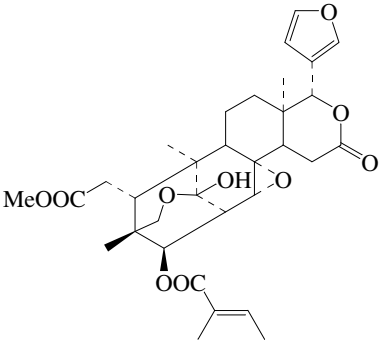


$C_{27}H_{34}O_8$ 486.561
Constit. of *Xylocarpus granatum*. Cryst. (EtOAc).
Mp 235-237°.

Kokpol, U. *et al., Phytochemistry*, 1996, **41**, 903 (*isol, pmr, cmr, cryst struct*)

Xyloccensin L X-64

[666216-93-9]

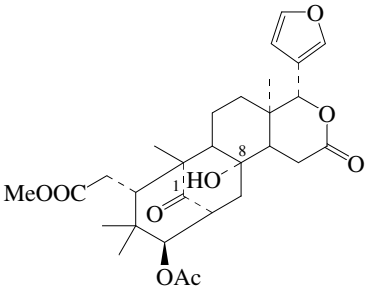


$C_{32}H_{40}O_{10}$ 584.662
Constit. of *Xylocarpus granatum*. Amorph. solid.
Mp 110-112°. $[\alpha]_D^{25}$ -56 (c, 0.6 in Me_2CO).

Wu, J. *et al., Tet. Lett.*, 2004, **45**, 591-593 (*isol, pmr, cmr*)

Xyloccensin N X-65

[758694-87-0]

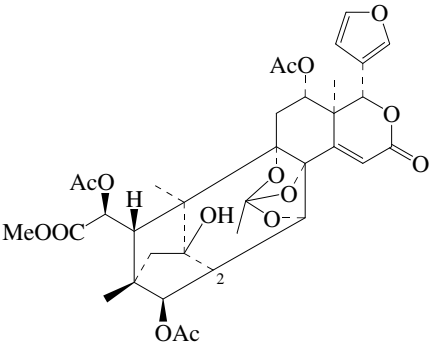


$C_{29}H_{38}O_9$ 530.614
Constit. of *Xylocarpus granatum*. Amorph. powder. $[\alpha]_D^{25}$ +10 (c, 0.5 in Me_2CO).

8→1 Hemiacetal: ***Xyloccensin M***
[758694-85-8]
$C_{29}H_{38}O_9$ 530.614
Constit. of *Xylocarpus granatum*. Amorph. powder. $[\alpha]_D^{25}$ -88 (c, 0.8 in Me_2CO).
Wu, J. *et al., Z. Naturforsch., B*, 2003, **58**, 1216-1219 (*isol, pmr, cmr*)

Xyloccensin O X-66

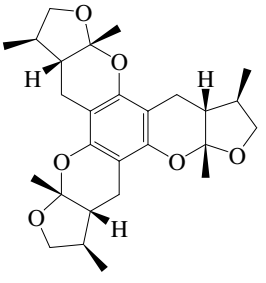
[713500-19-7]



$C_{35}H_{40}O_{15}$ 700.692
Constit. of *Xylocarpus granatum*. Cryst. $[\alpha]_D^{25}$ -22 (c, 0.8 in Me_2CO). λ_{max} 214 (MeCN).

2α-Acetoxy: ***Xyloccensin P***
[713500-21-1]
$C_{37}H_{42}O_{17}$ 758.729
Constit. of *Xylocarpus granatum*. Amorph. powder. $[\alpha]_D^{25}$ -36 (c, 0.6 in Me_2CO). λ_{max} 214 (MeCN).
Wu, J. *et al., Org. Lett.*, 2004, **6**, 1841-1844 (*isol, pmr, cmr, cryst struct*)

Xyloketal A X-67

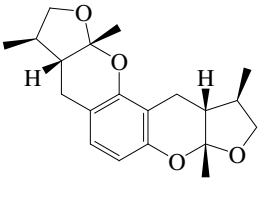


Absolute Configuration

$C_{27}H_{36}O_6$ 456.578
Prod. by the mangrove fungus *Xylaria* sp. No. 2508. Acetylcholinesterase inhibitor. Cryst.
Mp 164-166°. $[\alpha]_D^{25}$ -4.9 (c, 0.2 in $CHCl_3$). λ_{max} 222 (ϵ 14370); 224 (ϵ 14300); 228 (ϵ 14000) ($CHCl_3$).

Lin, Y.C. *et al., J.O.C.*, 2001, **66**, 6252-6256 (*isol, pmr, cmr, cryst struct*)
Krohn, K. *et al., Eur. J. Org. Chem.*, 2004, 1261-1270 (*synth, pmr, cmr*)
Pettigrew, J.D. *et al., Org. Lett.*, 2006, **8**, 1427-1429 (*synth*)

Xyloketal B X-68

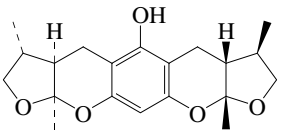


Absolute Configuration

$C_{20}H_{26}O_4$ 330.423
Prod. by the mangrove fungus *Xylaria* sp. No. 2508. Waxy solid.
Mp 84-86°. $[\alpha]_D^{25}$ +8.2 (c, 0.06 in $CHCl_3$). λ_{max} 215 (ϵ 68790); 228 (ϵ 41620); 274 (ϵ 9830) ($CHCl_3$).

Lin, Y.C. *et al., J.O.C.*, 2001, **66**, 6252-6256 (*isol, pmr, cmr, cryst struct*)
Krohn, K. *et al., Eur. J. Org. Chem.*, 2004, 1261-1270 (*synth, pmr, cmr*)

Xyloketal C X-69

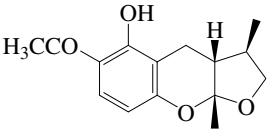


Absolute Configuration

$C_{20}H_{26}O_5$ 346.422
Prod. by the mangrove fungus *Xylaria* sp. No. 2508. Needles. $[\alpha]_D^{25}$ -52.4 (c, 0.04 in $CHCl_3$). Mp >260°. λ_{max} 215 (ϵ 15060); 227 (ϵ 9760); 275 (ϵ 1515) ($CHCl_3$).

Lin, Y.C. *et al., J.O.C.*, 2001, **66**, 6252-6256 (*isol, pmr, cmr, cryst struct*)

Xyloketal D X-70

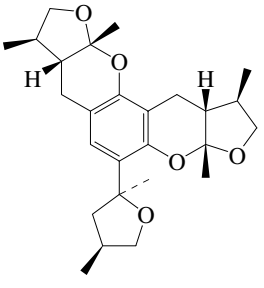


Absolute Configuration

$C_{15}H_{18}O_4$ 262.305
Prod. by the mangrove fungus *Xylaria* sp. No. 2508. Cryst. Mp 111-113°. $[\alpha]_D^{25}$ -119.5 (c, 0.11 in $CHCl_3$). λ_{max} 220 (ϵ 17450); 228 (ϵ 10720); 280 (ϵ 18040); 307 (ϵ 8770) ($CHCl_3$).

Lin, Y.C. *et al., J.O.C.*, 2001, **66**, 6252-6256 (*isol, cd, pmr, cmr, cryst struct*)
Krohn, K. *et al., Eur. J. Org. Chem.*, 2004, 1261-1270 (*synth, pmr, cmr*)
Pettigrew, J.D. *et al., Heterocycles*, 2004, **62**, 445-452 (*synth*)

Xyloketal E X-71

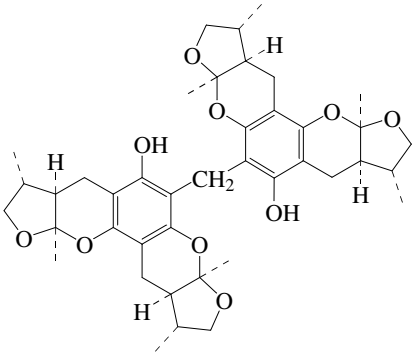


Absolute Configuration

$C_{26}H_{36}O_5$ 428.567
Prod. by the mangrove fungus *Xylaria* sp. No. 2508. Cryst. Mp 170-172°. $[\alpha]_D^{25}$ +5.3 (c, 0.37 in $CHCl_3$). λ_{max} 216 (ϵ 17510); 226 (ϵ 11390); 273 (ϵ 1450) ($CHCl_3$).

Lin, Y.C. *et al., J.O.C.*, 2001, **66**, 6252-6256 (*isol, pmr, cmr, cryst struct*)

Xyloketal F X-72

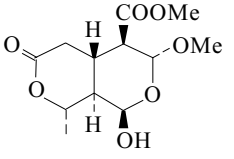


$C_{41}H_{52}O_{10}$ 704.856
Prod. by the mangrove fungus *Xylaria* sp. L-Calcium channel blocker. Needles (EtOAc/petrol).
Mp 160-162°. $[\alpha]_D^{25}$ -50.6 (c, 0.2 in MeOH). λ_{max} 226 (ϵ 15410); 273 (ϵ 2475) (MeOH).

Wu, X.-Y. *et al., Eur. J. Org. Chem.*, 2005, 4061-4064 (*isol, pmr, cmr, cryst struct*)

Xylomollin X-73

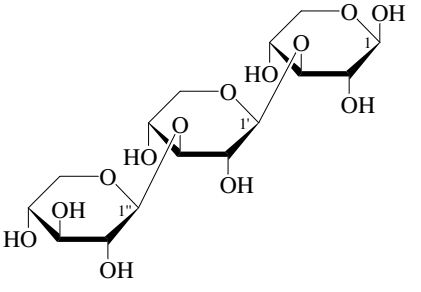
[61229-34-3]



$C_{12}H_{18}O_7$ 274.27
Constit. of the fruits of *Xylocarpus moluccensis*. Cryst. (EtOH). Mp 138-139°.

Kubo, I. *et al., J.A.C.S.*, 1976, **98**, 6704 (*isol*)
Nakare, M. *et al., J.A.C.S.*, 1978, **100**, 7079 (*cryst struct*)
Whitesell, J.K. *et al., J.O.C.*, 1983, **48**, 2511 (*synth*)
Whitesell, J.K. *et al., J.A.C.S.*, 1986, **108**, 6802 (*synth*)

β-D-Xylopyranosyl-(1 →3)-β-D-xylopyranosyl-(1 →3)-D-xylose, 9CI X-74



β-Pyranose-*form*

$C_{15}H_{26}O_{13}$ 414.363
Constit. of the cell walls of *Penicillus dumetosus*, *Rhodymenia palmata* and several other green algae.

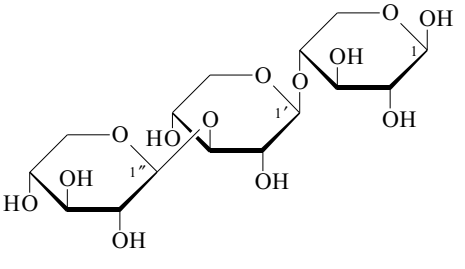
β-Pyranose-*form*

1,2,2′,2″,4,4′,4″-Hepta-Ac: [98264-08-5]
$C_{29}H_{40}O_{20}$ 708.623
Cryst. Mp 213°. $[\alpha]_D^{20}$ -70 (c, 1.0 in $CHCl_3$).

Percival, E.G.V. *et al., Nature (London)*, 1950, **166**, 787 (*isol*)
Freietal, E. *et al., Proc. R. Soc. London, B*, 1964, **160**, 293 (*occur*)
Dupeyre, D. *et al., Carbohydr. Res.*, 1984, **135**, C1 (*isol, hepta-Ac, pmr, cmr*)

β-D-Xylopyranosyl-(1 →3)-β-D-xylopyranosyl-(1 →4)-D-xylose, 9CI X-75

[32581-42-3]



$C_{15}H_{26}O_{13}$ 414.363

Obt. by the action of endoxylanases from *Cryptococcus albidus* and *Streptomyces* on Rhodymenan, a water sol. xylan isol. from the marine alga *Rhodymenia palmata*; also by action of β-xylosidase from *Penicillium wortmanni* IFO 7237 on β(1→4) xylobiose. Cryst.
Mp 224-225°. $[\alpha]_D^{20}$ -46 (c, 1.0 in H_2O) (-44.6°).

β-Pyranose-*form*

Me glycoside: [73654-66-7]
$C_{16}H_{28}O_{13}$ 428.389
Cryst. (MeOH). Mp 197-204°. $[\alpha]_D^{22}$ -82 (c, 1.0 in H_2O).

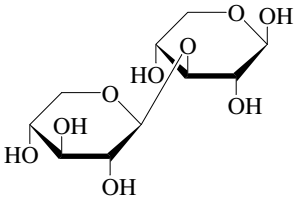
Me glycoside, hepta-Ac: [73654-64-5]
$C_{30}H_{42}O_{20}$ 722.65
Plates (MeOH). Mp 147-149°. $[\alpha]_D^{22}$ -99 (c, 1.0 in $CHCl_3$).

Me glycoside, hepta-Me: [73654-68-9]
$C_{23}H_{42}O_{13}$ 526.577
Cryst. (diisopropyl ether/hexane). Mp 106-107°. $[\alpha]_D^{22}$ -83.6 (c, 1.0 in $CHCl_3$).

Howard, B. *et al., Biochem. J.*, 1957, **67**, 643 (*enzymic synth*)
Kovac, P. *et al., Carbohydr. Res.*, 1980, **79**, 303 (*β-Me pyr derivs, pmr*)
Biely, P. *et al., Eur. J. Biochem.*, 1983, **129**, 645 (*cmr*)
Biely, P. *et al., J. Bacteriol.*, 1984, **160**, 408
Chen, W.P. *et al., Agric. Biol. Chem.*, 1986, **50**, 1183; 1195 (*enzymic synth*)
Win, M. *et al., Agric. Biol. Chem.*, 1988, **52**, 1151 (*enzymic synth, hplc*)

3-*O*-β-D-Xylopyranosyl-D-xylose X-76

Rhodymenabiose



β-Pyranose-*form*

$C_{10}H_{18}O_9$ 282.247
Isol. from a partial enzymatic hydrolysate of the seaweed polysaccharide rhodymenan from *Rhodymenia palmata*.
Mp 192-193°. $[\alpha]_D$ -22 (H_2O).

Phenylosazone: Mp 194-196°. $[\alpha]_D$ +47 (H_2O).

β-Pyranose-*form*

*Me glycoside: Methyl 3-*O*-β-D-xylopyranosyl-β-D-xylopyranoside*
[74405-67-7]
$C_{11}H_{20}O_9$ 296.274
Cryst. (2-propanol). Mp 161-162°. $[\alpha]_D^{22}$ -72 (c, 1.0 in H_2O).

*Me glycoside, penta-Ac: Methyl 2,4-di-*O*-acetyl-3-*O*-(2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl)-β-D-xylopyranoside*
[74405-65-5]
$C_{21}H_{30}O_{14}$ 506.46
Mp 131-132°. $[\alpha]_D^{22}$ -93 (c, 1.0 in $CHCl_3$).

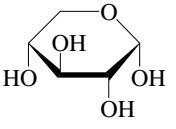
*Me glycoside, penta-Me: Methyl 2,4-di-*O*-methyl-3-*O*-(2,3,4-tri-*O*-methyl-β-D-xylopyranosyl)-β-D-xylopyranoside*
[74405-69-9]
$C_{16}H_{30}O_9$ 366.408
Cryst. (hexane). Mp 60-61°. $[\alpha]_D^{22}$ -73.7 (c, 1.0 in $CHCl_3$).

*Benzyl glycoside, 2′,3′,4′-tri-Ac: Benzyl 3-*O*-(2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl)-β-D-xylopyranoside*
$C_{23}H_{30}O_{12}$ 498.483
Mp 173-174.5°. $[\alpha]_D$ +47 ($CHCl_3$).

Howard, B.H. *et al., Biochem. J.*, 1957, **67**, 643; 1960, **74**, 173 (*isol, synth*)
Curtis, E.J.C. *et al., Can. J. Chem.*, 1960, **38**, 1305 (*synth*)
Ferrier, R.J. *et al., J.C.S.*, 1965, 7429 (*benzyl glycoside*)
Kovac, P. *et al., Coll. Czech. Chem. Comm.*, 1980, **45**, 892 (*Me glycoside*)

Xylose, 9CI, 8CI, USAN X-77

Wood sugar. Losan. Xylomed. Xylo-Pfan. FEMA 3606



α-D-Pyranose-*form*

$C_5H_{10}O_5$ 150.131
An aq. soln. at 31° contains 36.5% α-pyr, 63% β-pyr,

β-D-Pyranose-*form* [2460-44-8]

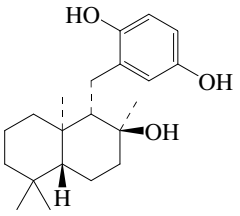
Hexadecyl glycoside: Hexadecyl β-D-xylopyranoside. Cetyl β-D-xylopyranoside
[115211-19-3]
$C_{21}H_{42}O_5$ 374.56
Constit. of the red alga *Laurencia karlae*. Solid.
Mp 94-95°. $[\alpha]_D$ -25 (c, 0.03 in $CHCl_3$).

[3154-36-7, 41546-29-6, 41546-30-9]

Zhong, Y.-L. *et al., CA*, 1996, **124**, 170194n (*hexadecyl glycoside*)

Yahazunol Y-1

[69809-36-5]



Absolute Configuration

$C_{21}H_{32}O_3$ 332.482
Constit. of *Dictyopteris undulata*. Cryst. (Me_2CO/Et_2O).
Mp 127-129°. $[\alpha]_D^{27}$ -12 (c, 0.1 in $CHCl_3$). λ_{max} 211 (ϵ 8400); 295 (ϵ 3150) (MeOH) (Derep).

ent-form
ent-*Yahazunol*
[852945-54-1]
Constit. of a *Dysidea* sp.
Oil. $[\alpha]_D^{25}$ +11.8 (c, 0.1 in $CHCl_3$).

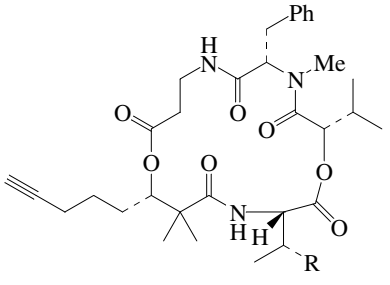
Ochi, N. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 629-630 (*isol, ir, pmr*)
Laube, T. *et al., Tetrahedron*, 2002, **58**, 4299-4309 (*synth*)
Pérez-Garcia, E. *et al., J. Nat. Prod.*, 2005, **68**, 653-658 (*ent-form*)

YAIVARPRF amide Y-2

Peptide tyrosine-phenylalanine
[144527-25-3]
Tyr-Ala-Ile-Val-Ala-Arg-Pro-Arg-Phe-NH_2
$C_{52}H_{82}N_{16}O_{10}$ 1091.321
Isol. from brain extracts of the squid *Loligo vulgaris*. Neuropeptide.

Smart, D. *et al., Biochem. Biophys. Res. Commun.*, 1992, **186**, 1616-1623 (*isol*)

Yanucamide A Y-3



R = CH_3

$C_{33}H_{47}N_3O_7$ 597.75
Depsipeptide. Stereochem. revised in 2003. Isol. from an assemblage of *Lyngbya majuscula* and a *Schizothrix* sp. Amorph. solid. $[\alpha]_D^{20}$ -33 (c, 0.1 in MeOH). λ_{max} 204 (ϵ 13000) (MeOH).

Sitachitta, N. *et al., J. Nat. Prod.*, 2000, **63**, 197-200 (*isol, pmr, cmr*)
Xu, Z. *et al., Org. Lett.*, 2003, **5**, 2821-2824 (*synth, abs config*)

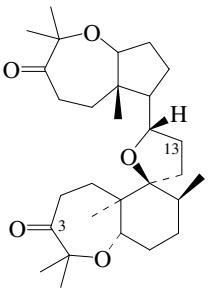
Yanucamide B Y-4

As Yanucamide A, Y-3 with
R = CH_2CH_3
$C_{34}H_{49}N_3O_7$ 611.777
Isol. from an assemblage of *Lyngbya majuscula* and a *Schizothrix* sp. Amorph. solid. $[\alpha]_D^{20}$ -31 (c, 0.1 in MeOH). λ_{max} 204 (ϵ 13000) (MeOH).

Sitachitta, N. *et al., J. Nat. Prod.*, 2000, **63**, 197-200 (*isol, pmr, cmr*)

Yardenone Y-5

[205750-25-0]



$C_{30}H_{48}O_5$ 488.706
Constit. of *Ptilocaulis spiculifer*.
$[\alpha]_D^{25}$ +2.38 (c, 1.05 in MeOH).

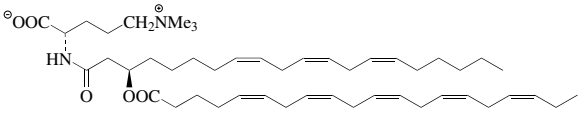
3α-Alcohol: ***Yardenone B***
[487016-98-8]
$C_{30}H_{50}O_5$ 490.722
Constit. of *Axinella* cf. *bidderi*. Cryst. $[\alpha]_D^{25}$ +2.38 (c, 1.05 in MeOH).

13β-Hydroxy: ***Yardenone A***
[487016-96-6]
$C_{30}H_{48}O_6$ 504.706
Constit. of *Axinella* cf. *bidderi*. Cryst. $[\alpha]_D^{25}$ +5.2 (c, 0.27 in MeOH).

Rudi, A. *et al., Tet. Lett.*, 1998, **39**, 1445-1448 (*isol, pmr, cmr, cryst struct*)
Carletti, I. *et al., J. Nat. Prod.*, 2003, **66**, 25-29 (*Yardenones A-B*)

Yendolipin Y-6

[160041-37-2]

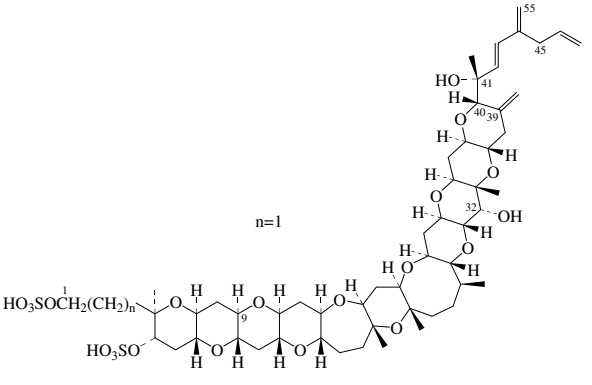


$C_{48}H_{78}N_2O_5$ 763.155
Lipobetaine. Isol. from the red alga *Neodilsea yendoana*. Pale yellow oil. $[\alpha]_D^{25}$ +6.7 (c,1 in CHCl3).

Ishida, R. *et al., Chem. Lett.*, 1994, 2427 (*isol, pmr, cmr*)
Matsuo, Y. *et al., Tetrahedron*, 1997, **53**, 869 (*isol, ir, pmr, cmr, ms*)

Yessotoxin Y-7

YTX
[112514-54-2]



$C_{55}H_{82}O_{21}S_2$ 1143.372
Toxic constit. of scallops (*Patinopecten yessoensis*) and mussels (*Mytilus galloprovincialis*), also *Protoceratium reticulatum* and *Gonyaulax spinifera*. Amorph. solid (as di-Na salt). Sol. MeOH,

butanol. $[\alpha]_D^{20}$ +3.01 (c, 0.45 in MeOH). λ_{max} 230 (ϵ 10600) (MeOH) (Derep).

▶ Toxic. LD_{50} (mus, ipr) 0.1 mg/kg. ZF9109000

1-Desulfo: ***1-Desulfoyessotoxin***
[255041-59-9]
$C_{55}H_{82}O_{18}S$ 1063.308
Isol. from mussels.

*32-*O*-β-D-Arabinofuranoside:* ***Glycoyessotoxin A***
$C_{60}H_{90}O_{25}S_2$ 1275.488
Isol. from *Protoceratium reticulatum*. Amorph. solid (as di-Na salt). $[\alpha]_D^{25}$ -6 (c, 0.29 in $CHCl_3$).

*32-*O*-[β-L-Arabinofuranosyl-(1→5)-β-L-arabinofuranoside]:*
$C_{65}H_{98}O_{29}S_2$ 1407.604
Isol. from *Protoceratium reticulatum*.

*45*R*-Hydroxy:* ***45-Hydroxyyessotoxin***
[124863-39-4]
$C_{55}H_{82}O_{22}S_2$ 1159.372
Constit. of toxic scallops *Patinopecten yessoensis* and mussels *Mytilus galloprovincialis*. Amorph. solid. λ_{max} 230 (ϵ 15600) (MeOH).

▶ LD_{50} (mus, ipr) 0.5 mg/kg.

44,55-Dihydro, 44ξ,55-dihydroxy: ***44,55-Dihydroxyyessotoxin***
[862783-86-6]
$C_{55}H_{84}O_{23}S_2$ 1177.387
Isol. from *Protoceratium reticulatum*.

*44-Demethylene, 44*R*-carboxy:* ***Carboxyyessotoxin***
[262842-91-1]
$C_{55}H_{82}O_{23}S_2$ 1175.371
Constit. of the mussel *Mytilus galloprovincialis*. Amorph. (as di-Na salt).

*44-Demethylene, 44*R*-carboxy, 45-hydroxy:* ***45-Hydroxycarboxyyessotoxin***
$C_{55}H_{82}O_{24}S_2$ 1191.37
Isol. from *Mytilus edulis*.

46,47-Dinor, 45-hydroxy: ***46,47-Dinor-45-hydroxyyessotoxin***.
45-Hydroxy-46,47-dinoryessotoxin
$C_{53}H_{80}O_{22}S_2$ 1133.334
Isol. from *Protoceratium reticulatum*.

45,46,47-Trinor: ***45,46,47-Trinoryessotoxin***
[181365-95-7]
$C_{52}H_{78}O_{21}S_2$ 1103.308
Constit. of the scallop (*Patinopecten yessoensis*). Amorph. solid. Lacks the 3 terminal carbons from the C-7 end chain, i.e. terminal group is 1-hydroxy-1-methyl-2,4-pentadienyl. λ_{max} 226 (ϵ 22600) (MeOH).

▶ Toxic; LD_{50} (mus, ipr) 0.22 mg/kg.

45,46,47-Trinor, 44,45-dihydro, 44-oxo: ***45,46,47-Trinor-44-oxoyessotoxin***
$C_{52}H_{78}O_{22}S_2$ 1119.307
Isol. from *Protoceratium reticulatum*.

42,43,44,45,46,47,55-Heptanor, 41-ketone: ***42,43,44,45,46,47,55-Heptanor-41-oxoyessotoxin***
[448238-76-4]
$C_{48}H_{72}O_{21}S_2$ 1049.216
Isol from *Mytilus galloprovincialis* and *Protoceratium reticulatum*.

42,43,44,45,46,47,55-Heptanor, $\Delta^{39,40}$-isomer, 41-ketone: ***Yessotoxin enone***
[803745-67-7]
$C_{48}H_{72}O_{21}S_2$ 1049.216
Isol. from *Protoceratium reticulatum*.

42,43,44,45,46,47,55-Heptanor, 40-epimer, 41-ketone: ***40-Epi-42,43,44,45,46,47,55-heptanor-41-oxoyessotoxin***
[803745-66-6]
$C_{48}H_{72}O_{21}S_2$ 1049.216
Isol. from *Protoceratium reticulatum*. Tentative identification.

42,43,44,45,46,47,55-Heptanor, 9-methyl, $\Delta^{39,40}$-isomer, 41-ketone: ***9-Methylyessotoxin enone***
$C_{49}H_{74}O_{21}S_2$ 1063.243
Isol. from *Protoceratium reticulatum*.

Homologue (n = 2): ***1a-Homoyessotoxin***. *Protoceratin I*
[196309-94-1]
$C_{56}H_{84}O_{21}S_2$ 1157.399
Isol. from mussels and *Protoceratium reticulatum*. Cytotoxic. Amorph. solid (as di-Na salt). $[\alpha]_D^{20}$ -5.5 (c, 1 in MeOH) (di-Na salt). λ_{max} 231 (log ϵ 4.29) (MeOH).

*Homologue (n = 2), 32-*O*-β-L-arabinofuranoside:* ***Protoceratin III***
$C_{61}H_{92}O_{25}S_2$ 1289.515
Isol. from *Protoceratium reticulatum*. Cytotoxic.

*Homologue (n = 2), 32-*O*-[β-L-arabinofuranosyl-(1→5)-β-L-arabinofuranoside]:* ***Protoceratin II***
$C_{66}H_{100}O_{29}S_2$ 1421.631
Isol. from *Protoceratium reticulatum*. Cytotoxic. $[\alpha]_D^{20}$ +12.1 (c, 0.2 in MeOH). λ_{max} 230 (log ϵ 4.24) (MeOH).

*Homologue (n = 2), 32-*O*-[β-L-arabinofuranosyl-(1→5)-β-L-arabinofuranosyl-(1→5)-β-L-arabinofuranoside]:* ***Protoceratin IV***
$C_{71}H_{108}O_{33}S_2$ 1553.746
Isol. from *Protoceratium reticulatum*. Cytotoxic.

Homologue (n = 2), 45-hydroxy: ***45-Hydroxy-1a-homoyessotoxin***
[196309-97-4]
$C_{56}H_{84}O_{22}S_2$ 1173.398
Constit. of *Mytilus* sp.

*Homologue (n = 2), 44-demethylene, 44*R*-carboxy:* ***Carboxy-1a-homoyessotoxin***
[292850-13-6]
$C_{56}H_{84}O_{23}S_2$ 1189.398
Isol. from Adriatic mussels.

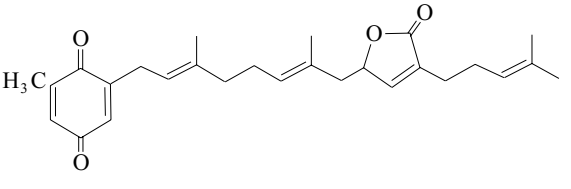
Homologue (n = 2), 41-de(3-methylene-1,5-hexadienyl), 41-ketone: ***42,43,44,45,46,47,55-Heptanor-41-oxo-1a-homoyessotoxin***
[346631-41-2]
$C_{49}H_{74}O_{21}S_2$ 1063.243
Isol. from *Mytilus galloprovincialis*.

[112574-50-2]

Murata, M. *et al., Tet. Lett.*, 1987, **28**, 5869-5872 (*isol, struct*)
Kumagai, M. *et al., CA*, 1988, **108**, 70214v (*isol, struct*)
Naoki, H. *et al., Rapid Commun. Mass Spectrom.*, 1993, **7**, 179 (*ms*)
Satake, M. *et al., Tet. Lett.*, 1996, **37**, 5955-5958 (*Trinoryessotoxin, 45-Hydroxyyessotoxin, config*)
Takahashi, H. *et al., Tet. Lett.*, 1996, **37**, 5955-5958; 7087-7090 (*abs config*)
Yasumoto, T. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1775-1777 (*hplc*)
Satake, M. *et al., Nat. Toxins*, 1997, **5**, 107-110; 164-167; 1998, **6**, 235-239 (*1-Desulfoyessotoxin, 2-Homoyessotoxin, 45-Hydroxy-1a-homoyessotoxin*)
Morohashi, A. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1761-1763 (*45-Hydroxyyessotoxin, abs config*)
Ciminiello, P. *et al., Chem. Res. Toxicol.*, 2000, **13**, 770-774; 2001, **14**, 596-599; 2002, **15**, 979-984 (*Carboxy-1a-homoyessotoxin, Noroxoyessotoxins*)
Ciminiello, P. *et al., Eur. J. Org. Chem.*, 2000, 291-295 (*Carboxyyessotoxin*)
Food Sci. Technol., Seafood and Freshwater Toxins, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**, (*rev*)
Ciminiello, P. *et al., Pure Appl. Chem.*, 2003, **75**, 325-336 (*rev*)
Ciminiello, P. *et al., Toxicon*, 2003, **42**, 7-14 (*Heptanoroxoyessotoxin*)
Ciminiello, P. *et al., Eur. J. Org. Chem.*, 2004, 2533-2551 (*rev*)
Konishi, M. *et al., J. Nat. Prod.*, 2004, **67**, 1309-1313 (*Protoceratins*)
Miles, C.O. *et al., Toxicon*, 2004, **44**, 325-336; 2005, **45**, 265-272; 2006, **47**, 229-240; 510-516 (*Yessotoxin enone, 45-Hydroxycarboxyyessotoxin, Trinoroxoyessotoxin, Dinorhydroxyyessotoxin, 9-Methylyessotoxin enone, 32-arabinosylarabinoside*)
Souto, M.L. *et al., J. Nat. Prod.*, 2005, **68**, 420-422 (*Glycoyessotoxin A*)
Finch, S.C. *et al., Toxicon*, 2005, **46**, 160-170 (*4S,5S-Dihydroxyyessotoxin*)
Rhodes, L. *et al., Harmful Algae*, 2006, **5**, 148-155 (*isol*)

Yezoquinolide Y-8

[110359-99-4]



$C_{27}H_{34}O_4$ 422.563

Plastoquinone constit. of brown alga *Sargassum sagamianum* var. *yezoense*. Pale-yellow oil. $[\alpha]_D^{24}$ -23.5 (c, 0.52 in $CHCl_3$). λ_{max} 252 (ϵ 17000) (MeOH) (Berdy).

Segawa, M. *et al., Chem. Lett.*, 1987, 1365

YIRF amide Y-9

[180048-91-3]

H-Tyr-Ile-Arg-Phe-NH_2

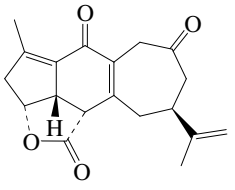
$C_{30}H_{44}N_8O_5$ 596.728

Isol. from the marine turbellarian *Bdelloura candida*. Neuropeptide.

Johnston, R.N. *et al., J. Neurochem.*, 1996, **67**, 814 (*isol, struct, props*)

Yonarolide Y-10

[171440-23-6]



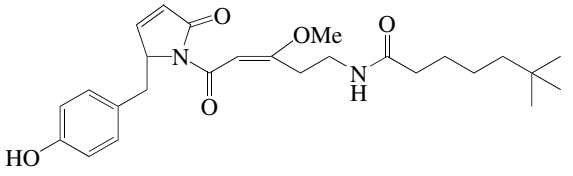
$C_{19}H_{20}O_4$ 312.365

Constit. of an Okinawan soft coral *Sinularia* sp. Pale yellow oil. $[\alpha]_D$ -109.2 (c, 0.13 in $CHCl_3$).

Iguchi, K. *et al., Tet. Lett.*, 1995, **36**, 8807-8808 (*isol, pmr, cmr*)

Ypaoamide Y-11

[180965-25-7]



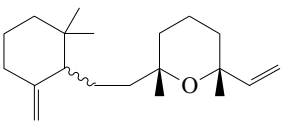
$C_{26}H_{36}N_2O_5$ 456.581

Isol. from a mixed cyanobacteria assemblage, actual source believed to be *Lyngbya majuscula*. Feeding deterrent. Ichthyotoxic. $[\alpha]_D^{19}$ +197 (c, 1.0 in $CHCl_3$). λ_{max} 222 (log ϵ 4.2); 270 (log ϵ 4.1) (MeOH).

Nagle, D.G. *et al., Tet. Lett.*, 1996, **37**, 6263 (*isol, uv, ir, pmr, cmr, struct*)

Zaatirin Z-1

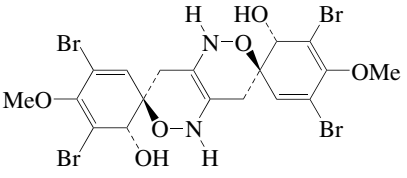
10,15-Cyclo-3,7-epoxy-1,11(18)-phytadiene
[145458-10-2]



$C_{20}H_{34}O$ 290.488
Constit. of *Chelonaplysilla erecta*. Oil.

Rudi, A. *et al., J. Nat. Prod.*, 1992, **55**, 1408-1414 (*isol, pmr, cmr*)

Zamamistatin Z-2



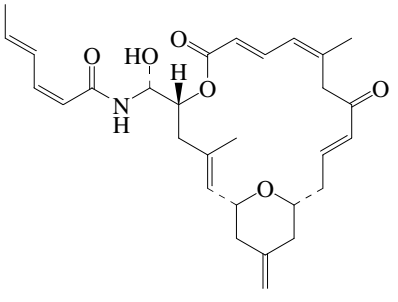
$C_{18}H_{18}Br_4N_2O_6$ 677.966

Struct. revised in 2006. Isol. from the sponge *Pseudoceratina purpurea*. Antibacterial agent. $[\alpha]_D^{29}$ +248 (c, 0.01 in $CHCl_3$).

Takada, N. *et al., Tet. Lett.*, 2001, **42**, 5265-5267 (*isol, pmr, cmr, abs config*)
Hayakawa, I. *et al., Tet. Lett.*, 2006, **47**, 155-158 (*cmr, struct*)

Zampanolide Z-3

[179730-36-0]



Absolute Configuration

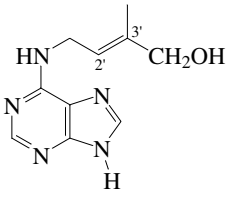
$C_{29}H_{37}NO_6$ 495.614

Macrolide antibiotic. Isol. from the sponge *Fasciospongia rimosa*. Cytotoxic agent. Amorph. solid. $[\alpha]_D^{29}$ -101 (c, 0.1 in CH_2Cl_2). λ_{max} 230 (ϵ 25000); 264 (ϵ 30000) (MeOH).

Tanaka, J. *et al., Tet. Lett.*, 1996, **37**, 5535-5538 (*isol, uv, ir, pmr, cmr*)
Smith, A.B. *et al., J.A.C.S.*, 2002, **124**, 11102-11113 (*synth, abs config*)
Hoye, T.R. *et al., J.A.C.S.*, 2003, **125**, 9576-9577 (*synth*)

Zeatin Z-4

*2-Methyl-4-(1*H*-purin-6-ylamino)-2-buten-1-ol, 9CI. 6-(4-Hydroxy-3-methyl-2-butenylamino)purine.* N^6*-(ω-Hydroxyisopentenyl)adenine*
[13114-27-7]



(*E*)-*form*

$C_{10}H_{13}N_5O$ 219.246

(*E*)-*form* [1637-39-4]

Isol. from sweet corn *Zea mays* (Gramineae) and numerous other plants. Also from algae, bacteria and basidiomycetes. Induces cell division; most effective of all known natural cytokinins. Sol. H_2O. Mp 212-213° (207-208°). λ_{max} 212 (ϵ 17050); 270 (ϵ 16150) (H_2O) (Berdy). λ_{max} 207 (ϵ 14500); 275 (ϵ 14650) (HCl) (Berdy). λ_{max} 220 (ϵ 15900); 276 (ϵ 14650) (NaOH) (Berdy).

▶ EM9506000

Picrate: Mp 180-190°.

O-*β-D-Glucopyranoside:* [56329-06-7]
$C_{16}H_{23}N_5O_6$ 381.388
Isol. from *Lupinus angustifolius* and other plants. Cryst. (1-butanol).
Mp 124-128°.

O-*Ac:* Mp 168-169°.

7-β-D-Glucopyranosyl: ***Raphanatin***
[38165-56-9]
$C_{16}H_{23}N_5O_6$ 381.388
Prod. by *Raphanus sativus* (radish) and crown galls of *Vinca rosea*. Cytokinin. Cryst. (MeOH).
Mp 266-271° (dec.). $[\alpha]_D^{26}$ -14.8 (c, 3.5 in DMSO).

9-β-D-Glucopyranosyl: [51255-96-0]
$C_{16}H_{23}N_5O_6$ 381.388
Cytokinin, widely distributed in plants. λ_{max} 269 (no solvent reported).

9-β-D-Ribofuranosyl: 9-(β-D-Ribofuranosyl)zeatin. Ribosylzeatin
[6025-53-2]
$C_{15}H_{21}N_5O_5$ 351.361
Isol. from many plants incl. bacteria. Cytokinin, phytotoxin, plant hormone. Sol. H_2O.
Mp 180-182°. λ_{max} 265 (ϵ 19200) (pH 1 H_2O) (Derep). λ_{max} 269 (ϵ 19400) (pH 13 H_2O) (Derep). λ_{max} 270 (ϵ 18400) (95% EtOH) (Derep).

9-β-D-Ribofuranosyl, 5″-phosphate: Ribosylzeatin phosphate
[25615-16-1]
[15075-52-2]
$C_{15}H_{22}N_5O_8P$ 431.341
Isol. from *Zea mays* (sweet corn). Cytokinin. Solid.

9-β-D-Ribofuranosyl, O-*β-D-glucopyranoside:* [62512-97-4]
$C_{21}H_{31}N_5O_{10}$ 513.503
Cytokinin, widely distributed in plants. No phys. props. accessible.

9-β-D-Ribofuranosyl, O-*[α-L-arabinopyranosyl-(1→4)-[β-D-galactopyranosyl-(1→2)-α-D-galactopyranosyl-(1→3)-α-L-arabinofuranosyl-(1→3)]-β-D-galactopyranoside]:* ***Gazer***
[171628-14-1]
$C_{43}H_{67}N_5O_{28}$ 1102.019
Constit. of coconut milk (*Cocos nucifera*). Cytokinin. $[\alpha]_D^{25}$ -5.2 (c, 1 in H_2O). λ_{max} 210 (ϵ 16600); 267 (ϵ 18200) (H_2O).

9-(2-Deoxy-β-D-ribofuranosyl): ***Zeatin 2-deoxyribofuranoside****. 2′-Deoxyzeatin riboside*
[124325-91-3]
$C_{15}H_{21}N_5O_4$ 335.362
Prod. by *Pseudomonas amygdali*. Cytokinin. Inhibitor of DNA polymerase I. Oil. $[\alpha]_D^{25}$ -13.5 (c, 0.35 in EtOH).

*2′,3′*S-*Dihydro: 2-Methyl-4-(1*H*-purin-6-ylamino)-1-butanol, 9CI. 6-[(4-Hydroxy-3-methylbutyl)amino]purine.* ***Dihydrozeatin***
[19272-91-4]
[23599759 general -no-.]
$C_{10}H_{15}N_5O$ 221.261
Cytokinin from immature *Lupinus luteus* seeds (Leguminosae). Constit. of numerous plant spp. Present in the brown alga *Sargassum heterophyllum*. Prisms (EtOH/MeCN).
Mp 165-166° (154-156°). $[\alpha]_D^{21}$ -12.1 (MeOH). $[\alpha]_D^{22}$ -15.4 (50% EtOH aq.).

*2′,3′*S-*Dihydro, picrate:*
Yellow needles (EtOH). Mp 187-189°.

2′,3′-Dihydro, O-*β-D-glucopyranoside: Dihydrozeatin* O-*glucoside*
[62512-96-3]
$C_{16}H_{25}N_5O_6$ 383.403
Constit. of various plant spp. incl. *Alnus* spp., *Lupinus* sp. and *Phaseolus* sp.

2′,3′-Dihydro, 9-β-D-ribofuranosyl: Dihydrozeatin riboside
[22663-55-4]
$C_{15}H_{23}N_5O_5$ 353.377
Constit. of numerous plants esp. in the Leguminosae. Prod. by *Pseudomonas* sp. Cytokinin. Sol. H_2O.

Deoxy: N-*(3-Methyl-2-butenyl)-1*H-*purin-6-amine. 6-(3-Methyl-2-butenylamino)purine.* **N^6-Prenyladenine**. *6-(γ,γ-Dimethylallylamino)purine.* N^6-*(3-Methyl-2-butenyl)adenine.* N^6-*Isopentenyladenine. 2iP*
[2365-40-4]
$C_{10}H_{13}N_5$ 203.246
Widespread in plant spp. Prod. by *Corynebacterium fascians* and *Pseudomonas amygdali* and prob. present in brown alga *Sargassum heterophyllum*. Potent cytokinin.
Mp 208-209° Mp 237-239° dec. Appears to be difficult to purify.
λ_{max} 269 (EtOH). λ_{max} 218; 275 (0.1*M* NaOH).

2-Hydroxy: ***2-Hydroxyzeatin***
[29736-32-1]
$C_{10}H_{13}N_5O_2$ 235.245
Prod. by *Pseudomonas syringae*. Cytokinin. Oil. Sol. H_2O.
λ_{max} 270 (MeOH).

(*Z*)-*form*
cis-*Zeatin*
[32771-64-5]
A modified nucleoside present in tRNAs. Isol. from *Corynebacterium fascians*. At least 50 times less active than the (*E*)-form.
Mp 206-208°.

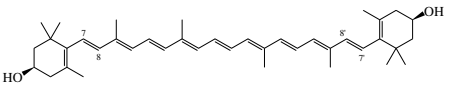
9-β-D-Glucopyranosyl: cis-*Zeatin 9-glucoside*
[169565-72-4]
$C_{16}H_{23}N_5O_6$ 381.388
Isol. from *Solanum tuberosum* (potatoes).

9-β-D-Ribofuranosyl: [15896-46-5]
Cryst. (EtOH). Mp 202-205°. λ_{max} 267 (ε 20280) (no solvent reported).

Shaw, G. *et al., J.C.S.(C)*, 1966, 921 (*synth, uv, ir*)
Letham, D.S. *et al., Life Sci.*, 1966, **5**, 1999-2004 (*isol, ribosylzeatin phosphate*)
Klambt, D. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1966, **56**, 52 (*isol, deriv*)
Helgeson, J.P. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1966, **56**, 60 (*deriv*)
Koshimizu, K. *et al., Tet. Lett.*, 1967, 1317 (*Dihydro, isol, synth*)
Letham, D.S. *et al., Tetrahedron*, 1967, **23**, 479 (*ms, uv, pmr, struct*)
Hecht, S.M. *et al., Phytochemistry*, 1970, **9**, 1173-1180 (*2-Hydroxyzeatin*)
Playtis, A.J. *et al., Biochem. Biophys. Res. Commun.*, 1971, **45**, 1-5 (*synth, 9-ribosyl*)
Leonard, N.J. *et al., J.A.C.S.*, 1971, **93**, 3056 (*synth, uv, pmr, ms*)
Bugg, C.E. *et al., Biochem. Biophys. Res. Commun.*, 1972, **46**, 779-784 (*deoxy, cryst struct*)
Corse, J. *et al., Synthesis*, 1972, **11**, 618 (*synth, pmr*)
Fujii, T. *et al., Tet. Lett.*, 1972, 3074 (*synth*)
Parker, C.W. *et al., Biochem. Biophys. Res. Commun.*, 1973, **55**, 1370-1376 (*synth, 9-glucoside*)
Scarbrough, E. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1973, **70**, 3825 (*cis-Zeatin*)
Parker, C.W. *et al., Planta*, 1974, **115**, 337-344 (*isol, 9-glucosyl*)
Parker, C.W. *et al., Ann. Bot. (London)*, 1975, **39**, 375-376 (*O-glucoside*)
Letham, D.S. *et al., Ann. Bot. (London)*, 1976, **41**, 261-263 (*9-ribosyl O-glucoside*)
Mackenzie, G. *et al., J.C.S. Perkin 1*, 1976, 1446 (*synth*)
Matsubara, S. *et al., Phytochemistry*, 1977, **16**, 933 (*synth*)
Wang, T.L. *et al., Planta*, 1977, **135**, 285; 1978, **140**, 151 (*glycosides*)
Cowley, D.E. *et al., Aust. J. Chem.*, 1978, **31**, 1095 (*Raphanatin*)
Duke, C.C. *et al., Aust. J. Chem.*, 1978, **31**, 1291-1301; 2219 (*glucopyranoside, dihydro, isol, synth, uv, pmr, cmr*)
Yokota, T. *et al., Phytochemistry*, 1980, **19**, 2367-2369 (*deoxy, isol*)
Chen, S.C. *et al., Agric. Biol. Chem.*, 1982, **46**, 2361 (*cmr*)
Corse, J. *et al., J. Plant Growth Regul.*, 1983, **2**, 47; *CA*, **00**, 34316 (*synth, resoln*)
Evidente, A. *et al., Phytochemistry*, 1989, **28**, 2603-2607 (*2-deoxyribosyl*)
De Napoli, L. *et al., Phytochemistry*, 1990, **29**, 701 (*2-deoxyribosyl*)
Shadid, B. *et al., Tetrahedron*, 1990, **46**, 901-912 (*synth, ribosylzeatin phosphate*)
Evidente, A. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1937 (*synth, 2-deoxyribosyl*)
Nicander, B. *et al., Plant Physiol.*, 1995, **109**, 513 (*9-glucoside*)
Kobayashi, H. *et al., Chem. Pharm. Bull.*, 1997, **45**, 260 (*Gazer*)
Jordis, U. *et al., Org. Prep. Proced. Int.*, 1997, **29**, 549-560 (*synth, pmr*)
Tsai, Y.-H. *et al., Helv. Chim. Acta*, 2003, **86**, 2452-2457 (*deoxy, isol*)

Zeaxanthin Z-5

β,β-Carotene-3,3′-diol. Anchovixanthin. Zeaxanthol



(3R,3′R,all-E)-form

$C_{40}H_{56}O_2$ 568.881

(3*R*,3′*R*, *all-E*)-*form* [144-68-3]
Constit. of crustaceans, fish, barley, maize (*Zea mays*), tomatoes, paprika pods, hen egg yolk and fruits. Found in cyanobacteria and most marine algae.
Yellow cryst. + ½MeOH (MeOH/C_6H_6).
Mp 215.5°. $[\alpha]_{656.3}^{20}$ -44 (c, 0.2 in $CHCl_3$).

3-O-α-L-Rhamnopyanoside: Zeaxanthin monorhamnoside
[55823-76-2]
$C_{46}H_{66}O_6$ 715.024
Constit. of *Sulfolobus shibatae* and from photosynthetic bacterium *Corynebacterium autotrophicum*. Ppt. (MeOH/C_6H_6/petrol).
Mp 149-150°. λ_{max} 428; 452; 480 (Me_2CO).

Di-O-α-L-rhamnopyranoside: Zeaxanthin dirhamnoside
[55823-75-1]
$C_{52}H_{76}O_{10}$ 861.166
Isol. from *Corynebacterium autotrophicum* and *Sulfolobus shibatae*. Red needles.
Mp 218-219°. λ_{max} 428; 452; 480 (Me_2CO).

3-O-[11-Methyldodecanoyl-(→6)-β-D-glucopyranoside]: ***Thermozeaxanthin 13***
[165525-68-8]
$C_{59}H_{90}O_8$ 927.355
Constit. of the thermophilic bacterium *Thermus thermophilus*.

3-O-[13-Methyltetradecanoyl-(→6)-β-D-glucopyranoside]: ***Thermozeaxanthin 15***
[165525-69-9]
$C_{61}H_{94}O_8$ 955.409
Constit. of the thermophilic bacterium *Thermus thermophilus*.

3-O-[15-Methylhexadecanoyl-(→6)-β-D-glucopyranoside]: ***Thermozeaxanthin 17***
[165525-70-2]
$C_{63}H_{98}O_8$ 983.462
Constit. of *Thermus thermophilus*.

Di-O-β-D-glucopyranoside: [53762-00-8]
$C_{52}H_{76}O_{12}$ 893.165
Constit. of *Sulfolobus shibatae*. λ_{max} 449; 477 (no solvent reported).

3,3′-Bis-O-[11-methyldodecanoyl-(→6)-β-D-glucopyranoside]: ***Thermozeaxanthin 13-13***
[165525-71-3]
$C_{78}H_{124}O_{14}$ 1285.829
Constit. of *Thermus thermophilus*.

3-O-[11-Methyldodecanoyl-(→6)-β-D-glucopyranoside], 3′-O-[13-methyltetradecanoyl-(→6)-β-D-glucopyranoside]: ***Thermozeaxanthin 13-15***
[165525-72-4]
$C_{80}H_{128}O_{14}$ 1313.883
Constit. of *Thermus thermophilus*.

3,3′-Bis[13-methyltetradecanoyl-(→6)-β-D-glucopyranoside]: ***Thermozeaxanthin 15-15***
[165525-73-5]
$C_{82}H_{132}O_{14}$ 1341.936
Constit. of *Thermus thermophilus*.

Dihexadecanoyl: ***Physalien***. *Zeaxanthin dipalmitate*
[144-67-2]
$C_{72}H_{116}O_4$ 1045.706
Constit. of *Physalis* spp., *Lycium* spp., asparagus (*Asparagus officinalis*) and others. Red cryst. (C_6H_6/MeOH).
Mp 98.5-99.5°. $[\alpha]_{Hg}$ -45 ($CHCl_3$).

Mono-Me ether: 3-Hydroxy-3′-methoxy-β-carotene. 3′-Methoxy-β,β-caroten-3-ol. Zeaxanthin monomethyl ether
[54200-44-1]

$C_{41}H_{58}O_2$ 582.908
Synthesized by methylation of zeaxanthin. Cryst. (MeOH). Mp 153°. Isol. not well documented.

Di-Me ether: 3,3′-Dimethoxy-β,β-carotene. Zeaxanthin dimethyl ether
[58526-52-6]
$C_{42}H_{60}O_2$ 596.935
Synth. by methylation of zeaxanthin. Glistening dark red needles (C_6H_6). Mp 176°. Isol. not well documented. λ_{max} 452; 480 (C_6H_{11}).

5,6-Epoxide: See Antheraxanthin, A-520

5,6:5′,6′-Diepoxide: See Violaxanthin, V-52

5,6-Dihydro, 5β,6α-dihydroxy: See 5,6-Dihydro-β,β-carotene-3,3′,5,6-tetrol in *The Combined Chemical Dictionary.*

(3*R*,3′*R*,9*Z*)-*form*

3-O-α-L-*Rhamnopyranoside:* [186525-05-3]
$C_{46}H_{66}O_6$ 715.024
Constit. of *Sulfolobus shibatae*. λ_{max} 335; 446; 472 (no solvent reported).

Di-O-α-L-*rhamnopyranoside:* [186525-04-2]
$C_{52}H_{76}O_{10}$ 861.166
Constit. of *Sulfolobus shibatae*. λ_{max} 442; 474 (no solvent reported).

(3*R*,3′*R*,13*Z*)-*form*

3-O-α-L-*Rhamnopyranoside:* [186525-06-4]
$C_{46}H_{66}O_6$ 715.024
Constit. of *Sulfolobus shibatae*. λ_{max} 339; 444; 470 (no solvent reported).

(3*R*,3′*R*,15*Z*)-*form*

3-O-α-L-*Rhamnopyranoside:* [186525-07-5]
$C_{46}H_{66}O_6$ 715.024
Constit. of *Sulfolobus shibatae*. λ_{max} 337; 448; 472 (no solvent reported).

(3*S*,3′*S*,*all-E*)-*form* [72002-36-9]
Constit. of *Paratya compressa compressa* (shrimp), integuments of bulkhead shark *Heterodontus japonicus*, pollack *Theragra chalcogramma* and other fish.
Mp 209-209.5°.

(3*RS*,3′*SR*,*all-E*)-*form*
meso-form
[31272-50-1]
Constit. of shrimp *Paratya compressa compressa*, loggerhead turtle *Caretta caretta*, green turtle *Chelonia mydas* and many fish.
Mp 212-213°.

(3ξ,3′ξ,all-*E*)-*form*

7′,8′-Dihydro: 7′,8′-Dihydro-β,β-carotene-3,3′-diol. ***Parasiloxanthin***
[62994-48-3]
$C_{40}H_{58}O_2$ 570.897
Isol. from skin and fin of Japanese catfish (*Parasilurus asotus*). Orange-yellow needles.
Mp 202°. Abs. config. not certain.

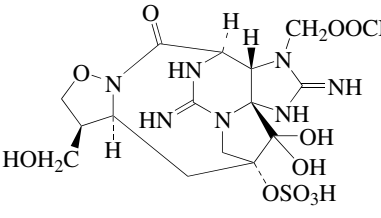
7,7′,8,8′-Tetrahydro: 7,7′,8,8′-Tetrahydro-β,β-carotene-3,3′-diol. ***7,8-Dihydroparasiloxanthin***
[62994-71-2]
$C_{40}H_{60}O_2$ 572.913
Constit. of skin and fin of Japanese catfish (*Parasilurus asotus*). Orange-yellow cryst.
Mp 197°.

[7756-97-0]

Curl, A.L. *et al., J. Food Sci.*, 1961, **26**, 106-111 (*isol*)
Cholnoky, L. *et al., J.C.S.(C)*, 1969, 1256-1263 (*struct*)
Loeber, D.E. *et al., J.C.S.(C)*, 1971, 404-408 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, 1972, nos. 1839; 1840 (*occur*)
McDermott, J.C.B. *et al., Biochem. J.*, 1973, **134**, 1115-1117 (*biosynth*)
Nybraaten, G. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 584-586; 1219-1224 (*isol, rhamnosides, Me ethers*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1974, **57**, 631-656 (*di-Me ether*)
Hlubucek, J.R. *et al., J.C.S. Perkin 1*, 1974, 848-852 (*abs config*)
Englert, G. *et al., Helv. Chim. Acta*, 1975, **58**, 2367-2390 (*cmr*)
Hertzberg, S. *et al., Arch. Microbiol.*, 1976, **110**, 95-99 (*abs config, rhamnosides*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97-102 (*cmr*)
Weedon, B.C.L. *et al., Pure Appl. Chem.*, 1976, **47**, 161-171 (*synth*)
Matsuno, T. *et al., Tet. Lett.*, 1976, 4601-4604 (*Parasiloxanthin, Dihydroparasiloxanthin*)
Britton, G. *et al., Chem. Comm.*, 1977, 655-656 (*biosynth*)
Rüttimann, A. *et al., Helv. Chim. Acta*, 1980, **63**, 1456-1462 (*3S,3′S-form, 3R,3′S-form, synth, pmr, cd*)
Widmer, E. *et al., Helv. Chim. Acta*, 1982, **65**, 944-957; 958-967 (*synth*)
Rüttimann, A. *et al., J. High Resolut. Chromatogr. Chromatogr. Commun.*, 1983, **6**, 612-616 (*chiral hplc*)
Maoka, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **83**, 121-124 (*stereoisomers, occur*)
Parkes, K.E.B. *et al., Tet. Lett.*, 1986, **27**, 2535-2538 (*epoxide, isol*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 119; 123 (*bibl*)
Widmer, E. *et al., Helv. Chim. Acta*, 1990, **73**, 861-867 (*synth*)
Soukup, M. *et al., Helv. Chim. Acta*, 1990, **73 /VOLN>868-873 (***synth*)
Palermo, J.A. *et al., Phytochemistry*, 1991, **30**, 2983-2986 (*isol, pmr, cmr*)
Yokoyama, A. *et al., Tet. Lett.*, 1995, **36**, 4901-4904 (*Thermozeaxanthins*)
Sliwka, H.-R. *et al., Acta Chem. Scand.*, 1996, **50**, 637-639 (*synth*)
Kull, D.R. *et al., J. Nat. Prod.*, 1997, **60**, 371-374 (*glycosides*)
Y, Yamano *et al., J.C.S. Perkin 1*, 2002, 2006-2013 (*synth*)
Eisenreich, W. *et al., J.O.C.*, 2002, **67**, 871-875 (*biosynth*)
Humphries, J.M. *et al., J. Agric. Food Chem.*, 2003, **51**, 1322-1327 (*occur, zeaxanthin*)
Linden, A. *et al., Helv. Chim. Acta*, 2004, **87**, 1254-1269 (*cryst struct, abs config*)
Eguchi, T. *et al., Tetrahedron*, 2005, **61**, 2027-2035 (*synth*)

Zetekitoxin AB Z-6

Atelopidtoxin



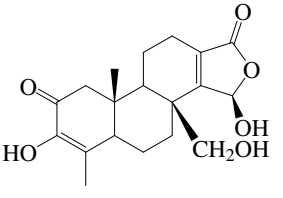
Relative Configuration

$C_{16}H_{24}N_8O_{12}S$ 552.478
Related to Saxitoxin, S-73. Toxin from the golden frog *Atelopus zeteki* of Panama. Extremely potent sodium channel blocker.

Yotsu-Yamashita, M. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2004, **101**, 4346-4351 (*isol, pmr, cmr, N-15 nmr, ms*)

Zimoclactone A Z-7

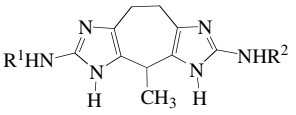
[565197-39-9]



$C_{19}H_{24}O_6$ 348.395
Constit. of *Spongia zimocca*.

Su, J.-Y. *et al., Gaodeng Xuexiao Huaxue Xuebao*, 2003, **24**, 817-819; *CA*, **139**, 114594r (*isol, pmr, cmr, cryst struct*)

Zoamides Z-8



	R^1	R^2
Zoamide A:	—COCH=C(CH_3)$_2$	—COCH=C(CH_3)$_2$
B:	—COPh	—COCH=C(CH_3)$_2$
C:	—COPh	—COCH(CH_3)$_2$
D:	—COPh	—COCH(CH_3)CH_2CH_3 (*S*-)

Related to Palyzoanthoxanthins.

Zoamide A [188558-01-2]

$C_{20}H_{26}N_6O_2$ 382.464

Alkaloid from an undescribed marine zoanthid, *Parazoanthus* sp., collected in the Philippines. Gummy solid. $[\alpha]_D$ 0. λ_{max} 200 (ϵ 20500); 290 (ϵ 18500) (MeOH).

Zoamide C [188558-97-6]

$C_{21}H_{24}N_6O_2$ 392.46

From *Parazoanthus* sp. Gummy solid. $[\alpha]_D$ 0. λ_{max} 225 (ϵ 19600); 270 (ϵ 13600) (MeOH).

Zoamide B [188558-50-1]

$C_{22}H_{24}N_6O_2$ 404.471

From *Parazoanthus* sp. Solid. $[\alpha]_D$ 0. λ_{max} 220 (ϵ 29000); 290 (ϵ 23500) (MeOH).

Zoamide D [188559-04-8]

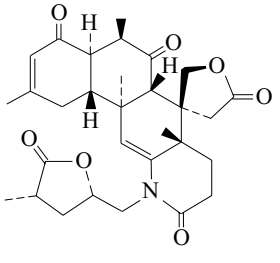
$C_{22}H_{26}N_6O_2$ 406.486

From *Parazoanthus* sp. Gummy solid. $[\alpha]_D$ +15.1. λ_{max} 230 (ϵ 17000); 270 (ϵ 14700) (MeOH).

D'Ambrosio, M. *et al., Tet. Lett.*, 1997, **38**, 717 (*isol, uv, ir, pmr, cmr, struct*)

Zoanthamide Z-9

[97877-70-8]



$C_{30}H_{37}NO_7$ 523.625

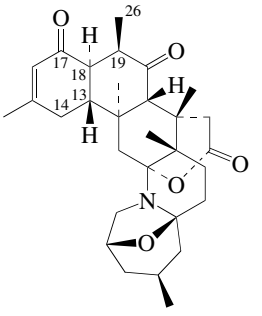
Alkaloid from an unidentified marine zoanthid, *Zoanthus* sp. Shows antiinflammatory props.

Mp 278-280°. $[\alpha]_D$ +133 (c, 0.83 in $CHCl_3$). λ_{max} 235 (ϵ 23900) (MeCN) (Derep).

Rao, C.B. *et al., J.O.C.*, 1985, **50**, 3757 (*isol, uv, ir, pmr, cmr, struct*)

Zoanthamine Z-10

[93426-90-5]



$C_{30}H_{41}NO_5$ 495.658

Alkaloid from a marine zoanthid, *Zoanthus* sp. Cytotoxic agent, antiinflammatory. Interleukin 6 production inhibitor.

Mp 306-308°. $[\alpha]_D$ +18 (c, 0.48 in $CHCl_3$). λ_{max} 233 (ϵ 11000) (MeCN) (Derep).

13,14,17,18-Tetradehydro, 17-alcohol: ***Zoanthenol***

[231945-73-6]

$C_{30}H_{39}NO_5$ 493.642

Alkaloid from a zoanthid. Amorph. solid. $[\alpha]_D^{25}$ +7.1 (c, 0.24 in $CHCl_3$).

11β-Hydroxy: ***11-Hydroxyzoanthamine***

$C_{30}H_{41}NO_6$ 511.657

Alkaloid from a zoanthid. Amorph. solid. $[\alpha]_D^{25}$ +1.8 (c, 0.23 in $CHCl_3$).

11-Oxo: ***Zoanthaminone***

[123853-69-0]

$C_{30}H_{39}NO_6$ 509.641

Alkaloid from a marine zoanthid, *Zoanthus* sp. Cryst. $[\alpha]_D$ +30 (c, 0.1 in $CHCl_3$). Mp not recorded. λ_{max} 235 (ϵ 23900) (MeCN) (Derep).

26-Hydroxy: 26-Hydroxyzoanthamine. ***Oxyzoanthamine***

[159509-36-1]

$C_{30}H_{41}NO_6$ 511.657

Alkaloid from a *Zoanthus* sp. Cytotoxic agent. Interleukin 6 production inhibitor. Oil.

17-Deoxo, 15β,16-dihydro, 16β-hydroxy: ***Zooxanthellamine***

[208256-91-1]

$C_{30}H_{45}NO_5$ 499.689

Alkaloid from cultures of the dinoflagellate *Symbiodinium* sp. Solid.

Mp >300°. $[\alpha]_D^{20}$ +40 (c, 0.05 in MeOH).

19-Epimer, 26-hydroxy: 26-Hydroxy-19-epizoanthamine. ***Epioxyzoanthamine***

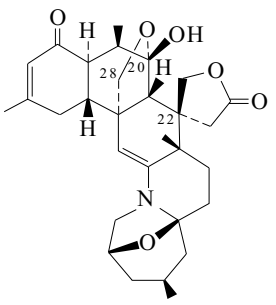
$C_{30}H_{41}NO_6$ 511.657

Alkaloid from a *Zoanthus* sp. Amorph. solid. $[\alpha]_D^{25}$ -17.5 (c, 0.24 in $CHCl_3$).

Rao, C.B. *et al., J.A.C.S.*, 1984, **106**, 7983 (*uv, ir, pmr, cmr, cryst struct*)
Atta-ur-Rahman, *et al., Tet. Lett.*, 1989, **30**, 6825 (*Zoanthaminone*)
Fukuzawa, S. *et al., Heterocycl. Commun.*, 1995, **1**, 207-214 (*Oxyzoanthamine*)
Nakamura, H. *et al., Bull. Chem. Soc. Jpn.*, 1998, **71**, 781-787 (*Zooxanthellamine*)
Daranas, A.H. *et al., Tetrahedron*, 1998, **54**, 7891-7896; 1999, **55**, 5539-5546 (*Epioxyzoanthamine, 11-Hydroxyzoanthamine, Zoanthenol*)

Zoanthenamine Z-11

[97877-69-5]



$C_{30}H_{39}NO_6$ 509.641
Alkaloid from the unidentified marine zoanthid, *Zoanthus* sp. Shows antiinflammatory props. Powder.
Mp 238-240°. Slowly dec. in soln. λ_{max} 233 (ϵ 11000) (CH_3CN) (Derep).

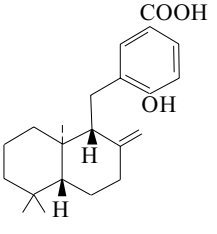
28-Deoxy, 20-oxo: ***28-Deoxyzoanthenamine***
[120314-15-0]
$C_{30}H_{39}NO_5$ 493.642
Alkaloid from an unidentified colonial zoanthid of the genus *Zoanthus*. Potent antiinflammatory and analgesic agent.
Mp 305-307°. $[\alpha]_D$ +216 (c, 3.7 in $CHCl_3$). λ_{max} 238 (ϵ 16250) (MeOH) (Berdy).

22-Epimer, 28-deoxy, 20-oxo: ***28-Deoxy-22-epizoanthenamine***.
22-Epi-28-deoxyzoanthenamine
[120409-36-1]
$C_{30}H_{39}NO_5$ 493.642
Alkaloid from the unidentified *Zoanthus* spp. Antiinflammatory and analgesic agent. Oil. $[\alpha]_D$ +85 (c, 2.36 in $CHCl_3$). λ_{max} 237 (ϵ 14200) (MeOH) (Berdy).

Rao, C.B. *et al., J.O.C.*, 1985, **50**, 3757 (*isol, uv, ir, pmr, cmr, struct*)
Rao, C.B. *et al., Heterocycles*, 1989, **28**, 103 (*Deoxyzoanthenamine, isol, uv, ir, pmr, cmr, struct*)

Zonaroic acid Z-12

[57765-74-9]



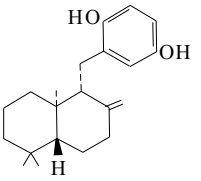
$C_{22}H_{30}O_3$ 342.477
Constit. of *Dictyopteris undulata*. Piscicide. Amorph. solid (cyclohexane). Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane.
Mp 81-85°. $[\alpha]_D$ -5.4 (c, 4 in $CHCl_3$). λ_{max} 257 (ϵ 10000) (MeOH) (Berdy). λ_{max} 288 (MeOH/NaOH) (Berdy).

Me ester:
Cryst. (Et_2O/petrol). Mp 182°.

Cimino, G. *et al., Experientia*, 1975, **31**, 1250

Zonarol Z-13

[39707-54-5]



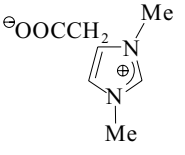
$C_{21}H_{30}O_2$ 314.467
Constit. of *Dictyopteris zonarioides* (*Dictyopteris undulata*). Phospholipase A2 inhibitor. Piscicide. Feeding inhibitor. Cryst. (Et_2O/petrol). Sol. MeOH, hexane; fairly sol. Et_2O; poorly sol. H_2O.
Mp 173.5-174.5°. $[\alpha]_D^{27}$ +18 (c, 0.1 in $CHCl_3$). λ_{max} 211 (ϵ 8400); 295 (ϵ 3150) (MeOH) (Derep). λ_{max} 211 (ϵ 6400); 293 (ϵ 3150) (MeOH) (Berdy).

Quinone: ***Zonarone***
[39707-56-7]
$C_{21}H_{28}O_2$ 312.451
Phospholipase A2 inhibitor. Piscicide. Antifeedant. Yellow needles (MeOH). Mp 125-127°. $[\alpha]_D^{30}$ +88.7 (MeOH). Poss. artifact. λ_{max} 248 (ϵ 12700); 331 (ϵ 790) (MeOH) (Berdy).

Fenical, W. *et al., J.O.C.*, 1973, **38**, 2383-2386 (*isol, struct*)
Welch, S.C. *et al., J.O.C.*, 1978, **43**, 1957-1961 (*synth*)
Ochi, M. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 629-630 (*isol*)
Mori, K. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 771-781 (*synth, abs config*)
Schöder, J. *et al., Tet. Lett.*, 2000, **41**, 5469-5473 (*synth, pmr, cmr*)
Laube, T. *et al., Tetrahedron*, 2002, **58**, 4299-4309 (*synth*)

Zooanemonin Z-14

*4-(Carboxymethyl)-1,3-dimethyl-1*H*-imidazolium hydroxide inner salt, 9CI. 1,3-Dimethyl-4-imidazoleacetic acid betaine. Anemonin*†
[584-91-8]



$C_7H_{10}N_2O_2$ 154.168
Isol. from the mussel *Arca noae*, the sea anemone *Anemonia sulcata* and the sponge *Axinella verrucosa*. Antibacterial, antineoplastic agent. Extremely hygroscopic.

Hydrochloride: Mp 184° (178°).

Picrate: Mp 149-153°.

Kutscher, F. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1933, **221**, 38 (*isol*)
Ackermann, D. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1953, **294**, 93; **295**, 1; 1954, **296**, 286; 1960, **318**, 281 (*synth, isol, nomencl, struct*)

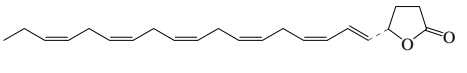
Zooanthellabetaine B Z-15

Betaine containing 4-hydroxybenzoyl and trimethylammonium groups, full struct. not determined. Isol. from cultures of a symbiotic dinoflagellate *Symbiodinium* sp.

Nakamura, H. *et al., Bull. Chem. Soc. Jpn.*, 1998, **71**, 781-787

Zooxanthellactone Z-16

*Dihydro-5-(1,3,6,9,12,15-octadecahexaenyl)-2(3*H*)-furanone. 5,7,10,13,16,19-Docosahexaen-4-olide*

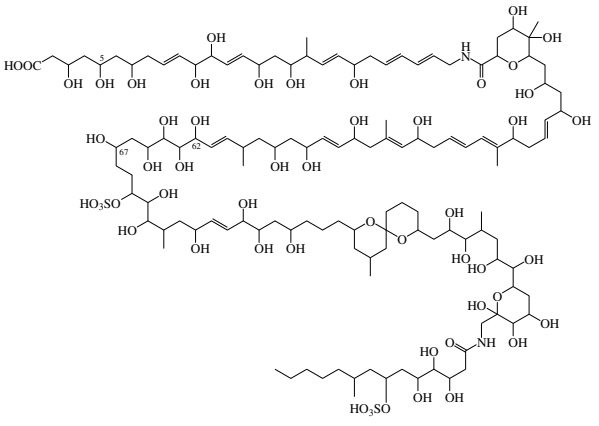


$C_{22}H_{30}O_2$ 326.478
Isol. from the dinoflagellates *Symbiodinium* spp. Cytotoxic. Oil.
$[\alpha]_D^{27}$ +64.6 (c, 0.24 in $CHCl_3$). λ_{max} 234 (ϵ 28500) (MeCN).

Onodera, K. *et al., Biosci., Biotechnol., Biochem.*, 2004, **68**, 848-852 (*isol, pmr, cmr*)

Zooxanthellamide A Z-17

[560131-35-3]



$C_{128}H_{222}N_2O_{54}S_2$ 2717.275

Isol. from *Symbiodinium* sp. Amorph. solid. $[\alpha]_D^{29}$ +1.9 (c, 0.36 in MeOH). λ_{max} 232 (ϵ 49000) (MeOH).

1→5-Lactone: ***Zooxanthellamide B***
[783322-76-9]
$C_{128}H_{220}N_2O_{53}S_2$ 2699.26
Isol. from *Symbiodinium* sp. Amorph. solid. $[\alpha]_D^{27}$ +4.5 (c, 0.08 in MeOH). λ_{max} 231 (ϵ 45000) (MeOH).

1→62-Lactone: ***Zooxanthellamide C_1***
[863644-66-0]
$C_{128}H_{220}N_2O_{53}S_2$ 2699.26
Isol. from *Symbiodinium* sp.

1→63-Lactone: ***Zooxanthellamide C_2***
[863644-67-1]
$C_{128}H_{220}N_2O_{53}S_2$ 2699.26
Isol. from *Symbiodinium* sp.

1→64-Lactone: ***Zooxanthellamide C_3***
[863644-68-2]
$C_{128}H_{220}N_2O_{53}S_2$ 2699.26
Isol. from *Symbiodinium* sp.

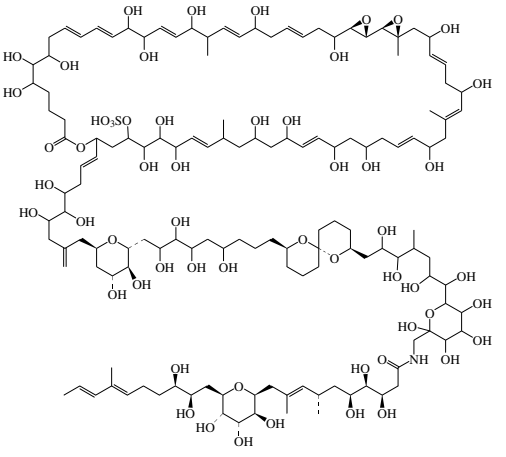
1→65-Lactone: ***Zooxanthellamide C_4***
[863644-69-3]
$C_{128}H_{220}N_2O_{53}S_2$ 2699.26
Isol. from *Symbiodinium* sp.

1→67-Lactone: ***Zooxanthellamide C_5***
[863644-70-6]
$C_{128}H_{220}N_2O_{53}S_2$ 2699.26
Isol. from *Symbiodinium* sp.

Onodera, K. *et al., Tetrahedron*, 2003, **59**, 1067-1071 (*Zooxanthellamide A*)
Onodera, K. *et al., Biosci., Biotechnol., Biochem.*, 2004, **68**, 955-958 (*Zooxanthellamide B*)
Onodera, K. *et al., J.A.C.S.*, 2005, **127**, 10406-10411 (*Zooxanthellamides C*)

Zooxanthellatoxin A Z-18

[146085-35-0]



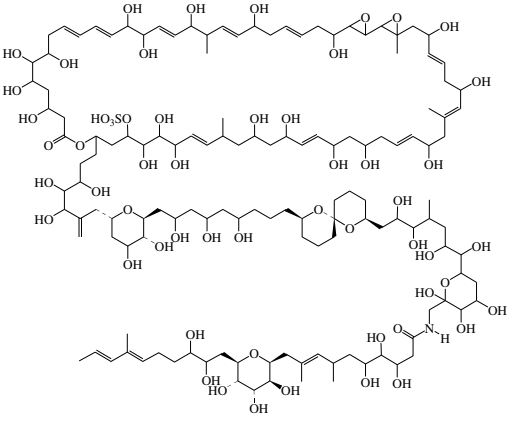
$C_{140}H_{233}NO_{57}S$ 2874.419

Highly unsaturated polyol toxin. Struct. revised in 1995. Isol. from *Symbiodinium* sp. Vasoconstrictive agent. Amorph. solid $+18H_2O$ (as Na salt). Sol. H_2O.
Mp 125-127° (Na salt). $[\alpha]_D^{24}$ +10 (c, 0.1 in MeOH). λ_{max} 233 (ϵ 29000) (MeOH).

Nakamura, H. *et al., J.O.C.*, 1993, **58**, 313 (*isol*)
Nakamura, H. *et al., J.A.C.S.*, 1995, **117**, 550 (*uv, ir, pmr, cmr, struct*)
Nakamura, H. *et al., Tet. Lett.*, 1996, **37**, 7267-7270; 2000, **41**, 1927-1930 (*partial config*)

Zooxanthellatoxin B Z-19

[148619-55-0]



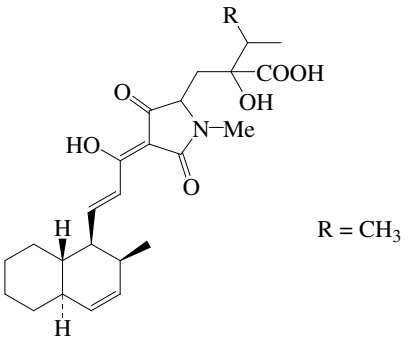
$C_{138}H_{231}NO_{56}S$ 2832.382

Highly unsaturated polyol toxin. Isol. from *Symbiodinium* sp. Vasoconstrictive agent.
Mp 127-129° (as Na salt). $[\alpha]_D^{24}$ +6.6 (c, 0.2 in MeOH) (Na salt). λ_{max} 234 (ϵ 28000) (MeOH).

Nakamura, H. *et al., Tet. Lett.*, 1995, **36**, 7255-7258 (*isol, uv, ir, pmr, cmr, ms*)

Zopfiellamide A Z-20

[478945-64-1]



$C_{25}H_{35}NO_6$ 445.555

Tetramic acid deriv. Incorr. MF given in the ref. Prod. by the marine fungus *Zopfiella latipes*. Yellowish cryst. (EtOH). Mp 225-230°. $[\alpha]_D^{22}$ +5.2 (c, 1.1 in $CHCl_3$). λ_{max} 247 (ϵ 11000); 320 (ϵ 10000) (MeOH).

Daferner, M. *et al., Tetrahedron*, 2002, **58**, 7781-7784 (*isol, pmr, cmr*)

Zopfiellamide B Z-21

[478945-65-2]

As Zopfiellamide A, Z-20 with

R = CH_2CH_3

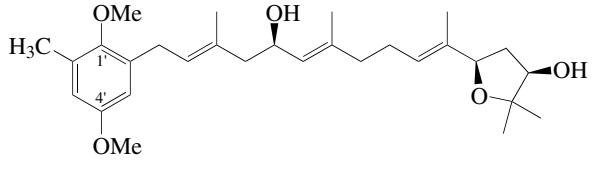
$C_{26}H_{37}NO_6$ 459.581

Tetramic acid deriv. Prod. by the marine fungus *Zopfiella latipes*. Yellowish oil. $[\alpha]_D^{22}$ -24 (c, 0.3 in $CHCl_3$). λ_{max} 247 (ϵ 3800); 321 (ϵ 3400) (MeOH).

Daferner, M. *et al., Tetrahedron*, 2002, **58**, 7781-7784 (*isol, pmr, cmr*)

Zosterdiol A Z-22

[120163-23-7]



$C_{29}H_{44}O_5$ 472.664

Constit. of *Cystoseira zosteroides*. Oil. $[\alpha]_D^{20}$ +0.5 (c, 2 in EtOH). λ_{max} 222 (ϵ 13800); 281 (ϵ 3200) (EtOH).

1′-De-Me, 5-Ac:

$C_{30}H_{44}O_6$ 500.674

Constit. of *Cystoseira crinita*. Oil. $[\alpha]_D^{25}$ +0.6 (c, 2 in CH_2Cl_2). λ_{max} 210 (ϵ 15220); 290 (ϵ 2800) (MeOH).

1′,4′-Di-de-Me, 5-Ac:

$C_{29}H_{42}O_6$ 486.647

Constit. of *Cystoseira crinita*. Oil. $[\alpha]_D^{25}$ +0.7 (c, 1.6 in CH_2Cl_2). λ_{max} 212 (ϵ 13650); 290 (ϵ 3440) (MeOH).

1′,4′-Di-de-Me, 1′,4′-quinone, 5-Ac:

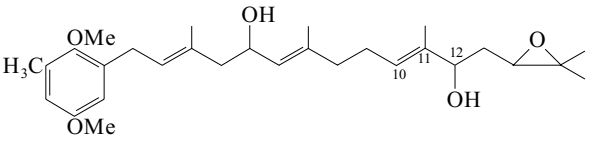
$C_{29}H_{40}O_6$ 484.631

Constit. of *Cystoseira crinita*. Oil. $[\alpha]_D^{25}$ +0.8 (c, 1.8 in CH_2Cl_2). λ_{max} 205 (ϵ 17350); 252 (ϵ 4380) (MeOH).

Amico, V. *et al., Phytochemistry*, 1989, **28**, 215-219 (*isol, pmr, cmr, ms*)
Praud, A. *et al., Phytochemistry*, 1995, **40**, 495-500 (*derivs, isol, pmr, cmr*)
Amico, V. *et al., J. Nat. Prod.*, 1997, **60**, 1088-1093 (*abs config*)

Zosterdiol B Z-23

[120163-24-8]



$C_{29}H_{44}O_5$ 472.664

Constit. of *Cystoseira zosteroides*. Oil. $[\alpha]_D^{20}$ +1.1 (c, 0.9 in EtOH). λ_{max} 222 (ϵ 12000); 284 (ϵ 3000) (EtOH).

10,11-Dihydro, 12-ketone: ***Zosteronol***

[120163-25-9]

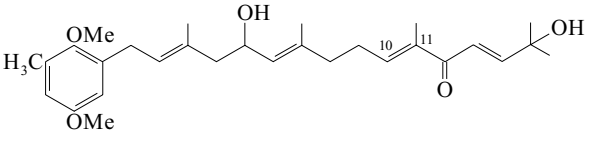
$C_{29}H_{44}O_5$ 472.664

Constit. of *Cystoseira zosteroides*. Oil. $[\alpha]_D^{20}$ +1.5 (c, 0.6 in EtOH). λ_{max} 222 (ϵ 10000); 282 (ϵ 2600) (EtOH).

Amico, V. *et al., Phytochemistry*, 1989, **28**, 215-219 (*isol, pmr, cmr, ms*)

Zosterondiol B Z-24

[120181-10-4]



$C_{29}H_{42}O_5$ 470.648

Constit. of *Cystoseira zosteroides*. Oil. $[\alpha]_D^{20}$ +0.9 (c, 0.4 in EtOH). λ_{max} 222 (ϵ 10800); 254 (ϵ 9200); 284 (ϵ 2800) (EtOH).

10,11-Dihydro: ***Zosterondiol A***

[120181-09-1]

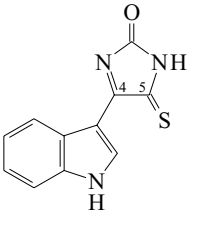
$C_{29}H_{44}O_5$ 472.664

Constit. of *Cystoseira zosteroides*. Oil. $[\alpha]_D^{20}$ +0.7 (c, 0.8 in EtOH). λ_{max} 222 (ϵ 18000); 234 (ϵ 11700); 280 (ϵ 2600) (EtOH).

Amico, V. *et al., Phytochemistry*, 1989, **28**, 215-219 (*isol, pmr, cmr, ms*)

Zyzzin Z-25

[159509-39-4]



$C_{11}H_7N_3OS$ 229.262

Metab. from the sponge *Zyzza massalis*. Deep orange amorph. solid. Undergoes exchange of the thioxo for the oxo group during aqueous workup. λ_{max} 212 (ϵ 15800); 270 (ϵ 5200); 345 (ϵ 2200); 420 (ϵ 1800); 475 (ϵ 1200) (MeOH) (Berdy).

*3,4-Dihydro, 4-hydroxy: 4-Hydroxy-4-(1*H*-indol-3-yl)-5-thioxo-2-imidazolidinone*

[159308-50-6]

$C_{11}H_9N_3O_2S$ 247.277

Artifact from *Zyzza massalis*. Racemic.

*3,4-Dihydro, 4-methoxy: 4-(1*H*-Indol-3-yl)-4-methoxy-5-thioxo-2-imidazolidinone*

[159308-48-2]

$C_{12}H_{11}N_3O_2S$ 261.304

Artifact from *Zyzza massalis*. Opt. inactive (racemic). The 5-thioxo analogue of Polyandrocarpamide D, P-519.

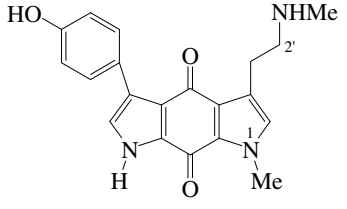
*5-Oxo analogue: 4-(1*H-*Indol-3-yl)-1*H-*imidazole-2,5-dione*
[159308-52-8]
$C_{11}H_7N_3O_2$ 213.195
Metab. from *Zyzza massalis*. Yellow amorph. solid. Almost certainly an artifact derived from Zyzzin during the isol. procedure.

5-Oxo analogue, C*(4),*N*-dihydro: 5-(1*H-*Indol-3-yl)-2,4-imidazolidinedione*
[159308-51-7]
$C_{11}H_9N_3O_2$ 215.211
Metab. of *Zyzza massalis*. Powder. $[\alpha]_D^{25}$ +10 (c, 0.13 in MeOH). Almost certainly a workup artifact originating from the corresp. thioamide.

*5-Oxo analogue, 3,4-dihydro, 4-hydroxy: 5-Hydroxy-5-(1*H-*indol-3-yl)-2,4-imidazolidinedione*
[159308-49-3]
$C_{11}H_9N_3O_3$ 231.21
Artifact from *Zyzza massalis*. Solid (EtOH/hexane).
Mp 140° dec. Racemic.

Mancini, I. *et al., Helv. Chim. Acta*, 1994, **77**, 1886-1894 (*isol, pmr, cmr, ms, struct, Zyzza massalis constits*)

Zyzzyanone A Z-26



$C_{20}H_{19}N_3O_3$ 349.388

Alkaloid from the sponge *Zyzzya fuliginosa*. Cytotoxic. Purple solid (as trifluoroacetate salt).
Mp 300° dec. (TFA salt). λ_{max} 242 (log ϵ 4.26); 286 (log ϵ 3.9); 342 (log ϵ 3.59); 484 (log ϵ 3.44) (MeOH) (TFA salt). λ_{max} 243 (log ϵ 4.28); 286 (log ϵ 3.96); 346 (log ϵ 3.6); 505 (log ϵ 3.48) (MeOH/KOH)(TFA salt).

N$^{2'}$*-Formyl:* ***Zyzzyanone C***
$C_{21}H_{19}N_3O_4$ 377.399
Alkaloid from *Zyzza fuliginosa*. Brownish-red solid (as TFA salt). λ_{max} 242 (log ϵ 3.67); 294 (log ϵ 3.24); 349 (log ϵ 2.49); 486 (log ϵ 2.85) (MeOH)(TFA salt).

N^{1}*De-Me:* ***Zyzzyanone B***
$C_{19}H_{17}N_3O_3$ 335.362
Alkaloid from *Zyzza fuliginosa*. Purple solid (as TFA salt). λ_{max} 240 (log ϵ 3.99); 281 (log ϵ 3.64); 328 (log ϵ 3.33); 483 (log ϵ 3.08) (MeOH)(TFA salt).

N^{1}*De-Me,* N$^{2'}$*-formyl:* ***Zyzzyanone D***
$C_{20}H_{17}N_3O_4$ 363.372
Alkaloid from *Zyzza fuliginosa*. Brownish-red solid (as TFA salt). λ_{max} 241 (log ϵ 3.67); 288 (log ϵ 3.23); 337 (log ϵ 2.95); 487 (log ϵ 2.84) (MeOH)(TFA salt).

Utkina, N.K. *et al., Tet. Lett.*, 2004, **45**, 7491-7494 (*isol, uv, ir, pmr, cmr*)
Utkina, N.K. *et al., J. Nat. Prod.*, 2005, **68**, 1424-1427 (*Zyzzyanones B,C,D*)

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Flavonols; six O substituents

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9,10-Anthraquinones with three O substituents

9,10-Anthraquinones with four O substituents

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12,6-Eudesmanolide sesquiterpenoids

12,8-Eudesmanolides and furanoeudesmane sesquiterpenoids

Agarofuran eudesmane sesquiterpenoids

Noreudesmane sesquiterpenoids

Emmotin sesquiterpenoids

Oppositane sesquiterpenoids

Cycloeudesmane sesquiterpenoids

Gorgonane sesquiterpenoids

Simple eremophilane sesquiterpenoids

Eremophilanolide and furanoeremophilane sesquiterpenoids

Noreremophilane sesquiterpenoids

Aristolane sesquiterpenoids

Nardosinane sesquiterpenoids

Brasilane sesquiterpenoids

Miscellaneous rearranged eudesmane sesquiterpenoids

Cadinane sesquiterpenoids

Nor- and secocadinane sesquiterpenoids

Alliacane sesquiterpenoids

Oplopane sesquiterpenoids

Drimane sesquiterpenoids

Nor- and secodrimane sesquiterpenoids

Simple guaiane sesquiterpenoids

12,8-Guaianolide sesquiterpenoids

Dimeric guiaiane sesquiterpenoids

Seco-, cyclo-, abeo- and norguaiane sesquiterpenoids

Aromadendrane sesquiterpenoids

Cycloaromadendrane sesquiterpenoids

Cubebane sesquiterpenoids

Valerenane sesquiterpenoids

Africanane sesquiterpenoids

Longifolane sesquiterpenoids

Fukinane sesquiterpenoids

Picrotoxane sesquiterpenoids

Daucane sesquiterpenoids

Isodaucane sesquiterpenoids

Perforane sesquiterpenoids

Pacifigorgiane sesquiterpenoids

Sterpurane sesquiterpenoids

Illudalane sesquiterpenoids

Furodysin sesquiterpenoids

Furodysinin sesquiterpenoids

Botrydial sesquiterpenoids

Chamigrane sesquiterpenoids

Secochamigrane sesquiterpenoids

Spiroaxane sesquiterpenoids

Miscellaneous spirosesquiterpenoids

Cedrane sesquiterpenoids

Zizaane sesquiterpenoids

Precapnellane sesquiterpenoids

Capnellane sesquiterpenoids

Hirsutane sesquiterpenoids

Rearranged hirsutane sesquiterpenoids

Silphiperfoliane sesquiterpenoids

Quadrane sesquiterpenoids

Sativane sesquiterpenoids

Sinularane sesquiterpenoids

Copaane sesquiterpenoids

Bourbonane sesquiterpenoids

Miscellaneous monocyclic sesquiterpenoids

Miscellaneous bicyclic sesquiterpenoids

Miscellaneous tricyclic sesquiterpenoids

Tetracyclic sesquiterpenoids

Phytane diterpenoids

Irregular linear diterpenoids

Linear homo- and nor- diterpenoids

Prenylbisabolane diterpenoids

10,15-Cyclophytane diterpenoids

Labdane diterpenoids

Secolabdane diterpenoids

Norlabdane diterpenoids

Halimane diterpenoids

Rearranged labdane diterpenoids

Clerodane diterpenoids

Nor-, seco- and abeoclerodane diterpenoids

Abietane diterpenoids

Pimarane diterpenoids

Erythroxylane diterpenoids

Parguerane diterpenoids

Isoparguerane diterpenoids

Isopimarane diterpenoids

Rearranged pimarane and isopimarane diterpenoids

Cleistanthane and isocleistanthane diterpenoids

Isocopalane and spongiane diterpenoids

Seco-, nor and abeospongiane diterpenoids

Podocarpane diterpenoids

Kaurane diterpenoids

Norkaurane diterpenoids

Beyerane diterpenoids

Atisane diterpenoids

Cembrane diterpenoids

Norcembrane diterpenoids

Rearranged cembrane diterpenoids

Pseudopterane diterpenoids

Eunicellane diterpenoids

Asbestinane diterpenoids

Sphaerane diterpenoids

Briarane diterpenoids

Dolabellane diterpenoids

Modified dolabellane diterpenoids

Dolastane diterpenoids

Modified dolastane diterpenoids

Cyathane diterpenoids

Sphaeroane diterpenoids

Modified verrucosane diterpenoids

Casbane diterpenoids

Fusicoccane diterpenoids

Spatane diterpenoids

Seco- and abeospatane diterpenoids

Verticillane diterpenoids

Amphilectane diterpenoids

Cycloamphilectane diterpenoids

Adociane diterpenoids

Xenicane diterpenoids

Nor-, seco- and cycloxenicane diterpenoids

Xeniaphyllane diterpenoids

Prenyleudesmane diterpenoids

Prenylgermacrane diterpenoids

Prenylbicyclogermacrane diterpenoids

Lobane diterpenoids

Pachydictyane diterpenoids

Cneorubine diterpenoids

Serrulatane and biflorane diterpenoids

Sacculatane diterpenoids

Obtusane diterpenoids

Irieol diterpenoids

Sphenolobane diterpenoids

Miscellaneous monocyclic diterpenoids

Miscellaneous bicyclic diterpenoids

Miscellaneous tricyclic diterpenoids

Miscellaneous tetracyclic diterpenoids

Acyclic sesterterpenoids

Noracyclic sesterterpenoids

Cyclohexane sesterterpenoids

Bicyclic sesterterpenoids

Cheilanthane sesterterpenoids

Ophiobolane sesterterpenoids

Scalarane sesterterpenoids

Methyl- and dimethylscalarane sesterterpenoids

Miscellaneous sesterterpenoids

Linear triterpenoids

Botryococcene triterpenoids

Protostane and fusidane triterpenoids

Lanostane triterpenoids

Cycloartane triterpenoids

Cucurbitane triterpenoids

Dammarane triterpenoids

Apotirucallane triterpenoids

Ring cleaved tetranortriterpenoids

Rearranged tetranortriterpenoids

Lupane triterpenoids

Oleanane triterpenoids

Nor-, seco- and abeooleanane triterpenoids

Taraxerane triterpenoids

Ursane triterpenoids

Nor-, seco- and abeohopane triterpenoids

Fernane triterpenoids

Gammacerane triterpenoids

Malabaricane and isomalabaricane triterpenoids

Miscellaneous triterpenoids

Iridal group norterpenoids

Sesquaterterpenes

Tetraterpenoids

Megastigmane norterpenoids

Apocarotenoids

Polyterpenoids

Meroterpenoids

Terpenoids of unknown structure

Nonaromatic 19-norandrostane steroids (estranes)

Androstane steroids

19-Norpregnane steroids

Pregnane steroids

Cholan-24-oic acid steroids

Other cholane steroids

Homocholane steroids (26,27-dinorcholestanes)

27-Norcholestane steroids

Neutral cholestane steroids

16,18,20-Trihydroxycholesta-1,4,22-trien-3-one; (16β,20*S*,22*E*)-*form*, T-581
3,5,6-Trihydroxycholest-8-ene-7,11-dione, C-587
3,5,26-Trihydroxycholest-24-en-6-one; (3β,5α,24*Z*)-*form*; 26-Ac, T-582
3,6,20-Trihydroxycholest-9(11)-en-23-one; (3β,5α,6α,20*S*)-*form*; 3-*O*-[β-D-Fucopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→4)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 6-*O*-sulfate, T-583
3,6,20-Trihydroxycholest-9(11)-en-23-one; (3β,5α,6α,20*S*)-*form*; 3-*O*-Sulfate, salt with, T-583
16,18,20-Trihydroxycholest-4-en-3-one, T-581
3,6,11-Trihydroxy-24-nor-9,11-secocholesta-7,22-dien-9-one; (3β,6α,22*E*)-*form*; 11-Ac, T-655
3,5,6-Trihydroxy-9-oxo-9,11-secocholest-7-en-11-al; (3β,5α,6β)-*form*; 3-Ac, T-661
3,6,11-Trihydroxy-9,11-secocholesta-7,22-dien-9-one; (3β,5α,6α,22*E*)-*form*; 11-Ac, T-675
3,6,11-Trihydroxy-9,11-secocholest-7-en-9-one; (3β,5α,6α)-*form*, T-676
24,26,26-Trimethylcholest-23-ene-2,3,6-triol; (2β,3α,5α,6α,23*E*,25ξ)-*form*; Tri-*O*-sulfate, T-706
24,27,27-Trimethylergosta-5,25-dien-3-ol; 3β-*form*, T-711
Trodusquemine, INN, USAN, S-356
Tumidoside A, D-1038
Tumidoside B, C-494
Validoside A, C-494
Validoside B, C-514
Verongulasterol, V-29
24-Vinyloxycholesta-5,23-dien-3-ol, H-507
Wondosterol B, C-454
Wondosterol C, C-457
Xestobergsterol A, X-40
Xestobergsterol B, X-40
Xestobergsterol C, X-40
Zoanthusterone, H-296
Zymostenol, C-626

Cholestanoic acid steroids

Carolisterol A, C-127
Carolisterol B, C-127
Carolisterol C, C-127
Dimorphoside A, D-1015
Dimorphoside B, D-1015
Isogosterone A, I-181
Isogosterone B, I-182
Isogosterone C, I-182
Isogosterone D, I-181
Tetrahydroxynorsterocholanic acid, T-234
Tetrahydroxysterocholanic acid, T-241
3,7,12-Trihydroxycoprostanic acid, T-578

Ecdysteroids

2-*O*-Acetylpinnasterol, T-205
Asterasterol C, D-627
Crustecdysone, H-297
4-Dehydroecdysterone, H-295
2-Deoxycrustecdysone, P-218
2-Deoxyecdysterone 25-acetate, P-218
3,26-Dihydroxycholest-7-ene-6-one 26-sulfate, D-627
α-Ecdysone, P-217
22-*O*-Hydroxyacetylponasterone A, P-216
Limnantheoside B, P-216
Makisterone B, H-300
Muristerone A, H-185
Palythoalone A, H-189
Palythoalone B, H-186
3,14,20,22,25-Pentahydroxycholest-7-en-6-one; (3β,5β,20*R*,22*R*)-*form*; 3-Benzoyl, P-218
3,14,20,22,25-Pentahydroxycholest-7-en-6-one; (3β,5β,20*R*,22*R*)-*form*; 3-*O*-β-D-Glucopyranoside, P-218
Pinnasterol, T-205
Ponasterone A, P-216
Ponasterone B, P-216
Ponasteroside A, P-216
Zoanthusterone, H-296

Furostane steroids

3-Acetyl-2-desacetyl-22-epihippurin 1, E-454
3-Acetyl-2-desacetylhippurin 1, E-454
3-Acetyl-22-epihippurin 1, E-454
3-Acetyl-22-epihippuristanol, E-455
Calicoferol B, C-45
11-Dehydroxy-22-epihippuristanol, E-453
2-Desacetyl-22-epihippurin 1, E-454
3,11-Diacetyl-22-epihippurin 1, E-454
3,11-Diacetylhippurin 1, E-454
18,20:22,25-Diepoxy-24-methylfurostane-2,3,11,18-tetrol; (2α,3α,5α,11β,18*R*,20*R*,22*S*,24*S*)-*form*; 2,3-Di-Ac, D-467
18,20:22,25-Diepoxy-24-methylfurostane-2,3,11,18-tetrol; (2α,3α,5α,11β,18*R*,20*R*,22*S*,24*S*)-*form*; 18-Ketone (lactone), 2-Ac, D-467
18,20:22,25-Diepoxy-24-methylfurostane-2,3,11,18-tetrol; (2α,3α,5α,11β,18*R*,20*R*,22*S*,24*S*)-*form*; 18-Ketone (lactone), 3-Ac, D-467
18,20:22,25-Diepoxy-24-methylfurostane-2,3,11,18-tetrol; (2α,3α,5α,11β,18*R*,20*R*,22*S*,24*S*)-*form*; 18-Ketone (lactone), 2,3-di-Ac, D-467
18,20:22,25-Diepoxy-24-methylfurostane-3,11,18-triol; (3α,5α,11β,18*R*,20*R*,22*S*,24*S*)-*form*; 3-Ac, D-468
22-Epihippurin 1, E-454
22-Epihippuristanol, E-455
22,25-Epoxy-3,11-dihydroxy-24-methylfurostan-18,20-olide; (3α,5α,11β,20*R*,22ξ,24ξ)-*form*; 3-Ac, E-222
22,25-Epoxy-3,11-dihydroxy-24-methylfurostan-18,20-olide; (3α,5α,11β,20*R*,22*S*,24*S*)-*form*, E-222
22,25-Epoxy-3,20-dihydroxy-24-methylfurostan-11-one, E-455
22,25-Epoxyfurost-1-en-3-one; (22*S*)-*form*, E-329
22,25-Epoxy-20-hydroxy-24-methylfurostan-3-one, E-453
22,25-Epoxy-24-methylfurost-5-ene-3,20-diol; (3β,20β,22*R*,24*S*)-*form*; 3-Ac, E-456
22,25-Epoxy-24-methylfurost-5-ene-3,20-diol; (3β,20β,22*S*,24*S*)-*form*; 3-Ac, E-456
22,25-Epoxy-24-methylfurost-5-ene-3,20-diol; (3β,20β,22*R*,24*S*)-*form*, E-456
22,25-Epoxy-24-methylfurost-5-ene-3,20-diol; (3β,20β,22*S*,24*S*)-*form*, E-456
22,25-Epoxy-2,3,11-trihydroxy-24-methylfurostan-18,20-olide, D-467
Hippurin 1, E-454
Hippurin 2, E-455
Hippuristanol, E-455
22-Hydroxyfurosta-1,4-dien-3-one; 22ξ-*form*, H-635
22-Hydroxyfurost-1-en-3-one; 22ξ-*form*, H-636
2α-Hydroxyhippuristanol, E-454
A-Nor-22-epihippurin-2-carboxylic acid, A-11
11,18:18,20:22,25-Triepoxy-24-methylfurostane-2,3-diol; (2α,3α,5α,11β,18*R*,22*S*,24*S*)-*form*; 2-Ac, T-541
11,18:18,20:22,25-Triepoxy-24-methylfurostane-2,3-diol; (2α,3α,5α,11β,18*R*,22*S*,24*S*)-*form*; 3-Ac, T-541
11,18:18,20:22,25-Triepoxy-24-methylfurostane-2,3-diol; (2α,3α,5α,11β,18*R*,22*S*,24*S*)-*form*; 2,3-Di-Ac, T-541
11,18:18,20:22,25-Triepoxy-24-methylfurostan-3-ol; (3α,5α,11β,18*R*,22*S*,24*S*)-*form*; 3-Ac, T-542

Ergostane steroids (excluding withanolides and brassinolides)

5(4→3)-Abeo-16,23-epoxyergostane-3,4,6,7,15-pentol; (3β,5α,6β,7β,15β,16α,23*R*,24*S*)-*form*; 15-(Methylphosphate), 3-sulfate, A-13
4(3→2)-Abeo-2-hydroxy-4-oxoergosta-5,22-dien-3-oic acid; (2β*OH*,22*E*,24ξ)-*form*; Et ester, A-17
Acanthaglycoside F, T-609
Acanthosterol sulfate D, E-289
Acanthosterol sulfate E, E-289
Acanthosterol sulfate F, E-289
Acanthosterol sulfate G, E-289
Acanthosterol sulfate I, E-289
Acanthosterol sulfate J, E-289
Acanthovagasteroid C, E-596
Acanthovagasteroid D, E-596
Acerosterol, T-705
11-Acetoxy-24-methylcholesta-7,22-diene-2α,3β,5α,6β,9α,19-hexol, E-609
3-Acetyl-2-desacetyl-22-epihippurin 1, E-454
3-Acetyl-2-desacetylhippurin 1, E-454
3-Acetyl-22-epihippurin 1, E-454
3-Acetyl-22-epihippuristanol, E-455
Acodontasteroside A, E-727
Acodontasteroside E, E-726
Acodontasteroside G, E-733
Acodontasteroside H, E-625
Agosterol A_4, E-612
Agosterol A_5, H-743
Agosterol C_7, E-613
Amphisterol, A-477
Amuresterol, N-193
Annasterol sulfate, E-597
Antarcticoside B, T-609
Antarcticoside J, E-733
Antarcticoside K, E-733
Antarcticoside L, E-733
Antarcticoside M, E-733
Antarcticoside N, E-663
Antarcticoside O, E-726
Antarcticoside P, E-726
Anthosterone B, A-526
Aplysterol, D-918
Arenicolsterol A, E-603
Armatinol A, E-599
Armatinol B, E-761
Asperoside A, E-725
Asperoside B, E-726
Asterasterol A, A-722
Asteriidoside B, E-640
Asteriidoside D, E-640
Asteriidoside G, E-730
Asteriidoside L, E-743
Asteroside B, E-250
Asteroside C, T-609
Asteroside D, E-640
Axinysterol, E-103
Biemnasterol, E-703
Bisconicasterone, B-135
Brassicasterol, E-643
Brevesterol, M-399
Campesta-7,22*E*-diene-3β,6α-diol, E-602
Campest-22-ene-3,4,5,6,8,14,15,25,26-nonol, E-735
Campest-22-ene-3,4,5,6,8,14,15,25-octol, H-733
Campest-5-ene-1,3,11-triol, E-765
Campest-7-en-3-ol, E-776
4-Campesten-3-one, E-780
Campesterol, E-775
Ceramasteroside C_1, E-720
Ceramasteroside C_4, E-726
Ceramasteroside C_3, E-731
Ceramasteroside C_2, E-731
Cerevisterol, E-638
Certonardoside A, E-733
Certonardoside B_3, E-756
Certonardoside B_2, E-756
Certonardoside B, E-763
Certonardoside C, E-748
Certonardoside D, E-726
Certonardoside E, E-742
Certonardoside H_2, E-675
Certonardosterol A_2, E-726
Certonardosterol A, E-733
Certonardosterol A_4, N-197
Certonardosterol B_4, E-668
Certonardosterol B_2, E-742

Withanolide and brassinolide steroids

Stigmastane steroids

Gorgostane and other cyclopropacholestane steroids

Vitamin D_3 (cholecalciferol) metabolites and analogues

Vitamin D_2 (ergocalciferol) metabolites and analogues

Steroids of unknown structure

Protein α-amino acids

Non-protein α-amino acids

β-Amino acids

Miscellaneous modified amino acids

Unsaturated amino acids

Diketopiperazines (dipeptide anhydrides)

Dipeptides

Tripeptides

Oligopeptides (4-10 residues)

Linear polypeptides

Cyclic oligo- and polypeptides

Aeruginosins

Larger depsipeptides

Small depsipeptides

Bicyclic/polycyclic depsipeptides

Actinomycin-type depsipeptides

Thiopeptin/siomycin-type depsipeptides (thiazole containing)

Monocyclic β-lactams (nocardicins and monobactams)

Enzymes

Other proteins

Glycopeptides and glycoproteins

Lipopeptides

Peptides of unknown structure

Simple acyclic amine alkaloids with one N

Simple acyclic amine alkaloids with two N

Simple guanidines

Nitriles and isonitriles

Simple amide alkaloids

Simple pyrrolidine alkaloids

Chromone alkaloids

Miscellaneous pyrrolidine alkaloids

Tetramic acids

Simple pyrrolizidine alkaloids

Anabasine-like alkaloids

Simple piperidine alkaloids incl. piperidides

Xestospongins

Aragupetrosine A, A-631
Araguspongine B, X-54
Araguspongine C, A-632
Araguspongine F, A-633
Araguspongine G, A-633
Araguspongine H, A-634
Araguspongine J, A-634
Araguspongine K, X-54
Araguspongine L, A-632
Araguspongine M, X-54
Demethylxestospongin B, X-55
3*R*,3′*R*-Dimethylxestospongin C, A-634
7*S*-Hydroxyxestospongin A, X-54
3α-Methylaragusponginе C, A-632
Petrosine A, P-287
Petrosine B, P-287
Petrosine, P-287
Upenamide, U-54
Xestosine A, P-287
Xestospongin A, X-54
Xestospongin B, X-55
Xestospongin C, X-54
Xestospongin D, X-54

Miscellaneous piperidine alkaloids

Anthosamine A, A-524
Anthosamine B, A-524
Arenosclerin A, A-655
Arenosclerin B, A-655
Arenosclerin C, A-655
Azaspiracid 8, A-792
Azaspiracid 3, A-792
Azaspiracid 4, A-792
Azaspiracid 5, A-792
Azaspiracid 2, A-792
Azaspiracid 11, A-792
Azaspiracid 6, A-792
Azaspiracid 9, A-792
Azaspiracid 10, A-792
Azaspiracid 1, A-792
Azaspiracid 7, A-792
Halichondramine, A-655
Haliclamine A, H-19
Haliclamine B, H-19
Haliclonacyclamine A, H-22
Haliclonacyclamine B, H-22
Haliclonacyclamine C, H-22
Haliclonacyclamine D, H-22
Haliclonacyclamine E, A-655
Halicyclamine A, H-27
Halicyclamine B, H-28
1,1,2,2,6,6-Hexamethyl-4-oxopiperidinium, 9CI, T-257
22-Hydroxyhalicyclamine A, H-27
Pinnaic acid, P-415
Pulcherrimine, P-704
Sesbanimide A; (+)-*form*, S-153
Sesbanimide B, S-153
Sesbanimide C, S-154
Sollasin B, S-254
Tauropinnaic acid, P-415
Tetradehydrohalicyclamine A, H-27
Tubastraine, T-788

Quinolizidine alkaloids (two rings)

Clathryimine A, C-682
Clavepictine A, C-686
Clavepictine B, C-686
Pictamine, P-403

Cylindricine alkaloids

Cylindricine A, C-1093
Cylindricine B, C-1094
Cylindricine C, C-1095
Cylindricine D, C-1095
Cylindricine E, C-1095
Cylindricine F, C-1096
Cylindricine G, C-1097
Cylindricine H, C-1098
Cylindricine I, C-1098
Cylindricine J, C-1099
Cylindricine K, C-1100
Fasicularine, F-20
Lepadiformine A, L-127
Lepadiformine B, L-128
Lepadiformine C, L-128
Polycitorol A, P-533
Polycitorol B, P-534

Miscellaneous quinolizidine alkaloids

Halichlorine, H-11
Isosaraine 1, S-25
Isosaraine 2, S-26
Isosaraine 3, S-27
Saraine 1, S-25
Saraine 2, S-26
Saraine 3, S-27

Azepine alkaloids

Aaptosamine, A-3
Bengamide A, B-49
Bengamide B, B-49
Bengamide C, B-49
Bengamide D, B-49
Bengamide E, B-49
Bengamide F, B-49
Bengamide G, B-49
Bengamide H, B-49
Bengamide I, B-49
Bengamide J, B-49
Bengamide K, B-48
Bengamide L, B-49
Bengamide M, B-49
Bengamide N, B-49
Bengamide O, B-49
Bengamide P, B-49
Bengamide Q, B-49
Bengamide R, B-49
Bengamide Y, B-49
Bengamide Z, B-49
Caprolactin A, A-315
Caprolactin B, A-315
13-Demethylspirolide C, S-322
13-Demethylspirolide D, S-322
13,19-Didemethylspirolide C, S-322
Isobengamide E, I-112
20-Methylspirolide G, S-324
Montiporyne E, M-622
Sollasin C, S-255
Spirolide A, S-321
Spirolide B, S-321
Spirolide C, S-322
Spirolide D, S-322

Nicotinic acid derived alkaloids

5-Amino-*N*,*N*,*N*-trimethylpentanaminium, 9CI, P-239
3-Carboxy-1-(carboxymethyl)pyridinium betaine, C-99
3-Carboxy-1-(2-hydroxyethyl)pyridinium betaine, P-743
3-Carboxy-1-methylpyridinium betaine, C-108
Humeic acid C, H-415
3-Pyridinecarboxamide, P-742
3-Pyridinecarboxylic acid, P-743
Tetrahydroanabasine, P-434

Pyridine alkaloids

4-Acetyl-6-methyl-2(1*H*)-pyridinone, A-78
Agelongine, A-167
Callyspongia fibrosa Alkaloid, A-200
Amphikuemin, A-468
Amphitoxin, A-478
Antibiotic B 90063, A-534
Aspernigrin A, A-717
Aspernigrin B, A-718
2,3′-Bipyridine, B-110
3-(2-Carboxyethyl)-1,4-dimethylpyridinium, C-102
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Indolizidine alkaloids

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Simple quinoline alkaloids

Miscellaneous quinoline alkaloids

Quinazoline alkaloids

Pyrido[2,3,4-*kl*]acridines

Benzodiazepine alkaloids

Simple phenethylamine alkaloids

α-Hydroxyphenethylamines

Halogenated tyrosinoids

Miscellaneous phenethylamines

Cinnamic acid amides

Simple isoquinoline alkaloids

Manzamine alkaloids

Miscellaneous isoquinoline alkaloids

Benzylisoquinoline alkaloids

Protoberberine alkaloids

Simple indole alkaloids

Simple biindoles

Monomeric tryptamine alkaloids

Physostigmine-like alkaloids

Chaetocin-like alkaloids

Evodia alkaloids

Tryptamine alkaloid dimers

Tryptamine alkaloid oligomers

β-Carboline alkaloids

Carbazole alkaloids

Indolo[2,3-*a*]carbazole and related alkaloids

Ergot alkaloids

Indoloquinolizine alkaloids

Ajmalicine-like alkaloids

Hapalindoles

Isoindoles

Pyrrolo[4,3,2-*de*]quinoline alkaloids

Miscellaneous indole alkaloids

Monoterpenoid alkaloids

Sesquiterpene alkaloids

C_{19}-Diterpenoid alkaloids and 4-nor analogues

Miscellaneous diterpene alkaloids

Sesterterpene alkaloids

Steroidal alkaloids (buxus type)

Steroidal alkaloids (pregnane type)

Miscellaneous steroidal alkaloids

Pyrazole alkaloids

Imidazole alkaloids

Cycloheptadiimidazoles

Oxazole and benzoxazole alkaloids

Isoxazole alkaloids

Spirobenzoxazoline alkaloids

Simple thiazole and benzothiazole alkaloids

Latrunculins

Macrocyclic thiazole alkaloids

Pyrazine and quinoxaline alkaloids

Pyrrolo[1,2-*a*]pyrazines

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Rhodophytes (red algae)

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3-Hydroxystigmasta-5,8,22-trien-7-one; (3β,22*E*,24ξ)-*form*, H-961
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4,6-Diethyl-3,6-dihydro-6-(2-methylhexyl)-1,2-dioxin-3-acetic acid; (3*S*,6*R*,8*S*)-*form*; Me ester, D-488
4,6-Diethyl-3,6-dihydro-6-(2-methylhexyl)-1,2-dioxin-3-acetic acid; (3*S*,6*R*,8*S*)-*form*, D-488
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Demosponges; Tetractinomorpha

Demosponges; Ceractinomorpha

Miscellaneous and unclassified sponges

Anthozoans; Octocorals

Anthozoans; Hexacorals

Medusozoans; Cubozoans

Medusozoans; Hydrozoans

Medusozoans; Scyphozoans

Miscellaneous and unclassified Cnidarians

Platyhelminths

Nematodes

Annelids

Rotifers

Smaller vermiform groups

Bryozoans

Brachiopods

Chitons

Gastropods; Prosobranchs

Gastropods; Ophisthobranchs

Gastropods; Pulmonates

Bivalve molluscs

Cephalopods

Miscellaneous and unclassified molluscs

Crinoids

Starfish (Asteroidea)

Sea urchins (Echinoidea)

Sea cucumbers (Holothuroidea)

Brittle stars (Ophiuroidea)

Arthropods

Arachnids

Acarids (mites and ticks)

Other non-insect arthropods

Insects; beetles (coleoptera)

Insects; Diptera

Insects; Lepidoptera

Insects; Hymenoptera

Bugs and aphids (Hemiptera, Homoptera, Heteroptera)

Other insects

Crustaceans

Hemichordates

Protochordates

Fish

Mammals

General Chemistry

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